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Synthases

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Chappell et al.

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(54) **SYNTHASES**

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Related U.S. Application Data

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(60) Provisional application No. 60/150,262, filed on Aug. 23, 1999, provisional application No. 60/130,628, filed on Apr. 22, 1999, and provisional application No. 60/100,993, filed on Sep. 18, 1998.

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(52) **U.S. Cl.** **435/183**; 435/4; 435/232; 435/468; 536/23.2; 536/1.11; 585/355; 524/9

(58) **Field of Search** 435/183, 193, 435/4, 232, 468; 536/1.11, 23.2; 585/355; 524/9; 558/12

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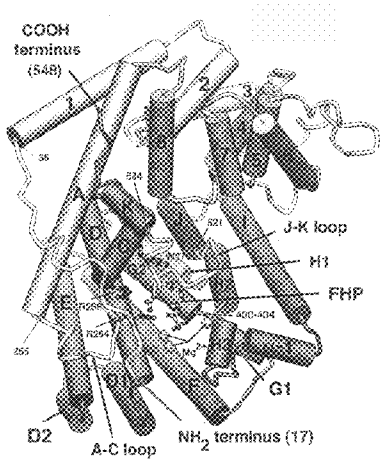
(57) **ABSTRACT**

Novel synthases and the corresponding nucleic acids encoding such synthases are disclosed herein. Such synthases possess an active site pocket that includes key amino acid residues that are modified to generate desired terpenoid reaction intermediates and products. Synthase modifications are designed based on, e.g., the three-dimensional coordinates of tobacco 5-epi-aristolochene synthase, with or without a substrate bound in the active site.

11 Claims, 4 Drawing Sheets



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Genbank Accession No: U20190.

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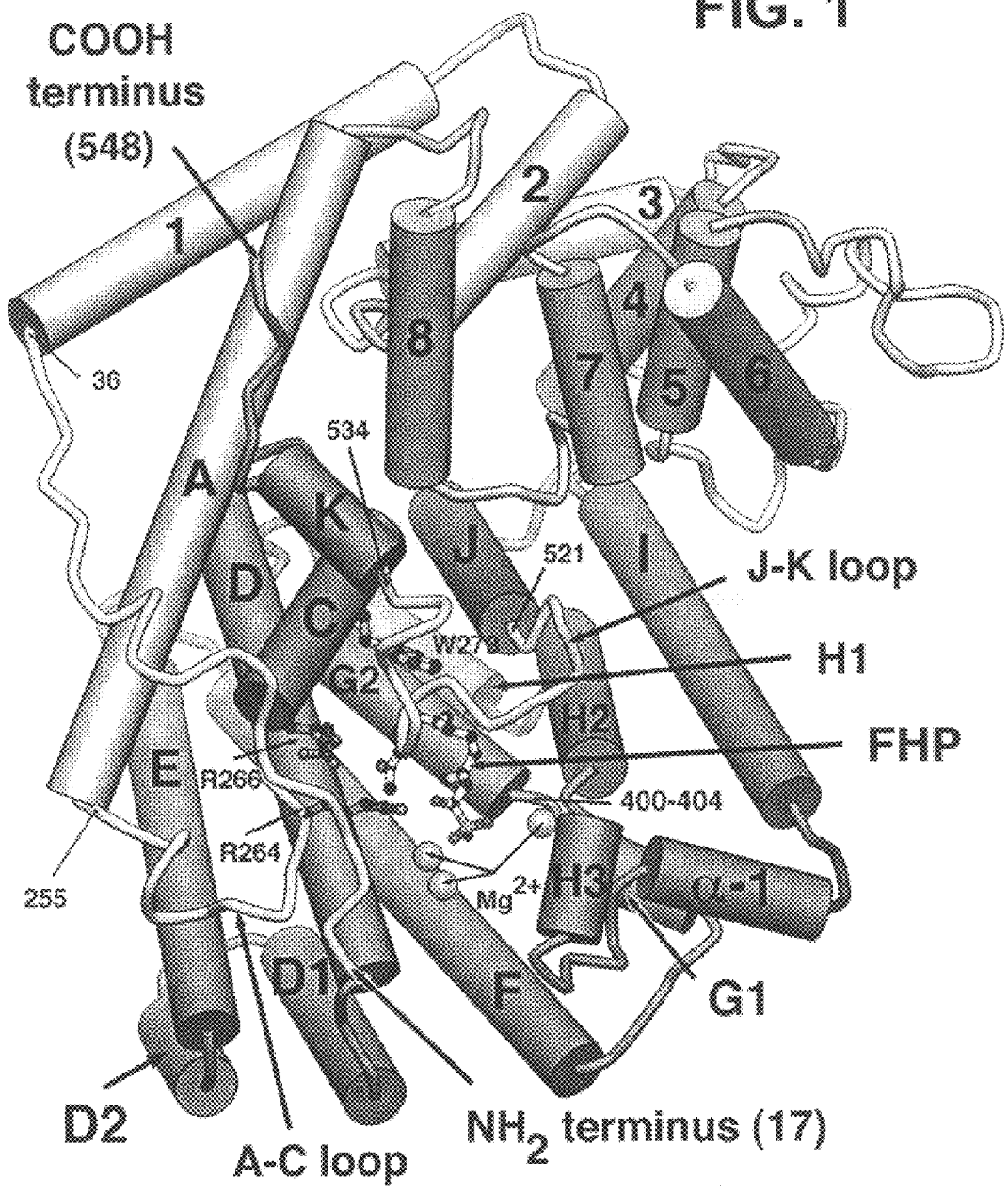
FIG. 1


COOH terminus (548)
1
2
3
4
5
6
7
8
36
534
A
K
J
I
D
C
521
J-K loop
W27
H1
G2
H2
FHP
E
R266
400-404
R264
255
Mg^{2+}
H3
α-1
D1
F
G1
D2
A-C loop
NH_2 terminus (17)

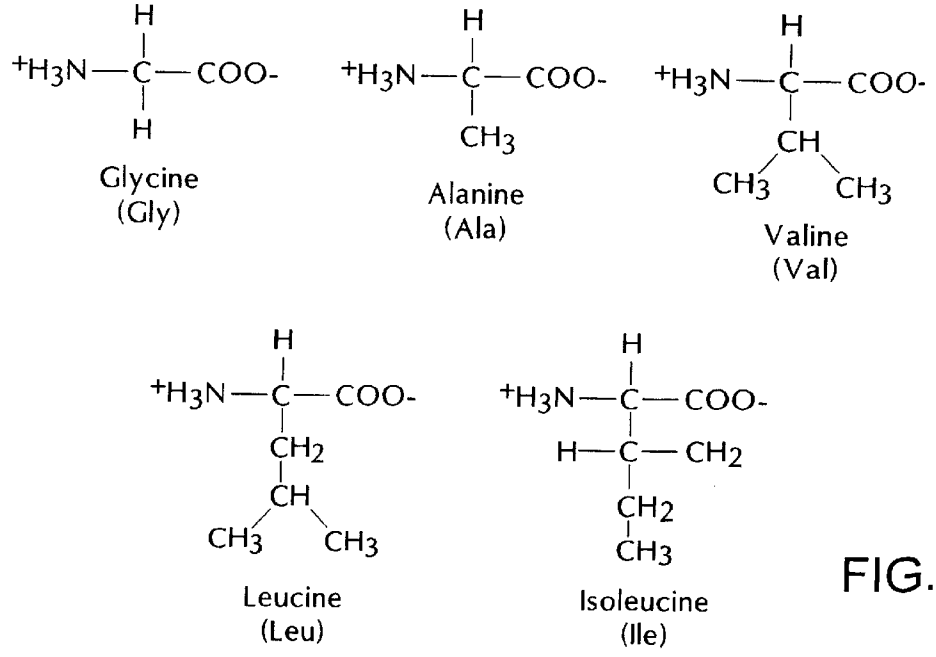
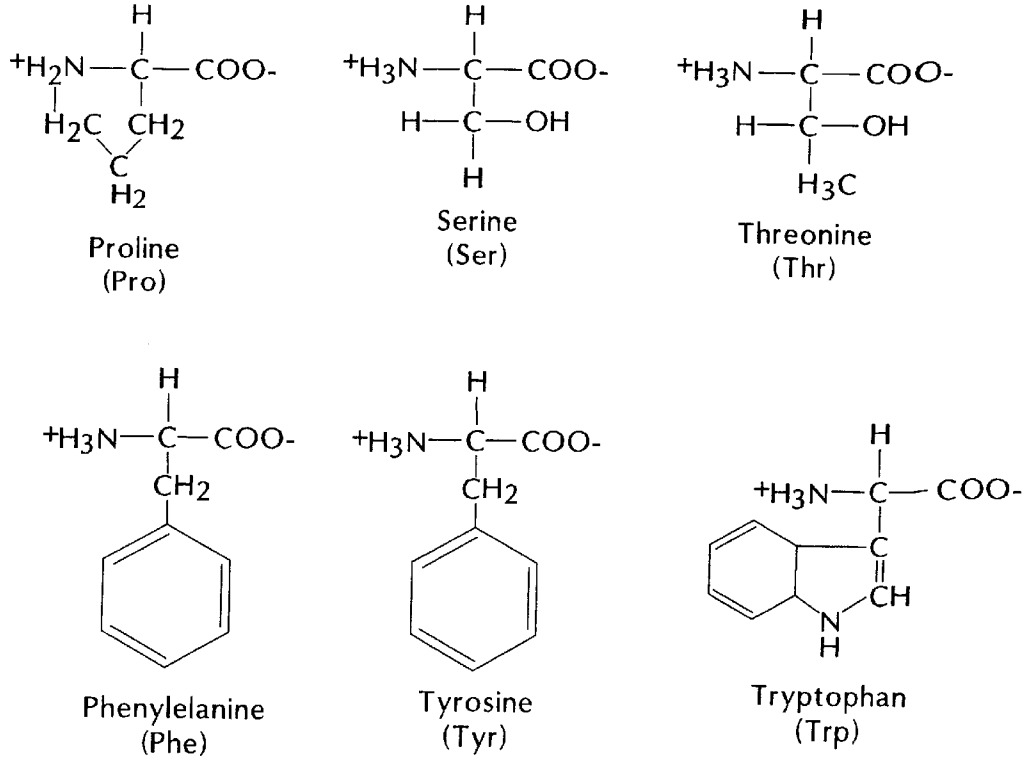

Glycine
(Gly)
Alanine
(Ala)
Valine
(Val)
Leucine
(Leu)
Isoleucine
(Ile)

FIG. 2-1


Proline
(Pro)
Serine
(Ser)
Threonine
(Thr)
Phenylelanine
(Phe)
Tyrosine
(Tyr)
Tryptophan
(Trp)

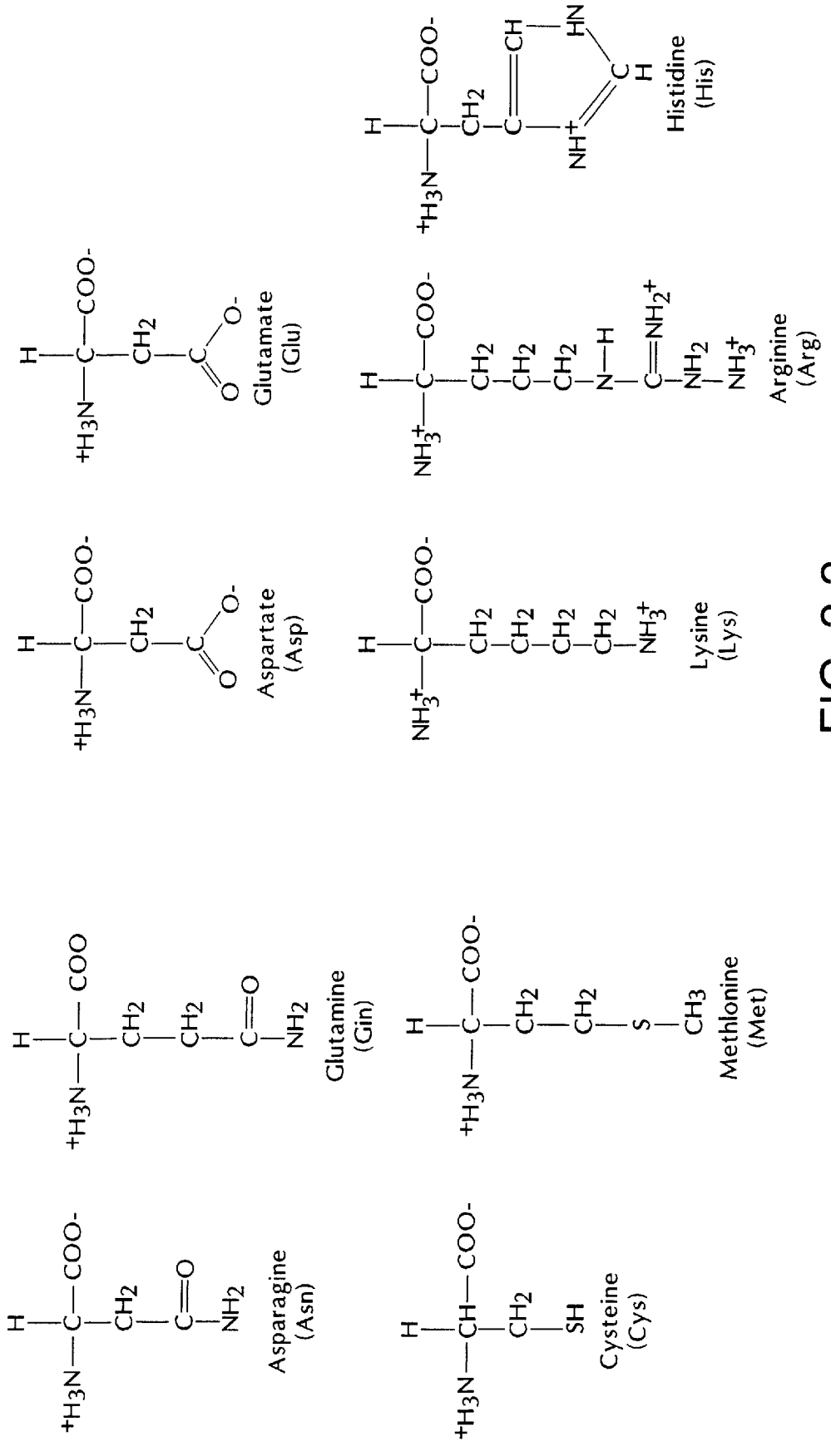

Asparagine (Asn)
Glutamine (Gin)
Cysteine (Cys)
Methlonine (Met)
Aspartate (Asp)
Glutamate (Glu)
Lysine (Lys)
Arginine (Arg)
Histidine (His)

FIG. 2-2

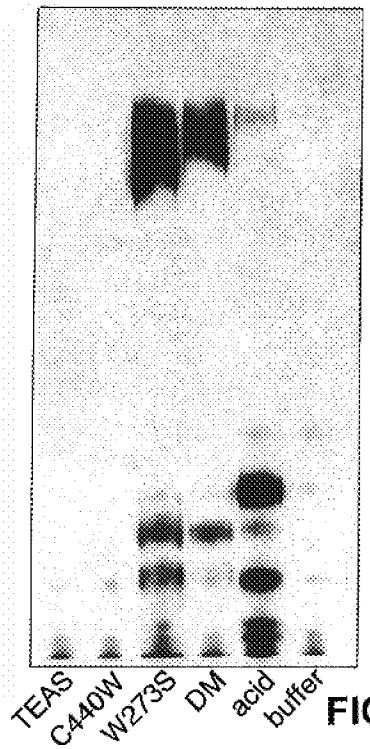

TEAS
C440W
W273S
DM
acid
buffer

FIG. 3

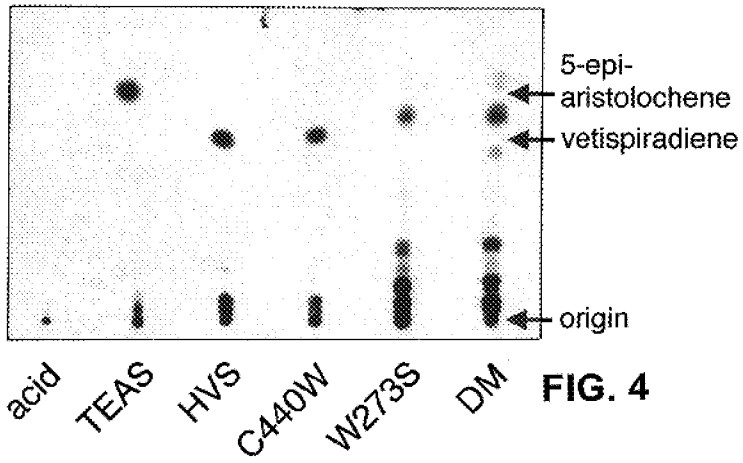

5-epi-
aristolochene
vetispiradiene
origin
acid
TEAS
HVS
C440W
W273S
DM

FIG. 4

SYNTHASES

CROSS REFERENCE TO RELATED APPLICATIONS

This application is a continuation of and claims priority under 35 U.S.C. §120 to U.S. application Ser. No. 09/398,395, filed Sep. 17, 1999 now U.S. Pat. No. 6,468,772, which claims benefit under 35 U.S.C. §119(e) of U.S. Provisional Application No. 60/150,252, filed Aug. 23, 1999, U.S. Provisional Application No. 60/130,628, filed Apr. 22, 1999, and U.S. Provisional Application No. 60/100,993, filed Sep. 18, 1998.

This work was supported, in part, with funding from NIH (GM54029 and GM07240) and NSF (IBW-9408152). Therefore, the United States Federal Government may have certain rights in the invention.

BACKGROUND OF THE INVENTION

Isoprenoid compounds are organic molecules produced by a wide range of organisms (e.g., plants, bacteria, fungi, etc). To date, over 23,000 individual isoprenoid molecules have been characterized with tens to hundreds of new structures identified each year. These molecules can fulfill a variety of roles. For example, monoterpenes can be used as fragrances and flavors. Sesquiterpenes and diterpenes can serve as pheromones, defensive agents, visual pigments, antitumor drugs, and components of signal transduction pathways. Triterpenes can serve important functions as membrane constituents and precursors of steroid hormones and bile acids. Polyprenols function as photoreceptive agents and cofactor side chains, and can also exist as natural polymers.

The diverse molecular compounds produced by the isoprenoid pathway are created from diphosphate esters of monounsaturated isoprene units.

Isoprenes are added together in multiples of 2, 3, or 4 by prenyl transferases to make C_{10}, C_{15}, and C_{20} units, respectively. The C_{10}, C_{15}, and C_{20} molecules, named geranyl diphosphate (GPP), farnesyl diphosphate (FPP), and geranylgeranyl diphosphate (GGPP), respectively, serve as substrates for terpene synthases.

Terpene synthases catalyze the production of isoprenoid compounds via one of the most complex reactions known in chemistry or biology. In general, terpene synthases are moderately sized enzymes having molecular weights of about 40 to 100 kD. As an enzyme, terpene synthases can be classified as having low to moderate turnover rates coupled with exquisite reaction specificity and preservation of chirality. Turnover comprises binding of substrate to the enzyme, establishment of substrate conformation, conversion of substrate to product and product release. Reactions can be performed in vitro in aqueous solvents, typically require magnesium ions as cofactors, and the resulting products, which are often highly hydrophobic, can be recovered by partitioning into an organic solvent.

Terpene synthase genes are found in a variety of organisms including bacteria, fungi and plants. Swapping regions approximating exons between different terpene synthases has identified functional domains responsible for terminal enzymatic steps. For example, work performed on 5-epi-aristolochene synthase (TEAS) from Nicotiana tabacum (tobacco) and Hyoscyamus muticus vetispiradiene synthase (HVS) from henbane revealed that exon 4 and exon 6, respectively, were responsible for reaction product specificity. Combining functional domains resulted in novel

enzymes capable of synthesizing new reaction products (U.S. Pat. No. 5,824,774).

Studies have led to proposed reaction mechanisms for isoprenoid production; see, e.g., Cane et al., 1985, Bioorg. Chem., 13:246–265; Wheeler and Croteau, 1987, Proc. Natl. Acad. Sci. USA, 84:4856–4859; and Pyun et al., 1994, Arch. Biochem. Biophys., 308:488–496. The studies used substrate analogs and suicide inhibitors (Croteau, 1994, Arch. Biochem. Biophys., 251:777–782; Cane et al., 1995, Biochemistry, 34:2471–2479; and Croteau et al., 1993, Arch. Biochem. Biophys., 307:397–404), as well as chemical-modifying reagents and site-directed mutagenesis in efforts to identify amino acids essential for catalysis (Cane et al., 1995, Biochemistry, 34:2480–2488; Rajaonarivony et al., 1992, Arch. Biochem. Biophys., 296:49–57; and Rajaonarivony et al., 1992, Arch. Biochem. Biophys., 299:77–82). However, these studies have resulted in limited success in defining the active site due to inherent limitations with these techniques.

SUMMARY OF THE INVENTION

The invention describes a method of identifying alpha-carbon atoms found in the active site of a terpene synthase and describes these atoms in three-dimensional space as well as the spatial relationships among them. The present invention also describes R-groups associated with such alpha-carbons and methods of altering these R-groups in order to create novel terpene synthases capable of generating novel reaction products.

Until the invention taught in this present application, the active site of synthase proteins, the amino acid residues located therein, the amino acid residues involved in catalysis, and the configuration of α-carbons and R-groups within the active site have not been known. The current invention now teaches the structure of synthases, as well as provides the means of making and using the information obtained therefrom to develop and produce new and novel synthases having new and novel synthetic capabilities. The data generated using the methods described herein are useful for creation and production of synthase mutants that can use a variety of isoprenoid substrates and produce a variety of isoprenoid products.

In one embodiment, the invention features an isolated terpene synthase having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2. Such a synthase comprises nine α-carbons having interatomic distances in Angstroms between the α-carbons that are ±2.3 Angstroms of the interatomic distances shown in Table 6. The center point of each α-carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center point of each such sphere has the structural coordinates given in Table 5. Each α-carbon has an associated R-group, and the synthase has an ordered arrangement of R-groups associated with each alpha-carbon other than the ordered arrangements of R-groups shown in Table 9. The synthase can have about 25% or greater sequence identity to residues 265 to 535 of SEQ ID 2, or about 35% or greater sequence identity to residues 265 to 535 of SEQ ID 2. Such a synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be a cyclic terpenoid hydrocarbon or an acydic terpenoid hydrocarbon. Either type of product can be hydroxylated or non-hydroxylated. The R-group associated with α-carbon 1 can be selected from one of the following groups: the group consisting of Cys, Ser, and Thr, the group consisting of Phe, Tyr and Trp, the group consist-

ing of Pro, Gly, and Ala, the group consisting of Glu and Asp, the group consisting of Met, Ile, Val and Leu, the group consisting of Arg and Lys, and the group consisting of Gin, Asn and His. R-groups associated with α-carbons 2 to 9 can be any amino acid except those having the ordered arrangements of Table 9. Similarly, the R-group associated with each of α-carbons 2–9 can be selected independently from the group consisting of Cys, Ser and Thr, the group consisting of Phe, Tyr and Trp, the group consisting of Pro, Gly, and Ala, the group consisting of Glu and Asp, the group consisting of Met, Ile, Val and Leu, the group consisting of Arg and Lys, and the group consisting of Gin, Asn and His. In these embodiments, R-groups associated with the remaining eight α-carbons except those having the ordered arrangements of Table 9.

In some embodiments, the ordered arrangement of R-groups associated with α-carbons 1 to 9 is Trp, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Phe, respectively, Ser, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Tyr, respectively, Trp, Ile, Thr, Thr, Tyr, Leu, Trp, Thr and Tyr, respectively, Ser, Ile, Thr, Thr, Tyr, Leu, Trp, Thr and Tyr, respectively, or Glu, Ile, Thr, Thr, Tyr, Leu, Cys, Thr and Tyr, respectively.

The invention also features a terpene synthase made by aligning the primary amino acid sequence of a preselected terpene synthase polypeptide to the amino acid sequence of residues 265 to 535 of SEQ ID NO:2, mutating a nucleic acid encoding the preselected polypepxide at one or more codons for nine amino acid residues in a region of the polypeptide primary amino acid sequence having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, the nine residues in the polypeptide aligning with residues 273, 294, 402, 403, 404, 407, 440, 519 and 520 of SEQ ID NO:2; and expressing the mutated nucleic acid so that a mutated terpene synthase is made.

The invention also features an isolated terpene synthase having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, the synthase comprising sixteen α-carbons having interatomic distances in Angstroms between the α-carbons that are ±2.3 Angstroms of the interatomic distances given in Table 4. The center point of each α-carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center point of each of the spheres has the structural coordinates given in Table 3. Each α-carbon has an associated R-group, and the synthase has an ordered arrangement of R-groups other than the ordered arrangements of R-groups given in Table 8. The synthase can have about 25% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, or about 35% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2. The synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be, for example, a cyclic terpenoid hydrocarbon. The ordered arrangement of R-groups in the synthase associated with α-carbons 1 to 16 can be Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu, Cys, Val, Thr, Tyr, Asp, Phe and Thr, respectively.

The invention also features an isolated terpene synthase having about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, the synthase comprising nineteen α-carbons having interatomic distances in Angstroms between the α-carbons that are ±2.3 Angstroms of the interatomic distances given in Table 2. The center point of each α-carbon is positioned within a sphere having a radius of 2.3 Angstroms. The center points of each sphere have the structural coordinates given in Table 1. Each α-carbon has an associated R-group, and the synthase has an ordered arrangement of the R-groups other than the ordered arrangements of R-groups given in Table 7. The synthase can have about 25% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, or about 35% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2. The synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be, for example, a cyclic terpenoid hydrocarbon.

The invention also features an isolated protein comprising a first domain having an amino terminal end and a carboxyl terminal end. The first domain comprises amino acids that align structurally in three-dimensional space with a glycosyl hydrolase catalytic core, the glycosyl hydrolase catalytic core selected from the group consisting of amino acids 36 to 230 of glucoamylase protein databank (PDB) code 3GLY of Aspergillus awamori and amino acids 36 to 230 of endoglucanase CelD PDB code 1 CLC. The isolated protein also comprises a second domain having an amino terminal end and carboxyl terminal end. The second domain comprises amino acids that align structurally in three-dimensional space with avian FPP synthase. The carboxyl terminal end of the first domain is linked to the amino terminal end of the second domain. The second domain has about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, and comprises nine α-carbons having interatomic distances in Angstroms between the α-carbons that are ±2.3 Angstroms of the interatomic distances given in Table 6. The center point of each α-carbon is positioned within a sphere having a radius of 2.3 Angstroms, the center point of each sphere having the structural coordinates given in Table 5. Each α-carbon has an associated R-group, and the synthase has an ordered arrangement of R-groups other than the ordered arrangements of R-groups given in Table 9. The protein can have about 25% or greater sequence identity to SEQ ID NO:2, or about 35% or greater sequence identity to SEQ ID NO:2. The synthase can catalyse the formation of a terpenoid product from a monoterpene substrate, a sesquiterpene substrate, or a diterpene substrate. The product can be, for example, a cyclic terpenoid hydrocarbon.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 343 to 606 of SEQ ID NO:20, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 348, 351, 372, 375, 376, 454, 479, 480, 481, 482, 485, 519, 523, 597, 600, 601, 605, 607 and 608 of SEQ ID NO:20 are residues other than amino acids Y, L, C, I, T, Y, S, C, G, H, S, L, G, F, G, Y, D, Y and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 316 to 586 of SEQ ID NO:22, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 321, 324, 345, 348, 349, 427, 452, 453, 454, 455, 458, 492. 496, 569, 572, 573, 577, 579 and 580 of SEQ ID NO:22 are residues other than amino acids C, W, N, I, T, Y, S, I, S, G, M, L, D, A, M, Y, D, H and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to

residues 352 to 622 of SEQ ID NO:58, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 357, 360, 381, 384, 385, 463, 487, 488, 489, 490, 493, 528, 532, 606, 609, 610, 614, 616 and 617 of SEQ ID NO:58 are residues other than amino acids Y, M, C, V, T, F, V, S, S, G, I, L, G, F, V, Y, D, Y and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to amino acid residues 272 to 540 encoded by SEQ ID NO:33, wherein one or more amino acid residues of the synthase that align with amino add residues at positions 277, 280, 301, 304, 305, 383, 408, 409, 410, 411, 414, 448, 452, 524, 527, 528, 532, 534 and 535 encoded by SEQ ID NO: 33 are residues other than amino acids G, W, I, A, S, Y, T, S, G, Y, L, C, D, M, L, Y, D, Y and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 319 to 571 of SEQ ID NO:42, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 324, 327, 348, 351, 352, 430, 455, 456, 457, 458, 461, 495, 499, 571, 574, 575, 579, 581 and 582 of SEQ ID NO:42 are residues other than amino acids I, W, V, I, S, Y, T, T, G, L, V, I, N, T, S, Y, D, Y, and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 579 to 847 of SEQ ID NO:44, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 584, 587, 606, 609, 610, 688, 713, 714, 715, 716, 719, 753, 757, 831, 834, 835, 839, 841 and 842 of SEQ ID NO:44 are residues other than amino acids V, S, G, Q, V, Y, S, V, G, L, C, W, N, V, F, Y, D, Y and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 495 to 767 of SEQ ID NO:46, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 500, 503, 524, 527, 528, 606, 631, 632, 633, 634, 637, 674, 678, 751, 754, 755, 759, 761 and 762 of SEQ ID NO:46 are residues other than amino acids F, L, A, Q, T, Y, S, I, G, Q, L, S, D, T, I, F, D, F and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 295 to 564 of SEQ ID NO:48, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 300, 303, 324, 327, 328, 406, 431, 432, 433, 434, 437, 471, 475, 548, 551, 552, 556, 558 and 559 of SEQ ID NO:48 are residues other than amino acids Y, W, A, C, T, Y, S, S, G, M, L, G, D, L, I, Y, D, L and Y, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 307 to 578 of SEQ ID NO:50, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 312, 315, 336, 339, 340, 419, 444, 445, 446, 447, 450, 484, 488, 562, 565, 566, 570, 572 and 573 of SEQ ID NO:50 are residues other than amino acids F, W, A, M, T, Y, N, T, G, M, L, S, D, I, M, Y, D, F and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 264 to 533 of SEQ ID NO:52, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 269, 272, 293, 296, 297, 375, 401, 402, 403, 404, 407, 441, 445, 517, 520, 521, 525, 527 and 528 of SEQ ID NO:52 are residues other than amino acids C, W, L, T, S, Y, S, A, G, Y, I, A, N, A, L, Y, D, Y and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 585 to 853 of SEQ ID NO:56, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 590, 593, 614, 617, 618, 696, 721, 722, 723, 724, 727, 761, 765, 837, 840, 841, 845, 847 and 848 of SEQ ID NO:56 are residues other than amino acids I, S, S, T, V, Y, S, I, A, L, V, G, N, M, F, Y, D, L and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 307 to 574 of SEQ ID NO:54, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 312, 315, 336, 339, 340, 418, 443, 444, 445, 446, 449, 483, 487, 560, 563, 564, 566, 568 and 569 of SEQ ID NO:54 are residues other than amino acids C, W, I, I, T, Y, S, I, S, A, I, L, D, A, I, Y, D, D and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 309 to 577 of SEQ ID NO:24, wherein one or more amino acid residues of the synthase that align with amino

acid residues at positions 314, 317, 338, 341, 342, 420, 446, 447, 448, 449, 452, 485, 489, 560, 563, 564, 569, 571 and 572 of SEQ ID NO:24 are residues other than amino acids C, W, N, V, T, Y, I, G, G, I, L, L, D, A, I, Y, D, F and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 315 to 584 of SEQ ID NO:26, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 320, 323, 344, 347, 348, 426, 451, 452, 453, 454, 457, 492, 496, 568, 571, 572, 576, 578 and 579 of SEQ ID NO:26 are residues other than amino acids S, W, I, A, T, Y, S, V, A, S, I, L, D, A, I, Y, D. F, and G, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 265 to 536 of SEQ ID NO:28, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 518, 521, 522, 528, 530 and 531 of SEQ ID NO:28 are residues other than amino acids A, W, V, C, G, F, T, S, C, I, M, G, N, C, S, Y, D, Y and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 342 to 612 of SEQ ID NO:30, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 347, 350, 371, 374, 375, 453, 478, 479, 480, 481, 483, 518, 522, 596, 599, 600, 604, 606 and 607 of SEQ ID NO:30 are residues other than amino acids F, L, C, V, T, Y, S, S, A, Y, V, L, G, L, L, Y, D, F and S, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more of the ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features an isolated synthase having a region with about 40% or greater sequence identity to residues 273 to 541 of SEQ ID NO:32, wherein one or more amino acid residues of the synthase that align with amino acid residues at positions 278, 281, 302, 305, 306, 384, 409, 410, 411, 412, 415, 448, 452, 524, 527, 528, 533, 535 and 536 of SEQ ID NO:32 are residues other than amino acids C, W, I, I, S, Y, T, S, T, Y, L, C, D, I, T, Y, D, Y and T, respectively. In some embodiments, the sequence identity can be about 20% or greater, 25% or greater, or 35% or greater. In some embodiments, one or more ordered arrangements of residues as given in Table 7 are not found in such a synthase.

The invention also features a method for making a terpene synthase, comprising identifying, in a preselected polypeptide having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, nine amino acid residues whose α-carbons have interatomic distances in Angstroms between the α-carbons that are ±2.3 Angstroms of the interatomic distances given in Table 6. The center point of each α-carbon is positioned with a sphere having a radius of 2.3 Angstroms. The center point of each sphere has the structural coordinates given in Table 5. The method then comprises synthesizing a polypeptide that is modified from the preselected polypeptide. The modified polypeptide has one or more R-groups associated with the nine α-carbons other than the R-groups associated with the α-carbons in the preselected polypeptide. The synthesizing step can comprise the formation of a nucleic acid encoding the preselected polypeptide in which the coding sequence for one or more amino acids corresponding to the nine α-carbons is replaced by a coding sequence that codes for an amino acid different from the amino acid present in the preselected polypeptide. The preselected polypeptide can be, for example, any one of the polypeptides given in SEQ ID NOS: 2, 4, 6, 8, 10, 12, 20, 22, 24, 26, 28, 30, 32, 34–40, 42, 44, 46, 48, 50, 52, 54, 56, or 58.

The invention also features a method of using a terpene synthase, comprising identifying, in a preselected polypeptide having a region with 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, amino acid residues at nine positions that align with amino acid residues 273, 294, 402, 403, 404, 407, 440, 519 and 520 of SEQ ID NO:2; and synthesizing a polypeptide that is modified from the preselected polypeptide. The novel polypeptide is modified by having amino acid residues at one or more of the nine positions other than the amino acid residues present in the preselected polypeptide. In some embodiments, the identifying step can comprise identifying sixteen amino acid residues in the preselected polypeptide that align with amino acid residues 270, 273, 294, 297, 298, 402, 403, 404, 407, 440, 516, 519, 520, 525, 527 and 528 of SEQ ID NO:2, and the synthesizing step can comprise synthesizing a polypeptide that is modified from the preselected polypeptide, the modified polypeptide having amino acid residues at one or more of the sixteen positions other than the amino add residues present in the preselected polypeptide. In some embodiments, the identifying step can comprise identifying nineteen amino acid residues in the preselected polypeptide that align with amino acid residues 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 516, 519, 520, 525, 527 and 528 of SEQ ID NO:2, and the synthesizing step can comprise synthesizing a polypeptide that is modified from the preselected polypeptide, the modified polypeptide having amino acid residues at one or more of the nineteen positions other than the amino acid residues present in the preselected polypeptide. The synthesizing step can comprise the formation of a nucleic acid encoding the preselected polypeptide in which the coding sequence in the nucleic acid coding for one or more of the identified amino acid residues is replaced by a coding sequence that encodes an amino acid different from the amino acid present in the preselected polypeptide. The preselected polypeptide can be, for example, any one of the polypeptides given in SEQ ID NOS: 2, 4, 6, 8, 10, 12, 20, 22, 24, 26, 28, 30, 32, 34–40, 42, 44, 46, 48, 50, 52, 54, 56, or 58. The method can further comprise: contacting the modified polypeptide with an isopreanoid substrate under conditions effective for the compound to bind the polypeptide; and measuring the ability of the modified polypeptide to catalyze the formation of a reaction product from the isoprenoid substrate. The isoprenoid substrate can be a monoterpene, a sesquiterpene, or a diterpene.

The invention also features a method of making a terpene synthase, comprising creating a population of nucleic acid

molecules that encode polypeptides, the population having members that differ from one another at one or more of nine codons specifying amino acids of a preselected terpene synthase having a region with about 20% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, α-carbons of the nine amino acids having interatomic distances in Angstroms between the α-carbons that are ±2.3 Angstroms of the interatomic distances given in Table 6. The center point of each α-carbon is positioned within a sphere having a radius of 2.3 Angstroms, and the center point of each sphere has the structural coordinates given in Table 5. In some embodiments, the codons specify amino acids as described in Tables 1–2 or 3–4 of a preselected terpene synthase. A portion, or all, of the nucleic acid population is expressed so that a population of polypeptides is made. At least one member of the population of polypeptides is a mutant terpene synthase. The expressing step can comprise in vitro transcription and in vitro translation of the nucleic acid population. In some embodiments, the expressing step comprises cloning members of the nucleic acid population into an expression vector, introducing the expression vector into host cells and expressing the cloned nucleic acid population members in the host cells so that the population of polypeptides is made. The preselected terpene synthase polypeptide can be a monoterpene synthase, a sesquiterpene synthase, or a diterpene synthase. The host cells can be prokaryotic cells or eukaryotic cells, including, without limitation, bacterial cells, fungal cells, and animal cells, e.g., mammalian cells or insect cells. The host cells can also be plant cells, e.g., a cell from a Graminaceae plant, a cell from a Legumineae plant, a cell from a Solanaceae plant, a cell from a Brassicaeae plant or a cell from a Conifereae plant.

The invention also features a nucleic acid encoding a synthase as described herein, and a host cell containing such a nucleic acid. The invention also features a transgenic plant containing such a nucleic acid, or a transgenic animal cell culture containing such a nucleic acid.

In some embodiments, a synthase polypeptide of the invention comprises a domain that contains an active site comprised of nine α-carbon atoms having the coordinates of Table 5, and interatomic distances between the α-carbons ±2.3 angstroms of the distances given in Table 6. The α-carbon atoms align structurally in three dimensional space in the presence or absence of bound substrate or substrate analogue, with avian FPP synthase. In another embodiment, a synthase of this invention comprises the following: (i) a first domain containing amino acid residues that align in three-dimensional space (in solution or crystal form, and either having a bound or unbound substrate) with a glycosyl hydrolase catalytic core selected from the group consisting of (a) amino acids 36–230 of glycosyl hydrolase (PDB code 3GLY) of *Aspergillus awarmori*, and (b) amino acids 36–230 of endogluconase CellB (PDB code 1CLC), and (ii) a second domain that aligns structurally in three dimensional space with or without substrate or substrate analogues bound in the active site with avian FPP synthase. The second domain contains an active site comprised of nine, sixteen or nineteen α-carbon atoms having the structural coordinates and interatomic distances of Tables 1–2, 3–4 or 5–6. These α-carbon atoms have R-groups attached thereto that can interact, either directly or indirectly, with an isoprenoid substrate.

The invention also features a method for generating mutant terpene synthases possessing catalytic activity. The method comprises the steps of (a) providing a crystallographic model of a preselected catalytically active terpene synthase having an active site, and (b) using the model to design a terpene synthase having at least one altered R-group in the active site relative to the preselected synthase. The invention also features terpene synthases having altered substrate specificity, methods of making the same, and procedures for generating three-dimensional structures thereof.

Although methods and materials similar or equivalent to those described herein can be used to practice the invention, suitable methods and materials are described below. All publications, patent applications, patents and other references mentioned herein are incorporated by reference in their entirety.

Other aspects, embodiments, advantages, and features of the present invention will become apparent from the specification.

BRIEF DESCRIPTION OF DRAWINGS

FIG. **1** Schematic representation of tobacco 5-epi-aristolochene synthase (TEAS) with bound farnesyl hydroxyphosphonate (FHP), prepared using the RIBBONS software program of Carson, M. and Bugg, C., J. Mol. Graphics 4:121 (1986). Cylinders 1–8 and A represent α-helices in the NH_2-terminal domain; cylinders C, D, D1, D2, E, F, G1, G2, H1, H2, H3, I and α-1 represent α-helices in the COOH-terminal domain.

FIG. **2**. Structure of twenty natural amino acids showing α-carbons and associated R-groups.

FIG. **3**. Autoradiogram of an argentation thin-layer chromatogram of terpenoid hydrocarbon products made by TEAS and mutant TEAS enzymes using GGPP as a substrate. DM: W273S/C440W mutant TEAS enzyme.

FIG. **4**. Autoradiogram of an argentation thin-layer chromatogram of terpenoid hydrocarbon products made by TEAS and mutant TEAS enzymes using FPP as a substrate.

BRIEF DESCRIPTION OF TABLES

Table 1. X-ray crystallographic structural coordinates for 19 α-carbons found in the active site of a terpene synthase.

Table 2. Interatomic distances in Angstroms between each α-carbon of Table 1. Each α-carbon occupies a sphere having a radius of 2.3 Angstroms. Interatomic distances are calculated from the center point of each sphere.

Table 3. X-ray crystallographic structural coordinates for 16 α-carbons found in the active site of a terpene synthase.

Table 4. Interatomic distances in Angstroms between each α-carbon of Table 3. Each α-carbon occupies a sphere having a radius of 2.3 Angstroms. Interatomic distances are calculated from the center point of each sphere.

Table 5. X-ray crystallographic structural coordinates for nine α-carbons found in the active site of a terpene synthase.

Table 6. Interatomic distances in Angstroms between each α-carbon of Table 5. Each α-carbon occupies a sphere having a radius of 2.3 Angstroms. Interatomic distances are calculated from the center point of each sphere.

Table 7. Ordered arrangement of R-groups not found associated with the α-carbons of Table 1.

Table 8. Ordered arrangement of R-groups not found associated with the α-carbons of Table 3.

Table 9. Ordered arrangement of R-groups not found associated with the α-carbons of Table 5.

Table 10. X-ray structural coordinates for TEAS having the substrate analog FHP bound in the active site.

Table 11. X-ray structural coordinates for TEAS in the absence of substrate.

Table 12. Alignment of residues 265–535 of TEAS with a limonene synthase, SEQ ID NO:22, using the BLASTp alignment program.

Table 13. Alignment of residues 579 to 847 of SEQ ID NO:44 with SEQ ID NO:26, using the BLASTp program.

Table 14. Alignment of residues 265 to 535 of TEAS with SEQ ID NO:48, using the BLASTp program.

Table 15. Alignment of residues 307 to 593 of SEQ ID NO:50 with SEQ ID NO:56 using the BLASTp program.

BRIEF DESCRIPTION OF THE SEQUENCE LISTING

SEQ ID NO:1 is the DNA coding sequence for a tobacco 5-epi-aristolochene synthase (TEAS) protein. Genbank No: Q40577.

SEQ ID NO:2 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:1.

SEQ ID NO:3 is the DNA coding sequence for a TEAS protein in which the codon for Trp273 has been changed to a codon for Glu.

SEQ ID NO:4 is the amino acid sequence for the W273E protein encoded by the TEAS DNA of SEQ ID NO:3.

SEQ ID NO:5 is the DNA coding sequence for a TEAS protein in which the codon for Tyr520 has been changed to a codon for Phe.

SEQ ID NO:6 is the amino add sequence for the Y520F protein encoded by the TEAS DNA of SEQ ID NO:5.

SEQ ID NO:7 is the DNA coding sequence for a TEAS protein in which the codon for Tyr527 has been changed to a codon for Phe.

SEQ ID NO:8 is the amino acid sequence for the Y527F protein encoded by the TEAS DNA of SEQ ID NO:7.

SEQ ID NO:9 is the DNA coding sequence for a TEAS protein in which the codon for Trp273 has been changed to a codon for Ser and the codon for Cys440 has been changed to a codon for Trp.

SEQ ID NO:10 is the amino acid sequence for the W273S/C440W protein encoded by the TEAS DNA of SEQ ID NO:9.

SEQ ID NO:11 is the DNA coding sequence for TEAS proteins in which the codons for Tyr406 and Leu407 have each been changed to the nucleotides NNS.

SEQ ID NO:12 is the amino acid sequence for the population of Y406X/L407X proteins encoded by the TEAS DNA of SEQ ID NO:11, where X is any naturally occurring amino acid.

SEQ ID NO:13 is a DNA primer sequence.

SEQ ID NO:14 is a DNA primer sequence.

SEQ ID NO:15 is a DNA primer sequence.

SEQ ID NO:16 is a DNA primer sequence.

SEQ ID NO:17 is a DNA primer sequence.

SEQ ID NO:18 is a DNA primer sequence.

SEQ ID NO:19 is the DNA coding sequence for a grand fir pinene synthase. Genbank Accession No: U87909.

SEQ ID NO:20 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:19.

SEQ ID NO:21 is the DNA coding sequence for a spearmint limonene synthase. Genbank Accession No: L13459.

SEQ ID NO:22 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:21.

SEQ ID NO:23 is the DNA coding sequence for a sage 1, 8 cineole synthase. Genbank Accession No: AF051899.

SEQ ID NO:24 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:23.

SEQ ID NO:25 is the DNA coding sequence for a sage bornyl diphosphate synthase. Genbank Accession No: AF051900.

SEQ ID NO:26 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:25.

SEQ ID NO:27 is the DNA coding sequence for a mint E-b-farnesene synthase. Genbank Accession No: AF024615.

SEQ ID NO:28 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:27.

SEQ ID NO:29 is the DNA coding sequence for a grand fir myrcene synthase. Genbank Accession No: U87908.

SEQ ID NO:30 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:29.

SEQ ID NO:31 is the DNA coding sequence for a potato vetaspiradiene synthase. Genbank Accession No: AB022598.

SEQ ID NO:32 is the amino acid sequence for the pratein encoded by the DNA of SEQ ID NO:31.

SEQ ID NO:33 is the genomic DNA coding sequence for a cotton delta-cadinene synthase. Genbank Accession No: Y18484.

SEQ ID NOS: 34–40 are the amino acid sequences for the exons encoded by the DNA of SEQ ID NO:33.

SEQ ID NO:41 is the DNA coding sequence for a castor bean casbene synthase. Genbank Accession No: L32134.

SEQ ID NO:42 is the amino add sequence for the protein encoded by the DNA of SEQ ID NO:41.

SEQ ID NO:43 is the DNA coding sequence for a yew taxadiene synthase. Genbank Accession No: U48796.

SEQ ID NO:44 is the amino add sequence for the protein encoded by the DNA of SEQ ID NO:43.

SEQ ID NO:45 is the DNA coding sequence for a grand fir E-alpha-bisabolene synthase. Genbank Accession No: AF006194.

SEQ ID NO:46 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:45.

SEQ ID NO:47 is the DNA coding sequence for a grand fir delta-selinene synthase. Genbank Accession No: U92266.

SEQ ID NO:48 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:47.

SEQ ID NO:49 is the DNA coding sequence for a grand fir gamma-humulene synthase. Genbank Accession No: U92267.

SEQ ID NO:50 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:49.

SEQ ID NO:51 is the DNA coding sequence for a tomato germacrene C synthase. Genbank Accession No: AF035631.

SEQ ID NO:52 is the amino add sequence for the protein encoded by the DNA of SEQ ID NO:51.

SEQ ID NO:53 is the DNA coding sequence for a sage +sabinene synthase. Genbank Accession No: AF051901.

SEQ ID NO:54 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:53.

SEQ ID NO:55 is the DNA coding sequence for a grand fir abietadiene synthase. Genbank Accession No: U50768.

SEQ ID NO:56 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:55.

SEQ ID NO:57 is the. DNA coding sequence for a grand fir limonene synthase. Genbank Accession No: AF06193.

SEQ ID NO:58 is the amino acid sequence for the protein encoded by the DNA of SEQ ID NO:57.

DETAILED DESCRIPTION

The following terms are used herein:

"α-carbon" refers to the chiral carbon atom found in an amino acid residue. Four substituents are covalently bound to the α-carbon, including an amino group, a carboxyl group, a hydrogen atom, and an R-group.

"R-group" refers to a substituent attached to the α-carbon of an amino acid residue that is not involved in peptide bond formation in a protein. An R-group is an important determinant of the overall chemical character of an amino acid. The twenty naturally occurring amino acids found in proteins and the R-groups associated with the α-carbon of each amino acid are listed in FIG. **2**. The three-letter and one-letter abbreviations for naturally occurring amino acids are sometimes used herein to refer to the R-group associated with a particular amino acid.

"Naturally occurring amino acid" includes L-isomers of the twenty amino acids naturally occurring in proteins. Naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, arginine, and lysine. Unless specially indicated, all amino acids referred to in this application are in the L-form. Three-letter and one-letter abbreviations are sometimes used herein to refer to naturally occurring amino acids. These abbreviations are known in the art.

"Unnatural amino add" includes amino acids that are not naturally found in proteins. Examples of unnatural amino acids included herein are racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of norleucine, para-nitrophenylalanine, homophenylalanine, para-fluorophenylalanine, 3-amino-2-benzylpropionic acid, homoarginine, D-phenylalanine, and the like.

"Positively charged amino acid" includes any naturally occurring or unnatural amino acid having an R-group that carries a positive charge under normal physiological conditions. Examples of positively charged, naturally occurring amino acids include arginine and lysine.

"Negatively charged amino acid" includes any naturally occurring or unnatural amino acid having an R-group that carries a negative charge under normal physiological conditions. Examples of negatively charged, naturally occurring amino acids include aspartic add and glutamic acid.

"Hydrophobic amino acid" includes any naturally occurring or unnatural amino acid having an uncharged, nonpolar side chain under normal physiological conditions. Examples of naturally occurring hydrophobic amino acids are leucine, isoleucine, valine and methionine.

"Hydrophilic amino acid" includes any naturally occurring or unnatural amino acid having a charged polar side chain. Examples of naturally occurring hydrophilic amino acids include serine, threonine and cysteine.

"Mutant terpene synthase" or "mutated terpene synthase" refers to a synthase polypeptide having a primary amino acid sequence. The center point of the α-carbon of nine residues of the polypeptide is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the nine spheres have the structural coordinates of Table 5 or coordinates which can be rotated and/or translated to coincide with the coordinates of Table 5. The relative interatomic distances between the nine α-carbons is ±2.3 angstroms of the interatomic distances given in Table 6. Each α-carbon has an associated R-group. A mutant synthase differs from a non-mutant synthase in the ordered arrangement of R-groups associated with the nine α-carbons. A mutant synthase has an ordered arrangement of R-groups on the nine α-carbons other than the ordered arrangements of R-groups listed in Table 9. R-groups associated with other carbons of the synthase primary amino acid sequence mayor may not be the same as in a non-mutated synthase.

In some embodiments, a mutant synthase refers to a synthase in which the center point of the α-carbon of sixteen residues of the polypeptide is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the sixteen spheres have the structural coordinates of Table 3 or coordinates which can be rotated and/or translated to coincide with the coordinates of Table 3. The relative interatomic distances between the nine α-carbons is ±2.3 angstroms of the interatomic distances given in Table 4. Each α-carbon has an associated R-group. A mutant synthase differs from a non-mutant synthase in the ordered arrangement of R-groups associated with the sixteen α-carbons. A mutant synthase has an ordered arrangement of R-groups on the sixteen α-carbons other than the ordered arrangements of R-groups listed in Table 8. R-groups associated with other α-carbons of the synthase primary amino acid sequence may or may not be the same as in a non-mutated synthase.

In some embodiments, a mutant synthase refers to a synthase in which the center point of the α-carbon of nineteen residues of the polypeptide is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the nineteen spheres have the three dimensional coordinates of Table 1 or coordinates which can be rotated and/or translated to coincide with the coordinates of Table 1. The relative interatomic distances between the nineteen α-carbons is ±2.3 angstroms of the interatomic distances given in Table 2. Each α-carbon has an associated R-group. A mutant synthase differs from a non-mutant synthase in the ordered arrangement of R-groups associated with the nineteen α-carbons. A mutant synthase has an ordered arrangement of R-groups on the nineteen α-carbons other than the ordered arrangements of R-groups listed in Table 7. R-groups associated with other α-carbons of the synthase primary amino acid sequence may or may not be the same as in a non-mutated synthase.

"Nonmutated synthase" or "non-mutant synthase" includes a synthase having a primary amino acid sequence comprising nine, sixteen, or nineteen amino acid residues. The center point of each α-carbon of these residues is positioned within a sphere having a radius of 2.3 Angstroms; the center points of the spheres have the three dimensional coordinates of Tables 5, 3, or 1, respectively, or coordinates which can be rotated and/or translated to coincide with the coordinates of Tables 5, 3, or 1. The relative interatomic distances between the nine, sixteen, or nineteen α-carbons is ±2.3 angstroms of the interatomic distances given in Tables 6, 4, or 2, respectively. Each α-carbon has an associated R-group. A non-mutant synthase has an ordered arrangement of R-groups on the nine, sixteen, or nineteen α-carbons as listed in Tables 9, 8, or 7, respectively.

"Degenerate variations thereof" refers to variants of a gene coding sequence by which the same polypeptide is encoded by different nucleotide sequences, due to the degeneracy of the genetic code. For example, synthases of the present invention have a primary amino acid sequence. Degenerate synthase variations are different nucleic acid coding sequences that nevertheless encode the same primary amino acid sequence due to the degeneracy of the genetic code.

"Expression" refers to transcription of a gene or nucleic acid molecule and the translation of that nucleic acid into a

polypeptide. Expression of genes also involves processing of RNA into mRNA in eukaryotic systems. It is not necessary for the genes to integrate into the genome of a cell in order to achieve expression. This definition is not limited to expression in a particular system or a particular cell type and includes, without limitation, stable, transient, in vitro, and in vivo expression.

"Promoter" and "promoter regulatory element", refers to a nucleic acid that is involved in controlling expression of a gene. Promoter regulatory elements, and the like, from a variety of sources can be used efficiently to promote gene expression. Promoter regulatory elements include constitutive, tissue-specific, developmental-specific, inducible, subgenomic promoters, and the like. Promoter regulatory elements may also include certain enhancer elements or silencing elements that improve or regulate transcriptional efficiency.

"Active Site" refers to a site in a terpene synthase that binds the hydrophobic portion of a terpene substrate, GPP, FPP, and/or GGPP. The active site can, under certain conditions, catalyze a biosynthetic reaction that allows one or more reaction products to be produced.

"Altered enzymatic specificity" includes an alteration in the ability of a mutant synthase to use a particular terpene substrate or a change in the profile of reaction product(s) from a mutant synthase, compared to the substrate specificity of and the reaction products made by a corresponding non-mutated synthase. Altered specificity may include the ability of a synthase to exhibit different enzymatic parameters relative to a non-mutated synthase (Km, Vmax, etc), and/or to produce products that are different from those that are produced by a corresponding non-mutant synthase.

"Structure coordinates" or "structural coordinates" refers to Cartesian coordinates (x, y, and z positions) derived from mathematical equations involving Fourier synthesis as determined from patterns obtained via diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a synthase molecule in crystal form. Diffraction data are used to calculate electron density maps of repeating protein units in the crystal (unit cell). Electron density maps are used to establish the positions of individual atoms within a crystal's unit cell. The absolute values for structural coordinates listed herein convey relative spatial relationships between atoms because the absolute values ascribed to structural coordinates can be changed by rotational and/or translational movement along the x, y and/or z axes, together or separately, while maintaining the same relative spatial relationships among atoms. Thus, a terpene synthase whose absolute values for a set of structural coordinates can be rotationally or translationally adjusted to coincide with the particular values listed in Tables 1, 3, or 5 is considered to have the same structural coordinates as those of Tables 1, 3 or 5. An example of structural coordinates that coincide with the absolute values listed herein after rotation and/or translation are the coordinates of Table 11.

"Heavy atom derivatization" refers to a method of Producing a chemically modified form of a synthase crystal. In practice, a crystal is soaked in a solution containing heavy atom salts or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal, uranyl acetate and the like, which can diffuse through the crystal and bind to the protein's surface. Locations of the bound heavy atoms can be determined by X-ray diffraction analysis of the soaked crystal. The information is then used to construct phase information which can then be used to construct three-dimensional structures of the enzyme as described in Blundel, T. L., and Johnson, N. L., Protein Crystallography, Academic Press (1976).

"Unit cell" refers to a basic parallelepiped shaped block. Regular assembly of such blocks may construct the entire volume of a crystal. Each unit cell comprises a complete representation of the unit pattern, the repetition of which builds up the crystal.

"Mutagenesis" refers to the substitution of a different amino acid residue at a particular position in the primary amino acid sequence of a protein, thereby changing the R-group present at that position. Mutagenesis can be most easily performed by changing the coding sequence of a nucleic acid encoding the protein so that the coding sequence in the nucleic acid specifies an amino acid residue different from the residue initially present at that position.

"Space Group" refers to the arrangement of symmetry elements within a crystal.

"Molecular replacement" refers to the generation of a preliminary model of a synthase whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, E., 1985, in Methods in Enzymology, 115:55–77; Rossmann, MG., ed., "The Molecular Replacement Method" 1972, Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York). Using structure coordinates and interatomic distance matrices, molecular replacement may be used to determine the structural coordinates of a crystalline mutant, homologue, or a different crystal form of terpene synthase.

"Recombinant protein" includes a protein that is chemically synthesized or derived biosynthetically from an isolated gene.

"Gene" includes naturally derived or genetically manipulated nucleic acids that contain the information needed to produce a polypeptide.

"Nucleic acid" includes any genetic material comprised of the nucleotides guanine, adenine, thymine, cytosine, uracil, inosine and the like. Nucleic acids may be single-, double, or triple stranded. Nucleic acids may be deoxyribonucleic acid or ribonucleic acid.

"Genetically manipulated" includes genes that have been modified to contain a different nucleotide sequence from that present in a preselected nucleic acid. Genes can be manipulated by synthetically or via traditional cloning, PCR, chemical gene synthesis, direct or random mutagenesis, and gene shuffling. Genetically manipulated also includes the process of making genes that are degenerate variations of nucleic acids encoding preselected proteins.

"First domain" includes polypeptides having a first and second end wherein the first end can have an amino terminal amino acid with a free amino group and can be linked by a peptide bond to a second amino acid. The first end may also be modified through acetylation and the like. The second end of the first domain may or may not have a free carboxyl terminal group.

"Second domain" includes polypeptides having a first and second end wherein the first end can have an amino terminal amino add and can be linked by a peptide bond to a second

amino acid. The second end of the second domain may or may not have a carboxyl terminal group. Typically, the first end of the second domain is linked to the second end of the first domain via a peptide bond.

"Isoprenoid substrate" refers to the C_{10}, C_{15}, and C_{20} molecules, named geranyl diphosphate (GPP), farnesyl diphosphate (FPP), and geranylgeranyl diphosphate (GGPP), respectively.

"Sequence identity" or "percent sequence identity" refers to the percentage of amino acids or nucleotides that occupy the same relative position when two protein sequences or nucleic acid sequences, a query sequence and a subject sequence, are aligned. The number of amino acid or nucleotide residues that are identical between both the subject and query sequences are counted, divided by the number of residues in the query sequence, and multiplied by 100. The process is repeated until the alignment resulting in the highest percent sequence identity is found. Percent sequence identity can be determined by visual inspection and/or by using various computer programs, e.g., MegAlign (DNASTAR, Inc., Madison, Wisconsin) or BLAST programs available on the world wide web from the National Center for Biotechnology Information (NCBI). Gaps of one or more residues may sometimes be inserted to maximize sequence alignments to structurally conserved domains of the query sequence, i.e., α-helices, β-sheets and loops.

"Monoterpene product" refers to linear, cyclized, and/or hydroxylated reaction products made from the substrate GPP. "Sesquiterpene product" refers to linear, cyclized, and/or hydroxylated reaction products made from the substrate FPP. "Diterpene product" refers to linear, cyclized, and/or hydroxylated reaction products made from the substrate GGPP.

The present invention relates to terpene synthases and mutants thereof from which the position of specific α-carbon atoms and R-groups associated therewith comprising the active site can be determined in three-dimensional space. The invention also relates to structural coordinates of the synthases, use of the structural coordinates to develop structural information related to synthase homologues, mutants, and the like, and to crystal forms of such synthases. Furthermore, the invention provides a method whereby α-carbon structural coordinates for atoms comprising the active site of a preselected terpene synthase can be used to develop synthases in which R-groups associated with active site α-carbon atoms are different from the R-groups found in the preselected terpene synthase. In addition, the present invention provides for the production of novel terpene synthases based on the structural information provided herein and for the use of such synthases to make a variety of isoprenoid compounds.

The present invention further provides, for the first time, crystals of a synthase, as exemplified by tobacco 5-epi-aristolochene synthase (TEAS), which are grown in the presence or absence of substrate and substrate analogues, thus allowing definition of the structural coordinates associated therewith. The structural coordinates allow determination of the carbon atoms comprising the active site and R-groups associated therewith. The crystals of the present invention belong to the tetragonal space group $P4_12_12$; the unit cell dimensions vary by a few angstroms between crystals but on average a=126 angstroms, c=122 angstroms, a=b, α=90°, β=90°, and γ=90°.

Structural coordinates are preferably obtained at a resolution of about 2.2 to about 2.8 angstroms for a synthase in the presence and in the absence of bound substrate or substrate analog. Coordinates for a synthase with a substrate analog bound in the active site are given in Table 10. Coordinates for a synthase in the absence of a substrate analog bound in the active site are given in Table 11. Those skilled in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. Therefore, for the purpose of this invention, any set of structure coordinates wherein the active site α-carbons of a synthase, synthase homologue, or mutants thereof, have a root mean square deviation less than ±2.3 angstroms when superimposed using the structural coordinates listed in Table 1–3, or 5, are considered identical.

A schematic representation of the three-dimensional shape of a synthase is shown in FIG. **1** which was prepared by RIBBONS (Carson and Bugg, 1986, J. Mol. Graphics, 4:121). The synthase shown in FIG. **1** consists entirely of α-helices and short connecting loops and turns, organized into first and second structural domains.

In one embodiment, an isolated synthase of the invention comprises sixteen active site carbons having the structural coordinates of Table 3 and the relative distances ±2.3 angstroms of the distances given in Table 4. The active site α-carbons of Table 3 generally are not all contiguous, i.e., are not adjacent to one another in the primary amino acid sequence of a synthase, due to intervening amino acid residues between various active site α-carbons. On the other hand, it should be appreciated that some of the active site α-carbons can be adjacent to one another in some instances. In the embodiment depicted in the TEAS Y527F protein (SEQ ID NO:8), for example, active site α-carbons are adjacent to one another in the primary amino acid sequence at positions 402, 403 and 404, respectively, whereas active site α-carbons at residues 273 and 294 are separated and thus are not adjacent. Thus, the numbering of active site α-carbons given in Tables 1, 2, 3, 4, 5, or 6 is merely for convenience and such α-carbons may reside at any position in the primary amino acid sequence that achieves the structural coordinates given in Tables 1, 3, or 5 and the relative interatomic distances ±2.3 angstroms given in Tables 2, 4, or 6.

An appropriate combination of R-groups, linked to active site α-carbons, can facilitate the formation of one or more desired reaction products. The combination of R-groups selected for use in a terpene synthase of the invention can be any combination other than the ordered arrangements of R-groups and corresponding active site α-carbons shown in Tables 7, 8, or 9. An illustrative example of a suitable arrangement of R-groups and α-carbons is Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu, Cys, Val, Thr, Phe, Asp, Tyr and Thr, associated with active site α-carbons 1 to 16, respectively, of Table 3. Another example of a suitable arrangement of R-groups and α-carbons is Cys, Trp, Ile, Ile, Ser, Thr, Thr, Tyr, Leu, Cys, Val, Thr, Tyr, Asp, Phe, and Thr at active site alpha-carbons 1 to 16, respectively, of Table 3. In some embodiments, a synthase of the invention may have primary amino acid sequences as listed in SEQ ID NO:4, SEQ ID NO:6, SEQ ID NO:8, and SEQ ID NO:10, DNA molecules encoding the same, which are listed in SEQ ID NO:3, SEQ ID NO:5, SEQ ID NO:7, and SEQ ID NO:9, respectively, and degenerate variations thereof. Typically, R-groups found on active site α-carbons are those found in naturally occurring amino acids. See, e.g., FIG. **2**. In some embodiments, however, R-groups other than naturally occurring amino acids can be used.

Some arrangements of R-groups and active site α-carbons result in mutant terpene synthases that form reaction products. Such enzymatically active synthases and their corre-

sponding genes are useful to make known terpenoid hydrocarbons, e.g., monoterpenes such as pinene, sesquiterpenes such as delta-cadinene and diterpenes such as abietadiene. Other enzymatically active synthases can be used to make novel terpenoid products.

Some arrangements of R-groups and active site α-carbons may result in mutant terpene synthases that do not form reaction product(s) at a desired rate. Such synthases and their genes are useful as controls in analyses of product formation by enzymatically active mutant synthases. Such synthases and their genes can also be useful in analyses of translation of enzymatically active mutant synthase genes, or as nutritional supplements. Such synthases can be attached to Sepharose beads and used for affinity purification of isoprenoid compounds from crude preparations. In addition, such synthases and their genes can also be useful to develop reagents for various purposes, e.g., immunological reagents to monitor expression of a terpene synthase protein or nucleic acid probes or primers to monitor inheritance of a terpene synthase gene in a plant breeding program.

In some embodiments, the α-carbon backbone of a synthase first domain aligns structurally with the catalytic core of glycosyl hydrolases, as exemplified by glucoamylase (Brookhaven Protein Database (PDB) code 3GLY) from Aspergillus awamori (Aleshin et al., 1994, J. Mol. Biol., 238:575) and endoglucanase CelD (PDB code ICLC) from Clostridium thermocelum (Juy et al., 1992, Nature, 357:89), and the α-carbon backbone of a synthase second domain, which contains the active site, aligns structurally with avian farnesyl diphosphate synthase (FPS), wherein the active site is comprised of 9, 16, or 19 amino acid residues with α-carbon structural coordinates as listed in Tables 1, 3, or 5 and interatomic distances as described in Tables 2, 4, or 6. Such α-carbons have an ordered arrangement of R-groups different from that observed in a non-mutated synthase.

In the present invention, the first domain forms a twisted α-barrel made up of eight short (10 to 15 amino acid residues) helices surrounding a surface cavity filled by ordered water molecules when hydrated. The second domain comprises a two-layered barrel of a-helices surrounding a hydrophobic and aromatic-rich active site pocket. Typically, the second domain contains a substrate binding site. As exemplified in FIG. **1**, helix H is disrupted between segments H1 and H2 by an amino acid such as proline, but its interhelical packing with helix G is accommodated by a corresponding kink in helix G between G1 and G2. Within this kink, hydrogen bonds between a hydroxyl group, such as that found on a threonine, and the carbonyl oxygen of other amino acids disrupt the main chain intrahelical hydrogen bonding of helix G thus assisting in producing the structure as determined.

As exemplified by TEAS, terpene synthases of the present invention can have a first domain segment comprising helices A and C (an A-C loop), and a second domain comprising helices J and K (a J-K loop) (FIG. **1**). The ordering of these loops upon substrate binding results in a closed, solvent-inaccessible active site pocket. As the J-K loop becomes ordered, a lid-type structure is formed that clamps down over the active site entrance in the presence of substrate and an extended aromatic patch deep within the active site pocket is formed. As the A-C loop becomes ordered, it translates inward toward the active site, positioning certain R groups in this loop at or near the active site. Thus, substrate binding to the active site results in a change in protein conformation.

To identify or create mutant terpene synthases, sequence alignments can be performed to locate specific residues and α-carbons in a preselected polypeptide that have the structural coordinates and interatomic distances of Tables 1–2, 3–4 or 5–6. The preselected polypeptide is used as the subject sequence in the alignment, e.g., the full-length primary amino acid sequence, a region 190 residues in length, a region 220 residues in length, or a region 300 residues in length. The alignment can use residues 265 to 535 of TEAS (SEQ ID NO:2), which includes the α-carbons of Tables 1, 3 or 5, as the query sequence to align with the preselected polypeptide. The preselected polypeptide and the query sequence can be aligned using the BLASTp 2.0.9 computer program with a BLOSUM 62 scoring matrix, an expect value of 10, a gap open value of 11, an x_dropoff value of 50, a gap extension value of 1, a wordsize of 3 and no filtering of low complexity sequences. As an alternative, the BLASTp 2.0.9 program can be used with a BLOSUM 50 scoring matrix, an expect value of 10, a gap open value 13, an x_dropoff value of 50, a gap extension value of 2, a wordsize of 3 and no filtering of low complexity sequences. Other parameter values can also be used, e.g., a gap extension value from 0 to 4. See Altschul, et al., Nucl. Acids Res. 25:3389–3402.

Regions of the preselected polypeptide with significant sequence identity to residues 265–535 of TEAS, e.g., 20% or greater sequence identity, 25% or greater sequence identity, 35% or greater sequence identity, 40% or greater sequence identity, 50% or greater sequence identity, 60% or greater sequence identity, 70% or greater sequence identity, or 80% or greater sequence identity are examined for specific residues that align with the TEAS residues corresponding to those listed in Tables 1, 3, or 5. In some cases, the output of the computer program alignment identifies a specific residue in the preselected polypeptide for each of the nine, sixteen, or nineteen residues in the query sequence having the structural coordinates and interatomic distances of Tables 1–2, 3–4 or 5–6, with or without gaps introduced by the alignment program. In other cases, a gap is introduced by the alignment program in either the query sequence or the subject sequence such that no direct alignment or a misalignment occurs between one or more of the nine, sixteen, or nineteen residues in the query sequence that are of interest In either case, the output can be visually inspected, and specific residues can be chosen in the subject sequence after adjusting the alignment so that alpha-helices and beta-sheet regions in the query sequence are maintained and that gaps or insertions in the subject sequence align with loop regions of the query sentence.

Sequence alignments suggest that other terpene synthases have regions with 20% or greater sequence identity to residues 265–535 of TEAS. Therefore, a region of a terpene synthase other than TEAS can be used as the query sequence, e.g., regions of terpene synthases given in SEQ ID NOS: 4, 6, 8, 10, 12, 20, 22, 24, 26, 28, 30, 32, 34–40, 42, 44, 46, 48, 50, 52, 54, 56, or 58, that have significant sequence identity to residues 265–535 of SEQ ID NO:2. For example, large sequence insertions are present at the amino terminus in taxadiene synthase (SEQ ID NO:44) with respect to TEAS, or are within solvent-exposed loops in the amino-terminal domain. Thus, regions of taxadiene synthase with greater than 20% sequence identity to SEQ ID NO:2 are doser to the carboxy-terminal end, e.g., from residue 579 to residue 847 of SEQ ID NO:44.

Useful regions of other terpene synthases that can be used as the query sequence include, without limitation, residues 343 to 606 of SEQ ID NO:20, 316 to 586 of SEQ ID NO:22, residues 352 to 622 of SEQ ID NO:58, residues 272 to 540 encoded by SEQ ID NO:33, residues 319 to 571 of SEQ ID

NO:42, residues 579 to 847 of SEQ ID NO:44, residues 495 to 767 of SEQ ID NO:46, residues 295 to 564 of SEQ ID NO:48, residues 307 to 578 of SEQ 10 NO:50, residues 264 to 533 of SEQ ID NO:52, residues 585 to 853 of SEQ ID NO:56, residues 307 to 574 of SEQ ID NO:54, residues 309 to 577 of SEQ ID NO:24, residues 315 to 584 of SEQ ID NO:26, residues 265 to 536 of SEQ ID NO:28, residues 342 to 612 of SEQ ID NO:30 and residues 273 to 541 of SEQ ID NO:32.

One or more of the specific residues in the subject sequence that align with residues in the query sequence are mutated in the preselected polypeptide, e.g, by making mutations in a nucleic acid encoding the polypeptide. The mutant terpene synthase thus created can then be expressed in a host cell and the protein evaluated for enzymatic activity, if desired.

Mutant proteins of the present invention may be prepared in a number of ways including but not limited to oligonucleotide-directed mutagenesis, deletion, chemical mutagenesis, and the like. One or more R-groups associated with the active site α-carbon atoms in a terpene synthase are changed by altering the nucleotide sequence of the corresponding gene. For example, a mutation can be introduced into SEQ ID NO:1, the nucleotide sequence for TEAS, at codons encoding one or more of the following sixteen α-carbons: α-carbon 1=Cys 270; α-carbon 2=Trp 273; α-carbon 3=Ile 294; α-carbon 4=Ile 297; α-carbon 5=Ser298; α-carbon 6=Thr 402; α-carbon 7=Thr 403; α-carbon 8=Tyr 404; α-carbon 9=Leu 407; α-carbon 10=Cys 440; α-carbon 11=Val 516; α-carbon 12=Thr 519; α-carbon 13=Tyr 520; α-carbon 14=Asp 525; α-carbon 15=Tyr 527; or α-carbon 16=Thr 528. The protein encoded by the mutant gene is then produced by expressing the gene in, for example, a bacterial or plant expression system. Alteratively, synthase mutants may be generated by site specific replacement of a particular amino acid with an unnaturally occurring amino acid. As such, synthase mutants may be generated through replacement of an amino acid residue or a particular cysteine or methionine residue with selenocysteine or selenomethionine. This may be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of natural cysteine or methionine or both and growing on medium enriched with either selenocysteine, selenomethionine, or both. These and similar techniques are described in Sambrook et al., (Molecular Cloning, A Laboratory Manual, 2nd Ed. (1989) Cold Spring Harbor Laboratory Press).

Another suitable method of creating mutant synthases of the present invention is based on a procedure described in Noel and Tsal (1989) J. Cell. Biochem., 40:309–320. In so doing, the nucleic acid encoding the synthase can be synthetically produced using oligonucleotides having overlapping regions, the oligonucleotides being degenerate at specific bases so that mutations are induced.

According to the present invention, nucleic acid sequences encoding a mutated synthase can be produced by the methods described herein, or any alternative methods available to the skilled artisan. In designing the nucleic acid sequence (gene) of interest, it may be desirable to reengineer the gene for improved expression in a particular expression system. For example, it has been shown that many bacterially derived genes do not express well in plant systems. In some cases, plant-derived genes do not express well in bacteria. This phenomenon may be due to the non-optimal G+C content or A+T content of the gene relative to the expression system being used. For example, the very low G+C content of many bacterial genes results in the generation of sequences mimicking or duplicating plant gene control sequences that are highly A+T rich. The presence of A+T rich sequences within the genes introduced into plants (e.g., TATA box regions normally found in gene promoters) may result in aberrant transcription of the gene(s). In addition, the presence of other regulatory sequences residing in the transcribed mRNA (e.g. polyadenylation signal sequences (AAUAAA) or sequences complementary to small nuclear RNAs involved in pre-mRNA splicing) may lead to RNA instability. Therefore, one goal in the design of genes is to generate nucleic acid sequences that have a G+C content that affords mRNA stability and translation accuracy for a particular expression system.

Due to the plasticity afforded by the redundancy of the genetic code (i.e., some amino acids are specified by more than one codon), evolution of the genomes of different organisms or classes of organisms has resulted in differential usage of redundant codons. This "codon bias" is reflected in the mean base composition of protein coding regions. For example, organisms with relatively low G+C contents utilize codons having A or T in the third position of redundant codons, whereas those having higher G+C contents utilize codons having G or C in the third position. Therefore, in reengineering genes for expression, one may wish to determine the codon bias of the organism in which the gene is to be expressed. Looking at the usage of the codons as determined for genes of a particular organism deposited in GenBank can provide this information. After determining the bias thereof, the new gene sequence can be analyzed for restriction enzyme sites as well as other sites that could affect transcription such as exon:intron junctions, polyA addition signals, or RNA polymerase termination signals.

Genes encoding synthases can be placed in an appropriate vector, depending on the artisan's interest, and can be expressed using a suitable expression system. An expression vector, as is well known in the art, typically includes elements that permit replication of said vector within the host cell and may contain one or more phenotypic markers for selection of cells containing said gene. The expression vector will typically contain sequences that control expression such as promoter sequences, ribosome binding sites, and translational initiation and termination sequences. Expression vectors may also contain elements such as subgenomic promoters, a repressor gene or various activator genes. The artisan may also choose to include nucleic acid sequences that result in secretion, of the gene product movement of said product to a particular organelle such as a plant plastid (see U.S. Pat. Nos. 4,762,785; 5,451,513 and 5,545,817), or other sequences that increase the ease of peptide purification, such as an affinity tag.

A wide variety of expression control sequences are useful in expressing mutated synthases when operably linked thereto. Such expression control sequences include, for example, the early and late promoters of SV40 for animal cells, the lac system, the trp system, major operator and promoter systems of phage λ, and the control regions of coat proteins, particularly those from RNA viruses in plants. In *E. coli*, a useful transcriptional control sequence is the T7 RNA polymerase binding promoter, which can be incorporated into a pET vector as described by Studier et al., (1990) Methods Enzymology, 185:60–89.

For expression, a desired gene should be operably linked to the expression control sequence and maintain the appropriate reading frame to permit production of the desired synthase. Any of a wide variety of well-known expression vectors are of use in the present invention. These include, for

example, vectors consisting of segments of chromosomal, non-chromosomal and synthetic DNA sequences such as those derived from SV40, bacterial plasmids (including those from *E. coli* such as col E1, pCR1, pBR322 and derivatives thereof, pMB9), wider host range plasmids such as RP4, phage DNA such as phage λ., NM989, M13, and other such systems as described by Sambrook et al., (Molecular Cloning, A Laboratory Manual, 2nd Ed. (1989) Cold Spring Harbor Laboratory Press).

A wide variety of host cells are available for expressing synthase mutants of the present invention. Such host cells include, without limitation, bacteria such as *E. coli*, Bacillus and Streptomyces, fungi, yeast, animal cells, plant cells, insect cells, and the like. Preferred embodiments of the present invention include terpene synthase mutants that are expressed in *E. coli* or in plant cells. Said plant cells can either be in suspension culture or a culture on a solid support such as an agar-based medium.

Genes encoding synthases of the present invention can also be expressed in transgenic plant cells. In order to produce transgenic plants, vectors containing a nucleic acid construct encoding a mutant terpene synthase are inserted into the plant genome. Preferably, these recombinant vectors are capable of stable integration into the plant genome. One variable in making a transgenic plant is the choice of a selectable marker gene. A selectable marker gene is used to identify transformed cells against a high background of untransformed cells. Such selectable marker genes include but are not limited to aminoglycoside phosphotransferase gene of transposon Tn5 (Aph II) which encodes resistance to the antibiotics kanamycin, neomycin, and G418, as well as those genes which encode for resistance or tolerance to glyphosate, hygromycin, methotrexate, phosphinothricin, imidazolinones, sulfonylureas, and triazolophyrimidine herbicides, such as chlorosulfuron, bromoxynil, dalapon and the like. In addition to a selectable marker gene, it may be desirable to use a reporter gene. In some instances a reporter gene may be used with a selectable marker. Reporter genes allow the detection of transformed cell and may be used at the discretion of the artisan. A list of these reporter genes is provided in K. Weising et al., 1988, Ann. Rev. Genetics, 22:421.

The genes are expressed either by promoters expressing in all tissues at all times (constitutive promoters), by promoters expressing in specific tissues (tissue-specific promoters), promoters expressing at specific stages of development (developmental promoters), and/or promoter expression in response to a stimulus or stimuli (inducible promoters). The choice of these is at the discretion of the artisan.

Several techniques exist for introducing foreign genes into plant cells, and for obtaining plants that stably maintain and express the introduced gene. Such techniques include acceleration of genetic material coated directly into cells (U.S. Pat. No. 4,945,050). Plant may also be transformed using Agrobacterium technology (U.S. Pat. Nos. 5,177,010, 5,104,310, 5,149,645, 5,469,976, 5,464,763, 4,940,838, 4,693,976, 5,591,616, 5,231,019, 5,463,174, 4,762,785, 5,004,863, and 5,159,135; European Patent Applications 116718, 290799, 320500, 604662, 627752, 0267159, and 0292435. Other transformation technologies include whiskers technology, see U.S. Pat. Nos. 5,302,523 and 5,464,765. Electroporation technology has also been used to transform plants, see WO 87/06614, WO 92/09696 and WO 93/21335 and U.S. Pat. Nos. 5,472,869 and 5,384,253. Viral vector expression systems can also be used such as those described in U.S. Pat. Nos. 5,316,931, 5,589,367, 5,811,653, and 5,866,785.

In addition to numerous technologies for transforming plants, the type of tissue that is contacted with the genes of interest may vary as well. Suitable tissue includes, but is not limited to, embryogenic tissue, callus tissue, hypocotyl, meristem and the like. Almost all plant tissues may be transformed during dedifferentiation using the appropriate techniques described herein.

Regardless of the transformation system used, a gene encoding a mutant synthase is preferably incorporated into a gene transfer vector adapted to express said gene in a plant cell by including in the vector an expression control sequence (plant promoter regulatory element). In addition to plant promoter regulatory elements, promoter regulatory elements from a variety of sources can be used efficiently in plant cells to express foreign genes. For example, promoter regulatory elements of bacterial origin, such as the octopine synthase promoter, the nopaline synthase promoter, the mannopine synthase promoter may be used. Promoters of viral origin, such as the cauliflower mosaic virus (35S and 19S) are also desirable. Plant promoter regulatory elements also include, but are not limited to, ribulose-1,6-bisphosphate carboxylase small subunit promoter, beta-conglycinin promoter, phaseolin promoter, ADH promoter, heat-shock promoters, and tissue specific promoters and the like. Numerous promoters are available to skilled artisans for use at their discretion.

It should be understood that not all expression vectors and expression systems function in the same way to express the mutated gene sequences of the present invention. Neither do all host cells function equally well with the same expression system. However, one skilled in the art may make a selection among these vectors, expression control sequences, and host without undue experimentation and without departing from the scope of this invention.

Once a synthase of the present invention is expressed, the protein obtained therefrom can be purified so that structural analysis, modeling, and/or biochemical analysis can be performed, as exemplified herein. The nature of the protein obtained can be dependent on the expression system used. For example, genes, when expressed in mammalian or other eukaryotic cells, may contain latent signal sequences that may result in glycosylation, phosphorylation, or other post-translational modifications, which may or may not alter function. Once the proteins are expressed, they can be easily isolated and purified using techniques common to the person having ordinary skill in the art of protein biochemistry and as described in Colligan et al., (1997) Current Protocols in Protein Science, Chanda, V. B., Ed., John Wiley & Sons, Inc. Such techniques often include the use of cation-exchange or anion-exchange chromatography, gel filtration-size exclusion chromatography, and the like. Another technique that may be commonly used is affinity chromatography. Affinity chromatography can include the use of antibodies, substrate analogs, or histidine residues (His-tag technology).

Once purified, mutants of the present invention may be characterized by any of several different properties. For example, such mutants may have altered active site surface charges of one or more charge units. In addition, the mutants may have an altered substrate specificity or spectrum of reaction product relative to a non-mutated synthase.

The present invention allows for the characterization of mutant terpene synthase by crystallization followed by X-ray diffraction. Polypeptide crystallization occurs in solutions where the polypeptide concentration exceeds it solubility maximum (i.e., the polypeptide solution is supersaturated). Such solutions may be restored to equilib-

rium by reducing the polypeptide concentration, preferably through precipitation of the polypeptide crystals. Often polypeptides may be induced to crystallize from supersaturated solutions by adding agents that alter the polypeptide surface charges or perturb the interaction between the polypeptide and bulk water to promote associations that lead to crystallization.

Compounds known as "precipitants" are often used to decrease the solubility of the polypeptide in a concentrated solution by forming an energetically unfavorable precipitating depleted layer around the polypeptide molecules (Weber, 1991, Advances in Protein Chemistry, 41:1–36). In addition to precipitants, other materials are sometimes added to the polypeptide crystallization solution. These include buffers to adjust the pH of the solution and salts to reduce the solubility of the polypeptide. Various precipitants are known in the art and include the following: ethanol, 3-ethyl-2–4 pentanediol, and many of the polyglycols, such as polyethylene glycol.

Commonly used polypeptide crystallization methods include the following techniques: batch, hanging drop, seed initiation, and dialysis. In each of these methods, it is important to promote continued crystallization after nucleation by maintaining a supersaturated solution. In the batch method, polypeptide is mixed with precipitants to achieve supersaturation, the vessel is sealed and set aside until crystals appear. In the dialysis method, polypeptide is retained in a sealed dialysis membrane that is placed into a solution containing precipitant. Equilibration across the membrane increases the polypeptide and precipitant concentrations thereby causing the polypeptide to reach supersaturation levels.

In the preferred hanging drop technique (McPherson, 1976, J. Biol. Chem., 6300–6306), an initial polypeptide mixture is created by adding a precipitant to a concentrated polypeptide solution. The concentrations of the polypeptide and precipitants are such that in this initial form, the polypeptide does not crystallize. A small drop of this mixture is placed on a glass slide that is inverted and suspended over a reservoir of a second solution. The system is then sealed. Typically, the second solution contains a higher concentration of precipitant or other dehydrating agent. The difference in the precipitant concentrations causes the protein solution to have a higher vapor pressure than the solution. Since the system containing the two solutions is sealed, an equilibrium is established, and water from the polypeptide mixture transfers to the second solution. This equilibrium increases the polypeptide and precipitant concentration in the polypeptide solution. At the critical concentration of polypeptide and precipitant, a crystal of the polypeptide may form.

Another method of crystallization introduces a nucleation site into a concentrated polypeptide solution. Generally, a concentrated polypeptide solution is prepared and a seed crystal of the polypeptide is introduced into this solution. If the concentration of the polypeptide and any precipitants are correct, the seed crystal will provide a nucleation site around which larger crystal forms. In preferred embodiments, the crystals of the present invention are formed in hanging drops with 15% PEG 8000; 200 mM magnesium acetate or magnesium chloride, 100 mM 3-(N-morpholino)-2-hydroxypropanesulfonic acid (pH 7.0), 1 mM dithiothreitol as precipitant.

Some proteins may be recalcitrant to crystallization. However, several techniques are available to the skilled artisan to induce crystallization. The removal of polypeptide segments at the amino or carboxyl terminal end of the protein may facilitate production of crystalline protein samples. Removal of such segments can be done using molecular biology techniques or treatment of the protein with proteases such as trypsin, chymotrypsin, subtlisin. Such procedures can result in the removal of flexible polypeptide segments that may negatively affect crystallization.

The crystals so produced have a wide range of uses. For example, high quality crystals are suitable for X-ray or neutron diffraction analysis to determine the three-dimensional structure of a mutant synthase and to design additional mutants thereof. In addition, crystallization can serve as a further purification method. In some instances, a polypeptide or protein will crystallize from a heterogeneous mixture into crystals. Isolation of such crystals by filtration, centrifugation, etc., followed by redissolving the polypeptide affords a purified solution suitable for use in growing the high-quality crystals needed for diffraction studies. The high-quality crystals may also be dissolved in water and then formulated to provide an aqueous solution having other uses as desired.

Because synthases may crystallize in more than one crystal form, the structural coordinates of α-carbons of an active site determined from a synthase or portions thereof, as provided by this invention, are particularly useful to solve the structure of other crystal forms of synthases. The structural coordinates, as provided herein, may also be used to solve the structure of synthases having α-carbons position within the active sites in a manner similar to the wild-type yet having R-groups that may or may not be identical. Furthermore, the structural coordinates disclosed herein may be used to determine the structure of the crystalline form of other proteins with significant amino acid or structural homology to any functional domain of a synthase. One method that may be employed for such purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of a synthase, a synthase having a mutated active site, or the crystal of some other protein with significant sequence identity and/or structural homology of a synthase may be determined using the coordinates given in Tables 10 and/or 11. This method provides sufficient structural form for the unknown crystal more efficiently than attempting to determine such information ab initio. In addition, this method can be used to determine whether or not a given synthase in question falls within the scope of this invention.

As further disclosed herein, synthases and mutants thereof may be crystallized in the presence or absence of substrates and substrate analogs. The crystal structures of a series of complexes may then be solved by molecular replacement and compared to that of the wild-type to assist in determination of suitable replacements for R-groups within the active site, thus making synthase mutants according to the present invention.

All mutants of the present inventions may be modeled using the information disclosed herein without necessarily having to crystallize and solve the structure for each and every mutant. For example, one skilled in the art may use one of several specialized computer programs to assist in the process of designing synthases having mutated active sites. Examples of such programs can be as follows: GRID (Goodford, 1985, J. Med. Chem., 28:849–857); MCSS (Miranker and Karplus, 1991, Proteins: Structure, Function and Genetics, 11:29–34); AUTODOCK (Goodsell and Olsen, 1990, Proteins: Structure, Function, and Genetics, 8:195202); and DOCK (Kuntz et al., 1982, J. Mol. Biol., 161:269–288). In addition, specific computer programs are also available to evaluate specific substrate-active site inter-

actions and the deformation energies and electrostatic interactions resulting therefrom. MODELLER is a computer program often used for homology or comparative modeling of the three-dimensional structure of a protein. A. Sali & T. L. Blundell. J. Mol. Biol. 234, 779–815,1993. A preselected polypeptide sequence to be modeled is aligned with one or more terpene synthases whose crystal structures are known and the MODELLER program is used to calculate a full-atom model, based on optimum satisfaction of spatial restraints. Such restraints can include, inter alia, homologous structures, fluorescence spectroscopy, NMR experiments, or atom—atom potentials of mean force.

The present invention enables synthase mutants to be made and crystal structures thereof to be solved. Moreover, by virtue of the present invention, the location of the active site and the interface of substrate therewith permit the identification of desirable R-groups for mutagenesis. The particular embodiments of this invention are further exemplified in the Examples. However, those skilled in the art will readily appreciate that the specific experiments detailed are only illustrative of the invention as described more fully in the claims, which follow thereafter.

EXAMPLE 1

Generation of Mutant TEAS Genes

Construct Generation and Expression.

All mutant enzymes were constructed by the QuickChange method (Stratagene). Manufacturer's instructions were followed, except as noted. Mutations were confirmed by DNA sequencing, and plasmids containing the desired mutation were used to transform BL-21 (DE3) expression cells. Protein was expressed, purified, and stored at −80° C.

TEAS W273S. The TEAS W273S mutant was generated from a TEAS-pET28b(+) template using the following primers: GTTGAATGCTACTTTTCGGCATTAGGAGTTTTAT (sense) (SEQ ID NO:13) and ATAAACTCCTAATGCCGAAAAGTAGCATTCAAC (antisense) (SEQ ID NO:14). Mutagenesis was carried out according to the manufacturer's instructions, except that sense and antisense strands were generated in separate reactions. For each, 30 plasmid-copying cycles of one minute, annealing at 55° C. and 16 minutes extension at 68° C. were carried out. The two reaction mixtures were then combined, heated to 95° C. for 2.5 minutes, and cooled to room temperature before DpnI treatment.

TEAS C440W The TEAS C440W mutant was generated from the TEAS-pET28b(+) template using the following primers: GCTAGTGTAATTATATGGCGAGTTATCGATGAC (sense) (SEQ ID NO:15) and GTCATCGATMCTCGCCATATMTTACACTAGC (antisense) (SEQ ID NO:16).

TEAS W273S/C440W. The TEAS C440W/W273S mutant was constructed from a TEAS W273S-pET28b(+) template using the primers described for generation of TEAS C440W.

TEAS 406/407 random library. For generation of a library of TEAS mutants with random amino acids at positions 406 and 407, two 50 microliter QuickChange reactions were carried out with the TEAS-pET28b(+) template and the primers GCACTAGCMCTACCACATATTACNNSNNSGCGACMCATCGTATTTGGGCATG (sense) (SEQ ID NO:17) and CATGCCCAAATACGATGTTGTCGCSNNSNNGTAATATGTGGTAGTTGCTAGTGC (antisense) (SEQ ID NO:18), in which N denotes A, C, G, or T and S denotes C or G. By this choice of nucleotides, the reaction included primers which coded for all possible amino acid combinations at positions 406 and 407. No adjustment was made for differing numbers of codons among amino acids. In order to ensure efficient reactions, and to minimize the preference for hybridization of wild-type primers to the template, the primers were designed to be longer than those used to generate the mutations described above. In addition, they were HPLC purified prior to use. After 18 cycles of plasmid copying, the reaction was incubated for two hours with DpnI, ethanol precipitated, and redissolved in 5 microliters water. Each of four 40 microliter aliquots of *E. coli* NovaBlue (Novagen) cells were electroporated with 1.5 microliters of the redissolved DNA. After a recovery period, the cells were plated on kanamycin-LB-agar plates. In order to transfer the newly constructed plasmids to expression cells, the colonies were scraped from all four plates, and used to start an 8 mL culture grown in liquid LB medium at 37° C. for 8 hours. Plasmid purified from this culture was used to transform 20 microliters of competent BL-21 (DE3) cells.

For storage of the constructs, each individual colony was used to inoculate 100 microliters of LB medium containing kanamycin (50 micrograms/mL) in 96-well culture plates. The cells were grown at 37° C. until the A_{600} reached approximately one; 100 microliters of 30% glycerol in LB were then added, and the plates were frozen at −80° C. A set of randomly selected colonies were grown from individual glycerol stocks of some colonies, and plasmids were extracted for sequencing. Approximately 30 percent of the colonies were found to be wild-type. Nudeotide and amino acid sequences for TEAS 406/407 mutant genes and proteins are shown in SEQ ID NOS: 11 and 12.

TEAS Y520F The tyrosine residue at position 520 of SEQ ID No: 2 was changed to a phenylalanine residue by site-directed mutagenesis with primers, in a manner similar to that described above. For Y520F the TAT codon was changed to TTC. The nucleotide sequence of the mutant gene is shown in SEQ ID No: 5.

TEAS Y527F The tyrosine residue at position 527 of SEQ ID No: 2 was changed to a phenylalanine residue by site-directed mutagenesis with primers, in a manner similar to that described above. For Y527F, the TAC codon at position 527 of the TEAS amino acid sequence was changed to TTC. The nucleotide sequence of the mutant TEAS Y527F gene is shown in SEQ ID No: 7.

TEAS W273E The tryptophan residue at position 273 of SEQ ID No: 2 was changed to a phenylalanine residue by site-directed mutagenesis with primers, in a manner similar to that described above. For W273E, the TGG codon at position 273 of the TEAS amino acid sequence was changed to GAG. The nucleotide sequence of the mutant gene is shown in SEQ ID No.: 3.

EXAMPLE 2

Expression and Isolation of Synthase Polypeptides

Unless otherwise noted, mutated and non-mutated TEAS proteins were expressed in Escherichia coli, purified by metal chelation, anion exchange, and gel filtration chromatography.

Constructs of TEAS and mutant TEAS proteins in the vector pET-28b(+) (Novagen) were expressed in *E. coli* cells. For a typical protein preparation of any of these enzymes, *E. coli* strain BL21 (DE3) cells containing the plasmid construct were grown at 37° C. in 4 X 1 L terrific broth to an A_{600}=1.0. The temperature was dropped to 22°

C., and protein expression was induced by adding IPTG to a final concentration of 0.1 mM. After 15–20 h, the cells were harvested by centrifugation, resuspended in 5 mL buffer A (20 mM Tris, 500 mM NaCl, 20 mM imidazole, pH 7.9) per 1 g cells (wet weight), and stirred for 0.5 h at 4° C. The cells were then lysed by sonication, and the resulting lysate was centrifuged for 0.7 h at 82,000×g. The supernatant, containing the protein, was loaded over a 2–3 mL Ni^{2+} chelating histidine affinity column (Qiagen) equilibrated in buffer A, and the column was washed with additional buffer A until the A_{280} of the eluent returned to baseline. The protein was then eluted with a 20–200 mM imidazole gradient in buffer A. Protein-containing fractions were pooled and dialyzed against buffer B (50 mM HEPES, 5 mM MgCl2, 1 mM DTT), then loaded onto an 8 mL MonoQ cation-exchange column (Pharmacia). The column was washed with 20 column volumes buffer B, and the protein was eluted with a 0–500 mM NaCl gradient in buffer B. The resulting protein was further purified by gel filtration on a Superdex-200 column (Pharmacia) in 50 mM Tris, 100 mM NaCl, 5 mM MgCl2, 1 mM DTT, pH 8.0. Purified protein was then dialyzed against 5 mM Tris, 5 mM NaCl, 1 mM DTT, pH 8.0, concentrated to 18–22 mg/mL, and stored at −80° C. in 100° L aliquots until needed.

EXAMPLE 3

Crystallization and Structural Analysis of Synthase Polypetides

Crystal Growth and Microseeding: All crystallization attempts were carried out by the hanging-drop vapor diffusion method. Concentrated protein was mixed with an equal volume (2–5 uL each) of reservoir solution on a plastic cover slip. The cover slip was then inverted over a well of a plastic 24-well tissue culture plate, containing 0.5–1.0 mL of reservoir solution, and sealed by a layer of vacuum grease between the well and cover slip. The plates were incubated at 4° C. while the protein concentration in the hanging drop slowly increased by vapor diffusion. Approximately 300 different reservoir solutions, ranging pH 4.5–9 with a variety of precipitants and added salts, were assayed for crystallization of TEAS (SEQ ID NO:2). TEAS crystallized with a reservoir solution of 15% PEG 8000, 100 mM MOPSO (3-[N-morpholino]-2-hydroxypropanesulfonic acid), 200 mM magnesium acetate, 1 mM DTT, pH 6.9–7.3. For microseeding, an existing crystal was crushed in a few uL of precipitant solution, then diluted to 50 microliters. After initial centrifugation to remove large partides, the suspension was serially diluted with additional precipitant solution, and a small volume of a diluted seed stock was added to each new crystallization drop. For macroseeding, crystals which were no longer rapidly growing (usually 2 weeks after drops were set up), were "rinsed" by serially transferring them through two to three drops of reservoir solution. The crystal was then transferred to a fresh drop containing protein and reservoir solution, and equilibrated against a reservoir solution as in the initial growth. Individual crystals varied in their degree of internal order. In some cases, several crystals were screened to identify a well-diffracting crystal with low mosaicity.

Data collection: Prior to data collection, crystals were transferred to a drop of reservoir solution, or reservoir solution containing a compound to be soaked into the crystal A small volume of cryoprotectant solution (15% PEG8000, 100 mM MOPSO, 200 mM Mg acetate, 20% ethylene glycol, 1 mM DTT, pH 7) was then added to the drop. After a short equilibration time (1–5 minutes), the crystal was transferred to a drop of cryoprotectant, or cryoprotectant with soaking compound added. After another short equilibration time, the crystal was picked up on a nylon loop, and quickly mounted for data collection in a stream of cold nitrogen gas (90–110 K).

The TEAS crystals belonged to the tetragonal space group $P4_12_12$; the unit cell dimensions varied by a few angstroms between crystals, but on average a=126 Å, c=122 Å. The uncomplexed TEAS structure was initially refined to 2.8 Å (Table 11) against data collected from a crystal grown in the presence of 2 mM FHP (Table 10). Electron density at the active site allowed unambiguous modeling of FHP, the A-C and J-K loops, and nine additional residues at the NH_2 terminus, The refined TEAS-FHP model consisted of residues 17 to 548, three Mg^2+ ions. 150 water molecules, and one FHP molecule. The three-dimensional coordinates, or TEAS in the presence of bound substrate is shown in Table 10. The three-dimensional coordinates for TEAS in the absence of FHP is shown in Table 11.

Crystals of TEAS complexed with trifluoro-farnesyl diphosphate (F3-FPP) were also prepared. In these crystals, a well-ordered diphosphate binding pocket was also observed. The A-C loop and the NH2-terminal segment exhibited well-defined electron density, the A-C loop was translated toward the active site, and there was strong electron density for the diphosphate moiety of F3-FPP. The hydrophobic pocket, however, remained flexible; the J-K loop and the farnesyl moiety of F3-FPP were disordered.

Homology models were created and energy-minimized using the Swiss PDB viewer interface of the SwissModel program (Peitsch MC (1996), Biochem. Soc. Trans., 24:274–279 and Guex N. and Peitsch MC, 1997, Electrophoresis., 18:2714–2723). Active site volumes were calculated with VOIDOO (Kleywegt, G. J., and Jones, T. A., CCP4/ESF-EACBM Newsletter on Protein Crystallography., 29, 26–28, 1993). To make dosed active site cavities, the energy-minimized diphosphate moiety from the modeled TEAS cyclase reaction was appended to the residue equivalent to TEAS D301.

TEAS W273S crystal structures. Two TEAS W273S structures, in the presence of FHP, were determined from different crystals; both crystals appeared to be well ordered, as dear main-chain and side-chain density were apparent for residues throughout the protein, including the frequently mobile helices D1, D2, and E. Initial difference electron density maps from both crystals immediately revealed the W273S mutations. The two crystals were designated W273S-1 and W273S-2.

In each structure, the loops surrounding the active site were ordered, resulting in a closed active site pocket. The A/C loop in each structure was translated toward the active site, forming part of its outer rim, as observed in the wild-type TEAS/FHP complex. However, while the JIK loop of W273S-1 adopted the same conformation observed in the wild-type TEAS/FHP complex, the same loop in W273S-2 adopted a different conformation. In this conformation of the J/K loop, Tyr527 moved away from the side chain of residue 273. In addition, Tyr520 and Asp525 were placed distal to the side chain of Asp444. Hydrogen bonds previously observed between the J/K loop, Arg266, and the N-terminal loop were also missing in the W273S-2 structure.

The W273S-2 conformation does not appear to be an effect of the W273S mutation, as it was also observed in a wild-type TEAS crystal soaked with the epi-aristolochene mimic deoxycapsidioi, despite the fact that no electron density was readily apparent for the deoxycapsidioi mol-

ecule in that structure. Further, the TEAS active site loops were distant from crystal contacts, and their conformations were not likely to be artifacts of crystal packing. It is possible that at different stages of the TEAS reaction, the enzyme's J/K loop exists in different, defined conformations, and that each of these crystal structures has captured an image of a different conformation. In both W273S structures, residues other than Arg266 and those on the J/K loop did not undergo significant rearrangement from the conformations observed in wild-type TEAS.

In each W273S crystal structure, electron density in the active site suggested that the substrate mimic FHP binds in multiple conformations. Some regions of this density possibly represented bound water molecules in the mutant active site. The presence of water molecules in the mutant active site is consistent with the observation that TEAS W273S gives rise to multiple hydroxylated terpenoid reaction products.

The FHP electron density in each W273S crystal structure was sufficient to suggest that FHP existed in a more extended conformation in the W273S structure, compared to the more tightly folded conformation of FHP in the wild-type TEAS/FHP complex. The observation that the active site of W273S binds multiple conformations of FHP is consistent with the fact that W273S converts FPP to multiple terpenoid hydrocarbon products.

TEAS C440W/W273S: TEAS C440W/W273S crystallized under conditions identical to wild-type TEAS. A 0.3 mm crystal was soaked for 20 minutes in reservoir solution saturated in farnesyl hydroxy phosphate (FHP). After cryoprotection and flash freezing as described for wild-type TEAS, data were collected on a laboratory source with Cu-Kα radiation (MacScience Corp., Japan). A starting model of uncomplexed TEAS (Table 11) (Brookhaven Protein Database Code 5EAT (PDB 5EAT), with waters and magnesiums removed, was positioned against the mutant data with the rigid body module of the software program X-PLOR (A. T. Brunge, X-PLOR Version 3.1—A System for X-Ray Crystallography and NMR Yale University Press, New Haven, 1992, pp. 187–207). Rounds of positional and restrained b-factor refinement with bulk solvent modeling were also carried out in X-PLOR, with manual model building and adjustment carried out in the software program O (Jones, TA, Zou, JY, Cowan, SW, and Kjeldgaard, M., Acta Cryst. D., 49:148–157, 1993). Additional rounds of refinement and map calculation using the CNS program suite resulted in significantly improved maps; this improvement was likely due to improved bulk solvent modeling.

TEAS C440W: TEAS C440W crystallized under conditions identical to wild-type TEAS, except that crystals nucleated less readily and were generally smaller. A mutant crystal was soaked for 6 hours in reservoir solution saturated in FHP before flash-freezing and data collection at SSRL beamline 7-1 (Stanford Synchrotoon Radiation Laboratory, Menlo Park, Calif.). A starting model of TEAS-FHP (Table 10), with water molecules, ligands, and residues 523–532 of SEQ ID NO:2 removed, was positioned against the data with the rigid body module of X-PLOR. Rounds of positional and restrained b-factor refinement with bulk solvent and overall anisotropic temperature factor modeling were also carried out in X-PLOR, and manual model building and adjustment were carried out in the software program O. As with the double mutant, electron density maps were noticeably improved after refinement and map calculation in CNS.

EXAMPLE 4

Terpene Synthase Enzyme Assays

Synthase activity assays were carried out based on the assay described in Vogeli and Chappell, Plant Physiol. 94:1860 (1990) and Vogeli, et al., Plant Physiol. 93:182 (1990). In general, radio-labeled (^{3}H or ^{14}C) substrate was incubated with enzyme at room temperature in a buffered magnesium salt solution (200 mM Tris, pH 8, 50 mM Mg chloride, 1 mM DTT, unless otherwise noted); hydrocarbon products were then selectively extracted into an organic solvent such as hexane. The hexane extract generally was treated with silica gel to remove prenyl alcohols and other oxygenated compounds generated by non-enzymatic hydrolysis of substrate, which partition inefficiently into hexane. Hydrocarbon products present in the hexane phase were quantitated by scintillation counting.

A subsequent extraction with a more polar organic solvent such as ethyl acetate was sometimes carried out. Oxygenated compounds more efficiently partition into ethyl acetate-type solvents. Compounds present in the ethyl acetate phase were also quantitated by scintillation counting.

Substrate concentrations typically ranged from 0.1 nanomolar to 100 micromolar. In some assays, the substrate was not radiolabeled. Reactions generally were carried out in triplicate for each substrate concentration. Protein concentration was determined by the Bradford method. For determination of steady-state kinetic parameters, enzyme concentrations were chosen such that generation of products over time was linear throughout the course of the reaction.

Diterpene synthase assays typically were earned out using ^{3}H geranylgeranyl diphosphate (GGPP) and enzyme in 250 mM Trs, 10 mM Mg chloride, 1 mM DTT, pH 8.0. Sesquiterpene synthase assays typically were carried out using ^{14}C or ^{3}H FPP and enzyme in 100 mM Tris, 30 mM Mg chloride, 1 mM DTT, pH 8.0. Monoterpene synthase assays typically were carried out using ^{3}H GPP and enzyme. As a control for nonspecific binding of GPP by protein, identical reactions were set up which contained BSA, rather than enzyme.

Product analysis of wild type and mutant TEAS enzymes by Ag-TLC. Terpenoid hydrocarbon products are not readily separated by thin layer chromatography on normal or reverse-phase plates; however, some can be separated by argentation TLC (Ag-TLC), in which silica plates are first treated with silver nitrate. Ag-TLC described here generally followed the procedure described by Back et al., Arch. Biochem. Biophys. 315:527 (1994). A silica TLC plate was dipped in 15% silver nitrate (aqueous), then dried for 3–5 hours at 110° C. After spotting of tritiated enzymatic products (solvent extract), the plate was developed in benzene:hexane, ethyl acetate (50:50:1, by volume), sprayed with En^{3}Hance (NEN) fluorography spray, placed on film, and exposed for several days to several weeks. Long exposure times were generally necessary, as silver-nitrate treatment of the TLC plate appeared to cause quenching of the fluorography reagent's fluorescence. Alternatively, ^{14}C labelled products were detected after one to two days without the use of fluorography spray.

EXAMPLE 5

Activity of TEAS W273S

Diterpene Synthase Activity of TEAS W273S. The TEAS W273S enzyme and radiolabelled GGPP were incubated as described above and hydrocarbon products were extracted with hexane. Oxygenated products were then extracted with ethyl acetate. Reactions using wild-type TEAS gave counts lower than buffer alone. TEAS W273S, on the other hand, gave counts that were significantly higher for both the hexane and ethyl acetate extracts. Hydrocarbon products formed from GGPP by W273S were distinct from the

products made by acid-catalyzed loss of diphosphates from GGPP. See FIG. **3**.

Sesquiterpene Synthase Activity of TEAS W273S. Products of FPP turnover by the purified TEAS W273S mutant were analyzed by argentation thin-layer chromatography (Ag-TLC). One major reaction product had an R_f of 0.7 by Ag-TLC, which was distinct from both 5-epi-aristolochene (R_f=0.78) and vetispiradiene (R_f=0.63). See FIG. **4**. Preliminary GC/MS data showed that hexane extracts from FPP turnover by TEAS W273S contained at least four terpene hydrocarbons, with mass spectra distinct from either 5-epi-aristolochene or vetispiradiene. One of these products had a mass spectrum similar to germacrene A.

EXAMPLE 6

Activity of TEAS C440W/W273S

Diterpene Synthase Activity of TEAS C440W/W273S. The mutant TEAS C440W/W273S protein contains a tryptophan residue at position 440 and a serine residue at position 273. Assays with GGPP were carried out using 0.5 micromolar ^{3}H GGPP, various concentrations of unlabelled GGPP (Echelon), and enzyme. Reactions were incubated for 60 minutes at room temperature. The TEAS C440W/W273S mutant protein converted GGPP to hexane-extractable products, whereas the wild-type enzyme did not. The results indicated that the product profile was altered compared to wild-type TEAS. Hexane-extractable products of GGPP turnover by the double mutant were analyzed by Ag-TLC. The products included two species (R_f=0.11 and 0.28) that were distinct from the hydrolysis product geranyl geraniol (R_f=0.0). To verify that products generated by TEAS C440W/W273S from GGPP were not the hydrolysis product, geranylgeraniol, a sample was analyzed by Ag-TLC. A reaction containing ^{3}H GGPP (5 μm) and enzyme (40 μm) in 100 microliters buffer was incubated overnight at room temperature. As controls, ^{3}H GGPP was incubated in reaction buffer alone and in reaction buffer adjusted to pH 1.5. Both the enzymatic and control reactions were extracted with hexane, which was spotted on an argentation TLC plate, and developed and exposed as described above. The results, shown in FIG. **3**, demonstrated that the products formed by TEAS C440W/W273S were different from those generated by non-enzymatic degradation of geranylgeranyl diphosphate.

Sesquiterpene Synthase Activity of TEAS C440W/W273S. Reactions with FPP as substrate were carried out with ^{14}C FPP (9 μm) and enzyme (160 μm) in reaction buffer (20 μl). After incubating for 30 minutes at room temperatures products made by TEAS C440W/W273S wee analyzed by Ag-TLC. The product profile of the double mutant was similar to that of TEAS W273S, with the addition of a major product having an R_f of 0.57. The new product was distinct from both 5-epi-aristolochene and vetispiradiene. Several other products were also formed, many of which migrated slowly upon argentation TLC. See FIG. **4**.

EXAMPLE 7

Activity of TEAS C440W

Diterpene Synthase Activity of TEAS C440W Enzyme assays with TEAS C440W were carried out as described in Example 6. As shown in FIG. **3**, no hexane-extractable products were detectable by Ag-TLC after an overnight incubation at room temperature with 160 μm of enzyme and 9 μm radiolabeled GGPP in 20 μl volume.

Sesquiterpene Synthase Activity of TEAS C440W. Ag-TLC analysis of the products made from radiolabelled by purified TEAS C440W detected the formation at least one major terpenoid hydrocarbon product (R_f 0.63) that was distinct from 5epi-aristolochene (R_f 0.78) and vetispiradiene. The reactions product profile on Ag-TLC is shown in FIG. **4**. Small amounts of slowly-migrating products (R_f 0–0.09) were also formed.

GC/MS analysis of the hexane extract of TEAS C440W terpenoid hydrocarbon reaction products confirmed that this mutant formed a single major sesquiterpene hydrocarbon product as well as a small number of minor hydroxylated products. The mass spectrum of the major product closely matched the published mass spectrum of the spirocydic compound hinesene. Hinesene differs from vetispiradiene in the stereochemistry at the C3 methyl group.

EXAMPLE 8

Activity of TEAS W273E

Sesquiterpene Synthase Activity of TEAS W273E. Reactions to determine the products made by TEAS W273E using FPP as substrate were carried out essentially as described above, using radiolabelled FPP. The results indicated that at least one product other than 5epi-aristolochene was formed. The results also indicated that alkylation of TEAS by FPP had occurred. The alkylation was dependent upon the presence of $MgCl_2$ in the reaction mixture. In control experiments, boiled W273E-TEAS, as well as wild-type TEAS and BSA, were not alkylated. These results indicate that alkylation had occurred at position 273 and that the amino acid residue at position 273 is part of the active site.

EXAMPLE 9

Activity of TEAS Y520F

Sesquiterpene Synthase Activity of TEAS Y520F. Reactions with radiolabeled FPP and TEAS Y520F enzyme were carried out essentially as described above. Reaction products were analysed by Ag-TLC and by GC/MS. A major product of the TEAS Y520F reaction had the same GC retention time as authentic germacrene A and the same mass spectrum as authentic germacrene A. The retention time and mass spectrum of this product were different from 5-epi-aristolochene.

EXAMPLE 10

Activity of TEAS Y527F

Enzymatic Activity of TEAS Y527F. A crude extract of TEAS Y527F enzyme was made by inducing expression in *E. coli* cells, and sonicating the cells. The sonicate was clarified and the supernatant used for enzyme assays. No products were observed in assays using GPP as a substrate, indicating that TEAS Y527F does not have monoterpene synthase activity. Reaction products were obtained using FPP as a substrate. Analysis of these products by Ag-TLC indicated that products other than 5epi-aristolochene were generated by the TEAS Y527F enzyme.

EXAMPLE 11

Alignment of Terpene Synthase Sequences

Residues 265 to 535 of the TEAS primary amino acid sequence (SEQ ID NO:2) were aligned with the full-length amino acid sequence of a limonene synthase (SEQ ID

NO:22), using the BLASTp program (NCBI) with a BLOSUM 62 scoring matrix, a gap open value of 11, a gap extension value of 1, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program, shown in Table 12, included a gap between residues 527 and 528 of the TEAS sequence (numbered as 263 and 264 in the alignment output). Residues 321, 324, 345, 348, 349, 427, 452, 453, 454, 455, 458, 492, 496, 569, 572, 573, 577, 579 and 580 were selected as having the most suitable alignment with the 19 TEAS residues. Residue 580 of limonene cyclase instead of residue 583 was selected as aligning with residue 528 of TEAS, in order to maintain the spatial orientation of structural aspects found in TEAS, i.e., α-helices, β-sheets and loops shown in FIG. **1** and Table 10.

A region including residues 579 to 847 of the taxadiene primary amino acid sequence of SEQ ID NO:44 was aligned with the full-length amino acid sequence of a bornyl diphosphate synthase (SEQ ID NO:26), using the BLASTp program (NCBI) with a BLOSUM 62 scoring matrix, a gap open value of 11, a gap extension value of 1, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program, shown in Table 13, included a gap between residues 453 and 454 of the bornyl diphosphate synthase sequence. Residues 321, 324, 344, 347, 348, 426, 451, 452, 453, 454, 457, 492, 496, 568, 571, 572, 576, 578 and 579 of the bornyl diphosphate synthase were selected as having the most suitable alignment with residues 584, 587, 606, 609, 610, 688, 713, 714, 715, 716, 719, 753, 757, 831, 834, 835, 839, 841 and 842 of the query region sequence of SEQ ID NO:44. Residues 453 and 454 of bornyl diphosphate synthase were selected to align with residues 715 and 716 of taxadiene synthase, in order to maintain the spatial orientation of structural aspects expected to be present in taxadiene synthase, i.e., α-helices, β-sheets and loops shown in FIG. **1** and Table 10.

Residues 265 to 535 of the TEAS primary amino acid sequence (SEQ ID NO:2) were aligned with the full-length amino acid sequence of a δ-selinene synthase (SEQ ID NO:48), using the BLASTp program (NCBI) with a BLOSUM 50 scoring matrix, a gap open value of 13, a gap extension value of 2, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program is shown in Table 14. Residues 300, 303, 324, 327, 328, 406, 431, 432, 433, 434, 437, 471, 475, 548, 551, 552, 556, 558 and 559 of SEQ ID NO:48 were selected as having the most suitable alignment with residues 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 516, 519, 520, 525, 527 and 528 of SEQ ID NO:2.

Residues 307 to 593 of the primary amino acid sequence of γ-humulene synthase (SEQ ID NO:50) were aligned with the full-length amino acid sequence of abietadiene synthase (SEQ ID NO:56), using the BLASTp program (NCBI) with a BLOSUM 62 scoring matrix, a gap open value of 11, a gap extension value of 1, an x_dropoff value of 50, an expect value of 10, a wordsize of 3 and no filtering of low complexity sequences. The output of the alignment program is shown in Table 15. Residues 590, 593, 614, 617, 618, 696, 721, 722, 723, 724, 727, 761, 765, 837, 840, 841, 845, 847 and 848 of the diterpene synthase (SEQ ID NO:56) were selected as having the most suitable alignment with residues 312, 315, 336, 339, 340, 419, 444, 445, 446, 447, 450, 484, 488, 562, 565, 566, 570, 572 and 573 of the sesquiterpene synthase query sequence (SEQ ID NO:50).

EXAMPLE 12

Generation of Novel Monoterpene Synthase Genes

A DNA sequence encoding a pinene synthase (SEQ ID NO:20) is used to construct a library of mutant pinene synthase genes. Random mutations are introduced at nucleotides encoding one or more of the following nine amino acid residues: L, C, C, G, H, S, L, G and Y, which correspond to positions 351, 372, 480, 481, 482, 485, 519, 600 and 601 of SEQ ID NO:20.

In some cases, the pinene synthase coding sequence is randomly mutated at nucleotides encoding one or more of amino acid residues 348, 375, 376, 597, 605, 607 and 608, which correspond to positions Y, I, T, F, D, Y and S of SEQ ID NO:20. The pinene synthase coding sequence is sometimes mutated at nucleotides encoding one or more of the following amino acid residues: Y, S and G, which correspond to positions 454, 479 and 523 of SEQ ID NO:20. In some cases, mutations at these ten positions are made in addition to mutations at nucleotides encoding the nine residues mentioned above. In other cases, mutations at these ten positions are made without introducing mutations at the nine residues mentioned above.

The pinene synthase coding sequence DNA is inserted in the pET28b(+) vector and mutagenized using the QuickChange® method, following a protocol similar to that described in Example 1 for the TEAS 406/407 random library. The primers used to generate mutations are synthesized as indicated in Example 1, using N or S as nucleotides in the desired codons in order to generate random mutants.

Specific mutations at one or more of the above 19 pinene synthase amino acid residues are made by site-directed mutagenesis using a protocol similar to that described in Example 1 for TEAS. Primers are made that have specific A, T, C or G substitutions in the codons to be mutated, in order to generate the desired mutant(s).

Random and/or specific mutations are prepared in a manner similar to that described above to alter amino acid residues of other monoterpene synthases, e.g., limonene synthase, (SEQ ID NOS: 22 or 58), myrcene synthase (SEQ ID NO:30), +sabinene synthase (SEQ ID NO:54), 1, 8 cineole synthase (SEQ ID NO:24) and +bornyl diphosphate synthase (SEQ ID NO:26), at residues whose α-carbons have the interatomic distances and structural coordinates described in Tables 1–6.

EXAMPLE 13

Generation of Novel Sesquiterpene Synthase Genes

A DNA sequence encoding a cadinene synthase (SEQ ID NO:33) is used construct a library of mutant cadinene synthases. Random mutations are introduced at nucleotides encoding one or more of the following nine amino acid residues: W, I, S, G, Y, L, C, L and Y, which correspond to amino acid residues 280, 301, 409, 410, 411, 414, 448, 527 and 528 encoded by SEQ ID NO:33.

In some cases, the cadinene synthase coding sequence is mutated at nucleotides encoding one or more of amino acid residues G, A, S, M, D, Y and T, which correspond to amino acid residues 277, 304, 305, 524, 532, 534 and 535 encoded by SEQ ID NO:33. In addition, the cadinene synthase coding sequence is sometimes mutated at nucleotides encoding one or more of the following amino acid residues: 383, 408 and 452, which correspond to amino acids Y, T and D encoded by SEQ ID NO:33. In some cases, these mutations are made in addition to mutations at the nine residues mentioned above. In other cases, mutations at these ten residues are made without introducing mutations at the nine residues mentioned above.

The cadinene synthase coding sequence is mutated using the QuickChange® method in the pET28b(+) vector, fol-

lowing a protocol similar to that described in Example 1 for the TEAS 406/407 random library. The primers used to generate mutations are synthesized as indicated in Example 11.

Specific mutations at one or more of the above cadinene synthase amino acid residues are made by site-directed mutagenesis using a protocol similar to that described in Example 1 for TEAS.

Random and/or specific mutations are prepared in a manner similar to that described above to alter amino acid residues of other sesquiterpene synthases, e.g., vetispiradiene synthase (SEQ ID NO:32), germacrene C synthase (SEQ ID NO:52), E-alpha-bisabolene synthase (SEQ ID NO:46), gamma-humulene synthase (SEQ ID NO:50), δ-selinene synthase (SEQ ID NO:48), e-b-farnesene synthase (SEQ ID NO:28), at residues whose α-carbons have the interatomic distances and structural coordinates described in Tables 1–6.

EXAMPLE 14

Generation of Novel Diterpene Synthase Genes

A DNA sequence encoding an abietadiene synthase (SEQ ID NO:56) is used construct a library of mutant abietadiene synthases. Random mutations are introduced at nucleotides encoding one or more of the following nine amino acid residues: S, S, I, A, L, V, G, F and Y, which correspond to positions 593, 614, 722, 723, 724, 727, 761, 840 and 841 of SEQ ID NO:56.

In some cases, the abietadiene synthase coding sequence is mutated at nucleotides encoding one or more of amino acid residues I, S, T, M, D, L and T, which correspond to positions 590, 617, 618, 837, 845, 847 and 848 of SEQ ID NO:56. The abietadiene synthase coding sequence is sometimes mutated at nucleotides encoding one or more of the following amino acid residues: Y, S and N, which correspond to positions 696, 721 and 765 of SEQ ID NO:56. In some cases, these mutations are made in addition to mutations at the nine residues mentioned above. In other cases, mutations are made at these ten residues without introducing mutations at the nine residues mentioned above.

The abietadiene synthase coding sequence is mutated using the QuickChange® method in the pET28b(+) vector, following a protocol similar to that described in Example 1 for the TEAS 406/407 random library. The primers used to generate mutations are synthesized as indicated in Example 11.

Specific mutations at one or more of the above abietadiene synthase amino acid residues are made by site-directed mutagenesis using a protocol similar to that described in Example 1 for TEAS.

Random and/or specific mutations are prepared in a manner similar to that described above to alter amino acid residues of other diterpene synthases at amino acid residues whose α-carbons have the interatomic distances and structural coordinates described in Tables 1–6, e.g., casbene synthase (SEQ ID NO:42) and taxadiene synthase (SEQ ID NO:44).

EXAMPLE 15

Expression of Mutant Synthases in Insect, Mammalian and Bacterial Cells

Constructs containing nucleic acids encoding mutant synthases of Examples 12, 13 and/or 14 are introduced into cultured cells of the insect *Spodoptera frugiperda* using a baculovirus expression vector. After expression of the gene, the mutant enzyme is isolated and purified from each done.

Constructs containing nucleic acids encoding mutant synthases of Examples 12, 13 and/or 14 are introduced into cultured HeLa cells using an expression vector having an SV40 promoter. After expression of the gene, the mutant enzyme is isolated and purified from each clone.

Constructs containing nucleic acids encoding mutant synthases of Examples 12, 13 and/or 14 are introduced into *E. coli* BL-21 on a plasmid vector as described in Example 1. The mutant synthase gene is expressed and the mutant enzyme is isolated and purified as described in Example 2.

Other Embodiments

To the extent not already indicated, it will be understood by those of ordinary skill in the art that any one of the various specific embodiments herein described and illustrated may be further modified to incorporate features shown in other of the specific embodiments.

It is to be understood that while the invention has been described in conjunction with the Detailed Description thereof, that the foregoing description is intended to illustrate, and not limit the scope of the invention, which is defined by the scope of the appended claims. Other aspects, advantages, and modifications are within the scope of the following claims.

TABLE 1

α-Carbon	X Position	Y Position	Z Position
1	119.144	43.487	44.133
2	120.203	38.695	43.506
3	114.058	43.884	41.015
4	109.327	46.145	41.743
5	110.682	46.410	45.284
6	99.381	42.920	45.148
7	103.445	38.054	44.605
8	106.807	36.336	45.151
9	107.629	38.010	41.804
10	109.375	34.842	40.617
11	111.944	37.854	37.602
12	110.233	31.098	47.361
13	109.178	33.314	52.875
14	115.915	32.218	48.369
15	118.846	34.443	51.796
16	116.461	32.848	54.290
17	114.100	38.006	55.620
18	116.617	41.285	51.702
19	114.855	43.486	54.238

TABLE 2

α-carbon	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	0.0	5.0	6.0	10.5	9.0	19.8	16.6	14.3	13.0	13.5	11.2	15.6	16.7	12.5	11.8	15.0	13.7	8.3	11.0
2	5.0	0.0	8.4	13.3	12.4	21.3	16.8	13.7	12.7	11.9	10.2	13.1	15.4	9.2	9.4	12.8	13.6	9.3	12.9
3	6.0	8.4	0.0	5.3	6.0	15.3	12.6	11.3	8.7	10.2	7.2	14.8	16.6	13.9	15.1	17.4	15.7	11.3	13.3
4	10.5	13.3	5.3	0.0	3.8	11.0	10.4	10.7	8.3	11.4	9.6	16.1	17.0	16.8	18.1	19.6	16.8	13.3	13.9
5	9.0	12.4	6.0	3.8	0.0	11.8	11.1	10.8	9.6	12.5	11.6	15.5	15.2	15.4	15.9	17.3	13.8	10.1	10.3
6	19.8	21.3	15.3	11.0	11.8	0.0	6.4	9.9	10.2	13.6	15.5	16.2	15.8	20.0	22.2	21.8	18.7	18.5	18.0
7	16.6	16.8	12.6	10.4	11.1	6.4	0.0	3.8	5.0	7.8	11.0	10.1	11.1	14.3	17.4	17.0	15.3	15.3	15.9
8	14.3	13.7	11.3	10.7	10.8	9.9	3.8	0.0	3.8	5.4	9.3	6.6	8.6	10.5	13.9	13.7	12.9	12.8	14.1
9	13.0	12.7	8.7	8.3	9.6	10.2	5.0	3.8	0.0	3.8	6.0	9.2	12.1	12.1	15.4	16.1	15.3	13.8	15.4
10	13.5	11.9	10.2	11.4	12.5	13.6	7.8	5.4	3.8	0.0	5.0	7.8	12.4	10.5	14.6	15.5	16.0	14.7	17.0
11	11.2	10.2	7.2	9.6	11.6	15.5	11.0	9.3	6.0	5.0	0.0	12.0	16.2	12.8	16.1	18.0	18.2	15.3	17.8
12	15.6	13.1	14.8	16.1	15.5	16.2	10.1	6.6	9.2	7.8	12.0	0.0	6.0	5.9	10.2	9.5	11.4	12.8	14.9
13	16.7	15.4	16.6	17.0	15.2	15.8	11.1	8.6	12.1	12.4	16.2	6.0	0.0	8.2	9.8	7.4	7.3	11.0	11.7
14	12.5	9.2	13.9	16.8	15.4	20.0	14.3	10.5	12.1	10.5	12.8	5.9	8.2	0.0	5.0	6.0	9.5	9.7	12.8
15	11.8	9.4	15.1	18.1	15.9	22.2	17.4	13.9	15.4	14.6	16.1	10.2	9.8	5.0	0.0	3.8	7.1	7.2	10.2
16	15.0	12.8	17.4	19.6	17.3	21.8	17.0	13.7	16.1	15.5	18.0	9.5	7.4	6.0	3.8	0.0	5.8	8.8	10.8
17	13.7	13.6	15.7	16.8	13.8	18.7	15.3	12.9	15.3	16.0	18.2	11.4	7.3	9.5	7.1	5.8	0.0	5.7	5.7
18	8.3	9.3	11.3	13.3	10.1	18.5	15.3	12.8	13.8	14.7	15.3	12.8	11.0	9.7	7.2	8.8	5.7	0.0	3.8
19	11.0	12.9	13.3	13.9	10.3	18.0	15.9	14.1	15.4	17.0	17.8	14.9	11.7	12.8	10.2	10.8	5.7	3.8	0.0

TABLE 3

α-Carbon	X Position	Y Position	Z Position
1	119.144	43.487	44.133
2	120.203	38.695	43.506
3	114.058	43.884	41.015
4	109.327	46.145	41.743
5	110.682	46.410	45.284
6	106.807	36.336	45.151
7	107.629	38.010	41.804
8	109.375	34.842	40.617
9	111.944	37.854	37.602
10	110.233	31.098	47.361
11	115.915	32.218	48.369
12	118.846	34.443	51.796
13	116.461	32.848	54.290
14	114.100	38.006	55.620
15	116.617	41.285	51.702
16	114.855	43.486	54.238

TABLE 5

α-Carbon	X Position	Y Position	Z Position
1	120.203	38.695	43.506
2	114.058	43.884	41.015
3	106.807	36.336	45.151
4	107.629	38.010	41.804
5	109.375	34.842	40.617
6	111.944	37.854	37.602
7	110.233	31.098	47.361
8	118.846	34.443	51.796
9	116.461	32.848	54.290

TABLE 4

α-Carbon	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0	5.0	6.0	10.5	9.0	14.3	13.0	13.5	11.2	15.6	12.5	11.8	15.0	13.7	8.3	11.0
2	5.0	0.0	8.4	13.3	12.4	13.7	12.7	11.9	10.2	13.1	9.2	9.4	12.8	13.6	9.3	12.9
3	6.0	8.4	0.0	5.3	6.0	11.3	8.7	10.2	7.2	14.8	13.9	15.1	17.4	15.7	11.3	13.3
4	10.5	13.3	5.3	0.0	3.8	10.7	8.3	11.4	9.6	16.1	16.8	18.1	19.6	16.8	13.3	13.9
5	9.0	12.4	6.0	3.8	0.0	10.8	9.6	12.5	11.6	15.5	15.4	15.9	17.3	13.8	10.1	10.3
6	14.3	13.7	11.3	10.7	10.8	0.0	3.8	5.4	9.3	6.6	10.5	13.9	13.7	12.9	12.8	14.1
7	13.0	12.7	8.7	8.3	9.6	3.8	0.0	3.8	6.0	9.2	12.1	15.4	16.1	15.3	13.8	15.4
8	13.5	11.9	10.2	11.4	12.5	5.4	3.8	0.0	5.0	7.8	10.5	14.6	15.5	16.0	14.7	17.0
9	11.2	10.2	7.2	9.6	11.6	9.3	6.0	5.0	0.0	12.0	12.8	16.1	18.0	18.2	15.3	17.8
10	15.6	13.1	14.8	16.1	15.5	6.6	9.2	7.8	12.0	0.0	5.9	12.2	9.5	11.4	12.8	14.9
11	12.5	9.2	13.9	16.8	15.4	10.5	12.1	10.5	12.8	5.9	0.0	5.0	6.0	9.5	9.7	12.8
12	11.8	9.4	15.1	18.1	15.9	13.9	15.4	14.6	16.1	12.2	5.0	0.0	3.8	7.1	7.2	10.2
13	15.0	12.8	17.4	19.6	17.3	13.7	16.1	15.5	18.0	9.5	6.0	3.8	0.0	5.8	8.8	10.8
14	13.7	13.6	15.7	16.8	13.8	12.9	15.3	16.0	18.2	11.4	9.5	7.1	5.8	0.0	5.7	5.7
15	8.3	9.3	11.3	13.3	10.1	12.8	13.8	14.7	15.3	12.8	9.7	7.2	8.8	5.7	0.0	3.8
16	11.0	12.9	13.3	13.9	10.3	14.1	15.4	17.0	17.8	14.9	12.8	10.2	10.8	5.7	3.8	0.0

TABLE 6

α-Carbon	1	2	3	4	5	6	7	8	9
1	0	8.4	13.7	12.7	11.9	10.2	13.1	9.4	12.8
2	8.4	0	11.3	8.7	10.2	7.2	14.8	15.1	17.4
3	13.7	11.3	0	3.8	5.4	9.3	6.6	13.9	13.7
4	12.7	8.7	3.8	0	3.8	6	9.2	15.4	16.1
5	11.9	10.2	5.4	3.8	0	5	7.8	14.6	15.5
6	10.2	7.2	9.3	6	5	0	12	16.1	18
7	13.1	14.8	6.6	9.2	7.8	12	0	10.2	9.5
8	9.4	15.1	13.9	15.4	14.6	16.1	10.2	0	3.8
9	12.8	17.4	13.7	16.1	15.5	18	9.5	3.8	0

TABLE 7

	Ordered Arrangement of R-Groups at α-carbons 1–19																		
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
A	C	W	I	I	S	Y	T	T	T	Y	L	C	D	V	T	Y	D	Y	T
B	C	W	I	I	S	Y	T	S	T	Y	L	C	D	I	T	Y	D	Y	T
C	G	W	I	A	S	Y	T	C	G	Y	L	C	D	M	L	Y	D	Y	T
D	G	W	I	A	S	Y	T	S	G	Y	L	C	D	M	L	Y	D	Y	T
E	C	W	L	T	S	Y	S	A	G	Y	I	A	N	A	L	Y	D	Y	T
F	G	W	L	L	S	Y	S	T	V	H	L	G	D	A	V	Y	D	Y	T
G	C	W	L	T	S	Y	S	A	G	Y	I	A	N	A	L	Y	D	Y	S
H	L	W	I	T	T	Y	S	V	G	N	L	F	D	V	L	Y	D	F	T
I	P	W	I	V	D	Y	S	T	A	G	L	S	D	A	C	Y	D	Y	T
J	A	W	V	C	G	F	T	S	C	I	M	G	N	C	S	Y	D	Y	S
K	N	F	F	L	G	A	E	I	T	A	T	G	N	I	T	Y	E	F	T
L	C	W	N	I	T	Y	S	I	S	G	M	L	D	A	M	Y	D	H	Q
M	S	W	V	L	T	Y	S	S	S	Y	L	G	G	V	L	Y	D	F	T
N	N	F	F	L	V	N	A	T	L	A	L	G	N	L	S	Y	E	F	T
O	C	W	N	I	T	Y	I	S	G	P	L	L	D	A	M	Y	D	H	G
P	C	W	N	V	T	Y	I	G	G	I	L	L	D	A	I	Y	D	F	G
Q	C	Y	L	L	T	F	A	V	T	M	T	G	N	I	T	Y	D	Y	T
R	C	W	I	I	T	Y	S	I	S	A	I	L	D	A	I	Y	D	D	G
S	S	W	F	I	V	F	S	S	S	V	I	L	N	V	I	Y	D	H	G
T	S	W	I	A	T	Y	S	V	A	S	I	L	D	A	I	Y	D	F	G
U	N	W	N	L	T	Y	S	I	S	S	I	F	N	S	M	Y	D	H	G
V	F	L	A	Q	T	Y	S	I	G	Q	L	S	D	T	I	F	D	F	G
W	I	S	S	T	V	Y	S	I	A	L	V	G	N	M	F	Y	D	L	T
X	Y	L	C	I	T	Y	S	C	G	H	S	L	G	F	G	Y	D	Y	S
Y	G	S	F	I	T	F	S	S	S	V	I	L	N	A	V	Y	D	H	G
Z	Y	W	A	C	T	Y	S	S	G	M	L	G	D	L	I	Y	D	L	Y
AA	A	A	N	L	T	N	A	L	T	S	T	C	M	L	L	Y	D	Y	N
BB	F	L	C	V	T	Y	S	S	A	Y	V	L	G	L	L	Y	D	F	S
CC	F	W	A	M	T	Y	N	T	G	M	L	S	D	I	M	Y	D	F	S
DD	Y	M	C	V	T	F	V	S	S	G	I	L	G	F	V	Y	D	Y	T
EE	V	S	G	Q	V	Y	S	V	G	L	C	W	N	V	F	Y	D	Y	G
FF	C	S	G	T	T	M	F	A	L	G	V	G	N	L	F	Y	D	F	T
GG	C	S	G	T	T	M	S	F	A	L	I	G	N	L	F	Y	D	F	T
HH	C	A	G	T	T	M	S	F	A	L	I	G	N	V	F	Y	D	Y	T
II	I	W	V	I	S	Y	T	T	G	L	V	I	N	T	S	Y	D	Y	T
JJ	Y	W	A	C	T	Y	S	S	G	M	L	G	D	L	I	Y	D	L	Y
KK	C	W	I	I	S	Y	T	S	T	Y	L	C	D	V	T	Y	D	Y	T
LL	C	W	I	I	S	Y	T	T	T	Y	L	C	D	I	T	Y	D	Y	T
MM	C	W	N	I	T	Y	S	I	S	G	M	L	D	A	M	Y	D	H	G
NN	F	A	A	Q	T	Y	S	I	G	Q	L	S	D	T	I	F	D	F	G
OO	F	A	I	A	T	Y	S	V	A	S	I	L	D	A	I	Y	D	F	G

TABLE 8

	Ordered Arrangement of R-Groups at α-carbons 1–16															
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
A	C	W	I	I	S	T	T	Y	L	C	V	T	Y	D	Y	T
B	C	W	I	I	S	S	T	Y	L	C	I	T	Y	D	Y	T
C	G	W	I	A	S	C	G	Y	L	C	M	L	Y	D	Y	T
D	G	W	I	A	S	S	G	Y	L	C	M	L	Y	D	Y	T
E	C	W	L	T	S	A	G	Y	I	A	A	L	Y	D	Y	T
F	G	W	L	L	S	T	V	H	L	G	A	V	Y	D	Y	T
G	C	W	L	T	S	A	G	Y	I	A	A	L	Y	D	Y	S
H	L	W	I	T	T	V	G	N	L	F	V	L	Y	D	F	T
I	P	W	I	V	D	T	A	G	L	S	A	C	Y	D	Y	T
J	A	W	V	C	G	S	C	I	M	G	C	S	Y	D	Y	S

TABLE 8-continued

	Ordered Arrangement of R-Groups at α-carbons 1–16															
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
K	N	F	F	L	G	I	T	A	T	G	I	T	Y	E	F	T
L	C	W	N	I	T	I	S	G	M	L	A	M	Y	D	H	Q
M	S	W	V	L	T	S	S	Y	L	G	V	L	Y	D	F	T
N	N	F	F	L	V	T	L	A	L	G	L	S	Y	E	F	T
O	C	W	N	I	T	S	G	P	L	L	A	M	Y	D	H	G
P	C	W	N	V	T	G	G	I	L	L	A	I	Y	D	F	G
Q	C	Y	L	L	T	V	T	M	T	G	I	T	Y	D	Y	T
R	C	W	I	I	T	I	S	A	I	L	A	I	Y	D	D	G
S	S	W	F	I	V	S	S	V	I	L	V	I	Y	D	H	G
T	S	W	I	A	T	V	A	S	I	L	A	I	Y	D	F	G
U	N	W	N	L	T	I	S	S	I	F	S	M	Y	D	H	G
V	F	L	A	Q	T	I	G	Q	L	S	T	I	F	D	F	G
W	I	S	S	T	V	I	A	L	V	G	M	F	Y	D	L	T
X	Y	L	C	I	T	C	G	H	S	L	F	G	Y	D	Y	S
Y	G	S	F	I	T	S	S	V	I	L	A	V	Y	D	H	G
Z	Y	W	A	C	T	S	G	M	L	G	L	I	Y	D	L	Y
AA	A	A	N	L	T	L	T	S	T	C	L	L	Y	D	Y	N
BB	F	L	C	V	T	S	A	Y	V	L	L	L	Y	D	F	S
CC	F	W	A	M	T	T	G	M	L	S	I	M	Y	D	F	S
DD	Y	M	C	V	T	S	S	G	I	L	F	V	Y	D	Y	T
EE	V	S	G	Q	V	V	G	L	C	W	V	F	Y	D	Y	G
FF	C	S	G	T	T	A	L	G	V	G	L	F	Y	D	F	T
GG	C	S	G	T	T	F	A	L	I	G	L	F	Y	D	F	T
HH	C	A	G	T	T	F	A	L	I	G	V	F	Y	D	Y	T
II	I	W	V	I	S	T	G	L	V	I	T	S	Y	D	Y	T
JJ	Y	W	A	C	T	S	G	M	L	G	L	I	Y	D	L	Y
KK	C	W	I	I	S	S	T	Y	L	C	V	T	Y	D	Y	T
LL	C	W	I	I	S	T	T	Y	L	C	I	T	Y	D	Y	T
MM	C	W	N	I	T	I	S	G	M	L	A	M	Y	D	H	G
NN	F	A	A	Q	T	I	G	Q	L	S	T	I	F	D	F	G
OO	F	A	I	A	T	V	A	S	I	L	A	I	Y	D	F	G

TABLE 9

	Ordered Arrangements of α-Carbons 1–9								
	1	2	3	4	5	6	7	8	9
A	W	I	T	T	Y	L	C	T	Y
B	W	I	S	T	Y	L	C	T	Y
C	W	I	C	G	Y	L	C	L	Y
D	W	I	S	G	Y	L	C	L	Y
E	W	L	A	G	Y	I	A	L	Y
F	W	L	T	V	H	L	G	V	Y
G	W	L	A	G	Y	I	A	L	Y
H	W	I	V	G	N	L	F	L	Y
I	W	I	T	A	G	L	S	C	Y
J	W	V	S	C	I	M	G	S	Y
K	F	F	I	T	A	T	G	T	Y
L	W	N	I	S	G	M	L	M	Y
M	W	V	S	S	Y	L	G	L	Y
N	F	F	T	L	A	L	G	S	Y
O	W	N	S	G	P	L	L	M	Y
P	W	N	G	G	I	L	L	I	Y
Q	Y	L	V	T	M	T	G	T	Y
R	W	I	I	S	A	I	L	I	Y
S	W	F	S	S	V	I	L	I	Y
T	W	I	V	A	S	I	L	I	Y
U	W	N	I	S	S	I	F	M	Y
V	L	A	I	G	Q	L	S	I	F
W	S	S	I	A	L	V	G	F	Y
X	L	C	C	G	H	S	L	G	Y
Y	S	F	S	S	V	I	L	V	Y
Z	W	A	S	G	M	L	G	I	Y
AA	A	N	L	T	S	T	C	L	Y
BB	L	C	S	A	Y	V	L	L	Y
CC	W	A	T	G	M	L	S	M	Y
DD	M	C	S	S	G	I	L	V	Y
EE	S	G	V	G	L	C	W	F	Y
FF	S	G	A	L	G	V	G	F	Y
GG	S	G	F	A	L	I	G	F	Y

TABLE 9-continued

	Ordered Arrangements of α-Carbons 1–9								
	1	2	3	4	5	6	7	8	9
HH	A	G	F	A	L	I	G	F	Y
II	W	V	T	G	L	V	I	S	Y
JJ	W	A	S	G	M	L	G	I	Y
KK	W	I	S	T	Y	L	C	T	Y
LL	W	I	T	T	Y	L	C	T	Y
MM	W	N	I	S	G	M	L	M	Y
NN	A	A	I	G	Q	L	S	I	F
OO	A	I	V	A	S	I	L	I	Y

TABLE 10

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1	CB	VAL	17	105.641	55.031	61.062	1.00	98.26
2	CG1	VAL	17	104.598	56.123	61.269	1.00	97.24
3	CG2	VAL	17	105.492	53.957	62.133	1.00	94.24
4	C	VAL	17	106.842	53.842	59.190	1.00	98.89
5	O	VAL	17	107.108	52.650	59.359	1.00	96.64
6	N	VAL	17	104.381	53.419	59.594	1.00	99.88
7	CA	VAL	17	105.495	54.412	59.646	1.00	99.06
8	N	ALA	18	107.671	54.719	58.615	1.00	98.95
9	CA	ALA	18	109.015	54.419	58.088	1.00	98.55
10	CB	ALA	18	110.007	55.478	58.572	1.00	97.57
11	C	ALA	18	109.570	53.012	58.346	1.00	99.86
12	O	ALA	18	109.580	52.170	57.447	1.00	100.00
13	N	ASP	19	110.068	52.793	59.562	1.00	99.07
14	CA	ASP	19	110.616	51.508	60.010	1.00	97.13

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
15	CB	ASP	19	109.507	50.447	60.064	1.00	96.62
16	CG	ASP	19	109.503	49.666	61.370	1.00	97.86
17	OD1	ASP	19	110.119	50.130	62.355	1.00	100.00
18	OD2	ASP	19	108.873	48.588	61.415	1.00	97.98
19	C	ASP	19	111.849	50.931	59.301	1.00	95.44
20	O	ASP	19	112.812	50.539	59.964	1.00	95.55
21	N	PHE	20	111.814	50.854	57.971	1.00	91.33
22	CA	PHE	20	112.925	50.297	57.190	1.00	84.17
23	CB	PHE	20	112.630	50.377	55.688	1.00	81.03
24	CG	PHE	20	111.437	49.572	55.251	1.00	77.17
25	CD1	PHE	20	110.691	49.971	54.147	1.00	74.72
26	CD2	PHE	20	111.056	48.422	55.939	1.00	77.18
27	CE1	PHE	20	109.581	49.239	53.733	1.00	72.36
28	CE2	PHE	20	109.947	47.681	55.535	1.00	78.10
29	CZ	PHE	20	109.207	48.092	54.428	1.00	75.86
30	C	PHE	20	114.280	50.942	57.465	1.00	82.49
31	O	PHE	20	114.400	52.167	57.517	1.00	84.00
32	N	SER	21	115.294	50.098	57.639	1.00	78.89
33	CA	SER	21	116.656	50.560	57.895	1.00	75.96
34	CB	SER	21	117.495	49.433	58.515	1.00	75.81
35	OG	SER	21	117.449	48.250	57.731	1.00	80.91
36	C	SER	21	117.305	51.063	56.602	1.00	69.67
37	O	SER	21	117.070	50.513	55.525	1.00	70.74
38	N	PRO	22	118.111	52.134	56.691	1.00	63.25
39	CD	PRO	22	118.421	52.939	57.887	1.00	60.39
40	CA	PRO	22	118.773	52.680	55.501	1.00	56.42
41	CB	PRO	22	119.362	53.994	56.018	1.00	53.56
42	CG	PRO	22	119.657	53.688	57.458	1.00	61.97
43	C	PRO	22	119.847	51.746	54.939	1.00	55.70
44	O	PRO	22	120.236	50.771	55.589	1.00	52.85
45	N	SER	23	120.301	52.038	53.724	1.00	56.69
46	CA	SER	23	121.327	51.233	53.065	1.00	53.59
47	CB	SER	23	121.600	51.775	51.660	1.00	51.37
48	OG	SER	23	122.574	50.995	50.991	1.00	45.40
49	C	SER	23	122.620	51.210	53.878	1.00	57.52
50	O	SER	23	123.161	52.258	54.236	1.00	61.76
51	N	LEU	24	123.101	50.004	54.168	1.00	58.09
52	CA	LEU	24	124.326	49.799	54.944	1.00	55.68
53	CB	LEU	24	124.545	48.301	55.191	1.00	60.64
54	CG	LEU	24	123.413	47.379	55.651	1.00	67.70
55	CD1	LEU	24	123.810	45.934	55.385	1.00	70.01
56	CD2	LEU	24	123.098	47.596	57.124	1.00	70.77
57	C	LEU	24	125.554	50.313	54.198	1.00	51.07
58	O	LEU	24	126.529	50.754	54.808	1.00	50.23
59	N	TRP	25	125.472	50.267	52.873	1.00	45.50
60	CA	TRP	25	126.563	50.636	51.977	1.00	44.42
61	CB	TRP	25	126.356	49.908	50.645	1.00	46.22
62	CG	TRP	25	125.853	48.510	50.867	1.00	47.97
63	CD2	TRP	25	126.604	47.407	51.384	1.00	50.67
64	CE2	TRP	25	125.700	46.331	51.553	1.00	50.91
65	CE3	TRP	25	127.948	47.219	51.729	1.00	45.66
66	CD1	TRP	25	124.567	48.070	50.732	1.00	49.99
67	NE1	TRP	25	124.466	46.765	51.147	1.00	47.16
68	CZ2	TRP	25	126.101	45.088	52.053	1.00	52.99
69	CZ3	TRP	25	128.347	45.983	52.227	1.00	47.77
70	CH2	TRP	25	127.423	44.934	52.384	1.00	51.93
71	C	TRP	25	126.893	52.110	51.744	1.00	44.49
72	O	TRP	25	127.997	52.550	52.063	1.00	43.75
73	N	GLY	26	125.958	52.862	51.172	1.00	47.80
74	CA	GLY	26	126.210	54.267	50.894	1.00	39.84
75	C	GLY	26	126.744	54.449	49.483	1.00	44.69
76	O	GLY	26	126.375	53.696	48.580	1.00	46.55
77	N	ASP	27	127.620	55.434	49.287	1.00	46.92
78	CA	ASP	27	128.200	55.708	47.966	1.00	50.38
79	CB	ASP	27	128.544	57.196	47.827	1.00	57.61
80	CG	ASP	27	127.307	58.091	47.770	1.00	66.06
81	OD1	ASP	27	126.168	57.582	47.895	1.00	64.78
82	OD2	ASP	27	127.482	59.318	47.597	1.00	67.46
83	C	ASP	27	129.441	54.857	47.686	1.00	46.14
84	O	ASP	27	130.165	55.082	46.711	1.00	47.50
85	N	GLN	28	129.642	53.855	48.536	1.00	40.05
86	CA	GLN	28	130.759	52.921	48.461	1.00	28.69
87	CB	GLN	28	130.591	51.884	49.575	1.00	25.72

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
88	CG	GLN	28	131.624	50.781	49.615	1.00	32.15
89	CD	GLN	28	131.331	49.745	50.688	1.00	33.15
90	OE1	GLN	28	131.873	48.643	50.665	1.00	41.21
91	NE2	GLN	28	130.467	50.097	51.638	1.00	18.55
92	C	GLN	28	130.904	52.221	47.108	1.00	27.55
93	O	GLN	28	131.974	51.709	46.787	1.00	21.99
94	N	PHE	29	129.840	52.223	46.307	1.00	27.43
95	CA	PHE	29	129.874	51.561	45.004	1.00	26.63
96	CB	PHE	29	128.840	50.432	44.956	1.00	33.69
97	CG	PHE	29	129.070	49.349	45.976	1.00	28.13
98	CD1	PHE	29	128.241	49.241	47.089	1.00	26.35
99	CD2	PHE	29	130.103	48.428	45.817	1.00	27.32
100	CE1	PHE	29	128.432	48.231	48.028	1.00	24.27
101	CE2	PHE	29	130.304	47.410	46.751	1.00	28.00
102	CZ	PHE	29	129.466	47.311	47.860	1.00	16.26
103	C	PHE	29	129.712	52.451	43.771	1.00	31.14
104	O	PHE	29	129.920	51.976	42.648	1.00	31.41
105	N	LEU	30	129.336	53.718	43.962	1.00	33.49
106	CA	LEU	30	129.164	54.658	42.844	1.00	39.53
107	CB	LEU	30	128.857	56.065	43.366	1.00	47.74
108	CG	LEU	30	127.443	56.556	43.658	1.00	54.63
109	CD1	LEU	30	127.508	58.033	44.036	1.00	54.01
110	CD2	LEU	30	126.568	56.378	42.429	1.00	53.57
111	C	LEU	30	130.433	54.764	42.009	1.00	40.75
112	O	LEU	30	130.384	54.947	40.787	1.00	34.99
113	N	SER	31	131.565	54.671	42.696	1.00	44.10
114	CA	SER	31	132.873	54.789	42.077	1.00	47.85
115	CB	SER	31	133.730	55.737	42.917	1.00	53.74
116	OG	SER	31	133.671	55.353	44.281	1.00	52.06
117	C	SER	31	133.669	53.515	41.851	1.00	45.38
118	O	SER	31	133.909	52.743	42.782	1.00	45.28
119	N	PHE	32	134.064	53.302	40.602	1.00	43.37
120	CA	PHE	32	134.905	52.172	40.232	1.00	45.26
121	CB	PHE	32	134.213	50.812	40.251	1.00	42.83
122	CG	PHE	32	135.181	49.670	40.073	1.00	33.22
123	CD1	PHE	32	136.098	49.365	41.075	1.00	29.45
124	CD2	PHE	32	135.266	48.984	38.858	1.00	32.90
125	CE1	PHE	32	137.096	48.407	40.875	1.00	28.42
126	CE2	PHE	32	136.261	48.023	38.647	1.00	27.39
127	CZ	PHE	32	137.179	47.737	39.655	1.00	28.24
128	C	PHE	32	135.601	52.358	38.896	1.00	50.87
129	O	PHE	32	134.988	52.256	37.829	1.00	43.81
130	N	SER	33	136.899	52.626	38.989	1.00	55.26
131	CA	SER	33	137.755	52.816	37.841	1.00	61.21
132	CB	SER	33	138.587	54.094	38.017	1.00	61.87
133	OG	SER	33	139.024	54.250	39.360	1.00	67.09
134	C	SER	33	138.641	51.583	37.731	1.00	59.75
136	O	SER	33	139.488	51.329	38.589	1.00	59.49
136	N	ILE	34	138.368	50.771	36.718	1.00	60.14
137	CA	ILE	34	139.128	49.552	36.486	1.00	66.15
138	CB	ILE	34	138.426	48.639	35.442	1.00	65.50
139	CG2	ILE	34	138.099	49.423	34.163	1.00	69.37
140	CG1	ILE	34	139.291	47.406	35.157	1.00	65.37
141	CD1	ILE	34	138.715	46.458	34.122	1.00	63.17
142	C	ILE	34	140.544	49.875	36.013	1.00	70.13
143	O	ILE	34	140.725	50.551	35.001	1.00	76.00
144	N	ASP	35	141.545	49.454	36.782	1.00	73.05
145	CA	ASP	35	142.935	49.673	36.388	1.00	70.88
146	CB	ASP	35	143.895	49.419	37.558	1.00	76.13
147	CG	ASP	35	143.288	48.547	38.638	1.00	84.32
148	OD1	ASP	35	142.931	47.387	38.344	1.00	92.06
149	OD2	ASP	35	143.155	49.030	39.784	1.00	86.08
150	C	ASP	35	143.198	48.714	35.227	1.00	68.52
151	O	ASP	35	143.555	47.552	35.425	1.00	65.76
152	N	ASN	36	142.940	49.214	34.019	1.00	66.53
153	CA	ASN	36	143.083	48.471	32.765	1.00	67.50
154	CB	ASN	36	142.949	49.430	31.577	1.00	72.78
155	CG	ASN	36	141.889	50.497	31.804	1.00	79.82
156	OD1	ASN	36	140.708	50.194	31.962	1.00	78.35
157	ND2	ASN	36	142.319	51.756	31.853	1.00	84.96
158	C	ASN	36	144.383	47.686	32.646	1.00	68.26
159	O	ASN	36	144.461	46.704	31.906	1.00	65.02
160	N	GLN	37	145.403	48.143	33.364	1.00	71.27

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
161	CA	GLN	37	146.709	47.500	33.370	1.00	71.18
162	CB	GLN	37	147.721	48.431	34.048	1.00	78.38
163	CG	GLN	37	149.005	47.761	34.524	1.00	90.52
164	CD	GLN	37	149.198	47.904	36.027	1.00	100.00
165	OE1	GLN	37	148.538	48.718	36.673	1.00	100.00
166	NE2	GLN	37	150.106	47.105	36.592	1.00	100.00
167	C	GLN	37	146.651	46.131	34.069	1.00	65.44
168	O	GLN	37	147.138	45.138	33.533	1.00	63.18
169	N	VAL	38	146.023	46.086	35.244	1.00	57.92
170	CA	VAL	38	145.883	44.849	36.021	1.00	51.76
171	CB	VAL	38	145.388	45.152	37.461	1.00	50.39
172	CG1	VAL	38	145.198	43.862	38.251	1.00	44.02
173	CG2	VAL	38	146.371	46.071	38.166	1.00	43.36
174	C	VAL	38	144.916	43.870	35.349	1.00	52.33
175	O	VAL	38	145.142	42.656	35.348	1.00	48.70
176	N	ALA	39	143.858	44.412	34.752	1.00	49.41
177	CA	ALA	39	142.848	43.610	34.068	1.00	48.03
178	CB	ALA	39	141.722	44.502	33.584	1.00	56.98
179	C	ALA	39	143.434	42.823	32.900	1.00	47.68
180	O	ALA	39	143.178	41.627	32.759	1.00	52.03
181	N	GLU	40	144.219	43.501	32.068	1.00	46.51
182	CA	GLU	40	144.855	42.881	30.908	1.00	40.96
183	CB	GLU	40	145.507	43.952	30.036	1.00	49.36
184	CG	GLU	40	144.507	44.896	29.383	1.00	62.86
185	CD	GLU	40	145.161	46.109	28.745	1.00	67.78
186	OE1	GLU	40	146.229	45.957	28.112	1.00	67.66
187	OE2	GLU	40	144.601	47.218	28.880	1.00	70.01
188	C	GLU	40	145.893	41.852	31.337	1.00	38.90
189	O	GLU	40	146.076	40.832	30.878	1.00	39.36
190	N	LYS	41	146.569	42.135	32.447	1.00	41.55
191	CA	LYS	41	147.584	41.243	32.998	1.00	38.43
192	CB	LYS	41	148.219	41.884	34.236	1.00	43.42
193	CG	LYS	41	149.304	41.056	34.903	1.00	55.00
194	CD	LYS	41	149.864	41.780	36.119	1.00	61.88
195	CE	LYS	41	151.040	41.028	36.721	1.00	62.99
196	NZ	LYS	41	151.665	41.794	37.835	1.00	69.92
197	C	LYS	41	146.914	39.926	33.373	1.00	36.30
198	O	LYS	41	147.362	38.855	32.966	1.00	34.80
199	N	TYR	42	145.823	40.027	34.132	1.00	35.61
200	CA	TYR	42	145.051	38.868	34.572	1.00	29.43
201	CB	TYR	42	143.880	39.307	35.457	1.00	29.64
202	CG	TYR	42	144.229	39.658	36.890	1.00	30.55
203	CD1	TYR	42	145.556	39.697	37.330	1.00	37.21
204	CE1	TYR	42	145.866	40.002	38.660	1.00	37.30
205	CD2	TYR	42	143.222	39.937	37.814	1.00	28.62
206	CE2	TYR	42	143.519	40.241	39.139	1.00	37.07
207	CZ	TYR	42	144.839	40.272	39.556	1.00	40.82
208	OH	TYR	42	145.121	40.567	40.869	1.00	43.81
209	C	TYR	42	144.499	38.097	33.377	1.00	30.40
210	O	TYR	42	144.603	36.872	33.318	1.00	29.10
211	N	ALA	43	143.920	38.827	32.426	1.00	24.33
212	CA	ALA	43	143.340	38.227	31.227	1.00	29.09
213	CB	ALA	43	142.713	39.308	30.356	1.00	19.04
214	C	ALA	43	144.358	37.423	30.421	1.00	29.23
215	O	ALA	43	144.074	36.308	29.984	1.00	29.14
216	N	LYS	44	145.559	37.972	30.260	1.00	37.81
217	CA	LYS	44	146.637	37.371	29.491	1.00	40.64
218	C	LYS	44	147.069	36.041	30.095	1.00	34.80
219	O	LYS	44	147.221	35.048	29.357	1.00	35.25
220	CB	LYS	44	147.824	38.329	29.396	1.00	54.18
221	CG	LYS	44	149.001	37.784	28.605	1.00	67.03
222	CD	LYS	44	150.141	38.787	28.552	1.00	79.04
223	CE	LYS	44	151.313	38.247	27.750	1.00	20.00
224	NZ	LYS	44	152.431	39.227	27.673	1.00	20.00
225	N	GLU	45	147.332	36.000	31.397	1.00	31.47
226	CA	GLU	45	147.771	34.779	32.070	1.00	30.36
227	CB	GLU	45	148.288	35.080	33.480	1.00	26.58
228	CG	GLU	45	149.071	33.920	34.105	1.00	19.97
229	CD	GLU	45	149.394	34.128	35.580	1.00	33.35
230	OE1	GLU	45	149.791	33.146	36.246	1.00	31.26
231	OE2	GLU	45	149.249	35.264	36.080	1.00	37.21
232	C	GLU	45	146.649	33.747	32.142	1.00	31.64
233	O	GLU	45	146.902	32.545	32.058	1.00	38.67

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
234	N	ILE	46	145.415	34.225	32.299	1.00	34.27
235	CA	ILE	46	144.239	33.358	32.373	1.00	30.12
236	CB	ILE	46	142.942	34.181	32.608	1.00	33.74
237	CG2	ILE	46	141.706	33.420	32.123	1.00	32.63
238	CG1	ILE	46	142.812	34.534	34.093	1.00	34.26
239	CD1	ILE	46	141.644	35.444	34.407	1.00	30.01
240	C	ILE	46	144.099	32.518	31.110	1.00	29.77
241	O	ILE	46	143.850	31.315	31.186	1.00	30.24
242	N	GLU	47	144.283	33.156	29.956	1.00	31.42
243	CA	GLU	47	144.185	32.482	28.666	1.00	37.34
244	CB	GLU	47	144.460	33.476	27.537	1.00	45.72
245	CG	GLU	47	144.290	32.896	26.137	1.00	68.61
246	CD	GLU	47	144.808	33.813	25.035	1.00	79.62
247	OE1	GLU	47	145.302	34.922	25.339	1.00	89.55
248	OE2	GLU	47	144.728	33.417	23.852	1.00	86.41
249	C	GLU	47	145.169	31.314	28.580	1.00	37.12
250	O	GLU	47	144.860	30.275	27.997	1.00	45.60
251	N	ALA	48	146.348	31.492	29.171	1.00	33.83
252	CA	ALA	48	147.378	30.459	29.170	1.00	30.76
253	CB	ALA	48	148.720	31.054	29.575	1.00	33.78
254	C	ALA	48	146.986	29.323	30.110	1.00	33.08
255	O	ALA	48	147.071	28.150	29.743	1.00	30.80
256	N	LEU	49	146.542	29.685	31.312	1.00	27.01
257	CA	LEU	49	146.110	28.720	32.321	1.00	23.68
258	CB	LEU	49	145.793	29.445	33.628	1.00	19.74
259	CG	LEU	49	146.936	30.167	34.337	1.00	15.12
260	CD1	LEU	49	146.368	31.161	35.328	1.00	8.67
261	CD2	LEU	49	147.844	29.164	35.033	1.00	12.64
262	C	LEU	49	144.862	27.985	31.836	1.00	24.27
263	O	LEU	49	144.610	26.842	32.214	1.00	31.26
264	N	LYS	50	144.101	28.663	30.983	1.00	27.77
265	CA	LYS	50	142.863	28.154	30.394	1.00	30.88
266	CB	LYS	50	142.247	29.263	29.548	1.00	31.45
267	CG	LYS	50	140.775	29.153	29.242	1.00	31.65
268	CD	LYS	50	140.333	30.468	28.621	1.00	33.98
269	CE	LYS	50	138.871	30.468	28.250	1.00	42.53
270	NZ	LYS	50	138.455	31.817	27.773	1.00	47.24
271	C	LYS	50	143.120	26.925	29.527	1.00	32.84
272	O	LYS	50	142.449	25.901	29.675	1.00	31.46
273	N	GLU	51	144.092	27.033	28.625	1.00	33.57
274	CA	GLU	51	144.439	25.927	27.741	1.00	38.44
275	CB	GLU	51	145.286	26.416	26.566	1.00	45.31
276	CG	GLU	51	145.241	25.501	25.339	1.00	54.99
277	CD	GLU	51	143.953	25.633	24.532	1.00	61.58
278	OE1	GLU	51	143.086	26.463	24.893	1.00	63.41
279	OE2	GLU	51	143.815	24.912	23.519	1.00	63.99
280	C	GLU	51	145.179	24.824	28.501	1.00	37.86
281	O	GLU	51	145.145	23.662	28.097	1.00	43.06
282	N	GLN	52	145.867	25.192	29.582	1.00	36.20
283	CA	GLN	52	146.592	24.212	30.397	1.00	38.10
284	CB	GLN	52	147.453	24.897	31.465	1.00	41.72
285	CG	GLN	52	148.691	25.615	30.943	1.00	47.34
286	CD	GLN	52	149.505	26.249	32.061	1.00	49.46
287	OE1	GLN	52	149.640	25.683	33.145	1.00	43.98
288	NE2	GLN	52	150.049	27.438	31.799	1.00	53.90
289	C	GLN	52	145.563	23.339	31.093	1.00	38.87
290	O	GLN	52	145.732	22.122	31.219	1.00	40.47
291	N	THR	53	144.501	23.991	31.554	1.00	37.87
292	CA	THR	53	143.407	23.323	32.236	1.00	32.77
293	CB	THR	53	142.541	24.347	32.992	1.00	31.08
294	OG1	THR	53	143.315	24.933	34.050	1.00	28.04
295	CG2	THR	53	141.296	23.685	33.569	1.00	32.90
296	C	THR	53	142.570	22.522	31.233	1.00	32.05
297	O	THR	53	142.013	21.476	31.573	1.00	29.73
298	N	ARG	54	142.529	22.992	29.988	1.00	28.01
299	CA	ARG	54	141.785	22.312	28.933	1.00	23.69
300	CB	ARG	54	141.723	23.176	27.673	1.00	23.31
301	CG	ARG	54	140.724	22.682	26.633	1.00	24.23
302	CD	ARG	54	140.755	23.527	25.360	1 00	30.78
303	NE	ARG	54	140.674	24.969	25.619	1.00	45.26
304	CZ	ARG	54	139.564	25.633	25.942	1.00	46.57
305	NH1	ARG	54	138.405	24.999	26.058	1.00	51.75
306	NH2	ARG	54	139.608	26.946	26.140	1.00	43.00

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
307	C	ARG	54	142.487	20.998	28.617	1.00	30.27
308	O	ARG	54	141.842	19.965	28.479	1.00	33.41
309	N	ASN	55	143.821	21.050	28.526	1.00	33.72
310	CA	ASN	55	144.648	19.899	28.240	1.00	33.22
311	C	ASN	55	144.538	18.872	29.348	1.00	35.28
312	O	ASN	55	144.679	17.660	29.105	1.00	35.19
313	CB	ASN	55	146.080	20.341	27.963	1.00	36.29
314	CG	ASN	55	146.150	21.264	26.761	1.00	20.00
315	OD1	ASN	55	145.473	21.038	25.754	1.00	20.00
316	ND2	ASN	55	146.963	22.307	26.857	1.00	20.00
317	N	MET	56	144.309	19.330	30.581	1.00	34.89
318	CA	MET	56	144.150	18.442	31.734	1.00	34.60
319	CB	MET	56	144.058	19.241	33.039	1.00	27.26
320	CG	MET	56	145.378	19.792	33.544	1.00	38.81
321	SD	MET	56	145.237	20.594	35.159	1.00	40.35
322	CE	MET	56	145.790	22.242	34.734	1.00	41.02
323	C	MET	56	142.880	17.606	31.560	1.00	38.38
324	O	MET	56	142.871	16.406	31.847	1.00	36.10
325	N	LEU	57	141.816	18.253	31.084	1.00	33.14
326	CA	LEU	57	140.535	17.593	30.852	1.00	33.61
327	CB	LEU	57	139.444	18.633	30.566	1.00	24.13
328	CG	LEU	57	138.939	19.472	31.742	1.00	25.14
329	CD1	LEU	57	138.092	20.624	31.235	1.00	18.69
330	CD2	LEU	57	138.143	18.604	32.703	1.00	10.16
331	C	LEU	57	140.610	16.611	29.686	1.00	37.09
332	O	LEU	57	139.922	15.588	29.679	1.00	34.95
333	N	LEU	58	141.453	16.924	28.703	1.00	35.34
334	CA	LEU	58	141.605	16.071	27.533	1.00	35.75
335	CB	LEU	58	141.930	16.926	26.304	1.00	33.37
336	CG	LEU	58	140.886	17.987	25.951	1.00	36.57
337	CD1	LEU	58	141.334	18.779	24.736	1.00	34.54
338	CD2	LEU	58	139.540	17.333	25.691	1.00	38.57
339	C	LEU	58	142.628	14.946	27.688	1.00	40.17
340	O	LEU	58	143.001	14.298	26.710	1.00	38.69
341	N	ALA	59	143.066	14.697	28.922	1.00	45.53
342	CA	ALA	59	144.038	13.637	29.198	1.00	52.73
343	CB	ALA	59	144.562	13.754	30.626	1.00	52.29
344	C	ALA	59	143.402	12.263	28.950	1.00	60.58
345	O	ALA	59	142.320	11.962	29.450	1.00	62.17
346	N	THR	60	144.084	11.432	28.168	1.00	63.55
347	CA	THR	60	143.575	10.109	27.794	1.00	63.50
348	CB	THR	60	144.405	9.528	26.641	1.00	63.61
349	OG1	THR	60	145.776	9.434	27.039	1.00	67.85
350	CG2	THR	60	144.302	10.426	25.420	1.00	59.57
351	C	THR	60	143.372	9.004	28.844	1.00	64.51
352	O	THR	60	142.237	8.681	29.198	1.00	69.94
353	N	GLY	61	144.470	8.435	29.337	1.00	59.72
354	CA	GLY	61	144.394	7.339	30.294	1.00	59.70
355	C	GLY	61	144.087	7.572	31.767	1.00	60.15
356	O	GLY	61	144.627	6.862	32.620	1.00	62.75
357	N	MET	62	143.233	8.546	32.098	1.00	62.09
358	CA	MET	62	142.904	8.860	33.482	1.00	62.20
359	C	MET	62	141.787	7.962	34.001	1.00	57.87
360	O	MET	62	140.858	7.592	33.304	1.00	60.93
361	CB	MET	62	142.512	10.333	33.619	1.00	65.78
362	CG	MET	62	142.374	10.806	35.057	1.00	71.62
363	SD	MET	62	141.924	12.547	35.177	1.00	20.00
364	CE	MET	62	141.630	12.940	33.455	1.00	20.00
365	N	LYS	63	141.877	7.621	35.308	1.00	53.67
366	CA	LYS	63	140.886	6.787	35.975	1.00	51.44
367	CB	LYS	63	141.401	6.323	37.342	1.00	55.26
368	CG	LYS	63	142.607	5.402	37.287	1.00	65.11
369	CD	LYS	63	142.968	4.915	38.682	1.00	69.24
370	CE	LYS	63	144.127	3.936	38.635	1.00	76.58
371	NZ	LYS	63	144.434	3.376	39.980	1.00	78.96
372	C	LYS	63	139.576	7.543	36.173	1.00	48.71
373	O	LYS	63	139.559	8.778	36.167	1.00	48.30
374	N	LEU	64	138.490	6.802	36.386	1.00	44.07
375	CA	LEU	64	137.182	7.413	36.586	1.00	38.53
376	CB	LEU	64	136.100	6.343	36.778	1.00	40.14
377	CG	LEU	64	134.671	6.886	36.899	1.00	35.60
378	CD1	LEU	64	134.283	7.589	35.606	1.00	32.53
379	CD2	LEU	64	133.689	5.773	37.203	1.00	30.12

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
380	C	LEU	64	137.184	8.363	37.778	1.00	32.66
381	O	LEU	64	136.773	9.515	37.650	1.00	32.91
382	N	ALA	65	137.664	7.881	38.923	1.00	26.30
383	CA	ALA	65	137.721	8.683	40.141	1.00	27.29
384	CB	ALA	65	138.362	7.885	41.265	1.00	26.12
385	C	ALA	65	138.482	9.988	39.919	1.00	33.96
386	O	ALA	65	138.019	11.057	40.318	1.00	35.01
387	N	ASP	66	139.630	9.897	39.250	1.00	35.46
388	CA	ASP	66	140.459	11.064	38.961	1.00	35.10
389	CB	ASP	66	141.776	10.646	38.298	1.00	36.60
390	CG	ASP	66	142.685	9.867	39.229	1.00	34.65
391	OD1	ASP	66	142.611	10.067	40.461	1.00	25.86
392	OD2	ASP	66	143.488	9.057	38.717	1.00	44.77
393	C	ASP	66	139.746	12.065	38.059	1.00	31.14
394	O	ASP	66	139.846	13.276	38.266	1.00	31.51
395	N	THR	67	139.045	11.552	37.051	1.00	26.69
396	CA	THR	67	138.316	12.392	36.105	1.00	26.40
397	CB	THR	67	137.793	11.571	34.918	1.00	26.70
398	OG1	THR	67	138.891	10.917	34.270	1.00	27.33
399	CG2	THR	67	137.095	12.474	33.918	1.00	28.90
400	C	THR	67	137.146	13.113	36.769	1.00	24.73
401	O	THR	67	136.899	14.290	36.502	1.00	27.41
402	N	LEU	68	136.425	12.401	37.629	1.00	23.13
403	CA	LEU	68	135.295	12.985	38.333	1.00	18.00
404	CB	LEU	68	134.504	11.909	39.078	1.00	13.23
405	CG	LEU	58	133.804	10.871	38.201	1.00	16.24
406	CD1	LEU	68	133.109	9.843	39.078	1.00	17.55
407	CD2	LEU	68	132.811	11.552	37.272	1.00	7.96
408	C	LEU	68	135.787	14.047	39.305	1.00	19.40
409	O	LEU	68	135.181	15.113	39.420	1.00	21.96
410	N	ASN	69	136.899	13.766	39.980	1.00	17.72
411	CA	ASN	69	137.471	14.714	40.931	1.00	23.29
412	CB	ASN	69	138.608	14.071	41.728	1.00	27.45
413	CG	ASN	69	138.102	13.102	42.783	1.00	44.15
414	OD1	ASN	69	137.171	13.413	43.530	1.00	45.05
415	ND2	ASN	69	138.709	11.921	42.846	1.00	48.60
416	C	ASN	69	137.954	15.985	40.240	1.00	21.73
417	O	ASN	69	137.784	17.083	40.764	1.00	19.56
418	N	LEU	70	138.526	15.834	39.050	1.00	19.22
419	CA	LEU	70	139.012	16.979	38.293	1.00	18.06
420	CB	LEU	70	139.736	16.522	37.025	1.00	14.83
421	CG	LEU	70	140.274	17.650	36.141	1.00	18.22
422	CD1	LEU	70	141.330	18.440	36.889	1.00	15.05
423	CD2	LEU	70	140.845	17.078	34.862	1.00	20.94
424	C	LEU	70	137.835	17.871	37.925	1.00	20.53
425	O	LEU	70	137.844	19.069	38.212	1.00	23.73
426	N	ILE	71	136.817	17.269	37.312	1.00	19.75
427	CA	ILE	71	135.613	17.986	36.901	1.00	16.33
428	CB	ILE	71	134.617	17.043	36.184	1.00	19.20
429	CG2	ILE	71	133.278	17.744	35.950	1.00	17.41
430	CG1	ILE	71	135.216	16.574	34.856	1.00	25.29
431	CD1	ILE	71	134.273	15.748	34.009	1.00	21.71
432	C	ILE	71	134.927	18.661	38.088	1.00	15.45
433	O	ILE	71	134.507	19.813	37.991	1.00	10.60
434	N	ASP	72	134.846	17.952	39.212	1.00	14.16
435	CA	ASP	72	134.222	18.477	40.425	1.00	13.13
436	CB	ASP	72	134.206	17.400	41.516	1.00	9.28
437	CG	ASP	72	133.456	17.828	42.766	1.00	8.19
438	OD1	ASP	72	132.472	18.591	42.660	1.00	19.56
439	OD2	ASP	72	133.842	17.381	43.865	1.00	24.87
440	C	ASP	72	134.969	19.709	40.926	1.00	20.93
441	O	ASP	72	134.357	20.734	41.230	1.00	31.87
442	N	THR	73	136.298	19.618	40.980	1.00	26.21
443	CA	THR	73	137.162	20.689	41.452	1.00	17.72
444	C	THR	73	137.051	21.912	40.558	1.00	16.99
445	O	THR	73	136.913	23.046	41.054	1.00	15.04
446	CB	THR	73	138.627	20.258	41.508	1.00	18.68
447	OG1	THR	73	138.771	19.152	42.406	1.00	20.00
448	CG2	THR	73	139.503	21.413	41.971	1.00	23.27
449	N	ILE	74	137.124	21.732	39.245	1.00	13.35
450	CA	ILE	74	137.024	22.837	38.298	1.00	15.24
451	CB	ILE	74	137.214	22.342	36.844	1.00	17.48
452	CG2	ILE	74	136.841	23.434	35.843	1.00	10.21

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
453	CG1	ILE	74	138.658	21.881	36.637	1.00	16.00
454	CD1	ILE	74	138.936	21.335	35.253	1.00	19.68
455	C	ILE	74	135.677	23.554	38.431	1.00	21.97
456	O	ILE	74	135.603	24.774	38.285	1.00	37.27
457	N	GLU	75	134.620	22.793	38.712	1.00	24.94
458	CA	GLU	75	133.283	23.362	38.869	1.00	17.86
459	CB	GLU	75	132.216	22.266	38.893	1.00	22.45
460	CG	GLU	75	131.998	21.565	37.557	1.00	23.19
461	CD	GLU	75	130.753	20.685	37.539	1.00	24.24
462	OE1	GLU	75	130.485	19.984	38.540	1.00	11.68
463	OE2	GLU	75	130.041	20.699	36.513	1.00	19.29
464	C	GLU	75	133.194	24.181	40.142	1.00	16.49
465	O	GLU	75	132.739	25.323	40.119	1.00	18.93
466	N	ARG	76	133.640	23.590	41.248	1.00	11.73
467	CA	ARG	76	133.626	24.248	42.552	1.00	15.45
468	CB	ARG	76	134.114	23.282	43.636	1.00	7.10
469	CG	ARG	76	133.198	22.097	43.899	1.00	15.61
470	CD	ARG	76	133.785	21.197	44.975	1.00	12.16
471	NE	ARG	76	132.824	20.231	45.508	1.00	16.00
472	CZ	ARG	76	132.467	20.165	46.789	1.00	19.23
473	NH1	ARG	76	132.982	21.010	47.670	1.00	26.80
474	NH2	ARG	76	131.618	19.234	47.202	1.00	29.06
475	C	ARG	76	134.488	25.519	42.564	1.00	20.45
476	O	ARG	76	134.214	26.454	43.319	1.00	19.47
477	N	LEU	77	135.525	25.539	41.732	1.00	20.12
478	CA	LEU	77	136.419	26.692	41.634	1.00	19.40
479	CB	LEU	77	137.756	26.281	41.014	1.00	12.91
480	CG	LEU	77	138.678	25.382	41.843	1.00	12.12
481	CD1	LEU	77	139.825	24.903	40.973	1.00	2.00
482	CD2	LEU	77	139.201	26.125	43.070	1.00	4.07
483	C	LEU	77	135.796	27.823	40.818	1.00	22.31
484	O	LEU	77	136.374	28.906	40.702	1.00	30.09
485	N	GLY	78	134.628	27.551	40.238	1.00	26.16
486	CA	GLY	78	133.915	28.542	39.447	1.00	20.26
487	C	GLY	78	134.496	28.855	38.082	1.00	16.66
488	O	GLY	78	134.185	29.898	37.504	1.00	19.22
489	N	ILE	79	135.323	27.959	37.553	1.00	13.23
490	CA	ILE	79	135.938	28.179	36.247	1.00	16.00
491	CB	ILE	79	137.488	28.083	36.321	1.00	14.32
492	CG2	ILE	79	138.055	29.257	37.111	1.00	9.65
493	CG1	ILE	79	137.909	26.751	36.944	1.00	15.84
494	CD1	ILE	79	139.413	26.574	37.082	1.00	20.69
495	C	ILE	79	135.420	27.216	35.185	1.00	17.13
496	O	ILE	79	135.860	27.256	34.033	1.00	20.55
497	N	SER	80	134.459	26.377	35.567	1.00	21.41
498	CA	SER	80	133.878	25.392	34.654	1.00	23.76
499	CB	SER	80	133.004	24.393	35.419	1.00	20.88
500	OG	SER	80	131.996	25.047	36.170	1.00	23.54
501	C	SER	80	133.093	25.977	33.485	1.00	20.44
502	O	SER	80	132.839	25.280	32.505	1.00	28.56
503	N	TYR	81	132.723	27.252	33.577	1.00	18.39
504	CA	TYR	81	131.972	27.907	32.507	1.00	19.66
505	CB	TYR	81	131.389	29.244	32.986	1.00	10.58
506	CG	TYR	81	132.396	30.362	33.170	1.00	19.55
507	CD1	TYR	81	132.635	31.285	32.151	1.00	26.56
508	CE1	TYR	81	133.540	32.331	32.320	1.00	23.18
509	CD2	TYR	81	133.092	30.513	34.367	1.00	12.72
510	CE2	TYR	81	133.998	31.555	34.546	1.00	18.75
511	CZ	TYR	81	134.218	32.460	33.519	1.00	21.59
512	OH	TYR	81	135.122	33.487	33.688	1.00	23.90
513	C	TYR	81	132.814	28.103	31.240	1.00	23.33
514	O	TYR	81	132.294	28.498	30.195	1.00	26.36
515	N	HIS	82	134.114	27.835	31.352	1.00	27.33
516	CA	HIS	82	135.044	27.955	30.229	1.00	28.77
517	CB	HIS	82	136.471	28.227	30.724	1.00	20.70
518	CG	HIS	82	136.676	29.592	31.301	1.00	18.33
519	CD2	HIS	82	137.002	29.989	32.553	1.00	7.90
520	ND1	HIS	82	136.574	30.742	30.548	1.00	14.62
521	CE1	HIS	82	136.829	31.788	31.312	1.00	11.77
522	NE2	HIS	82	137.091	31.359	32.533	1.00	13.85
523	C	HIS	82	135.085	26.654	29.440	1.00	28.78
524	O	HIS	82	135.456	26.643	28.265	1.00	31.36
525	N	PHE	83	134.719	25.557	30.098	1.00	30.57

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
526	CA	PHE	83	134.774	24.241	29.475	1.00	32.99
527	CB	PHE	83	135.829	23.389	30.191	1.00	38.74
528	CG	PHE	83	137.052	24.157	30.603	1.00	40.58
529	CD1	PHE	83	137.204	24.583	31.921	1.00	40.06
530	CD2	PHE	83	138.041	24.476	29.675	1.00	41.50
531	CE1	PHE	83	138.320	25.318	32.309	1.00	43.27
532	CE2	PHE	83	139.163	25.211	30.050	1.00	38.18
533	CZ	PHE	83	139.303	25.634	31.371	1.00	46.92
534	C	PHE	83	133.444	23.496	29.471	1.00	32.87
535	O	PHE	83	133.378	22.340	29.886	1.00	31.33
538	N	GLU	84	132.397	24.133	28.960	1.00	33.76
537	CA	GLU	84	131.086	23.496	28.929	1.00	38.03
538	CB	GLU	84	129.991	24.514	28.601	1.00	47.83
539	CG	GLU	84	129.901	25.690	29.578	1.00	58.57
540	CD	GLU	84	129.403	25.312	30.975	1.00	69.66
541	OE1	GLU	84	129.719	24.208	31.479	1.00	74.44
542	OE2	GLU	84	128.695	26.146	31.586	1.00	66.21
543	C	GLU	84	131.030	22.314	27.966	1.00	39.30
544	O	GLU	84	130.339	21.328	28.228	1.00	37.93
545	N	LYS	85	131.780	22.401	26.872	1.00	37.65
546	CA	LYS	85	131.815	21.329	25.886	1.00	40.19
547	CB	LYS	85	132.367	21.839	24.551	1.00	49.51
548	CG	LYS	85	132.443	20.770	23.469	1.00	57.11
549	CD	LYS	85	133.176	21.261	22.237	1.00	73.34
550	CE	LYS	85	133.280	20.160	21.180	1.00	81.58
551	NZ	LYS	85	134.029	20.532	19.952	1.00	94.03
552	C	LYS	85	132.661	20.151	26.381	1.00	37.98
553	O	LYS	85	132.200	19.018	26.404	1.00	43.86
554	N	GLU	86	133.894	20.461	26.784	1.00	36.06
555	CA	GLU	86	134.825	19.448	27.277	1.00	32.72
556	CB	GLU	86	136.122	20.102	27.774	1.00	36.71
557	CG	GLU	86	136.998	20.743	26.698	1.00	42.45
558	CD	GLU	86	136.500	22.103	26.219	1.00	44.54
559	OE1	GLU	86	135.646	22.720	26.891	1.00	49.68
560	OE2	GLU	86	136.977	22.566	25.162	1.00	47.77
561	C	GLU	86	134.213	18.618	28.402	1.00	29.96
562	O	GLU	86	134.254	17.389	28.370	1.00	32.06
563	N	ILE	87	133.638	19.303	29.388	1.00	28.21
564	CA	ILE	87	133.013	18.648	30.534	1.00	27.11
565	CB	ILE	87	132.618	19.672	31.617	1.00	28.37
566	CG2	ILE	87	131.813	18.996	32.729	1.00	28.34
567	CG1	ILE	87	133.880	20.338	32.179	1.00	22.12
568	CD1	ILE	87	133.613	21.386	33.241	1.00	21.16
569	C	ILE	87	131.795	17.815	30.150	1.00	27.00
570	O	ILE	87	131.581	16.735	30.700	1.00	29.31
571	N	ASP	88	131.007	18.309	29.200	1.00	31.52
572	CA	ASP	88	129.815	17.593	28.751	1.00	39.20
573	CB	ASP	88	129.009	18.445	27.764	1.00	40.43
574	CG	ASP	88	127.717	17.774	27.330	1.00	36.63
575	OD1	ASP	88	126.845	17.539	28.194	1.00	36.19
576	OD2	ASP	88	127.577	17.470	26.125	1.00	42.80
577	C	ASP	88	130.173	16.253	28.107	1.00	40.12
578	O	ASP	88	129.660	15.210	28.513	1.00	41.11
579	N	ASP	89	131.088	16.251	27.130	1.00	37.03
580	CA	ASP	89	131.496	15.096	26.397	1.00	33.87
581	C	ASP	89	132.107	14.047	27.304	1.00	33.85
582	O	ASP	89	132.047	12.832	26.978	1.00	33.37
583	CB	ASP	89	132.464	15.574	25.325	1.00	27.32
584	CG	ASP	89	131.779	16.561	24.391	1.00	34.13
585	OD1	ASP	89	130.528	16.553	24.341	1.00	20.00
586	OD2	ASP	89	132.481	17.345	23.721	1.00	20.00
587	N	ILE	90	132.765	14.453	28.372	1.00	31.52
588	CA	ILE	90	133.385	13.527	29.308	1.00	25.50
589	CB	ILE	90	134.370	14.245	30.258	1.00	22.28
590	CG2	ILE	90	134.861	13.285	31.328	1.00	22.91
591	CG1	ILE	90	135.549	14.818	29.465	1.00	31.26
592	CD1	ILE	90	136.543	15.620	30.301	1.00	31.23
593	C	ILE	90	132.297	12.836	30.124	1.00	23.61
594	O	ILE	90	132.331	11.620	30.316	1.00	27.20
595	N	LEU	91	131.331	13.622	30.593	1.00	23.72
596	CA	LEU	91	130.218	13.099	31.379	1.00	20.80
597	CB	LEU	91	129.469	14.238	32.071	1.00	20.19
598	CG	LEU	91	130.232	14.888	33.225	1.00	17.15

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
599	CD1	LEU	91	129.464	16.078	33.772	1.00	13.18
600	CD2	LEU	91	130.479	13.852	34.318	1.00	9.86
601	C	LEU	91	129.270	12.281	30.510	1.00	22.03
602	O	LEU	91	128.649	11.334	30.988	1.00	22.93
603	N	ASP	92	129.183	12.640	29.231	1.00	21.86
604	CA	ASP	92	128.337	11.930	28.276	1.00	23.86
605	CB	ASP	92	128.314	12.668	26.933	1.00	30.84
606	CG	ASP	92	127.282	12.105	25.973	1.00	37.16
607	OD1	ASP	92	126.182	12.690	25.879	1.00	34.52
608	OD2	ASP	92	127.568	11.083	25.309	1.00	45.02
609	C	ASP	92	128.928	10.539	28.090	1.00	30.87
610	O	ASP	92	128.208	9.542	28.106	1.00	38.64
611	N	GLN	93	130.247	10.490	27.914	1.00	33.31
612	CA	GLN	93	130.974	9.239	27.738	1.00	34.79
613	CB	GLN	93	132.454	9.531	27.466	1.00	46.61
614	CG	GLN	93	133.345	8.300	27.331	1.00	60.12
615	CD	GLN	93	134.831	8.640	27.354	1.00	75.57
616	OE1	GLN	93	135.217	9.801	27.510	1.00	79.60
617	NE2	GLN	93	135.672	7.621	27.208	1.00	81.92
618	C	GLN	93	130.833	8.380	28.994	1.00	35.74
619	O	GLN	93	130.620	7.171	28.906	1.00	39.97
620	N	ILE	94	130.933	9.019	30.159	1.00	32.85
621	CA	ILE	94	130.817	8.326	31.441	1.00	35.57
622	CB	ILE	94	131.191	9.266	32.625	1.00	33.17
623	CG2	ILE	94	130.909	8.588	33.969	1.00	25.21
624	CG1	ILE	94	132.671	9.652	32.538	1.00	32.16
625	CD1	ILE	94	133.120	10.631	33.603	1.00	32.74
626	C	ILE	94	129.407	7.770	31.645	1.00	38.37
627	O	ILE	94	129.224	6.716	32.260	1.00	45.31
628	N	TYR	95	128.421	8.477	31.102	1.00	38.86
629	CA	TYR	95	127.021	8.082	31.212	1.00	39.68
630	CB	TYR	95	126.122	9.249	30.784	1.00	34.17
631	CG	TYR	95	124.637	8.974	30.877	1.00	27.88
632	CD1	TYR	95	124.060	8.539	32.070	1.00	26.18
633	CE1	TYR	95	122.697	8.279	32.155	1.00	24.69
634	CD2	TYR	95	123.810	9.144	29.770	1.00	21.67
635	CE2	TYR	95	122.447	8.888	29.845	1.00	22.88
636	CZ	TYR	95	121.896	8.454	31.039	1.00	23.25
637	OH	TYR	95	120.546	8.185	31.112	1.00	32.19
638	C	TYR	95	126.715	6.846	30.369	1.00	40.10
639	O	TYR	95	125.987	5.953	30.803	1.00	41.67
640	N	ASN	96	127.291	6.796	29.173	1.00	40.40
641	CA	ASN	96	127.073	5.682	28.261	1.00	50.10
642	CB	ASN	96	127.273	6.146	26.815	1.00	50.46
643	CG	ASN	96	126.252	7.189	26.392	1.00	53.74
644	OD1	ASN	96	125.093	7.141	26.806	1.00	52.90
645	ND2	ASN	96	126.679	8.138	25.567	1.00	56.55
646	C	ASN	96	127.911	4.434	28.545	1.00	54.46
647	O	ASN	96	127.502	3.324	28.202	1.00	58.60
648	N	GLN	97	129.067	4.606	29.183	1.00	57.00
649	CA	GLN	97	129.933	3.469	29.494	1.00	62.35
650	CB	GLN	97	131.385	3.924	29.690	1.00	63.17
651	CG	GLN	97	131.622	4.834	30.885	1.00	68.59
652	CD	GLN	97	133.052	5.351	30.970	1.00	68.54
653	OE1	GLN	97	133.659	5.357	32.040	1.00	66.32
654	NE2	GLN	97	133.594	5.798	29.836	1.00	59.07
655	C	GLN	97	129.458	2.654	30.698	1.00	66.41
656	O	GLN	97	129.682	1.442	30.754	1.00	66.29
657	N	ASN	98	128.790	3.317	31.642	1.00	75.07
658	CA	ASN	98	128.274	2.676	32.854	1.00	85.32
659	CB	ASN	98	127.000	1.878	32.554	1.00	92.56
660	CG	ASN	98	125.798	2.771	32.325	1.00	97.44
661	OD1	ASN	98	125.273	3.375	33.262	1.00	97.63
662	ND2	ASN	98	125.357	2.865	31.074	1.00	98.68
663	C	ASN	98	129.314	1.791	33.535	1.00	89.40
664	O	ASN	98	129.073	0.612	33.812	1.00	88.19
665	N	SER	99	130.486	2.369	33.779	1.00	94.53
666	CA	SER	99	131.560	1.640	34.435	1.00	98.60
667	CB	SER	99	132.918	2.248	34.106	1.00	99.63
668	OG	SER	99	132.996	3.591	34.559	1.00	100.00
669	C	SER	99	131.332	1.673	35.926	1.00	99.96
670	O	SER	99	131.030	2.717	36.500	1.00	98.72
671	N	ASN	100	131.508	0.532	36.566	1.00	100.00

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
672	CA	ASN	100	131.294	0.473	37.995	1.00	100.00
673	CB	ASN	100	130.733	−0.892	38.382	1.00	97.11
674	CG	ASN	100	129.297	−1.056	37.956	1.00	95.75
675	OD1	ASN	100	128.429	−0.279	38.360	1.00	86.86
676	ND2	ASN	100	129.028	−2.069	37.139	1.00	94.51
677	C	ASN	100	132.513	0.784	38.857	1.00	100.00
678	O	ASN	100	133.196	−0.133	39.303	1.00	100.00
679	N	CYS	101	132.829	2.068	39.047	1.00	98.98
680	CA	CYS	101	133.942	2.429	39.953	1.00	94.29
681	CB	CYS	101	134.350	3.905	39.872	1.00	96.36
682	SG	CYS	101	135.708	4.382	41.017	1.00	100.00
683	C	CYS	101	133.151	2.160	41.226	1.00	90.03
684	O	CYS	101	132.261	2.914	41.595	1.00	89.78
685	N	ASN	102	133.483	1.057	41.870	1.00	85.97
686	CA	ASN	102	132.753	0.573	43.043	1.00	81.73
687	CB	ASN	102	133.072	−0.902	43.238	1.00	86.41
688	CG	ASN	102	132.971	−1.688	41.962	1.00	88.71
689	OD1	ASN	102	133.978	−2.107	41.412	1.00	90.82
690	ND2	ASN	102	131.750	−1.869	41.462	1.00	81.79
691	C	ASN	102	132.652	1.257	44.413	1.00	74.07
692	O	ASN	102	131.770	0.881	45.187	1.00	77.40
693	N	ASP	103	133.474	2.260	44.713	1.00	58.82
694	CA	ASP	103	133.377	2.904	46.037	1.00	48.91
695	CB	ASP	103	134.746	3.418	46.524	1.00	50.06
696	CG	ASP	103	135.346	4.487	45.622	1.00	54.31
697	OD1	ASP	103	135.589	4.210	44.429	1.00	68.60
698	OD2	ASP	103	135.616	5.599	46.128	1.00	47.23
699	C	ASP	103	132.290	3.974	46.178	1.00	38.98
700	O	ASP	103	131.875	4.585	45.198	1.00	30.42
701	N	LEU	104	131.820	4.168	47.408	1.00	25.79
702	CA	LEU	104	130.764	5.139	47.702	1.00	26.09
703	CB	LEU	104	130.414	5.114	49.195	1.00	14.86
704	CG	LEU	104	129.294	6.042	49.674	1.00	13.82
705	CD1	LEU	104	127.971	5.654	49.031	1.00	10.36
706	CD2	LEU	104	129.171	5.996	51.191	1.00	7.52
707	C	LEU	104	131.082	6.567	47.274	1.00	26.59
708	O	LEU	104	130.232	7.240	46.696	1.00	27.23
709	N	CYS	105	132.297	7.021	47.574	1.00	28.20
710	CA	CYS	105	132.735	8.370	47.225	1.00	24.21
711	CB	CYS	105	134.164	8.606	47.721	1.00	29.54
712	SG	CYS	105	134.889	10.178	47.188	1.00	32.14
713	C	CYS	105	132.659	8.634	45.724	1.00	20.98
714	O	CYS	105	132.062	9.618	45.285	1.00	24.94
715	N	THR	106	133.258	7.744	44.941	1.00	22.03
716	CA	THR	106	133.261	7.890	43.489	1.00	23.52
717	CB	THR	106	134.197	6.858	42.823	1.00	18.21
718	OG1	THR	106	135.481	6.893	43.461	1.00	20.18
719	CG2	THR	106	134.372	7.183	41.349	1.00	18.22
720	C	THR	106	131.858	7.739	42.906	1.00	22.72
721	O	THR	106	131.481	8.465	41.984	1.00	21.14
722	N	SER	107	131.092	6.802	43.461	1.00	26.53
723	CA	SER	107	129.730	6.532	43.009	1.00	24.15
724	CB	SER	107	129.158	5.312	43.735	1.00	24.72
725	OG	SER	107	129.913	4.147	43.453	1.00	34.14
726	C	SER	107	128.818	7.731	43.228	1.00	20.49
727	O	SER	107	128.128	8.170	42.306	1.00	15.26
728	N	ALA	108	128.822	8.254	44.453	1.00	18.95
729	CA	ALA	108	128.002	9.408	44.810	1.00	16.79
730	CB	ALA	108	128.168	9.732	46.282	1.00	13.84
731	C	ALA	108	128.349	10.623	43.953	1.00	15.33
732	O	ALA	108	127.455	11.340	43.499	1.00	19.47
733	N	LEU	109	129.644	10.836	43.722	1.00	10.72
734	CA	LEU	109	130.106	11.954	42.907	1.00	11.35
735	CB	LEU	109	131.627	12.093	42.993	1.00	15.00
736	CG	LEU	109	132.277	13.237	42.203	1.00	19.48
737	CD1	LEU	109	131.670	14.577	42.596	1.00	15.00
738	CD2	LEU	109	133.778	13.239	42.442	1.00	17.22
739	C	LEU	109	129.673	11.754	41.459	1.00	15.76
740	O	LEU	109	129.216	12.692	40.807	1.00	28.55
741	N	GLN	110	129.813	10.526	40.966	1.00	19.50
742	CA	GLN	110	129.417	10.184	39.600	1.00	20.50
743	CB	GLN	110	129.679	8.699	39.339	1.00	24.06
744	CG	GLN	110	129.287	8.221	37.949	1.00	31.51

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
745	CD	GLN	110	129.373	6.711	37.797	1.00	31.57
746	OE1	GLN	110	129.661	5.990	38.756	1.00	35.16
747	NE2	GLN	110	129.117	6.225	36.586	1.00	34.19
748	C	GLN	110	127.926	10.478	39.414	1.00	21.12
749	O	GLN	110	127.508	11.009	38.389	1.00	20.13
750	N	PHE	111	127.139	10.140	40.431	1.00	23.63
751	CA	PHE	111	125.699	10.356	40.409	1.00	21.06
752	CB	PHE	111	125.065	9.729	41.655	1.00	21.44
753	CG	PHE	111	123.565	9.806	41.685	1.00	18.29
754	CD1	PHE	111	122.795	8.933	40.924	1.00	18.70
755	CD2	PHE	111	122.921	10.744	42.483	1.00	14.43
756	CE1	PHE	111	121.404	8.990	40.959	1.00	18.31
757	CE2	PHE	111	121.533	10.810	42.523	1.00	21.91
758	CZ	PHE	111	120.773	9.929	41.758	1.00	17.47
759	C	PHE	111	125.373	11.846	40.345	1.00	19.49
760	O	PHE	111	124.731	12.305	39.399	1.00	17.88
761	N	ARG	112	125.857	12.598	41.332	1.00	16.34
762	CA	ARG	112	125.606	14.033	41.407	1.00	8.21
763	CB	ARG	112	126.326	14.651	42.608	1.00	7.94
764	CG	ARG	112	126.081	16.153	42.745	1.00	14.61
765	CD	ARG	112	126.507	16.703	44.100	1.00	22.36
766	NE	ARG	112	127.955	16.745	44.291	1.00	19.69
767	CZ	ARG	112	128.777	17.561	43.639	1.00	22.41
768	NH1	ARG	112	128.300	18.407	42.737	1.00	29.76
769	NH2	ARG	112	130.073	17.555	43.915	1.00	26.92
770	C	ARG	112	125.961	14.808	40.145	1.00	13.57
771	O	ARG	112	125.113	15.505	39.588	1.00	17.92
772	N	LEU	113	127.205	14.676	39.693	1.00	11.94
773	CA	LEU	113	127.671	15.385	38.504	1.00	14.83
774	CB	LEU	113	129.151	15.088	38.239	1.00	20.65
775	CG	LEU	113	130.149	15.516	39.322	1.00	16.72
776	CD1	LEU	113	131.568	15.259	38.847	1.00	15.77
777	CD2	LEU	113	129.970	16.985	39.651	1.00	21.06
778	C	LEU	113	126.840	15.108	37.256	1.00	19.17
779	O	LEU	113	126.484	16.034	36.532	1.00	26.79
780	N	LEU	114	126.516	13.841	37.014	1.00	23.83
781	CA	LEU	114	125.717	13.464	35.849	1.00	14.66
782	CB	LEU	114	125.668	11.943	35.703	1.00	18.52
783	CG	LEU	114	126.969	11.251	35.287	1.00	19.65
784	CD1	LEU	114	126.800	9.746	35.362	1.00	22.06
785	CD2	LEU	114	127.352	11.666	33.882	1.00	21.06
786	C	LEU	114	124.300	14.030	35.939	1.00	15.67
787	O	LEU	114	123.787	14.596	34.972	1.00	18.67
788	N	ARG	115	123.678	13.883	37.104	1.00	9.26
789	CA	ARG	115	122.328	14.387	37.328	1.00	7.86
790	CB	ARG	115	121.849	14.021	38.736	1.00	10.49
791	CG	ARG	115	121.450	12.562	38.901	1.00	12.35
792	CD	ARG	115	120.323	12.202	37.949	1.00	17.12
793	NE	ARG	115	119.807	10.857	38.179	1.00	21.26
794	CZ	ARG	115	118.803	10.570	39.000	1.00	15.94
795	NH1	ARG	115	118.199	11.537	39.676	1.00	8.20
796	NH2	ARG	115	118.406	9.314	39.152	1.00	17.38
797	C	ARG	115	122.250	15.899	37.126	1.00	13.44
798	O	ARG	115	121.379	16.390	36.402	1.00	8.27
799	N	GLN	116	123.180	16.629	37.743	1.00	14.35
800	CA	GLN	116	123.225	18.086	37.629	1.00	11.93
801	CB	GLN	116	124.364	18.664	38.471	1.00	4.12
802	CG	GLN	116	124.165	18.534	39.968	1.00	5.13
803	CD	GLN	116	125.303	19.142	40.768	1.00	11.78
804	OE1	GLN	116	125.080	19.950	41.669	1.00	21.37
805	NE2	GLN	116	126.530	18.747	40.451	1.03	11.47
806	C	GLN	116	123.392	18.530	36.183	1.00	15.48
807	O	GLN	116	123.126	19.682	35.851	1.00	19.88
808	N	HIS	117	123.827	17.607	35.328	1.00	19.55
809	CA	HIS	117	124.031	17.893	33.912	1.00	15.02
810	CB	HIS	117	125.405	17.392	33.460	1.00	13.78
811	CG	HIS	117	126.538	18.253	33.925	1.00	17.44
812	CD2	HIS	117	126.999	18.525	35.169	1.00	18.38
813	ND1	HIS	117	127.322	18.983	33.059	1.00	19.26
814	CE1	HIS	117	128.216	19.668	33.748	1.00	20.36
815	NE2	HIS	117	128.042	19.408	35.031	1.00	17.37
816	C	HIS	117	122.930	17.349	33.006	1.00	16.42
817	O	HIS	117	123.036	17.419	31.780	1.00	15.29

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
818	N	GLY	118	121.872	16.813	33.613	1.00	17.98
819	CA	GLY	118	120.756	16.292	32.839	1.00	21.36
820	C	GLY	118	120.761	14.808	32.521	1.00	21.11
821	O	GLY	118	119.760	14.284	32.032	1.00	23.89
822	N	PHE	119	121.880	14.134	32.773	1.00	20.97
823	CA	PHE	119	121.994	12.702	32.510	1.00	15.97
824	CB	PHE	119	123.465	12.282	32.477	1.00	13.26
825	CG	PHE	119	124.281	13.007	31.439	1.00	19.34
826	CD1	PHE	119	125.155	14.025	31.808	1.00	18.10
827	CD2	PHE	119	124.160	12.686	30.090	1.00	17.78
828	CE1	PHE	119	125.896	14.714	30.850	1.00	14.61
829	CE2	PHE	119	124.896	13.370	29.122	1.00	16.11
830	CZ	PHE	119	125.765	14.386	29.503	1.00	22.05
831	C	PHE	119	121.238	11.917	33.576	1.00	20.90
832	O	PHE	119	121.620	11.910	34.749	1.00	17.99
833	N	ASN	120	120.157	11.263	33.161	1.00	20.78
834	CA	ASN	120	119.326	10.494	34.078	1.00	23.46
835	CB	ASN	120	117.928	10.307	33.477	1.00	23.75
836	CG	ASN	120	116.919	9.766	34.481	1.00	23.50
837	OD1	ASN	120	117.147	9.782	35.695	1.00	18.94
838	ND2	ASN	120	115.786	9.295	33.973	1.00	24.72
839	C	ASN	120	119.940	9.145	34.447	1.00	29.37
840	O	ASN	120	119.467	8.092	34.011	1.00	37.56
841	N	ILE	121	120.999	9.183	35.251	1.00	30.57
842	CA	ILE	121	121.674	7.965	35.691	1.00	28.30
843	CB	ILE	121	123.118	8.250	36.202	1.00	31.51
844	CG2	ILE	121	123.116	9.395	37.212	1.00	18.33
845	CG1	ILE	121	123.734	6.970	36.784	1.00	34.25
846	CD1	ILE	121	125.160	7.119	37.270	1.00	35.18
847	C	ILE	121	120.862	7.263	36.774	1.00	24.20
848	O	ILE	121	120.435	7.888	37.746	1.00	29.58
849	N	SER	122	120.654	5.963	36.594	1.00	28.31
850	CA	SER	122	119.886	5.158	31.538	1.00	31.22
851	CB	SER	122	119.782	3.711	37.040	1.00	37.94
852	OG	SER	122	119.046	2.907	37.948	1.00	37.31
853	C	SER	122	120.471	5.193	38.942	1.00	26.25
854	O	SER	122	121.690	5.086	39.121	1.00	36.49
855	N	PRO	123	119.606	5.367	39.956	1.00	25.72
856	CD	PRO	123	118.162	5.626	39.787	1.00	24.10
857	CA	PRO	123	119.995	5.427	41.367	1.00	24.12
858	CB	PRO	123	118.807	6.139	42.015	1.00	14.52
859	CG	PRO	123	117.635	5.620	41.222	1.00	18.26
860	C	PRO	123	120.266	4.057	41.978	1.00	26.29
861	O	PRO	123	120.649	3.957	43.143	1.00	26.93
862	N	GLU	124	120.106	3.007	41.176	1.00	31.58
863	CA	GLU	124	120.362	1.656	41.665	1.00	42.38
864	CB	GLU	124	119.734	0.614	40.749	1.00	52.63
865	CG	GLU	124	118.661	−0.182	41.472	1.00	66.87
866	CD	GLU	124	117.857	−1.078	40.558	1.00	84.70
867	OE1	GLU	124	118.072	−1.045	39.323	1.00	92.92
868	OE2	GLU	124	116.995	−1.820	41.075	1.00	95.72
869	C	GLU	124	121.850	1.396	41.860	1.00	40.43
870	O	GLU	124	122.243	0.345	42.359	1.00	40.69
871	N	ILE	125	122.685	2.383	41.493	1.00	40.56
872	CA	ILE	125	124.113	2.311	41.658	1.00	33.74
873	CB	ILE	125	124.796	3.532	40.995	1.00	34.47
874	CG2	ILE	125	124.231	4.828	41.567	1.00	35.94
875	CG1	ILE	125	126.317	3.471	41.176	1.00	33.47
876	CD1	ILE	125	127.051	4.648	40.560	1.00	33.54
877	C	ILE	125	124.397	2.311	43.166	1.00	27.96
878	O	ILE	125	125.450	1.867	43.612	1.00	32.46
879	N	PHE	126	123.422	2.783	43.938	1.00	24.55
880	CA	PHE	126	123.518	2.850	45.393	1.00	31.56
881	CB	PHE	126	122.701	4.034	45.925	1.00	31.55
882	CG	PHE	126	123.245	5.377	45.536	1.00	36.38
883	CD1	PHE	126	122.701	6.079	44.465	1.00	32.78
884	CD2	PHE	126	124.300	5.946	46.245	1.00	35.39
885	CE1	PHE	126	123.197	7.328	44.105	1.00	32.25
886	CE2	PHE	126	124.805	7.194	45.894	1.00	31.56
887	CZ	PHE	126	124.252	7.889	44.820	1.00	28.07
888	C	PHE	126	123.042	1.568	46.079	1.00	37.75
889	O	PHE	126	122.939	1.520	47.308	1.00	36.32
890	N	SER	127	122.730	0.542	45.289	1.00	42.49

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
891	CA	SER	127	122.268	−0.732	45.836	1.00	43.38
892	CB	SER	127	121.659	−1.601	44.733	1.00	48.30
893	OG	SER	127	120.465	−1.025	44.233	1.00	59.77
894	C	SER	127	123.401	−1.482	46.527	1.00	39.67
895	O	SER	127	123.228	−2.001	47.632	1.00	35.01
896	N	LYS	128	124.567	−1.503	45.886	1.00	35.16
897	CA	LYS	128	125.743	−2.179	46.426	1.00	36.47
898	CB	LYS	128	126.877	−2.180	45.389	1.00	33.52
899	CG	LYS	128	127.146	−0.834	44.732	1.00	37.85
900	CD	LYS	128	128.170	−0.947	43.606	1.00	37.35
901	CE	LYS	128	128.353	0.388	42.892	1.00	50.12
902	NZ	LYS	128	129.338	0.328	41.776	1.00	54.36
903	C	LYS	128	126.233	−1.623	47.769	1.00	38.71
904	O	LYS	128	127.102	−2.217	48.412	1.00	46.49
905	N	PHE	129	125.656	−0.501	48.199	1.00	38.63
906	CA	PHE	129	126.028	0.135	49.466	1.00	31.98
907	CB	PHE	129	126.309	1.626	49.256	1.00	24.98
908	CG	PHE	129	127.324	1.904	48.191	1.00	20.86
909	CD1	PHE	129	126.946	2.506	46.997	1.00	19.33
910	CD2	PHE	129	128.653	1.537	48.368	1.00	17.79
911	CE1	PHE	129	127.877	2.735	45.988	1.00	22.73
912	CE2	PHE	129	129.590	1.760	47.368	1.00	19.77
913	CZ	PHE	129	129.201	2.361	46.174	1.00	17.69
914	C	PHE	129	124.929	−0.024	50.509	1.00	31.84
915	O	PHE	129	125.051	0.462	51.635	1.00	32.60
916	N	GLN	130	123.854	−0.700	50.123	1.00	40.45
917	CA	GLN	130	122.720	−0.922	51.010	1.00	47.58
918	CB	GLN	130	121.456	−0.310	50.403	1.00	51.16
919	CG	GLN	130	121.515	1.197	50.231	1.00	50.70
920	CD	GLN	130	120.308	1.755	49.505	1.00	54.25
921	OE1	GLN	130	119.310	1.063	49.303	1.00	62.26
922	NE2	GLN	130	120.394	3.017	49.105	1.00	58.79
923	C	GLN	130	122.496	−2.405	51.263	1.00	51.99
924	O	GLN	130	122.818	−3.245	50.419	1.00	55.44
925	N	ASP	131	121.945	−2.723	52.431	1.00	53.38
926	CA	ASP	131	121.665	−4.108	52.789	1.00	60.28
927	CB	ASP	131	121.556	−4.258	54.314	1.00	58.61
928	CG	ASP	131	120.311	−3.596	54.892	1.00	62.05
929	OD1	ASP	131	119.749	−4.145	55.860	1.00	69.31
930	OD2	ASP	131	119.893	−2.532	54.391	1.00	65.85
931	C	ASP	131	120.382	−4.583	52.103	1.00	64.98
932	O	ASP	131	119.762	−3.837	51.341	1.00	64.40
933	N	GLU	132	119.989	−5.823	52.383	1.00	70.50
934	CA	GLU	132	118.786	−6.415	51.803	1.00	72.09
935	CB	GLU	132	118.735	−7.913	52.120	1.00	78.41
936	CG	GLU	132	119.098	−8.253	53.562	1.00	92.85
937	CD	GLU	132	117.997	−8.995	54.303	1.00	100.00
938	OE1	GLU	132	116.803	−8.735	54.037	1.00	100.00
939	OE2	GLU	132	118.331	−9.837	55.165	1.00	100.00
940	C	GLU	132	117.486	−5.729	52.236	1.00	69.60
941	O	GLU	132	116.424	−5.985	51.666	1.00	67.84
942	N	ASN	133	117.575	−4.849	53.230	1.00	69.95
943	CA	ASN	133	116.408	−4.124	53.726	1.00	71.81
944	CB	ASN	133	116.540	−3.882	55.235	1.00	76.32
945	CG	ASN	133	115.238	−3.425	55.873	1.00	85.38
946	OD1	ASN	133	114.202	−4.076	55.731	1.00	89.18
947	ND2	ASN	133	115.288	−2.303	56.583	1.00	85.57
948	C	ASN	133	116.214	−2.794	52.982	1.00	70.23
949	O	ASN	133	115.184	−2.132	53.136	1.00	67.90
950	N	GLY	134	117.204	−2.414	52.176	1.00	67.24
951	CA	GLY	134	117.120	−1.177	51.416	1.00	63.86
952	C	GLY	134	117.758	0.036	52.072	1.00	61.93
953	O	GLY	134	117.712	1.138	51.520	1.00	64.71
954	N	LYS	135	118.332	−0.158	53.257	1.00	57.80
955	CA	LYS	135	118.989	0.921	53.993	1.00	52.54
956	CB	LYS	135	118.628	0.565	55.482	1.00	54.50
957	CG	LYS	135	117.298	1.519	55.845	1.00	58.81
958	CD	LYS	135	116.106	0.776	55.259	1.00	65.64
959	CE	LYS	135	114.795	1.428	55.666	1.00	66.94
960	NZ	LYS	135	114.629	1.450	57.145	1.00	67.92
961	C	LYS	135	120.505	0.859	53.827	1.00	46.30
962	O	LYS	135	121.062	−0.191	53.506	1.00	39.34
963	N	PHE	136	121.168	1.988	54.058	1.00	40.70

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
964	CA	PHE	136	122.619	2.066	53.929	1.00	37.70
965	CB	PHE	136	123.082	3.525	53.941	1.00	30.32
966	CG	PHE	136	122.848	4.238	52.644	1.00	18.97
967	CD1	PHE	136	121.752	5.079	52.485	1.00	16.88
968	CD2	PHE	136	123.708	4.044	51.569	1.00	2.95
969	CE1	PHE	136	121.512	5.714	51.269	1.00	9.36
970	CE2	PHE	138	123.478	4.674	50.350	1.00	8.37
971	CZ	PHE	136	122.376	5.510	50.200	1.00	11.64
972	C	PHE	136	123.368	1.280	54.992	1.00	40.03
973	O	PHE	136	123.007	1.310	56.173	1.00	36.07
974	N	LYS	137	124.404	0.564	54.554	1.00	35.20
975	CA	LYS	137	125.232	−0.232	55.451	1.00	37.62
976	CB	LYS	137	126.333	−0.957	54.670	1.00	36.07
977	CG	LYS	137	125.845	−2.039	53.721	1.00	43.95
978	CD	LYS	137	127.016	−2.672	52.985	1.00	45.68
979	CE	LYS	137	126.558	−3.745	52.011	1.00	46.97
980	NZ	LYS	137	127.709	−4.340	51.276	1.00	45.41
981	C	LYS	137	125.872	0.698	56.472	1.00	42.74
982	O	LYS	137	126.612	1.614	56.108	1.00	49.71
983	N	GLU	138	125.569	0.472	57.747	1.00	44.30
984	CA	GLU	138	126.116	1.290	58.824	1.00	43.35
985	CB	GLU	138	125.482	0.895	60.157	1.00	48.22
986	CG	GLU	138	123.997	1.184	60.285	1.00	55.55
987	CD	GLU	138	123.703	2.650	60.528	1.00	59.82
988	OE1	GLU	138	124.127	3.180	61.577	1.00	58.06
989	OE2	GLU	138	123.040	3.272	59.674	1.00	70.04
990	C	GLU	138	127.641	1.172	58.913	1.00	46.10
991	O	GLU	138	128.283	1.909	59.662	1.00	51.05
992	N	SER	139	128.210	0.242	58.149	1.00	40.33
993	CA	SER	139	129.653	0.027	58.122	1.00	37.26
994	CB	SER	139	129.975	−1.354	57.541	1.00	42.99
995	OG	SER	139	129.518	−1.477	56.204	1.00	42.44
996	C	SER	139	130.384	1.114	57.326	1.00	38.83
997	O	SER	139	131.606	1.247	57.423	1.00	44.35
998	N	LEU	140	129.633	1.875	56.531	1.00	35.64
999	CA	LEU	140	130.191	2.960	55.721	1.00	26.87
1000	CB	LEU	140	129.289	3.244	54.514	1.00	27.15
1001	CG	LEU	140	129.037	2.148	53.476	1.00	27.17
1002	CD1	LEU	140	127.955	2.607	52.511	1.00	23.24
1003	CD2	LEU	140	130.317	1.814	52.726	1.00	21.35
1004	C	LEU	140	130.325	4.241	56.547	1.00	23.48
1005	O	LEU	140	130.817	5.254	56.054	1.00	18.12
1006	N	ALA	141	129.883	4.178	57.803	1.00	21.14
1007	CA	ALA	141	129.916	5.311	58.725	1.00	23.07
1008	CB	ALA	141	129.182	4.951	60.007	1.00	13.93
1009	C	ALA	141	131.316	5.829	59.053	1.00	29.68
1010	O	ALA	141	131.465	6.917	59.614	1.00	34.02
1011	N	SER	142	132.334	5.045	58.710	1.00	31.98
1012	CA	SER	142	133.723	5.413	58.963	1.00	25.78
1013	CB	SER	142	134.482	4.211	59.534	1.00	27.76
1014	OG	SER	142	134.293	3.059	58.731	1.00	23.34
1015	C	SER	142	134.436	5.957	57.719	1.00	26.37
1016	O	SER	142	135.629	6.255	57.761	1.00	36.05
1017	N	ASP	143	133.699	6.078	56.617	1.00	19.43
1018	CA	ASP	143	134.237	6.596	55.361	1.00	13.45
1019	CB	ASP	143	133.794	5.701	54.194	1.00	12.41
1020	CG	ASP	143	134.284	6.196	52.835	1.00	22.67
1021	OD1	ASP	143	133.710	5.759	51.811	1.00	21.93
1022	OD2	ASP	143	135.239	7.004	52.778	1.00	35.17
1023	C	ASP	143	133.727	8.025	55.162	1.00	19.69
1024	O	ASP	143	132.675	8.238	54.559	1.00	21.70
1025	N	VAL	144	134.485	8.997	55.664	1.00	21.88
1026	CA	VAL	144	134.120	10.411	55.566	1.00	19.30
1027	CB	VAL	144	135.093	11.295	56.376	1.00	16.67
1028	CG1	VAL	144	134.789	12.769	56.155	1.00	22.12
1029	CG2	VAL	144	134.978	10.961	57.857	1.00	20.43
1030	C	VAL	144	133.997	10.942	54.136	1.00	18.93
1031	O	VAL	144	133.012	11.603	53.801	1.00	23.53
1032	N	LEU	145	134.984	10.657	53.293	1.00	15.19
1033	CA	LEU	145	134.940	11.122	51.912	1.00	18.54
1034	CB	LEU	145	136.238	10.780	51.181	1.00	22.93
1035	CG	LEU	145	137.524	11.410	51.722	1.00	23.25
1038	CD1	LEU	145	138.647	11.189	50.715	1.00	24.40

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1037	CD2	LEU	145	137.327	12.898	51.968	1.00	18.75
1038	C	LEU	145	133.744	10.535	51.168	1.00	23.90
1039	O	LEU	145	133.236	11.135	50.219	1.00	26.81
1040	N	GLY	146	133.303	9.358	51.610	1.00	24.92
1041	CA	GLY	146	132.159	8.705	50.999	1.00	21.44
1042	C	GLY	146	130.868	9.313	51.512	1.00	19.58
1043	O	GLY	146	129.953	9.591	50.740	1.00	22.50
1044	N	LEU	147	130.805	9.524	52.823	1.00	9.20
1045	CA	LEU	147	129.643	10.116	53.467	1.00	7.33
1046	CB	LEU	147	129.849	10.163	54.980	1.00	7.87
1047	CG	LEU	147	129.927	8.831	55.721	1.00	12.02
1048	CD1	LEU	147	130.341	9.066	57.157	1.00	8.20
1049	CD2	LEU	147	128.583	8.122	55.656	1.00	15.08
1050	C	LEU	147	129.388	11.527	52.945	1.00	20.24
1051	O	LEU	147	128.244	11.900	52.680	1.00	27.36
1052	N	LEU	148	130.462	12.333	52.795	1.00	20.47
1053	CA	LEU	148	130.371	13.676	52.304	1.00	20.11
1054	CB	LEU	148	131.751	14.347	52.330	1.00	16.79
1055	CG	LEU	148	131.829	15.805	51.857	1.00	13.41
1066	CD1	LEU	148	130.897	16.833	52.683	1.00	6.32
1057	CD2	LEU	148	133.256	16.306	51.961	1.00	9.98
1058	C	LEU	148	129.777	13.758	50.895	1.00	16.22
1059	O	LEU	148	128.838	14.520	50.657	1.00	19.05
1060	N	ASN	149	130.332	12.985	49.965	1.00	14.19
1061	CA	ASN	149	129.840	12.986	48.592	1.00	19.68
1062	CB	ASN	149	130.776	12.199	47.678	1.00	17.57
1063	CG	ASN	149	132.009	12.987	47.306	1.00	21.68
1064	OD1	ASN	149	132.904	13.181	48.129	1.00	27.23
1065	ND2	ASN	149	132.055	13.469	46.067	1.00	17.93
1066	C	ASN	149	128.414	12.461	48.486	1.00	24.02
1067	O	ASN	149	127.676	12.829	47.571	1.00	25.30
1068	N	LEU	150	128.033	11.596	49.424	1.00	23.15
1069	CA	LEU	150	126.685	11.049	49.449	1.00	19.85
1070	CB	LEU	150	126.606	9.844	50.391	1.00	15.00
1071	CG	LEU	150	125.224	9.198	50.548	1.00	14.74
1072	CD1	LEU	150	124.735	8.634	49.215	1.00	8.02
1073	CD2	LEU	150	125.287	8.115	51.600	1.00	2.00
1074	C	LEU	150	125.745	12.153	49.925	1.00	20.18
1075	O	LEU	150	124.640	12.304	49.404	1.00	22.47
1076	N	TYR	151	126.209	12.930	50.904	1.00	18.20
1077	CA	TYR	151	125.440	14.041	51.455	1.00	18.43
1078	CB	TYR	151	126.226	14.739	52.569	1.00	10.57
1079	CG	TYR	151	125.598	16.032	53.044	1.00	11.49
1080	CD1	TYR	151	124.759	16.056	54.156	1.00	5.47
1081	CE1	TYR	151	124.171	17.242	54.586	1.00	8.73
1082	CD2	TYR	151	125.835	17.234	52.372	1.00	10.72
1083	CE2	TYR	151	125.250	18.421	52.791	1.00	9.08
1084	CZ	TYR	151	124.421	18.420	53.898	1.00	11.39
1085	OH	TYR	151	123.845	19.598	54.316	1.00	11.19
1086	C	TYR	151	125.117	15.041	50.355	1.00	17.39
1087	O	TYR	151	123.990	15.521	50.256	1.00	26.93
1088	N	GLU	152	126.121	15.374	49.552	1.00	15.23
1089	CA	GLU	152	125.937	16.316	48.455	1.00	18.45
1090	CB	GLU	152	127.282	16.649	47.798	1.00	14.61
1091	CG	GLU	152	128.316	17.293	48.727	1.00	17.73
1092	CD	GLU	152	127.962	18.712	49.169	1.00	16.74
1093	OE1	GLU	152	126.980	19.292	48.662	1.00	16.63
1094	OE2	GLU	152	128.681	19.252	50.034	1.00	22.78
1095	C	GLU	152	124.977	15.750	47.413	1.00	13.63
1096	O	GLU	152	124.114	16.463	46.904	1.00	20.19
1097	N	ALA	153	125.115	14.458	47.125	1.00	18.04
1098	CA	ALA	153	124.271	13.778	48.143	1.00	14.37
1099	CB	ALA	153	124.859	12.417	45.794	1.00	13.44
1100	C	ALA	153	122.815	13.624	46.580	1.00	13.36
1101	O	ALA	153	121.921	13.577	45.738	1.00	11.20
1102	N	SER	154	122.574	13.568	47.889	1.00	16.02
1103	CA	SER	154	121.218	13.413	48.416	1.00	13.22
1104	CB	SER	154	121.250	13.157	49.928	1.00	8.73
1105	CG	SER	154	121.581	14.330	50.651	1.00	16.49
1106	C	SER	154	120.312	14.607	48.118	1.00	14.26
1107	O	SER	154	119.087	14.504	48.207	1.00	26.54
1108	N	HIS	155	120.915	15.735	47.757	1.00	14.00
1109	CA	HIS	155	120.154	16.942	47.457	1.00	8.22

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1110	CB	HIS	155	120.920	18.177	47.928	1.00	2.00
1111	CG	HIS	155	120.932	18.340	49.415	1.00	2.00
1112	CD2	HIS	155	120.036	18.914	50.255	1.00	3.97
1113	ND1	HIS	155	121.946	17.856	50.211	1.00	3.74
1114	CE1	HIS	155	121.676	18.123	51.476	1.00	12.80
1115	NE2	HIS	155	120.522	18.764	51.529	1.00	11.17
1116	C	HIS	155	119.742	17.092	45.997	1.00	10.18
1117	O	HIS	155	119.025	18.030	45.645	1.00	16.07
1118	N	VAL	156	120.182	16.163	45.152	1.00	6.86
1119	CA	VAL	156	119.843	16.202	43.733	1.00	7.09
1120	CB	VAL	156	121.109	16.099	42.823	1.00	5.97
1121	CG1	VAL	156	122.161	17.113	43.248	1.00	2.00
1122	CG2	VAL	156	121.678	14.682	42.841	1.00	4.04
1123	C	VAL	156	118.866	15.087	43.354	1.00	11.84
1124	O	VAL	156	118.644	14.827	42.170	1.00	13.76
1125	N	ARG	157	118.264	14.443	44.351	1.00	12.59
1126	CA	ARG	157	117.329	13.357	44.074	1.00	21.43
1127	CB	ARG	157	117.224	12.398	45.271	1.00	17.56
1128	CG	ARG	157	116.482	12.908	46.491	1.00	22.45
1129	CD	ARG	157	116.525	11.846	47.583	1.00	26.00
1130	NE	ARG	157	115.512	12.037	48.620	1.00	35.19
1131	CZ	ARG	157	114.360	11.370	48.676	1.00	40.41
1132	NH1	ARG	157	114.064	10.465	47.753	1.00	42.25
1133	NH2	ARG	157	113.505	11.598	49.664	1.00	42.66
1134	C	ARG	157	115.945	13.815	43.609	1.00	22.46
1135	O	ARG	157	115.473	14.885	43.985	1.00	28.62
1136	N	THR	158	115.334	13.012	42.740	1.00	30.57
1137	CA	THR	158	114.003	13.287	42.200	1.00	23.48
1138	CB	THR	158	113.951	13.012	40.675	1.00	18.85
1139	OG1	THR	158	114.132	11.613	40.424	1.00	23.14
1140	CG2	THR	158	115.044	13.781	39.959	1.00	5.29
1141	C	THR	158	112.962	12.409	42.911	1.00	26.07
1142	O	THR	158	113.258	11.786	43.936	1.00	29.73
1143	N	HIS	159	111.745	12.362	42.373	1.00	25.85
1144	CA	HIS	159	110.681	11.551	42.967	1.00	24.71
1145	CB	HIS	159	109.312	11.987	42.435	1.00	24.02
1146	CG	HIS	159	108.903	13.358	42.872	1.00	20.05
1147	CD2	HIS	159	108.888	14.538	42.209	1.00	14.66
1148	ND1	HIS	159	108.453	13.629	44.147	1.00	22.06
1149	CE1	HIS	159	108.179	14.917	44.250	1.00	20.70
1150	NE2	HIS	159	108.434	15.492	43.088	1.00	18.69
1151	C	HIS	159	110.893	10.054	42.723	1.00	28.82
1152	O	HIS	159	110.377	9.211	43.464	1.00	29.90
1153	N	ALA	160	111.674	9.733	41.695	1.00	22.36
1154	CA	ALA	160	111.966	8.351	41.341	1.00	16.69
1155	CB	ALA	160	112.118	8.233	39.835	1.00	12.78
1156	C	ALA	160	113.218	7.821	42.038	1.00	24.25
1157	O	ALA	160	113.748	6.775	41.655	1.00	30.58
1158	N	ASP	161	113.679	8.531	43.066	1.00	27.69
1159	CA	ASP	161	114.880	8.134	43.800	1.00	24.25
1160	CB	ASP	161	115.968	9.212	43.669	1.00	22.91
1161	CG	ASP	161	116.356	9.495	42.222	1.00	29.35
1162	OD1	ASP	161	116.405	8.550	41.404	1.00	29.54
1163	OD2	ASP	161	116.623	10.672	41.906	1.00	19.16
1164	C	ASP	161	114.626	7.840	45.281	1.00	26.01
1165	O	ASP	161	115.308	8.380	46.154	1.00	34.22
1166	N	ASP	162	113.670	6.957	45.561	1.00	28.71
1167	CA	ASP	162	113.339	6.590	46.939	1.00	28.70
1168	CB	ASP	162	111.999	5.859	46.993	1.00	34.90
1169	CG	ASP	162	110.851	6.726	46.536	1.00	42.80
1170	OD1	ASP	162	110.426	7.600	47.322	1.00	36.44
1171	OD2	ASP	162	110.386	6.543	45.389	1.00	43.54
1172	C	ASP	162	114.423	5.728	47.573	1.00	27.14
1173	O	ASP	162	114.386	5.441	48.769	1.00	28.39
1174	N	ILE	163	115.378	5.302	46.756	1.00	26.67
1175	CA	ILE	163	116.485	4.486	47.229	1.00	27.39
1176	CB	ILE	163	117.250	3.866	46.030	1.00	24.84
1177	CG2	ILE	163	118.201	4.881	45.412	1.00	29.37
1178	CG1	ILE	163	118.015	2.623	46.471	1.00	30.57
1179	CD1	ILE	163	118.639	1.863	45.323	1.00	43.90
1180	C	ILE	163	117.407	5.372	48.078	1.00	28.12
1181	O	ILE	163	118.169	4.881	48.912	1.00	29.38
1182	N	LEU	164	117.277	6.686	47.890	1.00	30.46

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1183	CA	LEU	164	118.070	7.684	48.607	1.00	24.33
1184	CB	LEU	164	118.646	8.695	47.612	1.00	16.04
1185	CG	LEU	164	119.602	8.181	46.538	1.00	20.33
1186	CD1	LEU	164	119.864	9.271	45.514	1.00	22.74
1187	CD2	LEU	164	120.894	7.720	47.184	1.00	17.92
1188	C	LEU	164	117.259	8.441	49.658	1.00	23.88
1189	O	LEU	164	117.667	9.518	50.101	1.00	32.16
1190	N	GLU	165	116.120	7.882	50.061	1.00	21.56
1191	CA	GLU	165	115.256	8.529	51.043	1.00	18.89
1192	CB	GLU	165	113.947	7.755	51.202	1.00	24.79
1193	CG	GLU	165	114.127	6.324	51.689	1.00	48.18
1194	CD	GLU	165	112.819	5.561	51.814	1.00	57.24
1195	OE1	GLU	165	111.765	6.076	51.375	1.00	63.77
1196	OE2	GLU	165	112.850	4.434	52.353	1.00	62.32
1197	C	GLU	165	115.907	8.727	52.405	1.00	16.81
1198	O	GLU	165	115.598	9.687	53.106	1.00	18.04
1199	N	ASP	166	116.817	7.828	52.771	1.00	23.03
1200	CA	ASP	166	117.497	7.914	54.061	1.00	27.94
1201	CB	ASP	166	117.383	6.579	54.811	1.00	35.23
1202	CG	ASP	166	115.936	6.177	55.082	1.00	50.03
1203	OD1	ASP	166	115.565	5.024	54.771	1.00	57.17
1204	OD2	ASP	166	115.169	7.013	55.606	1.00	53.93
1205	C	ASP	166	118.966	8.330	53.943	1.00	24.13
1206	O	ASP	166	119.674	8.409	54.950	1.00	23.24
1207	N	ALA	167	119.401	8.638	52.721	1.00	14.78
1208	CA	ALA	167	120.780	9.044	52.443	1.00	16.72
1209	CB	ALA	167	120.993	9.169	50.948	1.00	12.70
1210	C	ALA	167	121.215	10.333	53.136	1.00	24.13
1211	O	ALA	167	122.355	10.443	53.590	1.00	29.67
1212	N	LEU	168	120.317	11.313	53.193	1.00	27.80
1213	CA	LEU	168	120.614	12.590	53.831	1.00	19.27
1214	CB	LEU	168	119.540	13.623	53.487	1.00	23.80
1215	CG	LEU	168	119.706	15.016	54.099	1.00	18.12
1216	CD1	LEU	168	121.006	15.642	53.626	1.00	19.21
1217	CD2	LEU	168	118.524	15.890	53.719	1.00	17.36
1218	C	LEU	168	120.730	12.450	55.343	1.00	20.39
1219	O	LEU	168	121.663	12.973	55.943	1.00	26.94
1220	N	ALA	169	119.776	11.755	55.954	1.00	22.95
1221	CA	ALA	169	119.784	11.555	57.400	1.00	28.99
1222	CB	ALA	169	118.472	10.934	57.856	1.00	26.34
1223	C	ALA	169	120.959	10.676	57.816	1.00	31.11
1224	O	ALA	169	121.529	10.855	58.895	1.00	32.24
1225	N	PHE	170	121.319	9.736	56.944	1.00	26.27
1226	CA	PHE	170	122.423	8.819	57.197	1.00	22.01
1227	CB	PHE	170	122.448	7.714	56.135	1.00	20.64
1228	CG	PHE	170	123.592	6.747	56.284	1.00	28.63
1229	CD1	PHE	170	123.622	5.837	57.338	1.00	28.29
1230	CD2	PHE	170	124.642	6.745	55.368	1.00	25.46
1231	CE1	PHE	170	124.683	4.938	57.479	1.00	27.46
1232	CE2	PHE	170	125.706	5.850	55.500	1.00	24.24
1233	CZ	PHE	170	125.726	4.945	56.558	1.00	22.35
1234	C	PHE	170	123.752	9.564	57.205	1.00	20.63
1235	O	PHE	170	124.440	9.610	58.224	1.00	23.76
1236	N	SER	171	124.095	10.156	56.066	1.00	16.15
1237	CA	SER	171	125.340	10.899	55.918	1.00	12.93
1238	CB	SER	171	125.476	11.429	54.488	1.00	12.97
1239	OG	SER	171	124.397	12.281	54.152	1.00	12.50
1240	C	SER	171	125.479	12.047	56.912	1.00	13.92
1241	O	SER	171	126.567	12.297	57.420	1.00	15.50
1242	N	THR	172	124.372	12.726	57.205	1.00	16.38
1243	CA	THR	172	124.383	13.854	58.137	1.00	16.69
1244	CB	THR	172	123.000	14.564	58.196	1.00	14.70
1245	OG1	THR	172	122.758	15.259	56.966	1.00	12.00
1246	CG2	THR	172	122.946	15.559	59.348	1.00	6.76
1247	C	THR	172	124.813	13.486	59.556	1.00	19.18
1248	O	THR	172	125.759	14.067	60.086	1.00	22.93
1249	N	ILE	173	124.129	12.516	60.160	1.00	22.35
1250	CA	ILE	173	124.439	12.112	61.529	1.00	26.29
1251	CB	ILE	173	123.428	11.061	62.070	1.00	29.19
1252	CG2	ILE	173	123.553	9.747	61.305	1.00	26.89
1253	CG1	ILE	173	123.657	10.844	63.572	1.00	34.59
1254	CD1	ILE	173	122.655	9.928	64.240	1.00	35.92
1255	C	ILE	173	125.868	11.602	61.702	1.00	27.07

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1256	O	ILE	173	126.481	11.801	62.754	1.00	30.04
1257	N	HIS	174	126.404	10.972	60.662	1.00	18.99
1258	CA	HIS	174	127.757	10.441	60.721	1.00	26.30
1259	CB	HIS	174	127.895	9.228	59.799	1.00	36.54
1260	CG	HIS	174	127.114	8.034	60.257	1.00	41.37
1261	CD2	HIS	174	126.355	7.147	59.571	1.00	35.65
1262	ND1	HIS	174	127.057	7.644	61.579	1.00	39.38
1263	CE1	HIS	174	126.295	6.569	61.687	1.00	33.20
1264	NE2	HIS	174	125.857	6.248	60.483	1.00	35.00
1265	C	HIS	174	128.804	11.504	60.407	1.00	27.93
1266	O	HIS	174	129.945	11.419	60.872	1.00	25.80
1267	N	LEU	175	128.410	12.508	59.626	1.00	25.88
1268	CA	LEU	175	129.312	13.600	59.280	1.00	17.20
1269	CB	LEU	175	128.804	14.376	58.066	1.00	12.92
1270	CG	LEU	175	129.069	13.747	56.696	1.00	4.37
1271	CD1	LEU	175	128.472	14.624	55.606	1.00	2.00
1272	CD2	LEU	175	130.566	13.572	56.482	1.00	6.69
1273	C	LEU	175	129.459	14.530	60.470	1.00	17.96
1274	O	LEU	175	130.534	15.074	60.705	1.00	30.10
1275	N	GLU	176	128.375	14.699	61.225	1.00	17.67
1276	CA	GLU	176	128.386	15.550	62.412	1.00	27.17
1277	CB	GLU	176	126.969	15.740	62.959	1.00	26.19
1278	CG	GLU	176	125.997	16.452	62.037	1.00	39.91
1279	CD	GLU	176	124.606	16.584	62.645	1.00	51.08
1280	OE1	GLU	176	124.184	15.676	63.398	1.00	49.19
1281	OE2	GLU	176	123.932	17.600	62.368	1.00	52.29
1282	C	GLU	176	129.241	14.913	63.505	1.00	29.58
1283	O	GLU	176	129.953	15.604	64.237	1.00	37.29
1284	N	SER	177	129.156	13.589	63.604	1.00	31.69
1285	CA	SER	177	129.883	12.816	64.607	1.00	28.71
1286	CB	SER	177	129.310	11.395	64.678	1.00	24.94
1287	OG	SER	177	129.868	10.660	65.755	1.00	27.40
1288	C	SER	177	131.392	12.758	64.370	1.00	25.55
1289	O	SER	177	132.177	12.795	65.324	1.00	17.66
1290	N	ALA	178	131.787	12.682	63.102	1.00	17.70
1291	CA	ALA	178	133.195	12.600	62.723	1.00	19.27
1292	CB	ALA	178	133.330	11.789	61.441	1.00	22.41
1293	C	ALA	178	133.897	13.948	62.558	1.00	24.31
1294	O	ALA	178	135.107	14.054	62.769	1.00	24.74
1295	N	ALA	179	133.124	14.975	62.214	1.00	25.32
1296	CA	ALA	179	133.630	16.326	61.971	1.00	25.36
1297	CB	ALA	179	132.460	17.289	61.779	1.00	32.63
1298	C	ALA	179	134.658	16.943	62.928	1.00	23.67
1299	O	ALA	179	135.706	17.420	62.487	1.00	23.47
1300	N	PRO	180	134.384	16.929	64.244	1.00	21.48
1301	CD	PRO	180	133.196	16.355	64.900	1.00	20.79
1302	CA	PRO	180	135.291	17.505	65.247	1.00	20.21
1303	CB	PRO	180	134.601	17.155	66.568	1.00	10.68
1304	CG	PRO	180	133.162	17.108	66.203	1.00	16.34
1305	C	PRO	180	136.747	17.040	65.264	1.00	21.05
1306	O	PRO	180	137.623	17.772	65.722	1.00	30.38
1307	N	HIS	181	137.015	15.846	64.750	1.00	24.41
1308	CA	HIS	181	138.372	15.310	64.785	1.00	20.38
1309	CB	HIS	181	138.359	13.955	65.498	1.00	22.19
1310	CG	HIS	181	137.686	13.989	66.837	1.00	20.19
1311	CD2	HIS	181	138.077	14.524	68.018	1.00	22.10
1312	ND1	HIS	181	136.437	13.448	67.055	1.00	24.79
1313	CE1	HIS	181	136.086	13.649	68.313	1.00	28.39
1314	NE2	HIS	181	137.064	14.300	68.919	1.00	34.90
1315	C	HIS	181	139.073	15.184	63.443	1.00	16.56
1316	O	HIS	181	140.138	14.575	63.351	1.00	20.78
1317	N	LEU	182	138.496	15.775	62.407	1.00	19.38
1318	CA	LEU	182	139.095	15.698	61.082	1.00	19.81
1319	CB	LEU	182	138.023	15.838	59.999	1.00	12.64
1320	CG	LEU	182	136.883	14.822	60.017	1.00	9.36
1321	CD1	LEU	182	135.883	15.191	58.946	1.00	6.26
1322	CD2	LEU	182	137.414	13.405	59.808	1.00	5.44
1323	C	LEU	182	140.164	16.760	60.884	1.00	23.01
1324	O	LEU	182	140.177	17.787	61.567	1.00	24.75
1325	N	LYS	183	141.071	16.492	59.953	1.00	23.75
1326	CA	LYS	183	142.139	17.426	59.648	1.00	25.95
1327	CB	LYS	183	143.300	16.712	58.948	1.00	25.08
1328	CG	LYS	183	142.946	16.106	57.600	1.00	32.88

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1329	CD	LYS	183	144.157	15.465	56.949	1.00	39.75
1330	CE	LYS	183	143.804	14.905	55.581	1.00	45.64
1331	NZ	LYS	183	144.980	14.277	54.913	1.00	50.66
1332	C	LYS	183	141.590	18.522	58.747	1.00	26.52
1333	O	LYS	183	140.579	18.333	58.068	1.00	31.05
1334	N	SER	184	142.247	19.675	58.769	1.00	25.24
1335	CA	SER	184	141.842	20.806	57.949	1.00	18.75
1336	CB	SER	184	142.202	22.111	58.656	1.00	15.62
1337	OG	SER	184	141.536	22.192	59.906	1.00	17.72
1338	C	SER	184	142.553	20.707	56.605	1.00	13.85
1339	O	SER	184	143.666	20.186	56.528	1.00	23.56
1340	N	PRO	185	141.930	21.221	55.526	1.00	14.69
1341	CD	PRO	185	142.636	21.342	54.235	1.00	6.08
1342	CA	PRO	185	140.622	21.886	55.462	1.00	13.32
1343	CB	PRO	185	140.758	22.747	54.213	1.00	7.14
1344	CG	PRO	185	141.553	21.860	53.309	1.00	4.25
1345	C	PRO	185	139.378	20.990	55.368	1.00	19.26
1346	O	PRO	185	138.268	21.502	55.198	1.00	22.11
1347	N	LEU	186	139.547	19.671	55.478	1.00	15.43
1348	CA	LEU	186	138.410	18.757	55.385	1.00	7.82
1349	CB	LEU	186	138.859	17.304	55.533	1.00	10.45
1350	CG	LEU	186	137.743	16.259	55.379	1.00	14.68
1351	CD1	LEU	186	137.199	16.257	53.953	1.00	2.00
1352	CD2	LEU	186	138.269	14.885	55.744	1.00	10.39
1353	C	LEU	186	137.339	19.061	56.424	1.00	14.43
1354	O	LEU	186	136.147	19.062	56.114	1.00	15.11
1355	N	ARG	187	137.774	19.318	57.653	1.00	11.19
1356	CA	ARG	187	136.868	19.626	58.755	1.00	10.77
1357	CB	ARG	187	137.675	19.929	60.019	1.00	9.64
1358	CG	ARG	187	136.839	20.202	61.251	1.00	12.29
1359	CD	ARG	187	137.724	20.530	62.429	1.00	17.99
1360	NE	ARG	187	136.944	20.796	63.633	1.00	40.99
1361	CZ	ARG	187	137.468	20.982	64.841	1.00	53.63
1362	NH1	ARG	187	138.785	20.931	65.014	1.00	54.42
1363	NH2	ARG	187	136.674	21.217	65.879	1.00	49.07
1364	C	ARG	187	135.949	20.804	58.424	1.00	19.68
1365	O	ARG	187	134.754	20.771	58.731	1.00	20.19
1366	N	GLU	188	136.512	21.831	57.789	1.00	19.04
1367	CA	GLU	188	135.758	23.026	57.405	1.00	14.75
1368	CB	GLU	188	136.708	24.179	57.052	1.00	18.38
1369	CG	GLU	188	137.416	24.825	58.248	1.00	25.44
1370	CD	GLU	188	138.326	23.865	59.000	1.00	37.02
1371	OE1	GLU	188	138.143	23.708	60.228	1.00	36.96
1372	OE2	GLU	188	139.224	23.271	58.362	1.00	33.70
1373	C	GLU	188	134.819	22.758	56.236	1.00	15.06
1374	O	GLU	188	133.720	23.317	56.176	1.00	16.38
1375	N	GLN	189	135.263	21.920	55.301	1.00	12.50
1376	CA	GLN	189	134.458	21.567	54.134	1.00	10.80
1377	CB	GLN	189	135.269	20.711	53.153	1.00	10.38
1378	CG	GLN	189	134.529	20.384	51.856	1.00	9.35
1379	CD	GLN	189	135.415	19.722	50.811	1.00	16.04
1380	OE1	GLN	189	135.319	20.022	49.617	1.00	8.08
1381	NE2	GLN	189	136.277	18.812	51.254	1.00	11.78
1382	C	GLN	189	133.204	20.814	54.574	1.00	12.51
1383	O	GLN	189	132.117	21.057	54.059	1.00	19.40
1384	N	VAL	190	133.363	19.920	55.546	1.00	11.87
1385	CA	VAL	190	132.250	19.139	56.070	1.00	14.05
1386	CB	VAL	190	132.750	17.975	56.967	1.00	18.34
1384	CG1	VAL	190	131.574	17.265	57.637	1.00	19.94
1388	CG2	VAL	190	133.556	16.986	56.135	1.00	2.59
1389	C	VAL	190	131.300	20.031	56.865	1.00	12.69
1390	O	VAL	190	130.091	20.012	56.642	1.00	16.38
1391	N	THR	191	131.858	20.822	57.777	1.00	19.11
1392	CA	THR	191	131.065	21.727	58.606	1.00	20.76
1393	CB	THR	191	131.964	22.557	59.551	1.00	23.59
1394	OG1	THR	191	132.681	21.675	60.424	1.00	29.20
1395	CG2	THR	191	131.130	23.511	50.391	1.00	29.68
1396	C	THR	191	130.241	22.664	57.731	1.00	19.82
1397	O	THR	191	129.073	22.927	58.023	1.00	24.05
1398	N	HIS	192	130.843	23.136	56.641	1.00	11.94
1399	CA	HIS	192	130.160	24.032	55.719	1.00	13.13
1400	CB	HIS	192	131.148	24.658	54.741	1.00	14.49
1401	CG	HIS	192	130.512	25.600	53.764	1.00	13.85

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1402	CD2	HIS	192	130.320	25.503	52.428	1.00	14.30
1403	ND1	HIS	192	129.981	26.814	54.141	1.00	17.04
1404	CE1	HIS	192	129.488	27.425	53.078	1.00	22.40
1405	NE2	HIS	192	129.681	26.651	52.025	1.00	9.94
1406	C	HIS	192	129.061	23.321	54.939	1.00	15.72
1407	O	HIS	192	128.002	23.896	54.696	1.00	19.37
1408	N	ALA	193	129.331	22.085	54.524	1.00	22.40
1409	CA	ALA	193	128.367	21.288	53.766	1.00	17.47
1410	CB	ALA	193	128.993	19.976	53.333	1.00	13.16
1411	C	ALA	193	127.104	21.027	54.584	1.00	18.46
1412	O	ALA	193	125.991	21.093	54.063	1.00	20.11
1413	N	LEU	194	127.285	20.747	55.870	1.00	13.26
1414	CA	LEU	194	126.165	20.488	56.763	1.00	18.67
1415	CB	LEU	194	126.669	19.948	58.103	1.00	22.98
1416	CG	LEU	194	127.424	18.615	58.050	1.00	17.83
1417	CD1	LEU	194	127.913	18.249	59.439	1.00	22.28
1418	CD2	LEU	194	126.526	17.524	57.494	1.00	9.41
1419	C	LEU	194	125.325	21.745	56.977	1.00	20.18
1420	O	LEU	194	124.169	21.662	57.390	1.00	28.31
1421	N	GLU	195	125.913	22.906	56.701	1.00	23.69
1422	CA	GLU	195	125.217	24.182	56.845	1.00	23.91
1423	CB	GLU	195	126.145	25.235	57.459	1.00	28.38
1424	CG	GLU	195	126.558	24.930	58.897	1.00	48.57
1425	CD	GLU	195	127.591	25.905	59.449	1.00	61.92
1426	OE1	GLU	195	128.341	26.515	58.652	1.00	66.87
1427	OE2	GLU	195	127.658	26.052	60.690	1.00	55.96
1428	C	GLU	195	124.693	24.670	55.497	1.00	14.54
1429	O	GLU	195	123.721	25.422	55.436	1.00	17.77
1430	N	GLN	196	125.327	24.207	54.422	1.00	10.51
1431	CA	GLN	196	124.951	24.584	53.064	1.00	9.57
1432	CB	GLN	196	125.488	25.984	52.740	1.00	9.74
1433	CG	GLN	196	125.212	26.461	51.321	1.00	13.51
1434	CD	GLN	196	123.737	26.672	51.051	1.00	18.27
1435	OE1	GLN	196	123.111	27.556	51.633	1.00	31.94
1436	NE2	GLN	196	123.174	25.862	50.162	1.00	21.35
1437	C	GLN	196	125.484	23.583	52.039	1.00	8.87
1438	O	GLN	196	126.695	23.481	51.830	1.00	16.57
1439	N	CYS	197	124.577	22.837	51.415	1.00	11.72
1440	CA	CYS	197	124.963	21.865	50.398	1.00	13.36
1441	CB	CYS	197	123.821	20.882	50.114	1.00	20.25
1442	SG	CYS	197	122.310	21.605	49.432	1.00	16.36
1443	C	CYS	197	125.351	22.614	49.126	1.00	11.32
1444	O	CYS	197	124.948	23.758	48.924	1.00	16.69
1445	N	LEU	198	126.134	21.965	48.274	1.00	14.40
1446	CA	LEU	198	126.594	22.580	47.038	1.00	14.31
1447	CB	LEU	198	127.688	21.717	46.394	1.00	14.46
1448	CG	LEU	198	128.283	22.186	45.060	1.00	13.58
1449	CD1	LEU	198	128.949	23.541	45.225	1.00	9.55
1450	CD2	LEU	198	129.279	21.162	44.547	1.00	12.33
1451	C	LEU	198	125.478	22.848	46.034	1.00	18.46
1452	O	LEU	198	125.389	23.945	45.481	1.00	26.64
1453	N	HIS	199	124.614	21.857	45.829	1.00	20.84
1454	CA	HIS	199	123.519	21.965	44.869	1.00	13.67
1455	CB	HIS	199	122.756	20.640	44.781	1.00	11.33
1456	CG	HIS	199	121.733	20.603	43.688	1.00	6.17
1457	CD2	HIS	199	120.389	20.445	43.729	1.00	12.38
1458	ND1	HIS	199	122.061	20.738	42.356	1.00	10.08
1459	CE1	HIS	199	120.964	20.663	41.624	1.00	10.18
1460	NE2	HIS	199	119.935	20.486	42.432	1.00	2.01
1461	C	HIS	199	122.540	23.111	45.108	1.00	14.52
1462	O	HIS	199	122.174	23.813	44.166	1.00	13.39
1463	N	LYS	200	122.120	23.300	46.357	1.00	15.92
1464	CA	LYS	200	121.161	24.353	46.698	1.00	14.65
1465	CB	LYS	200	120.205	23.859	47.789	1.00	15.18
1466	CG	LYS	200	119.425	22.609	47.416	1.00	12.45
1467	CD	LYS	200	118.523	22.158	48.554	1.00	3.23
1468	CE	LYS	200	117.827	20.849	48.213	1.00	14.66
1469	NZ	LYS	200	116.966	20.369	49.332	1.00	22.03
1470	C	LYS	200	121.786	25.688	47.120	1.00	22.11
1471	O	LYS	200	121.101	26.541	47.693	1.00	20.41
1472	N	GLY	201	123.078	25.860	46.844	1.00	21.90
1473	CA	GLY	201	123.764	27.097	47.191	1.00	14.85
1474	C	GLY	201	124.040	27.969	45.978	1.00	16.72

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1475	O	GLY	201	123.992	27.489	44.842	1.00	12.09
1476	N	VAL	202	124.329	29.253	46.209	1.00	11.53
1477	CA	VAL	202	124.627	30.183	45.114	1.00	11.31
1478	CB	VAL	202	124.437	31.661	45.555	1.00	9.93
1479	CG1	VAL	202	124.960	32.617	44.491	1.00	2.00
1480	CG2	VAL	202	122.964	31.937	45.803	1.00	6.34
1481	C	VAL	202	126.054	29.940	44.612	1.00	10.17
1482	O	VAL	202	126.997	29.883	45.405	1.00	8.95
1483	N	PRO	203	126.222	29.774	43.286	1.00	2.10
1484	CD	PRO	203	125.136	29.796	42.290	1.00	5.19
1485	CA	PRO	203	127.509	29.524	42.628	1.00	8.34
1486	CB	PRO	203	127.168	29.704	41.154	1.00	5.82
1487	CG	PRO	203	125.785	29.152	41.087	1.00	2.00
1488	C	PRO	203	128.699	30.381	43.069	1.00	18.54
1489	O	PRO	203	129.709	29.836	43.516	1.00	26.42
1490	N	ARG	204	128.591	31.704	42.951	1.00	11.17
1491	CA	ARG	204	129.687	32.582	43.357	1.00	5.94
1492	CB	ARG	204	129.366	34.047	43.061	1.00	4.29
1493	CG	ARG	204	129.405	34.440	41.587	1.00	10.69
1494	CD	ARG	204	130.821	34.543	41.033	1.00	8.35
1495	NE	ARG	204	131.410	33.242	40.725	1.00	21.05
1496	CZ	ARG	204	132.555	33.071	40.068	1.00	20.78
1497	NH1	ARG	204	133.250	34.121	39.644	1.00	14.75
1498	NH2	ARG	204	132.996	31.844	39.818	1.00	16.69
1499	C	ARG	204	130.016	32.420	44.836	1.00	6.43
1500	O	ARG	204	131.185	32.304	45.207	1.00	15.01
1501	N	VAL	205	128.983	32.380	45.672	1.00	2.00
1502	CA	VAL	205	129.159	32.238	47.116	1.00	3.42
1503	CB	VAL	205	127.809	32.238	47.855	1.00	2.00
1504	CG1	VAL	205	128.027	32.047	49.342	1.00	13.49
1505	CG2	VAL	205	127.064	33.530	47.594	1.00	2.00
1506	C	VAL	205	129.904	30.963	47.488	1.00	7.19
1507	O	VAL	205	130.785	30.982	48.342	1.00	17.39
1508	N	GLU	206	129.543	29.854	46.851	1.00	11.33
1509	CA	GLU	206	130.188	28.579	47.136	1.00	11.44
1510	CB	GLU	206	129.348	27.417	46.606	1.00	10.75
1511	CG	GLU	206	128.033	27.237	47.340	1.00	4.42
1512	CD	GLU	206	128.208	27.226	48.845	1.00	7.68
1513	OE1	GLU	206	128.858	26.298	49.366	1.00	15.79
1514	OE2	GLU	206	127.700	28.153	49.509	1.00	12.42
1515	C	GLU	206	131.598	28.528	46.568	1.00	13.88
1516	O	GLU	206	132.484	27.897	47.144	1.00	16.22
1517	N	THR	207	131.792	29.199	45.438	1.00	9.73
1518	CA	THR	207	133.090	29.268	44.785	1.00	13.84
1519	CB	THR	207	132.970	29.928	43.400	1.00	15.72
1520	OG1	THR	207	132.272	29.045	42.513	1.00	13.12
1521	CG2	THR	207	134.338	30.250	42.827	1.00	11.92
1522	C	THR	207	134.059	30.066	45.658	1.00	19.41
1523	O	THR	207	135.177	29.623	45.917	1.00	27.17
1524	N	ARG	208	133.608	31.226	46.133	1.00	22.15
1525	CA	ARG	208	134.417	32.091	46.988	1.00	17.49
1526	CB	ARG	208	133.595	33.309	47.429	1.00	23.71
1527	CG	ARG	208	134.349	34.352	48.264	1.00	24.20
1528	CD	ARG	208	135.532	34.935	47.501	1.00	35.41
1529	NE	ARG	208	136.060	36.169	48.090	1.00	40.81
1530	CZ	ARG	208	136.736	36.242	49.235	1.00	40.71
1531	NH1	ARG	208	136.978	35.150	49.947	1.00	42.82
1532	NH2	ARG	208	137.194	37.412	49.658	1.00	37.98
1533	C	ARG	208	134.906	31.313	48.208	1.00	19.76
1534	O	ARG	208	136.075	31.395	48.576	1.00	27.03
1535	N	PHE	209	134.010	30.534	48.809	1.00	16.90
1536	CA	PHE	209	134.350	29.734	49.979	1.00	12.93
1537	CB	PHE	209	133.090	29.165	50.632	1.00	3.91
1538	CG	PHE	209	133.377	28.292	51.818	1.00	8.27
1539	CD1	PHE	209	133.605	28.852	53.070	1.00	5.35
1540	CD2	PHE	209	133.472	26.912	51.676	1.00	11.24
1541	CE1	PHE	209	133.928	28.052	54.162	1.00	10.99
1542	CE2	PHE	209	133.794	26.105	52.760	1.00	7.23
1543	CZ	PHE	209	134.023	26.677	54.007	1.00	2.00
1544	C	PHE	209	135.305	28.581	49.664	1.00	16.94
1545	O	PHE	209	136.176	28.248	50.473	1.00	13.43
1546	N	PHE	210	135.112	27.942	48.514	1.00	11.91
1547	CA	PHE	210	135.960	26.823	48.126	1.00	12.01

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1548	CB	PHE	210	135.384	26.105	46.901	1.00	5.35
1549	CG	PHE	210	136.131	24.854	46.525	1.00	2.00
1550	CD1	PHE	210	136.182	23.773	47.392	1.00	7.13
1551	CD2	PHE	210	136.794	24.763	45.307	1.00	13.50
1552	CE1	PHE	210	136.883	22.617	47.052	1.00	13.12
1553	CE2	PHE	210	137.498	23.613	44.956	1.00	10.64
1554	CZ	PHE	210	137.542	22.539	45.830	1.00	12.55
1555	C	PHE	210	137.380	27.297	47.844	1.00	15.50
1556	O	PHE	210	138.339	26.801	48.436	1.00	21.01
1557	N	ILE	211	137.500	28.290	46.970	1.00	11.89
1558	CA	ILE	211	138.798	28.834	46.601	1.00	14.18
1559	CB	ILE	211	138.663	30.000	45.604	1.00	13.95
1560	CG2	ILE	211	140.040	30.517	45.218	1.00	23.94
1561	CG1	ILE	211	137.925	29.547	44.346	1.00	14.06
1562	CD1	ILE	211	137.734	30.656	43.335	1.00	19.84
1563	C	ILE	211	139.622	29.318	47.790	1.00	11.48
1564	O	ILE	211	140.730	28.838	48.010	1.00	22.99
1565	N	SER	212	139.069	30.238	48.574	1.00	11.99
1566	CA	SER	212	139.799	30.797	49.708	1.00	19.48
1567	CB	SER	212	139.279	32.205	50.044	1.00	10.83
1568	OG	SER	212	137.939	32.174	50.500	1.00	32.56
1569	C	SER	212	139.902	29.954	50.979	1.00	15.60
1570	O	SER	212	140.992	29.800	51.530	1.00	26.35
1571	N	SER	213	138.785	29.398	51.437	1.00	18.79
1572	CA	SER	213	138.780	28.607	52.665	1.00	15.21
1573	CB	SER	213	137.426	28.737	53.372	1.00	13.39
1574	OG	SER	213	137.168	30.074	53.766	1.00	19.66
1575	C	SER	213	139.141	27.126	52.543	1.00	21.19
1576	O	SER	213	139.540	26.503	53.534	1.00	22.69
1577	N	ILE	214	139.021	26.558	51.345	1.00	16.22
1578	CA	ILE	214	139.308	25.138	51.177	1.00	12.65
1579	CB	ILE	214	138.047	24.354	50.712	1.00	17.01
1580	CG2	ILE	214	138.343	22.853	50.628	1.00	14.54
1581	CG1	ILE	214	136.879	24.602	51.673	1.00	7.09
1582	CD1	ILE	214	137.175	24.247	53.124	1.00	2.16
1583	C	ILE	214	140.477	24.759	50.276	1.00	14.51
1584	O	ILE	214	141.486	24.247	50.759	1.00	20.94
1585	N	TYR	215	140.342	25.006	48.975	1.00	10.71
1586	CA	TYR	215	141.378	24.634	48.016	1.00	16.76
1587	CB	TYR	215	140.914	24.914	46.587	1.00	10.15
1588	CG	TYR	215	141.523	23.975	45.569	1.00	16.49
1589	CD1	TYR	215	141.526	22.595	45.777	1.00	14.36
1590	CE1	TYR	215	142.079	21.722	44.837	1.00	16.84
1591	CD2	TYR	215	142.090	24.463	44.393	1.00	18.93
1592	CE2	TYR	215	142.645	23.601	43.447	1.00	14.61
1593	CZ	TYR	215	142.636	22.232	43.676	1.00	18.72
1594	OH	TYR	215	143.191	21.375	42.749	1.00	21.97
1595	C	TYR	215	142.753	25.251	48.256	1.00	22.56
1596	O	TYR	215	143.772	24.567	48.154	1.00	21.88
1597	N	ASP	216	142.780	26.538	48.582	1.00	25.86
1598	CA	ASP	216	144.032	27.239	48.841	1.00	28.90
1599	CB	ASP	216	143.745	28.708	49.155	1.00	35.55
1600	CG	ASP	216	145.000	29.514	49.373	1.00	32.91
1601	OD1	ASP	216	145.170	30.035	50.494	1.00	33.80
1602	OD2	ASP	216	145.811	29.630	48.427	1.00	38.29
1603	C	ASP	216	144.782	26.590	50.002	1.00	28.68
1604	O	ASP	216	146.013	26.552	50.017	1.00	35.11
1605	N	LYS	217	144.026	26.052	50.954	1.00	24.04
1606	CA	LYS	217	144.604	25.406	52.129	1.00	25.31
1607	CB	LYS	217	143.768	25.741	53.368	1.00	17.45
1608	CG	LYS	217	143.687	27.234	53.646	1.00	28.42
1609	CD	LYS	217	142.811	27.551	54.844	1.00	36.77
1610	CE	LYS	217	142.729	29.057	55.071	1.00	36.92
1611	NZ	LYS	217	141.758	29.426	56.143	1.00	37.10
1612	C	LYS	217	144.754	23.892	51.973	1.00	25.97
1613	O	LYS	217	145.170	23.201	52.905	1.00	23.71
1614	N	GLU	218	144.429	23.385	50.788	1.00	30.40
1615	CA	GLU	218	144.528	21.958	50.504	1.00	34.37
1616	CB	GLU	218	143.655	21.603	49.297	1.00	41.93
1617	CG	GLU	218	143.462	20.114	49.073	1.00	45.33
1618	CD	GLU	218	142.740	19.451	50.226	1.00	52.39
1619	OE1	GLU	218	141.553	19.780	50.449	1.00	49.41
1620	OE2	GLU	218	143.364	18.612	50.918	1.00	46.07

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1621	C	GLU	218	145.982	21.585	50.228	1.00	34.68
1622	O	GLU	218	146.624	22.166	49.356	1.00	31.92
1623	N	GLN	219	146.493	20.611	50.974	1.00	37.87
1624	CA	GLN	219	147.872	20.156	50.827	1.00	41.61
1625	CB	GLN	219	148.180	19.105	51.896	1.00	52.08
1626	CG	GLN	219	149.617	18.615	51.900	1.00	67.09
1627	CD	GLN	219	149.709	17.102	51.943	1.00	78.27
1628	OE1	GLN	219	149.305	16.470	52.917	1.00	81.71
1629	NE2	GLN	219	150.233	16.510	50.870	1.00	80.10
1630	C	GLN	219	148.173	19.583	49.438	1.00	38.79
1631	O	GLN	219	149.260	19.789	48.893	1.00	34.89
1632	N	SER	220	147.205	18.867	48.874	1.00	39.35
1633	CA	SER	220	147.359	18.252	47.556	1.00	36.65
1634	CB	SER	220	146.658	16.891	47.537	1.00	48.69
1635	OG	SER	220	145.291	17.018	47.899	1.00	58.57
1636	C	SER	220	146.824	19.117	46.418	1.00	30.45
1637	O	SER	220	146.651	18.639	45.297	1.00	31.98
1638	N	LYS	221	146.581	20.392	46.704	1.00	25.39
1639	CA	LYS	221	146.052	21.327	45.716	1.00	18.20
1640	CB	LYS	221	145.949	22.731	46.316	1.00	17.94
1641	CG	LYS	221	147.292	23.352	46.659	1.00	24.63
1642	CD	LYS	221	147.136	24.772	47.155	1.00	32.69
1643	CE	LYS	221	148.444	25.312	47.716	1.00	42.07
1644	NZ	LYS	221	149.547	25.257	46.720	1.00	42.25
1645	C	LYS	221	146.879	21.412	44.444	1.00	15.22
1646	O	LYS	221	148.097	21.243	44.467	1.00	21.32
1647	N	ASN	222	146.196	21.660	43.333	1.00	11.20
1648	CA	ASN	222	146.853	21.818	42.048	1.00	9.54
1649	CB	ASN	222	145.993	21.250	40.919	1.00	2.46
1650	CG	ASN	222	146.599	21.488	39.550	1.00	12.07
1651	OD1	ASN	222	146.698	22.626	39.097	1.00	10.03
1652	ND2	ASN	222	147.003	20.414	38.881	1.00	11.12
1653	C	ASN	222	147.032	23.322	41.885	1.00	17.59
1654	O	ASN	222	146.060	24.061	41.717	1.00	21.24
1655	N	ASN	223	148.281	23.765	41.958	1.00	18.52
1656	CA	ASN	223	148.619	25.175	41.850	1.00	9.91
1657	CB	ASN	223	150.127	25.349	41.972	1.00	11.52
1658	CG	ASN	223	150.664	24.821	43.282	1.00	23.77
1659	OD1	ASN	223	150.579	25.491	44.311	1.00	21.40
1660	ND2	ASN	223	151.208	23.605	43.258	1.00	21.52
1661	C	ASN	223	148.104	25.870	40.594	1.00	15.35
1662	O	ASN	223	147.668	27.019	40.662	1.00	21.88
1663	N	VAL	224	148.157	25.184	39.455	1.00	10.58
1664	CA	VAL	224	147.677	25.755	38.195	1.00	18.60
1665	CB	VAL	224	147.957	24.811	37.001	1.00	24.63
1666	CG1	VAL	224	147.405	25.406	35.709	1.00	25.94
1667	CG2	VAL	224	149.449	24.558	36.873	1.00	17.27
1668	C	VAL	224	146.177	26.049	38.259	1.00	23.24
1669	O	VAL	224	145.716	27.071	37.746	1.00	25.12
1670	N	LEU	225	145.423	25.146	38.886	1.00	23.80
1671	CA	LEU	225	143.980	25.313	39.032	1.00	18.51
1672	CB	LEU	225	143.314	23.994	39.434	1.00	18.23
1673	CG	LEU	225	143.337	22.844	38.424	1.00	20.30
1674	CD1	LEU	225	142.613	21.645	39.010	1.00	18.77
1675	CD2	LEU	225	142.691	23.270	37.115	1.00	10.44
1676	C	LEU	225	143.652	26.392	40.061	1.00	18.24
1677	O	LEU	225	142.710	27.162	39.872	1.00	22.06
1678	N	LEU	226	144.431	26.448	41.141	1.00	18.51
1679	CA	LEU	226	144.230	27.445	42.197	1.00	17.64
1680	CB	LEU	226	145.128	27.149	43.401	1.00	15.88
1681	CG	LEU	226	145.013	28.096	44.605	1.00	19.63
1682	CD1	LEU	226	143.633	27.996	45.235	1.00	8.24
1683	CD2	LEU	226	146.086	27.764	45.627	1.00	2.89
1684	C	LEU	226	144.507	28.855	41.681	1.00	15.54
1685	O	LEU	226	143.753	29.785	41.966	1.00	28.19
1686	N	ARG	227	145.595	29.002	40.927	1.00	22.25
1687	CA	ARG	227	145.995	30.282	40.338	1.00	21.24
1688	CB	ARG	227	147.320	30.108	39.587	1.00	25.23
1689	CG	ARG	227	147.831	31.335	38.844	1.00	26.56
1690	CD	ARG	227	148.575	32.292	39.760	1.00	33.23
1691	NE	ARG	227	149.114	33.433	39.021	1.00	27.48
1692	CZ	ARG	227	149.516	34.568	39.585	1.00	29.44
1693	NH1	ARG	227	149.447	34.722	40.902	1.00	31.95

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1694	NH2	ARG	227	149.963	35.561	38.831	1.00	19.58
1695	C	ARG	227	144.911	30.745	39.367	1.00	17.48
1696	O	ARG	227	144.475	31.894	39.402	1.00	22.08
1697	N	PHE	228	144.474	29.822	38.516	1.00	17.49
1698	CA	PHE	228	143.439	30.073	37.516	1.00	20.78
1699	CB	PHE	228	143.484	28.770	36.741	1.00	17.58
1700	CG	PHE	228	142.261	28.908	35.556	1.00	10.74
1701	CD1	PHE	228	141.685	30.128	35.214	1.00	18.32
1702	CD2	PHE	228	141.958	27.791	34.785	1.00	13.57
1703	CE1	PHE	228	140.819	30.230	34.122	1.00	18.76
1704	CE2	PHE	228	141.095	27.883	33.692	1.00	18.93
1705	CZ	PHE	228	140.525	29.106	33.361	1.00	12.22
1706	C	PHE	228	142.158	30.552	38.205	1.00	20.33
1707	O	PHE	228	141.585	31.580	37.834	1.00	17.12
1708	N	ALA	229	141.746	29.817	39.233	1.00	15.85
1709	CA	ALA	229	140.541	30.125	39.989	1.00	14.57
1710	CB	ALA	229	140.320	29.069	41.059	1.00	11.49
1711	C	ALA	229	140.572	31.513	40.619	1.00	22.21
1712	O	ALA	229	139.606	32.272	40.505	1.00	26.82
1713	N	LYS	230	141.683	31.841	41.278	1.00	17.14
1714	CA	LYS	230	141.836	33.136	41.933	1.00	13.72
1715	CB	LYS	230	143.118	33.168	42.766	1.00	17.71
1716	CG	LYS	230	143.067	32.332	44.030	1.00	14.07
1717	CD	LYS	230	144.343	32.505	44.835	1.00	23.37
1718	CE	LYS	230	144.253	31.802	46.177	1.00	31.01
1719	NZ	LYS	230	145.477	32.021	46.994	1.00	32.57
1720	C	LYS	230	141.816	34.310	40.956	1.00	16.07
1721	O	LYS	230	141.111	35.292	41.176	1.00	15.73
1722	N	LEU	231	142.585	34.202	39.876	1.00	17.93
1723	CA	LEU	231	142.646	35.260	38.872	1.00	20.80
1724	CB	LEU	231	143.653	34.911	37.775	1.00	18.38
1725	CG	LEU	231	145.141	34.870	38.116	1.00	16.32
1726	CD1	LEU	231	145.920	34.518	36.863	1.00	14.82
1727	CD2	LEU	231	145.593	36.212	38.658	1.00	15.83
1728	C	LEU	231	141.287	35.506	38.233	1.00	24.81
1729	O	LEU	231	140.828	36.647	38.151	1.00	28.14
1730	N	ASP	232	140.648	34.427	37.790	1.00	28.52
1731	CA	ASP	232	139.344	34.503	37.139	1.00	23.60
1732	CB	ASP	232	138.878	33.104	36.736	1.00	20.22
1733	CG	ASP	232	137.737	33.137	35.742	1.00	29.93
1734	OD1	ASP	232	138.019	33.223	34.527	1.00	24.38
1735	OD2	ASP	232	136.564	33.079	36.174	1.00	26.36
1736	C	ASP	232	138.300	35.170	38.032	1.00	20.67
1737	O	ASP	232	137.622	36.111	37.612	1.00	15.86
1738	N	PHE	233	138.203	34.707	39.274	1.00	12.27
1739	CA	PHE	233	137.244	35.260	40.219	1.00	12.59
1740	CB	PHE	233	137.355	34.549	41.569	1.00	14.20
1741	CG	PHE	233	136.243	34.887	42.524	1.00	30.75
1742	CD1	PHE	233	135.130	34.058	42.634	1.00	33.32
1743	CD2	PHE	233	136.298	36.042	43.302	1.00	29.41
1744	CE1	PHE	233	134.088	34.372	43.502	1.00	34.63
1745	CE2	PHE	233	135.263	36.365	44.172	1.00	31.81
1746	CZ	PHE	233	134.155	35.528	44.272	1.00	32.38
1747	C	PHE	233	137.452	36.760	40.407	1.00	18.84
1748	O	PHE	233	136.495	37.534	40.394	1.00	24.79
1749	N	ASN	234	138.710	37.160	40.572	1.00	25.72
1750	CA	ASN	234	139.057	38.563	40.770	1.00	20.56
1751	CB	ASN	234	140.509	38.694	41.239	1.00	25.13
1752	CG	ASN	234	140.702	38.249	42.683	1.00	30.65
1753	OD1	ASN	234	139.738	37.996	43.406	1.00	21.26
1754	ND2	ASN	234	141.957	38.162	43.109	1.00	35.99
1755	C	ASN	234	138.818	39.427	39.536	1.00	18.33
1756	O	ASN	234	138.457	40.599	39.662	1.00	15.79
1757	N	LEU	235	139.019	38.848	38.353	1.00	17.45
1758	CA	LEU	235	138.814	39.567	37.097	1.00	16.13
1759	CB	LEU	235	139.402	38.789	35.920	1.00	14.09
1760	CG	LEU	235	139.233	39.426	34.534	1.00	25.16
1761	CD1	LEU	235	139.947	40.774	34.472	1.00	16.26
1762	CD2	LEU	235	139.762	38.487	33.458	1.00	11.51
1763	C	LEU	235	137.329	39.812	36.866	1.00	23.53
1764	O	LEU	235	136.929	40.918	36.502	1.00	30.18
1765	N	LEU	236	136.517	38.773	37.065	1.00	26.97
1766	CA	LEU	236	135.071	38.894	36.900	1.00	21.97

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1767	CB	LEU	236	134.375	37.538	37.041	1.00	22.99
1768	CG	LEU	236	134.550	36.506	35.931	1.00	24.74
1769	CD1	LEU	236	133.601	35.347	36.187	1.00	22.83
1770	CD2	LEU	236	134.259	37.133	34.579	1.00	26.05
1771	C	LEU	236	134.511	39.858	37.935	1.00	15.40
1772	O	LEU	236	133.581	40.602	37.646	1.00	21.06
1773	N	GLN	237	135.080	39.837	39.139	1.00	13.42
1774	CA	GLN	237	134.645	40.721	40.217	1.00	14.55
1775	CB	GLN	237	135.477	40.481	41.475	1.00	14.51
1776	CG	GLN	237	135.051	41.318	42.671	1.00	12.72
1777	CD	GLN	237	135.967	41.131	43.862	1.00	12.21
1778	OE1	GLN	237	137.121	41.566	43.847	1.00	18.76
1779	NE2	GLN	237	135.460	40.483	44.900	1.00	4.88
1780	C	GLN	237	134.760	42.180	39.788	1.00	22.23
1781	O	GLN	237	133.950	43.011	40.192	1.00	28.74
1782	N	MET	238	135.770	42.481	38.970	1.00	29.92
1783	CA	MET	238	135.985	43.833	38.458	1.00	23.66
1784	CB	MET	238	137.275	43.906	37.638	1.00	25.72
1785	CG	MET	238	138.552	43.791	38.454	1.00	26.38
1786	SD	MET	238	140.030	43.684	37.408	1.00	30.42
1787	CE	MET	238	141.233	43.058	38.580	1.00	23.83
1788	C	MET	238	134.801	44.227	37.584	1.00	20.92
1789	O	MET	238	134.344	45.367	37.628	1.00	20.70
1790	N	LEU	239	134.310	43.274	36.792	1.00	23.17
1791	CA	LEU	239	133.159	43.509	35.920	1.00	21.15
1792	CB	LEU	239	132.938	42.323	34.978	1.00	10.92
1793	CG	LEU	239	131.684	42.381	34.100	1.00	20.20
1794	CD1	LEU	239	131.748	43.579	33.166	1.00	9.66
1795	CD2	LEU	239	131.541	41.089	33.309	1.00	10.55
1796	C	LEU	239	131.908	43.732	36.764	1.00	14.68
1797	O	LEU	239	131.129	44.645	36.501	1.00	23.63
1798	N	HIS	240	131.735	42.904	37.788	1.00	15.07
1799	CA	HIS	240	130.587	43.015	38.680	1.00	19.33
1800	CB	HIS	240	130.619	41.913	39.746	1.00	16.76
1801	CG	HIS	240	130.661	40.525	39.185	1.00	12.10
1802	CD2	HIS	240	130.296	40.039	37.973	1.00	12.51
1803	ND1	HIS	240	131.144	39.449	39.897	1.00	8.57
1834	CE1	HIS	240	131.077	38.362	39.150	1.00	16.05
1805	NE2	HIS	240	130.567	38.692	37.979	1.00	13.30
1806	C	HIS	240	130.610	44.383	39.344	1.00	21.46
1807	O	HIS	240	129.572	45.034	39.481	1.00	28.61
1808	N	LYS	241	131.809	44.819	39.728	1.00	24.98
1809	CA	LYS	241	132.008	46.118	40.364	1.00	19.85
1810	CB	LYS	241	133.469	46.281	40.782	1.00	18.41
1811	CG	LYS	241	133.855	45.556	42.057	1.00	18.41
1812	CD	LYS	241	135.348	45.688	42.297	1.00	29.39
1813	CE	LYS	241	135.667	45.861	43.769	1.00	43.69
1814	NZ	LYS	241	137.131	45.987	43.991	1.00	46.04
1815	C	LYS	241	131.604	47.252	39.419	1.00	23.69
1816	O	LYS	241	130.983	48.229	39.845	1.00	14.81
1817	N	GLN	242	131.954	47.107	38.140	1.00	20.70
1818	CA	GLN	242	131.615	48.099	37.120	1.00	28.94
1819	CB	GLN	242	132.262	47.748	35.775	1.00	29.06
1820	CG	GLN	242	133.775	47.862	35.748	1.00	39.14
1821	CD	GLN	242	134.359	47.517	34.392	1.00	42.97
1822	OE1	GLN	242	134.324	46.363	33.962	1.00	48.36
1823	NE2	GLN	242	134.904	48.519	33.710	1.00	39.66
1824	C	GLN	242	130.103	48.163	36.943	1.00	33.40
1825	O	GLN	242	129.514	49.246	36.938	1.00	40.80
1826	N	GLU	243	129.487	46.992	36.807	1.00	33.80
1827	CA	GLU	243	128.044	46.884	36.631	1.00	22.54
1828	CB	GLU	243	127.647	45.420	36.466	1.00	15.53
1829	CG	GLU	243	128.204	44.778	35.210	1.00	15.70
1830	CD	GLU	243	127.938	43.290	35.137	1.00	18.78
1831	OE1	GLU	243	127.639	42.675	36.178	1.00	18.01
1832	OE2	GLU	243	128.040	42.727	34.032	1.00	15.89
1833	C	GLU	243	127.290	47.495	37.806	1.00	20.49
1834	O	GLU	243	126.351	48.266	37.611	1.00	18.81
1835	N	LEU	244	127.715	47.159	39.022	1.00	12.97
1836	CA	LEU	244	127.079	47.675	40.231	1.00	15.01
1837	CB	LEU	244	127.676	46.999	41.467	1.00	12.34
1838	CG	LEU	244	127.144	47.436	42.832	1.00	12.62
1839	CD1	LEU	244	125.628	47.332	42.881	1.00	24.09

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1840	CD2	LEU	244	127.780	46.582	43.908	1.00	9.05
1841	C	LEU	244	127.213	49.191	40.335	1.00	22.78
1842	O	LEU	244	126.328	49.868	40.863	1.00	27.46
1843	N	ALA	245	128.325	49.725	39.838	1.00	31.72
1844	CA	ALA	245	128.560	51.167	39.856	1.00	30.71
1845	CB	ALA	245	129.998	51.476	39.466	1.00	26.12
1846	C	ALA	245	127.589	51.860	38.893	1.00	29.98
1847	O	ALA	245	127.005	52.887	39.226	1.00	32.44
1848	N	GLN	246	127.410	51.256	37.718	1.00	29.03
1849	CA	GLN	246	126.528	51.754	36.668	1.00	31.14
1850	CB	GLN	246	126.689	50.868	35.430	1.00	31.92
1851	CG	GLN	246	125.845	51.244	34.232	1.00	41.36
1852	CD	GLN	246	125.970	50.235	33.109	1.00	48.09
1853	OE1	GLN	246	127.023	49.627	32.919	1.00	49.29
1854	NE2	GLN	246	124.887	50.043	32.361	1.00	55.11
1855	C	GLN	246	125.074	51.762	37.119	1.00	34.84
1856	O	GLN	246	124.297	52.637	36.732	1.00	42.31
1857	N	VAL	247	124.719	50.762	37.921	1.00	39.27
1858	CA	VAL	247	123.360	50.631	38.441	1.00	38.03
1859	CB	VAL	247	123.069	49.138	38.742	1.00	38.04
1860	CG1	VAL	247	122.330	48.954	40.059	1.00	39.31
1861	CG2	VAL	247	122.270	48.526	37.603	1.00	37.60
1862	C	VAL	247	123.144	51.507	39.667	1.00	37.49
1863	O	VAL	247	122.012	51.862	39.998	1.00	33.11
1864	N	SER	248	124.231	51.871	40.340	1.00	39.80
1865	CA	SER	248	124.173	52.736	41.515	1.00	43.54
1866	CB	SER	248	125.456	52.604	42.352	1.00	41.35
1867	OG	SER	248	125.482	51.368	43.057	1.00	23.81
1868	C	SER	248	123.963	54.195	41.093	1.00	41.56
1869	O	SER	248	123.288	54.976	41.783	1.00	39.28
1870	N	ARG	249	124.591	54.559	39.974	1.00	40.01
1871	CA	ARG	249	124.467	55.901	39.421	1.00	47.97
1872	CB	ARG	249	125.475	56.127	38.290	1.00	51.84
1873	CG	ARG	249	126.912	56.292	38.747	1.00	62.62
1874	CD	ARG	249	127.836	56.501	37.563	1.00	69.45
1875	NE	ARG	249	129.065	55.731	37.713	1.00	78.07
1876	CZ	ARG	249	129.491	54.824	36.840	1.00	81.11
1877	NH1	ARG	249	128.795	54.570	35.737	1.00	75.69
1878	NH2	ARG	249	130.602	54.145	37.087	1.00	86.20
1879	C	ARG	249	123.051	56.058	38.890	1.00	43.68
1880	O	ARG	249	122.402	57.072	39.127	1.00	45.81
1881	N	TRP	250	122.588	55.030	38.183	1.00	38.57
1882	CA	TRP	250	121.247	55.000	37.613	1.00	34.46
1883	CB	TRP	250	121.060	53.682	36.851	1.00	37.42
1884	CG	TRP	250	119.635	53.325	36.531	1.00	37.50
1885	CD2	TRP	250	118.745	52.545	37.341	1.00	32.98
1886	CE2	TRP	250	117.516	52.464	36.652	1.00	39.28
1887	CE3	TRP	250	118.867	51.909	38.585	1.00	32.90
1888	CD1	TRP	250	118.931	53.672	35.413	1.00	28.29
1889	NE1	TRP	250	117.658	53.159	35.479	1.00	36.07
1890	CZ2	TRP	250	116.411	51.771	37.167	1.00	40.28
1891	CZ3	TRP	250	117.770	51.221	39.098	1.00	33.00
1892	CH2	TRP	250	116.557	51.159	38.388	1.00	34.10
1893	C	TRP	250	120.215	55.131	38.731	1.00	31.76
1894	O	TRP	250	119.207	55.820	38.583	1.00	38.62
1895	N	TRP	251	120.499	54.493	39.861	1.00	29.34
1896	CA	TRP	251	119.611	54.513	41.017	1.00	28.23
1897	CB	TRP	251	120.041	53.431	42.003	1.00	24.43
1898	CG	TRP	251	119.164	53.309	43.196	1.00	27.54
1899	CD2	TRP	251	117.813	52.824	43.224	1.00	28.47
1900	CE2	TRP	251	117.394	52.848	44.576	1.00	30.61
1901	CE3	TRP	251	116.921	52.373	42.246	1.00	22.56
1902	CD1	TRP	251	119.493	53.603	44.486	1.00	29.85
1903	NE1	TRP	251	118.439	53.127	45.321	1.00	28.21
1904	CZ2	TRP	251	116.117	52.434	44.974	1.00	27.80
1905	CZ3	TRP	251	115.646	51.959	42.641	1.00	16.40
1906	CH2	TRP	251	115.261	51.995	43.993	1.00	23.32
1907	C	TRP	251	119.675	55.877	41.703	1.00	37.98
1908	O	TRP	251	118.564	56.243	42.309	1.00	45.16
1909	N	LYS	252	120.685	56.610	41.636	1.00	42.00
1910	CA	LYS	252	120.758	57.938	42.238	1.00	42.12
1911	CB	LYS	252	122.198	58.328	42.551	1.00	47.95
1912	CG	LYS	252	122.598	58.028	43.975	1.00	54.42

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1913	CD	LYS	252	123.720	58.943	44.418	1.00	63.61
1914	CE	LYS	252	123.889	58.896	45.923	1.00	76.47
1915	NZ	LYS	252	124.827	59.944	46.407	1.00	82.00
1916	C	LYS	252	120.113	58.992	41.348	1.00	43.32
1917	O	LYS	252	119.528	59.955	41.845	1.00	40.24
1918	N	ASP	253	120.220	58.802	40.033	1.00	41.81
1919	CA	ASP	253	119.621	59.715	39.061	1.00	42.20
1920	CB	ASP	253	119.991	59.305	37.632	1.00	46.23
1921	CG	ASP	253	121.475	59.448	37.340	1.00	56.62
1922	OD1	ASP	253	122.222	59.973	38.197	1.00	59.66
1923	OD2	ASP	253	121.896	59.029	36.240	1.00	59.43
1924	C	ASP	253	118.100	59.701	39.208	1.00	46.95
1925	O	ASP	253	117.404	60.508	38.597	1.00	47.82
1926	N	LEU	254	117.600	58.743	39.987	1.00	50.43
1927	CA	LEU	254	116.172	58.596	40.253	1.00	52.57
1928	CB	LEU	254	115.777	57.116	40.236	1.00	51.09
1929	CG	LEU	254	116.036	56.357	38.930	1.00	52.73
1930	CD1	LEU	254	115.673	54.894	39.102	1.00	50.16
1931	CD2	LEU	254	115.244	56.974	37.788	1.00	48.48
1932	C	LEU	254	115.867	59.205	41.619	1.00	50.66
1933	O	LEU	254	114.780	59.735	41.848	1.00	48.89
1934	N	ASP	255	116.838	59.099	42.522	1.00	54.73
1935	CA	ASP	255	116.750	59.641	43.875	1.00	59.42
1936	CB	ASP	255	116.930	61.167	43.829	1.00	63.16
1937	CG	ASP	255	117.232	61.774	45.193	1.00	70.47
1938	OD1	ASP	255	117.674	61.045	46.110	1.00	70.14
1939	OD2	ASP	255	117.030	62.997	45.344	1.00	79.11
1940	C	ASP	255	115.476	59.260	44.640	1.00	56.10
1941	O	ASP	255	114.834	60.106	45.263	1.00	54.97
1942	N	PHE	256	115.127	57.977	44.602	1.00	55.78
1943	CA	PHE	256	113.946	57.486	45.308	1.00	55.28
1944	CB	PHE	256	113.556	56.093	44.808	1.00	51.79
1945	CG	PHE	256	113.024	56.079	43.407	1.00	52.55
1946	CD1	PHE	256	113.356	55.051	42.537	1.00	55.14
1947	CD2	PHE	256	112.186	57.091	42.955	1.00	58.21
1948	CE1	PHE	256	112.862	55.028	41.236	1.00	57.90
1949	CE2	PHE	256	111.687	57.077	41.656	1.00	60.53
1950	CZ	PHE	256	112.026	56.042	40.796	1.00	57.76
1951	C	PHE	256	114.199	57.438	46.812	1.00	60.70
1952	O	PHE	256	113.292	57.162	47.596	1.00	62.84
1953	N	VAL	257	115.442	57.704	47.203	1.00	64.41
1954	CA	VAL	257	115.834	57.697	48.606	1.00	64.01
1955	CB	VAL	257	117.373	57.799	48.757	1.00	62.36
1956	CG1	VAL	257	117.789	57.482	50.187	1.00	60.29
1957	CG2	VAL	257	118.068	56.864	47.774	1.00	58.27
1958	C	VAL	257	115.179	58.870	49.333	1.00	65.72
1959	O	VAL	257	114.849	58.771	50.517	1.00	64.55
1960	N	THR	258	114.977	59.971	48.609	1.00	66.40
1961	CA	THR	258	114.364	61.171	49.175	1.00	65.40
1962	CB	THR	258	115.200	62.437	48.870	1.00	65.98
1963	CG1	THR	258	115.282	62.633	47.453	1.00	65.25
1964	CG2	THR	258	116.608	62.302	49.442	1.00	64.28
1965	C	THR	258	112.919	61.399	48.716	1.00	62.28
1966	O	THR	258	112.066	61.769	49.524	1.00	62.30
1967	N	THR	259	112.649	61.182	47.428	1.00	58.00
1968	CA	THR	259	111.303	61.372	46.879	1.00	53.45
1969	CB	THR	259	111.300	61.402	45.332	1.00	48.24
1970	OG1	THR	259	111.730	60.136	44.818	1.00	47.10
1971	CG2	THR	259	112.221	62.496	44.817	1.00	44.78
1972	C	THR	259	110.320	60.303	47.358	1.00	54.85
1973	O	THR	259	109.147	60.593	47.593	1.00	58.40
1974	N	LEU	260	110.802	59.069	47.492	1.00	54.85
1975	CA	LEU	260	109.977	57.952	47.958	1.00	57.07
1976	CB	LEU	260	109.811	56.907	46.845	1.00	54.53
1977	CG	LEU	260	109.191	57.346	45.511	1.00	54.02
1978	CD1	LEU	260	109.216	56.192	44.523	1.00	47.30
1979	CD2	LEU	260	107.765	57.838	45.715	1.00	53.62
1980	C	LEU	260	110.655	57.326	49.183	1.00	59.06
1981	O	LEU	260	111.135	56.190	49.132	1.00	61.18
1982	N	PRO	261	110.672	58.057	50.314	1.00	59.80
1983	CD	PRO	261	110.004	59.362	50.474	1.00	57.03
1984	CA	PRO	261	111.281	57.634	51.582	1.00	60.02
1985	CB	PRO	261	111.144	58.883	52.452	1.00	59.64

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
1986	CG	PRO	261	109.865	59.476	51.972	1.00	61.83
1987	C	PRO	261	110.685	56.401	52.265	1.00	56.67
1988	O	PRO	261	111.317	55.811	53.143	1.00	54.94
1989	N	TYR	262	109.475	56.019	51.869	1.00	55.28
1990	CA	TYR	262	108.813	54.855	52.455	1.00	52.74
1991	CB	TYR	262	107.309	54.898	52.167	1.00	46.52
1992	CG	TYR	262	106.954	54.869	50.695	1.00	38.58
1993	CD1	TYR	262	106.624	53.671	50.062	1.00	30.09
1994	CE1	TYR	262	106.295	53.636	48.711	1.00	29.27
1995	CD2	TYR	262	106.944	56.039	49.936	1.00	34.60
1996	CE2	TYR	262	106.614	56.015	48.581	1.00	37.08
1997	CZ	TYR	262	106.290	54.809	47.974	1.00	32.64
1998	OH	TYR	262	105.961	54.776	46.635	1.00	17.43
1999	C	TYR	262	109.398	53.534	51.956	1.00	52.07
2000	O	TYR	262	109.356	52.522	52.658	1.00	51.95
2001	N	ALA	263	109.957	53.565	50.748	1.00	48.22
2002	CA	ALA	263	110.545	52.386	50.120	1.00	49.01
2003	CB	ALA	263	110.701	52.527	48.623	1.00	44.24
2004	C	ALA	263	111.879	51.943	50.723	1.00	52.04
2005	O	ALA	263	112.458	52.631	51.567	1.00	52.30
2006	N	ARG	264	112.333	50.766	50.297	1.00	53.43
2007	CA	ARG	264	113.592	50.196	50.752	1.00	48.17
2008	CB	ARG	264	113.499	48.670	50.889	1.00	40.34
2009	CG	ARG	264	112.624	48.166	52.030	1.00	43.53
2010	CD	ARG	264	112.450	46.639	51.998	1.00	35.92
2011	NE	ARG	264	111.772	46.200	50.774	1.00	44.75
2012	CZ	ARG	264	110.964	45.144	50.679	1.00	49.82
2013	NH1	ARG	264	110.714	44.385	51.738	1.00	51.07
2014	NH2	ARG	264	110.385	44.857	49.518	1.00	37.04
2015	C	ARG	264	114.676	50.512	49.742	1.00	49.03
2016	O	ARG	264	114.453	50.444	48.527	1.00	47.55
2017	N	ASP	265	115.848	50.870	50.252	1.00	50.80
2018	CA	ASP	265	116.987	51.164	49.392	1.00	51.29
2019	CB	ASP	265	117.728	52.418	49.877	1.00	52.76
2020	CG	ASP	265	118.690	52.955	48.843	1.00	54.37
2021	OD1	ASP	265	118.782	52.363	47.747	1.00	50.00
2022	OD2	ASP	265	119.358	53.972	49.120	1.00	60.30
2023	C	ASP	265	117.903	49.933	49.419	1.00	45.08
2024	O	ASP	265	118.824	49.846	50.238	1.00	39.53
2025	N	ARG	266	117.614	48.973	48.541	1.00	41.67
2026	CA	ARG	266	118.377	47.732	48.482	1.00	37.99
2027	CB	ARG	266	117.528	48.574	48.983	1.00	38.78
2028	CG	ARG	266	116.957	46.771	50.372	1.00	29.99
2029	CD	ARG	266	118.028	48.593	51.418	1.00	37.48
2030	NE	ARG	266	117.503	46.781	52.764	1.00	38.27
2031	CZ	ARG	266	117.416	47.958	53.376	1.00	45.66
2032	NH1	ARG	266	117.822	49.066	52.763	1.00	38.28
2033	NH2	ARG	266	116.920	48.027	54.603	1.00	42.90
2034	C	ARG	266	118.826	47.429	47.034	1.00	33.86
2035	O	ARG	266	118.671	46.306	46.542	1.00	40.81
2036	N	VAL	267	119.392	48.431	48.371	1.00	25.69
2037	CA	VAL	267	119.845	48.257	45.000	1.00	20.97
2038	CB	VAL	267	120.143	49.611	44.326	1.00	21.69
2039	CG1	VAL	267	121.384	50.264	44.933	1.00	20.36
2040	CG2	VAL	267	120.292	49.420	42.828	1.00	8.30
2041	C	VAL	267	121.058	47.333	44.913	1.00	27.40
2042	O	VAL	267	121.231	46.616	43.926	1.00	36.12
2043	N	VAL	268	121.889	47.347	45.952	1.00	30.76
2044	CA	VAL	268	123.080	46.503	46.008	1.00	32.68
2045	CB	VAL	268	123.998	46.904	47.190	1.00	35.53
2046	CG1	VAL	268	125.220	46.001	47.245	1.00	32.24
2047	CG2	VAL	268	124.420	48.355	47.058	1.00	33.69
2048	C	VAL	268	122.623	45.058	46.196	1.00	29.06
2049	O	VAL	268	123.119	44.144	45.533	1.00	25.58
2050	N	GLU	269	121.662	44.878	47.100	1.00	24.94
2051	CA	GLU	269	121.087	43.573	47.406	1.00	22.59
2052	CB	GLU	269	120.083	43.692	48.558	1.00	16.86
2053	CG	GLU	269	120.705	43.939	49.942	1.00	22.84
2054	CD	GLU	269	121.136	45.385	50.200	1.00	25.18
2055	OE1	GLU	269	121.417	45.713	51.374	1.00	24.26
2056	OE2	GLU	269	121.194	46.198	49.255	1.00	23.69
2057	C	GLU	269	120.404	43.001	46.167	1.00	21.52
2058	O	GLU	269	120.423	41.789	45.941	1.00	22.99

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2059	N	CYS	270	119.814	43.885	45.365	1.00	16.93
2060	CA	CYS	270	119.144	43.487	44.133	1.00	15.61
2061	CB	CYS	270	118.305	44.637	43.577	1.00	14.26
2062	SG	CYS	270	116.923	45.097	44.637	1.00	24.62
2063	C	CYS	270	120.191	43.065	43.117	1.00	19.83
2064	O	CYS	270	119.922	42.239	42.245	1.00	25.94
2065	N	TYR	271	121.382	43.648	43.220	1.00	25.82
2066	CA	TYR	271	122.464	43.290	42.315	1.00	22.31
2067	CB	TYR	271	123.616	44.296	42.366	1.00	15.29
2068	CG	TYR	271	124.715	43.914	41.408	1.00	11.26
2069	CD1	TYR	271	124.592	44.174	40.043	1.00	9.23
2070	CE1	TYR	271	125.534	43.705	39.135	1.00	12.75
2071	CD2	TYR	271	125.821	43.184	41.844	1.00	6.39
2072	CE2	TYR	271	126.767	42.709	40.946	1.00	6.94
2073	CZ	TYR	271	126.615	42.970	39.594	1.00	11.07
2074	OH	TYR	271	127.525	42.467	38.702	1.00	9.47
2075	C	TYR	271	122.973	41.904	42.692	1.00	23.07
2076	O	TYR	271	123.318	41.104	41.820	1.00	22.92
2077	N	PHE	272	123.037	41.639	43.997	1.00	17.89
2078	CA	PHE	272	123.484	40.344	44.500	1.00	17.87
2079	CB	PHE	272	123.481	40.329	46.033	1.00	20.14
2080	CG	PHE	272	123.722	38.967	46.625	1.00	18.24
2081	CD1	PHE	272	124.998	38.409	46.631	1.00	20.70
2082	CD2	PHE	272	122.669	38.232	47.160	1.00	19.50
2083	CE1	PHE	272	125.219	37.139	47.159	1.00	15.25
2084	CE2	PHE	272	122.881	36.961	47.690	1.00	17.71
2085	CZ	PHE	272	124.159	36.414	47.689	1.00	12.72
2086	C	PHE	272	122.540	39.273	43.972	1.00	20.61
2087	O	PHE	272	122.974	38.200	43.550	1.00	26.50
2088	N	TRP	273	121.248	39.594	43.982	1.00	24.31
2089	CA	TRP	273	120.203	38.695	43.506	1.00	20.50
2090	CB	TRP	273	118.831	39.335	43.724	1.00	22.07
2091	CG	TRP	273	117.820	38.395	44.280	1.00	22.11
2092	CD2	TRP	273	117.499	38.205	45.661	1.00	17.16
2093	CE2	TRP	273	116.513	37.193	45.726	1.00	18.77
2094	CE3	TRP	273	117.949	38.789	46.851	1.00	16.10
2095	OD1	TRP	273	117.036	37.522	43.580	1.00	22.90
2096	NE1	TRP	273	116.250	36.794	44.442	1.00	15.33
2097	CZ2	TRP	273	115.969	36.750	46.938	1.00	8.52
2098	CZ3	TRP	273	117.408	38.351	48.057	1.00	19.38
2099	CH2	TRP	273	116.428	37.339	48.088	1.00	25.09
2100	C	TRP	273	120.401	38.389	42.024	1.00	19.25
2101	O	TRP	273	120.291	37.239	41.596	1.00	26.32
2102	N	ALA	274	120.705	39.424	41.247	1.00	15.42
2103	CA	ALA	274	120.925	39.267	39.815	1.00	17.00
2104	CB	ALA	274	120.927	40.622	39.138	1.00	8.15
2105	C	ALA	274	122.240	38.538	39.553	1.00	21.87
2106	O	ALA	274	122.394	37.858	38.535	1.00	24.79
2107	N	LEU	275	123.188	38.694	40.474	1.00	18.76
2108	CA	LEU	275	124.487	38.045	40.354	1.00	20.76
2109	CB	LEU	275	125.505	38.712	41.281	1.00	15.67
2110	CG	LEU	275	126.937	38.176	41.221	1.00	6.06
2111	CD1	LEU	275	127.475	38.257	39.798	1.00	5.14
2112	CD2	LEU	275	127.812	38.960	42.179	1.00	9.22
2113	C	LEU	275	124.351	36.560	40.684	1.00	19.71
2114	O	LEU	275	125.130	35.731	40.206	1.00	17.59
2115	N	GLY	276	123.356	36.239	41.507	1.00	22.38
2116	CA	GLY	276	123.098	34.860	41.880	1.00	15.02
2117	C	GLY	276	122.429	34.101	40.747	1.00	8.27
2118	O	GLY	276	122.574	32.885	40.641	1.00	21.39
2119	N	VAL	277	121.693	34.825	39.904	1.00	9.55
2120	CA	VAL	277	120.992	34.245	38.758	1.00	6.19
2121	CB	VAL	277	119.950	35.238	38.201	1.00	4.45
2122	CG1	VAL	277	119.236	34.660	36.994	1.00	2.00
2123	CG2	VAL	277	118.946	35.576	39.284	1.00	2.00
2124	C	VAL	277	122.003	33.848	37.686	1.00	9.32
2125	O	VAL	277	121.872	32.807	37.042	1.00	17.27
2126	N	TYR	278	122.992	34.711	37.481	1.00	13.83
2127	CA	TYR	278	124.082	34.466	36.543	1.00	17.57
2128	CB	TYR	278	123.644	34.476	35.067	1.00	14.31
2129	CG	TYR	278	122.485	35.368	34.675	1.00	21.92
2130	CD1	TYR	278	122.304	36.630	35.242	1.00	28.06
2131	CE1	TYR	278	121.249	37.454	34.839	1.00	17.69

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2132	CD2	TYR	278	121.581	34.952	33.698	1.00	10.48
2133	CE2	TYR	278	120.532	35.762	33.290	1.00	15.32
2134	CZ	TYR	278	120.371	37.012	33.860	1.00	20.32
2135	OH	TYR	278	119.341	37.820	33.432	1.00	16.49
2136	C	TYR	278	125.236	35.423	36.790	1.00	22.42
2137	O	TYR	278	125.024	36.609	37.052	1.00	24.68
2138	N	PHE	279	126.454	34.883	36.756	1.00	20.65
2139	CA	PHE	279	127.665	35.662	36.998	1.00	24.23
2140	CB	PHE	279	128.474	35.036	38.140	1.00	19.97
2141	CG	PHE	279	129.063	33.694	37.800	1.00	27.50
2142	CD1	PHE	279	130.278	33.600	37.124	1.00	27.56
2143	CD2	PHE	279	128.387	32.523	38.120	1.00	26.31
2144	CE1	PHE	279	130.804	32.363	36.770	1.00	27.48
2145	CE2	PHE	279	128.906	31.283	37.770	1.00	27.51
2146	CZ	PHE	279	130.116	31.202	37.093	1.00	26.58
2147	C	PHE	279	128.564	35.797	35.773	1.00	22.60
2148	O	PHE	279	129.420	36.681	35.727	1.00	29.14
2149	N	GLU	280	128.404	34.893	34.811	1.00	26.53
2150	CA	GLU	280	129.217	34.909	33.599	1.00	25.23
2151	CB	GLU	280	128.759	33.832	32.608	1.00	31.74
2152	CG	GLU	280	129.004	32.392	33.056	1.00	26.55
2153	CD	GLU	280	127.873	31.806	33.899	1.00	40.41
2154	CE1	GLU	280	127.909	30.581	34.149	1.00	41.01
2155	CE2	GLU	280	126.949	32.549	34.307	1.00	31.27
2156	C	GLU	280	129.195	36.276	32.928	1.00	28.72
2157	O	GLU	280	128.169	36.958	32.918	1.00	21.31
2158	N	PRO	281	130.346	36.702	32.382	1.00	31.20
2159	CD	PRO	281	131.607	35.942	32.368	1.00	29.80
2160	CA	PRO	281	130.511	37.988	31.697	1.00	31.18
2161	CB	PRO	281	131.976	37.949	31.246	1.00	36.16
2162	CG	PRO	281	132.274	36.479	31.137	1.00	35.87
2163	C	PRO	281	129.561	38.213	30.522	1.00	29.70
2164	O	PRO	281	129.196	39.352	30.226	1.00	29.95
2165	N	GLN	282	129.161	37.126	29.866	1.00	27.63
2166	CA	GLN	282	128.252	37.194	28.722	1.00	28.39
2167	CB	GLN	282	128.174	35.832	28.028	1.00	34.10
2168	CG	GLN	282	127.630	34.717	28.912	1.00	45.80
2169	CD	GLN	282	127.714	33.351	28.264	1.00	47.83
2170	OE1	GLN	282	128.543	32.523	28.647	1.00	54.06
2171	NE2	GLN	282	126.848	33.101	27.285	1.00	41.38
2172	C	GLN	282	126.851	37.640	29.133	1.00	25.75
2173	O	GLN	282	126.061	38.071	28.294	1.00	34.41
2174	N	TYR	283	126.553	37.521	30.425	1.00	26.54
2175	CA	TYR	283	125.254	37.910	30.972	1.00	26.30
2176	CB	TYR	283	124.765	36.853	31.966	1.00	19.61
2177	CG	TYR	283	124.537	35.506	31.323	1.00	13.47
2178	CD1	TYR	283	125.030	34.339	31.901	1.00	13.33
2179	CE1	TYR	283	124.852	33.099	31.286	1.00	15.49
2180	CD2	TYR	283	123.853	35.402	30.112	1.00	18.67
2181	CE2	TYR	283	123.669	34.173	29.490	1.00	23.42
2182	CZ	TYR	283	124.172	33.026	30.079	1.00	14.24
2183	OH	TYR	283	124.002	31.817	29.448	1.00	22.41
2184	C	TYR	283	125.304	39.287	31.632	1.00	29.24
2185	O	TYR	283	124.504	39.599	32.517	1.00	27.80
2186	N	SER	284	126.244	40.108	31.170	1.00	29.09
2187	CA	SER	284	126.438	41.401	31.673	1.00	24.35
2188	CB	SER	284	127.644	42.103	30.981	1.00	29.60
2189	OG	SER	284	127.873	43.418	31.456	1.00	29.67
2190	C	SER	284	125.192	42.315	31.451	1.00	23.95
2191	O	SER	284	124.647	42.882	32.396	1.00	16.24
2192	N	GLN	285	124.743	42.393	30.199	1.00	29.77
2193	CA	GLN	285	123.556	43.173	29.852	1.00	36.37
2194	CB	GLN	285	123.313	43.138	28.339	1.00	36.36
2195	CG	GLN	285	122.119	43.974	27.883	1.00	42.33
2196	CD	GLN	285	121.887	43.913	26.382	1.00	47.38
2197	OE1	GLN	285	122.208	42.919	25.727	1.00	45.82
2198	NE2	GLN	285	121.321	44.981	25.832	1.00	47.01
2199	C	GLN	285	122.328	42.638	30.588	1.00	40.35
2200	O	GLN	285	121.503	43.413	31.076	1.00	46.67
2201	N	ALA	286	122.242	41.312	30.686	1.00	38.34
2202	CA	ALA	286	121.136	40.637	31.356	1.00	27.14
2203	CB	ALA	286	121.252	39.136	31.170	1.00	34.43
2204	C	ALA	286	121.067	40.983	32.837	1.00	24.71

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2205	O	ALA	286	119.996	41.319	33.346	1.00	32.18
2206	N	ARG	287	122.203	40.891	33.526	1.00	17.67
2207	CA	ARG	287	122.261	41.212	34.951	1.00	17.77
2208	CB	ARG	287	123.680	41.046	35.504	1.00	14.04
2209	CG	ARG	287	124.013	39.659	36.008	1.00	21.57
2210	CD	ARG	287	125.294	39.673	36.828	1.00	20.38
2211	NE	ARG	287	126.451	40.078	36.033	1.00	14.48
2212	CZ	ARG	287	127.080	39.293	35.162	1.00	22.09
2213	NH1	ARG	287	126.670	38.049	34.959	1.00	17.96
2214	NH2	ARG	287	128.132	39.749	34.497	1.00	25.61
2215	C	ARG	287	121.802	42.642	35.207	1.00	24.30
2216	O	ARG	287	120.942	42.877	36.046	1.00	22.53
2217	N	VAL	288	122.358	43.583	34.449	1.00	32.79
2218	CA	VAL	288	122.031	45.001	34.586	1.00	35.93
2219	CB	VAL	288	122.800	45.853	33.543	1.00	42.80
2220	CG1	VAL	288	122.484	47.329	33.718	1.00	45.42
2221	CG2	VAL	288	124.294	45.622	33.682	1.00	39.26
2222	C	VAL	288	120.525	45.246	34.470	1.00	30.79
2223	O	VAL	288	119.927	45.888	35.339	1.00	27.62
2224	N	MET	289	119.914	44.698	33.422	1.00	25.59
2225	CA	MET	289	118.473	44.837	33.202	1.00	20.40
2226	CB	MET	289	118.055	44.123	31.908	1.00	11.02
2227	CG	MET	289	118.675	44.684	30.646	1.00	17.69
2228	SD	MET	289	118.236	43.769	29.151	1.00	29.61
2229	CE	MET	289	117.076	44.873	28.424	1.00	23.00
2230	C	MET	289	117.692	44.240	34.383	1.00	20.89
2231	O	MET	289	116.762	44.861	34.901	1.00	25.06
2232	N	LEU	290	118.104	43.063	34.825	1.00	20.72
2233	CA	LEU	290	117.448	42.379	35.935	1.00	15.74
2234	CB	LEU	290	118.020	40.969	36.078	1.00	14.98
2235	CG	LEU	290	117.497	40.044	37.174	1.00	16.12
2236	CD1	LEU	290	115.981	39.981	37.142	1.00	16.37
2237	CD2	LEU	290	118.098	38.659	36.964	1.00	19.76
2238	C	LEU	290	117.530	43.139	37.261	1.00	21.50
2239	O	LEU	290	116.561	43.172	38.019	1.00	23.53
2240	N	VAL	291	118.675	43.761	37.534	1.00	24.67
2241	CA	VAL	291	118.858	44.518	38.773	1.00	28.92
2242	CB	VAL	291	120.280	45.113	38.893	1.00	30.77
2243	CG1	VAL	291	120.439	45.822	40.234	1.00	27.10
2244	CG2	VAL	291	121.324	44.033	38.742	1.00	35.91
2245	C	VAL	291	117.872	45.679	38.826	1.00	33.69
2246	O	VAL	291	117.266	45.950	39.867	1.00	38.64
2247	N	LYS	292	117.722	46.360	37.693	1.00	32.65
2248	CA	LYS	292	116.819	47.500	37.589	1.00	29.16
2249	CB	LYS	292	116.961	48.155	36.213	1.00	28.67
2250	CG	LYS	292	118.314	48.814	35.986	1.00	28.14
2251	CD	LYS	292	118.440	49.353	34.575	1.00	36.09
2252	CE	LYS	292	119.765	50.059	34.370	1.00	37.49
2253	NZ	LYS	292	119.962	50.417	32.940	1.00	42.24
2254	C	LYS	292	115.369	47.102	37.849	1.00	25.46
2255	O	LYS	292	114.633	47.829	38.514	1.00	23.99
2256	N	THR	293	114.984	45.922	37.365	1.00	28.08
2257	CA	THR	293	113.627	45.401	37.536	1.00	20.11
2258	CB	THR	293	113.385	44.183	36.617	1.00	19.93
2259	OG1	THR	293	113.325	44.619	35.252	1.00	19.22
2260	CG2	THR	293	112.095	43.472	36.972	1.00	14.44
2261	C	THR	293	113.326	45.026	38.987	1.00	22.63
2262	O	THR	293	112.286	45.405	39.524	1.00	30.10
2263	N	ILE	294	114.239	44.295	39.621	1.00	23.15
2264	CA	ILE	294	114.058	43.884	41.015	1.00	22.01
2265	CB	ILE	294	115.232	43.007	41.522	1.00	19.34
2266	CG2	ILE	294	114.962	42.546	42.958	1.00	19.45
2267	CG1	ILE	294	115.430	41.799	40.604	1.00	12.44
2268	CD1	ILE	294	116.564	40.876	41.017	1.00	23.70
2269	C	ILE	294	113.959	45.113	41.910	1.00	21.14
2270	O	ILE	294	113.097	45.193	42.789	1.00	23.19
2271	N	SER	295	114.841	46.075	41.664	1.00	27.23
2272	CA	SER	295	114.879	47.310	42.435	1.00	36.44
2273	CB	SER	295	116.063	48.167	41.979	1.00	38.02
2274	OG	SER	295	116.508	49.015	43.021	1.00	50.33
2275	C	SER	295	113.566	48.077	42.265	1.00	33.20
2276	O	SER	295	112.984	48.562	43.239	1.00	27.63
2277	N	MET	296	113.083	48.124	41.026	1.00	32.18

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2278	CA	MET	296	111.843	48.816	40.685	1.00	33.20
2279	CB	MET	296	111.659	48.829	39.165	1.00	33.02
2280	CG	MET	296	110.820	49.978	38.637	1.00	34.84
2281	SD	MET	296	111.653	51.571	38.807	1.00	40.22
2282	CE	MET	296	110.937	52.162	40.336	1.00	31.58
2283	C	MET	296	110.617	48.181	41.343	1.00	36.25
2284	O	MET	296	109.831	48.871	41.997	1.00	35.27
2285	N	ILE	297	110.462	46.867	41.172	1.00	36.41
2286	CA	ILE	297	109.327	46.145	41.743	1.00	31.22
2287	CB	ILE	297	109.240	44.681	41.222	1.00	30.61
2288	CG2	ILE	297	110.401	43.850	41.748	1.00	32.13
2289	CG1	ILE	297	107.915	44.039	41.647	1.00	25.21
2290	CD1	ILE	297	106.681	44.725	41.088	1.00	9.77
2291	C	ILE	297	109.362	46.151	43.266	1.00	28.01
2292	O	ILE	297	108.333	45.964	43.914	1.00	33.37
2293	N	SER	298	110.544	46.369	43.834	1.00	26.49
2294	CA	SER	298	110.682	46.410	45.284	1.00	31.31
2295	CB	SER	298	112.152	46.511	45.692	1.00	36.65
2296	OG	SER	298	112.281	46.533	47.106	1.00	34.52
2297	C	SER	298	109.921	47.616	45.810	1.00	31.13
2298	O	SER	298	109.331	47.567	46.888	1.00	32.44
2299	N	ILE	299	109.932	48.693	45.029	1.00	31.80
2300	CA	ILE	299	109.239	49.023	45.390	1.00	37.55
2301	CB	ILE	299	109.648	51.086	44.462	1.00	44.76
2302	CG2	ILE	299	108.809	52.326	44.753	1.00	45.64
2303	CG1	ILE	299	111.135	51.390	44.645	1.00	46.63
2304	CD1	LE	299	111.656	52.438	43.707	1.00	51.58
2305	C	ILE	299	107.735	49.710	45.315	1.00	31.48
2306	O	ILE	299	107.008	50.072	46.238	1.00	32.42
2307	N	VAL	300	107.277	49.101	44.224	1.00	27.09
2308	CA	VAL	300	105.855	43.824	44.037	1.00	23.95
2309	CB	VAL	300	105.598	48.080	42.709	1.00	22.51
2310	CG1	VAL	300	104.108	47.876	42.494	1.00	20.37
2311	CG2	VAL	300	106.190	48.867	41.552	1.00	20.21
2312	C	VAL	300	105.349	47.990	45.211	1.00	23.59
2313	O	VAL	300	104.247	48.204	45.714	1.00	30.31
2314	N	ASP	301	106.186	47.072	45.674	1.00	24.66
2315	CA	ASP	301	105.837	46.226	46.802	1.00	31.65
2316	CB	ASP	301	106.879	45.121	46.975	1.00	25.48
2317	CG	ASP	301	106.523	44.163	48.087	1.00	24.95
2318	OD1	ASP	301	105.672	43.277	47.869	1.00	37.24
2319	OD2	ASP	301	107.075	44.309	49.193	1.00	32.62
2320	C	ASP	301	105.762	47.078	48.065	1.00	33.30
2321	O	ASP	301	104.847	46.930	48.874	1.00	36.41
2322	N	ASP	302	106.737	47.971	48.218	1.00	41.65
2323	CA	ASP	302	106.805	48.866	49.369	1.00	43.94
2324	CB	ASP	302	108.124	49.650	49.353	1.00	49.38
2325	CG	ASP	302	109.322	48.798	49.744	1.00	55.74
2326	OD1	ASP	302	109.246	48.101	50.780	1.00	59.49
2327	OD2	ASP	302	110.344	48.833	49.024	1.00	52.10
2328	C	ASP	302	105.619	49.831	49.416	1.00	43.11
2329	O	ASP	302	105.198	50.257	50.493	1.00	44.18
2330	N	THR	303	105.081	50.159	48.243	1.00	38.88
2331	CA	THR	303	103.945	51.069	48.123	1.00	33.20
2332	CB	THR	303	103.745	51.514	46.660	1.00	41.14
2333	OG1	THR	303	104.965	52.075	46.158	1.00	39.42
2334	CG2	THR	303	102.643	52.555	46.564	1.00	44.39
2335	C	THR	303	102.652	50.426	48.624	1.00	36.28
2336	O	THR	303	101.930	51.016	49.425	1.00	44.91
2337	N	PHE	304	102.367	49.218	48.143	1.00	33.21
2338	CA	PHE	304	101.167	48.478	48.532	1.00	26.28
2339	CB	PHE	304	101.005	47.234	47.653	1.00	23.04
2340	CG	PHE	304	100.431	47.509	46.293	1.00	14.95
2341	CD1	PHE	304	101.250	47.901	45.239	1.00	16.64
2342	CD2	PHE	304	99.068	47.352	46.059	1.00	16.64
2343	CE1	PHE	304	100.720	48.132	43.968	1.00	20.58
2344	CE2	PHE	304	98.527	47.580	44.793	1.00	13.24
2345	CZ	PHE	304	99.355	47.971	43.746	1.00	15.28
2346	C	PHE	304	101.183	48.032	49.993	1.00	34.53
2347	O	PHE	304	100.135	47.926	50.632	1.00	38.46
2348	N	ASP	305	102.379	47.778	50.515	1.00	40.19
2349	CA	ASP	305	102.544	47.300	51.881	1.00	46.42
2350	CB	ASP	305	103.774	46.399	51.968	1.00	58.96

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2351	CG	ASP	305	103.431	44.933	51.845	1.00	70.39
2352	OD1	ASP	305	102.647	44.572	50.940	1.00	75.74
2353	OD2	ASP	305	103.957	44.140	52.656	1.00	75.60
2354	C	ASP	305	102.605	48.324	53.001	1.00	47.79
2355	O	ASP	305	101.936	48.161	54.022	1.00	46.25
2356	N	ALA	306	103.425	49.357	52.831	1.00	52.07
2357	CA	ALA	306	103.574	50.362	53.875	1.00	54.53
2358	CB	ALA	306	104.958	50.240	54.518	1.00	57.28
2359	C	ALA	306	103.312	51.807	53.462	1.00	53.39
2360	O	ALA	306	103.971	52.718	53.965	1.00	58.62
2361	N	TYR	307	102.345	52.030	52.576	1.00	51.30
2362	CA	TYR	307	102.045	53.395	52.165	1.00	53.81
2363	CB	TYR	307	103.107	53.918	51.195	1.00	48.52
2364	CG	TYR	307	103.396	55.388	51.392	1.00	55.69
2365	CD1	TYR	307	103.963	55.847	52.581	1.00	59.86
2366	CE1	TYR	307	104.206	57.200	52.789	1.00	62.54
2367	CD2	TYR	307	103.077	56.324	50.411	1.00	56.20
2368	CE2	TYR	307	103.315	57.683	50.608	1.00	59.89
2369	CZ	TYR	307	103.878	58.112	51.801	1.00	62.92
2370	OH	TYR	307	104.112	59.451	52.009	1.00	66.19
2371	C	TYR	307	100.647	53.640	51.597	1.00	59.33
2372	O	TYR	307	99.752	54.078	52.320	1.00	66.09
2373	N	GLY	308	100.473	53.364	50.307	1.00	59.69
2374	CA	GLY	308	99.199	53.580	49.636	1.00	58.39
2375	C	GLY	308	97.924	53.122	50.326	1.00	60.86
2376	O	GLY	308	97.925	52.163	51.101	1.00	61.04
2377	N	THR	309	96.833	53.833	50.044	1.00	60.72
2378	CA	THR	309	95.522	53.524	50.609	1.00	57.07
2379	CB	THR	309	94.751	54.807	50.989	1.00	55.19
2380	OG1	THR	309	94.651	55.667	49.847	1.00	47.62
2381	CG2	THR	309	95.461	55.538	52.117	1.00	46.57
2382	C	THR	309	94.693	52.722	49.609	1.00	59.08
2383	O	THR	309	94.996	52.709	48.415	1.00	56.21
2384	N	VAL	310	93.631	52.089	50.107	1.00	60.80
2385	CA	VAL	310	92.737	51.264	49.295	1.00	62.84
2386	CB	VAL	310	91.430	50.932	50.059	1.00	64.23
2387	CG1	VAL	310	90.667	49.821	49.351	1.00	66.80
2388	CG2	VAL	310	91.737	50.534	51.498	1.00	61.87
2389	C	VAL	310	92.390	51.903	47.947	1.00	63.74
2390	O	VAL	310	92.469	51.244	46.904	1.00	60.65
2391	N	LYS	311	92.038	53.189	47.972	1.00	65.40
2392	CA	LYS	311	91.687	53.926	46.755	1.00	65.81
2393	CB	LYS	311	91.121	55.301	47.105	1.00	70.45
2394	CG	LYS	311	89.696	55.305	47.621	1.00	74.65
2395	CD	LYS	311	89.175	56.734	47.692	1.00	77.16
2396	CE	LYS	311	87.719	56.787	48.120	1.00	75.45
2397	NZ	LYS	311	87.239	58.194	48.137	1.00	78.70
2398	C	LYS	311	92.889	54.116	45.842	1.00	63.97
2399	O	LYS	311	92.840	53.788	44.658	1.00	64.41
2400	N	GLU	312	93.961	54.670	46.403	1.00	60.54
2401	CA	GLU	312	95.195	54.931	45.665	1.00	57.43
2402	CB	GLU	312	96.263	55.516	46.596	1.00	59.85
2403	CG	GLU	312	95.900	56.859	47.194	1.00	66.27
2404	CD	GLU	312	97.024	57.438	48.033	1.00	69.45
2405	OE1	GLU	312	97.396	56.817	49.051	1.00	71.29
2406	OE2	GLU	312	97.544	58.514	47.666	1.00	70.23
2407	C	GLU	312	95.750	53.679	44.989	1.00	53.28
2408	O	GLU	312	96.133	53.715	43.815	1.00	44.50
2409	N	LEU	313	95.787	52.577	45.736	1.00	45.10
2410	CA	LEU	313	96.290	51.310	45.222	1.00	40.42
2411	CB	LEU	313	96.361	50.267	46.343	1.00	35.64
2412	CG	LEU	313	97.263	50.614	47.534	1.00	32.14
2413	CD1	LEU	313	97.226	49.501	48.569	1.00	28.15
2414	CD2	LEU	313	98.687	50.861	47.061	1.00	26.11
2415	C	LEU	313	95.430	50.800	44.071	1.00	41.37
2416	O	LEU	313	95.950	50.275	43.085	1.00	39.82
2417	N	GLU	314	94.116	50.981	44.193	1.00	41.16
2418	CA	GLU	314	93.180	50.553	43.156	1.00	41.35
2419	CB	GLU	314	91.737	50.728	43.636	1.00	45.36
2420	CG	GLU	314	90.674	50.326	42.612	1.00	51.16
2421	CD	GLU	314	90.717	48.848	42.251	1.00	56.61
2422	OE1	GLU	314	90.469	48.007	43.144	1.00	55.46
2423	OE2	GLU	314	90.988	48.530	41.071	1.00	49.16

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2424	C	GLU	314	93.417	51.357	41.880	1.00	38.64
2425	O	GLU	314	93.315	50.828	40.772	1.00	41.77
2426	N	ALA	315	93.742	52.634	42.047	1.00	37.56
2427	CA	ALA	315	94.012	53.513	40.917	1.00	37.09
2428	CB	ALA	315	94.024	54.961	41.375	1.00	41.02
2429	C	ALA	315	95.354	53.146	40.292	1.00	37.51
2430	O	ALA	315	95.522	53.222	39.074	1.00	40.72
2431	N	TYR	316	96.301	52.741	41.138	1.00	37.47
2432	CA	TYR	316	97.641	52.351	40.698	1.00	36.60
2433	CB	TYR	316	98.567	52.189	41.908	1.00	42.76
2434	CG	TYR	316	100.045	52.214	41.576	1.00	47.70
2435	CD1	TYR	316	100.701	53.421	41.323	1.00	50.35
2436	CE1	TYR	316	102.064	53.456	41.029	1.00	47.09
2437	CD2	TYR	316	100.792	51.038	41.526	1.00	50.58
2438	CE2	TYR	316	102.158	51.063	41.232	1.00	51.96
2439	CZ	TYR	316	102.785	52.276	40.988	1.00	46.31
2440	OH	TYR	316	104.130	52.308	40.697	1.00	45.69
2441	C	TYR	316	97.582	51.047	39.909	1.00	38.30
2442	O	TYR	316	98.142	50.949	38.812	1.00	29.96
2443	N	THR	317	96.890	50.058	40.473	1.00	34.49
2444	CA	THR	317	96.731	48.752	39.839	1.00	33.58
2445	CB	THR	317	95.811	47.831	40.671	1.00	29.35
2446	OG1	THR	317	96.347	47.676	41.990	1.00	30.19
2447	CG2	THR	317	95.691	46.460	40.020	1.00	28.64
2448	C	THR	317	96.125	48.922	38.448	1.00	38.84
2449	O	THR	317	96.624	48.363	37.470	1.00	37.70
2450	N	ASP	318	95.070	49.731	38.369	1.00	39.63
2451	CA	ASP	318	94.385	49.987	37.110	1.00	43.25
2452	CB	ASP	318	93.115	50.806	37.351	1.00	53.81
2453	CG	ASP	318	92.282	50.972	36.094	1.00	64.26
2454	OD1	ASP	318	91.830	49.947	35.538	1.00	68.93
2455	OD2	ASP	318	92.088	52.126	35.656	1.00	69.91
2456	C	ASP	318	95.292	50.706	36.118	1.00	38.89
2457	O	ASP	318	95.280	50.406	34.922	1.00	35.65
2458	N	ALA	319	96.081	51.651	36.622	1.00	39.85
2459	CA	ALA	319	97.001	52.409	35.783	1.00	39.48
2460	CB	ALA	319	97.716	53.462	36.610	1.00	45.21
2461	C	ALA	319	98.007	51.469	35.123	1.00	36.47
2462	O	ALA	319	98.261	51.564	33.920	1.00	28.06
2463	N	ILE	320	98.547	50.541	35.912	1.00	36.88
2464	CA	ILE	320	99.514	49.560	35.422	1.00	35.98
2465	CB	ILE	320	99.994	48.620	36.561	1.00	43.40
2466	CG2	ILE	320	100.784	47.443	35.991	1.00	44.99
2467	CG1	ILE	320	100.834	49.397	37.582	1.00	45.58
2468	CD1	ILE	320	102.173	49.891	37.054	1.00	39.26
2469	C	ILE	320	98.911	48.712	34.307	1.00	31.85
2470	O	ILE	320	99.544	48.506	33.271	1.00	32.45
2471	N	GLN	321	97.680	48.245	34.518	1.00	27.13
2472	CA	GLN	321	96.980	47.414	33.538	1.00	29.80
2473	CB	GLN	321	95.592	47.021	34.053	1.00	37.41
2474	CG	GLN	321	95.581	46.336	35.422	1.00	37.33
2475	CD	GLN	321	96.510	45.136	35.508	1.00	42.33
2476	OE1	GLN	321	96.690	44.398	34.536	1.00	43.16
2477	NE2	GLN	321	97.108	44.938	36.679	1.00	35.06
2478	C	GLN	321	96.856	48.101	32.180	1.00	30.46
2479	O	GLN	321	97.066	47.474	31.139	1.00	25.13
2480	N	ARG	322	96.519	49.390	32.199	1.00	36.61
2481	CA	ARG	322	96.384	50.171	30.971	1.00	40.97
2482	CB	ARG	322	95.779	51.549	31.264	1.00	48.13
2483	CG	ARG	322	94.261	51.612	31.176	1.00	58.29
2484	CD	ARG	322	93.581	50.838	32.290	1.00	66.64
2485	NE	ARG	322	92.125	50.822	32.134	1.00	76.38
2486	CZ	ARG	322	91.326	51.868	32.344	1.00	74.78
2487	NH1	ARG	322	91.827	53.035	32.727	1.00	73.98
2488	NH2	ARG	322	90.019	51.751	32.157	1.00	73.84
2489	C	ARG	322	97.737	50.347	30.290	1.00	39.65
2490	O	ARG	322	97.848	50.233	29.067	1.00	46.16
2491	N	TRP	323	98.757	50.635	31.094	1.00	37.39
2492	CA	TRP	323	100.118	50.828	30.607	1.00	35.58
2493	CB	TRP	323	100.663	49.535	29.990	1.00	36.83
2494	CG	TRP	323	102.169	49.447	29.979	1.00	41.47
2495	CD2	TRP	323	103.017	49.048	31.063	1.00	38.37
2496	CE2	TRP	323	104.351	49.089	30.594	1.00	38.29

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2497	CE3	TRP	323	102.779	48.656	32.390	1.00	36.27
2498	CD1	TRP	323	103.003	49.714	28.922	1.00	40.25
2499	NE1	TRP	323	104.312	49.500	29.286	1.00	39.37
2500	CZ2	TRP	323	105.439	48.753	31.402	1.00	30.80
2501	CZ3	TRP	323	103.863	48.322	33.192	1.00	34.06
2502	CH2	TRP	323	105.178	48.374	32.691	1.00	37.92
2503	C	TRP	323	100.182	51.976	29.606	1.00	36.88
2504	O	TRP	323	100.522	51.788	28.437	1.00	30.80
2505	N	ASP	324	99.781	53.157	30.066	1.00	48.71
2506	CA	ASP	324	99.797	54.366	29.249	1.00	54.17
2507	CB	ASP	324	98.462	54.586	28.537	1.00	56.16
2508	CG	ASP	324	98.585	55.547	27.366	1.00	58.43
2509	OD1	ASP	324	98.956	56.724	27.575	1.00	59.06
2510	OD2	ASP	324	98.328	55.120	26.222	1.00	57.24
2511	C	ASP	324	100.076	55.543	30.165	1.00	57.09
2512	O	ASP	324	99.468	55.671	31.230	1.00	54.89
2513	N	ILE	325	100.977	56.414	29.729	1.00	60.16
2514	CA	ILE	325	101.377	57.584	30.495	1.00	64.12
2515	CB	ILE	325	102.559	58.286	29.788	1.00	67.78
2516	CG2	ILE	325	102.072	59.013	28.542	1.00	68.84
2517	CG1	ILE	325	103.325	59.185	30.768	1.00	71.40
2518	CD1	ILE	325	104.716	59.579	30.273	1.00	78.93
2519	C	ILE	325	100.219	58.560	30.760	1.00	62.87
2520	O	ILE	325	100.248	59.325	31.723	1.00	55.53
2521	N	ASN	326	99.181	58.489	29.931	1.00	63.16
2522	CA	ASN	326	98.008	59.347	30.075	1.00	60.43
2523	CB	ASN	326	97.060	59.157	28.891	1.00	58.85
2524	CG	ASN	326	97.208	60.240	27.858	1.00	58.26
2525	OD1	ASN	326	97.005	61.420	28.150	1.00	61.96
2526	ND2	ASN	326	97.564	59.854	26.640	1.00	59.50
2527	C	ASN	326	97.247	59.093	31.370	1.00	61.39
2528	O	ASN	326	96.561	59.982	31.875	1.00	62.82
2529	N	GLU	327	97.378	57.881	31.904	1.00	59.66
2530	CA	GLU	327	96.691	57.498	33.136	1.00	62.98
2531	CB	GLU	327	96.563	55.973	33.216	1.00	64.39
2532	CG	GLU	327	96.087	55.299	31.933	1.00	69.30
2533	CD	GLU	327	94.708	55.750	31.491	1.00	70.48
2534	OE1	GLU	327	93.784	55.783	32.335	1.00	72.78
2535	OE2	GLU	327	94.548	56.067	30.291	1.00	63.31
2536	C	GLU	327	97.414	58.011	34.380	1.00	62.97
2537	O	GLU	327	96.972	57.771	35.505	1.00	62.71
2538	N	ILE	328	98.510	58.734	34.169	1.00	64.24
2539	CA	ILE	328	99.316	59.270	35.264	1.00	67.30
2540	CB	ILE	328	100.636	59.886	34.729	1.00	69.70
2541	CG2	ILE	328	100.372	61.245	34.069	1.00	69.85
2542	CG1	ILE	328	101.657	60.013	35.863	1.00	72.49
2543	CD1	ILE	328	103.047	60.424	35.409	1.00	71.67
2544	C	ILE	328	98.577	60.298	36.122	1.00	66.37
2545	O	ILE	328	98.763	60.349	37.340	1.00	61.63
2546	N	ASP	329	97.711	61.082	35.485	1.00	70.35
2547	CA	ASP	329	96.950	62.128	36.163	1.00	73.14
2548	CB	ASP	329	96.212	62.987	35.134	1.00	73.34
2549	CG	ASP	329	97.154	63.620	34.123	1.00	75.99
2550	OD1	ASP	329	97.861	64.584	34.486	1.00	75.75
2551	OD2	ASP	329	97.193	63.140	32.970	1.00	74.82
2552	C	ASP	329	95.978	61.611	37.219	1.00	73.26
2553	O	ASP	329	95.637	62.332	38.159	1.00	73.84
2554	N	ARG	330	95.539	60.366	37.065	1.00	70.87
2555	CA	ARG	330	94.616	59.756	38.019	1.00	70.53
2556	CB	ARG	330	93.932	58.535	37.393	1.00	71.49
2557	CG	ARG	330	93.145	58.845	36.129	1.00	73.19
2558	CD	ARG	330	92.435	57.612	35.591	1.00	85.11
2559	NE	ARG	330	91.756	57.889	34.326	1.00	94.74
2560	CZ	ARG	330	90.865	57.082	33.754	1.00	98.54
2561	NH1	ARG	330	90.532	55.934	34.331	1.00	100.00
2562	NH2	ARG	330	90.309	57.424	32.599	1.00	94.40
2563	C	ARG	330	95.358	59.345	39.291	1.00	67.20
2564	O	ARG	330	94.749	59.145	40.345	1.00	61.95
2565	N	LEU	331	96.681	59.252	39.183	1.00	66.11
2566	CA	LEU	331	97.539	58.857	40.295	1.00	65.38
2567	CB	LEU	331	98.727	58.047	39.768	1.00	70.15
2568	CG	LEU	331	98.430	56.802	38.933	1.00	71.98
2569	CD1	LEU	331	99.710	56.289	38.300	1.00	67.56

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2570	CD2	LEU	331	97.789	55.739	39.806	1.00	72.35
2571	C	LEU	331	98.081	60.056	41.057	1.00	59.96
2572	O	LEU	331	98.432	61.069	40.456	1.00	60.57
2573	N	PRO	332	98.145	59.962	42.397	1.00	56.66
2574	CD	PRO	332	97.661	58.870	43.257	1.00	52.18
2575	CA	PRO	332	98.666	61.070	43.204	1.00	60.33
2576	CB	PRO	332	98.458	60.578	44.640	1.00	54.14
2577	CG	PRO	332	98.462	59.090	44.507	1.00	53.96
2578	C	PRO	332	100.144	61.294	42.871	1.00	65.03
2579	O	PRO	332	100.817	60.386	42.381	1.00	68.68
2580	N	ASP	333	100.637	62.500	43.138	1.00	70.86
2581	CA	ASP	333	102.021	62.876	42.839	1.00	72.50
2582	CB	ASP	333	102.362	64.220	43.489	1.00	76.30
2583	CG	ASP	333	101.737	65.396	42.760	1.00	73.02
2584	OD1	ASP	333	101.290	66.343	43.438	1.00	75.36
2585	OD2	ASP	333	101.700	65.378	41.510	1.00	70.83
2586	C	ASP	333	103.146	61.873	43.105	1.00	69.45
2587	O	ASP	333	104.019	61.694	42.254	1.00	64.53
2588	N	TYR	334	103.139	61.226	44.269	1.00	65.65
2589	CA	TYR	334	104.195	60.267	44.590	1.00	64.14
2590	CB	TYR	334	104.180	59.900	48.080	1.00	67.04
2591	CG	TYR	334	103.162	58.858	46.484	1.00	71.84
2592	CD1	TYR	334	101.827	59.199	46.688	1.00	74.21
2593	CE1	TYR	334	100.895	58.243	47.086	1.00	74.47
2594	CD2	TYR	334	103.542	57.531	46.685	1.00	72.86
2595	CE2	TYR	334	102.620	56.570	47.081	1.00	72.07
2596	CZ	TYR	334	101.299	56.932	47.281	1.00	72.74
2597	OH	TYR	334	100.386	55.962	47.675	1.00	69.90
2598	C	TYR	334	104.143	59.015	43.714	1.00	59.49
2599	O	TYR	334	105.181	58.466	43.341	1.00	58.89
2600	N	MET	335	102.933	58.575	43.379	1.00	51.53
2601	CA	MET	335	102.762	57.401	42.533	1.00	48.12
2602	CB	MET	335	101.340	56.854	42.637	1.00	45.40
2603	CG	MET	335	100.979	56.325	44.006	1.00	34.82
2604	SD	MET	335	99.387	55.502	44.005	1.00	37.30
2605	CE	MET	335	99.776	53.904	44.867	1.00	41.41
2606	C	MET	335	103.082	57.727	41.081	1.00	48.13
2607	O	MET	335	103.354	56.826	40.287	1.00	55.57
2608	N	LYS	336	103.032	59.013	40.738	1.00	48.65
2609	CA	LYS	336	103.332	59.465	39.380	1.00	50.84
2610	CB	LYS	336	103.004	60.953	39.213	1.00	55.94
2611	CG	LYS	336	101.524	61.301	39.255	1.00	63.40
2612	CD	LYS	336	101.298	62.758	38.857	1.00	63.31
2613	CE	LYS	336	99.820	63.092	38.764	1.00	60.22
2614	NZ	LYS	336	99.580	64.473	38.271	1.00	62.57
2615	C	LYS	336	104.810	59.237	39.080	1.00	51.33
2616	O	LYS	336	105.187	58.938	37.943	1.00	47.74
2617	N	ILE	337	105.638	59.382	40.114	1.00	45.10
2618	CA	ILE	337	107.079	59.195	39.996	1.00	46.36
2619	CB	ILE	337	107.805	59.607	41.297	1.00	48.91
2620	CG2	ILE	337	109.309	59.641	41.067	1.00	50.47
2621	CG1	ILE	337	107.330	60.986	41.759	1.00	50.88
2622	OD1	ILE	337	107.888	61.407	43.105	1.00	47.89
2623	C	ILE	337	107.380	57.725	39.712	1.00	47.32
2624	O	ILE	337	108.140	57.402	38.795	1.00	52.27
2625	N	SER	338	106.755	56.844	40.491	1.00	42.57
2626	CA	SER	338	106.928	55.401	40.351	1.00	32.89
2627	CB	SER	338	106.120	54.663	41.424	1.00	29.02
2628	OG	SER	338	106.339	55.198	42.718	1.00	33.47
2629	C	SER	338	106.465	54.933	38.975	1.00	31.60
2630	O	SER	338	107.214	54.287	38.243	1.00	27.59
2631	N	TYR	339	105.239	55.311	38.621	1.00	33.89
2632	CA	TYR	339	104.622	54.932	37.353	1.00	39.75
2633	CB	TYR	339	103.204	55.508	37.265	1.00	42.11
2634	CG	TYR	339	102.367	54.908	36.157	1.00	46.50
2635	CD1	TYR	339	101.682	53.709	36.348	1.00	48.25
2636	CE1	TYR	339	100.924	53.144	35.327	1.00	52.79
2637	CD2	TYR	339	102.270	55.530	34.915	1.00	42.98
2638	CE2	TYR	339	101.515	54.976	33.890	1.00	51.56
2639	CZ	TYR	339	100.845	53.784	34.100	1.00	54.29
2640	OH	TYR	339	100.100	53.236	33.080	1.00	56.73
2641	C	TYR	339	105.414	55.309	36.101	1.00	43.13
2642	O	TYR	339	105.531	54.502	35.174	1.00	41.07

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2643	N	LYS	340	105.941	56.531	36.064	1.00	49.11
2644	CA	LYS	340	106.706	56.989	34.903	1.00	49.74
2645	CB	LYS	340	106.894	58.508	34.934	1.00	58.08
2646	CG	LYS	340	107.553	59.059	33.674	1.00	64.41
2647	CD	LYS	340	107.642	60.573	33.694	1.00	69.77
2648	CE	LYS	340	108.246	61.097	32.403	1.00	73.44
2649	NZ	LYS	340	108.256	62.584	32.365	1.00	82.14
2650	C	LYS	340	108.062	56.297	34.800	1.00	44.71
2651	O	LYS	340	108.506	55.938	33.703	1.00	34.93
2652	N	ALA	341	108.712	56.114	35.948	1.00	36.45
2653	CA	ALA	341	110.013	55.456	36.003	1.00	36.97
2654	CB	ALA	341	110.517	55.415	37.439	1.00	35.42
2655	C	ALA	341	109.897	54.041	35.444	1.00	35.71
2656	O	ALA	341	110.791	53.561	34.746	1.00	34.74
2657	N	ILE	342	108.766	53.399	35.734	1.00	29.99
2658	CA	ILE	342	108.487	52.041	35.283	1.00	21.08
2659	CB	ILE	342	107.231	51.472	35.982	1.00	16.81
2660	CG2	ILE	342	106.786	50.171	35.309	1.00	10.96
2661	CG1	ILE	342	107.523	51.275	37.476	1.00	10.78
2662	CD1	ILE	342	106.333	50.884	38.324	1.00	2.00
2663	C	ILE	342	108.336	51.939	33.771	1.00	28.67
2664	O	ILE	342	108.949	51.071	33.150	1.00	32.50
2665	N	LEU	343	107.530	52.821	33.180	1.00	33.81
2666	CA	LEU	343	107.320	52.809	31.732	1.00	37.97
2667	CB	LEU	343	106.208	53.774	31.317	1.00	41.50
2668	CG	LEU	343	104.822	53.594	31.932	1.00	46.77
2669	CD1	LEU	343	103.831	54.537	31.267	1.00	48.11
2670	CD2	LEU	343	104.375	52.165	31.759	1.00	43.32
2671	C	LEU	343	108.596	53.177	30.995	1.00	41.41
2672	O	LEU	343	108.880	52.626	29.932	1.00	43.16
2673	N	ASP	344	109.348	54.126	31.552	1.00	45.08
2674	CA	ASP	344	110.601	54.563	30.942	1.00	51.08
2675	CB	ASP	344	111.144	55.820	31.628	1.00	57.96
2676	OG	ASP	344	110.754	57.098	30.903	1.00	64.16
2677	CD1	ASP	344	110.680	57.090	29.654	1.00	69.36
2678	OD2	ASP	344	110.526	58.117	31.588	1.00	65.04
2679	C	ASP	344	111.643	53.461	30.980	1.00	50.69
2680	O	ASP	344	112.415	53.301	30.034	1.00	53.80
2681	N	LEU	345	111.661	52.709	32.078	1.00	47.98
2682	CA	LEU	345	112.594	51.599	32.242	1.00	43.23
2683	CB	LEU	345	112.384	50.925	33.599	1.00	45.16
2684	CG	LEU	345	113.317	49.773	33.977	1.00	44.62
2685	CD1	LEU	345	114.752	50.267	34.070	1.00	45.63
2686	CD2	LEU	345	112.875	49.186	35.307	1.00	42.33
2687	C	LEU	345	112.364	50.585	31.129	1.00	42.19
2688	O	LEU	345	113.315	50.068	30.541	1.00	47.47
2689	N	TYR	346	111.094	50.311	30.844	1.00	38.09
2690	CA	TYR	346	110.731	49.372	29.793	1.00	36.61
2691	CB	TYR	346	109.298	48.878	29.983	1.00	32.28
2692	CG	TYR	346	109.211	47.802	31.038	1.00	30.73
2693	CD1	TYR	346	108.903	48.110	32.361	1.00	22.11
2694	CE1	TYR	346	108.895	47.122	33.346	1.00	24.69
2695	CD2	TYR	346	109.503	46.477	30.722	1.00	35.15
2696	CE2	TYR	346	109.499	45.484	31.694	1.00	26.34
2697	CZ	TYR	346	109.198	45.809	33.000	1.00	27.54
2698	OH	TYR	346	109.224	44.812	33.948	1.00	22.51
2699	C	TYR	346	110.954	49.953	28.403	1.00	39.45
2700	O	TYR	346	111.086	49.213	27.429	1.00	37.79
2701	N	LYS	347	110.995	51.281	28.320	1.00	44.42
2702	CA	LYS	347	111.256	51.958	27.056	1.00	45.72
2703	CB	LYS	347	110.797	53.418	27.105	1.00	49.09
2704	CG	LYS	347	109.313	53.604	26.824	1.00	54.73
2705	CD	LYS	347	108.959	53.084	25.433	1.00	58.88
2706	CE	LYS	347	107.471	53.195	25.149	1.00	58.70
2707	NZ	LYS	347	107.129	52.632	23.816	1.00	45.34
2708	C	LYS	347	112.756	51.874	26.810	1.00	44.56
2709	O	LYS	347	113.201	51.803	25.666	1.00	44.20
2710	N	ASP	348	113.524	51.865	27.901	1.00	45.25
2711	CA	ASP	348	114.977	51.748	27.829	1.00	43.43
2712	CB	ASP	348	115.630	52.041	29.188	1.00	41.08
2713	CG	ASP	348	115.545	53.509	29.584	1.00	45.56
2714	OD1	ASP	348	115.741	54.388	28.716	1.00	50.29
2715	OD2	ASP	348	115.293	53.787	30.775	1.00	46.84

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2716	C	ASP	348	115.308	50.325	27.394	1.00	44.57
2717	O	ASP	348	116.186	50.116	26.555	1.00	45.03
2718	N	TYR	349	114.586	49.355	27.959	1.00	43.55
2719	CA	TYR	349	114.773	47.943	27.627	1.00	42.30
2720	CB	TYR	349	113.813	47.054	28.429	1.00	41.29
2721	CG	TYR	349	114.128	46.916	29.906	1.00	37.24
2722	CD1	TYR	349	113.181	46.393	30.785	1.00	30.06
2723	CE1	TYR	349	113.458	46.247	32.142	1.00	36.46
2724	CD2	TYR	349	115.368	47.293	30.424	1.00	41.76
2725	CE2	TYR	349	115.656	47.151	31.783	1.00	40.50
2726	CZ	TYR	349	114.694	46.627	32.633	1.00	36.99
2727	OH	TYR	349	114.960	46.491	33.975	1.00	36.59
2728	C	TYR	349	114.520	47.741	26.139	1.00	42.51
2729	O	TYR	349	115.308	47.094	25.446	1.00	42.03
2730	N	GLU	350	113.411	48.296	25.656	1.00	44.24
2731	CA	GLU	350	113.053	48.199	24.244	1.00	46.89
2732	CB	GLU	350	111.734	48.929	23.969	1.00	49.81
2733	CG	GLU	350	110.509	48.270	24.589	1.00	54.69
2734	CD	GLU	350	109.214	49.033	24.347	1.00	58.54
2735	OE1	GLU	350	108.144	48.491	24.695	1.00	62.24
2736	OE2	GLU	350	109.253	50.168	23.822	1.00	64.71
2737	C	GLU	350	114.162	48.811	23.397	1.00	48.29
2738	O	GLU	350	114.491	48.294	22.334	1.00	45.94
2739	N	LYS	351	114.763	49.884	23.909	1.00	53.89
2740	CA	LYS	351	115.841	50.591	23.222	1.00	58.14
2741	CB	LYS	351	116.053	51.971	23.855	1.00	63.43
2742	CG	LYS	351	116.916	52.921	23.031	1.00	71.72
2743	CD	LYS	351	116.247	53.286	21.711	1.00	77.97
2744	CE	LYS	351	117.122	54.218	20.885	1.00	83.68
2745	NZ	LYS	351	116.483	54.588	19.591	1.00	83.73
2746	C	LYS	351	117.155	49.795	23.215	1.00	57.54
2747	O	LYS	351	117.873	49.784	22.209	1.00	56.27
2748	N	GLU	352	117.465	49.142	24.336	1.00	56.46
2749	CA	GLU	352	118.684	48.334	24.458	1.00	52.60
2750	CB	GLU	352	118.847	47.801	25.390	1.00	50.25
2751	CG	GLU	352	119.239	48.828	26.943	1.00	58.10
2752	CD	GLU	352	119.464	48.194	28.311	1.00	59.00
2753	OE1	GLU	352	118.655	48.447	29.232	1.00	57.55
2754	OE2	GLU	352	120.447	47.435	28.468	1.00	53.94
2755	C	GLU	352	118.645	47.140	23.508	1.00	49.57
2756	O	GLU	352	119.671	46.735	22.957	1.00	45.55
2757	N	LEU	353	117.448	46.587	23.327	1.00	44.88
2758	CA	LEU	353	117.239	45.432	22.463	1.00	44.80
2759	CB	LEU	353	116.116	44.561	23.034	1.00	35.61
2760	CG	LEU	353	116.304	44.125	24.489	1.00	30.68
2761	CD1	LEU	353	115.030	43.507	25.030	1.00	31.93
2762	CD2	LEU	353	117.468	43.156	24.597	1.00	32.93
2763	C	LEU	353	116.937	45.806	21.011	1.00	48.25
2764	O	LEU	353	116.878	44.933	20.140	1.00	48.95
2765	N	SER	354	116.756	47.101	20.751	1.00	54.12
2766	CA	SER	354	116.468	47.595	19.403	1.00	58.83
2767	CB	SER	354	116.358	49.122	19.395	1.00	64.47
2768	OG	SER	354	115.196	49.571	20.072	1.00	73.04
2769	C	SER	354	117.534	47.171	18.400	1.00	58.85
2770	O	SER	354	117.228	46.900	17.237	1.00	60.25
2771	N	SER	355	118.784	47.119	18.857	1.00	59.55
2772	CA	SER	355	119.918	46.731	18.022	1.00	60.93
2773	CB	SER	355	121.219	46.840	18.823	1.00	58.82
2774	OG	SER	355	122.333	46.392	18.071	1.00	61.05
2775	C	SER	355	119.772	45.316	17.455	1.00	67.50
2776	O	SER	355	119.753	45.125	16.239	1.00	72.60
2777	N	ALA	356	119.640	44.338	18.345	1.00	68.57
2778	CA	ALA	356	119.501	42.943	17.946	1.00	67.55
2779	CB	ALA	356	119.690	42.040	19.152	1.00	63.74
2780	C	ALA	356	118.163	42.642	17.278	1.00	69.18
2781	O	ALA	356	118.071	41.754	16.434	1.00	70.23
2782	N	GLY	357	117.131	43.385	17.661	1.00	69.13
2783	CA	GLY	357	115.811	43.152	17.102	1.00	62.21
2784	C	GLY	357	115.027	42.258	18.039	1.00	59.93
2785	O	GLY	357	114.203	41.443	17.604	1.00	60.71
2786	N	ARG	358	115.322	42.391	19.332	1.00	54.34
2787	CA	ARG	358	114.669	41.616	20.385	1.00	52.71
2788	CB	ARG	358	115.713	40.882	21.231	1.00	45.26

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2789	CG	ARG	358	116.561	39.896	20.442	1.00	47.78
2790	CD	ARG	358	117.644	39.275	21.309	1.00	47.12
2791	NE	ARG	358	117.083	38.456	22.383	1.00	44.42
2792	CZ	ARG	358	117.206	38.724	23.681	1.00	39.46
2793	NH1	ARG	358	117.871	39.797	24.083	1.00	37.90
2794	NH2	ARG	356	116.684	37.905	24.583	1.00	43.78
2795	C	ARG	358	113.817	42.522	21.282	1.00	55.62
2796	O	ARG	358	113.676	42.268	22.479	1.00	60.74
2797	N	SER	359	113.286	43.596	20.699	1.00	54.17
2798	CA	SER	359	112.440	44.548	21.419	1.00	49.75
2799	CB	SER	359	112.373	45.887	20.671	1.00	46.10
2800	OG	SER	359	113.659	46.424	20.441	1.00	39.24
2801	C	SER	359	111.030	43.979	21.584	1.00	51.35
2802	O	SER	359	110.321	44.294	22.549	1.00	51.03
2803	N	HIS	360	110.642	43.145	20.619	1.00	48.18
2804	CA	HIS	360	109.339	42.484	20.566	1.00	49.55
2805	CB	HIS	360	109.165	41.769	19.214	1.00	55.45
2806	CG	HIS	360	110.191	40.706	18.955	1.00	57.94
2807	CD2	HIS	360	111.485	40.791	18.565	1.00	58.70
2808	ND1	HIS	360	109.933	39.363	19.134	1.00	62.62
2809	CE1	HIS	360	111.028	38.668	18.875.	1.00	63.83
2810	NE2	HIS	360	111.985	39.511	18.527	1.00	63.77
2811	C	HIS	360	109.105	41.483	21.705	1.00	51.67
2812	O	HIS	360	108.023	40.886	21.795	1.00	56.00
2813	N	ILE	361	110.115	41.294	22.552	1.00	44.35
2814	CA	ILE	361	110.005	40.352	23.659	1.00	40.02
2815	CB	ILE	361	111.217	39.396	23.719	1.00	40.34
2816	CG2	ILE	361	111.350	38.631	22.412	1.00	38.81
2817	CG1	ILE	361	112.490	40.174	24.052	1.00	45.99
2818	CD1	ILE	361	113.742	39.324	24.096	1.00	38.31
2819	C	ILE	361	109.837	41.012	25.022	1.00	38.58
2820	O	ILE	361	109.629	40.323	26.018	1.00	46.53
2821	N	VAL	362	109.920	42.339	25.068	1.00	34.37
2822	CA	VAL	362	109.784	43.073	26.323	1.00	36.05
2823	CB	VAL	362	110.133	44.567	26.131	1.00	44.38
2824	CG1	VAL	362	110.157	45.290	27.474	1.00	28.09
2825	CG2	VAL	362	111.470	44.705	25.420	1.00	50.90
2826	C	VAL	362	108.372	42.959	26.899	1.00	35.07
2827	O	VAL	362	108.187	43.012	28.113	1.00	27.77
2828	N	CYS	363	107.383	42.770	26.025	1.00	37.13
2829	CA	CYS	363	105.980	42.653	26.437	1.00	34.16
2830	CB	CYS	363	105.066	42.483	25.215	1.00	29.73
2831	SG	CYS	363	105.447	41.051	24.179	1.00	41.96
2832	C	CYS	363	105.730	41.520	27.434	1.00	32.61
2833	O	CYS	363	104.887	41.646	28.325	1.00	25.38
2834	N	HIS	364	106.481	40.429	27.292	1.00	28.31
2835	CA	HIS	364	106.356	39.267	28.168	1.00	20.38
2836	CB	HIS	364	107.304	38.159	27.713	1.00	19.91
2837	CG	HIS	364	107.064	37.696	26.309	1.00	25.64
2838	CD2	HIS	364	107.777	37.887	25.173	1.00	29.90
2839	ND1	HIS	364	105.976	36.929	25.954	1.00	34.65
2840	CE1	HIS	364	106.028	36.667	24.659	1.00	33.79
2841	NE2	HIS	364	107.111	37.237	24.162	1.00	27.05
2842	C	HIS	364	106.646	39.635	29.622	1.00	28.17
2843	O	HIS	364	105.942	39.200	30.537	1.00	27.54
2844	N	ALA	365	107.685	40.440	29.826	1.00	30.22
2845	CA	ALA	365	108.067	40.880	31.163	1.00	30.86
2846	CB	ALA	365	109.427	41.574	31.120	1.00	34.60
2847	C	ALA	365	107.007	41.822	31.725	1.00	31.03
2848	O	ALA	365	106.752	41.838	32.931	1.00	31.19
2849	N	ILE	366	106.389	42.596	30.835	1.00	36.30
2850	CA	ILE	366	105.347	43.550	31.208	1.00	36.55
2851	CB	ILE	366	105.016	44.504	30.034	1.00	41.23
2852	CG2	ILE	366	103.857	45.419	30.403	1.00	40.62
2853	CG1	ILE	366	106.253	45.331	29.668	1.00	35.62
2854	CD1	ILE	366	106.065	46.231	28.468	1.00	29.32
2855	C	ILE	366	104.070	42.845	31.667	1.00	30.85
2856	O	ILE	366	103.524	43.173	32.722	1.00	28.50
2857	N	GLU	367	103.613	41.867	30.886	1.00	25.21
2858	CA	GLU	367	102.404	41.117	31.223	1.00	22.77
2859	CB	GLU	367	102.095	40.069	30.153	1.00	32.06
2860	CG	GLU	367	101.926	40.626	28.736	1.00	41.69
2861	CD	GLU	367	100.870	41.721	28.629	1.00	48.62

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2862	OE1	GLU	367	99.829	41.633	29.321	1.00	48.68
2863	OE2	GLU	367	101.083	42.670	27.841	1.00	43.16
2864	C	GLU	367	102.539	40.448	32.585	1.00	20.02
2865	O	GLU	367	101.555	40.297	33.314	1.00	20.91
2866	N	ARG	368	103.766	40.057	32.923	1.00	21.53
2867	CA	ARG	368	104.055	39.422	34.205	1.00	14.50
2868	CB	ARG	368	105.406	38.709	34.159	1.00	17.59
2869	CG	ARG	368	105.427	37.442	33.319	1.00	13.40
2870	CD	ARG	368	104.602	36.338	33.960	1.00	17.58
2871	NE	ARG	368	104.843	35.044	33.325	1.00	25.37
2872	CZ	ARG	368	104.380	33.884	33.784	1.00	29.88
2873	NH1	ARG	368	103.641	33.847	34.887	1.00	15.72
2874	NH2	ARG	368	104.669	32.757	33.146	1.00	25.60
2875	C	ARG	368	104.058	40.473	35.306	1.00	22.28
2876	O	ARG	368	103.674	40.193	36.444	1.00	25.28
2877	N	MET	369	104.489	41.686	34.965	1.00	23.23
2878	CA	MET	369	104.513	42.774	35.933	1.00	22.69
2879	CB	MET	369	105.234	44.001	35.371	1.00	21.94
2880	CG	MET	369	105.216	45.178	36.332	1.00	33.04
2881	SD	MET	369	106.226	46.580	35.855	1.00	30.05
2882	CE	MET	369	106.788	47.105	37.492	1.00	22.46
2883	C	MET	369	103.088	43.138	36.329	1.00	21.30
2884	O	MET	369	102.794	43.316	37.513	1.00	25.30
2885	N	LYS	370	102.207	43.230	35.332	1.00	22.42
2886	CA	LYS	370	100.798	43.555	35.562	1.00	21.17
2887	CB	LYS	370	100.033	43.596	34.237	1.00	18.37
2888	CG	LYS	370	100.498	44.679	33.272	1.00	19.38
2889	CD	LYS	370	99.724	44.628	31.959	1.00	22.90
2890	CE	LYS	370	100.144	45.754	31.026	1.00	25.30
2891	NZ	LYS	370	99.370	45.760	29.753	1.00	26.14
2892	C	LYS	370	100.184	42.503	36.480	1.00	22.60
2893	O	LYS	370	99.433	42.830	37.404	1.00	22.82
2894	N	GLU	371	100.540	41.243	36.233	1.00	20.87
2895	CA	GLU	371	100.060	40.117	37.027	1.00	17.91
2896	CB	GLU	371	100.633	38.805	36.473	1.00	17.04
2897	CG	GLU	371	100.291	37.558	37.281	1.00	14.89
2898	CD	GLU	371	100.951	36.307	36.737	1.00	33.96
2899	OE1	GLU	371	100.246	35.281	36.624	1.00	49.48
2900	OE2	GLU	371	102.162	36.342	36.433	1.00	39.35
2901	C	GLU	371	100.459	40.291	38.491	1.00	14.70
2902	O	GLU	371	99.629	40.146	39.389	1.00	15.00
2903	N	VAL	372	101.727	40.624	38.718	1.00	16.52
2904	CA	VAL	372	102.246	40.830	40.066	1.00	17.45
2905	CB	VAL	372	103.747	41.232	40.043	1.00	17.58
2906	CG1	VAL	372	104.258	41.453	41.450	1.00	3.56
2907	CG2	VAL	372	104.575	40.156	39.365	1.00	18.80
2908	C	VAL	372	101.455	41.919	40.782	1.00	21.27
2909	O	VAL	372	101.101	41.767	41.952	1.00	23.46
2910	N	VAL	373	101.155	43.000	40.063	1.00	26.12
2911	CA	VAL	373	100.407	44.123	40.629	1.00	29.37
2912	CB	VAL	373	100.425	45.356	39.694	1.00	33.84
2913	CG1	VAL	373	99.736	46.537	40.366	1.00	27.54
2914	CG2	VAL	373	101.861	45.724	39.335	1.00	29.76
2915	C	VAL	373	98.962	43.754	40.969	1.00	29.64
2916	O	VAL	373	98.462	44.135	42.030	1.00	27.43
2917	N	ARG	374	98.298	43.015	40.078	1.00	27.06
2918	CA	ARG	374	96.916	42.587	40.315	1.00	22.92
2919	CB	ARG	374	96.438	41.626	39.225	1.00	20.10
2920	CG	ARG	374	96.101	42.257	37.897	1.00	18.80
2921	CD	ARG	374	95.627	41.191	36.924	1.00	11.40
2922	NE	ARG	374	96.410	41.194	35.692	1.00	20.17
2923	CZ	ARG	374	96.956	40.112	35.146	1.00	19.94
2924	NH1	ARG	374	96.810	38.924	35.720	1.00	26.31
2925	NH2	ARG	374	97.655	40.218	34.025	1.00	24.45
2926	C	ARG	374	96.835	41.858	41.646	1.00	26.89
2927	O	ARG	374	95.964	42.134	42.472	1.00	32.47
2928	N	ASN	375	97.766	40.931	41.842	1.00	27.68
2929	CA	ASN	375	97.827	40.133	43.055	1.00	25.57
2930	CB	ASN	375	98.776	38.955	42.850	1.00	30.36
2931	CG	ASN	375	98.299	38.009	41.756	1.00	32.94
2932	OD1	ASN	375	97.594	38.415	40.827	1.00	25.76
2933	ND2	ASN	375	98.677	36.741	41.865	1.00	30.37
2934	C	ASN	375	98.213	40.958	44.279	1.00	26.96

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
2935	O	ASN	375	97.819	40.632	45.399	1.00	21.31
2936	N	TYR	376	98.980	42.026	44.062	1.00	33.99
2937	CA	TYR	376	99.381	42.920	45.148	1.00	33.87
2938	CB	TYR	376	100.382	43.986	44.645	1.00	39.17
2939	CG	TYR	376	101.823	43.579	44.628	1.00	42.30
2940	CD1	TYR	376	102.765	44.344	43.940	1.00	40.53
2941	CE1	TYR	376	104.111	43.997	43.934	1.00	45.46
2942	CD2	TYR	376	102.268	42.446	45.312	1.00	43.05
2943	CE2	TYR	376	103.614	42.088	45.313	1.00	42.63
2944	CZ	TYR	376	104.531	42.868	44.623	1.00	48.37
2945	OH	TYR	376	105.865	42.523	44.621	1.00	39.23
2946	C	TYR	376	98.122	43.605	45.668	1.00	29.88
2947	O	TYR	376	97.942	43.773	46.874	1.00	27.89
2948	N	ASN	377	97.252	43.984	44.733	1.00	29.64
2949	CA	ASN	377	95.987	44.642	45.043	1.00	31.75
2950	CB	ASN	377	95.304	45.094	43.748	1.00	34.90
2951	CG	ASN	377	94.116	45.999	43.999	1.00	40.49
2952	OD1	ASN	377	92.992	45.532	44.178	1.00	42.59
2953	ND2	ASN	377	94.360	47.303	44.011	1.00	34.81
2954	C	ASN	377	95.084	43.674	45.804	1.00	28.41
2955	O	ASN	377	94.538	44.015	46.857	1.00	30.58
2956	N	VAL	378	94.952	42.460	45.274	1.00	17.90
2957	CA	VAL	378	94.131	41.426	45.900	1.00	17.33
2958	CB	VAL	378	94.186	40.112	45.086	1.00	10.51
2959	CG1	VAL	378	93.423	39.012	45.789	1.00	11.35
2960	CG2	VAL	378	93.612	40.332	43.698	1.00	13.48
2961	C	VAL	378	94.616	41.163	47.327	1.00	25.35
2962	O	VAL	378	93.813	40.997	48.248	1.00	27.43
2963	N	GLU	379	95.936	41.176	47.497	1.00	31.20
2964	CA	GLU	379	96.575	40.938	48.787	1.00	33.04
2965	CB	GLU	379	98.100	40.924	48.613	1.00	40.56
2966	CG	GLU	379	98.888	40.454	49.836	1.00	52.37
2967	CD	GLU	379	100.392	40.399	49.591	1.00	57.31
2968	OE1	GLU	379	101.158	40.762	50.510	1.00	59.83
2969	OE2	GLU	379	100.810	39.986	48.485	1.00	55.53
2970	C	GLU	379	96.166	41.984	49.825	1.00	31.53
2971	O	GLU	379	95.922	41.650	50.987	1.00	29.16
2972	N	SER	380	96.092	43.245	49.402	1.00	32.96
2973	CA	SER	380	95.706	44.331	50.300	1.00	37.42
2974	CB	SER	380	96.066	45.695	49.698	1.00	38.70
2975	OG	SER	380	95.348	45.945	48.504	1.00	49.17
2976	C	SER	380	94.212	44.264	50.604	1.00	38.16
2977	O	SER	380	93.789	44.512	51.737	1.00	31.46
2978	N	THR	381	93.424	43.915	49.587	1.00	36.08
2979	CA	THR	381	91.976	43.790	49.729	1.00	27.53
2980	CB	THR	381	91.320	43.333	48.413	1.00	22.85
2981	OG1	THR	381	91.706	44.212	47.350	1.00	16.53
2982	CG2	THR	381	89.812	43.351	48.543	1.00	23.91
2983	C	THR	381	91.662	42.762	50.814	1.00	27.68
2984	O	THR	381	90.813	42.996	51.670	1.00	29.54
2985	N	TRP	382	92.375	41.637	50.779	1.00	28.31
2986	CA	TRP	382	92.199	40.563	51.755	1.00	28.12
2987	CB	TRP	382	93.063	39.353	51.386	1.00	36.50
2988	CG	TRP	382	92.583	38.570	50.195	1.00	38.50
2989	CD2	TRP	382	93.258	37.475	49.565	1.00	42.33
2990	CE2	TRP	382	92.430	37.022	48.516	1.00	44.37
2991	CE3	TRP	382	94.483	36.830	49.787	1.00	47.90
2992	CD1	TRP	382	91.408	38.735	49.518	1.00	36.49
2993	NE1	TRP	382	91.308	31.808	48.511	1.00	36.31
2994	CZ2	TRP	382	92.787	35.951	47.688	1.00	51.17
2995	CZ3	TRP	382	94.838	35.764	48.963	1.00	43.35
2996	CH2	TRP	382	93.991	35.337	47.927	1.00	45.79
2997	C	TRP	382	92.567	41.030	53.157	1.00	30.09
2998	O	TRP	382	91.926	40.651	54.137	1.00	31.61
2999	N	PHE	383	93.617	41.841	53.240	1.00	36.62
3000	CA	PHE	383	94.092	42.378	54.510	1.00	38.24
3001	CB	PHE	383	95.411	43.138	54.298	1.00	36.46
3002	CG	PHE	383	95.885	43.880	55.516	1.00	32.91
3003	CD1	PHE	383	96.157	43.202	56.701	1.00	32.24
3004	CD2	PHE	383	96.020	45.264	55.490	1.00	33.47
3005	CE1	PHE	383	96.553	43.892	57.843	1.00	34.44
3006	CE2	PHE	383	96.415	45.963	56.628	1.00	34.81
3007	CZ	PHE	383	96.081	45.275	57.807	1.00	35.83

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3008	C	PHE	383	93.045	43.296	55.144	1.00	38.45
3009	O	PHE	383	92.793	43.223	56.351	1.00	36.37
3010	N	ILE	384	92.436	44.144	54.315	1.00	36.46
3011	CA	ILE	384	91.410	45.091	54.756	1.00	34.56
3012	CB	ILE	384	91.025	46.062	53.615	1.00	27.26
3013	CG2	ILE	384	89.917	46.996	54.066	1.00	33.92
3014	CG1	ILE	384	92.249	46.870	53.171	1.00	30.39
3015	CD1	ILE	384	92.881	47.691	54.278	1.00	31.10
3016	C	ILE	384	90.145	44.391	55.255	1.00	34.50
3017	O	ILE	384	89.634	44.702	56.333	1.00	36.61
3018	N	GLU	385	89.643	43.453	54.460	1.00	26.50
3019	CA	GLU	385	88.443	42.703	54.811	1.00	26.95
3020	CB	GLU	385	87.937	41.926	53.595	1.00	21.63
3021	CG	GLU	385	87.650	42.790	52.375	1.00	29.50
3022	CD	GLU	385	87.418	41.976	51.115	1.00	38.78
3023	OE1	GLU	385	87.706	40.758	51.124	1.00	42.45
3024	OE2	GLU	385	86.955	42.560	50.110	1.00	36.35
3025	C	GLU	385	88.711	41.732	55.954	1.00	32.21
3026	O	GLU	385	87.778	41.289	56.629	1.00	43.97
3027	N	GLY	386	89.985	41.419	56.184	1.00	30.98
3028	CA	GLY	386	90.341	40.486	57.238	1.00	29.71
3029	C	GLY	386	90.069	39.071	56.767	1.00	29.59
3030	O	GLY	386	89.738	38.178	57.557	1.00	27.61
3031	N	TYR	387	90.238	38.877	55.461	1.00	23.79
3032	CA	TYR	387	89.999	37.595	54.816	1.00	27.24
3033	CB	TYR	387	89.744	37.802	53.319	1.00	29.04
3034	CG	TYR	387	89.248	36.570	52.580	1.00	23.98
3035	CD1	TYR	387	88.361	35.675	53.179	1.00	22.30
3036	CE1	TYR	387	87.891	34.552	52.493	1.00	29.04
3037	CD2	TYR	387	89.657	36.311	51.271	1.00	26.35
3038	CE2	TYR	387	89.192	35.194	50.575	1.00	24.90
3039	CZ	TYR	387	88.311	34.320	51.191	1.00	29.66
3040	OH	TYR	387	87.848	33.218	50.510	1.00	26.42
3041	C	TYR	387	91.127	36.591	55.014	1.00	30.82
3042	O	TYR	387	92.311	36.917	54.874	1.00	39.13
3043	N	THR	388	90.721	35.375	55.364	1.00	37.65
3044	CA	THR	388	91.623	34.247	55.568	1.00	31.40
3045	CB	THR	388	91.576	33.728	57.025	1.00	33.01
3046	OG1	THR	388	92.090	34.729	57.911	1.00	35.43
3047	CG2	THR	388	92.416	32.482	57.179	1.00	38.16
3048	C	THR	388	91.140	33.148	54.609	1.00	31.72
3049	O	THR	388	90.343	32.282	54.981	1.00	39.68
3050	N	PRO	389	91.581	33.203	53.335	1.00	25.34
3051	CD	PRO	389	92.494	34.204	52.755	1.00	23.99
3052	CA	PRO	389	91.190	32.214	52.323	1.00	26.01
3053	CB	PRO	389	91.717	32.829	51.030	1.00	21.95
3054	CG	PRO	389	92.953	33.531	51.475	1.00	17.85
3055	C	PRO	389	91.779	30.825	52.537	1.00	30.44
3056	O	PRO	389	92.711	30.651	53.324	1.00	28.62
3057	N	PRO	390	91.177	29.805	51.909	1.00	32.36
3058	CD	PRO	390	89.921	29.814	51.135	1.00	26.81
3059	CA	PRO	390	91.691	28.442	52.047	1.00	33.56
3060	CB	PRO	390	90.600	27.601	51.379	1.00	32.56
3061	CG	PRO	390	90.024	28.532	50.356	1.00	23.42
3062	C	PRO	390	93.016	28.383	51.277	1.00	34.49
3063	O	PRO	390	93.222	29.160	50.335	1.00	30.76
3064	N	VAL	391	93.920	27.494	51.689	1.00	29.65
3065	CA	VAL	391	95.230	27.360	51.046	1.00	25.79
3066	CB	VAL	391	95.943	26.061	51.479	1.00	23.80
3067	CG1	VAL	391	97.314	25.969	50.831	1.00	20.24
3068	CG2	VAL	391	96.078	26.017	52.981	1.00	16.75
3069	C	VAL	391	95.155	27.393	49.523	1.00	25.32
3070	O	VAL	391	95.944	28.075	48.868	1.00	27.66
3071	N	SER	392	94.178	26.683	48.970	1.00	25.00
3072	CA	SER	392	93.993	26.621	47.527	1.00	25.90
3073	CB	SER	392	92.727	25.827	47.194	1.00	26.67
3074	OG	SER	392	92.570	25.684	45.794	1.00	47.32
3075	C	SER	392	93.911	28.015	46.918	1.00	18.85
3076	O	SER	392	94.671	28.350	46.011	1.00	19.28
3077	N	GLU	393	93.013	28.837	47.450	1.00	16.74
3078	CA	GLU	393	92.827	30.191	46.949	1.00	24.04
3079	CB	GLU	393	91.579	30.821	47.565	1.00	27.67
3080	CG	GLU	393	91.105	32.067	46.831	1.00	20.67

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3081	CD	GLU	393	90.095	32.873	47.618	1.00	19.63
3082	OE1	GLU	393	89.550	32.362	48.619	1.00	20.04
3083	OE2	GLU	393	89.853	34.032	47.232	1.00	26.17
3084	C	GLU	393	94.044	31.071	47.226	1.00	27.53
3085	O	GLU	393	94.474	31.837	46.361	1.00	22.89
3086	N	TYR	394	94.590	30.960	48.435	1.00	26.05
3087	CA	TYR	394	95.762	31.736	48.829	1.00	26.22
3088	CB	TYR	394	96.252	31.293	50.211	1.00	32.15
3089	CG	TYR	394	97.597	31.868	50.595	1.00	37.24
3090	CD1	TYR	394	97.739	33.224	50.890	1.00	37.33
3091	CE1	TYR	394	98.980	33.762	51.214	1.00	33.89
3092	CD2	TYR	394	98.733	31.061	50.639	1.00	35.64
3093	CE2	TYR	394	99.979	31.590	50.961	1.00	31.95
3094	CZ	TYR	394	100.095	32.941	51.248	1.00	34.89
3095	OH	TYR	394	101.324	33.471	51.562	1.00	35.44
3096	C	TYR	394	96.900	31.615	47.813	1.00	27.71
3097	O	TYR	394	97.400	32.622	47.310	1.00	30.17
3098	N	LEU	395	97.278	30.379	47.496	1.00	19.47
3099	CA	LEU	395	98.356	30.112	46.551	1.00	18.70
3100	CB	LEU	395	98.664	28.615	46.506	1.00	23.07
3101	CG	LEU	395	99.219	28.005	47.796	1.00	25.20
3102	CD1	LEU	395	99.416	26.512	47.609	1.00	19.35
3103	CD2	LEU	395	100.532	28.681	48.180	1.00	17.74
3104	C	LEU	395	98.106	30.630	45.140	1.00	19.62
3105	O	LEU	395	99.030	31.112	44.485	1.00	19.16
3106	N	SER	396	96.862	30.549	44.676	1.00	25.13
3107	CA	SER	396	96.521	31.018	43.332	1.00	19.88
3108	CB	SER	396	95.047	30.749	43.022	1.00	25.09
3109	OG	SER	396	94.196	31.513	43.858	1.00	39.87
3110	C	SER	396	96.828	32.504	43.165	1.00	19.03
3111	O	SER	396	96.920	33.005	42.040	1.00	15.70
3112	N	ASN	397	96.999	33.198	44.290	1.00	14.51
3113	CA	ASN	397	97.308	34.624	44.281	1.00	20.25
3114	CB	ASN	397	96.252	35.401	45.072	1.00	21.33
3115	CG	ASN	397	96.348	36.901	44.858	1.00	25.70
3116	OD1	ASN	397	95.985	37.411	43.795	1.00	26.44
3117	ND2	ASN	397	96.840	37.617	45.868	1.00	14.18
3118	C	ASN	397	98.702	34.926	44.844	1.00	21.44
3119	O	ASN	397	99.446	35.727	44.277	1.00	16.68
3120	N	ALA	398	99.053	34.263	45.944	1.00	21.43
3121	CA	ALA	398	100.339	34.463	48.611	1.00	18.24
3122	CB	ALA	398	100.303	33.853	47.996	1.00	9.21
3123	C	ALA	398	101.576	33.973	45.861	1.00	22.03
3124	O	ALA	398	102.693	34.375	48.183	1.00	27.40
3125	N	LEU	399	101.392	33.099	44.878	1.00	24.29
3126	CA	LEU	399	102.530	32.590	44.123	1.00	21.14
3127	CB	LEU	399	102.133	31.379	43.276	1.00	16.51
3128	CG	LEU	399	101.814	30.092	44.047	1.00	22.47
3129	CD1	LEU	399	101.475	28.979	43.068	1.00	23.59
3130	CD2	LEU	399	102.986	29.686	44.929	1.00	24.50
3131	C	LEU	399	103.189	33.656	43.256	1.00	21.08
3132	O	LEU	399	104.414	33.724	43.181	1.00	27.40
3133	N	ALA	400	102.384	34.499	42.618	1.00	23.35
3134	CA	ALA	400	102.921	35.556	41.762	1.00	25.45
3135	CB	ALA	400	101.860	36.050	40.782	1.00	20.16
3138	C	ALA	400	103.500	36.724	42.562	1.00	21.72
3137	O	ALA	400	104.438	37.380	42.109	1.00	16.17
3138	N	THR	401	102.960	36.966	43.757	1.00	16.96
3139	CA	THR	401	103.445	38.054	44.605	1.00	19.18
3140	CB	THR	401	102.535	38.294	45.832	1.00	15.54
3141	OG1	THR	401	102.407	37.090	46.592	1.00	24.65
3142	CG2	THR	401	101.167	38.752	45.393	1.00	12.23
3143	C	THR	401	104.893	37.842	45.055	1.00	25.46
3144	O	THR	401	105.512	38.743	45.624	1.00	34.91
3145	N	THR	402	105.421	36.644	44.813	1.00	25.90
3146	CA	THR	402	106.807	36.336	45.151	1.00	21.29
3147	CB	THR	402	107.092	34.812	45.138	1.00	19.71
3148	OG1	THR	402	106.944	34.300	43.806	1.00	12.44
3149	CG2	THR	402	106.152	34.080	46.070	1.00	17.92
3150	C	THR	402	107.674	36.988	44.076	1.00	22.11
3151	O	THR	402	108.881	37.135	44.245	1.00	21.20
3152	N	THR	403	107.022	37.366	42.974	1.00	21.28
3153	CA	THR	403	107.629	38.010	41.804	1.00	18.85

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3154	CB	THR	403	108.446	39.288	42.167	1.00	15.80
3155	OG1	THR	403	109.662	38.922	42.827	1.00	16.98
3156	CG2	THR	403	107.647	40.210	43.071	1.00	14.55
3157	C	THR	403	108.515	37.084	40.980	1.00	17.52
3158	O	THR	403	109.136	37.523	40.013	1.00	14.77
3159	N	TYR	404	108.533	35.799	41.326	1.00	19.57
3160	CA	TYR	404	109.375	34.842	40.617	1.00	16.03
3161	CB	TYR	404	109.560	33.560	41.431	1.00	23.52
3162	CG	TYR	404	110.799	33.611	42.295	1.00	19.00
3163	CD1	TYR	404	111.271	34.828	42.785	1.00	20.18
3164	CE1	TYR	404	112.430	34.903	43.536	1.00	26.20
3165	CD2	TYR	404	111.527	32.459	42.586	1.00	21.26
3166	CE2	TYR	404	112.695	32.523	43.345	1.00	26.60
3167	CZ	TYR	404	113.139	33.753	43.813	1.00	25.95
3168	OH	TYR	404	114.291	33.853	44.553	1.00	17.83
3169	C	TYR	404	109.040	34.545	39.164	1.00	16.09
3170	O	TYR	404	109.945	34.265	38.375	1.00	15.20
3171	N	TYR	405	107.760	34.593	38.803	1.00	14.07
3172	CA	TYR	405	107.375	34.360	37.411	1.00	18.64
3173	CB	TYR	405	105.852	34.353	37.250	1.00	21.43
3174	CG	TYR	405	105.096	33.276	37.991	1.00	14.20
3175	CD1	TYR	405	104.458	33.557	39.196	1.00	25.61
3176	CE1	TYR	405	103.687	32.599	39.844	1.00	26.54
3177	CD2	TYR	405	104.949	31.998	37.452	1.00	18.03
3178	CE2	TYR	405	104.178	31.031	38.094	1.00	15.71
3179	CZ	TYR	405	103.550	31.341	39.290	1.00	17.50
3180	OH	TYR	405	102.785	30.404	39.941	1.00	14.13
3181	C	TYR	405	107.922	35.558	36.638	1.00	16.83
3182	O	TYR	405	108.450	35.433	35.532	1.00	12.99
3183	N	TYR	406	107.784	36.718	37.271	1.00	19.05
3184	CA	TYR	406	108.213	38.005	36.749	1.00	20.07
3185	CB	TYR	406	107.708	39.095	37.709	1.00	20.76
3186	CG	TYR	406	108.060	40.523	37.365	1.00	13.44
3187	CD1	TYR	406	108.092	40.965	36.044	1.00	16.24
3188	CE1	TYR	406	108.412	42.284	35.739	1.00	19.34
3189	CD2	TYR	406	108.355	41.436	38.373	1.00	2.00
3190	CE2	TYR	406	108.673	42.751	38.081	1.00	7.86
3191	CZ	TYR	406	108.701	43.171	36.764	1.00	14.60
3192	OH	TYR	406	109.015	44.481	36.481	1.00	12.74
3193	C	TYR	406	109.735	38.068	36.570	1.00	18.51
3194	O	TYR	406	110.222	38.302	35.462	1.00	20.47
3195	N	LEU	407	110.478	37.822	37.647	1.00	18.49
3196	CA	LEU	407	111.944	37.854	37.602	1.00	17.48
3197	CB	LEU	407	112.536	37.617	38.994	1.00	9.18
3198	CG	LEU	407	112.066	38.535	40.125	1.00	11.41
3199	CD1	LEU	407	112.894	38.261	41.366	1.00	4.35
3200	CD2	LEU	407	112.179	40.001	39.714	1.00	14.20
3201	C	LEU	407	112.533	36.843	36.619	1.00	17.93
3202	O	LEU	407	113.506	37.142	35.925	1.00	23.70
3203	N	ALA	408	111.944	35.650	36.568	1.00	17.24
3204	CA	ALA	408	112.402	34.603	35.662	1.00	15.77
3205	CB	ALA	408	111.636	33.320	35.913	1.00	20.39
3206	C	ALA	408	112.233	35.046	34.214	1.00	15.32
3207	O	ALA	408	113.108	34.820	33.383	1.00	19.31
3208	N	THR	409	111.106	35.685	33.919	1.00	18.97
3209	CA	THR	409	110.830	36.174	32.570	1.00	20.42
3210	CB	THR	409	109.382	36.705	32.455	1.00	12.64
3211	OG1	THR	409	108.465	35.679	32.853	1.00	23.03
3212	CG2	THR	409	109.074	37.116	31.023	1.00	8.86
3213	C	THR	409	111.804	37.302	32.233	1.00	18.76
3214	O	THR	409	112.269	37.426	31.096	1.00	14.71
3215	N	THR	410	112.118	38.105	33.245	1.00	23.19
3216	CA	THR	410	113.031	39.232	33.105	1.00	22.03
3217	CB	THR	410	113.060	40.078	34.390	1.00	17.23
3218	OG1	THR	410	111.751	40.600	34.652	1.00	20.47
3219	CG2	THR	410	114.043	41.228	34.251	1.00	18.91
3220	C	THR	410	114.453	38.781	32.790	1.00	25.12
3221	O	THR	410	115.109	39.356	31.918	1.00	24.94
3222	N	SER	411	114.913	37.741	33.486	1.00	18.76
3223	CA	SER	411	116.264	37.221	33.298	1.00	11.15
3224	CB	SER	411	116.517	36.026	34.224	1.00	9.23
3225	OG	SER	411	115.722	34.911	33.871	1.00	10.06
3226	C	SER	411	116.586	36.859	31.848	1.00	15.22

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3227	O	SER	411	117.744	36.915	31.431	1.00	22.78
3228	N	TYR	412	115.555	36.525	31.078	1.00	12.29
3229	CA	TYR	412	115.715	36.165	29.673	1.00	14.56
3230	CB	TYR	412	114.473	35.428	29.160	1.00	21.66
3231	CG	TYR	412	114.284	34.000	29.630	1.00	31.85
3232	CD1	TYR	412	113.510	33.110	28.884	1.00	25.46
3233	CE1	TYR	412	113.285	31.807	29.315	1.00	25.33
3234	CD2	TYR	412	114.837	33.544	30.829	1.00	33.63
3235	CE2	TYR	412	114.617	32.236	31.271	1.00	30.87
3236	CZ	TYR	412	113.837	31.377	30.508	1.00	30.43
3237	OH	TYR	412	113.589	30.095	30.941	1.00	25.14
3238	C	TYR	412	115.938	37.382	28.775	1.00	18.89
3239	O	TYR	412	116.473	37.252	27.672	1.00	21.47
3240	N	LEU	413	115.501	38.553	29.235	1.00	22.06
3241	CA	LEU	413	115.620	39.790	28.460	1.00	21.99
3242	CB	LEU	413	115.120	40.988	29.274	1.00	21.82
3243	CG	LEU	413	113.623	40.999	29.600	1.00	28.58
3244	CD1	LEU	413	113.286	42.192	30.481	1.00	24.87
3245	CD2	LEU	413	112.806	41.026	28.316	1.00	20.55
3246	C	LEU	413	117.008	40.081	27.901	1.00	23.58
3247	O	LEU	413	117.157	40.329	26.702	1.00	27.31
3248	N	GLY	414	118.018	40.041	28.764	1.00	17.88
3249	CA	GLY	414	119.376	40.309	28.324	1.00	19.54
3250	C	GLY	414	120.063	39.141	27.644	1.00	21.66
3251	O	GLY	414	121.088	39.319	26.981	1.00	32.10
3252	N	MET	415	119.500	37.947	27.804	1.00	20.71
3253	CA	MET	415	120.062	36.741	27.209	1.00	18.08
3254	CB	MET	415	119.440	35.504	27.850	1.00	15.67
3255	CG	MET	415	119.705	35.424	29.345	1.00	19.68
3256	SD	MET	415	118.883	34.052	30.144	1.00	21.56
3257	CE	MET	415	119.945	32.725	29.700	1.00	15.56
3258	C	MET	415	119.870	36.734	25.702	1.00	23.08
3259	O	MET	415	118.808	36.379	25.199	1.00	35.78
3260	N	LYS	416	120.930	37.112	24.996	1.00	32.44
3261	CA	LYS	416	120.953	37.207	23.538	1.00	38.05
3262	CB	LYS	416	122.360	37.608	23.090	1.00	47.08
3263	CG	LYS	416	122.865	38.875	23.776	1.00	61.44
3264	CD	LYS	416	124.358	39.084	23.581	1.00	67.69
3265	CE	LYS	416	124.846	40.273	24.399	1.00	67.49
3266	NZ	LYS	416	126.319	40.457	24.297	1.00	75.93
3267	C	LYS	416	120.486	35.970	22.767	1.00	39.94
3268	O	LYS	416	120.113	36.070	21.597	1.00	44.84
3269	N	SER	417	120.493	34.813	23.422	1.00	39.76
3270	CA	SER	417	120.071	33.571	22.780	1.00	39.16
3271	CB	SER	417	120.900	32.398	23.304	1.00	38.83
3272	OG	SER	417	122.282	32.610	23.076	1.00	46.53
3273	C	SER	417	118.581	33.270	22.956	1.00	40.99
3274	O	SER	417	118.040	32.385	22.289	1.00	41.33
3275	N	ALA	418	117.925	34.005	23.853	1.00	38.28
3276	CA	ALA	418	116.501	33.814	24.122	1.00	31.24
3277	CB	ALA	418	116.087	34.610	25.348	1.00	30.62
3278	C	ALA	418	115.628	34.186	22.930	1.00	31.48
3279	O	ALA	418	115.674	35.317	22.440	1.00	35.02
3280	N	THR	419	114.841	33.219	22.468	1.00	27.95
3281	CA	THR	419	113.942	33.409	21.332	1.00	26.20
3282	CB	THR	419	113.996	32.197	20.370	1.00	26.76
3283	OG1	THR	419	113.511	31.027	21.039	1.00	27.32
3284	CG2	THR	419	115.424	31.945	19.901	1.00	18.56
3285	C	THR	419	112.502	33.595	21.806	1.00	30.31
3286	O	THR	419	112.241	33.693	23.005	1.00	33.17
3287	N	GLU	420	111.573	33.662	20.857	1.00	35.12
3288	CA	GLU	420	110.158	33.818	21.183	1.00	39.51
3289	CB	GLU	420	109.349	34.179	19.935	1.00	46.05
3290	CG	GLU	420	108.972	35.653	19.828	1.00	51.65
3291	CD	GLU	420	108.013	36.104	20.919	1.00	54.36
3292	OE1	GLU	420	107.027	35.384	21.192	1.00	55.36
3293	OE2	GLU	420	108.245	37.186	21.500	1.00	58.01
3294	C	GLU	420	109.620	32.527	21.781	1.00	37.05
3295	O	GLU	420	108.852	32.550	22.742	1.00	36.79
3296	N	GLN	421	110.050	31.404	21.215	1.00	37.04
3297	CA	GLN	421	109.624	30.090	21.676	1.00	33.78
3298	CB	GLN	421	110.218	28.999	20.792	1.00	40.49
3299	CG	GLN	421	109.711	29.009	19.363	1.00	57.72

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3300	CD	GLN	421	110.206	27.813	18.564	1.00	74.05
3301	OE1	GLN	421	110.596	26.786	19.128	1.00	68.24
3302	NE2	GLN	421	110.190	27.941	17.242	1.00	83.42
3303	C	GLN	421	109.999	29.826	23.128	1.00	31.12
3304	O	GLN	421	109.336	29.041	23.807	1.00	35.81
3305	N	ASP	422	111.071	30.466	23.592	1.00	27.52
3306	CA	ASP	422	111.527	30.304	24.971	1.00	25.90
3307	CB	ASP	422	112.963	30.821	25.137	1.00	25.75
3308	CG	ASP	422	113.985	29.971	24.396	1.00	29.11
3309	OD1	ASP	422	114.983	30.537	23.902	1.00	33.41
3310	OD2	ASP	422	113.800	28.736	24.311	1.00	32.66
3311	C	ASP	422	110.590	31.020	25.936	1.00	21.80
3312	O	ASP	422	110.282	30.502	27.011	1.00	19.43
3313	N	PHE	423	110.145	32.213	25.545	1.00	24.75
3314	CA	PHE	423	109.223	33.004	26.357	1.00	26.23
3315	CB	PHE	423	109.117	34.432	25.818	1.00	30.85
3316	CG	PHE	423	110.290	35.306	26.166	1.00	32.84
3317	CD1	PHE	423	111.336	35.482	25.268	1.00	34.61
3318	CD2	PHE	423	110.338	35.972	27.388	1.00	33.51
3319	CE1	PHE	423	112.412	36.312	25.579	1.00	30.52
3320	CE2	PHE	423	111.410	36.805	27.708	1.00	35.27
3321	CZ	PHE	423	112.448	36.974	26.801	1.00	23.59
3322	C	PHE	423	107.849	32.354	26.330	1.00	24.84
3323	O	PHE	423	107.106	32.392	27.311	1.00	31.10
3324	N	GLU	424	107.530	31.751	25.191	1.00	29.70
3325	CA	GLU	424	106.261	31.070	24.982	1.00	36.07
3326	CB	GLU	424	106.187	30.588	23.535	1.00	40.70
3327	CG	GLU	424	104.785	30.391	22.992	1.00	63.10
3328	CD	GLU	424	104.759	30.296	21.473	1.00	75.17
3329	OE1	GLU	424	105.781	29.898	20.867	1.00	75.10
3330	OE2	GLU	424	103.710	30.630	20.880	1.00	85.30
3331	C	GLU	424	106.164	29.892	25.949	1.00	31.83
3332	O	GLU	424	105.138	29.687	26.595	1.00	35.87
3333	N	TRP	425	107.258	29.148	26.066	1.00	29.46
3334	CA	TRP	425	107.339	27.999	26.958	1.00	23.86
3335	CB	TRP	425	108.680	27.285	26.753	1.00	25.55
3336	CG	TRP	425	108.991	26.265	27.803	1.00	29.41
3337	CD2	TRP	425	109.808	26.455	28.965	1.00	27.61
3338	CE2	TRP	425	109.779	25.249	29.697	1.00	24.31
3339	CE3	TRP	425	110.557	27.529	29.460	1.00	30.25
3340	CD1	TRP	425	108.521	24.984	27.871	1.00	28.89
3341	NE1	TRP	425	108.987	24.369	29.007	1.00	29.83
3342	CZ2	TRP	425	110.473	25.087	30.900	1.00	16.37
3343	CZ3	TRP	425	111.245	27.367	30.658	1.00	25.72
3344	CH2	TRP	425	111.196	26.154	31.363	1.00	19.53
3345	C	TRP	425	107.205	28.437	28.414	1.00	25.64
3346	O	TRP	425	106.523	27.792	29.213	1.00	26.99
3347	N	LEU	426	107.852	29.553	28.739	1.00	26.42
3348	CA	LEU	426	107.853	30.103	30.088	1.00	21.18
3349	CB	LEU	426	108.922	31.191	30.195	1.00	21.43
3350	CG	LEU	426	109.379	31.600	31.595	1.00	14.19
3351	CD1	LEU	426	110.106	30.441	32.251	1.00	14.14
3352	CD2	LEU	426	110.297	32.798	31.499	1.00	12.82
3353	C	LEU	426	106.504	30.664	30.523	1.00	23.80
3354	O	LEU	426	106.153	30.596	31.702	1.00	31.77
3355	N	SER	427	105.754	31.221	29.575	1.00	28.08
3356	CA	SER	427	104.444	31.802	29.871	1.00	30.28
3357	CB	SER	427	103.915	32.592	28.665	1.00	26.14
3358	OG	SER	427	103.742	31.763	27.528	1.00	29.08
3359	C	SER	427	103.406	30.773	30.325	1.00	29.36
3360	O	SER	427	102.497	31.099	31.088	1.00	31.12
3361	N	LYS	428	103.558	29.530	29.873	1.00	27.92
3362	CA	LYS	428	102.637	28.455	30.230	1.00	20.58
3363	CB	LYS	428	102.770	27.290	29.251	1.00	23.24
3364	CG	LYS	428	102.454	27.613	27.801	1.00	22.85
3365	CD	LYS	428	102.509	26.335	26.976	1.00	42.29
3366	CE	LYS	428	102.338	26.597	25.493	1.00	49.89
3367	NZ	LYS	428	102.345	25.316	24.727	1.00	62.04
3368	C	LYS	428	102.844	27.935	31.654	1.00	20.72
3369	O	LYS	428	102.183	26.980	32.067	1.00	29.09
3370	N	ASN	429	103.762	28.557	32.391	1.00	20.35
3371	CA	ASN	429	104.072	28.170	33.770	1.00	14.44
3372	CB	ASN	429	102.868	28.406	34.685	1.00	13.93

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3373	CG	ASN	429	102.581	29.876	34.910	1.00	21.29
3374	OD1	ASN	429	103.306	30.747	34.431	1.00	26.38
3375	ND2	ASN	429	101.522	30.159	35.657	1.00	28.12
3376	C	ASN	429	104.545	26.724	33.900	1.00	19.87
3377	O	ASN	429	103.831	25.868	34.426	1.00	27.89
3378	N	PRO	430	105.764	26.433	33.418	1.00	18.35
3379	CD	PRO	430	106.650	27.362	32.701	1.00	19.00
3380	CA	PRO	430	106.358	25.096	33.468	1.00	11.22
3381	CB	PRO	430	107.711	25.309	32.808	1.00	15.49
3382	CG	PRO	430	107.444	26.425	31.859	1.00	26.05
3383	C	PRO	430	106.518	24.612	34.902	1.00	17.61
3384	O	PRO	430	106.617	25.416	35.828	1.00	19.92
3385	N	LYS	431	106.569	23.294	35.073	1.00	18.71
3386	CA	LYS	431	106.699	22.681	36.389	1.00	14.83
3387	CB	LYS	431	106.682	21.157	36.256	1.00	15.08
3388	CG	LYS	431	106.353	20.409	37.539	1.00	26.85
3389	CD	LYS	431	106.103	18.937	37.244	1.00	41.27
3390	CE	LYS	431	105.561	18.195	38.455	1.00	49.80
3391	NZ	LYS	431	105.297	16.760	38.140	1.00	45.04
3392	C	LYS	431	107.959	23.137	37.121	1.00	19.80
3393	O	LYS	431	107.937	23.333	38.338	1.00	20.81
3394	N	ILE	432	109.051	23.316	36.380	1.00	15.93
3395	CA	ILE	432	110.306	23.757	36.979	1.00	16.86
3396	CB	ILE	432	111.497	23.632	35.994	1.00	20.40
3397	CG2	ILE	432	111.278	24.502	34.756	1.00	16.63
3398	CG1	ILE	432	112.804	23.985	36.709	1.00	14.19
3399	CD1	ILE	432	114.048	23.649	35.920	1.00	13.37
3400	C	ILE	432	110.182	25.187	37.499	1.00	17.42
3401	O	ILE	432	113.681	25.508	38.579	1.00	24.54
3402	N	LEU	433	109.488	26.035	36.742	1.00	15.09
3403	CA	LEU	433	109.277	27.420	37.146	1.00	14.83
3404	CB	LEU	433	108.728	28.245	35.978	1.00	13.49
3405	CG	LEU	433	108.378	29.708	36.272	1.00	10.45
3406	CD1	LEU	433	109.564	30.430	36.896	1.00	15.23
3407	CD2	LEU	433	107.939	30.400	34.993	1.00	9.30
3408	C	LEU	433	108.289	27.433	38.304	1.00	18.07
3409	O	LEU	433	108.481	28.140	39.295	1.00	21.14
3410	N	GLU	434	107.245	26.621	38.173	1.00	21.38
3411	CA	GLU	434	106.209	26.503	39.188	1.00	16.25
3412	CB	GLU	434	105.184	25.452	38.753	1.00	23.52
3413	CG	GLU	434	103.812	25.605	39.385	1.00	38.66
3414	CD	GLU	434	103.161	26.933	39.037	1.00	42.62
3415	OE1	GLU	434	102.828	27.148	37.851	1.00	32.73
3416	OE2	GLU	434	102.993	27.765	39.953	1.00	37.72
3417	C	GLU	434	106.850	26.095	40.511	1.00	14.12
3418	O	GLU	434	106.561	26.676	41.556	1.00	14.76
3419	N	ALA	435	107.753	25.120	40.440	1.00	17.75
3420	CA	ALA	435	108.465	24.610	41.610	1.00	16.67
3421	CB	ALA	435	109.303	23.410	41.214	1.00	8.83
3422	C	ALA	435	109.344	25.683	42.254	1.00	11.99
3423	O	ALA	435	109.372	25.827	43.477	1.00	7.99
3424	N	SER	436	110.057	26.435	41.422	1.00	15.97
3425	CA	SER	436	110.924	27.508	41.900	1.00	21.95
3426	CB	SER	436	111.636	28.163	40.713	1.00	24.20
3427	OG	SER	436	112.489	29.212	41.135	1.00	40.93
3428	C	SER	436	110.110	28.554	42.674	1.00	21.39
3429	O	SER	436	110.519	29.009	43.748	1.00	24.40
3430	N	VAL	437	108.951	28.912	42.125	1.00	18.68
3431	CA	VAL	437	108.054	29.889	42.739	1.00	8.95
3432	CB	VAL	437	106.855	30.188	41.818	1.00	11.54
3433	CG1	VAL	437	105.917	31.169	42.478	1.00	11.34
3434	CG2	VAL	437	107.339	30.734	40.486	1.00	5.44
3435	C	VAL	437	107.533	29.401	44.092	1.00	9.21
3436	O	VAL	437	107.452	30.176	45.048	1.00	12.18
3437	N	ILE	438	107.185	28.115	44.161	1.00	9.76
3438	CA	ILE	438	106.673	27.504	45.388	1.00	8.03
3439	CB	ILE	438	106.309	26.015	45.171	1.00	14.49
3440	CG2	ILE	438	105.931	25.380	46.500	1.00	10.62
3441	CG1	ILE	438	105.162	25.896	44.164	1.00	23.13
3442	CD1	ILE	438	104.753	24.468	43.853	1.00	31.20
3443	C	ILE	438	107.692	27.603	46.520	1.00	12.21
3444	O	ILE	438	107.349	27.982	47.639	1.00	18.63
3445	N	ILE	439	108.941	27.258	46.216	1.00	14.08

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3446	CA	ILE	439	110.033	27.307	47.188	1.00	9.89
3447	CB	ILE	439	111.369	26.901	46.525	1.00	12.54
3448	CG2	ILE	439	112.540	27.161	47.459	1.00	11.31
3449	CG1	ILE	439	111.321	25.424	46.136	1.00	2.00
3450	CD1	ILE	439	112.441	24.990	45.233	1.00	14.05
3451	C	ILE	439	110.152	28.706	47.783	1.00	9.52
3452	O	ILE	439	110.213	28.871	49.003	1.00	10.13
3453	N	CYS	440	110.135	29.714	46.918	1.00	8.13
3454	CA	CYS	440	110.233	31.098	47.361	1.00	12.62
3455	CB	CYS	440	110.267	32.036	46.153	1.00	5.84
3456	SG	CYS	440	110.449	33.774	46.599	1.00	11.97
3457	C	CYS	440	109.073	31.482	48.283	1.00	17.47
3458	O	CYS	440	109.264	32.175	49.287	1.00	18.40
3459	N	ARG	441	107.875	31.012	47.940	1.00	18.94
3460	CA	ARG	441	106.669	31.296	48.714	1.00	11.76
3461	CB	ARG	441	105.433	30.810	47.949	1.00	10.60
3462	CG	ARG	441	104.093	31.083	48.629	1.00	6.45
3463	CD	ARG	441	103.718	32.559	48.590	1.00	19.08
3464	NE	ARG	441	104.454	33.353	49.571	1.00	23.16
3465	CZ	ARG	441	104.623	34.670	49.500	1.00	20.47
3466	NH1	ARG	441	104.108	35.353	48.489	1.00	12.16
3467	NH2	ARG	441	105.307	35.307	50.441	1.00	30.69
3468	C	ARG	441	106.716	30.637	50.089	1.00	17.00
3469	O	ARG	441	106.629	31.307	51.120	1.00	25.77
3470	N	VAL	442	106.858	29.317	50.086	1.00	22.16
3471	CA	VAL	442	106.920	28.518	51.306	1.00	22.25
3472	CB	VAL	442	107.112	27.032	50.959	1.00	23.82
3473	CG1	VAL	442	107.624	26.261	52.164	1.00	26.50
3474	CG2	VAL	442	105.796	26.450	50.471	1.00	31.37
3475	C	VAL	442	108.004	28.969	52.283	1.00	21.17
3476	O	VAL	442	107.765	29.058	53.488	1.00	25.05
3477	N	ILE	443	109.195	29.243	51.761	1.00	22.99
3478	CA	ILE	443	110.305	29.685	52.596	1.00	27.94
3479	CB	ILE	443	111.628	29.710	51.805	1.00	34.71
3480	CG2	ILE	443	112.721	30.396	52.612	1.00	32.63
3481	CG1	ILE	443	112.041	28.279	51.458	1.00	35.15
3482	CD1	ILE	443	113.322	28.183	50.669	1.00	41.45
3483	C	ILE	443	110.024	31.054	53.208	1.00	24.50
3484	O	ILE	443	110.253	31.263	54.400	1.00	25.69
3485	N	ASP	444	109.500	31.972	52.398	1.00	24.21
3486	CA	ASP	444	109.178	33.314	52.875	1.00	26.25
3487	CB	ASP	444	108.695	34.203	51.721	1.00	29.76
3488	CG	ASP	444	108.365	35.624	52.169	1.00	39.45
3489	OD1	ASP	444	109.179	36.535	51.910	1.00	45.87
3490	OD2	ASP	444	107.288	35.841	52.768	1.00	45.57
3491	C	ASP	444	108.103	33.247	53.952	1.00	28.37
3492	O	ASP	444	108.228	33.883	54.995	1.00	29.64
3493	N	ASP	445	107.061	32.458	53.700	1.00	30.42
3494	CA	ASP	445	105.950	32.318	54.637	1.00	32.30
3495	CB	ASP	445	104.797	31.544	53.994	1.00	33.98
3496	CG	ASP	445	104.151	32.302	52.838	1.00	37.92
3497	OD1	ASP	445	104.356	33.532	52.717	1.00	38.86
3498	OD2	ASP	445	103.429	31.662	52.047	1.00	28.07
3499	C	ASP	445	106.335	31.690	55.970	1.00	33.30
3500	O	ASP	445	105.762	32.030	57.009	1.00	42.91
3501	N	THR	446	107.302	30.778	55.946	1.00	33.28
3502	CA	THR	446	107.758	30.124	57.168	1.00	30.88
3503	CB	THR	446	108.625	28.887	56.855	1.00	26.02
3504	OG1	THR	446	107.873	27.969	56.050	1.00	21.99
3505	CG2	THR	446	109.046	28.188	58.143	1.00	25.74
3506	C	THR	446	108.570	31.110	58.014	1.00	32.83
3507	O	THR	446	108.459	31.131	59.238	1.00	33.61
3508	N	ALA	447	109.357	31.944	57.339	1.00	40.56
3509	CA	ALA	447	110.202	32.937	57.996	1.00	45.46
3510	CB	ALA	447	111.313	33.374	57.056	1.00	42.21
3511	C	ALA	447	109.434	34.155	58.468	1.00	46.97
3512	O	ALA	447	109.596	34.617	59.599	1.00	54.11
3513	N	THR	448	108.599	34.690	57.581	1.00	47.28
3514	CA	THR	448	107.832	35.884	57.879	1.00	46.44
3515	CB	THR	448	107.689	36.787	56.618	1.00	41.12
3516	OG1	THR	448	106.943	36.112	55.607	1.00	30.26
3517	CG2	THR	448	109.064	37.170	56.071	1.00	32.60
3518	C	THR	448	106.446	35.694	58.497	1.00	51.30

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3519	O	THR	448	105.708	36.657	58.620	1.00	53.69
3520	N	TYR	449	106.080	34.481	58.912	1.00	53.28
3521	CA	TYR	449	104.751	34.282	59.492	1.00	58.27
3522	CB	TYR	449	104.497	32.811	59.888	1.00	58.98
3523	CG	TYR	449	103.175	32.661	60.637	1.00	61.56
3524	CD1	TYR	449	101.973	33.066	60.055	1.00	66.72
3525	CE1	TYR	449	100.772	33.026	60.769	1.00	64.98
3526	CD2	TYR	449	103.147	32.198	61.957	1.00	62.94
3527	CE2	TYR	449	101.956	32.155	62.672	1.00	66.76
3528	CZ	TYR	449	100.773	32.575	62.080	1.00	67.45
3529	OH	TYR	449	99.601	32.590	62.810	1.00	73.04
3530	C	TYR	449	104.462	35.189	60.691	1.00	59.96
3531	O	TYR	449	103.576	36.051	60.638	1.00	60.11
3532	N	GLU	450	105.199	34.975	61.771	1.00	61.73
3533	CA	GLU	450	105.029	35.733	62.995	1.00	61.61
3534	CB	GLU	450	106.071	35.308	64.025	1.00	65.21
3535	CG	GLU	450	105.833	33.912	64.589	1.00	75.41
3536	CD	GLU	450	106.887	33.502	65.610	1.00	85.43
3537	OE1	GLU	450	107.416	34.375	66.331	1.00	91.32
3538	OE2	GLU	450	107.196	32.293	65.686	1.00	90.42
3539	C	GLU	450	105.026	37.251	62.841	1.00	59.86
3540	O	GLU	450	104.144	37.918	63.377	1.00	59.89
3541	N	VAL	451	105.995	37.787	62.098	1.00	61.44
3542	CA	VAL	451	106.092	39.234	61.873	1.00	63.11
3543	CB	VAL	451	107.408	39.596	61.116	1.00	64.01
3544	CG1	VAL	451	107.256	40.886	60.304	1.00	63.92
3545	CG2	VAL	451	108.541	39.761	62.123	1.00	71.39
3546	C	VAL	451	104.881	39.809	61.152	1.00	62.77
3547	O	VAL	451	104.336	40.841	61.555	1.00	65.95
3548	N	GLU	452	104.450	39.118	60.103	1.00	62.77
3549	CA	GLU	452	103.304	39.545	59.315	1.00	57.61
3550	CB	GLU	452	103.275	38.782	57.991	1.00	56.30
3551	CG	GLU	452	104.444	39.130	57.058	1.00	59.48
3552	CD	GLU	452	104.469	38.317	55.787	1.00	60.10
3553	OE1	GLU	452	104.787	38.899	54.728	1.00	62.60
3554	OE2	GLU	452	104.183	37.106	55.843	1.00	61.28
3555	C	GLU	452	101.984	39.392	60.081	1.00	56.17
3556	O	GLU	452	101.034	40.136	59.838	1.00	51.59
3557	N	LYS	453	101.946	38.486	61.040	1.00	58.80
3558	CA	LYS	453	100.753	38.241	61.858	1.00	58.04
3559	CB	LYS	453	100.863	36.913	62.611	1.00	59.76
3560	CG	LYS	453	99.644	36.565	63.453	1.00	60.02
3561	CD	LYS	453	99.925	35.384	64.366	1.00	58.67
3562	CE	LYS	453	98.732	35.093	65.262	1.00	61.72
3563	NZ	LYS	453	99.013	33.991	66.222	1.00	58.55
3564	C	LYS	453	100.584	39.385	62.863	1.00	57.99
3565	O	LYS	453	99.461	39.769	63.195	1.00	57.81
3566	N	SER	454	101.709	39.920	63.339	1.00	62.23
3567	CA	SER	454	101.712	41.026	64.295	1.00	61.09
3568	CB	SER	454	103.125	41.265	64.837	1.00	60.66
3569	OG	SER	454	103.548	40.191	65.654	1.00	66.36
3570	C	SER	454	101.185	42.311	63.665	1.00	58.28
3571	O	SER	454	100.632	43.163	64.360	1.00	56.27
3572	N	ARG	455	101.373	42.447	62.354	1.00	58.50
3573	CA	ARG	455	100.916	43.623	61.619	1.00	62.35
3574	CB	ARG	455	101.827	43.885	60.414	1.00	67.55
3575	CG	ARG	455	103.261	44.228	60.797	1.00	76.19
3576	CD	ARG	455	104.115	44.547	59.581	1.00	85.72
3577	NE	ARG	455	105.444	45.024	59.964	1.00	96.37
3578	CZ	ARG	455	106.292	45.634	59.140	1.00	100.00
3579	NH1	ARG	455	105.960	45.845	57.872	1.00	100.00
3580	NH2	ARG	455	107.470	46.051	59.587	1.00	99.29
3581	C	ARG	455	99.457	43.503	61.176	1.00	60.13
3582	O	ARG	455	98.922	44.399	60.519	1.00	58.35
3583	N	GLY	456	98.824	42.391	61.546	1.00	60.37
3584	CA	GLY	456	97.432	42.164	61.201	1.00	62.20
3585	C	GLY	456	97.183	41.378	59.925	1.00	67.18
3586	O	GLY	456	96.036	41.048	59.626	1.00	70.98
3587	N	GLN	457	98.238	41.091	59.166	1.00	69.31
3588	CA	GLN	457	98.108	40.340	57.917	1.00	68.54
3589	CB	GLN	457	99.397	40.438	57.089	1.00	69.51
3590	CG	GLN	457	99.764	41.859	56.671	1.00	74.48
3591	CD	GLN	457	101.105	41.941	55.965	1.00	78.04

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3592	OE1	GLN	457	102.099	41.389	56.428	1.00	87.45
3593	NE2	GLN	457	101.140	42.651	54.840	1.00	80.41
3594	C	GLN	457	97.755	38.879	58.197	1.00	66.56
3595	O	GLN	457	98.645	38.020	58.262	1.00	70.53
3596	N	ILE	458	96.475	38.616	58.384	1.00	64.43
3597	CA	ILE	458	95.976	37.272	58.664	1.00	60.84
3598	CB	ILE	458	94.652	37.317	59.458	1.00	62.21
3599	CG2	ILE	458	94.940	37.397	60.958	1.00	64.20
3600	CG1	ILE	458	93.769	38.462	58.943	1.00	60.42
3601	CD1	ILE	458	92.437	38.608	59.656	1.00	66.77
3602	C	ILE	458	95.768	36.440	57.403	1.00	55.84
3603	O	ILE	458	95.281	35.310	57.468	1.00	51.58
3604	N	ALA	459	96.145	37.005	56.259	1.00	58.27
3605	CA	ALA	459	96.011	36.318	54.979	1.00	56.90
3606	CB	ALA	459	95.609	37.305	53.888	1.00	56.20
3607	C	ALA	459	97.296	35.587	54.579	1.00	54.74
3608	O	ALA	459	97.434	35.158	53.433	1.00	54.48
3609	N	THR	460	98.236	35.455	55.513	1.00	49.39
3610	CA	THR	460	99.494	34.779	55.224	1.00	47.02
3611	CB	THR	460	100.603	35.180	56.200	1.00	50.43
3612	OG1	THR	460	100.077	35.259	57.532	1.00	52.34
3613	CG2	THR	460	101.194	36.507	55.781	1.00	56.05
3614	C	THR	460	99.399	33.264	55.164	1.00	45.28
3615	O	THR	460	98.566	32.651	55.832	1.00	47.09
3616	N	GLY	461	100.303	32.676	54.386	1.00	45.02
3617	CA	GLY	461	100.351	31.238	54.190	1.00	41.47
3618	C	GLY	461	100.107	30.318	55.367	1.00	38.12
3619	O	GLY	461	99.172	29.516	55.341	1.00	41.90
3620	N	ILE	462	100.962	30.399	56.380	1.00	36.28
3621	CA	ILE	462	100.825	29.545	57.552	1.00	41.08
3622	CB	ILE	462	101.954	29.813	58.580	1.00	34.80
3623	CG2	ILE	462	101.814	28.893	59.792	1.00	33.01
3624	CG1	ILE	462	103.319	29.613	57.917	1.00	21.22
3625	CD1	ILE	462	103.525	28.231	57.322	1.00	17.74
3626	C	ILE	462	99.444	29.683	58.197	1.00	47.74
3627	O	ILE	462	98.823	28.682	58.556	1.00	53.27
3628	N	GLU	463	98.940	30.915	58.266	1.00	49.04
3629	CA	GLU	463	97.626	31.178	58.852	1.00	46.29
3630	CB	GLU	463	97.358	32.687	58.929	1.00	44.06
3631	CG	GLU	463	96.076	33.063	59.677	1.00	51.03
3632	CD	GLU	463	96.101	32.673	61.150	1.00	55.15
3633	OE1	GLU	463	96.861	33.290	61.931	1.00	50.13
3634	OE2	GLU	463	95.348	31.752	61.529	1.00	55.86
3635	C	GLU	463	96.530	30.483	58.041	1.00	44.39
3636	O	GLU	463	95.690	29.774	58.600	1.00	47.37
3637	N	CYS	464	96.559	30.680	56.723	1.00	39.81
3638	CA	CYS	464	95.589	30.068	55.816	1.00	37.44
3639	CB	CYS	464	95.916	30.426	54.362	1.00	29.94
3640	SG	CYS	464	95.879	32.186	53.990	1.00	33.66
3641	C	CYS	464	95.630	28.556	55.973	1.00	39.78
3642	O	CYS	464	94.594	27.903	56.091	1.00	43.58
3643	N	CYS	465	96.846	28.016	55.995	1.00	44.06
3644	CA	CYS	465	97.072	26.583	56.133	1.00	43.89
3645	CB	CYS	465	98.568	26.275	56.009	1.00	39.41
3646	SG	CYS	465	98.961	24.513	55.936	1.00	40.79
3647	C	CYS	465	96.532	26.052	57.454	1.00	44.77
3648	O	CYS	465	95.883	25.004	57.490	1.00	43.29
3649	N	MET	466	96.788	26.794	58.530	1.00	50.46
3650	CA	MET	466	96.342	26.418	59.870	1.00	59.83
3651	CB	MET	466	96.838	27.429	60.916	1.00	58.39
3652	CG	MET	466	98.343	27.424	61.149	1.00	55.57
3653	SD	MET	466	98.825	28.416	62.560	1.00	56.88
3654	CE	MET	466	98.266	29.965	62.036	1.00	50.47
3655	C	MET	466	94.825	26.271	59.979	1.00	64.16
3656	O	MET	466	94.334	25.227	60.409	1.00	65.97
3657	N	ARG	467	94.094	27.319	59.598	1.00	67.84
3658	CA	ARG	467	92.631	27.320	59.654	1.00	69.35
3659	CB	ARG	467	92.083	28.744	59.512	1.00	75.34
3660	CG	ARG	467	92.397	29.655	60.684	1.00	84.97
3661	CD	ARG	467	91.640	30.965	60.560	1.00	96.41
3662	NE	ARG	467	92.020	31.944	61.578	1.00	100.00
3663	CZ	ARG	467	91.475	33.152	61.696	1.00	100.00
3664	NH1	ARG	467	90.515	33.541	60.862	1.00	100.00

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3665	NH2	ARG	467	91.901	33.982	62.639	1.00	100.00
3666	C	ARG	467	91.965	26.415	58.620	1.00	64.55
3667	O	ARG	467	90.863	25.907	58.853	1.00	66.78
3668	N	ASP	468	92.631	26.222	57.485	1.00	52.01
3669	CA	ASP	468	92.108	25.383	56.412	1.00	45.50
3670	CB	ASP	468	92.825	25.707	55.097	1.00	38.83
3671	CG	ASP	468	92.140	25.103	53.886	1.00	38.56
3672	OD1	ASP	468	92.817	24.928	52.852	1.00	35.49
3673	OD2	ASP	468	90.925	24.814	53.953	1.00	52.91
3674	C	ASP	468	92.201	23.882	56.718	1.00	49.65
3675	O	ASP	468	91.302	23.120	56.358	1.00	53.89
3676	N	TYR	469	93.271	23.469	57.397	1.00	48.30
3677	CA	TYR	469	93.475	22.059	57.740	1.00	47.34
3678	CB	TYR	469	94.887	21.611	57.345	1.00	49.69
3679	CG	TYR	469	95.110	21.555	55.851	1.00	50.72
3680	CD1	TYR	469	95.085	20.339	55.169	1.00	53.63
3681	CE1	TYR	469	95.255	20.284	53.787	1.00	51.76
3682	CD2	TYR	469	95.318	22.719	55.113	1.00	50.18
3683	CE2	TYR	469	95.489	22.675	53.732	1.00	50.61
3684	CZ	TYR	469	95.455	21.456	53.075	1.00	54.80
3685	OH	TYR	469	95.615	21.407	51.708	1.00	57.11
3686	C	TYR	469	93.230	21.743	59.215	1.00	46.62
3687	O	TYR	469	93.180	20.573	59.605	1.00	47.10
3688	N	GLY	470	93.069	22.788	60.026	1.00	43.51
3689	CA	GLY	470	92.837	22.610	61.449	1.00	43.21
3690	C	GLY	470	94.055	22.038	62.146	1.00	45.56
3691	O	GLY	470	93.952	21.077	62.912	1.00	44.25
3692	N	ILE	471	95.215	22.624	61.860	1.00	50.47
3693	CA	ILE	471	96.488	22.188	62.433	1.00	49.97
3694	CB	ILE	471	97.415	21.596	61.342	1.00	47.18
3695	CG2	ILE	471	96.844	20.285	60.811	1.00	47.32
3696	CG1	ILE	471	97.613	22.611	60.211	1.00	41.43
3697	CD1	ILE	471	98.427	22.094	59.049	1.00	46.18
3698	C	ILE	471	97.217	23.339	63.124	1.00	49.28
3699	O	ILE	471	96.894	24.508	62.907	1.00	49.58
3700	N	SER	472	98.204	23.000	63.949	1.00	49.04
3701	CA	SER	472	98.986	23.998	64.674	1.00	52.64
3702	CB	SER	472	99.748	23.340	65.829	1.00	54.48
3703	OG	SER	472	100.699	22.404	65.351	1.00	56.26
3704	C	SER	472	99.969	24.716	63.753	1.00	53.26
3705	O	SER	472	100.101	24.369	62.578	1.00	53.95
3706	N	THR	473	100.650	25.725	64.292	1.00	53.55
3707	CA	THR	473	101.634	26.491	63.531	1.00	54.18
3708	CB	THR	473	102.233	27.639	64.384	1.00	60.37
3709	OG1	THR	473	101.180	28.490	64.855	1.00	61.07
3710	CG2	THR	473	103.210	28.469	63.562	1.00	58.84
3711	C	THR	473	102.760	25.550	63.105	1.00	51.25
3712	O	THR	473	103.203	25.573	61.956	1.00	44.22
3713	N	LYS	474	103.173	24.697	64.038	1.00	49.57
3714	CA	LYS	474	104.236	23.722	63.821	1.00	51.50
3715	CB	LYS	474	104.440	22.903	65.098	1.00	55.84
3716	CG	LYS	474	105.605	21.930	65.063	1.00	60.97
3717	CD	LYS	474	105.778	21.266	66.421	1.00	66.81
3718	CE	LYS	474	107.011	20.382	66.482	1.00	71.89
3719	NZ	LYS	474	107.261	19.853	67.832	1.00	72.76
3720	C	LYS	474	103.924	22.797	62.646	1.00	53.47
3721	O	LYS	474	104.759	22.603	61.759	1.00	56.55
3722	N	GLU	475	102.712	22.249	62.637	1.00	54.30
3723	CA	GLU	475	102.271	21.342	61.578	1.00	54.12
3724	CB	GLU	475	100.921	20.719	61.946	1.00	49.93
3725	CG	GLU	475	100.940	19.925	63.244	1.00	54.09
3726	CD	GLU	475	99.559	19.471	63.673	1.00	56.55
3727	OE1	GLU	475	99.055	18.476	63.111	1.00	59.40
3728	OE2	GLU	475	98.977	20.109	54.577	1.00	54.88
3729	C	GLU	475	102.170	22.043	60.224	1.00	48.29
3730	O	GLU	475	102.514	21.485	59.192	1.00	43.53
3731	N	ALA	476	101.706	23.291	60.240	1.00	47.85
3732	CA	ALA	476	101.556	24.085	59.023	1.00	48.40
3733	CB	ALA	476	100.857	25.400	59.335	1.00	44.20
3734	C	ALA	476	102.906	24.348	58.367	1.00	45.69
3735	O	ALA	476	103.043	24.246	57.148	1.00	40.88
3736	N	MET	477	103.897	24.690	59.185	1.00	46.31
3737	CA	MET	477	105.241	24.956	58.687	1.00	47.60

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3738	CB	MET	477	106.097	25.600	59.777	1.00	41.69
3739	CG	MET	477	105.533	26.906	60.286	1.00	40.46
3740	SD	MET	477	106.643	27.743	61.402	1.00	51.90
3741	CE	MET	477	106.373	29.438	60.922	1.00	53.11
3742	C	MET	477	105.882	23.659	58.213	1.00	47.15
3743	O	MET	477	106.580	23.637	57.196	1.00	43.34
3744	N	ALA	478	105.617	22.580	58.948	1.00	44.29
3745	CA	ALA	478	106.146	21.262	58.617	1.00	43.92
3746	CB	ALA	478	105.808	20.264	59.716	1.00	37.80
3747	C	ALA	478	105.601	20.732	57.272	1.00	43.29
3748	O	ALA	478	106.312	20.127	56.509	1.00	44.64
3749	N	LYS	479	104.346	21.116	56.981	1.00	45.34
3750	CA	LYS	479	103.736	20.723	55.715	1.00	50.82
3751	CB	LYS	479	102.214	20.847	55.762	1.00	57.75
3752	CG	LYS	479	101.555	20.268	54.522	1.00	65.44
3753	CD	LYS	479	100.167	20.814	54.286	1.00	68.93
3754	CE	LYS	479	99.651	20.332	52.943	1.00	68.91
3755	NZ	LYS	479	93.384	20.999	52.566	1.00	74.62
3756	C	LYS	479	104.283	21.581	54.581	1.00	47.22
3757	O	LYS	479	104.451	21.109	53.455	1.00	50.00
3758	N	PHE	480	104.526	22.854	54.878	1.00	43.15
3759	CA	PHE	480	105.076	23.776	53.894	1.00	41.41
3760	CB	PHE	480	105.089	25.204	54.443	1.00	41.63
3761	CG	PHE	480	103.894	26.021	54.033	1.00	44.23
3762	CD1	PHE	480	102.638	25.432	53.905	1.00	41.42
3763	CD2	PHE	480	104.026	27.379	53.756	1.00	39.25
3764	CE1	PHE	480	101.535	26.182	53.503	1.00	36.23
3765	CE2	PHE	480	102.929	28.136	53.353	1.00	32.42
3766	CZ	PHE	480	101.682	27.536	53.227	1.00	29.83
3767	C	PHE	480	106.485	23.334	53.515	1.00	41.98
3768	O	PHE	480	106.881	23.434	52.353	1.00	37.95
3769	N	GLN	481	107.229	22.824	54.495	1.00	41.79
3770	CA	GLN	481	108.585	22.342	54.256	1.00	41.10
3771	CB	GLN	481	109.238	21.868	55.559	1.00	39.98
3772	CG	GLN	481	109.603	22.993	56.513	1.00	47.39
3773	CD	GLN	481	110.507	24.034	55.870	1.00	56.58
3774	OE1	GLN	481	111.605	23.720	55.406	1.00	55.49
3775	NE2	GLN	481	110.042	25.279	55.834	1.00	58.30
3776	C	GLN	481	108.553	21.204	53.245	1.00	38.69
3777	O	GLN	481	109.386	21.148	52.340	1.00	37.55
3778	N	ASN	482	107.564	20.324	53.391	1.00	35.14
3779	CA	ASN	482	107.394	19.189	52.491	1.00	35.59
3780	CB	ASN	482	106.302	18.250	53.009	1.00	41.18
3781	CG	ASN	482	106.647	17.642	54.355	1.00	52.28
3782	OD1	ASN	482	107.756	17.148	54.560	1.00	53.57
3783	ND2	ASN	482	105.697	17.678	55.282	1.00	61.08
3784	C	ASN	482	107.057	19.657	51.081	1.00	32.00
3785	O	ASN	482	107.358	18.971	50.105	1.00	35.80
3786	N	MET	483	106.421	20.822	50.981	1.00	30.00
3787	CA	MET	483	106.063	21.391	49.687	1.00	29.42
3788	CB	MET	483	105.092	22.562	49.855	1.00	33.61
3789	CG	MET	483	103.693	22.173	50.303	1.00	33.22
3790	SD	MET	483	102.589	23.605	50.374	1.00	34.18
3791	CE	MET	483	102.294	23.881	48.638	1.00	31.57
3792	C	MET	483	107.330	21.870	48.991	1.00	26.58
3793	O	MET	483	107.453	21.778	47.769	1.00	26.98
3794	N	ALA	484	108.267	22.386	49.782	1.00	24.14
3795	CA	ALA	484	109.539	22.874	49.261	1.00	20.18
3796	CB	ALA	484	110.260	23.687	50.323	1.00	15.48
3797	C	ALA	484	110.399	21.694	48.812	1.00	18.99
3798	O	ALA	484	111.070	21.762	47.777	1.00	18.13
3799	N	GLU	485	110.360	20.610	49.587	1.00	15.88
3800	CA	GLU	485	111.115	19.398	49.274	1.00	22.72
3301	CB	GLU	485	110.965	18.367	50.391	1.00	26.33
3802	CG	GLU	485	111.571	18.811	51.719	1.00	57.96
3803	CD	GLU	485	111.355	17.814	52.853	1.00	66.33
3804	OE1	GLU	485	110.840	16.702	52.602	1.00	74.62
3805	OE2	GLU	485	111.704	18.149	54.006	1.00	72.14
3806	C	GLU	485	110.625	18.806	47.962	1.00	19.07
3807	O	GLU	485	111.422	18.403	47.114	1.00	23.09
3808	N	THR	486	109.306	13.768	47.802	1.00	18.34
3809	CA	THR	486	108.680	18.247	46.594	1.00	13.68
3810	CB	THR	486	107.132	18.239	46.724	1.00	19.42

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3811	OG1	THR	486	106.740	17.320	47.753	1.00	18.34
3812	CG2	THR	486	106.474	17.832	45.409	1.00	7.13
3813	C	THR	486	109.084	19.126	45.418	1.00	12.40
3814	O	THR	486	109.432	18.628	44.347	1.00	12.64
3815	N	ALA	487	109.054	20.437	45.641	1.00	18.37
3816	CA	ALA	487	109.420	21.406	44.618	1.00	14.12
3817	CB	ALA	487	109.224	22.812	45.137	1.00	12.83
3818	C	ALA	487	110.863	21.195	44.178	1.00	11.72
3819	O	ALA	487	111.182	21.312	42.993	1.00	14.71
3820	N	TRP	488	111.731	20.860	45.128	1.00	11.21
3821	CA	TRP	488	113.129	20.616	44.801	1.00	9.48
3822	CB	TRP	488	113.985	20.541	46.061	1.00	2.00
3823	CG	TRP	488	114.586	21.864	46.394	1.00	10.22
3824	CD2	TRP	488	115.535	22.596	45.602	1.00	8.75
3825	CE2	TRP	488	115.798	23.807	46.279	1.00	8.09
3826	CE3	TRP	488	116.186	22.345	44.384	1.00	8.76
3827	CD1	TRP	488	114.322	22.636	47.488	1.00	2.81
3828	NE1	TRP	488	115.045	23.807	47.425	1.00	14.28
3829	CZ2	TRP	488	116.686	24.768	45.780	1.00	4.43
3830	CZ3	TRP	488	117.072	23.301	43.885	1.00	8.98
3831	CH2	TRP	488	117.312	24.497	44.585	1.00	9.72
3832	C	TRP	488	113.306	19.378	43.936	1.00	9.87
3833	O	TRP	488	114.112	19.380	43.005	1.00	11.24
3834	N	LYS	489	112.526	18.335	44.214	1.00	7.93
3835	CA	LYS	489	112.601	17.110	43.427	1.00	2.00
3836	CB	LYS	489	111.815	15.987	44.096	1.00	7.82
3837	CG	LYS	489	112.350	15.603	45.470	1.00	9.24
3838	CD	LYS	489	111.550	14.471	46.069	1.00	2.14
3839	CE	LYS	489	111.921	14.248	47.517	1.00	16.24
3840	NZ	LYS	489	111.056	13.208	48.146	1.00	26.26
3841	C	LYS	489	112.051	17.390	42.037	1.00	7.99
3842	O	LYS	489	112.480	16.784	41.055	1.00	11.24
3843	N	ASP	490	111.115	18.333	41.960	1.00	9.24
3844	CA	ASP	490	110.518	18.716	40.687	1.00	12.50
3845	CB	ASP	490	109.234	19.514	40.901	1.00	15.83
3846	CG	ASP	490	108.083	18.648	41.360	1.00	23.66
3847	OD1	ASP	490	107.949	17.509	40.856	1.00	20.17
3848	OD2	ASP	490	107.308	19.111	42.221	1.00	28.73
3849	C	ASP	490	111.501	19.522	39.856	1.00	11.20
3850	O	ASP	490	111.519	19.409	38.629	1.00	17.78
3851	N	ILE	491	112.308	20.345	40.523	1.00	16.49
3852	CA	ILE	491	113.311	21.149	39.831	1.00	15.96
3853	CB	ILE	491	113.973	22.183	40.766	1.00	14.10
3854	CG2	ILE	491	115.138	22.870	40.058	1.00	17.39
3855	CG1	ILE	491	112.938	23.221	41.209	1.00	20.61
3856	CD1	ILE	491	113.493	24.319	42.097	1.00	6.59
3857	C	ILE	491	114.372	20.207	39.279	1.00	11.72
3858	O	ILE	491	114.802	20.342	38.132	1.00	18.27
3859	N	ASN	492	114.744	19.217	40.084	1.00	9.30
3860	CA	ASN	492	115.739	18.232	39.684	1.00	8.49
3861	CB	ASN	492	116.078	17.320	40.866	1.00	8.53
3862	CG	ASN	492	116.793	18.062	41.986	1.00	2.00
3863	OD1	ASN	492	117.444	19.081	41.756	1.00	2.00
3864	ND2	ASN	492	116.674	17.554	43.204	1.00	9.30
3865	C	ASN	492	115.296	17.421	38.458	1.00	6.69
3866	O	ASN	492	116.120	17.067	37.618	1.00	15.10
3867	N	GLU	493	113.994	17.157	38.345	1.00	11.11
3868	CA	GLU	493	113.452	16.420	37.203	1.00	6.79
3869	CB	GLU	493	112.036	15.929	37.490	1.00	14.43
3870	CG	GLU	493	111.966	14.681	38.344	1.00	35.11
3871	CD	GLU	493	110.554	14.143	38.504	1.00	39.54
3872	OE1	GLU	493	109.669	14.505	37.695	1.00	36.96
3873	OE2	GLU	493	110.335	13.345	39.441	1.00	44.74
3874	C	GLU	493	113.420	17.284	35.947	1.00	15.20
3875	O	GLU	493	113.539	16.777	34.828	1.00	19.79
3876	N	GLY	494	113.234	18.588	36.140	1.00	15.92
3877	CA	GLY	494	113.176	19.512	35.021	1.00	13.61
3878	C	GLY	494	114.488	19.613	34.276	1.00	18.91
3879	O	GLY	494	114.507	19.822	33.061	1.00	23.19
3880	N	LEU	495	115.583	19.437	35.008	1.00	18.93
3881	CA	LEU	495	116.927	19.508	34.445	1.00	18.10
3882	CB	LEU	495	117.955	19.662	35.571	1.00	12.15
3883	CG	LEU	495	117.764	20.846	36.527	1.00	11.37

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3884	CD1	LEU	495	118.788	20.781	37.650	1.00	2.00
3885	CD2	LEU	495	117.866	22.164	35.771	1.00	6.14
3886	C	LEU	495	117.279	18.289	33.593	1.00	21.97
3887	O	LEU	495	118.146	18.366	32.717	1.00	20.13
3888	N	LEU	496	116.602	17.171	33.849	1.00	21.91
3889	CA	LEU	496	116.851	15.931	33.118	1.00	15.41
3890	CB	LEU	496	116.126	14.760	33.784	1.00	8.37
3891	CG	LEU	496	116.604	14.435	35.204	1.00	10.05
3892	CD1	LEU	496	115.819	13.269	35.769	1.00	2.00
3893	CD2	LEU	496	118.094	14.121	35.206	1.00	5.54
3894	C	LEU	496	116.492	16.017	31.641	1.00	14.28
3895	O	LEU	496	115.471	16.593	31.269	1.00	19.94
3896	N	ARG	497	117.360	15.454	30.808	1.00	16.05
3897	CA	ARG	497	117.184	15.456	29.359	1.00	18.50
3898	CB	ARG	497	118.516	15.107	28.682	1.00	19.50
3899	CG	ARG	497	119.665	16.035	29.066	1.00	28.42
3900	CD	ARG	497	121.024	15.363	28.908	1.00	24.39
3901	NE	ARG	497	121.803	15.905	27.797	1.00	27.16
3902	CZ	ARG	497	122.978	16.517	27.927	1.00	26.59
3903	NH1	ARG	497	123.525	16.677	29.125	1.00	14.53
3904	NH2	ARG	497	123.618	16.955	26.850	1.00	32.59
3905	C	ARG	497	116.099	14.471	28.922	1.00	23.25
3906	O	ARG	497	115.890	13.441	29.566	1.00	25.86
3907	N	PRO	498	115.369	14.793	27.838	1.00	22.25
3908	CD	PRO	498	114.524	13.808	27.150	1.00	25.52
3909	CA	PRO	498	115.491	16.003	27.017	1.00	25.55
3910	CB	PRO	498	114.781	15.612	25.715	1.00	17.40
3911	CG	PRO	498	114.819	14.122	25.715	1.00	25.69
3912	C	PRO	498	114.785	17.192	27.662	1.00	28.98
3913	O	PRO	498	113.609	17.104	28.021	1.00	33.06
3914	N	THR	499	115.506	18.299	27.804	1.00	24.14
3915	CA	THR	499	114.949	19.511	28.391	1.00	15.92
3916	CB	THR	499	116.070	20.473	28.835	1.00	16.49
3917	OG1	THR	499	116.946	20.735	27.730	1.00	6.47
3918	CG2	THR	499	116.870	19.862	29.983	1.00	10.26
3919	C	THR	499	114.043	20.205	27.374	1.00	19.26
3920	O	THR	499	114.329	20.205	26.174	1.00	30.87
3921	N	PRO	500	112.919	20.776	27.836	1.00	16.60
3922	CD	PRO	500	112.472	20.794	29.239	1.00	9.65
3923	CA	PRO	500	111.959	21.473	26.971	1.00	19.15
3924	CB	PRO	500	110.870	21.907	27.954	1.00	16.41
3925	CG	PRO	500	111.599	22.004	29.267	1.00	14.64
3926	C	PRO	500	112.569	22.656	26.213	1.00	26.43
3927	O	PRO	500	112.131	23.001	25.111	1.00	28.97
3928	N	VAL	501	113.580	23.266	26.824	1.00	27.74
3929	CA	VAL	501	114.317	24.393	26.253	1.00	27.33
3930	CB	VAL	501	113.874	25.749	26.867	1.00	25.49
3931	CG1	VAL	501	112.495	26.136	26.367	1.00	27.78
3932	CG2	VAL	501	113.880	25.675	28.386	1.00	25.11
3933	C	VAL	501	115.792	24.149	26.572	1.00	27.50
3934	O	VAL	501	116.118	23.190	27.268	1.00	34.26
3935	N	SER	502	116.685	24.991	26.059	1.00	27.56
3936	CA	SER	502	118.111	24.821	26.336	1.00	26.62
3937	CB	SER	502	118.942	25.802	25.513	1.00	31.78
3938	OG	SER	502	118.853	25.497	24.133	1.00	55.84
3939	C	SER	502	118.407	25.000	27.823	1.00	30.86
3940	O	SER	502	117.759	25.801	28.505	1.00	31.25
3941	N	THR	503	119.387	24.247	28.318	1.00	31.45
3942	CA	THR	503	119.785	24.296	29.726	1.00	32.20
3943	CB	THR	503	121.008	23.389	29.989	1.00	33.25
3944	OG1	THR	503	120.732	22.067	29.511	1.00	46.44
3945	CG2	THR	503	121.316	23.320	31.478	1.00	33.35
3946	C	THR	503	120.119	25.722	30.162	1.00	25.43
3947	O	THR	503	119.955	26.087	31.331	1.00	17.17
3948	N	GLU	504	120.569	26.522	29.200	1.00	21.60
3949	CA	GLU	504	120.931	27.914	29.433	1.00	21.35
3950	CB	GLU	504	121.355	28.549	28.104	1.00	16.54
3951	CG	GLU	504	121.779	30.009	28.189	1.00	26.78
3952	CD	GLU	504	122.043	30.642	26.825	1.00	35.29
3953	OE1	GLU	504	121.832	29.971	25.789	1.00	38.25
3954	OE2	GLU	504	122.460	31.821	26.793	1.00	34.16
3955	C	GLU	504	119.747	28.680	30.028	1.00	20.56
3956	O	GLU	504	119.924	29.595	30.837	1.00	14.15

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
3957	N	PHE	505	118.541	28.251	29.665	1.00	18.81
3958	CA	PHE	505	117.320	28.896	30.126	1.00	15.87
3959	CB	PHE	505	116.330	28.995	28.966	1.00	13.36
3960	CG	PHE	505	116.892	29.710	27.769	1.00	20.57
3961	CD1	PHE	505	117.193	29.013	26.602	1.00	24.10
3962	CD2	PHE	505	117.183	31.070	27.831	1.00	20.76
3963	CE1	PHE	505	117.782	29.658	25.517	1.00	19.64
3964	CE2	PHE	505	117.772	31.724	26.754	1.00	25.52
3965	CZ	PHE	505	118.072	31.015	25.595	1.00	26.72
3966	C	PHE	505	116.675	28.274	31.358	1.00	15.98
3967	O	PHE	505	115.703	28.808	31.886	1.00	16.03
3968	N	LEU	506	117.232	27.162	31.829	1.00	16.47
3969	CA	LEU	506	116.712	26.492	33.018	1.00	10.03
3970	CB	LEU	506	116.774	24.972	32.856	1.00	19.45
3971	CG	LEU	506	115.962	24.330	31.729	1.00	25.84
3972	CD1	LEU	506	116.268	22.852	31.690	1.00	29.46
3973	CD2	LEU	506	114.473	24.557	31.928	1.00	24.50
3974	C	LEU	506	117.503	26.895	34.254	1.00	11.68
3975	O	LEU	506	116.967	26.926	35.365	1.00	15.18
3976	N	THR	507	118.781	27.210	34.054	1.00	10.27
3977	CA	THR	507	119.662	27.601	35.151	1.00	7.47
3978	CB	THR	507	121.108	27.838	34.671	1.00	10.86
3979	OG1	THR	507	121.492	26.798	33.762	1.00	20.06
3980	CG2	THR	507	122.058	27.824	35.852	1.00	2.66
3981	C	THR	507	119.181	28.824	35.936	1.00	10.65
3982	O	THR	507	119.229	28.821	37.167	1.00	14.58
3983	N	PRO	508	118.718	29.887	35.242	1.00	8.73
3984	CD	PRO	508	118.680	30.110	33.784	1.00	7.34
3985	CA	PRO	508	118.244	31.080	35.956	1.00	5.70
3986	CB	PRO	508	117.717	31.959	34.826	1.00	8.88
3987	CG	PRO	508	118.630	31.616	33.688	1.00	2.00
3988	C	PRO	508	117.141	30.742	36.955	1.00	16.13
3989	O	PRO	508	117.109	31.282	38.064	1.00	19.06
3990	N	ILE	509	116.254	29.831	36.555	1.00	12.82
3991	CA	ILE	509	115.149	29.390	37.401	1.00	7.60
3992	CB	ILE	509	114.201	28.444	36.635	1.00	13.85
3993	CG2	ILE	509	113.160	27.865	37.577	1.00	3.89
3994	CG1	ILE	509	113.533	29.189	35.477	1.00	8.63
3995	CD1	ILE	509	112.681	28.301	34.597	1.00	16.09
3996	C	ILE	509	115.723	28.657	38.604	1.00	10.09
3997	O	ILE	509	115.320	28.906	39.744	1.00	13.81
3998	N	LEU	510	116.670	27.759	38.335	1.00	10.69
3999	CA	LEU	510	117.347	26.983	39.376	1.00	8.28
4000	CB	LEU	510	118.381	26.047	38.738	1.00	13.30
4001	CG	LEU	510	119.429	25.349	39.612	1.00	10.83
4002	CD1	LEU	510	118.781	24.553	40.736	1.00	9.01
4003	CD2	LEU	510	120.267	24.444	38.728	1.00	2.40
4004	C	LEU	510	118.033	27.927	40.358	1.00	4.13
4005	O	LEU	510	117.860	27.806	41.570	1.00	2.43
4006	N	ASN	511	118.778	28.890	39.819	1.00	12.14
4007	CA	ASN	511	119.487	29.875	40.627	1.00	11.57
4008	CB	ASN	511	120.347	30.773	39.743	1.00	12.88
4009	CG	ASN	511	121.567	30.054	39.208	1.00	18.35
4010	OD1	ASN	511	122.137	29.196	39.881	1.00	15.86
4011	ND2	ASN	511	121.972	30.396	37.991	1.00	27.20
4012	C	ASN	511	118.553	30.710	41.487	1.00	11.23
4013	O	ASN	511	118.883	31.018	42.634	1.00	9.07
4014	N	LEU	512	117.387	31.058	40.941	1.00	13.33
4015	CA	LEU	512	116.393	31.837	41.683	1.00	8.79
4016	CB	LEU	512	115.168	32.131	40.814	1.00	13.75
4017	CG	LEU	512	115.255	33.332	39.865	1.00	12.09
4018	CD1	LEU	512	114.100	33.306	38.884	1.00	2.00
4019	CD2	LEU	512	115.256	34.623	40.667	1.00	2.00
4020	C	LEU	512	115.975	31.083	42.940	1.00	10.14
4021	O	LEU	512	115.810	31.682	44.002	1.00	13.04
4022	N	ALA	513	115.836	29.764	42.819	1.00	10.74
4023	CA	ALA	513	115.464	28.916	43.951	1.00	12.16
4024	CB	ALA	513	115.097	27.523	43.464	1.00	14.93
4025	C	ALA	513	116.621	28.842	44.947	1.00	13.31
4026	O	ALA	513	116.408	28.757	46.157	1.00	9.13
4027	N	ARG	514	117.846	28.879	44.424	1.00	19.25
4028	CA	ARG	514	119.048	28.834	45.253	1.00	17.40
4029	CB	ARG	514	120.294	28.644	44.382	1.00	14.56

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4030	CG	ARG	514	120.493	27.229	43.863	1.00	4.10
4031	CD	ARG	514	121.602	27.170	42.823	1.00	9.06
4032	NE	ARG	514	121.943	15.793	42.471	1.00	17.13
4033	CZ	ARG	514	122.653	25.434	41.403	1.00	16.59
4034	NH1	ARG	514	123.107	26.346	40.554	1.00	8.47
4035	NH2	ARG	514	122.929	24.154	41.197	1.00	15.58
4036	C	ARG	514	119.190	30.106	46.084	1.00	13.80
4037	O	ARG	514	119.522	30.051	47.270	1.00	10.51
4038	N	ILE	515	118.901	31.247	45.466	1.00	15.59
4039	CA	ILE	515	119.011	32.535	46.147	1.00	20.36
4040	CB	ILE	515	118.764	33.718	45.194	1.00	12.70
4041	CG2	ILE	515	119.221	35.007	45.851	1.00	25.50
4042	CG1	ILE	515	119.567	33.534	43.910	1.00	19.52
4043	CD1	ILE	515	119.220	34.523	42.828	1.00	29.86
4044	C	ILE	515	118.085	32.672	47.353	1.00	17.44
4045	O	ILE	515	118.477	33.257	48.359	1.00	19.69
4046	N	VAL	516	116.868	32.136	47.258	1.00	21.26
4047	CA	VAL	516	115.915	32.218	48.369	1.00	23.09
4048	CB	VAL	516	114.504	31.679	48.008	1.00	32.21
4049	CG1	VAL	516	113.444	32.441	48.787	1.00	27.43
4050	CG2	VAL	516	114.244	31.755	46.526	1.00	29.34
4051	C	VAL	516	116.424	31.382	49.535	1.00	20.11
4052	O	VAL	516	116.429	31.835	50.681	1.00	22.46
4053	N	GLU	517	116.833	30.154	49.229	1.00	21.26
4054	CA	GLU	517	117.352	29.230	50.231	1.00	23.87
4055	CB	GLU	517	117.859	27.949	49.555	1.00	24.13
4056	CG	GLU	517	116.765	27.008	49.049	1.00	27.64
4057	CD	GLU	517	116.153	26.132	50.143	1.00	36.07
4058	OE1	GLU	517	116.480	26.314	51.336	1.00	40.38
4059	OE2	GLU	517	115.338	25.248	49.804	1.00	38.38
4060	C	GLU	517	118.484	29.872	51.024	1.00	25.33
4061	O	GLU	517	118.488	29.840	52.255	1.00	28.96
4062	N	VAL	518	119.411	30.492	50.297	1.00	22.43
4063	CA	VAL	518	120.577	31.156	50.874	1.00	22.95
4064	CB	VAL	518	121.605	31.482	49.762	1.00	24.42
4065	CG1	VAL	518	122.767	32.289	50.313	1.00	23.12
4066	CG2	VAL	518	122.105	30.194	49.125	1.00	20.43
4067	C	VAL	518	120.239	32.436	51.649	1.00	24.42
4068	O	VAL	518	120.850	32.725	52.683	1.00	23.34
4069	N	THR	519	119.267	33.192	51.145	1.00	22.60
4070	CA	THR	519	118.846	34.443	51.769	1.00	20.24
4071	CB	THR	519	118.044	35.305	50.773	1.00	23.46
4072	OG1	THR	519	118.872	35.615	49.648	1.00	23.28
4073	CG2	THR	519	117.597	36.601	51.410	1.00	22.46
4074	C	THR	519	118.051	34.232	53.058	1.00	25.34
4075	O	THR	519	118.164	35.020	54.000	1.00	24.48
4076	N	TYR	520	117.261	33.162	53.105	1.00	30.17
4077	CA	TYR	520	116.461	32.848	54.290	1.00	34.43
4078	CB	TYR	520	115.017	32.528	53.892	1.00	35.49
4079	CG	TYR	520	114.238	33.696	53.330	1.00	32.60
4080	CD1	TYR	520	114.481	34.171	52.041	1.00	27.24
4081	CE1	TYR	520	113.758	35.242	51.520	1.00	34.38
4082	CD2	TYR	520	113.247	34.321	54.087	1.00	30.57
4083	CE2	TYR	520	112.516	35.392	53.577	1.00	22.83
4084	CZ	TYR	520	112.777	35.848	52.294	1.00	34.91
4085	OH	TYR	520	112.070	36.916	51.787	1.00	38.85
4086	C	TYR	520	117.047	31.663	55.058	1.00	37.02
4087	O	TYR	520	116.321	30.937	55.740	1.00	41.01
4088	N	ILE	521	118.361	31.483	54.956	1.00	39.45
4089	CA	ILE	521	119.048	30.380	55.621	1.00	41.53
4090	CB	ILE	521	120.561	30.363	55.251	1.00	34.97
4091	CG2	ILE	521	121.263	31.607	55.775	1.00	33.59
4092	CG1	ILE	521	121.228	29.087	55.770	1.00	32.90
4093	CD1	ILE	521	122.620	28.865	55.224	1.00	16.56
4094	C	ILE	521	118.841	30.384	57.140	1.00	51.61
4095	O	ILE	521	118.649	29.329	57.750	1.00	55.56
4096	N	HIS	522	118.840	31.573	57.737	1.00	57.98
4097	CA	HIS	522	118.634	31.715	59.176	1.00	63.52
4098	CB	HIS	522	119.500	32.851	59.730	1.00	73.38
4099	CG	HIS	522	120.971	32.581	59.659	1.00	84.65
4100	CD2	HIS	522	122.020	33.405	59.421	1.00	85.52
4101	ND1	HIS	522	121.508	31.324	59.848	1.00	37.86
4102	CE1	HIS	522	122.822	31.386	59.729	1.00	88.53

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4103	NE2	HIS	522	123.158	32.637	59.470	1.00	88.81
4104	C	HIS	522	117.159	31.977	59.482	1.00	63.87
4105	O	HIS	522	116.816	32.500	60.546	1.00	62.90
4106	N	ASN	523	116.300	31.606	58.534	1.00	61.66
4107	CA	ASN	523	114.850	31.771	58.635	1.00	60.61
4108	CB	ASN	523	114.273	30.822	59.691	1.00	60.04
4109	CG	ASN	523	112.807	30.509	59.453	1.00	59.80
4110	OD1	ASN	523	112.388	30.266	58.319	1.00	62.26
4111	ND2	ASN	523	112.021	30.510	60.522	1.00	59.58
4112	C	ASN	523	114.434	33.220	58.910	1.00	60.32
4113	O	ASN	523	113.481	33.486	59.649	1.00	55.47
4114	N	LEU	524	115.162	34.149	58.295	1.00	61.14
4115	CA	LEU	524	114.905	35.577	58.436	1.00	59.79
4116	CB	LEU	524	115.935	36.223	59.371	1.00	62.62
4117	CG	LEU	524	115.945	35.764	60.835	1.00	65.24
4118	CD1	LEU	524	117.147	36.347	61.567	1.00	65.21
4119	CD2	LEU	524	114.642	36.163	61.521	1.00	62.62
4120	C	LEU	524	114.966	36.235	57.065	1.00	59.79
4121	O	LEU	524	115.721	35.800	56.189	1.00	56.91
4122	N	ASP	525	114.156	37.274	56.882	1.00	62.76
4123	CA	ASP	525	114.100	38.006	55.620	1.00	59.59
4124	CB	ASP	525	112.987	39.055	55.670	1.00	58.10
4125	CG	ASP	525	112.641	39.608	54.302	1.00	60.27
4126	OD1	ASP	525	113.331	39.276	53.315	1.00	58.07
4127	OD2	ASP	525	111.660	40.374	54.210	1.00	64.63
4128	C	ASP	525	115.448	38.668	55.332	1.00	59.32
4129	O	ASP	525	115.753	39.740	55.854	1.00	63.36
4130	N	GLY	526	116.239	38.028	54.478	1.00	58.65
4131	CA	GLY	526	117.557	38.536	54.149	1.00	55.69
4132	C	GLY	526	117.641	39.797	53.316	1.00	53.62
4133	O	GLY	526	118.648	40.502	53.372	1.00	60.05
4134	N	TYR	527	116.607	40.085	52.534	1.00	51.88
4135	CA	TYR	527	116.617	41.285	51.702	1.00	55.73
4136	CB	TYR	527	115.648	41.119	50.545	1.00	55.31
4137	CG	TYR	527	115.562	42.295	49.598	1.00	57.45
4138	CD1	TYR	527	116.330	42.336	48.433	1.00	58.75
4139	CE1	TYR	527	116.193	43.375	47.518	1.00	59.49
4140	OD2	TYR	527	114.656	43.332	49.824	1.00	58.17
4141	CE2	TYR	527	114.511	44.373	48.917	1.00	56.67
4142	CZ	TYR	527	115.282	44.388	47.767	1.00	57.63
4143	OH	TYR	527	115.159	45.420	46.868	1.00	55.43
4144	C	TYR	527	116.266	42.524	52.517	1.00	58.54
4145	O	TYR	527	116.862	43.593	52.342	1.00	58.64
4146	N	THR	528	115.271	42.383	53.386	1.00	59.24
4147	CA	THR	528	114.855	43.486	54.238	1.00	59.20
4148	CB	THR	528	113.447	43.253	54.836	1.00	54.20
4149	OG1	THR	528	112.504	43.053	53.776	1.00	47.41
4150	CG2	THR	528	113.010	44.458	55.655	1.00	54.59
4151	C	THR	528	115.887	43.653	55.356	1.00	60.28
4152	O	THR	528	116.168	44.773	55.787	1.00	63.64
4153	N	HIS	529	116.464	42.533	55.792	1.00	61.45
4154	CA	HIS	529	117.484	42.512	56.842	1.00	66.52
4155	CB	HIS	529	116.984	41.721	58.060	1.00	66.73
4156	CG	HIS	529	115.652	42.169	58.576	1.00	71.41
4157	CD2	HIS	529	115.119	43.407	58.721	1.00	72.13
4158	ND1	HIS	529	114.688	41.286	59.010	1.00	74.46
4159	CE1	HIS	529	113.618	41.958	59.398	1.00	72.55
4160	NE2	HIS	529	113.856	43.248	59.232	1.00	70.77
4161	C	HIS	529	118.743	41.844	56.273	1.00	66.01
4162	O	HIS	529	119.005	40.665	56.528	1.00	68.54
4163	N	PRO	530	119.540	42.598	55.492	1.00	63.94
4164	CD	PRO	530	119.254	43.981	55.082	1.00	59.34
4165	CA	PRO	530	120.778	42.128	54.856	1.00	66.66
4166	CB	PRO	530	121.137	43.284	53.914	1.00	62.98
4167	CG	PRO	530	119.837	44.009	53.711	1.00	59.02
4168	C	PRO	530	121.952	41.819	55.784	1.00	70.87
4169	O	PRO	530	122.567	40.757	55.682	1.00	73.58
4170	N	GLU	531	122.248	42.762	56.676	1.00	73.21
4171	CA	GLU	531	123.365	42.683	57.621	1.00	73.20
4172	CB	GLU	531	123.107	43.597	58.822	1.00	75.84
4173	CG	GLU	531	124.335	43.811	59.703	1.00	84.33
4174	CD	GLU	531	124.108	44.832	60.799	1.00	87.41
4175	OE1	GLU	531	123.904	46.021	60.474	1.00	95.89

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4176	OE2	GLU	531	124.142	44.448	61.986	1.00	83.48
4177	C	GLU	531	123.843	41.312	58.106	1.00	71.16
4178	O	GLU	531	125.042	41.026	58.066	1.00	69.83
4179	N	GLU	532	122.923	40.470	58.563	1.00	69.84
4180	CA	GLU	532	123.299	39.151	59.064	1.00	69.95
4181	CB	GLU	532	122.239	38.621	60.028	1.00	76.12
4182	CG	GLU	532	122.200	39.350	61.360	1.00	90.10
4183	CD	GLU	532	121.231	38.719	62.343	1.00	99.66
4184	OE1	GLU	532	121.294	37.485	62.540	1.00	100.00
4185	OE2	GLU	532	120.407	39.460	62.922	1.00	100.00
4186	C	GLU	532	123.601	38.095	58.006	1.00	65.98
4187	O	GLU	532	124.484	37.257	58.202	1.00	65.68
4188	N	VAL	533	122.878	38.136	56.891	1.00	60.94
4189	CA	VAL	533	123.071	37.152	55.829	1.00	51.25
4190	CB	VAL	533	121.727	36.491	55.419	1.00	57.84
4191	CG1	VAL	533	121.983	35.305	54.492	1.00	49.96
4192	CG2	VAL	533	120.942	36.054	56.655	1.00	58.45
4193	C	VAL	533	123.741	37.704	54.574	1.00	44.33
4194	O	VAL	533	124.834	37.270	54.208	1.00	42.16
4195	N	LEU	534	123.085	38.662	53.925	1.00	37.63
4196	CA	LEU	534	123.590	39.249	52.687	1.00	27.92
4197	CB	LEU	534	122.499	40.068	52.002	1.00	24.48
4198	CG	LEU	534	121.258	39.299	51.554	1.00	25.70
4199	CD1	LEU	534	120.395	40.207	50.696	1.00	29.78
4200	CD2	LEU	534	121.657	38.064	50.769	1.00	19.34
4201	C	LEU	534	124.864	40.076	52.770	1.00	29.24
4202	O	LEU	534	125.661	40.069	51.834	1.00	31.85
4203	N	LYS	535	125.053	40.793	53.875	1.00	30.62
4204	CA	LYS	535	126.239	41.632	54.047	1.00	30.24
4205	CB	LYS	535	126.251	42.276	55.439	1.00	33.69
4206	CG	LYS	535	127.412	43.232	55.692	1.00	38.92
4207	CD	LYS	535	127.429	43.699	57.142	1.00	43.85
4208	CE	LYS	535	128.605	44.617	57.425	1.00	46.39
4209	NZ	LYS	535	128.657	45.016	58.861	1.00	46.21
4210	C	LYS	535	127.548	40.881	53.784	1.00	30.84
4211	O	LYS	535	128.328	41.286	52.918	1.00	28.96
4212	N	PRO	536	127.790	39.759	54.495	1.00	26.98
4213	CD	PRO	536	126.965	39.148	55.554	1.00	30.04
4214	CA	PRO	536	129.018	38.982	54.302	1.00	22.09
4215	CB	PRO	536	128.796	37.772	55.206	1.00	22.33
4216	CG	PRO	536	127.975	38.330	56.312	1.00	25.59
4217	C	PRO	536	129.213	38.551	52.853	1.00	23.63
4218	O	PRO	536	130.313	38.660	52.315	1.00	34.37
4219	N	HIS	537	128.137	38.082	52.226	1.00	21.41
4220	CA	HIS	537	128.180	37.635	50.836	1.00	16.74
4221	CB	HIS	537	126.812	37.108	50.393	1.00	17.36
4222	CG	HIS	537	126.392	35.849	51.086	1.00	26.82
4223	CD2	HIS	537	125.171	35.406	51.467	1.00	19.54
4224	ND1	HIS	537	127.289	34.872	51.465	1.00	20.86
4225	CE1	HIS	537	126.638	33.883	52.050	1.00	21.91
4226	NE2	HIS	537	125.351	34.182	52.064	1.00	18.99
4227	C	HIS	537	128.611	38.757	49.910	1.00	19.57
4228	O	HIS	537	129.477	38.569	49.060	1.00	24.18
4229	N	ILE	538	128.003	39.927	50.091	1.00	25.84
4230	CA	ILE	538	128.307	41.101	49.279	1.00	25.72
4231	CB	ILE	538	127.331	42.262	49.600	1.00	25.90
4232	CG2	ILE	538	127.739	43.536	48.856	1.00	21.31
4233	CG1	ILE	538	125.905	41.849	49.219	1.00	14.44
4234	CD1	ILE	538	124.847	42.872	49.559	1.00	19.77
4235	C	ILE	538	129.760	41.545	49.467	1.00	24.83
4236	O	ILE	538	130.419	41.957	46.510	1.00	17.63
4237	N	ILE	539	130.255	41.440	50.698	1.00	19.39
4238	CA	ILE	539	131.632	41.809	51.002	1.00	25.84
4239	CB	ILE	539	131.882	41.864	52.532	1.00	31.48
4240	CG2	ILE	539	133.375	41.923	52.835	1.00	28.38
4241	CG1	ILE	539	131.172	43.078	53.137	1.00	26.00
4242	CD1	ILE	539	131.381	43.224	54.633	1.00	28.00
4243	C	ILE	539	132.598	40.819	50.355	1.00	24.71
4244	O	ILE	539	133.587	41.218	49.742	1.00	30.21
4245	N	ASN	540	132.286	39.531	50.461	1.00	22.80
4246	CA	ASN	540	133.132	38.487	49.892	1.00	16.68
4247	CB	ASN	540	132.802	37.135	50.525	1.00	17.40
4248	CG	ASN	540	133.009	37.126	52.032	1.00	26.52

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4249	OD1	ASN	540	132.357	36.371	52.755	1.00	29.34
4250	ND2	ASN	540	133.918	37.969	52.511	1.00	25.48
4251	C	ASN	540	133.039	38.386	48.371	1.00	16.85
4252	O	ASN	540	133.933	37.832	47.733	1.00	18.60
4253	N	LEU	541	131.979	38.944	47.789	1.00	16.65
4254	CA	LEU	541	131.791	38.889	46.340	1.00	19.54
4255	CB	LEU	541	130.393	38.360	46.001	1.00	16.13
4256	CG	LEU	541	130.003	36.954	46.463	1.00	16.63
4257	CD1	LEU	541	128.588	36.662	46.017	1.00	9.71
4258	CD2	LEU	541	130.960	35.919	45.901	1.00	11.40
4259	C	LEU	541	132.016	40.198	45.585	1.00	22.24
4260	O	LEU	541	132.528	40.186	44.464	1.00	22.51
4261	N	LEU	542	131.642	41.321	46.192	1.00	23.86
4262	CA	LEU	542	131.774	42.619	45.531	1.00	27.26
4263	CB	LEU	542	130.392	43.266	45.412	1.00	30.85
4264	CG	LEU	542	129.374	42.454	44.608	1.00	33.63
4265	CD1	LEU	542	127.960	42.968	44.844	1.00	33.98
4266	CD2	LEU	542	129.741	42.505	43.137	1.00	30.60
4267	C	LEU	542	132.770	43.621	46.124	1.00	30.35
4268	O	LEU	542	133.102	44.615	45.474	1.00	32.15
4269	N	VAL	543	133.234	43.373	47.348	1.00	20.35
4270	CA	VAL	543	134.192	44.263	48.008	1.00	17.15
4271	CB	VAL	543	133.758	44.564	49.466	1.00	22.13
4272	CG1	VAL	543	134.761	45.485	50.147	1.00	18.99
4273	CG2	VAL	543	132.369	45.184	49.485	1.00	25.56
4274	C	VAL	543	135.608	43.670	48.012	1.00	20.12
4275	O	VAL	543	136.484	44.106	47.259	1.00	14.30
4276	N	ASP	544	135.813	42.667	48.860	1.00	22.55
4277	CA	ASP	544	137.102	41.999	48.992	1.00	17.64
4278	CB	ASP	544	137.183	41.240	50.326	1.00	10.56
4279	CG	ASP	544	137.103	42.164	51.532	1.00	22.81
4280	OD1	ASP	544	136.839	41.648	52.639	1.00	23.90
4281	OD2	ASP	544	137.313	43.390	51.385	1.00	33.46
4282	C	ASP	544	137.389	41.018	47.868	1.00	18.71
4283	O	ASP	544	136.548	40.191	47.517	1.00	20.02
4284	N	SER	545	138.590	41.116	47.310	1.00	23.60
4285	CA	SER	545	139.022	40.215	46.253	1.00	27.74
4286	CB	SER	545	139.900	40.957	45.243	1.00	27.70
4287	OG	SER	545	141.043	41.512	45.871	1.00	32.50
4288	C	SER	545	139.823	39.098	46.920	1.00	31.23
4289	O	SER	545	140.409	39.303	47.987	1.00	32.16
4290	N	ILE	546	139.816	37.913	46.317	1.00	30.36
4291	CA	ILE	546	140.558	36.780	40.863	1.00	33.30
4292	CB	ILE	546	140.281	35.475	46.072	1.00	33.46
4293	CG2	ILE	546	141.051	34.310	46.686	1.00	27.25
4294	CG1	ILE	546	138.783	35.165	46.072	1.00	27.20
4295	CD1	ILE	546	138.418	33.915	45.319	1.00	23.76
4296	C	ILE	546	142.041	37.113	46.765	1.00	35.94
4297	O	ILE	546	142.559	37.332	45.668	1.00	34.27
4298	N	LYS	547	142.708	37.200	47.913	1.00	37.96
4299	CA	LYS	547	144.131	37.518	47.929	1.00	45.36
4300	CB	LYS	547	144.581	37.989	49.318	1.00	53.18
4301	CG	LYS	547	144.193	37.086	50.476	1.00	62.91
4302	CD	LYS	547	144.627	37.709	51.796	1.00	73.57
4303	CE	LYS	547	144.241	36.839	52.982	1.00	81.58
4304	NZ	LYS	547	144.683	37.440	54.274	1.00	85.95
4305	C	LYS	547	144.986	36.359	47.425	1.00	43.05
4306	O	LYS	547	144.897	35.236	47.921	1.00	34.62
4307	N	ILE	548	145.778	36.648	46.396	1.00	45.90
4308	CA	ILE	548	146.656	35.666	45.771	1.00	45.52
4309	CB	ILE	548	147.148	36.170	44.394	1.00	41.81
4310	CG2	ILE	548	147.927	35.073	43.679	1.00	45.55
4311	CG1	ILE	548	145.951	36.603	43.540	1.00	39.14
4312	CD1	ILE	548	146.327	37.269	42.238	1.00	45.90
4313	C	ILE	548	147.856	35.342	46.659	1.00	48.55
4314	OT1	ILE	548	148.019	34.153	47.005	1.00	46.58
4315	OT2	ILE	548	148.606	36.278	47.012	1.00	59.90
4316	OH2	WAT	601	109.544	21.898	33.684	1.00	2.00
4317	OH2	WAT	602	132.108	38.577	42.342	1.00	3.74
4318	OH2	WAT	603	121.652	22.556	52.348	1.00	5.90
4319	OH2	WAT	604	136.076	10.222	44.594	1.00	31.07
4320	OH2	WAT	605	131.497	21.852	51.678	1.00	7.22
4321	OH2	WAT	606	128.656	14.200	45.316	1.00	17.90

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4322	OH2	WAT	607	124.677	19.198	47.081	1.00	15.60
4323	OH2	WAT	608	125.455	29.812	49.014	1.00	8.48
4324	OH2	WAT	609	105.474	36.871	39.547	1.00	9.05
4325	OH2	WAT	610	133.536	36.915	40.513	1.00	19.37
4326	OH2	WAT	611	126.730	22.375	41.980	1.00	17.96
4327	OH2	WAT	612	133.379	23.457	50.388	1.00	16.43
4328	OH2	WAT	613	136.836	31.698	39.273	1.00	23.48
4329	OH2	WAT	614	130.615	20.278	41.368	1.00	11.16
4330	OH2	WAT	615	127.633	29.682	51.807	1.00	16.49
4331	OH2	WAT	616	100.533	31.281	26.832	1.00	34.28
4332	OH2	WAT	617	121.692	21.167	34.150	1.00	25.91
4333	OH2	WAT	618	131.226	32.257	50.439	1.00	34.81
4334	OH2	WAT	619	88.365	35.120	57.147	1.00	33.73
4335	OH2	WAT	620	118.147	18.317	26.341	1.00	21.70
4336	OH2	WAT	621	113.190	8.087	35.703	1.00	36.62
4337	OH2	WAT	622	125.312	30.072	37.791	1.00	30.00
4338	OH2	WAT	623	92.432	24.852	50.099	1.00	25.65
4339	OH2	WAT	624	108.974	15.165	49.075	1.00	21.10
4340	OH2	WAT	625	135.431	14.884	45.393	1.00	46.74
4341	OH2	WAT	626	115.012	4.805	43.826	1.00	30.43
4342	OH2	WAT	627	88.415	44.463	58.820	1.00	30.86
4343	OH2	WAT	628	125.976	25.755	43.265	1.00	27.75
4344	OH2	WAT	629	117.921	5.153	51.682	1.00	34.87
4345	OH2	WAT	630	91.157	43.104	44.532	1.00	27.09
4346	OH2	WAT	631	114.902	63.428	42.828	1.00	30.49
4347	OH2	WAT	632	99.150	43.135	52.476	1.00	17.32
4348	OH2	WAT	633	116.849	14.286	50.256	1.00	20.41
4349	OH2	WAT	634	136.092	41.410	33.663	1.00	26.72
4350	OH2	WAT	635	104.683	23.377	25.808	1.00	36.55
4351	OH2	WAT	636	133.163	25.808	57.616	1.00	29.75
4352	OH2	WAT	637	130.650	30.337	40.643	1.00	11.08
4353	OH2	WAT	638	141.018	40.362	50.563	1.00	27.14
4354	OH2	WAT	639	126.744	19.348	30.510	1.00	20.69
4355	OH2	WAT	640	99.257	26.859	66.394	1.00	32.76
4356	OH2	WAT	641	107.042	13.044	38.812	1.00	37.53
4357	OH2	WAT	642	111.411	17.702	31.576	1.00	25.63
4358	OH2	WAT	643	136.247	16.841	49.081	1.00	26.74
4359	OH2	WAT	644	130.107	34.877	51.432	1.00	22.05
4360	OH2	WAT	645	131.572	27.845	36.507	1.00	33.61
4361	OH2	WAT	646	139.273	18.921	51.935	1.00	18.69
4362	OH2	WAT	647	102.180	34.258	26.188	1.00	38.28
4363	OH2	WAT	648	123.655	36.667	26.709	1.00	23.51
4364	OH2	WAT	649	126.661	35.233	55.363	1.00	32.41
4365	OH2	WAT	650	106.153	21.764	42.249	1.00	20.34
4366	OH2	WAT	651	135.834	34.833	30.691	1.00	52.17
4367	OH2	WAT	652	103.106	38.892	25.426	1.00	26.00
4368	OH2	WAT	653	140.880	35.431	50.226	1.00	26.45
4369	OH2	WAT	654	112.327	13.971	50.722	1.00	46.47
4370	OH2	WAT	655	142.876	32.708	49.617	1.00	38.19
4371	OH2	WAT	656	136.448	11.686	63.277	1.00	31.93
4372	OH2	WAT	657	128.522	28.120	35.575	1.00	25.65
4373	OH2	WAT	658	124.837	30.666	35.131	1.00	22.56
4374	OH2	WAT	659	130.833	34.205	29.481	1.00	42.51
4375	OH2	WAT	660	112.306	35.037	18.431	1.00	22.73
4376	OH2	WAT	661	121.695	49.220	48.983	1.00	34.50
4377	OH2	WAT	662	134.850	24.747	24.896	1.00	61.06
4378	OH2	WAT	663	120.492	22.780	56.510	1.00	33.74
4379	OH2	WAT	664	145.265	41.024	28.023	1.00	26.03
4380	OH2	WAT	665	92.325	61.829	41.100	1.00	63.45
4381	OH2	WAT	666	122.583	51.518	33.284	1.00	48.58
4382	OH2	WAT	667	134.126	51.766	45.296	1.00	19.94
4383	OH2	WAT	668	99.217	28.001	33.331	1.00	36.10
4384	OH2	WAT	669	116.117	48.969	45.889	1.00	27.24
4385	OH2	WAT	670	90.118	37.836	45.821	1.00	21.42
4386	OH2	WAT	671	140.530	43.280	48.000	1.00	25.45
4387	OH2	WAT	672	91.812	21.421	53.465	1.00	25.28
4388	OH2	WAT	673	133.156	24.02	49.442	1.00	44.64
4389	OH2	WAT	674	124.710	30.183	52.286	1.00	27.01
4390	OH2	WAT	675	108.046	22.156	30.804	1.00	29.23
4391	OH2	WAT	676	141.812	18.051	53.703	1.00	33.60
4392	OH2	WAT	677	122.438	4.780	34.061	1.00	22.75
4393	OH2	WAT	678	106.890	50.310	27.843	1.00	27.59
4394	OH2	WAT	679	99.813	44.123	49.703	1.00	35.15

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4395	OH2	WAT	680	114.424	25.540	53.859	1.00	59.82
4396	OH2	WAT	681	120.122	17.036	61.627	1.00	33.13
4397	OH2	WAT	682	123.491	39.726	28.595	1.00	39.84
4398	OH2	WAT	683	120.197	47.611	55.219	1.00	29.64
4399	OH2	WAT	684	103.132	41.401	52.472	1.00	31.67
4400	OH2	WAT	685	95.409	27.232	43.768	1.00	40.36
4401	OH2	WAT	686	93.494	47.869	47.074	1.00	41.27
4402	OH2	WAT	687	101.201	66.857	39.062	1.00	78.46
4403	OH2	WAT	688	117.640	29.026	61.987	1.00	47.48
4404	OH2	WAT	689	125.779	23.773	30.324	1.00	37.41
4405	OH2	WAT	690	118.394	14.351	39.712	1.00	8.48
4406	OH2	WAT	691	115.774	17.384	46.942	1.00	55.16
4407	OH2	WAT	692	125.846	32.742	40.650	1.00	30.56
4408	OH2	WAT	693	134.539	32.766	51.897	1.00	52.33
4409	OH2	WAT	694	132.231	24.088	46.766	1.00	63.16
4410	OH2	WAT	695	120.423	11.828	28.871	1.00	44.89
4411	OH2	WAT	696	109.529	18.849	35.510	1.00	41.86
4412	OH2	WAT	697	126.344	22.049	35.670	1.00	37.93
4413	OH2	WAT	698	140.761	46.564	40.929	1.00	36.10
4414	OH2	WAT	699	149.712	28.211	43.996	1.00	63.77
4415	OH2	WAT	700	122.788	19.483	59.019	1.00	46.07
4416	OH2	WAT	701	133.230	48.486	44.266	1.00	36.68
4417	OH2	WAT	702	121.294	17.890	56.388	1.00	45.00
4418	OH2	WAT	703	129.924	31.321	53.670	1.00	28.12
4419	OH2	WAT	704	130.041	22.759	34.128	1.00	58.80
4420	OH2	WAT	705	120.990	14.019	62.153	1.00	90.42
4421	OH2	WAT	706	144.565	20.274	60.540	1.00	57.31
4422	OH2	WAT	707	122.007	30.989	34.128	1.00	74.81
4423	OH2	WAT	708	136.782	18.854	45.912	1.00	38.89
4424	OH2	WAT	709	148.608	25.064	51.823	1.00	69.75
4425	OH2	WAT	710	129.546	23.547	49.088	1.00	59.55
4426	OH2	WAT	711	98.361	36.814	48.633	1.00	48.61
4427	OH2	WAT	712	135.173	8.831	61.117	1.00	57.62
4428	OH2	WAT	713	125.025	32.134	55.885	1.00	46.77
4429	OH2	WAT	714	109.222	19.287	57.955	1.00	58.38
4430	OH2	WAT	715	137.206	8.347	56.384	1.00	48.16
4431	OH2	WAT	716	105.467	21.522	45.303	1.00	55.42
4432	OH2	WAT	717	108.946	9.853	39.154	1.00	73.91
4433	OH2	WAT	718	96.255	23.880	48.000	1.00	73.23
4434	OH2	WAT	719	101.728	36.619	50.363	1.00	57.83
4435	OH2	WAT	720	116.536	13.569	56.095	1.00	62.99
4436	OH2	WAT	721	128.739	23.611	38.616	1.00	70.69
4437	OH2	WAT	722	126.664	3.370	36.233	1.00	79.09
4438	OH2	WAT	723	120.338	3.428	58.493	1.00	86.19
4439	OH2	WAT	724	132.490	26.185	26.764	1.00	67.03
4440	OH2	WAT	725	119.137	22.564	24.070	1.00	75.84
4441	OH2	WAT	726	98.004	28.038	42.458	1.00	72.19
4442	OH2	WAT	727	99.674	33.037	41.131	1.00	69.00
4443	OH2	WAT	728	113.394	11.413	52.820	1.00	69.11
4444	OH2	WAT	729	129.629	27.848	38.891	1.00	31.80
4445	OH2	WAT	730	138.391	3.193	36.697	1.00	88.33
4446	OH2	WAT	731	101.751	58.675	54.521	1.00	69.41
4447	OH2	WAT	732	146.260	39.908	45.702	1.00	71.98
4448	OH2	WAT	733	99.632	27.238	39.217	1.00	65.15
4449	OH2	WAT	734	139.029	16.241	44.768	1.00	76.36
4450	OH2	WAT	735	93.410	43.367	39.907	1.00	51.51
4451	OH2	WAT	736	99.833	50.411	52.960	1.00	40.10
4452	OH2	WAT	737	121.822	63.145	36.945	1.00	88.71
4453	OH2	WAT	738	123.231	52.111	47.051	1.00	59.41
4454	OH2	WAT	739	112.095	2.568	44.854	1.00	87.55
4455	OH2	WAT	740	105.823	21.588	32.912	1.00	65.78
4456	OH2	WAT	741	112.121	15.677	29.574	1.00	63.57
4457	OH2	WAT	742	116.006	23.098	23.234	1.00	66.58
4458	OH2	WAT	743	101.396	34.063	30.976	1.00	67.78
4459	OH2	WAT	744	105.307	25.170	29.199	1.00	41.04
4460	OH2	WAT	745	138.659	10.582	45.837	1.00	59.51
4461	OH2	WAT	746	114.904	60.800	37.648	1.00	51.77
4462	OH2	WAT	747	124.430	21.295	33.036	1.00	63.60
4463	OH2	WAT	748	107.809	9.528	45.664	1.00	96.91
4464	OH2	WAT	749	129.675	48.310	54.546	1.00	50.35
4465	OH2	WAT	750	104.938	42.943	50.401	1.00	73.99
4466	OH2	WAT	751	127.598	19.431	38.063	1.00	50.28
4467	OH2	WAT	752	107.804	42.960	53.690	1.00	100.00

TABLE 10-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase With Farnesyl Hydroxyphosphonate Bound

Atom	Atom Type	Residue	Residue #	X	Y	Z	OCC	B-factor
4468	OH2	WAT	753	106.996	46.067	52.208	1.00	80.89
4469	OH2	WAT	754	115.697	53.285	33.391	1.00	88.83
4470	OH2	WAT	755	107.557	43.929	23.164	1.00	97.00
4471	OH2	WAT	756	104.503	37.526	36.972	1.00	58.13
4472	MG	MG	757	105.326	36.717	53.406	1.00	29.00
4473	MG	MG	758	103.375	43.256	48.861	1.00	41.96
4474	MG	MG	759	106.905	43.906	51.594	1.00	60.57
4475	PA	HPH	900	106.514	40.269	50.769	1.00	64.84
4476	O1A	HPH	900	106.467	39.079	51.657	1.00	56.34
4477	O2A	HPH	900	106.738	41.560	51.467	1.00	62.50
4478	O3A	HPH	900	105.506	40.292	49.674	1.00	62.63
4479	O1	HPH	900	108.952	41.335	50.186	1.00	61.96
4480	C1	HPH	900	108.025	40.315	49.769	1.00	64.00
4481	C2	HPH	900	108.690	38.930	49.523	1.00	61.37
4482	C3	HPH	900	109.069	38.562	48.285	1.00	51.27
4483	C4	HPH	900	109.443	37.123	48.011	1.00	49.88
4484	C5	HPH	900	110.870	36.593	48.349	1.00	48.79
4485	C6	HPH	900	112.049	37.566	48.069	1.00	37.71
4486	C7	HPH	900	112.320	38.019	46.829	1.00	34.33
4487	C8	HPH	900	113.476	38.969	46.623	1.00	35.58
4488	C9	HPH	900	113.227	40.333	47.247	1.00	56.66
4489	C10	HPH	900	113.089	40.275	48.776	1.00	68.86
4490	C11	HPH	900	112.157	41.010	49.392	1.00	73.13
4491	C12	HPH	900	112.037	40.934	50.893	1.00	66.86
4492	C15	HPH	900	108.853	39.500	47.137	1.00	54.81
4493	C13	HPH	900	111.421	42.067	48.641	1.00	68.76
4494	C14	HPH	900	111.753	37.299	45.656	1.00	41.06

TABLE 11

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1	N	LEU	24	121.956	50.261	52.247	1.00	124.05
2	CA	LEU	24	122.946	50.852	53.202	1.00	125.60
3	C	LEU	24	124.286	50.797	52.493	1.00	125.95
4	O	LEU	24	125.338	50.615	53.099	1.00	126.05
5	CB	LEU	24	123.008	50.020	54.477	1.00	127.81
6	CG	LEU	24	121.748	50.062	55.337	1.00	127.97
7	CD1	LEU	24	121.898	49.121	56.526	1.00	126.52
8	CD2	LEU	24	121.487	51.490	55.822	1.00	127.81
9	1H	LEU	24	122.251	49.292	51.984	1.00	25.00
10	2H	LEU	24	121.021	50.239	52.677	1.00	25.00
11	3H	LEU	24	121.929	50.798	51.366	1.00	25.00
12	N	TRP	25	124.208	51.008	51.190	1.00	128.26
13	CA	TRP	25	125.348	50.953	50.308	1.00	126.64
14	C	TRP	25	125.910	52.322	49.937	1.00	128.50
15	O	TRP	25	127.131	52.480	49.824	1.00	130.12
16	CB	TRP	25	124.945	50.134	49.078	1.00	122.57
17	CG	TRP	25	124.537	48.725	49.460	1.00	116.55
18	CD1	TRP	25	123.263	48.214	49.513	1.00	111.25
19	CD2	TRP	25	125.407	47.685	49.877	1.00	114.36
20	NE1	TRP	25	123.302	46.911	49.947	1.00	109.76
21	CE2	TRP	25	124.612	46.556	50.178	1.00	113.64
22	CE3	TRP	25	126.801	47.577	50.036	1.00	114.01
23	CZ2	TRP	25	125.146	45.346	50.624	1.00	114.93
24	CZ3	TRP	25	127.340	46.387	50.476	1.00	112.58
25	CH2	TRP	25	126.515	45.282	50.767	1.00	114.08
26	H	TRP	25	123.358	51.275	50.804	1.00	25.00
27	HE1	TRP	25	122.575	46.258	50.073	1.00	25.00
28	N	GLY	26	125.028	53.306	49.785	1.00	129.69
29	CA	GLY	26	125.460	54.647	49.432	1.00	129.22
30	C	GLY	26	126.079	54.744	48.049	1.00	128.72
31	O	GLY	26	125.794	53.929	47.177	1.00	128.98
32	H	GLY	26	124.083	53.132	49.888	1.00	25.00
33	N	ASP	27	126.962	55.721	47.868	1.00	128.05

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
34	CA	ASP	27	127.635	55.946	46.589	1.00	126.16
35	C	ASP	27	128.786	54.971	46.340	1.00	122.14
36	O	ASP	27	129.641	55.215	45.485	1.00	121.90
37	CB	ASP	27	128.154	57.390	46.495	1.00	128.56
38	CG	ASP	27	127.036	58.414	46.382	1.00	129.57
39	OD1	ASP	27	126.092	58.200	45.590	1.00	129.32
40	OD2	ASP	27	127.109	59.446	47.083	1.00	128.42
41	H	ASP	27	127.188	56.294	48.627	1.00	25.00
42	N	GLN	28	128.786	53.863	47.075	1.00	117.67
43	CA	GLN	28	129.811	52.833	46.950	1.00	112.25
44	C	GLN	28	129.807	52.195	45.554	1.00	112.76
45	O	GLN	28	130.803	51.612	45.131	1.00	110.25
46	CB	GLN	28	129.581	51.764	48.025	1.00	106.94
47	CG	GLN	28	130.657	50.691	48.117	1.00	101.12
48	CD	GLN	28	130.380	49.637	49.179	1.00	99.15
49	OE1	GLN	28	131.021	48.585	49.199	1.00	98.20
50	NE2	GLN	28	129.431	49.911	50.072	1.00	95.39
51	H	GLN	28	128.073	53.736	47.724	1.00	25.00
52	1HE2	GLN	28	129.287	49.206	50.749	1.00	25.00
53	2HE2	GLN	28	128.922	50.738	50.067	1.00	25.00
54	N	PHE	29	128.696	52.349	44.833	1.00	116.96
55	CA	PHE	29	128.536	51.766	43.496	1.00	118.70
56	C	PHE	29	128.026	52.717	42.398	1.00	122.05
57	O	PHE	29	127.643	52.249	41.318	1.00	123.10
58	CB	PHE	29	127.570	50.572	43.539	1.00	114.02
59	CG	PHE	29	127.906	49.532	44.568	1.00	111.57
60	CD1	PHE	29	128.928	48.614	44.349	1.00	109.61
61	CD2	PHE	29	127.148	49.429	45.731	1.00	108.83
62	CE1	PHE	29	129.193	47.609	45.274	1.00	102.49
63	CE2	PHE	29	127.401	48.432	46.663	1.00	101.60
64	CZ	PHE	29	128.425	47.514	46.434	1.00	101.60
65	H	PHE	29	127.985	52.899	45.209	1.00	25.00
66	N	LEU	30	127.984	54.022	42.669	1.00	124.46
67	CA	LEU	30	127.509	55.009	41.689	1.00	127.15
68	C	LEU	30	128.208	54.874	40.335	1.00	128.12
69	O	LEU	30	127.578	54.916	39.277	1.00	126.56
70	CB	LEU	30	127.732	56.433	42.230	1.00	128.23
71	CG	LEU	30	127.357	57.672	41.388	1.00	129.74
72	CD1	LEU	30	126.987	58.843	42.316	1.00	126.98
73	CD2	LEU	30	128.437	58.089	40.428	1.00	126.72
74	H	LEU	30	128.261	54.333	43.538	1.00	25.00
75	N	SER	331	129.527	54.725	40.400	1.00	129.78
76	CA	SER	31	130.384	54.608	39.222	1.00	130.48
77	C	SER	31	131.618	53.722	39.458	1.00	129.14
78	O	SER	31	132.211	53.745	40.535	1.00	127.41
79	CB	SER	31	130.831	56.004	38.781	1.00	133.08
80	OG	SER	31	131.461	56.700	39.845	1.00	136.17
81	H	SER	31	129.890	54.673	41.303	1.00	25.00
82	HG	SER	31	130.880	56.771	40.611	1.00	25.00
83	N	PHE	32	132.004	52.973	38.423	1.00	127.29
84	CA	PHE	32	133.156	52.065	38.458	1.00	126.38
85	C	PHE	32	134.056	52.249	37.231	1.00	129.92
88	O	PHE	32	133.693	51.847	36.122	1.00	131.71
87	CB	PHE	32	132.683	50.601	38.531	1.00	120.86
88	CG	PHE	32	133.805	49.581	38.475	1.00	117.02
89	CD1	PHE	32	134.736	49.488	39.507	1.00	114.77
90	CD2	PHE	32	133.912	48.701	37.396	1.00	113.67
91	CE1	PHE	32	135.755	48.533	39.472	1.00	111.21
92	CE2	PHE	32	134.927	47.742	37.349	1.00	111.87
93	CZ	PHE	32	135.851	47.658	38.389	1.00	111.43
94	H	PHE	32	131.485	53.046	37.602	1.00	25.00
95	N	SER	33	135.219	52.861	37.434	1.00	129.98
96	CA	SER	33	136.179	53.082	36.355	1.00	128.55
97	C	SER	33	137.014	51.819	36.136	1.00	128.72
98	O	SER	33	137.973	51.561	36.865	1.00	128.38
99	CB	SER	33	137.079	54.277	36.684	1.00	130.20
100	OG	SER	33	137.554	54.211	38.019	1.00	130.89
101	H	SER	33	135.440	53.163	38.329	1.00	25.00
102	HG	SER	33	136.817	54.182	38.626	1.00	25.00
103	N	ILE	34	136.616	51.017	35.153	1.00	128.06
104	CA	ILE	34	137.313	49.773	34.842	1.00	127.26

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
105	C	ILE	34	138.715	50.001	34.268	1.00	123.81
106	O	ILE	34	138.869	50.556	33.177	1.00	132.56
107	CB	ILE	34	136.483	48.884	33.865	1.00	125.22
108	CG1	ILE	34	137.227	47.570	33.595	1.00	124.19
109	CG2	ILE	34	136.174	49.640	32.570	1.00	123.27
110	CD1	ILE	34	136.518	46.611	32.665	1.00	121.43
111	H	ILE	34	135.838	51.274	34.627	1.00	25.00
112	N	ASP	35	139.738	49.600	35.020	1.00	125.91
113	CA	ASP	35	141.105	49.749	34.548	1.00	120.92
114	C	ASP	35	141.437	48.728	33.464	1.00	116.38
115	O	ASP	35	141.993	47.661	33.726	1.00	115.56
116	CB	ASP	35	142.122	49.709	35.700	1.00	122.56
117	CG	ASP	35	141.780	48.684	36.761	1.00	123.82
118	OD1	ASP	35	141.342	47.566	36.414	1.00	129.46
119	OD2	ASP	35	141.952	49.002	37.955	1.00	123.01
120	H	ASP	35	139.577	49.234	35.909	1.00	25.00
121	N	ASN	36	141.017	49.067	32.254	1.00	111.08
122	CA	ASN	36	141.237	48.307	31.037	1.00	107.72
123	C	ASN	38	142.508	47.482	30.983	1.00	104.04
124	O	ASN	36	142.486	46.361	30.443	1.00	103.31
125	CB	ASN	36	141.160	49.215	29.783	1.00	108.78
126	CG	ASN	38	141.378	50.742	30.076	1.00	113.72
127	OD1	ASN	36	141.308	51.535	29.156	1.00	115.16
128	ND2	ASN	36	141.666	51.127	31.309	1.00	113.86
129	H	ASN	36	140.490	49.899	32.196	1.00	25.00
130	1HD2	ASN	36	141.642	52.070	31.558	1.00	25.00
131	2HD2	ASN	38	141.817	50.557	32.067	1.00	25.00
132	N	GLN	37	143.593	47.958	31.571	1.00	101.33
133	CA	GLN	37	144.857	47.226	31.576	1.00	97.84
134	C	GLN	37	144.752	45.887	32.306	1.00	91.48
135	O	GLN	37	145.120	44.848	31.756	1.00	87.36
138	CB	GLN	37	145.964	48.079	32.204	1.00	104.38
137	CG	GLN	37	147.329	47.907	31.541	1.00	109.27
138	CD	GLN	37	147.433	48.643	30.213	1.00	112.48
139	OE1	GLN	37	148.192	49.604	30.088	1.00	116.42
140	NE2	GLN	37	146.670	48.202	29.220	1.00	113.85
141	H	GLN	37	143.558	48.839	31.989	1.00	25.00
142	1HE2	GLN	37	146.735	48.687	28.371	1.00	25.00
143	2HE2	GLN	37	146.083	47.436	29.358	1.00	25.00
144	N	VAL	38	144.242	45.916	33.538	1.00	85.52
145	CA	VAL	38	144.092	44.702	34.337	1.00	79.25
146	C	VAL	38	143.148	43.731	33.634	1.00	77.63
147	O	VAL	38	143.416	42.529	33.568	1.00	78.06
148	CB	VAL	38	143.542	45.018	35.752	1.00	78.16
149	CG1	VAL	38	143.484	43.754	36.593	1.00	75.39
150	CG2	VAL	38	144.409	46.061	36.437	1.00	78.10
151	H	VAL	38	143.943	46.770	33.907	1.00	25.00
152	N	ALA	39	142.060	44.268	33.086	1.00	71.24
153	CA	ALA	39	141.071	43.463	32.379	1.00	66.46
154	C	ALA	39	141.694	42.736	31.191	1.00	65.26
155	O	ALA	39	141.519	41.527	31.038	1.00	59.37
156	CB	ALA	39	139.910	44.338	31.916	1.00	64.84
157	H	ALA	39	141.924	45.233	33.161	1.00	25.00
158	N	GLU	40	142.436	43.472	30.366	1.00	66.68
159	CA	GLU	40	143.086	42.896	29.190	1.00	69.85
160	C	GLU	40	144.107	41.828	29.559	1.00	66.85
161	O	GLU	40	144.233	40.818	28.859	1.00	65.59
162	CB	GLU	40	143.744	43.985	28.342	1.00	75.56
163	CG	GLU	40	142.752	44.836	27.560	1.00	89.79
164	CD	GLU	40	143.409	45.993	26.828	1.00	98.34
165	OE1	GLU	40	144.515	45.807	26.273	1.00	101.87
166	OE2	GLU	40	142.814	47.092	26.808	1.00	102.72
167	H	GLU	40	142.551	44.427	30.550	1.00	25.00
168	N	LYS	41	144.830	42.048	30.656	1.00	62.69
169	CA	LYS	41	145.821	41.079	31.112	1.00	60.33
170	C	LYS	41	145.081	39.798	31.478	1.00	56.90
171	O	LYS	41	145.440	38.707	31.024	1.00	56.12
172	CB	LYS	41	146.588	41.603	32.331	1.00	64.30
173	CG	LYS	41	147.689	40.655	32.802	1.00	70.61
174	CD	LYS	41	148.373	41.137	34.070	1.00	74.86
175	CE	LYS	41	149.449	40.152	34.505	1.00	79.07

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
176	NZ	LYS	41	150.138	40.584	35.753	1.00	86.06
177	H	LYS	41	144.700	42.879	31.160	1.00	25.00
178	1HZ	LYS	41	150.588	41.510	35.601	1.00	25.00
179	2HZ	LYS	41	149.443	40.661	36.524	1.00	25.00
180	3HZ	LYS	41	150.864	39.885	36.010	1.00	25.00
181	N	TYR	42	144.027	39.951	32.278	1.00	54.48
182	CA	TYR	42	143.200	38.831	32.712	1.00	49.46
183	C	TYR	42	142.687	38.048	31.508	1.00	49.51
184	O	TYR	42	142.886	36.837	31.418	1.00	46.83
185	CB	TYR	42	142.011	39.332	33.535	1.00	49.09
186	CG	TYR	42	142.316	39.665	34.981	1.00	51.81
187	CD1	TYR	42	143.609	39.555	35.498	1.00	55.25
188	CD2	TYR	42	141.297	40.067	35.844	1.00	51.34
189	CE1	TYR	42	143.873	39.836	36.843	1.00	60.63
190	CE2	TYR	42	141.548	40.347	37.180	1.00	51.18
191	CZ	TYR	42	142.832	40.231	37.677	1.00	57.44
192	OH	TYR	42	143.064	40.503	39.009	1.00	57.29
193	H	TYR	42	143.796	40.855	32.582	1.00	25.00
194	HH	TYR	42	142.245	40.765	39.435	1.00	25.00
195	N	ALA	43	142.067	38.756	30.568	1.00	48.90
196	CA	ALA	43	141.514	38.150	29.359	1.00	49.75
197	C	ALA	43	142.560	37.363	28.576	1.00	49.98
198	O	ALA	43	142.331	36.209	28.204	1.00	49.38
199	CB	ALA	43	140.897	39.223	28.477	1.00	46.66
200	H	ALA	43	141.980	39.722	30.693	1.00	25.00
201	N	GLN	44	143.711	37.987	22.344	1.00	52.04
202	CA	GLN	44	144.796	37.352	27.607	1.00	51.53
203	C	GLN	44	145.219	36.030	28.257	1.00	45.51
204	O	GLN	44	145.304	35.002	27.582	1.00	43.18
205	CB	GLN	44	145.994	38.299	27.506	1.00	58.59
206	CG	GLN	44	147.101	37.804	26.583	1.00	74.05
207	CD	GLN	44	148.364	38.649	26.658	1.00	84.03
208	OE1	GLN	44	148.343	39.734	27.132	1.00	90.02
209	NE2	GLN	44	149.475	38.092	26.167	1.00	84.98
210	H	GLN	44	143.837	38.900	28.677	1.00	25.00
211	1HE2	GLN	44	150.290	38.631	26.238	1.00	25.00
212	2HE2	GLN	44	149.438	37.187	25.820	1.00	25.00
213	N	GLU	45	145.468	36.047	29.565	1.00	40.03
214	CA	GLU	45	145.874	34.831	30.261	1.00	37.78
215	C	GLU	45	144.740	33.813	30.320	1.00	41.99
216	O	GLU	45	144.970	32.609	30.153	1.00	43.40
217	CB	GLU	45	146.374	35.134	31.673	1.00	38.09
218	CG	GLU	45	147.037	33.924	32.334	1.00	41.87
219	CD	GLU	45	147.595	34.209	33.718	1.00	52.34
220	OE1	GLU	45	147.678	35.393	34.116	1.00	58.77
221	OE2	GLU	45	147.962	33.235	34.409	1.00	53.14
222	H	GLU	45	145.372	36.890	30.064	1.00	25.00
223	N	ILE	46	143.521	34.296	30.553	1.00	38.09
224	CA	ILE	46	142.352	33.428	30.622	1.00	35.19
225	C	ILE	46	142.239	32.630	29.328	1.00	37.05
226	O	ILE	46	141.923	31.441	29.360	1.00	40.60
227	CB	ILE	46	141.054	34.236	30.886	1.00	33.29
228	CG1	ILE	46	140.992	34.650	32.357	1.00	25.99
229	CG2	ILE	46	139.817	33.420	30.528	1.00	33.03
230	CD1	ILE	46	139.889	35.630	32.667	1.00	27.20
231	H	ILE	46	143.414	35.255	30.675	1.00	25.00
232	N	GLU	47	142.548	33.263	28.199	1.00	37.32
233	CA	GLU	47	142.485	32.581	26.910	1.00	43.87
234	C	GLU	47	143.420	31.379	26.870	1.00	44.27
235	O	GLU	47	143.061	30.324	26.341	1.00	48.49
236	CB	GLU	47	142.817	33.537	25.765	1.00	50.83
237	CG	GLU	47	141.700	34.516	25.422	1.00	72.13
238	CD	GLU	47	140.408	33.833	24.970	1.00	80.45
239	OE1	GLU	47	140.440	32.643	24.577	1.00	82.39
240	OE2	GLU	47	139.353	34.501	25.001	1.00	87.14
241	H	GLU	47	142.813	34.208	28.233	1.00	25.00
242	N	ALA	48	144.610	31.538	27.444	1.00	41.56
243	CA	ALA	48	145.597	30.464	27.489	1.00	36.13
244	C	ALA	48	145.078	29.340	28.375	1.00	38.33
245	O	ALA	48	145.027	28.176	27.964	1.00	40.71
246	CB	ALA	48	146.917	30.990	28.031	1.00	33.18

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
247	H	ALA	48	144.824	32.404	27.853	1.00	25.00
248	N	LEU	49	144.662	29.708	29.583	1.00	37.02
249	CA	LEU	49	144.136	28.757	30.554	1.00	34.21
250	C	LEU	49	142.894	28.044	30.029	1.00	33.34
251	O	LEU	49	142.694	26.860	30.296	1.00	34.71
252	CB	LEU	49	143.816	29.477	31.862	1.00	32.92
253	OG	LEU	49	145.013	30.132	32.551	1.00	29.78
254	CD1	LEU	49	144.541	31.096	33.621	1.00	28.55
255	CD2	LEU	49	145.915	29.062	33.139	1.00	31.11
256	H	LEU	49	144.717	30.657	29.827	1.00	25.00
257	N	LYS	50	142.083	28.759	29.254	1.00	35.43
258	CA	LYS	50	140.858	28.208	28.681	1.00	36.99
259	C	LYS	50	141.193	27.105	27.687	1.00	39.13
260	O	LYS	50	140.643	26.004	27.762	1.00	39.46
261	CB	LYS	50	140.056	29.307	27.981	1.00	38.20
262	CG	LYS	50	138.670	28.882	27.520	1.00	37.82
263	CD	LYS	50	138.021	29.947	26.638	1.00	41.56
264	CE	LYS	50	137.926	31.297	27.341	1.00	44.73
265	NZ	LYS	50	137.282	32.342	26.489	1.00	40.08
266	H	LYS	50	142.323	29.682	29.055	1.00	25.00
267	1HZ	LYS	50	136.318	32.042	26.239	1.00	25.00
268	2HZ	LYS	50	137.245	33.240	27.012	1.00	25.00
269	3HZ	LYS	50	137.841	32.474	25.620	1.00	25.00
270	N	GLU	51	142.106	27.396	26.765	1.00	41.23
271	CA	GLU	51	142.516	26.419	25.762	1.00	44.62
272	C	GLU	51	143.174	25.226	26.446	1.00	42.95
273	O	GLU	51	142.931	24.073	26.091	1.00	43.13
274	CB	GLU	51	143.489	27.055	24.766	1.00	52.90
275	CG	GLU	51	143.846	26.162	23.581	1.00	70.21
276	CD	GLU	51	142.623	25.709	22.792	1.00	79.98
277	OE1	GW	51	141.917	26.575	22.226	1.00	86.16
278	OE2	GLU	51	142.368	24.486	22.739	1.00	81.08
279	H	GLU	51	142.510	28.293	26.751	1.00	25.00
280	N	GLN	52	143.965	25.514	27.471	1.00	48.21
281	CA	GLN	52	144.662	24.480	28.223	1.00	49.28
282	C	GLN	52	143.657	23.563	28.933	1.00	44.99
283	O	GLN	52	143.817	22.337	28.936	1.00	42.93
284	CB	GLN	52	145.609	25.138	29.230	1.00	51.94
285	CG	GLN	52	146.728	24.247	29.736	1.00	57.86
286	CD	GLN	52	147.655	24.973	30.696	1.00	61.66
287	OE1	GLN	52	147.719	26.205	30.711	1.00	53.55
288	NE2	GLN	52	148.372	24.211	31.511	1.00	66.48
289	H	GLN	52	144.095	26.453	27.720	1.00	25.00
290	1HE2	GLN	52	148.989	24.676	32.114	1.00	25.00
291	2HE2	GLN	52	148.283	23.237	31.480	1.00	25.00
292	N	THR	53	142.615	24.160	29.512	1.00	42.37
293	CA	THR	53	141.578	23.404	30.214	1.00	41.44
294	C	THR	53	140.753	22.584	29.220	1.00	40.96
295	O	THR	53	140.334	21.462	29.519	1.00	38.12
296	CB	THR	53	140.648	24.338	31.027	1.00	42.33
297	OG1	THR	53	141.420	25.054	32.001	1.00	42.93
298	OG2	THR	53	139.569	23.534	31.746	1.00	41.61
299	H	THR	53	142.537	25.134	29.467	1.00	25.00
300	HG1	THR	53	142.088	25.586	31.555	1.00	25.00
301	N	ARG	54	140.553	23.138	28.027	1.00	42.45
302	CA	ARG	54	139.802	22.461	26.9976	1.00	41.46
303	C	ARG	54	140.516	21.152	26.653	1.00	43.94
304	O	ARG	54	139.891	20.088	26.607	1.00	41.93
305	CB	ARG	54	139.731	23.344	25.727	1.00	43.17
306	CG	ARG	54	138.759	22.861	24.658	1.00	49.52
307	CD	ARG	54	138.792	23.763	23.428	1.00	55.06
308	NE	ARG	54	138.600	25.176	23.764	1.00	65.13
309	CZ	ARG	54	137.416	25.758	23.951	1.00	73.50
310	NH1	ARG	54	136.293	25.058	23.836	1.00	78.69
311	NH2	ARG	54	137.353	27.046	24.263	1.00	72.72
312	H	ARG	54	140.919	24.030	27.846	1.00	25.00
313	HE	ARG	54	139.400	25.734	23.857	1.00	25.00
314	1HH1	ARG	54	136.328	24.086	23.604	1.00	25.00
315	2HH1	ARG	54	135.410	25.505	23.976	1.00	25.00
316	1HH2	ARG	54	138.196	27.578	24.357	1.00	25.00
317	2HH2	ARG	54	136.466	27.484	24.403	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
318	N	SER	55	141.834	21.233	26.480	1.00	41.53
319	CA	SER	55	142.645	20.062	26.176	1.00	41.04
320	C	SER	55	142.550	19.010	27.284	1.00	42.34
321	O	SER	55	142.587	17.810	27.005	1.00	42.66
322	CB	SER	55	144.100	20.469	25.916	1.00	46.50
323	OG	SER	55	144.208	21.230	24.719	1.00	41.12
324	H	SER	55	142.280	22.107	26.538	1.00	25.00
325	HG	SER	55	143.898	20.704	23.977	1.00	25.00
326	N	MET	56	142.399	19.458	28.531	1.00	41.33
327	CA	MET	56	142.265	18.544	29.668	1.00	40.87
328	C	MET	56	141.003	17.703	29.501	1.00	43.46
329	O	MET	56	141.017	16.489	29.711	1.00	41.72
330	CB	MET	56	142.164	19.312	30.989	1.00	44.45
331	CG	MET	56	143.461	19.894	31.500	1.00	46.36
332	SD	MET	56	143.231	20.659	33.118	1.00	45.60
333	CE	MET	56	143.715	22.320	32.763	1.00	44.30
334	H	MET	56	142.383	20.426	28.690	1.00	25.00
335	N	LEU	57	139.910	18.365	29.132	1.00	42.82
336	CA	LEU	57	138.632	17.696	28.929	1.00	41.38
337	C	LEU	57	138.684	16.700	27.779	1.00	43.36
338	O	LEU	57	138.042	15.653	27.831	1.00	45.75
339	CB	LEU	57	137.531	18.726	28.670	1.00	34.91
340	CG	LEU	57	137.047	19.512	29.887	1.00	31.36
341	CD1	LEU	57	136.174	20.663	29.441	1.00	31.29
342	CD2	LEU	57	136.287	18.592	30.833	1.00	25.33
343	H	LEU	57	139.968	19.335	28.990	1.00	25.00
344	N	LEU	58	139.466	17.016	26.754	1.00	43.66
345	CA	LEU	58	139.577	16.145	25.591	1.00	48.27
346	C	LEU	58	140.659	15.059	25.683	1.00	53.11
347	O	LEU	58	141.005	14.441	24.672	1.00	54.87
348	CB	LEU	58	139.762	16.987	24.325	1.00	45.38
349	CG	LEU	58	138.682	18.051	24.083	1.00	48.84
350	CD1	LEU	58	138.936	18.772	22.772	1.00	46.56
351	CD2	LEU	58	137.303	17.413	24.074	1.00	49.64
352	H	LEU	58	139.978	17.851	26.781	1.00	25.00
353	N	ALA	59	141.180	14.813	26.884	1.00	58.17
354	CA	ALA	59	142.208	13.788	27.078	1.00	61.28
355	C	ALA	59	141.605	12.397	26.874	1.00	66.17
356	O	ALA	59	140.672	11.998	27.572	1.00	65.17
357	CB	ALA	59	142.830	13.908	28.460	1.00	61.08
358	H	ALA	59	140.859	15.316	27.661	1.00	25.00
359	N	THR	60	142.188	11.651	25.943	1.00	71.93
360	CA	THR	60	141.717	10.317	25.572	1.00	78.50
361	C	THR	60	141.721	9.179	26.599	1.00	77.85
362	O	THR	60	140.694	8.536	26.812	1.00	82.48
363	CB	THR	60	142.443	9.828	24.304	1.00	80.20
364	OG1	THR	60	143.852	10.053	24.449	1.00	82.38
365	OG2	THR	60	141.933	10.573	23.076	1.00	82.60
366	H	THR	60	142.957	12.026	25.478	1.00	25.00
367	HG1	THR	60	144.029	10.991	24.540	1.00	25.00
368	N	GLY	61	142.866	8.914	27.217	1.00	74.94
369	CA	GLY	61	142.942	7.813	28.165	1.00	75.87
370	C	GLY	61	142.662	8.104	29.626	1.00	73.64
371	O	GLY	61	143.494	7.804	30.484	1.00	73.89
372	H	GLY	61	143.654	9.465	27.047	1.00	25.00
373	N	ARG	62	141.491	8.651	29.925	1.00	70.85
374	CA	ARG	62	141.149	8.960	31.307	1.00	67.41
375	C	ARG	62	140.068	8.054	31.870	1.00	61.77
376	O	ARG	62	139.147	7.654	31.160	1.00	63.43
377	CB	ARG	62	140.755	10.429	31.444	1.00	69.30
378	CG	ARG	62	141.883	11.309	31.967	1.00	75.81
379	CD	ARG	62	141.666	12.780	31.647	1.00	78.22
380	NE	ARG	62	140.334	13.254	32.009	1.00	79.69
381	CZ	ARG	62	139.335	13.405	31.143	1.00	88.12
382	NH1	ARG	62	139.508	13.118	29.859	1.00	90.62
383	NH2	ARG	62	138.160	13.852	31.559	1.00	92.99
384	H	ARG	62	140.835	8.835	29.218	1.00	25.00
385	HE	ARG	62	140.163	13.477	32.948	1.00	25.00
386	1HH1	ARG	62	140.393	12.785	29.534	1.00	25.00
387	2HH1	ARO	62	138.752	13.233	29.216	1.00	25.00
388	1HH2	ARG	62	138.022	14.076	32.524	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
389	2HH2	ARG	62	137.408	13.963	30.909	1.00	25.00
390	N	LYS	63	140.214	7.702	33.143	1.00	56.71
391	CA	LYS	63	139.258	6.840	33.830	1.00	53.88
392	C	LYS	63	137.986	7.614	34.170	1.00	49.91
393	O	LYS	63	138.024	8.831	34.377	1.00	43.13
394	CB	LYS	63	139.876	6.284	35.114	1.00	60.17
395	CG	LYS	63	141.181	5.544	34.901	1.00	72.02
396	CD	LYS	63	141.807	5.141	36.225	1.00	82.26
397	CE	LYS	63	143.131	4.428	36.004	1.00	90.54
398	NZ	LYS	63	143.764	4.015	37.286	1.00	94.67
399	H	LYS	63	140.988	8.042	33.633	1.00	25.00
400	1HZ	LYS	63	143.130	3.366	37.795	1.00	25.00
401	2HZ	LYS	63	144.664	3.533	37.085	1.00	25.00
402	3HZ	LYS	63	143.945	4.857	37.868	1.00	25.00
403	N	LEU	64	136.877	6.890	34.289	1.00	44.28
404	CA	LEU	64	135.583	7.487	34.603	1.00	40.75
405	C	LEU	64	135.650	8.425	35.805	1.00	38.00
406	O	LEU	64	135.273	9.592	35.708	1.00	38.34
407	CB	LEU	64	134.539	6.395	34.858	1.00	37.20
408	CG	LEU	64	133.128	6.897	35.170	1.00	35.50
409	CD1	LEU	64	132.563	7.618	33.964	1.00	30.93
410	CD2	LEU	64	132.232	5.741	35.572	1.00	32.83
411	H	LEU	64	136.930	5.926	34.145	1.00	25.00
412	N	ALA	65	136.149	7.915	36.927	1.00	34.87
413	CA	ALA	65	136.264	8.700	38.152	1.00	33.63
414	C	ALA	65	136.977	10.022	37.909	1.00	32.94
415	O	ALA	65	136.508	11.073	38.342	1.00	31.36
416	CB	ALA	65	136.991	7.000	39.222	1.00	26.54
417	H	ALA	65	136.437	6.983	36.932	1.00	25.00
418	N	ASP	66	138.094	9.965	37.188	1.00	36.39
419	CA	ASP	66	138.887	11.151	36.882	1.00	34.98
420	C	ASP	66	138.127	12.136	36.002	1.00	34.90
421	O	ASP	66	138.200	13.352	36.210	1.00	34.81
422	CB	ASP	66	140.202	10.755	36.202	1.00	42.66
423	CG	ASP	66	141.054	9.825	37.059	1.00	51.98
424	OD1	ASP	66	141.008	9.934	38.306	1.00	48.05
425	OD2	ASP	66	141.774	8.982	36.479	1.00	59.40
426	H	ASP	66	138.390	9.103	36.840	1.00	25.00
427	N	THR	67	137.400	11.607	35.023	1.00	32.76
428	CA	THR	67	136.617	12.433	34.110	1.00	29.98
429	C	THR	67	135.486	13.131	34.869	1.00	27.93
430	O	THR	67	135.262	14.337	34.708	1.00	26.55
431	CB	THR	67	136.033	11.582	32.963	1.00	33.36
432	OG1	THR	67	137.102	10.914	32.278	1.00	32.56
433	OG2	THR	67	135.272	12.460	31.972	1.00	24.21
434	H	THR	67	137.385	10.635	34.900	1.00	25.00
435	HG1	THR	67	136.746	10.375	31.566	1.00	25.00
436	N	LEU	68	134.806	12.382	35.730	1.00	24.35
437	CA	LEU	68	133.717	12.938	36.513	1.00	23.41
438	C	LEU	68	134.223	14.025	37.449	1.00	28.28
439	O	LEU	68	133.644	15.112	37.507	1.00	26.82
440	CB	LEU	68	133.004	11.842	37.301	1.00	24.43
441	CG	LEU	68	132.221	10.841	136.447	1.00	32.03
442	CD1	LEU	68	131.651	9.744	37.330	1.00	23.28
443	CD2	LEU	68	131.112	11.556	35.680	1.00	27.61
444	H	LEU	68	135.049	11.442	35.844	1.00	25.00
445	N	ASN	69	135.323	13.750	38.147	1.00	26.79
446	CA	ASN	69	135.894	14.724	39.072	1.00	30.78
447	C	ASN	69	136.341	15.981	38.340	1.00	28.43
448	O	ASN	69	136.165	17.092	38.837	1.00	30.31
449	CB	ASN	69	137.061	14.125	39.867	1.00	40.14
450	CG	ASN	69	136.597	13.165	40.959	1.00	53.22
451	OD1	ASN	69	135.478	13.271	41.467	1.00	52.67
452	ND2	ASN	69	137.460	12.224	41.326	1.00	60.05
453	H	ASN	69	135.750	12.874	38.043	1.00	25.00
454	1HD2	ASN	69	137.165	11.608	42.027	1.00	25.00
455	2HD2	ASN	69	138.335	12.185	40.893	1.00	25.00
456	N	LEU	70	136.884	15.813	37.140	1.00	26.00
457	CA	LEU	70	137.327	16.958	36.358	1.00	27.21
458	C	LEU	70	136.135	17.867	36.053	1.00	29.79
459	O	LEU	70	136.192	19.076	36.287	1.00	27.18

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
460	CB	LEU	70	137.990	16.498	35.058	1.00	23.13
461	CG	LEU	70	138.417	17.624	34.109	1.00	30.77
462	CD1	LEU	70	139.366	18.580	34.821	1.00	21.76
463	CD2	LEU	70	139.062	17.045	32.860	1.00	27.07
464	H	LEU	70	136.995	14.908	36.777	1.00	25.00
465	N	ILE	71	135.053	17.272	35.553	1.00	30.05
466	CA	ILE	71	133.840	18.012	35.217	1.00	24.54
467	C	ILE	71	133.221	18.663	36.456	1.00	23.02
468	O	ILE	71	132.849	19.839	36.429	1.00	23.20
469	CB	ILE	71	132.809	17.095	34.516	1.00	26.68
470	CG1	ILE	71	133.338	16.693	33.136	1.00	25.05
471	CG2	ILE	71	131.459	17.795	34.383	1.00	23.87
472	CD1	ILE	71	132.442	15.736	32.400	1.00	27.35
473	H	ILE	71	135.073	16.300	35.409	1.00	25.00
474	N	ASP	72	133.140	17.910	37.546	1.00	19.38
475	CA	ASP	72	132.585	18.429	38.789	1.00	22.68
476	C	ASP	72	133.376	19.657	39.266	1.00	25.06
477	O	ASP	72	132.784	20.680	39.626	1.00	24.92
478	CB	ASP	72	132.593	17.335	39.861	1.00	23.74
479	CG	ASP	72	131.900	17.760	41.147	1.00	27.65
480	OD1	ASP	72	130.953	18.575	41.086	1.00	29.89
481	OD2	ASP	72	132.303	17.268	42.223	1.00	30.37
482	H	ASP	72	133.459	16.986	37.512	1.00	25.00
483	N	ILE	73	134.705	19.565	39.228	1.00	26.02
484	CA	ILE	73	135.589	20.656	39.654	1.00	21.86
485	C	ILE	73	135.431	21.918	38.797	1.00	23.60
486	O	ILE	73	135.270	23.019	39.329	1.00	25.70
487	CB	ILE	73	137.075	20.198	39.671	1.00	20.21
488	CG1	ILE	73	137.245	19.066	40.684	1.00	22.84
489	CG2	ILE	73	137.992	21.351	40.058	1.00	17.62
490	CD1	ILE	73	138.659	18.513	40.788	1.00	53.34
491	H	ILE	73	135.108	18.732	38.902	1.00	25.00
492	N	ILE	74	135.450	21.755	37.476	1.00	22.39
493	CA	ILE	74	135.297	22.884	36.556	1.00	22.15
494	C	ILE	74	133.955	23.581	36.784	1.00	24.59
495	O	ILE	74	133.858	24.807	36.702	1.00	29.58
496	CB	ILE	74	135.415	22.426	35.079	1.00	24.24
497	CG1	ILE	74	136.835	21.909	34.811	1.00	25.85
498	CG2	ILE	74	135.071	23.571	34.132	1.00	19.61
499	CD1	ILE	74	137.054	21.340	33.420	1.00	23.74
500	H	ILE	74	135.571	20.851	37.109	1.00	25.00
501	N	GLU	75	132.925	22.797	37.083	1.00	23.15
502	CA	GLU	75	131.599	23.343	37.338	1.00	23.53
503	C	GLU	75	131.548	24.092	38.658	1.00	21.84
504	O	GLU	75	131.040	25.208	38.722	1.00	25.34
505	CB	GLU	75	130.550	22.237	37.342	1.00	26.71
506	CG	GLU	75	130.274	21.647	35.978	1.00	30.84
507	CD	GLU	75	129.073	20.720	35.969	1.00	36.10
508	OE1	GLU	75	128.644	20.253	37.051	1.00	29.89
509	OE2	GLU	75	128.559	20.460	34.865	1.00	31.50
510	H	GLU	75	133.056	21.822	37.122	1.00	25.00
511	N	ARG	76	132.060	23.474	39.717	1.00	19.68
512	CA	ARG	76	132.066	24.115	41.028	1.00	20.75
513	C	ARG	76	132.925	25.385	41.017	1.00	22.83
514	O	ARG	76	132.699	26.303	41.803	1.00	21.89
515	CB	ARG	76	132.581	23.148	42.091	1.00	16.07
516	CG	ARG	76	131.653	21.989	42.411	1.00	20.22
517	CD	ARG	76	132.331	21.061	43.395	1.00	21.08
518	NE	ARG	76	131.498	19.939	43.819	1.00	18.53
519	CZ	ARG	76	130.847	19.891	44.977	1.00	24.53
520	NH1	ARG	76	130.917	20.907	45.829	1.00	17.48
521	NH2	ARG	76	130.170	18.802	45.311	1.00	26.65
522	H	ARG	76	132.440	22.577	39.618	1.00	25.00
523	HE	ARG	76	131.417	19.172	43.218	1.00	25.00
524	1HH1	ARG	76	131.459	21.717	45.606	1.00	25.00
525	2HH1	ARG	76	130.423	20.865	46.697	1.00	25.00
526	1HH2	ARG	76	130.146	18.021	44.691	1.00	25.00
527	2HH2	ARG	76	129.678	18.766	46.181	1.00	25.00
528	N	LEU	77	133.913	25.425	40.126	1.00	22.29
529	CA	LEU	77	134.798	26.579	40.001	1.00	23.34
530	C	LEU	77	134.156	27.710	39.193	1.00	26.64

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
531	O	LEU	77	134.752	28.777	39.026	1.00	25.27
532	CB	LEU	77	136.131	26.167	39.372	1.00	18.34
533	CG	LEU	77	137.076	25.352	40.258	1.00	18.25
534	CD1	LEU	77	138.266	24.893	39.443	1.00	15.60
535	CD2	LEU	77	137.531	26.182	41.459	1.00	17.00
536	H	LEU	77	134.063	24.649	39.546	1.00	25.00
537	N	GLY	78	132.958	27.455	38.668	1.00	24.42
538	CA	GLY	78	132.228	28.464	37.914	1.00	20.32
539	C	GLY	78	132.741	28.807	38.531	1.00	20.16
540	O	GLY	78	132.375	29.841	35.970	1.00	22.90
541	H	GLY	78	132.553	26.576	38.793	1.00	25.00
542	N	ILE	79	133.550	27.927	335.952	1.00	22.82
543	CA	ILE	79	134.099	28.170	34.623	1.00	24.96
544	C	ILE	79	133.577	27.204	33.560	1.00	29.01
545	O	ILE	79	133.991	27.273	32.398	1.00	28.78
546	CB	ILE	79	135.646	28.133	34.635	1.00	24.44
547	CG1	ILE	79	136.142	26.920	35.429	1.00	27.37
548	CG2	ILE	79	136.195	29.426	35.210	1.00	25.45
549	CD1	ILE	79	137.632	26.715	35.381	1.00	25.03
550	H	ILE	79	133.782	27.105	36.435	1.00	25.00
551	N	SER	80	132.629	26.347	33.935	1.00	27.52
552	CA	SER	80	132.079	25.381	32.986	1.00	29.32
553	C	SER	80	131.317	26.012	31.816	1.00	31.74
554	O	SER	80	131.187	25.391	30.761	1.00	34.93
555	CB	SEER	80	131.205	24.338	33.694	1.00	26.24
556	OG	SER	80	130.096	24.932	34.338	1.00	29.78
557	H	SER	80	132.308	26.358	34.857	1.00	25.00
558	HG	SER	80	130.432	25.530	34.992	1.00	25.00
559	N	TYR	81	130.869	27.258	31.966	1.00	25.77
560	CA	TYR	81	130.134	27.914	30.887	1.00	23.28
561	C	TYR	81	130.965	28.063	29.605	1.00	30.16
562	O	TYR	81	130.418	28.302	28.527	1.00	32.12
563	CB	TYR	81	129.556	29.261	31.344	1.00	24.86
564	CG	TYR	81	130.557	30.381	31.543	1.00	29.19
565	CD1	TYR	81	131.260	30.519	32.740	1.00	27.27
566	CD2	TYR	81	130.768	31.329	30.545	1.00	28.18
567	CE1	TYR	81	132.148	31.575	32.935	1.00	29.22
568	CE2	TYR	81	131.649	32.384	30.729	1.00	29.85
569	CZ	TYR	81	132.336	32.504	31.923	1.00	29.78
570	OH	TYR	81	133.220	33.547	32.084	1.00	28.93
571	H	TYR	81	131.028	27.734	32.805	1.00	25.00
572	HH	TYR	81	133.196	34.121	31.313	1.00	25.00
573	N	HIS	82	132.284	27.904	29.727	1.00	32.51
574	CA	HIS	82	133.194	27.991	28.581	1.00	29.34
575	C	HIS	82	133.237	26.669	27.828	1.00	28.19
576	O	HIS	82	133.658	26.620	26.672	1.00	28.93
577	CB	HIS	82	134.631	28.280	29.038	1.00	27.19
578	CG	HIS	82	134.839	29.654	29.589	1.00	22.31
579	ND1	HIS	82	134.702	30.793	28.825	1.00	24.56
580	CD2	HIS	82	135.195	30.071	30.827	1.00	20.64
581	CE1	HIS	82	134.964	31.853	29.568	1.00	22.72
582	NE2	HIS	82	135.265	31.442	30.786	1.00	23.06
583	H	HIS	82	132.658	27.714	30.612	1.00	25.00
584	HD1	HIS	82	134.458	30.815	27.872	1.00	25.00
585	HE2	HIS	82	135.465	32.016	31.549	1.00	25.00
586	N	PHE	83	132.820	25.596	28.493	1.00	26.84
587	CA	PHE	83	132.878	24.266	27.903	1.00	33.10
588	C	PHE	83	131.549	23.521	27.811	1.00	36.98
589	O	PHE	83	131.511	22.296	27.973	1.00	34.23
590	CB	PHE	83	133.895	23.426	28.683	1.00	32.26
591	CG	PHE	83	135.171	24.159	28.985	1.00	36.23
592	CD1	PHE	83	136.138	24.336	27.998	1.00	36.38
993	CD2	PHE	83	135.381	24.724	30.241	1.00	34.95
594	CE1	PHE	83	137.295	25.067	28.254	1.00	36.74
595	CE2	PHE	83	136.533	25.457	30.509	1.00	39.63
596	CZ	PHE	83	137.492	25.630	29.511	1.00	41.21
597	H	PHE	83	132.457	25.694	29.394	1.00	25.00
598	N	GLU	84	130.478	24.241	27.484	1.00	40.92
599	CA	GLU	84	129.146	23.641	27.365	1.00	46.14
600	C	GLU	84	129.159	22.422	26.431	1.00	42.13
601	O	GLU	84	128.753	21.325	26.819	1.00	38.24

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
602	CB	GLU	84	128.128	24.674	26.851	1.00	56.77
603	CG	GLU	84	128.042	25.978	27.660	1.00	74.38
604	CD	GLU	84	127.252	25.853	28.960	1.00	81.74
605	OE1	GLU	84	127.654	25.066	29.847	1.00	85.56
606	OE2	GLU	84	126.233	26.564	29.101	1.00	84.80
607	H	GLU	84	130.590	25.203	27.330	1.00	25.00
608	N	LYS	85	129.674	22.614	25.218	1.00	40.25
609	CA	LYS	85	129.740	21.544	24.224	1.00	41.41
610	C	LYS	85	130.590	20.348	24.663	1.00	36.27
611	O	LYS	85	130.138	19.204	24.595	1.00	35.16
612	CB	LYS	85	130.268	22.085	22.890	1.00	46.40
613	CG	LYS	85	130.364	21.025	21.801	1.00	58.06
614	CD	LYS	85	131.176	21.498	20.605	1.00	70.05
615	CE	LYS	85	131.305	20.389	19.565	1.00	70.91
616	NZ	LYS	85	132.101	20.809	18.379	1.00	79.32
617	H	LYS	85	130.016	23.501	24.992	1.00	25.00
618	1HZ	LYS	85	133.059	21.080	18.678	1.00	25.00
619	2HZ	LYS	85	132.157	20.018	17.706	1.00	25.00
620	3HZ	LYS	85	131.636	21.619	17.922	1.00	25.00
621	N	GLU	86	131.812	20.620	25.115	1.00	37.17
622	CA	GLU	86	132.736	19.573	25.545	1.00	35.98
623	C	GLU	86	132.162	18.714	26.663	1.00	36.73
624	O	GLU	86	132.156	17.483	26.571	1.00	38.05
625	CB	GLU	86	134.077	20.173	25.990	1.00	36.51
626	CG	GLU	86	134.938	20.773	24.866	1.00	40.91
627	CD	GLU	86	134.439	22.124	24.349	1.00	43.71
628	OE1	GLU	86	133.728	22.840	25.085	1.00	42.43
629	OE2	GLU	86	134.776	22.480	23.201	1.00	50.53
630	H	GLU	86	132.086	21.551	25.172	1.00	25.00
631	N	ILE	87	131.666	19.368	27.708	1.00	35.80
632	CA	ILE	87	131.092	18.662	28.845	1.00	30.66
633	C	ILE	87	129.871	17.844	28.428	1.00	32.98
634	O	ILE	87	129.692	16.711	28.887	1.00	32.50
635	CB	ILE	87	130.739	19.640	29.986	1.00	30.27
636	CG1	ILE	87	132.027	20.253	30.546	1.00	29.89
637	CG2	ILE	87	129.972	18.926	31.091	1.00	29.25
638	CD1	ILE	87	131.814	21.264	31.654	1.00	25.52
639	H	ILE	87	131.681	20.348	27.719	1.00	25.00
640	N	ASP	88	129.054	18.393	27.534	1.00	32.95
641	CA	ASP	88	127.870	17.679	27.070	1.00	36.69
642	C	ASP	88	128.256	16.407	26.309	1.00	39.28
643	O	ASP	88	127.745	15.324	26.6601	1.00	40.13
644	CB	ASP	88	126.994	18.573	26.191	1.00	40.42
645	CG	ASP	88	125.682	17.901	25.800	1.00	49.09
646	OD1	ASP	88	124.874	17.586	26.702	1.00	48.29
647	OD2	ASP	88	125.464	17.677	24.590	1.00	57.24
648	H	ASP	88	129.245	19.291	27.185	1.00	25.00
649	N	GLU	89	129.178	16.532	25.359	1.00	38.92
650	CA	GLU	89	129.621	15.385	24.573	1.00	38.06
651	C	GLU	89	130.258	14.303	25.433	1.00	35.90
652	O	GLU	89	130.077	13.115	25.168	1.00	39.91
653	CB	GLU	89	130.572	15.829	23.466	1.00	44.42
654	CG	GLU	89	129.871	16.622	22.379	1.00	61.34
655	CD	GLU	89	130.822	17.159	21.333	1.00	75.40
656	OE1	GLU	89	131.776	17.873	21.707	1.00	80.47
657	OE2	GLU	89	130.609	16.878	20.134	1.00	86.74
658	H	GLU	89	129.569	17.416	25.185	1.00	25.00
659	N	ILE	90	130.985	14.708	26.470	1.00	32.75
660	CA	ILE	90	131.619	13.749	27.368	1.00	31.62
661	C	ILE	90	130.556	13.052	28.215	1.00	33.52
662	O	ILE	90	130.580	11.830	28.376	1.00	35.53
663	CB	ILE	90	132.646	14.427	28.302	1.00	31.23
664	CG1	ILE	90	133.815	14.983	27.485	1.00	32.25
665	CG2	ILE	90	133.153	13.431	29.340	1.00	23.52
666	CD1	ILE	90	134.794	15.802	28.300	1.00	27.90
667	H	ILE	90	131.105	15.670	26.630	1.00	25.00
668	N	LEU	91	129.617	13.828	28.749	1.00	33.39
669	CA	LEU	91	128.551	13.266	29.569	1.00	33.57
670	C	LEU	91	127.642	12.351	28.756	1.00	35.23
671	O	LEU	91	127.145	11.346	29.269	1.00	32.55
672	CB	LEU	91	127.741	14.373	30.244	1.00	30.86

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
673	CG	LEU	91	128.430	15.017	31.447	1.00	28.62
674	CD1	LEU	91	127.538	16.084	32.040	1.00	25.02
675	CD2	LEU	91	128.752	13.952	32.490	1.00	25.28
676	H	LEU	91	129.643	14.796	28.591	1.00	25.00
677	N	ASP	92	127.445	12.692	27.486	1.00	34.80
678	CA	ASP	92	126.620	11.889	26.595	1.00	37.65
679	C	ASP	92	127.273	10.516	26.446	1.00	38.72
680	O	ASP	92	126.594	9.490	26.494	1.00	41.65
681	CB	ASP	92	126.491	12.569	25.231	1.00	44.12
682	CG	ASP	92	125.426	11.931	24.358	1.00	48.79
683	OD1	ASP	92	124.235	12.268	24.531	1.00	49.33
684	OD2	ASP	92	125.781	11.098	23.498	1.00	52.21
685	H	ASP	92	127.856	13.512	27.149	1.00	25.00
686	N	GLN	93	128.595	10.499	26.286	1.00	40.62
687	CA	GLN	93	129.337	9.247	26.155	1.00	41.87
688	C	GLN	93	129.209	8.415	27.424	1.00	41.38
689	O	GLN	93	129.038	7.198	27.356	1.00	44.29
690	CB	GLN	93	130.817	9.504	25.883	1.00	47.84
691	CG	GLN	93	131.124	10.061	24.511	1.00	65.26
692	CD	GLN	93	132.618	10.230	24.286	1.00	76.60
693	OE1	GLN	93	133.402	9.308	24.532	1.00	78.42
694	NE2	GLN	93	133.023	11.413	23.829	1.00	78.28
695	H	GLN	93	129.082	11.351	26.254	1.00	25.00
696	1HE2	GLN	93	133.983	11.522	23.685	1.00	25.00
697	2HE2	GLN	93	132.356	12.108	23.664	1.00	25.00
698	N	ILE	94	129.302	9.065	28.580	1.00	38.08
699	CA	ILE	94	129.186	8.360	29.851	1.00	38.56
700	C	ILE	94	127.783	7.763	30.011	1.00	37.25
701	O	ILE	94	127.631	6.623	30.464	1.00	40.45
702	CB	ILE	94	129.519	9.284	31.051	1.00	38.10
703	CG1	ILE	94	130.982	9.729	30.973	1.00	33.78
704	CG2	ILE	94	129.265	8.559	32.372	1.00	39.54
705	CD1	ILE	94	131.426	10.590	32.131	1.00	28.73
706	H	ILE	94	129.455	10.035	28.576	1.00	25.00
707	N	TYR	95	126.769	8.527	29.616	1.00	35.79
708	CA	TYR	95	125.383	8.080	29.702	1.00	36.92
709	C	TYR	95	125.219	6.814	28.869	1.00	40.95
710	O	TYR	95	124.681	5.812	29.340	1.00	39.72
711	CB	TYR	95	124.438	9.170	29.176	1.00	31.04
712	CG	TYR	95	122.969	8.799	29.213	1.00	35.51
713	CD1	TYR	95	122.356	8.420	30.407	1.00	37.94
714	CD2	TYR	95	122.189	8.826	28.054	1.00	40.35
715	CE1	TYR	95	121.002	8.073	30.452	1.00	42.00
716	CE2	TYR	95	120.827	8.481	28.088	1.00	44.29
717	CZ	TYR	95	120.245	8.107	29.294	1.00	43.88
718	OH	TYR	95	118.912	7.763	29.351	1.00	49.08
719	H	TYR	95	126.959	9.421	29.265	1.00	25.00
720	HH	TYR	95	118.668	7.513	30.254	1.00	25.00
721	N	ASN	96	125.744	6.861	27.649	1.00	42.27
722	CA	ASN	96	125.664	5.749	26.711	1.00	45.67
723	C	ASN	96	126.430	4.484	27.088	1.00	53.96
724	O	ASN	96	125.949	3.383	26.831	1.00	58.48
725	CB	ASN	96	126.068	6.215	25.310	1.00	41.30
726	CG	ASN	96	125.004	7.072	24.656	1.00	45.95
727	OD1	ASN	96	123.922	6.590	24.339	1.00	50.40
728	ND2	ASN	96	125.299	3.349	24.459	1.00	47.53
729	H	ASN	96	128.205	7.682	27.378	1.00	25.00
730	1HD2	ASN	96	124.616	8.910	24.040	1.00	25.00
731	2HD2	ASN	96	126.172	8.686	24.743	1.00	25.00
732	N	GLN	97	127.604	4.625	27.702	1.00	62.59
733	CA	GLN	97	128.397	3.453	28.081	1.00	69.96
734	C	GLN	97	127.898	2.701	29.320	1.00	74.06
735	O	GLN	97	128.255	1.540	29.521	1.00	71.27
736	CB	GLN	97	129.885	3.804	28.219	1.00	74.21
737	CG	GLN	97	130.227	4.801	29.315	1.00	82.49
738	CD	GLN	97	131.723	5.065	29.415	1.00	85.73
739	OE1	GLN	97	132.336	4.837	30.456	1.00	88.41
740	NE2	GLN	97	132.316	5.548	28.329	1.00	82.49
741	H	GLN	97	127.943	5.524	27.899	1.00	25.00
742	1HE2	GLN	97	133.277	5.711	28.402	1.00	25.00
743	2HE2	GLN	97	131.787	5.714	27.528	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
744	N	ASN	98	127.091	3.367	30.147	1.00	83.07
745	CA	ASN	98	126.517	2.769	31.360	1.00	95.02
746	C	ASN	98	127.459	1.854	32.148	1.00	101.68
747	O	ASN	98	127.088	0.737	32.517	1.00	106.47
748	CB	ASN	98	125.233	1.997	31.019	1.00	98.06
749	CG	ASN	98	124.034	2.902	30.830	1.00	100.62
750	OD1	ASN	98	123.390	3.307	31.799	1.00	107.25
751	ND2	ASN	98	123.711	3.207	29.580	1.00	100.51
752	H	ASN	98	126.876	4.301	29.938	1.00	25.00
753	1HD2	ASN	98	122.944	3.798	29.449	1.00	25.00
754	2HD2	ASN	98	124.241	2.849	28.838	1.00	25.00
755	N	SER	99	128.671	2.326	32.415	1.00	105.86
756	CA	SER	99	129.649	1.533	33.153	1.00	108.38
757	C	SER	999	129.389	1.528	34.659	1.00	109.53
758	O	SER	99	129.054	2.561	35.243	1.00	110.32
759	CB	SER	99	131.057	2.049	32.859	1.00	107.06
760	OG	SER	99	131.078	3.405	32.861	1.00	109.07
761	H	SER	99	128.927	3.224	32.122	1.00	25.00
762	HG	SER	99	130.810	3.805	33.720	1.00	25.00
763	N	ASN	100	129.534	0.361	35.280	1.00	111.83
764	CA	ASN	100	129.325	0.223	36.720	1.00	115.28
765	C	ASN	100	130.612	0.548	37.462	1.00	114.16
766	O	ASN	100	131.577	−0.213	37.402	1.00	114.16
767	CB	ASN	100	128.873	−1.195	37.072	1.00	117.88
768	CG	ASN	100	127.451	−1.473	36.640	1.00	122.11
769	OD1	ASN	100	126.518	−0.785	37.056	1.00	119.89
770	ND2	ASN	100	127.274	−2.485	35.799	1.00	124.85
771	H	ASN	100	129.794	−0.423	34.757	1.00	25.00
772	1HD2	ASN	100	126.354	−2.663	35.510	1.00	25.00
773	2HD2	ASN	100	128.048	−3.001	35.500	1.00	25.00
774	N	CYS	101	130.622	1.678	38.162	1.00	112.97
775	CA	CYS	101	131.804	2.103	38.902	1.00	109.49
776	C	CYS	101	132.046	1.309	40.184	1.00	104.47
777	O	CYS	101	133.178	1.226	40.662	1.00	107.64
778	CB	CYS	101	131.735	3.593	39.218	1.00	112.66
779	SG	CYS	101	133.273	4.224	39.908	1.00	125.35
780	H	CYS	101	129.822	2.244	38.153	1.00	25.00
781	N	ASN	102	130.976	0.765	40.756	1.00	95.01
782	CA	ASN	102	131.043	−0.0488	41.975	1.00	88.33
783	C	ASN	102	131.235	0.673	43.315	1.00	78.73
784	O	ASN	102	131.005	0.074	44.367	1.00	78.57
785	CB	ASN	102	132.071	−1.182	41.831	1.00	94.60
786	CG	ASN	102	131.727	−2.147	40.704	1.00	99.33
787	OD1	ASN	102	130.667	−2.774	40.706	1.00	97.79
788	ND2	ASN	102	132.618	−2.256	39.727	1.00	103.54
789	H	ASN	102	130.102	0.912	40.350	1.00	25.00
790	1HD2	ASN	102	132.412	−2.867	38.993	1.00	25.00
791	2HD2	ASN	102	133.439	−1.721	39.766	1.00	25.00
792	N	ASP	103	131.684	1.926	43.301	1.00	65.57
793	CA	ASP	103	131.845	2.657	44.560	1.00	56.22
794	C	ASP	103	130.870	3.833	44.638	1.00	46.49
795	O	ASP	103	130.659	4.550	43.657	1.00	41.71
796	CB	ASP	103	133.296	3.102	44.796	1.00	56.91
797	CG	ASP	103	133.767	4.133	43.802	1.00	64.49
798	OD1	ASP	103	134.215	3.735	42.707	1.00	74.22
799	OD2	ASP	103	133.707	5.339	44.124	1.00	67.65
800	H	ASP	103	131.912	2.367	42.461	1.00	25.00
801	N	LEU	104	130.281	4.015	45.816	1.00	38.89
802	CA	LEU	104	129.291	5.060	40.071	1.00	36.92
803	C	LEU	104	129.672	6.457	45.591	1.00	36.45
804	O	LEU	104	128.898	7.109	44.895	1.00	35.19
805	CB	LEU	104	128.943	5.092	47.561	1.00	33.67
806	CG	LEU	104	127.824	6.031	48.011	1.00	36.34
807	CD1	LEU	104	126.538	5.713	47.269	1.00	35.38
808	CD2	LEU	104	127.622	5.893	49.510	1.00	35.29
809	H	LEU	104	130.509	3.401	46.542	1.00	25.00
810	N	CYS	105	130.872	6.895	45.951	1.00	36.36
811	CA	CYS	105	131.376	8.212	45.581	1.00	35.11
812	C	CYS	105	131.220	8.537	44.092	1.00	34.06
813	O	CYS	105	130.596	9.536	43.725	1.00	37.28
814	CB	CYS	105	132.847	8.325	45.993	1.00	35.03

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
815	SG	CYS	105	133.614	9.885	45.573	1.00	53.55
816	H	CYS	105	131.437	6.307	46.484	1.00	25.00
817	N	THR	106	131.761	7.679	43.236	1.00	30.74
818	CA	THR	106	131.697	7.890	41.797	1.00	28.00
819	C	THR	106	130.301	7.663	41.227	1.00	25.73
820	O	THR	106	129.870	8.396	40.339	1.00	28.92
821	CB	THR	106	132.714	7.000	41.074	1.00	33.61
822	OG1	THR	106	134.000	7.172	41.684	1.00	38.24
823	CG2	THR	106	132.807	7.369	39.598	1.00	30.78
824	H	THR	106	132.208	6.874	43.564	1.00	25.00
825	HG1	THR	106	134.270	8.093	41.602	1.00	25.00
826	N	SER	107	129.592	6.670	41.751	1.00	23.29
827	CA	SER	107	128.237	6.371	41.294	1.00	27.37
828	C	SER	107	127.268	7.540	41.539	1.00	25.50
829	O	SER	107	126.518	7.932	40.643	1.00	25.99
830	CB	SER	107	127.721	5.101	41.978	1.00	26.16
831	OG	SER	107	128.552	3.993	41.676	1.00	34.57
832	H	SER	107	129.981	6.113	42.456	1.00	25.00
833	HG	SER	107	128.501	3.864	40.726	1.00	25.00
834	N	ALA	108	127.298	8.096	42.749	1.00	23.90
835	CA	ALA	108	126.441	9.219	43.121	1.00	23.63
836	C	ALA	108	126.779	10.466	42.307	1.00	25.62
837	O	ALA	108	125.887	11.189	41.861	1.00	27.88
838	CB	ALA	108	126.566	9.509	44.608	1.00	18.25
839	H	ALA	108	127.913	7.734	43.418	1.00	25.00
840	N	LEU	109	128.069	10.709	42.099	1.00	21.86
841	CA	LEU	109	128.493	11.861	41.322	1.00	21.96
842	C	LEU	109	128.009	11.704	39.881	1.00	25.59
843	O	LEU	109	127.458	12.640	39.297	1.00	26.33
844	CB	LEU	109	130.017	12.002	41.359	1.00	21.29
845	CG	LEU	109	130.611	13.186	40.550	1.00	23.03
846	CD1	LEU	109	129.969	14.480	40.962	1.00	15.35
847	CD2	LEU	109	132.111	13.210	40.751	1.00	17.60
848	H	LEU	109	128.742	10.101	42.475	1.00	25.00
849	N	GLN	110	128.205	10.509	39.325	1.00	27.12
850	CA	GLN	110	127.796	10.199	37.954	1.00	28.41
851	C	GLN	110	126.302	10.449	37.803	1.00	24.05
852	O	GLN	110	125.849	11.049	36.825	1.00	23.84
853	CB	GLN	110	128.098	8.732	37.632	1.00	26.80
854	CG	GLN	110	127.790	8.333	36.197	1.00	34.89
855	CD	GLN	110	127.942	6.843	35.947	1.00	37.60
856	OE1	GLN	110	128.418	6.098	36.804	1.00	43.99
857	NE2	GLN	110	127.538	6.401	34.765	1.00	38.91
858	H	GLN	110	128.641	9.810	39.852	1.00	25.00
859	1HE2	GLN	110	127.636	5.440	34.604	1.00	25.00
860	2HE2	GLN	110	127.167	7.030	34.117	1.00	25.00
861	N	PHE	111	125.543	9.970	38.779	1.00	20.86
862	CA	PHE	111	124.104	10.140	38.783	1.00	24.95
863	C	PHE	111	123.760	11.633	38.792	1.00	24.87
864	O	PHE	111	123.037	12.113	37.917	1.00	27.29
865	CB	PHE	111	123.511	9.442	40.008	1.00	21.47
866	CG	PHE	111	122.019	9.568	40.120	1.00	28.99
867	CD1	PHE	111	121.183	8.649	39.494	1.00	24.39
868	CD2	PHE	111	121.448	10.600	40.865	1.00	26.46
869	CE1	PHE	111	119.799	8.753	39.610	1.00	26.64
870	CE2	PHE	111	120.072	10.713	40.985	1.00	25.60
871	CZ	PHE	111	119.243	9.787	40.356	1.00	30.12
872	H	PHE	111	125.966	9.482	39.513	1.00	25.00
873	N	ARG	112	124.323	12.372	39.747	1.00	23.80
874	CA	ARG	112	124.055	13.802	39.858	1.00	18.05
875	C	ARG	112	124.384	14.598	38.601	1.00	22.05
876	O	ARG	112	123.539	15.341	38.103	1.00	28.69
877	CB	ARG	112	124.771	14.417	41.066	1.00	18.30
878	CG	ARG	112	124.503	15.911	41.209	1.00	16.54
879	CD	ARG	112	125.077	16.519	42.479	1.00	17.13
880	NE	ARG	112	126.540	16.520	42.517	1.00	19.87
881	CZ	ARG	112	127.323	17.379	41.866	1.00	22.23
882	NH1	ARG	112	126.808	18.328	41.099	1.00	19.31
883	NH2	ARG	112	128.636	17.311	42.012	1.00	25.31
884	H	ARO	112	124.923	11.945	40.387	1.00	25.00
885	HE	ARG	112	126.982	15.846	43.063	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
886	1HH1	ARG	112	125.815	18.407	40.998	1.00	25.00
887	2HH1	ARG	112	127.408	13.960	40.612	1.00	25.00
888	1HH2	ARG	112	129.037	16.615	42.608	1.00	25.00
889	2HH2	ARG	112	129.219	17.950	41.520	1.00	25.00
890	N	LEU	113	125.596	14.445	38.077	1.00	22.19
891	CA	LEU	113	125.994	15.192	36.883	1.00	23.19
892	C	LEU	113	125.112	14.907	35.665	1.00	27.49
893	O	LEU	113	124.752	15.828	34.921	1.00	24.19
894	CB	LEU	113	127.465	14.937	36.532	1.00	26.29
895	CG	LEU	113	128.547	15.323	37.546	1.00	28.48
896	CD1	LEEU	113	129.911	15.110	36.905	1.00	21.83
897	CD2	LEU	113	128.391	16.772	37.993	1.00	17.87
898	H	LEU	113	126.225	13.821	38.492	1.00	25.00
899	N	LEU	114	124.776	13.638	35.451	1.00	24.90
900	CA	LEU	114	123.932	13.268	34.321	1.00	25.28
901	C	LEU	114	122.537	13.867	34.485	1.00	23.09
902	O	LEU	114	122.038	14.534	33.580	1.00	26.40
903	CB	LEU	114	123.866	11.746	34.168	1.00	23.58
904	CG	LEU	114	125.167	11.101	33.671	1.00	25.79
905	CD1	LEU	114	125.043	9.591	33.660	1.00	24.20
906	CD2	LEU	114	125.504	11.607	32.280	1.00	23.62
907	H	LEU	114	125.095	12.937	36.062	1.00	25.00
908	N	ARG	115	121.948	13.694	35.665	1.00	23.30
909	CA	ARG	115	120.620	14.228	35.955	1.00	21.07
910	C	ARG	115	120.551	15.748	35.787	1.00	26.37
911	O	ARG	115	119.628	16.267	35.148	1.00	26.34
912	CB	ARG	115	120.178	13.844	37.372	1.00	20.95
913	CG	ARG	115	119.749	12.394	37.528	1.00	21.24
914	CD	ARG	115	118.588	12.057	36.595	1.00	24.51
915	NE	ARG	115	118.086	10.702	36.813	1.00	20.45
916	CZ	ARG	115	117.090	10.394	37.639	1.00	25.55
917	NH1	ARG	115	116.475	11.347	38.327	1.00	26.55
918	NH2	ARG	115	116.729	9.128	37.807	1.00	21.55
919	H	ARG	115	122.416	13.187	36.361	1.00	25.00
920	HE	ARG	115	118.508	9.978	36.314	1.00	25.00
921	1HH1	ARG	115	116.757	12.300	38.232	1.00	25.00
922	2HH1	ARG	115	115.725	11.114	38.942	1.00	25.00
923	1HH2	ARG	115	117.205	8.402	37.314	1.00	25.00
924	2HH2	ARG	115	115.980	8.901	38.425	1.00	25.00
925	N	GLN	116	121.537	16.458	36.333	1.00	24.98
926	CA	GLN	116	121.573	17.917	36.235	1.00	21.36
927	C	CLN	116	121.696	18.366	34.792	1.00	23.11
928	O	GLN	116	121.331	19.491	34.450	1.00	20.94
929	CB	GLN	116	122.718	18.501	37.066	1.00	21.35
930	CG	GLN	116	122.536	18.322	38.561	1.00	24.02
931	CD	GLN	116	123.594	19.035	39.371	1.00	23.65
932	OE1	CLN	116	123.278	19.835	40.252	1.00	30.06
933	NE2	GLN	116	124.855	18.744	39.088	1.00	21.53
934	H	GLN	116	122.246	15.983	36.814	1.00	25.00
935	1HE2	GLN	116	125.538	19.210	39.609	1.00	25.00
936	2HE2	GLN	116	125.046	18.089	38.391	1.00	25.00
937	N	HIS	117	122.232	17.490	33.950	1.00	21.29
938	CA	HIS	117	122.381	17.804	32.537	1.00	21.02
939	C	HIS	117	121.264	17.235	31.366	1.00	23.62
940	O	HIS	117	121.389	17.192	30.445	1.00	22.85
941	CB	HIS	117	123.755	17.366	32.031	1.00	23.58
942	CG	HIS	117	124.863	18.267	32.475	1.00	27.17
943	ND1	HIS	117	125.477	19.165	31.628	1.00	28.70
944	CD2	HIS	117	125.421	18.456	33.693	1.00	26.70
945	CE1	HIS	117	126.361	19.874	32.307	1.00	25.66
946	NE2	HIS	117	126.346	19.464	33.562	1.00	29.17
947	H	HIS	117	122.526	16.612	34.277	1.00	25.00
948	HD1	HIS	117	125.301	19.252	30.671	1.00	25.00
949	HE2	HIS	117	126.861	19.825	34.298	1.00	25.00
950	N	GLY	118	120.183	16.784	32.301	1.00	24.12
951	CA	GLY	118	119.050	16.258	31.562	1.00	25.68
952	C	GLY	118	119.037	14.786	31.193	1.00	30.13
953	O	GLY	118	118.028	14.303	30.676	1.00	35.12
954	H	GLY	118	120.143	16.804	33.279	1.00	25.00
955	N	PHE	119	120.130	14.068	31.432	1.00	29.49
956	CA	PHE	119	120.184	12.644	31.102	1.00	26.30

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
957	C	PHE	119	119.435	11.867	32.172	1.00	28.96
958	O	PHE	119	119.836	11.861	33.337	1.00	25.84
959	CB	PHE	119	121.633	12.156	31.019	1.00	24.99
960	CG	PHE	119	122.447	12.845	29.964	1.00	23.43
961	CD1	PHE	119	122.392	12.421	28.640	1.00	22.02
962	CD2	PHE	119	123.267	13.922	30.291	1.00	23.36
963	CE1	PHE	119	123.145	13.063	27.650	1.00	26.82
964	CE2	PHE	119	124.023	14.572	29.312	1.00	20.73
965	CZ	PHE	119	123.962	14.141	27.988	1.00	22.11
966	H	PHE	119	120.902	14.496	31.856	1.00	25.00
967	N	ASN	120	118.351	11.207	31.779	1.00	31.42
968	CA	ASN	120	117.551	10.447	32.733	1.00	36.20
969	C	ASN	120	118.208	9.117	33.088	1.00	36.85
970	O	ASN	120	117.727	8.048	32.707	1.00	39.49
971	CB	ASN	120	116.126	10.232	32.200	1.00	33.41
972	CG	ASN	120	115.142	9.796	33.286	1.00	35.58
973	OD1	ASN	120	115.481	9.721	34.465	1.00	38.24
974	ND2	ASN	120	113.907	9.531	32.886	1.00	40.30
975	H	ASN	120	118.092	11.226	30.839	1.00	25.00
976	1HD2	ASN	120	113.277	9.246	33.576	1.00	25.00
977	2HD2	ASN	120	113.672	9.626	31.940	1.00	25.00
978	N	ILE	121	119.347	9.194	33.770	1.00	36.98
979	CA	ILE	121	120.054	7.997	34.192	1.00	29.59
980	C	ILE	121	119.207	7.323	35.264	1.00	29.55
981	O	ILE	121	118.647	7.984	36.134	1.00	30.63
982	CB	ILE	121	121.478	8.319	34.745	1.00	35.93
983	CG1	ILE	121	122.130	7.046	35.300	1.00	34.57
984	CG2	LE	121	121.419	9.425	35.7798	1.00	27.62
985	CD1	ILE	121	123.558	7.221	35.775	1.00	37.39
986	H	ILE	121	119.696	10.074	34.313	1.00	25.00
987	N	SER	122	119.086	6.007	35.172	1.00	32.39
968	CA	SER	122	118.299	5.245	36.129	1.00	27.80
989	C	SER	122	118.912	5.243	37.526	1.00	27.11
990	O	SER	122	120.130	5.143	37.685	1.00	30.59
991	CB	SER	122	118.145	3.801	35.642	1.00	28.47
992	OG	SER	122	117.529	2.993	36.633	1.00	27.99
993	H	SER	122	119.540	5.535	34.444	1.00	25.00
994	HG	SER	122	117.442	2.098	36.275	1.00	25.00
995	N	PRO	123	118.065	5.325	38.564	1.00	27.95
996	CA	PRO	123	118.542	5.323	39.949	1.00	27.26
997	C	PRO	123	118.941	3.904	40.372	1.00	33.55
998	O	PRO	123	119.325	3.664	41.521	1.00	34.51
999	CB	PRO	123	117.323	5.823	40.723	1.00	26.86
1000	CG	PRO	123	116.184	5.252	39.938	1.00	26.05
1001	CD	PRO	123	116.605	5.531	38.510	1.00	24.97
1002	N	GLU	124	118.849	2.967	39.431	1.00	34.65
1003	CA	GLU	124	119.199	1.569	39.673	1.00	42.28
1004	C	GLU	124	120.673	1.441	40.056	1.00	39.18
1005	O	GLU	124	121.072	0.492	40.735	1.00	41.59
1006	CB	GLU	124	118.902	0.732	38.424	1.00	48.21
1007	CG	GLU	124	119.074	−0.773	38.601	1.00	61.85
1008	CD	GLU	124	118.112	−1.379	39.615	1.00	71.29
1009	OE1	GLU	124	117.022	−0.803	39.851	1.00	70.67
1010	OE2	GLU	124	118.450	−2.447	40.170	1.00	76.93
1011	H	GLU	124	118.522	3.203	38.539	1.00	25.00
1012	N	ILE	125	121.466	2.430	39.657	1.00	36.76
1013	CA	ILE	125	122.892	2.458	39.955	1.00	35.15
1014	C	ILE	125	123.155	2.401	41.472	1.00	35.83
1015	O	ILE	125	124.237	2.016	41.900	1.00	36.05
1016	CB	ILE	125	123.557	3.718	39.319	1.00	33.60
1017	CG1	ILE	125	125.082	3.610	39.368	1.00	32.56
1018	CG2	ILE	125	123.087	4.988	40.017	1.00	28.43
1019	CD1	ILE	125	125.789	4.705	38.586	1.00	28.58
1020	H	ILE	125	121.080	3.169	39.141	1.00	25.00
1021	N	PHE	126	122.145	2.733	42.276	1.00	33.20
1022	CA	PHE	126	122.276	2.717	43.731	1.00	33.30
1023	C	PHE	126	121.902	1.394	44.402	1.00	38.46
1024	O	PHE	126	122.171	1.211	45.591	1.00	38.34
1025	CB	PHE	126	121.444	3.843	44.362	1.00	29.75
1026	CG	PHE	126	121.937	5.218	44.030	1.00	32.61
1027	CD1	PHE	126	123.084	5.724	44.631	1.00	29.30

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1028	CD2	PHE	126	121.263	6.007	43.103	1.00	33.58
1029	CE1	PHE	126	123.558	6.997	44.310	1.00	31.83
1030	CE2	PHE	126	121.726	7.279	42.775	1.00	36.03
1031	CZ	PHE	126	122.877	7.776	43.380	1.00	34.15
1032	H	PHE	126	121.286	3.004	41.891	1.00	25.00
1033	N	SER	127	121.285	0.477	43.662	1.00	37.94
1034	CA	SER	127	120.871	−0.806	44.236	1.00	37.24
1035	C	SER	127	122.012	−1.601	44.855	1.00	37.05
1036	O	SER	127	121.842	−2.210	45.908	1.00	37.94
1037	CB	SER	127	120.141	−1.658	43.201	1.00	34.22
1038	OG	SER	127	118.885	−1.087	42.887	1.00	44.36
1039	H	SER	127	121.104	0.658	42.719	1.00	25.00
1040	HG	SER	127	119.018	−0.202	42.539	1.00	25.00
1041	N	LYS	128	123.184	−1.557	44.228	1.00	37.17
1042	CA	LYS	128	124.348	−2.280	44.737	1.00	39.88
1043	C	LYS	128	124.840	−1.783	46.097	1.00	42.69
1044	O	LYS	128	125.690	−2.417	46.720	1.00	48.65
1045	CB	LYS	128	125.492	−2.257	43.715	1.00	39.92
1046	CG	LYS	128	125.877	−0.882	43.210	1.00	41.79
1047	CD	LYS	128	126.864	−0.983	42.061	1.00	45..38
1048	CE	LYS	128	127.112	0.380	41.430	1.00	57.33
1049	NZ	LYS	128	128.057	0.329	40.278	1.00	63.77
1050	H	LYS	128	123.266	−1.028	43.408	1.00	25.00
1051	1HZ	LYS	128	128.971	−0.047	40.597	1.00	25.00
1052	2HZ	LYS	128	127.667	−0.293	39.541	1.00	25.00
1053	3HZ	LYS	128	128.187	1.285	39.892	1.00	25.00
1054	N	PHE	129	124.305	−0.656	46.556	1.00	41.03
1055	CA	PHE	129	124.697	−0.090	47.844	1.00	38.56
1056	C	PHE	129	123.574	−0.255	48.848	1.00	42.42
1057	O	PHE	129	123.617	0.319	49.940	1.00	44.74
1058	CB	PHE	129	125.013	1.396	47.695	1.00	32.52
1059	CG	PHE	129	125.984	1.691	46.604	1.00	28.29
1060	CD1	PHE	129	127.291	1.225	46.677	1.00	27.71
1061	CD2	PHE	129	125.585	2.402	45.481	1.00	27.23
1062	CE1	PHE	129	128.186	1.461	45.645	1.00	27.92
1063	CE2	PHE	129	126.473	2.644	44.442	1.00	29.82
1064	CZ	PHE	129	127.776	2.172	44.523	1.00	29.88
1065	H	PHE	129	123.617	−0.193	46.037	1.00	25.00
1066	N	GLN	130	122.566	−1.036	48.482	1.00	46.51
1067	CA	GLN	130	121.425	−1.242	49.356	1.00	52.21
1068	C	GLN	130	121.181	−2.700	49.659	1.00	60.08
1069	O	GLN	130	121.565	−3.588	48.891	1.00	57.60
1070	CB	GLN	130	120.173	−0.638	48.736	1.00	50.11
1071	CG	GLN	130	120.247	0.860	48.526	1.00	50.91
1072	CD	GLN	130	119.025	1.399	47.840	1.00	51.21
1073	OE1	GLN	130	118.339	0.677	47.117	1.00	52.53
1074	NE2	GLN	130	118.737	2.677	48.061	1.00	47.70
1075	H	GLN	130	122.585	−1.533	47.632	1.00	25.00
1076	1HE2	GLN	130	117.922	2.996	47.623	1.00	25.00
1077	2HE2	GLN	130	119.296	3.221	48.627	1.00	25.00
1078	N	ASP	131	120.531	−2.944	50.790	1.00	67.42
1079	CA	ASP	131	120.236	−4.306	51.203	1.00	74.82
1080	C	ASP	131	118.975	−4.746	50.421	1.00	79.83
1081	O	ASP	131	118.273	−3.905	49.822	1.00	81.73
1082	CB	ASP	131	120.046	4.394	52.745	1.00	75.37
1083	CG	ASP	131	118.894	−3.558	53.284	1.00	79.54
1084	OD1	ASP	131	118.173	−2.911	52.501	1.00	89.69
1085	OD2	ASP	131	118.707	−3.540	54.511	1.00	80.32
1086	H	ASP	131	120.203	−2.147	51.259	1.00	25.00
1087	N	GLU	132	118.671	−6.041	50.521	1.00	86.92
1088	CA	GLU	132	117.492	−6.620	49.865	1.00	93.82
1089	C	GLU	132	116.183	−5.970	50.310	1.00	94.42
1090	O	GLU	132	115.084	−6.369	49.910	1.00	95.34
1091	CB	GLU	132	117.414	−8.108	50.165	1.00	99.58
1092	CG	GLU	132	118.603	−8.893	49.626	1.00	110.72
1093	CD	GLU	132	118.550	−10.369	49.968	1.00	117.77
1094	OE1	GLU	132	118.100	−10.716	51.082	1.00	122.96
1095	OE2	GLU	132	118.962	−11.187	49.117	1.00	118.79
1096	H	GLU	132	119.347	−6.569	50.930	1.00	25.00
1097	N	ASN	133	116.318	−4.957	51.145	1.00	94.58
1098	CA	ASN	1333	115.214	4.208	51.715	1.00	92.72

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1099	C	ASN	133	115.107	−2.839	51.042	1.00	90.09
1100	O	ASN	133	114.134	−2.112	51.210	1.00	90.03
1101	CB	ASN	133	115.492	−4.043	53.214	1.00	99.96
1102	CG	ASN	133	114.389	−3.337	53.923	1.00	106.41
1103	OD1	ASN	133	113.275	−3.847	54.016	1.00	108.32
1104	ND2	ASN	133	114.683	−2.159	54.447	1.00	111.37
1105	H	ASN	133	117.175	−4.667	51.437	1.00	25.00
1106	1HD2	ASN	133	113.925	−1.736	54.889	1.00	25.00
1107	2HD2	ASN	133	115.561	−1.741	54.365	1.00	25.00
1108	N	GLY	134	116.139	−2.501	50.284	1.00	84.16
1109	CA	GLY	134	116.195	−1.224	49.597	1.00	77.66
1110	C	GLY	134	116.752	−0.121	50.479	1.00	73.68
1111	O	GLY	134	116.780	1.040	50.072	1.00	72.39
1112	H	GLY	134	116.840	−3.192	50.233	1.00	25.00
1113	N	LYS	135	117.141	−0.462	51.704	1.00	70.01
1114	CA	LYS	135	117.724	0.524	52.606	1.00	61.88
1115	C	LYS	135	119.229	0.556	52.361	1.00	58.01
1116	O	LYS	135	119.831	−0.473	52.038	1.00	52.64
1117	CB	LYS	135	117.429	0.190	54.069	1.00	52.54
1118	CG	LYS	135	116.279	0.994	54.661	1.00	69.58
1119	CD	LYS	135	114.935	0.594	54.062	1.00	74.13
1120	CE	LYS	136	113.799	1.517	54.474	1.00	77.90
1121	NZ	LYS	135	113.779	1.824	55.931	1.00	77.60
1122	H	LYS	135	117.045	−1.379	52.010	1.00	25.00
1123	1HZ	LYS	135	113.687	0.959	956.498	1.00	25.00
1124	2HZ	LYS	135	114.669	2.310	56.155	1.00	25.00
1125	3HZ	LYS	135	112.977	2.401	56.110	1.00	25.00
1126	N	PHE	136	119.834	1.731	52.491	1.00	53.56
1127	CA	PHE	136	121.268	1.864	52.261	1.00	46.60
1128	C	PHE	136	122.075	1.074	53.275	1.00	46.58
1129	O	PHE	136	121.797	1.118	54.473	1.00	47.43
1130	CB	PHE	136	121.686	3.336	52.270	1.00	39.21
1131	CG	PHE	136	121.382	4.056	50.990	1.00	32.34
1132	CD1	PHE	136	122.171	3.854	49.863	1.00	31.37
1133	CD2	PHE	136	120.282	4.898	50.896	1.00	32.38
1134	CE1	PHE	136	121.876	4.491	48.657	1.00	25.70
1135	CE2	PHE	136	119.976	5.540	49.701	1.00	34.62
1136	CZ	PHE	136	120.771	5.330	48.573	1.00	28.91
1137	H	PHE	136	119.315	2.505	52.789	1.00	25.00
1138	N	LYS	137	123.046	0.315	52.776	1.00	48.31
1139	CA	LYS	137	123.910	−0.487	53.829	1.00	53.52
1140	C	LYS	137	124.551	0.429	54.656	1.00	59.01
1141	O	LYS	137	125.408	1.247	54.316	1.00	64.30
1142	CB	LYS	137	125.007	−1.160	52.801	1.00	48.57
1143	CG	LYS	137	124.526	−2.258	51.872	1.00	52.37
1144	CD	LYS	137	125.683	−2.796	51.049	1.00	56.61
1145	CE	LYS	137	125.266	−3.980	50.199	1.00	55.76
1146	NZ	LYS	137	126.388	4.433	49.330	1.00	62.73
1147	H	LYS	137	123.197	0.306	51.808	1.00	25.00
1148	1HZ	LYS	137	127.197	−4.714	49.920	1.00	25.00
1149	2HZ	LYS	137	126.377	−5.245	48.758	1.00	25.00
1150	3HZ	LYS	137	126.670	−3.656	48.699	1.00	25.00
1151	N	GLU	138	124.151	0.281	55.914	1.00	61.30
1152	CA	GLU	138	124.688	1.107	56.991	1.00	62.65
1153	C	GLU	138	126.219	1.035	57.078	1.00	60.08
1154	O	GLU	138	126.855	1.862	57.732	1.00	61.14
1155	CB	GLU	138	124.049	0.720	58.324	1.00	63.46
1156	CG	GLU	138	122.561	1.033	58.457	1.00	67.41
1157	CD	GLU	138	122.276	2.499	58.743	1.00	68.98
1158	OE1	GLU	138	122.994	3.105	59.568	1.00	67.92
1159	OE2	GLU	138	121.317	3.043	58.154	1.00	72.44
1160	H	GLU	138	123.462	−0.385	56.115	1.00	25.00
1161	N	SER	139	126.807	0.062	56.390	1.00	54.50
1162	CA	SER	139	128.255	−0.105	56.357	1.00	54.27
1163	C	SER	139	128.960	1.037	55.609	1.00	51.34
1164	O	SER	139	130.144	1.292	55.828	1.00	53.27
1165	CB	SER	139	128.600	−1.453	55.722	1.00	59.61
1166	OG	SER	139	127.596	−1.846	54.800	1.00	67.84
1167	H	SER	139	126.266	−0.582	55.893	1.00	25.00
1168	HG	SER	139	127.548	−1.203	54.087	1.00	25.00
1169	N	LEU	140	128.225	1.714	54.728	1.00	46.50

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1170	CA	LEU	140	128.751	2.839	53.953	1.00	37.91
1171	C	LEU	140	128.861	4.092	54.826	1.00	33.78
1172	O	LEU	140	129.454	5.090	54.422	1.00	30.69
1173	CB	LEU	140	127.821	3.151	52.777	1.00	39.38
1174	CG	LEU	140	127.643	2.142	51.639	1.00	42.09
1175	CD1	LEU	140	126.330	2.417	50.919	1.00	38.48
1176	CD2	LEU	140	128.819	2.212	50.672	1.00	38.39
1177	H	LEU	140	127.290	1.456	54.590	1.00	25.00
1178	N	ALA	141	128.295	4.024	56.026	1.00	28.75
1179	CA	ALA	141	128.288	5.141	56.964	1.00	29.20
1180	C	ALA	141	129.646	5.737	57.310	1.00	30.53
1881	O	ALA	141	129.713	6.825	57.882	1.00	30.24
1182	CS	ALA	141	127.565	4.742	58.235	1.00	28.51
1183	H	ALA	141	127.860	3.193	56.303	1.00	25.00
1184	N	SER	142	130.719	5.018	57.002	1.00	28.14
1185	CA	SER	142	132.062	5.500	57.297	1.00	30.43
1186	C	SER	142	132.788	6.004	56.051	1.00	30.66
1187	O	SER	142	133.961	6.371	56.107	1.00	39.46
1188	CB	SER	142	132.879	4.409	58.011	1.00	30.29
1189	OG	SER	142	132.790	3.146	57.358	1.00	26.69
1190	H	SER	142	130.627	4.148	56.569	1.00	25.00
1191	HG	SER	142	133.417	2.568	57.780	1.00	25.00
1192	N	ASP	143	132.069	6.053	54.937	1.00	27.41
1193	CA	ASP	143	132.614	6.512	53.663	1.00	28.00
1194	C	ASP	143	132.168	7.966	53.447	1.00	33.02
1195	O	ASP	143	131.211	8.232	52.714	1.00	34.43
1196	CB	ASP	143	132.085	5.603	52.540	1.00	26.21
1197	CG	ASP	143	132.609	5.978	51.160	1.00	32.37
1198	OD1	ASP	143	133.578	6.762	51.045	1.00	34.10
1199	OD2	ASP	143	132.041	5.465	50.174	1.00	37.80
1200	H	ASP	143	131.130	5.700	54.969	1.00	25.30
1201	N	VAL	144	132.884	8.906	54.060	1.00	31.09
1202	CA	VAL	144	132.548	10.328	53.958	1.00	27.23
1203	C	VAL	144	132.392	10.873	52.534	1.00	27.59
1204	O	VAL	144	131.404	11.545	52.243	1.00	25.91
1205	CB	VAL	144	133.541	11.204	54.758	1.00	27.72
1206	CG1	VAL	144	133.183	12.684	54.621	1.00	21.28
1207	CG2	VAL	144	133.509	10.804	56.227	1.00	34.69
1208	H	VAL	144	133.643	8.619	54.609	1.00	25.00
1209	N	LEU	145	133.344	10.580	51.649	1.00	25.30
1210	CA	LEU	145	133.266	11.063	50.268	1.00	27.68
1211	C	LEU	145	132.039	10.510	49.544	1.00	29.04
1212	O	LEU	145	131.392	11.218	48.773	1.00	26.76
1213	CB	LEU	145	134.541	10.722	49.487	1.00	27.26
1214	CG	LEU	145	135.839	11.375	49.970	1.00	29.50
1215	CD1	LEU	145	136.956	11.087	48.983	1.00	25.10
1216	CD2	LEU	145	135.648	12.875	50.113	1.00	31.66
1217	H	LEU	145	134.098	10.040	51.931	1.00	25.00
1218	N	GLY	146	131.717	9.247	49.806	1.00	27.11
1219	CA	GLY	146	130.552	8.643	49.185	1.00	25.43
1220	C	GLY	146	129.288	9.290	49.726	1.00	27.86
1221	O	GLY	146	128.373	9.621	48.968	1.00	24.45
1222	H	GLY	146	132.255	8.727	50.431	1.00	25.00
1223	N	LEU	147	129.251	9.485	51.043	1.00	21.13
1224	CA	LEU	147	128.114	10.102	551.712	1.00	23.48
1225	C	LEU	147	127.867	11.519	51.202	1.00	23.64
1226	O	LEU	147	126.722	11.922	51.002	1.00	25.30
1227	CB	LEU	147	128.338	10.140	53.226	1.00	23.15
1228	CG	LEU	147	128.286	8.821	54.003	1.00	30.78
1229	CD1	LEU	147	128.667	9.059	55.455	1.00	24.16
1230	CD2	LEU	147	126.892	8.210	53.911	1.00	22.86
1231	H	LEU	147	130.010	9.196	51.584	1.00	25.00
1232	N	LEU	148	128.943	12.265	50.978	1.00	20.29
1233	CA	LEU	148	128.831	13.633	50.498	1.00	24.04
1234	C	LEU	148	128.217	13.664	49.106	1.00	23.69
1235	O	LEU	148	127.267	14.408	48.855	1.00	26.51
1236	CB	LEU	148	130.198	14.328	50.506	1.00	22.43
1237	CG	LEU	148	130.240	15.787	50.033	1.00	24.68
1238	CD1	LEU	148	129.285	16.649	50.853	1.00	16.95
1239	CD2	LEU	148	131.662	16.314	50.136	1.00	19.49
1240	H	LEU	148	129.830	11.885	51.143	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1241	N	ASN	149	128.742	12.845	48.203	1.00	23.38
1242	CA	ASN	149	128.210	12.801	46.850	1.00	20.71
1243	C	ASN	149	126.761	12.269	46.809	1.00	25.14
1244	O	ASN	149	125.990	12.678	45.956	1.00	25.34
1245	CB	ASN	149	129.125	12.008	45.932	1.00	15.21
1246	CG	ASN	149	130.320	12.817	45.489	1.00	19.96
1247	OD1	ASN	149	131.340	12.856	46.167	1.00	34.43
1248	ND2	ASN	149	130.185	13.505	44.369	1.00	25.72
1249	H	ASN	149	129.509	12.271	48.444	1.00	25.00
1250	1HD2	ASN	149	130.969	14.021	44.090	1.00	25.00
1251	2HD2	ASN	149	129.340	13.468	43.887	1.00	25.00
1252	N	LEU	150	126.445	11.379	47.743	1.00	21.91
1253	CA	LEU	150	125.096	10.829	47.827	1.00	24.64
1254	C	LEU	150	124.171	11.938	48.330	1.00	22.13
1255	O	LEU	150	123.058	12.104	47.831	1.00	27.92
1256	CB	LEU	150	125.051	9.630	48.780	1.00	17.59
1257	CG	LEU	150	123.659	9.057	49.062	1.00	21.25
1258	CD1	LEU	150	123.054	8.510	47.780	1.00	18.26
1259	CD2	LEU	150	123.739	7.976	50.118	1.00	19.18
1260	H	LEU	150	127.125	11.076	48.382	1.00	25.00
1261	N	TYR	151	124.652	12.706	49.301	1.00	20.18
1262	CA	TYR	151	123.892	13.818	49.858	1.00	20.96
1263	C	TYR	151	123.533	14.798	48.738	1.00	19.39
1264	O	TYR	151	122.380	15.204	48.592	1.00	21.76
1265	CB	TYR	151	124.723	14.535	50.929	1.00	20.29
1266	CG	TYR	151	124.115	15.828	51.418	1.00	22.32
1267	CD1	TYR	151	123.202	15.834	52.470	1.00	20.29
1268	CD2	TYR	151	124.432	17.047	50.811	1.00	21.17
1269	CE1	TYR	151	122.614	17.021	52.907	1.00	20.42
1270	CE2	TYR	151	123.850	18.236	51.237	1.00	21.39
1271	CZ	TYR	151	122.940	18.214	52.285	1.00	22.07
1272	OH	TYR	151	122.337	19.377	52.696	1.00	21.54
1273	H	TYR	151	125.542	12.522	49.655	1.00	25.00
1274	HH	TYR	151	121.769	19.210	53.457	1.00	25.00
12775	N	GLU	152	124.532	15.194	47.959	1.00	21.41
1276	CA	GLU	152	124.316	16.128	46.863	1.00	19.05
1277	C	GLU	152	123.388	15.546	45.800	1.00	23.34
1278	O	GLU	152	122.540	16.259	45.260	1.00	21.99
1279	CB	GLU	152	125.653	16.544	46.235	1.00	23.58
1280	CG	GLU	152	126.641	17.236	47.198	1.00	23.54
1281	CD	GLU	152	126.245	18.662	47.577	1.00	27.07
1282	OE1	GLU	152	125.046	19.009	47.529	1.00	30.35
1283	OE2	GLU	152	127.145	19.444	47.935	1.00	23.20
1284	H	GLU	152	125.434	14.851	48.136	1.00	25.00
1285	N	ALA	153	123.530	14.248	45.526	1.00	24.42
1286	CA	ALA	153	122.706	13.565	44.526	1.00	22.61
1287	C	ALA	153	121.251	13.409	44.964	1.00	19.49
1288	O	ALA	153	120.342	13.450	44.138	1.00	21.30
1289	CB	ALA	153	123.300	12.203	44.186	1.00	21.47
1290	H	ALA	153	124.211	13.731	46.006	1.00	25.00
1291	N	SER	154	121.026	13.262	46.264	1.00	16.33
1292	CA	SER	154	119.672	13.105	46.776	1.00	21.77
1293	C	SER	154	118.822	14.343	46.464	1.00	27.62
1294	O	SER	154	117.603	14.258	46.351	1.00	29.95
1295	CB	SER	154	119.688	12.820	48.288	1.00	15.72
1296	OG	SER	154	119.902	13.991	49.060	1.00	20.33
1297	H	SER	154	121.776	13.256	46.901	1.00	25.00
1298	HG	SER	154	119.193	14.609	48.898	1.00	25.00
1299	N	HIS	155	119.470	15.489	46.291	1.00	24.50
1300	CA	HIS	155	118.751	16.720	46.001	1.00	20.74
1301	C	HIS	155	118.320	16.907	44.552	1.00	22.52
1302	O	HIS	155	117.682	17.905	44.224	1.00	23.13
1303	CB	HIS	155	119.543	17.929	46.487	1.00	19.93
1304	CG	HiS	155	119.439	18.154	47.961	1.00	14.77
1305	ND1	HIS	155	120.456	17.843	48.838	1.00	20.63
1306	CD2	HIS	155	118.431	18.652	48.716	1.00	13.91
1307	CE1	HIS	155	120.080	18.142	50.069	1.00	21.57
1308	NE2	HIS	155	118.855	18.634	50.022	1.00	17.34
1309	H	HIS	155	120.451	15.494	46.346	1.00	25.00
1310	HD1	HIS	155	121.317	17.420	48.603	1.00	25.00
1311	HE2	HIS	155	118.336	18.952	50.793	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1312	N	VAL	156	118.686	15.972	43.678	1.00	22.99
1313	CA	VAL	156	118.283	16.063	42.276	1.00	22.09
1314	C	VAL	156	117.265	14.970	41.940	1.00	22.99
1315	O	VAL	156	116.954	14.741	40.768	1.00	22.80
1316	CB	VAL	156	119.491	15.956	41.299	1.00	18.92
1317	CG1	VAL	156	120.541	16.999	41.636	1.00	20.34
1318	CG2	VAL	156	120.089	14.560	41.329	1.00	20.67
1319	H	VAL	156	119.229	15.207	43.966	1.00	25.00
1320	N	ARG	157	116.729	14.317	42.968	1.00	19.28
1321	CA	ARG	157	115.766	13.239	42.762	1.00	25.29
1322	C	ARG	157	114.394	13.708	42.272	1.00	26.91
1323	O	ARG	157	113.988	14.850	42.498	1.00	27.10
1324	CB	ARG	157	115.625	12.380	44.024	1.00	19.93
1325	CG	ARG	157	114.831	13.011	45.1144	1.00	19.14
1326	CD	ARG	157	114.914	12.156	46.397	1.00	20.33
1327	NE	ARG	157	114.069	12.674	47.473	1.00	30.46
1328	CZ	ARG	157	114.373	13.717	48.242	1.00	36.78
1329	NH1	ARG	157	115.515	14.371	48.071	1.00	39.31
1330	NH2	ARG	157	113.523	14.119	49.176	1.00	36.74
1331	H	ARG	157	116.972	14.566	43.881	1.00	25.00
1332	HE	ARG	157	113.214	12.230	47.643	1.00	25.00
1333	1HH1	ARG	157	116.149	14.079	47.364	1.00	25.00
1334	2HH1	ARG	157	115.736	15.154	48.652	1.00	25.00
1335	1HH2	ARG	157	112.655	13.643	49.305	1.00	25.00
1336	2HH2	ARG	157	113.751	14.905	49.753	1.00	25.00
1337	N	THR	158	113.709	12.813	41.569	1.00	30.13
1338	CA	THR	158	112.385	13.066	41.015	1.00	27.65
1339	C	THR	158	111.374	12.189	41.763	1.00	25.41
1340	O	THR	158	111.751	11.413	42.642	1.00	23.51
1341	CB	THR	158	112.350	12.703	39.513	1.00	24.84
1342	OG1	THR	158	112.630	11.307	39.355	1.00	27.71
1343	CG2	THR	158	113.391	13.496	38.738	1.00	19.09
1344	H	THR	158	114.102	11.937	41.427	1.00	25.00
1345	HG1	THR	158	111.995	10.771	39.817	1.00	25.00
1346	N	HIS	159	110.103	12.268	41.377	1.00	26.77
1347	CA	HIS	159	109.051	11.473	42.016	1.00	27.30
1348	C	HIS	159	109.196	9.971	41.741	1.00	33.58
1349	O	HIS	159	108.630	9.150	42.462	1.00	33.82
1360	CB	HIS	159	107.663	11.939	41.557	1.00	26.01
1351	CG	HIS	159	107.337	13.350	41.941	1.00	23.00
1352	ND1	HIS	159	106.999	13.711	43.226	1.00	24.86
1353	CD2	HIS	159	107.311	14.490	41.210	1.00	18.70
1354	CE1	HIS	159	106.782	15.012	43.275	1.00	24.72
1355	NE2	HIS	159	106.966	15.509	42.064	1.00	23.55
1356	H	HIS	159	109.879	12.878	40.646	1.00	25.00
1357	HD1	HIS	159	106.924	13.094	43.988	1.00	25.00
1358	HE2	HIS	159	106.880	16.460	41.845	1.00	25.00
1359	N	ALA	160	109.948	9.624	40.697	1.00	32.77
1360	CA	ALA	160	110.167	8.229	40.315	1.00	31.64
1361	C	ALA	160	111.364	7.581	41.009	1.00	36.31
1362	O	ALA	160	111.509	6.361	41.002	1.00	37.53
1363	CB	ALA	160	110.326	8.130	38.803	1.00	25.40
1364	H	ALA	160	110.358	10.319	40.160	1.00	25.00
1365	N	ASP	161	112.217	8.401	41.612	1.00	40.41
1366	CA	ASP	161	113.415	7.904	42.281	1.00	40.26
1367	C	ASP	161	113.123	7.414	43.689	1.00	41.77
1368	O	ASP	161	113.634	7.937	44.678	1.00	41.48
1369	CB	ASP	161	114.508	8.976	42.291	1.00	34.22
1370	CG	ASP	161	114.959	9.354	40.898	1.00	34.94
1371	OD1	ASP	161	114.954	8.486	40.002	1.00	33.51
1372	OD2	ASP	161	115.319	10.532	40.697	1.00	32.35
1373	H	ASP	161	112.014	9.350	41.663	1.00	25.00
1374	N	ASP	162	112.353	6.342	43.742	1.00	46.26
1375	CA	ASP	162	111.932	5.726	44.985	1.00	46.59
1376	C	ASP	162	113.108	5.156	45.760	1.00	44.37
1377	O	ASP	162	113.127	5.172	46.990	1.00	37.28
1378	CB	ASP	162	110.916	4.630	44.670	1.00	56.78
1379	CG	ASP	162	109.654	5.185	44.046	1.00	69.65
1380	OD1	ASP	162	108.899	5.870	44.766	1.00	67.08
1381	OD2	ASP	162	109.435	4.978	42.830	1.00	79.19
1382	H	ASP	162	112.114	5.949	42.869	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1383	N	ILE	163	114.106	4.699	45.015	1.00	41.87
1384	CA	ILE	163	115.314	4.112	45.575	1.00	43.77
1385	C	ILE	163	116.093	5.124	46.426	1.00	42.36
1386	O	ILE	163	116.764	4.757	47.385	1.00	45.56
1387	CB	ILE	163	116.200	3.561	44.433	1.00	47.25
1388	CG1	ILE	163	115.385	2.571	43.595	1.00	56..48
1389	CG2	ILE	163	117.433	2.870	44.986	1.00	49.93
1390	CD1	ILE	163	116.134	1.994	42.404	1.00	60.37
1391	H	ILE	163	114.031	4.781	44.043	1.00	25.00
1392	N	LEU	164	115.955	6.404	46.097	1.00	37.87
1393	CA	LEU	164	116.650	7.473	46.805	1.00	33.53
1394	C	LEU	164	115.828	8.132	47.897	1.00	32.57
1395	O	LEU	164	116.206	9.192	48.400	1.00	36.58
1396	CB	LEU	164	117.102	8.542	45.815	1.00	30.53
1397	CG	LEU	164	118.184	8.139	44.815	1.00	36.53
1398	CD1	LEU	164	118.416	9.266	43.820	1.00	26.74
1399	CD2	LEU	164	119.468	7.794	45.562	1.00	30.59
1400	H	LEU	164	115.309	6.641	45.397	1.00	25.00
1401	N	GLU	165	114.737	7.489	48.290	1.00	32.57
1402	CA	GLU	165	113.854	8.022	49.320	1.00	32.62
1403	C	GLU	165	114.537	8.326	50.655	1.00	35.56
1404	O	GUi	135	114.298	9.338	51.267	1.00	35.70
1405	CB	GLU	165	112.683	7.058	49.551	1.00	39.90
1406	CG	GLU	165	111.645	7.571	50.549	1.00	50.03
1407	CD	GLU	165	111.021	8.886	50.115	1.00	59.83
1408	OE1	GLU	165	110.492	8.952	48.983	1.00	63.90
1409	OE2	GLU	165	111.069	9.862	50.899	1.00	58.42
1410	H	GLU	165	114.553	6.614	47.898	1.00	25.00
1411	N	ASP	166	115.411	7.431	51.091	1.00	37.81
1412	CA	ASP	168	116.079	7.609	52.369	1.00	43.12
1413	C	ASP	166	117.546	8.030	52.268	1.00	40.48
1414	O	ASP	166	118.274	8.039	53.262	1.00	40.91
1415	CB	ASP	166	115.899	6.352	53.234	1.00	51.99
1416	CG	ASP	166	114.532	6.303	53.902	1.00	67.29
1417	OD1	ASP	166	114.268	7.173	54.761	1.00	74.04
1418	OD2	ASP	166	113.712	5.423	53.552	1.00	74.06
1419	H	ASP	166	115.669	6.693	50.506	1.00	25.00
1420	N	ALA	167	117.939	8.459	51.075	1.00	34.07
1421	CA	ALA	167	119.298	8.902	50.806	1.00	30.06
1422	C	ALA	167	119.664	10.182	51.554	1.00	33.12
1423	O	ALA	167	120.759	10.292	52.103	1.00	34.41
1424	CB	ALA	167	119.488	9.090	49.308	1.00	25.56
1425	H	ALA	167	117.260	8.486	50.375	1.00	25.00
1426	N	LEU	168	118.737	11.134	51.593	1.00	34.35
1427	CA	LEU	168	118.975	12.403	52.268	1.00	29.26
1428	C	LEU	168	119.184	12.226	53.764	1.00	32.06
1429	O	LEU	168	120.199	12.656	54.311	1.00	34.07
1430	CB	LEU	168	117.820	13.381	52.024	1.00	25.73
1431	CG	LEU	168	117.980	14.767	52.671	1.00	29.40
1432	CD1	LEU	168	119.241	15.454	52.153	1.00	22.56
1433	CD2	LEU	168	116.765	15.635	52.397	1.00	28.30
1434	H	LEU	168	117.879	10.944	51.168	1.00	25.00
1435	N	ALA	169	118.224	11.593	54.425	1.00	32.55
1438	CA	ALA	169	118.317	11.372	55.885	1.00	37.53
1437	C	ALA	169	119.561	10.552	56.227	1.00	37.81
1438	O	ALA	169	120.273	10.873	57.185	1.00	38.90
1439	CB	ALA	1669	117.058	10.680	56.370	1.00	36.88
1440	H	ALA	169	117.444	11.265	53.938	1.00	25.00
144i	N	PHE	170	119.830	9.520	55.429	1.00	30.70
1442	CA	PHE	170	120.976	8.640	55.635	1.00	29.14
1443	C	PHE	170	122.296	9.413	55.592	1.00	31.93
1444	O	PHE	170	123.048	9.432	56.573	1.00	35.80
1445	CB	PHE	170	120.978	7.538	54.569	1.00	27.52
1446	CG	PHE	170	122.093	6.538	54.719	1.00	29.21
1447	CD1	PHE	170	122.055	5.576	55.722	1.00	32.25
1448	CD2	PHE	170	123.178	6.553	53.850	1.00	31.23
1449	CE1	PHE	170	123.085	4.642	55.854	1.00	35.77
1450	CE2	PHE	170	124.213	5.624	53.974	1.00	28.29
1451	CZ	PHE	170	124.166	4.668	54.977	1.00	33.63
1452	H	PHE	170	119.237	9.336	54.671	1.00	25.00
1453	N	SER	171	122.572	10.054	54.460	1.00	29.96

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1454	CA	SER	171	123.803	10.817	54.297	1.00	23.74
1455	C	SER	171	123.888	11.970	55.293	1.00	25.49
1456	O	SER	171	124.951	12.232	55.845	1.00	30.00
1457	CB	SER	171	123.927	11.333	52.860	1.00	25.16
1458	OG	SER	171	122.818	12.137	52.501	1.00	31.46
1459	H	SER	171	121.937	10.029	53.708	1.00	25.00
1460	HG	SER	171	122.754	12.902	53.078	1.00	25.00
1461	N	THR	172	122.761	12.025	55.557	1.00	25.72
1462	CA	THR	172	122.728	13.746	56.490	1.00	25.18
1463	C	THR	172	123.183	13.367	57.902	1.00	30.69
1464	O	THR	172	124.122	13.961	58.438	1.00	29.76
1465	CB	THR	172	121.311	14.390	56.574	1.00	24.33
1466	OG1	THR	172	120.958	14.958	55.307	1.00	19.73
1467	CG2	THR	172	121.282	15.499	57.620	1.00	16.92
1468	H	THR	172	121.932	12.351	55.113	1.00	25.00
1469	HG1	THR	172	120.938	14.264	54.646	1.00	25.00
1470	N	ILE	173	122.542	12.363	58.489	1.00	34.29
1471	CA	ILE	173	122.875	11.951	59.848	1.00	37.02
1472	C	ILE	173	124.319	11.488	60.017	1.00	31.30
1473	O	ILE	173	124.958	11.777	61.032	1.00	34.03
1474	CB	ILE	173	121.894	10.870	60.384	1.00	42.89
1475	CG1	ILE	173	122.082	10.702	61.893	1.00	46.46
1476	CG2	ILE	173	122.115	9.539	59.673	1.00	43.32
1477	CD11	ILE	173	121.040	9.829	62.553	1.00	58.82
1478	H	ILE	173	121.833	11.884	58.002	1.00	25.00
1479	N	HIS	174	124.848	10.790	59.020	1.00	27.02
1480	CA	HIS	174	126.220	10.309	59.100	1.00	30.73
1481	C	HIS	174	127.251	11.412	58.870	1.00	30.72
1482	O	HIS	174	128.261	11.477	59.574	1.00	32.05
1483	CB	HIS	174	126.431	9.118	58.166	1.00	32.72
1484	CG	HIS	174	125.701	7.884	58.603	1.00	42.58
1485	ND1	HIS	174	125.738	7.418	59.902	1.00	43.81
1486	CD2	HIS	174	124.891	7.036	57.925	1.00	39.61
1487	CE1	HIS	174	124.981	6.339	60.005	1.00	38.39
1488	NE2	HIS	174	124.457	6.086	58.820	1.00	38.65
1489	H	HIS	174	124.304	10.608	58.221	1.00	25.00
1490	HD1	HIS	174	126.233	7.787	60.656	1.00	25.00
1491	HE2	HIS	174	123.858	5.338	58.611	1.00	25.00
1492	N	LEU	175	126.970	12.310	57.931	1.00	30.47
1493	CA	LEU	175	127.874	13.420	57.655	1.00	24.51
1494	C	LEU	175	127.926	14.333	58.880	1.00	23.90
1495	O	LEU	175	128.999	14.803	59.267	1.00	27.49
1496	CB	LEU	175	127.429	14.193	56.408	1.00	18.74
1497	CG	LEU	175	127.687	13.517	55.054	1.00	19.75
1498	CD1	LEU	175	127.007	14.295	53.935	1.00	19.14
1499	CD2	LEU	175	129.187	13.404	54.789	1.00	13.66
1500	H	LEU	175	126.143	12.235	57.409	1.00	25.00
1501	N	GLU	176	126.781	14.535	59.524	1.00	23.45
1502	CA	GLU	176	126.7221	15.374	60.717	1.00	29.31
1503	C	GLU	176	127.596	14.788	61.814	1.00	29.58
1504	O	GLU	176	128.222	15.519	62.580	1.00	30.33
1505	CB	GLU	176	125.292	15.477	61.247	1.00	28.86
1506	CG	GLU	176	124.338	16.265	60.381	1.00	41.02
1507	CD	GLU	176	122.976	16.431	61.032	1.00	50.96
1508	OE1	GLU	176	122.409	15.422	61.511	1.00	58.24
1509	OE2	GLU	176	122.474	17.574	61.069	1.00	53.02
1510	H	GLU	176	125.956	14.127	69.182	1.00	25.00
1511	N	SER	177	127.615	13.461	61.890	1.00	31.99
1512	CA	SER	177	128.394	12.746	62.894	1.00	33.70
1513	C	SER	177	129.905	12.777	62.620	1.00	29.73
1514	O	SER	177	130.710	12.952	63.541	1.00	31.31
1515	CB	SER	177	127.896	11.299	62.986	1.00	33.08
1516	OG	SER	177	128.446	10.626	64.103	1.00	42.66
1517	H	SER	177	127.077	12.944	61.259	1.00	25.00
1518	HG	SER	177	128.220	11.094	64.907	1.00	25.00
1519	N	ALA	178	130.283	12.652	61.352	1.00	26.67
1520	CA	ALA	178	131.692	12.641	60.970	1.00	25.61
1521	C	ALA	178	132.351	14.013	60.858	1.00	28.58
1522	O	ALA	178	133.540	14.162	61.153	1.00	23.60
1523	CB	ALA	178	131.862	11.884	59.665	1.00	22.60
1524	H	ALA	178	129.599	12.566	60.656	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1525	N	ALA	179	131.568	15.018	60.475	1.00	25.11
1526	CA	ALA	179	132.068	16.376	60.268	1.00	25.17
1527	C	ALA	179	133.071	16.983	61.254	1.00	25.37
1528	O	ALA	179	134.141	17.430	60.844	1.00	25.58
1529	CB	ALA	179	130.903	17.340	60.044	1.00	21.50
1530	H	ALA	179	130.617	14.840	60.325	1.00	25.00
1531	N	PRO	180	132.771	16.963	62.564	1.00	27.61
1532	CA	PRO	180	133.680	17.541	63.565	1.00	28.57
1533	C	PRO	180	135.132	17.058	63.584	1.00	30.64
1534	O	PRO	180	135.994	17.724	64.155	1.00	37.22
1535	CB	PRO	180	132.988	17.206	64.889	1.00	25.80
1536	CG	PRO	180	131.540	17.118	64.518	1.00	31.06
1537	CD	PRO	180	131.597	16.360	63.221	1.00	30.35
1538	N	HIS	181	135.414	15.910	62.980	1.00	28.35
1539	CA	HIS	181	136.772	15.377	63.013	1.00	27.57
1540	C	HIS	181	137.470	15.237	61.672	1.00	26.99
1541	O	HIS	181	138.529	14.611	61.584	1.00	29.22
1542	CB	HIS	181	136.764	14.035	63.740	1.00	30.76
1543	CG	HIS	181	136.153	14.103	65.104	1.00	32.51
1544	ND1	HIS	181	134.893	13.619	65.379	1.00	34.64
1545	CD2	HIS	181	136.607	14.652	66.257	1.00	34.04
1548	CE1	HIS	181	134.593	13.870	66.641	1.00	35.16
1547	NE2	HIS	181	135.615	14.495	67.196	1.00	38.60
1548	H	HIS	181	134.717	15.429	62.478	1.00	25.00
1549	HD1	HIS	181	134.298	13.158	64.739	1.00	25.00
1550	HE2	HIS	181	135.666	14.802	68.128	1.00	25.00
1551	N	LEU	182	136.890	15.827	60.635	1.00	22.56
1552	CA	LEU	182	137.488	15.750	59.303	1.00	22.65
1553	C	LEU	182	138.532	16.821	59.103	1.00	24.98
1554	O	LEU	182	138.494	17.878	59.741	1.00	22.99
1555	CB	LEU	182	136.372	15.900	58.243	1.00	25.05
1556	CG	LEU	182	135.271	14.835	58.205	1.00	23.65
1557	CD1	LEU	182	134.178	15.274	57.249	1.00	17.28
1558	CD2	LEU	182	135.849	13.483	57.786	1.00	20.03
1559	H	LEU	182	136.072	16.351	60.762	1.00	25.00
1560	N	LYS	183	139.494	16.528	58.236	1.00	22.16
1561	CA	LYS	183	140.556	17.469	57.926	1.00	25.90
1562	C	LYS	183	139.982	18.573	57.045	1.00	30.39
1563	O	LYS	183	138.898	18.429	56.468	1.00	31.71
1564	CB	LYS	183	141.696	16.767	57.183	1.00	27.62
1565	CG	LYS	183	141.274	16.122	555.871	1.00	37.10
1566	CD	LYS	183	142.437	15.441	55.169	1.00	45.13
1567	CE	LYS	183	141.974	14.764	53.885	1.00	50.33
1568	NZ	LYS	183	143.088	14.040	53.210	1.00	57.79
1569	H	LYS	183	139.473	15.658	57.786	1.00	25.00
1570	1HZ	LYS	183	143.846	14.713	52.975	1.00	25.00
1571	2HZ	LYS	183	143.463	13.311	53.852	1.00	25.00
1572	3HZ	LYS	183	142.736	13.592	52.341	1.00	25.00
1573	N	SER	184	140.714	19.674	56.944	1.00	27.77
1574	CA	SER	184	140.304	20.802	56.122	1.00	28.80
1575	C	SER	184	140.970	20.675	54.752	1.00	27.61
1576	O	SER	184	142.084	20.158	54.645	1.00	26.37
1577	CB	SER	184	140.702	22.109	56.805	1.00	28.03
1578	OG	SEER	184	140.003	22.254	58.031	1.00	32.93
1579	H	SER	184	141.565	19.725	57.420	1.00	25.00
1580	HG	SER	184	140.193	21.517	58.620	1.00	25.00
1581	N	PRO	185	140.312	21.171	53.689	1.00	26.21
1582	CA	PRO	185	139.003	21.834	53.680	1.00	23.45
1583	C	PRO	185	137.767	20.926	53.597	1.00	24.54
1584	O	PRO	185	136.638	21.425	53.589	1.00	23.22
1585	CB	PRO	185	139.109	22.737	52.458	1.00	21.98
1586	CG	PRO	185	139.858	21.876	51.503	1.00	21.03
1587	CD	PRO	185	140.949	21.263	52.381	1.00	21.80
1588	N	LEU	186	137.969	19.608	53.570	1.00	21.43
1589	CA	LEU	186	136.852	18.666	53.483	1.00	21.42
1590	C	LEU	186	135.780	18.964	54.522	1.00	22.24
1591	O	LEU	186	134.586	18.987	54.210	1.00	20.84
1592	CS	LEU	186	137.331	17.220	53.654	1.00	23.63
1593	CG	LEU	186	136.217	16.160	53.646	1.00	21.09
1594	CD1	LEU	186	135.491	16.145	52.292	1.00	20.03
1595	CD2	LEU	186	136.800	14.800	53.943	1.00	21.57

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1596	H	LEU	186	138.882	19.259	53.605	1.00	25.00
1597	N	ARG	187	136.221	19.208	55.751	1.00	16.73
1598	CA	ARO	187	135.326	19.515	56.859	1.00	22.57
1599	C	ARG	187	134.427	20.723	56.564	1.00	27.49
1600	O	ARG	187	133.225	20.693	56.848	1.00	26.35
1601	CB	ARG	187	136.146	19.777	58.117	1.00	17.71
1602	CG	ARG	187	135.325	20.087	59.343	1.00	21.93
1603	CD	ARG	187	136.235	20.478	60.483	1.00	31.75
1604	NE	ARG	187	135.507	20.685	61.727	1.00	46.15
1605	CZ	ARG	187	136.087	20.961	62.89	1.00	58.70
1606	NH1	ARG	187	137.412	21.066	62.970	1.00	57.84
1607	NH2	ARG	187	135.344	21.111	63.982	1.00	58.69
1608	H	ARG	187	137.182	19.161	55.923	1.00	25.00
1609	HE	ARG	187	134.530	20.613	61.708	1.00	25.00
1610	1HH1	ARG	187	137.977	20.941	62.156	1.00	25.00
1611	2HH1	ARG	187	137.843	21.275	63.848	1.00	25.00
1612	1HH2	ARG	187	134.351	21.012	63.926	1.00	25.00
1613	2HH2	ARG	187	135.779	21.316	64.858	1.00	25.00
1614	N	GLU	188	135.010	21.782	56.001	1.00	28.09
1615	CA	GLU	188	134.255	22.993	55.667	1.00	26.62
16116	C	GLU	188	133.293	22.726	54.516	1.00	22.97
1617	O	GLU	188	132.203	23.296	54.462	1.00	21.14
1618	CB	GLU	188	135.192	24.153	55.305	1.00	24.01
1619	CG	GLU	188	135.934	24.768	56.482	1.00	32.71
1620	CD	GLU	188	137.045	23.878	57.014	1.00	42.50
1621	OE1	GLU	188	138.030	23.657	56.279	1.00	43.53
1622	OE2	GLU	188	136.936	23.403	58.165	1.00	47.38
1623	H	GLU	188	135.965	21.747	55.798	1.00	25.00
1624	N	GLN	189	133.702	21.853	53.601	1.00	19.36
1625	CA	GLN	189	132.872	21.496	52.460	1.00	20.62
1626	C	GLN	189	131.636	20.728	52.927	1.00	22.47
1627	O	GLN	189	130.522	21.010	52.483	1.00	25.58
1628	CB	GLN	189	133.672	20.662	51.461	1.00	17.31
1629	CG	GLN	189	132.915	20.359	50.187	1.00	24.12
1630	CD	GLN	189	133.796	19.780	49.104	1.00	25.67
1631	OE1	GLN	189	133.691	20.162	47.939	1.00	28.92
1632	NE2	GLN	189	134.666	18.850	49.477	1.00	28.68
1633	H	GLN	189	134.590	21.445	53.695	1.00	25.00
1634	1HE2	GLN	189	135.235	18.480	48.773	1.00	25.00
1635	2HE2	GLN	189	134.704	18.576	50.413	1.00	25.00
1636	N	VAL	190	131.833	19.783	53.846	1.00	22.03
1637	CA	VAL	190	130.734	18.983	54.388	1.00	22.50
1638	C	VAL	190	129.778	19.864	55.198	1.00	22.00
1639	O	VAL	190	128.565	19.846	54.977	1.00	26.49
1640	CB	VAL	190	131.255	17.808	55.274	1.00	18.21
1641	CG1	VAL	190	130.093	17.093	55.947	1.00	19.13
1642	CG2	VAL	190	132.037	16.815	54.422	1.00	13.74
1643	H	VAL	190	132.742	19.618	54.168	1.00	25.00
1644	N	THR	191	130.335	20.638	56.124	1.00	20.35
1645	CA	THR	191	129.555	21.541	56.967	1.00	23.43
1646	C	THR	191	128.733	22.504	56.116	1.00	23.79
1647	O	THR	191	127.564	22.772	56.410	1.00	27.12
1648	CB	THR	191	130.478	22.350	57.903	1.00	29.00
1649	CG1	THR	191	131.124	21.454	58.814	1.00	35.12
1650	CG2	THR	191	129.688	23.385	58.691	1.00	32.22
1651	H	THR	191	131.304	20.599	56.257	1.00	25.00
1652	HG1	THR	191	131.661	20.824	58.321	1.00	25.00
1653	N	HIS	192	129.345	23.015	55.054	1.00	22.27
1654	CA	HIS	192	128.658	23.935	54.168	1.00	24.21
1655	C	HIS	192	127.530	23.226	53.417	1.00	24.78
1656	O	HIS	192	126.421	23.756	53.326	1.00	20.41
1657	CB	HIS	192	129.632	24.564	53.173	1.00	17.98
1658	CG	HIS	192	128.965	25.446	52.169	1.00	21.55
1659	ND1	HIS	192	128.506	26.707	52.480	1.00	21.86
1660	CD2	HIS	192	128.637	25.234	50.872	1.00	20.40
1661	CE1	HIS	192	127.919	27.234	51.420	1.00	20.03
1662	NE2	HIS	192	127.985	26.360	50.432	1.00	20.23
1663	H	HIS	192	130.278	22.766	54.870	1.00	25.00
1664	HD1	HIS	192	128.594	27.143	53.355	1.00	25.00
1665	HE2	HIS	192	127.614	26.486	49.551	1.00	25.00
1666	N	ALA	193	127.826	22.038	52.8888	1.00	22.45

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1667	CA	ALA	193	126.854	21.242	52.139	1.00	20.56
1668	C	ALA	193	125.601	20.963	52.964	1.00	22.26
1669	O	ALA	193	124.485	21.072	52.459	1.00	21.49
1670	CB	ALA	193	127.483	19.938	51.679	1.00	18.73
1671	H	ALA	193	128.729	21.672	53.002	1.00	25.00
1672	N	LEU	194	125.791	20.623	54.236	1.00	23.86
1673	CA	LEU	194	124.678	20.344	55.136	1.00	25.16
1674	C	LEU	194	123.757	21.551	55.298	1.00	26.76
1675	O	LEU	194	122.573	21.391	55.579	1.00	28.61
1676	CB	LEU	194	125.194	19.902	56.509	1.00	23.10
1677	CG	LEU	194	125.924	18.556	56.579	1.00	26.60
1678	CD1	LEU	194	126.426	18.319	57.992	1.00	20.06
1679	CD2	LEU	194	124.998	17.433	56.149	1.00	18.24
1680	H	LEU	194	126.710	20.552	54.574	1.00	25.00
1681	N	GLU	195	124.309	22.754	55.149	1.00	33.01
1682	CA	GLU	195	123.529	23.987	55.277	1.00	34.61
1683	C	GLU	195	123.005	24.448	53.923	1.00	26.09
1684	O	GLU	195	121.952	25.074	53.834	1.00	29.66
1685	CB	GLU	195	124.385	25.102	55.884	1.00	38.35
1686	CG	GLU	195	124.885	24.816	57.288	1.00	59.66
1687	CD	GLU	195	125.945	25.803	57.751	1.00	72.22
1688	OE1	GLU	195	126.800	26.203	56.927	1.00	75.42
1689	OE2	GLU	195	125.931	26.169	58.947	1.00	82.70
1690	H	GLU	195	125.263	22.814	54.944	1.00	25.00
1691	N	GLN	196	123.747	24.130	52.871	1.00	22.78
1692	CA	GLN	196	123.376	24.529	51.527	1.00	20.33
1693	C	GLN	196	123.891	23.520	50.515	1.00	19.79
1694	O	GLN	196	125.094	23.463	50.258	1.00	24.78
1695	CB	GLN	196	123.980	25.903	51.219	1.00	20.38
1696	CG	GLN	196	123.727	26.397	49.807	1.00	24.47
1697	CD	GLN	196	122.253	26.591	49.524	1.00	28.74
1698	OE1	GLN	196	121.622	27.490	50.074	1.00	32.30
1699	NE2	GLN	196	121.694	25.744	48.667	1.00	21.06
1700	H	GLN	196	124.554	23.592	52.995	1.00	25.00
1701	1HE2	GLN	196	120.741	25.876	48.480	1.00	25.00
1702	2HE2	GLN	196	122.247	25.045	48.258	1.00	25.00
1703	N	CYS	197	122.992	22.727	49.942	1.00	19.52
1704	CA	CYS	197	123.399	21.749	48.944	1.00	17.94
1705	C	CYS	197	123.782	22.497	47.669	1.00	18.82
1706	O	CYS	197	123.316	23.614	47.428	1.00	19.62
1707	CB	CYS	197	122.278	20.743	48.669	1.00	21.42
1708	SG	CYS	197	120.832	21.394	47.800	1.00	42.82
1709	H	CYS	197	122.056	22.808	50.202	1.00	25.00
1710	N	LEU	198	124.626	21.878	46.856	1.00	19.01
1711	CA	LEU	198	125.094	22.489	45.620	1.00	20.23
1712	C	LEU	198	123.986	22.760	44.610	1.00	23.18
1713	O	LEU	198	123.868	23.867	44.096	1.00	26.68
1714	CB	LEU	198	126.174	21.608	44.981	1.00	13.53
1715	CG	LEU	198	126.762	22.058	43.640	1.00	20.37
1716	CD1	LEU	198	127.386	23.440	43.773	1.00	19.35
1717	CD2	LEU	198	127.789	21.044	43.158	1.00	18.28
1718	H	LEU	198	124.968	21.004	47.109	1.00	25.00
1719	N	HiS	199	123.160	21.752	44.354	1.00	24.27
1720	CA	HIS	199	122.079	21.859	43.379	1.00	22.48
1721	C	HiS	199	121.089	23.001	43.608	1.00	19.15
1722	O	HIS	199	120.586	23.582	42.653	1.00	19.66
1723	CB	HIS	199	121.327	20.523	43.277	1.00	22.51
1724	CG	HIS	199	120.225	20.519	42.261	1.00	16.72
1725	ND1	HIS	199	120.452	20.697	40.911	1.00	19.56
1726	CD2	HIS	199	118.885	20.360	42.396	1.00	15.14
1727	CE1	HIS	199	119.303	20.648	40.261	1.00	15.68
1728	NE2	HIS	199	118.338	20.444	41.138	1.00	19.96
1729	H	HIS	199	123.297	20.912	44.822	1.00	25.00
1730	HD1	HIS	199	121.340	20.834	40.498	1.00	25.00
1731	HE2	HIS	199	117.376	20.343	40.929	1.00	25.00
1732	N	LYS	200	120.811	23.323	44.864	1.00	18.06
1733	CA	LYS	200	119.853	24.377	45.170	1.00	19.34
1734	C	LYS	200	120.463	25.726	45.548	1.00	21.28
1735	O	LYS	200	119.755	26.617	46.012	1.00	20.62
1736	CB	LYS	200	118.898	23.893	46.264	1.00	17.06
1737	CG	LYS	200	118.144	22.630	45.875	1.00	17.06

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1738	CD	LYS	200	117.287	22.086	47.005	1.00	18.82
1739	CE	LYS	200	116.597	20.804	46.559	1.00	16.83
1740	NZ	LYS	200	115.820	20.155	47.645	1.00	19.41
1741	H	LYS	200	121.264	22.869	45.599	1.00	25.00
1742	1HZ	LYS	200	1166.454	19.923	48.438	1.00	25.00
1743	2HZ	LYS	200	115.081	20.807	47.978	1.00	25.00
1744	3HZ	LYS	200	115.377	19.285	47.288	1.00	25.00
1745	N	GLY	201	121.768	25.881	45.343	1.00	23.54
1746	CA	GLY	201	122.424	27.136	45.675	1.00	19.60
1747	C	GLY	201	122.583	28.062	44.482	1.00	19.35
1748	O	GLY	201	122.569	27.613	43.338	1.00	21.61
1749	H	GLY	201	122.299	25.166	44.933	1.00	25.00
1750	N	VAL	202	122.685	29.363	44.734	1.00	17.34
1751	CA	VAL	202	122.871	30.327	43.653	1.00	17.16
1752	C	VAL	202	124.281	30.084	43.108	1.00	20.63
1753	O	VAL	202	125.248	30.059	43.874	1.00	22.87
1754	CB	VAL	202	122.722	31.778	44.168	1.00	17.85
1755	CG1	VAL	202	123.062	32.782	43.071	1.00	19.32
1756	CG2	VAL	202	121.301	32.003	44.645	1.00	15.75
1757	H	VAL	202	122.625	29.676	45.655	1.00	25.00
1758	N	PRO	203	124.414	29.905	41.780	1.00	18.06
1759	CA	PRO	203	125.705	29.652	41.128	1.00	19.86
1760	C	PRO	203	126.889	30.506	41.588	1.00	23.15
1761	O	PRO	203	127.827	29.974	42.172	1.00	27.00
1762	CB	PRO	203	125.378	29.840	39.650	1.00	21.47
1763	CG	PRO	203	123.982	29.300	39.574	1.00	19.55
1764	CD	PRO	203	123.332	29.952	40.780	1.00	17.62
1765	N	ARG	204	126.844	31.817	41.365	1.00	21.91
1766	CA	ARG	204	127.949	32.683	41.781	1.00	20.91
1767	C	ARG	204	128.283	32.568	43.265	1.00	20.45
1758	O	ARG	204	129.455	22.598	43.638	1.00	25.04
1769	CB	ARG	204	127.681	34.149	41.426	1.00	22.61
1770	CG	ARG	204	127.940	34.519	39.972	1.00	18.14
1771	CD	ARG	204	129.420	34.487	39.618	1.00	21.69
1772	NE	ARG	204	129.852	33.202	39.074	1.00	23.42
1773	CZ	ARG	204	130.953	33.027	38.345	1.00	28.33
1774	NH1	ARG	204	131.747	34.055	38.069	1.00	25.07
1775	NH2	ARG	204	131.248	31.827	37.862	1.00	26.89
1776	H	ARG	204	126.071	32.201	40.913	1.00	25.00
1777	HE	ARG	204	129.297	32.416	39.258	1.00	25.00
1778	1HH1	ARG	204	131.521	34.967	38.404	1.00	25.00
1779	2HHI	ARG	204	132.570	33.921	37.522	1.00	25.00
1780	1HH2	ARG	2004	130.647	31.051	38.047	1.00	25.00
1781	2HH2	ARG	204	132.077	31.699	37.316	1.00	25.00
1782	N	VAL	205	127.264	32.431	44.108	1.00	17.32
1783	CA	VAL	205	127.496	32.312	45.545	1.00	18.99
1784	C	VAL	205	128.267	31.034	45.866	1.00	20.53
1785	O	VAL	205	129.220	31.048	46.647	1.00	24.18
1786	CB	VAL	205	126.175	32.309	46.339	1.00	19.83
1787	CG1	VAL	205	126.442	32.022	47.811	1.00	14.97
1788	CG2	VAL	205	125.473	33.642	46.190	1.00	21.52
1789	H	VAL	205	126.353	32.398	43.764	1.00	25.00
1790	N	GLU	206	127.862	29.933	45.249	1.00	22.23
1791	CA	GLU	206	128.519	28.649	45.478	1.00	22.70
1792	C	GLU	206	129.919	28.601	44.876	1.00	18.65
1793	O	GLU	206	130.838	28.029	45.469	1.00	20.84
1794	CB	GLU	206	127.648	27.506	44.957	1.00	17.73
1795	CG	GLU	206	126.317	27.413	45.683	1.00	20.17
1796	CD	GLU	206	126.478	27.407	47.201	1.00	26.03
1797	OE1	GLU	206	127.190	26.523	47.721	1.00	21.64
1798	OE2	GLU	206	125.895	28.283	47.876	1.00	20.28
1799	H	GLU	206	127.111	29.981	44.620	1.00	25.00
1800	N	THR	207	130.081	29.223	43.714	1.00	18.09
1801	CA	THR	207	131.369	29.291	43.038	1.00	21.23
1802	C	THR	207	132.373	30.057	43.909	1.00	25.71
1803	O	THR	207	133.474	29.568	44.179	1.00	28.93
1804	CB	THR	207	131.219	29.984	41.672	1.00	24.22
1805	OG1	THR	207	130.529	29.1077	40.770	1.00	28.95
1806	CG2	THR	207	132.573	30.379	41.088	1.00	23.10
1807	H	THR	207	129.311	29.644	43.289	1.00	25.00
1808	HG1	THR	207	131.030	28.287	40.685	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1809	N	ARG	208	131.973	31.238	44.374	1.00	24.65
1810	CA	ARG	208	132.825	32.070	45.221	1.00	25.56
1811	C	ARG	208	133.292	31.273	46.432	1.00	25.87
1812	O	ARG	208	134.472	31.289	46.780	1.00	27.73
1813	CB	ARG	208	132.059	33.314	45.682	1.00	25.72
1814	CG	ARG	208	132.836	34.258	46.588	1.00	31.65
1815	CD	ARG	208	134.062	34.826	45.892	1.00	39.53
1816	NE	ARG	208	134.374	36.184	46.344	1.00	46.43
1817	CZ	ARG	208	135.283	36.488	47.266	1.00	47.18
1818	NH11	ARG	208	135.991	35.534	47.858	1.00	54.31
1819	NH2	ARG	208	135.492	37.754	47.592	1.00	54.01
1820	H	ARG	208	131.077	31.566	44.139	1.00	25.00
1821	HE	ARG	208	133.881	36.924	45.937	1.00	25.00
1822	1HH1	ARG	208	135.847	34.577	47.610	1.00	25.00
1823	2HH1	ARG	208	136.673	35.775	48.548	1.00	25.00
1824	1HH2	ARG	208	134.962	38.478	47.150	1.00	25.00
1825	2HH2	ARG	208	136.172	37.986	48.287	1.00	25.00
1826	N	PHE	209	132.364	30.556	47.056	1.00	25.17
1827	CA	PHE	209	132.688	29.750	48.224	1.00	23.72
1828	C	PHE	209	133.677	28.632	47.908	1.00	24.69
1829	O	PHE	209	134.656	28.442	48.626	1.00	24.23
1830	CB	PHE	209	131.430	29.135	48.838	1.00	22.94
1831	CG	PHE	209	131.721	28.195	49.976	1.00	22.62
1832	CD1	PHE	209	132.019	28.691	51.242	1.00	22.83
1833	CD2	PHE	209	131.745	26.817	49.773	1.00	20.76
1834	CE1	PHE	209	132.336	27.824	52.293	1.00	22.43
1835	CE2	PHE	209	132.060	25.946	50.813	1.00	24.13
1836	CZ	PHE	209	132.358	26.450	52.075	1.00	22.16
1837	H	PHE	209	131.439	30.580	46.728	1.00	25.00
1838	N	PHE	210	133.399	27.872	46.856	1.00	24.89
1839	CA	PHE	210	134.263	26.765	46.486	1.00	21.48
1840	C	PHE	210	135.671	27.241	48.172	1.00	23.23
1841	O	PHE	210	138.645	26.676	46.671	1.00	24.15
1842	CB	PHE	210	133.688	25.989	45.296	1.00	18.25
1843	CG	PHE	210	134.4776	24.754	44.944	1.00	20.04
1844	CD1	PHE	210	134.506	23.661	45.811	1.00	17.95
1845	CD2	PHE	210	135.212	24.694	43.763	1.00	19.06
1846	CE1	PHE	210	135.260	22.525	45.510	1.00	17.28
1847	CE2	PHE	210	135.972	23.563	43.450	1.00	21.18
1848	CZ	PHE	210	135.995	22.476	44.329	1.00	18.42
1849	H	PHE	210	132.602	28.062	46.315	1.00	25.00
1850	N	ILE	211	135.781	28.290	45.368	1.00	26.53
1851	CA	ILE	211	137.086	28.818	44.997	1.00	27.06
1852	C	ILE	211	137.917	29.248	46.205	1.00	27.01
1853	O	ILE	211	138.953	28.652	46.490	1.00	25.02
1854	CB	ILE	211	136.967	30.015	44.023	1.00	23.08
1855	CG1	ILE	211	136.317	29.574	42.713	1.00	22.07
1856	CG2	ILE	211	138.344	30.603	43.737	1.00	18.73
1857	CD1	ILE	211	136.163	30.700	41.701	1.00	22.59
1858	H	ILE	211	134.968	28.712	45.022	1.00	25.00
1859	N	SER	212	137.430	30.233	46.949	1.00	26.45
1860	CA	SER	212	138.174	30.758	48.087	1.00	29.47
1861	C	SER	212	138.263	29.914	49.355	1.00	29.82
1862	O	SER	212	139.317	29.873	49.993	1.00	31.08
1863	CB	SER	212	137.691	32.173	48.425	1.00	28.90
1864	OG	SER	212	136.311	32.186	48.742	1.00	48.04
1865	H	SER	212	136.550	30.622	46.740	1.00	25.00
1866	HG	SER	212	136.156	31.647	49.517	1.00	25.00
1867	N	SER	213	137.175	29.249	49.728	1.00	25.54
1868	CA	SER	213	137.173	28.447	50.949	1.00	25.42
1869	C	SER	213	137.555	26.969	50.823	1.00	23.90
1870	O	SER	213	138.019	26.371	51.794	1.00	29.58
1871	CB	SER	213	135.820	28.566	51.662	1.00	19.77
1872	OG	SER	213	135.503	29.920	51.942	1.00	36.00
1873	H	SER	213	136.366	29.279	49.173	1.00	25.00
1874	HG	SER	213	135.449	30.406	51.120	1.00	25.00
1875	N	ILE	214	137.390	26.376	49.645	1.00	20.94
1876	CA	ILE	214	137.701	24.958	49.502	1.00	20.03
1877	C	ILE	214	138.869	24.617	48.591	1.00	20.98
1878	O	ILE	214	139.914	24.174	49.065	1.00	23.05
1879	CB	ILE	214	136.463	24.144	49.041	1.00	20.03

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1880	CG1	ILE	214	135.255	24.455	49.932	1.00	15.38
1881	CG2	ILE	214	136.778	22.640	49.046	1.00	14.86
1882	CD1	ILE	214	135.488	24.207	51.418	1.00	14.56
1883	H	ILE	214	137.066	26.887	48.873	1.00	25.00
1884	N	TYR	215	138.696	24.823	47.289	1.00	18.70
1885	CA	TYR	215	139.733	24.490	46.323	1.00	22.93
1886	C	TYR	215	141.076	25.168	46.582	1.00	25.73
1887	O	TYR	215	142.128	24.545	46.450	1.00	25.96
1888	CB	TYR	215	139.258	24.777	44.899	1.00	19.89
1889	CG	TYR	215	139.859	23.834	43.884	1.00	17.39
1890	CD1	TYR	215	139.726	22.455	44.030	1.00	18.08
1891	CD2	TYR	215	140.557	24.315	42.782	1.00	19.17
1892	CE1	TYR	215	140.275	21.575	43.102	1.00	17.39
1893	CE2	TYR	215	141.113	23.445	41.843	1.00	16.77
1894	CZ	TYR	215	140.967	22.076	42.010	1.00	21.36
1895	OH	TYR	215	141.517	21.212	41.088	1.00	25.91
1896	H	TYR	215	137.858	25.217	46.973	1.00	25.00
1897	HH	TYR	215	141.317	20.302	41.340	1.00	25.00
1898	N	ASP	216	141.037	26.434	46.969	1.00	26.71
1899	CA	ASP	216	142.254	27.184	47.250	1.00	32.33
1900	C	ASP	216	143.057	26.532	48.377	1.00	32.46
1901	O	ASP	216	144.288	26.589	48.387	1.00	33.87
1902	CB	ASP	216	141.895	28.621	47.636	1.00	35.77
1903	CG	ASP	216	143.111	29.514	47.769	1.00	36.73
1904	OD1	ASP	216	143.842	29.670	46.769	1.00	37.16
1905	OD2	ASP	216	143.327	30.062	48.871	1.00	41.08
1906	H	ASP	216	140.170	26.885	447.054	1.00	25.00
1907	N	LYS	217	142.350	25.910	49.316	1.00	31.70
1908	CA	LYS	217	142.978	25.255	50.459	1.00	29.37
1909	C	LYS	217	143.134	23.745	50.269	1.00	30.32
1910	O	LYS	217	143.506	23.029	51.200	1.00	31.00
1911	CB	LYS	217	142.170	25.553	51.724	1.00	26.09
1912	CG	LYS	217	142.062	27.033	52.017	1.00	27.73
1913	CD	LYS	217	141.185	27.312	53.213	1.00	35.35
1914	CE	LYS	217	141.091	28.807	53.463	1.00	40.60
1915	NZ	LYS	217	140.124	29.115	54.551	1.00	49.88
1916	H	LYS	217	141.376	25.876	49.235	1.00	25.00
1917	1HZ	LYS	217	140.429	28.650	55.430	1.00	25.00
1918	2HZ	LYS	217	140.083	30.143	54.698	1.00	25.00
1919	3HZ	LYS	217	139.181	28.767	54.284	1.00	25.00
1920	N	GLU	218	142.864	23.271	49.057	1.00	31.03
1921	CA	GLU	218	142.961	21.855	48.750	1.00	33.23
1922	C	GLU	218	144.391	21.489	48.357	1.00	42.71
1923	O	GLU	218	144.932	22.012	47.381	1.00	41.53
1924	CB	GLU	218	141.983	21.492	47.626	1.00	32.79
1925	CG	GLU	218	141.873	20.007	47.345	1.00	49.16
1926	CD	GLU	218	141.324	19.228	48.526	1.00	61.57
1927	OE1	GLU	218	140.147	19.456	48.886	1.00	66.99
1928	OE2	GLU	218	142.066	18.391	49.092	1.00	62.96
1929	H	GLU	218	142.616	23.896	48.343	1.00	25.00
1930	N	GLN	219	144.974	20.551	49.098	1.00	48.16
1931	CA	GLN	219	146.339	20.089	48.858	1.00	52.73
1932	C	GLN	219	146.533	19.487	47.467	1.00	49.21
1933	O	GLN	219	147.594	19.622	46.870	1.00	51.36
1934	CB	GLN	219	146.733	19.063	49.929	1.00	62.56
1935	CG	GLN	219	148.127	19.262	50.531	1.00	81.40
1936	CD	GLN	219	148.498	18.186	51.534	1.00	90.93
1937	OE1	GLN	219	148.863	17.072	51.156	1.00	97.11
1938	NE2	GLN	219	148.408	18.512	52.825	1.00	96.41
1939	H	GLN	219	144.450	20.162	49.821	1.00	25.00
1940	1HE2	GLN	219	148.113	19.389	53.115	1.00	25.00
1941	2HE2	GLN	219	148.656	17.793	53.455	1.00	25.00
1942	N	SER	220	145.496	18.842	46.950	1.00	47.51
1943	CA	SER	220	145.552	18.199	45.636	1.00	47.04
1944	C	SER	220	144.945	19.020	44.487	1.00	45.29
1945	O	SER	220	144.577	18.407	43.446	1.00	47.02
1946	CB	SER	220	144.862	16.833	45.713	1.00	51.73
1947	OG	SER	220	143.585	16.948	46.327	1.00	55.26
1948	H	SER	220	144.658	18.796	47.447	1.00	25.00
1949	HG	SER	220	143.671	17.280	47.217	1.00	25.00
1950	N	LYS	221	144.849	20.332	44.679	1.00	38.03

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
1951	CA	LYS	221	144.270	21.233	43.682	1.00	32.98
1952	C	LYS	221	145.037	21.284	42.363	1.00	30.63
1953	O	LYS	221	146.249	21.077	42.328	1.00	33.91
1954	CB	LYS	221	144.206	22.649	44.255	1.00	33.08
1955	CG	LYS	221	145.584	23.257	44.500	1.00	40.24
1956	CD	LYS	221	145.512	24.563	45.257	1.00	53.13
19557	CE	LYS	221	146.902	25.093	45.561	1.00	55.90
1958	NZ	LYS	221	146.843	26.358	46.344	1.00	67.32
1959	H	LYS	221	145.198	20.720	45.508	1.00	25.00
1960	1HZ	LYS	221	146.350	26.191	47.244	1.00	25.00
1961	2HZ	LYS	221	147.807	26.698	46.533	1.00	25.00
1962	3HZ	LYS	221	146.326	27.080	45.800	1.00	25.00
1963	N	ASN	222	144.322	21.536	41.273	1.00	28.13
1964	CA	ASN	222	144.958	21.675	39.970	1.00	25.27
1965	C	ASN	222	145.154	23.174	39.816	1.00	30.00
1966	O	ASN	222	144.187	23.933	39.707	1.00	29.84
1967	CB	ASN	222	144.077	21.149	38.843	1.00	22.73
1968	CG	ASN	222	144.688	21.390	37.473	1.00	24.93
1969	OD1	ASN	222	144.914	22.534	37.072	1.00	31.82
1970	ND2	ASN	222	144.973	20.317	36.755	1.00	23.78
1971	H	ASN	222	143.353	21.640	41.343	1.00	25.00
1972	1HD2	ASN	222	145.364	20.460	35.868	1.00	25.00
1973	2HD2	ASN	222	144.734	19.432	37.125	1.00	25.00
1974	N	ASN	223	146.412	23.596	39.819	1.00	31.07
1975	CA	ASN	223	146.759	25.009	39.726	1.00	26.94
1976	C	ASN	223	146.273	25.730	38.477	1.00	25.82
1977	O	ASN	223	145.933	28.910	38.538	1.00	27.88
1978	CB	ASN	223	148.261	25.185	39.915	1.00	23.98
1979	CG	ASN	223	148.739	24.633	41.242	1.00	28.15
1980	OD1	ASN	223	143.586	25.271	42.281	1.00	30.20
1981	ND2	ASN	223	149.291	23.423	41.219	1.00	25.49
1982	H	ASN	223	147.118	22.925	39.901	1.00	25.00
1983	1HD2	ASN	223	149.595	23.063	42.082	1.00	25.00
1984	2HD2	ASN	223	149.377	22.938	40.382	1.00	25.00
1985	N	VAL	224	146.224	25.036	37.346	1.00	24.73
1986	CA	VAL	224	145.743	25.667	36.124	1.00	27.15
1987	C	VAL	224	144.263	26.026	36.304	1.00	28.87
1988	O	VAL	224	143.852	27.150	36.019	1.00	29.97
1989	CB	VAL	224	145.914	24.742	34.900	1.00	31.17
1990	CG1	VAL	224	145.359	25.404	33.651	1.00	30.27
1991	CG2	VAL	224	147.382	24.400	34.707	1.00	30.28
1992	H	VAL	224	146.488	24.096	37.329	1.00	25.00
1993	N	LEU	225	143.486	25.089	36.843	1.00	25.78
1994	CA	LEU	225	142.057	25.303	37.069	1.00	25.90
1995	C	LEU	225	141.792	26.380	38.125	1.00	26.51
1996	O	LEU	225	140.900	27.214	37.956	1.00	26.55
1997	CB	LEU	225	141.366	23.991	37.463	1.00	20.07
1998	CG	LEU	225	141.398	22.848	36.441	1.00	21.81
1999	CD1	LEU	225	140.664	21.638	36.991	1.00	10.56
2000	CD2	LEU	225	140.780	23.295	35.126	1.00	19.02
2001	H	LEU	225	143.883	24.229	37.092	1.00	25.00
2002	N	LEU	226	142.566	26.369	39.207	1.00	22.12
2003	CA	LEU	226	142.400	27.367	40.261	1.00	27.39
2004	C	LEU	228	142.724	28.775	39.743	1.00	28.78
2005	O	LEU	226	141.967	29.720	39.969	1.00	34.36
2006	CB	LEU	226	143.282	27.033	41.468	1.00	25.60
2007	CG	LEU	226	143.170	27.984	42.6665	1.00	26.39
2008	CD1	LEU	226	141.731	28.037	43.183	1.00	20.17
2009	CD2	LEU	226	144.110	27.532	43.763	1.00	26.04
2010	H	LEU	226	143.249	25.673	39.298	1.00	25.00
2011	N	ARG	227	143.842	28.904	39.036	1.00	28.64
2012	CA	ARG	227	144.270	30.183	38.473	1.00	30.51
2013	C	ARG	227	143.186	30.688	37.508	1.00	29.19
2014	O	ARG	227	142.770	31.849	37.567	1.00	25.86
2015	CB	ARG	227	145.607	29.989	37.742	1.00	30.51
2016	CG	ARG	227	146.171	31.215	37.037	1.00	32.00
2017	CD	ARG	227	146.883	32.162	37.981	1.00	35.49
2018	NE	ARG	227	147.414	33.314	37.256	1.00	34.46
2019	CZ	ARG	227	147.799	34.454	37.822	1.00	32.62
2020	NH1	ARG	227	147.727	34.611	39.136	1.00	33.39
2021	NH2	ARG	227	148.214	35.460	37.066	1.00	35.87

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2022	H	ARG	227	144.402	28.114	38.884	1.00	25.00
2023	HE	ARG	227	147.480	33.245	36.292	1.00	25.00
2024	1HH1	ARG	227	147.381	33.871	39.712	1.00	25.00
2025	2HH1	ARG	227	148.020	35.470	39.554	1.00	25.00
2026	1HH2	ARG	227	148.236	35.359	36.073	1.00	25.00
2027	2HH2	ARG	227	148.505	36.315	37.491	1.00	25.00
2028	N	PHE	228	142.723	29.788	36.645	1.00	23.49
2029	CA	PHE	228	141.678	30.063	35.656	1.00	30.24
2030	C	PHE	228	140.411	30.575	36.369	1.00	29.56
2031	O	PHE	228	139.909	31.662	36.068	1.00	31.17
2032	CB	PHE	228	141.394	28.752	34.892	1.00	32.31
2033	CG	PHE	228	140.441	28.879	33.721	1.00	30.15
2034	CD1	PHE	228	139.889	30.103	33.348	1.00	29.90
2035	CD2	PHE	228	140.084	27.740	32.999	1.00	24.53
2036	CE1	PHE	228	138.994	30.188	32.277	1.00	28.21
2037	CE2	PHE	228	139.193	27.811	31.930	1.00	23.61
2038	CZ	PHE	228	138.646	29.036	31.568	1.00	29.31
2039	H	PHE	228	143.108	28.886	36.672	1.00	25.00
2040	N	ALA	229	139.935	29.809	37.344	1.00	25.42
2041	CA	ALA	229	138.737	30.156	38.099	1.00	25.11
2042	C	ALA	229	138.808	31.533	38.764	1.00	29.20
2043	O	ALA	229	137.847	32.310	38.703	1.00	26.99
2044	CB	ALA	229	138.456	29.085	39.135	1.00	20.89
2045	H	ALA	229	140.406	28.982	37.565	1.00	25.00
2046	N	LYS	230	139.944	31.838	39.389	1.00	29.21
2047	CA	LYS	230	140.127	33.121	40.068	1.00	29.75
2048	C	LYS	230	140.100	34.306	39.109	1.00	30.11
2049	O	LYS	230	139.405	35.298	39.350	1.00	30.69
2050	CB	LYS	230	141.434	33.138	40.866	1.00	30.27
2051	CG	LYS	230	141.422	32.247	42.100	1.00	29.79
2052	CD	LYS	230	142.686	32.430	42.923	1.00	24.40
2053	CE	LYS	230	142.595	31.664	44.227	1.00	29.55
2054	NZ	LYS	230	143.790	31.883	45.079	1.00	36.37
2055	H	LYS	230	140.676	31.183	39.394	1.00	25.00
2056	1HZ	LYS	230	143.881	32.896	45.296	1.00	25.00
2057	2HZ	LYS	230	143.689	31.356	45.965	1.00	25.00
2058	33HZ	LYS	230	144.640	31.560	44.573	1.00	25.00
2059	N	LEU	231	140.852	34.201	38.016	1.00	31.56
2060	CA	LEU	231	140.911	35.275	37.032	1.00	30.17
2061	C	LEU	231	139.549	35.506	36.394	1.00	30.20
2062	O	LEU	231	139.085	36.645	36.299	1.00	26.72
2063	CB	LEU	231	141.941	34.959	35.941	1.00	29.21
2064	CG	LEU	231	143.408	34.790	36.340	1.00	26.11
2065	CD1	LEU	231	144.232	34.631	35.077	1.00	22.49
2066	CD2	LEU	231	143.890	35.990	37.139	1.00	22.48
2067	H	LEU	231	141.374	33.380	37.869	1.00	25.00
2068	N	ASP	232	138.898	34.417	35.995	1.00	29.28
2069	CA	ASP	232	137.593	34.490	35.351	1.00	28.41
2070	C	ASP	232	136.549	35.149	36.247	1.00	25.56
2071	O	ASP	232	135.820	36.044	35.813	1.00	25.21
2072	CB	ASP	232	137.131	33.097	34.932	1.00	26.05
2073	CG	ASP	232	136.143	33.143	33.793	1.00	33.93
2074	OD1	ASP	232	136.587	33.188	32.627	1.00	32.45
2075	OD2	ASP	232	134.927	33.157	34.060	1.00	29.97
2076	H	ASP	232	139.310	33.539	36.141	1.00	25.00
2077	N	PHE	233	136.510	34.730	37.507	1.00	24.45
2078	CA	PHE	233	135.569	35.286	38.466	1.00	22.77
2079	C	PHE	233	135.788	36.788	38.603	1.00	28.10
2080	O	PHE	233	134.835	37.568	38.516	1.00	31.99
2081	CB	PHE	233	135.732	34.605	39.831	1.00	19.36
2082	CG	PHE	233	134.714	35.035	40.854	1.00	22.51
2083	CD1	PHE	233	1344.857	36.241	41.540	1.00	22.18
2084	CD2	PHE	233	133.604	34.237	41.127	1.00	23.90
2085	CE1	PHE	233	133.906	36.646	42.481	1.00	26.05
2088	CE2	PHE	233	132.650	34.631	42.065	1.00	23.08
2087	CZ	PHE	233	132.801	35.839	42.743	1.00	24.51
2088	H	PHE	233	137.126	34.022	37.802	1.00	25.00
2089	N	ASN	234	137.044	37.189	38.801	1.00	28.39
2090	CA	ASN	234	137.393	38.602	38.965	1.00	28.37
2091	C	ASN	234	137.079	39.446	37.743	1.00	27.25
2092	O	ASN	234	136.606	40.575	37.868	1.00	32.70

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2093	CB	ASN	234	138.867	38.762	39.342	1.00	27.32
2094	CG	ASN	234	139.152	38.353	40.776	1.00	30.63
2095	OD1	ASN	234	138.242	38.219	41.595	1.00	29.34
2096	ND2	ASN	234	140.426	38.166	41.092	1.00	37.28
2097	H	ASN	234	137.753	38.513	38.851	1.00	25.00
2098	1HD2	ASN	234	140.628	37.901	42.015	1.00	25.00
2099	2HD2	ASN	234	141.114	38.292	40.408	1.00	25.00
2100	N	LEU	235	137.339	38.902	36.561	1.00	28.66
2101	CA	LEU	235	137.059	39.616	35.321	1.00	29.93
2102	C	LEU	235	135.551	39.830	35.167	1.00	30.84
2103	O	LEU	235	135.106	40.949	34.908	1.00	31.89
2104	CB	LEU	235	137.625	38.852	34.119	1.00	29.05
2105	CG	LEU	235	137.476	39.509	32.742	1.00	30.21
2106	CD1	LEU	235	138.045	40.922	32.769	1.00	29.02
2107	CD2	LEU	235	138.173	38.667	31.684	1.00	31.45
2108	H	LEU	235	137.721	38.001	36.525	1.00	25.00
2109	N	LEU	236	134.766	38.769	35.352	1.00	29.90
2110	CA	LEU	236	133.311	38.875	35.245	1.00	28.94
2111	C	LEU	236	132.774	39.874	36.263	1.00	28.31
2112	O	LEU	236	131.833	40.623	35.979	1.00	29.04
2113	CB	LEU	236	132.632	37.518	35.463	1.00	26.96
2114	CG	LEU	236	132.722	36.463	34.359	1.00	32.49
2115	CD1	LEU	236	131.797	35.299	34.694	1.00	28.63
2116	CD2	LEU	236	132.326	37.068	33.026	1.00	30.07
2117	H	LEU	236	135.173	37.900	35.561	1.00	25.00
2118	N	GLN	237	133.362	39.870	37.454	1.00	25.46
2119	CA	GLN	237	132.953	40.777	38.521	1.00	25.58
2120	C	GLN	237	133.059	42.231	38.062	1.00	27.92
2121	O	GLN	2337	132.201	43.054	38.387	1.00	29.65
2122	CB	GLN	237	133.807	40.549	39.769	1.00	20.55
2123	CG	GLN	237	133.342	41.314	40.993	1.00	23.60
2124	CD	GLN	237	134.216	41.046	42.197	1.00	31.25
2125	OE1	GLN	237	135.435	41.196	42.134	1.00	31.93
2126	NE2	GLN	237	133.602	40.634	43.298	1.00	28.03
2127	H	GLN	237	134.094	39.237	37.625	1.00	25.00
2128	1HE2	GLN	237	134.156	40.446	44.081	1.00	25.00
2129	2HE2	GLN	237	132.635	40.519	43.287	1.00	25.00
2130	N	MET	238	134.096	42.537	37.286	1.00	28.91
2131	CA	MET	238	134.288	43.888	36.776	1.00	33.08
2132	C	MET	238	133.084	44.282	35.924	1.00	33.53
2133	O	MET	238	132.562	45.391	36.049	1.00	37.31
2134	CB	MET	238	135.573	43.976	35.954	1.00	32.86
2135	CG	MET	238	136.836	43.837	36.782	1.00	39.06
2136	SD	MET	238	138.318	43.815	35.763	1.00	43.74
2137	CE	MET	238	139.508	43.186	36.929	1.00	46.28
2138	H	MET	238	134.751	41.842	37.055	1.00	25.00
2139	N	LEU	239	132.624	43.356	35.087	1.00	31.84
2140	CA	LEU	239	131.465	43.599	34.233	1.00	30.89
2141	C	LEU	239	130.219	43.801	35.097	1.00	28.36
2142	O	LEU	239	129.450	44.742	34.885	1.00	32.90
2143	CB	LEU	239	131.255	42.427	33.271	1.00	29.61
2144	CG	LEU	239	129.969	42.432	32.436	1.00	29.85
2145	CD1	LEU	239	129.929	43.636	31.499	1.00	25.22
2146	CD2	LEU	239	129.870	41.138	31.649	1.00	26.65
2147	H	LEU	239	133.084	42.491	35.043	1.00	25.00
2148	N	HIS	240	130.042	42.942	36.095	1.00	25.85
2149	CA	HIS	240	128.891	43.042	36.990	1.00	28.32
2150	C	HIS	240	128.885	44.406	37.671	1.00	30.20
2151	O	HIS	240	127.824	44.974	37.940	1.00	30.10
2152	CB	HIS	240	128.925	41.926	38.036	1.00	25.55
2153	CG	HIS	240	128.881	40.545	37.448	1.00	24.20
2154	ND1	HIS	240	129.449	39.456	38.058	1.00	25.29
2155	CD2	HIS	240	128.358	40.103	38.283	1.00	21.44
2156	CE1	HIS	240	129.289	38.394	37.302	1.00	27.58
2157	NE2	HIS	240	128.627	38.750	36.209	1.00	21.74
2158	H	HIS	240	130.713	42.244	36.233	1.00	25.00
2159	HD11	HIS	240	129.918	39.455	38.924	1.00	25.00
2160	HE2	HIS	240	128.362	38.151	35.470	1.00	25.00
2181	N	LYS	241	130.079	44.926	37.935	1.00	34.60
2162	CA	LYS	241	130.239	46.230	38.563	1.00	32.03
2163	C	LYS	241	129.855	47.374	37.613	1.00	31.99

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2164	O	LYS	241	129.280	48.374	38.045	1.00	29.66
2165	CB	LYS	241	131.675	46.391	39.072	1.00	32.10
2166	CG	LYS	241	131.984	45.614	40.356	1.00	34.40
2167	CD	LYS	241	133.447	45.807	40.758	1.00	41.19
2168	CE	LYS	241	133.701	45.417	42.208	1.00	49.51
2169	NZ	LYS	241	135.044	45.881	42.698	1.00	56.06
2170	H	LYS	241	130.875	44.403	37.703	1.00	25.00
2171	1HZ	LYS	241	135.111	46.916	42.625	1.00	25.00
2172	2HZ	LYS	241	135.179	45.610	43.698	1.00	25.00
2173	3HZ	LYS	241	135.803	45.446	42.135	1.00	25.00
2174	N	GLN	242	130.121	47.201	36.316	1.00	34.13
2175	CA	GLN	242	129.799	48.211	35.303	1.00	38.39
2176	C	GLN	242	128.288	48.278	35.161	1.00	39.98
2177	O	GLN	242	127.702	49.353	34.990	1.00	45.19
2178	CB	GLN	242	130.376	47.827	33.942	1.00	42.52
2179	CG	GLN	242	131.883	47.683	33.920	1.00	60.88
2180	CD	GLN	242	132.417	47.252	32.574	1.00	69.61
2181	OE1	GLN	242	131.663	47.052	31.620	1.00	75.13
2182	NE2	GLN	242	133.730	47.102	32.488	1.00	78.40
2183	H	GLN	242	130.490	46.358	35.996	1.00	25.00
2184	1HE2	GLN	242	134.0772	46.820	31.621	1.00	25.00
2185	2HE2	GLN	242	134.282	47.272	33.272	1.00	25.00
2186	N	GLU	243	127.674	47.105	35.219	1.00	33.89
2187	CA	GLU	243	126.233	46.975	35.107	1.00	28.66
2188	C	GLU	243	125.568	47.591	36.325	1.00	28.27
2189	O	GLU	243	124.635	48.381	36.193	1.00	32.26
2190	CB	GLU	243	125.857	45.505	34.982	1.00	25.09
2191	CG	GLU	243	126.416	44.820	33.741	1.00	24.03
2192	CD	GLU	243	126.182	43.329	33.738	1.00	26.58
2193	OE1	GLU	243	125.633	42.810	34.726	1.00	24.63
2194	OE2	GLU	243	126.556	42.665	32.750	1.00	29.69
2195	H	GLU	243	128.248	46.333	35.341	1.00	25.00
2196	N	LEU	244	126.078	47.267	37.508	1.00	24.94
2197	CA	LEU	244	125.522	47.798	38.745	1.00	30.48
2198	C	LEU	244	125.635	49.324	38.766	1.00	36.45
2199	O	LEU	244	124.700	50.021	39.163	1.00	35.07
2200	CB	LEU	244	126.233	47.185	39.957	1.00	28.96
2201	CG	LEU	244	125.765	47.658	41.339	1.00	29.10
2202	CD1	LEU	244	124.249	47.527	41.484	1.00	25.23
2203	CD2	LEU	244	126.484	48.859	42.423	1.00	27.57
2204	H	LEU	244	126.855	48.662	37.535	1.00	25.00
2205	N	ALA	245	126.778	49.832	38.318	1.00	37.15
2206	CA	ALA	245	127.023	51.268	38.270	1.00	38.62
2207	C	ALA	245	126.030	51.937	37.325	1.00	39.57
2208	O	ALA	245	125.352	52.902	37.692	1.00	43.21
2209	CB	ALA	245	128.452	51.539	37.802	1.00	35.23
2210	H	ALA	245	127.477	49.215	38.032	1.00	25.00
2211	N	GLN	246	125.920	51.380	36.123	1.00	35.82
2212	CA	GLN	246	125.025	51.888	35.088	1.00	40.78
2213	C	GLN	246	123.577	51.989	35.566	1.00	43.61
2214	O	GLN	246	122.907	53.016	35.404	1.00	43.37
2215	CB	GLN	246	125.088	50.963	33.872	1.00	42.45
2216	CG	GLN	246	124.151	51.350	32.733	1.00	59.73
2217	CD	GLN	246	124.146	50.338	31.610	1.00	65.77
2218	OE1	GLN	246	125.149	49.663	31.357	1.00	67.95
2219	NE2	GLN	246	123.009	50.223	30.920	1.00	66.48
2220	H	GLN	246	126.450	50.576	35.964	1.00	25.00
2221	1HE2	GLN	246	123.038	49.559	30.198	1.00	25.00
2222	2HE2	GLN	246	122.232	50.763	31.132	1.00	25.00
2223	N	VAL	247	123.115	50.916	38.185	1.00	39.07
2224	CA	VAL	247	121.762	50.830	36.692	1.00	37.02
2225	C	VAL	247	121.538	51.732	37.908	1.00	40.33
2226	O	VAL	247	120.435	52.248	38.106	1.00	39.92
2227	CB	VAL	247	121.387	49.341	36.948	1.00	35.95
2228	CG1	VAL	247	120.417	49.201	38.091	1.00	37.82
2229	CG2	VAL	247	120.794	48.754	35.686	1.00	32.90
2230	H	VAL	247	123.730	50.170	36.340	1.00	25.00
2231	N	SER	248	122.579	51.926	38.715	1.00	44.51
2232	CA	SER	248	122.483	52.798	39.887	1.00	46.80
2233	C	SER	248	122.250	54.234	39.410	1.00	47.29
2234	O	SER	248	121.454	54.976	39.997	1.00	46.67

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2235	CB	SER	248	123.759	52.727	40.726	1.00	44.77
2236	OG	SER	243	123.859	51.479	41.381	1.00	45.74
2237	H	SER	248	123.423	51.465	38.531	1.00	25.00
2238	HG	SER	248	123.876	50.777	40.722	1.00	25.00
2239	N	ARG	249	122.938	54.015	38.334	1.00	44.35
2240	CA	ARG	249	122.789	55.943	37.750	1.00	48.22
2241	C	ARG	249	121.354	56.097	37.256	1.00	47.00
2242	O	ARG	249	120.710	57.119	37.504	1.00	47.12
2243	CB	ARG	249	123.785	56.147	36.604	1.00	52.69
2244	CG	ARG	249	125.165	56.590	37.075	1.00	66.38
2245	CD	ARG	249	126.154	56.712	35.924	1.00	73.20
2246	NE	ARG	249	126.919	55.484	35.712	1.00	75.40
2247	CZ	ARG	249	126.922	54.778	334.584	1.00	77.33
2248	NH1	ARG	249	126.194	55.165	33.542	1.00	74.66
2249	NH2	ARG	249	127.669	53.686	34.493	1.00	83.65
2250	H	ARG	249	123.579	53.986	37.936	1.00	25.00
2251	HE	ARG	249	127.471	55.153	36.453	1.00	25.00
2252	1HH1	ARG	249	125.633	55.990	33.598	1.00	25.00
2253	2HH1	ARG	249	126.203	54.625	32.700	1.00	25.00
2254	1HH2	ARG	249	128.229	53.396	35.269	1.00	25.00
2255	2HH2	ARG	249	127.675	53.153	33.646	1.00	25.00
2256	N	TRP	250	120.848	55.053	36.603	1.00	46.33
2257	CA	TRP	250	119.480	55.024	36.092	1.00	43.84
2258	C	TRP	250	118.488	55.311	37.230	1.00	46.38
2259	O	TRP	250	117.566	56.118	37.075	1.00	44.72
2260	CB	TRRP	250	119.201	53.652	35.456	1.00	38.48
2261	CG	TRP	250	117.747	53.324	35.232	1.00	37.37
2262	CD1	TRP	250	116.986	53.661	34.150	1.00	33.31
2263	CD2	TRP	250	116.891	52.569	36.105	1.00	36.85
2264	NE1	TRP	250	115.713	53.164	34.293	1.00	34.01
2265	CE2	TRP	250	115.626	52.490	35.483	1.00	36.82
2266	CE3	TRP	250	117.070	51.952	37.352	1.00	34.91
2267	CZ2	TRP	250	114.543	51.816	36.065	1.00	39.04
2268	CZ3	TRP	250	115.992	51.281	37.932	1.00	39.64
2269	CH2	TRP	250	114.746	51.220	37.286	1.00	39.49
2270	H	TRP	250	121.423	54.272	36.448	1.00	25.00
2271	HE1	TRP	250	114.984	53.281	33.650	1.00	25.00
2272	N	TRP	251	118.718	54.683	38.382	1.00	46.65
2272	CA	TRP	251	117.859	54.851	39.551	1.00	54.20
2274	C	TRP	251	117.864	56.279	40.089	1.00	59.43
2275	O	TRP	251	116.814	56.823	40.445	1.00	62.13
2276	CB	TRP	251	118.284	53.889	40.657	1.00	51.89
2277	CG	TRP	251	117.358	53.872	41.836	1.00	58.17
2278	CD1	TRP	251	117.596	54.402	43.071	1.00	60.91
2279	CD2	TRP	251	116.069	53.246	41.908	1.00	60.72
2280	NE1	TRP	251	116.541	54.136	43.912	1.00	64.22
2281	CE2	TRP	251	115.589	53.429	43.225	1.00	60.87
2282	CE3	TRP	251	115.274	52.546	40.989	1.00	56.90
2283	CZ2	TRP	251	114.351	52.934	43.648	1.00	58.08
2284	CZ3	TRP	251	114.042	52.054	41.410	1.00	53.15
2285	CH2	TRP	251	113.594	52.252	42.729	1.00	53.35
2286	H	TRP	251	119.485	54.076	38.442	1.00	25.00
2287	HE1	TRP	251	116.481	54.409	44.851	1.00	25.00
2288	N	LYS	252	119.049	56.875	40.167	1.00	64.71
2289	CA	LYS	252	119.191	58.241	40.661	1.00	68.07
2290	C	LYS	252	118.440	59.227	39.779	1.00	65.20
2291	O	LYS	252	117.831	60.169	40.283	1.00	65.28
2292	CB	LYS	252	120.668	58.621	40.755	1.00	75.64
2293	CG	LYS	252	121.400	57.815	41.803	1.00	85.57
2294	CD	LYS	252	122.890	57.818	41.588	1.00	92.92
2295	CE	LYS	252	123.526	56.776	42.486	1.00	95.43
2296	NZ	LYS	252	124.902	56.526	42.101	1.00	94.64
2297	H	LYS	252	119.849	56.379	39.887	1.00	25.00
22998	1HZ	LYS	252	125.056	56.256	41.101	1.00	25.00
2299	2HZ	LYS	252	125.376	57.437	42.219	1.00	25.00
2300	3HZ	LYS	252	125.417	55.867	42.716	1.00	25.00
2301	N	ASP	253	118.453	58.983	38.469	1.00	63.40
2302	CA	ASP	253	117.762	59.846	37.515	1.00	63.30
2303	C	ASP	253	116.265	59.872	37.796	1.00	63.95
2304	O	ASP	253	115.635	60.925	37.729	1.00	68.15
2305	CB	ASP	253	118.003	59.376	36.077	1.00	68.18

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2306	CG	ASP	253	119.467	59.453	35.664	1.00	76.46
2307	OD1	ASP	253	120.293	60.015	36.419	1.00	78.84
2308	OD2	ASP	253	119.793	58.943	34.570	1.00	79.35
2309	H	ASP	253	118.948	58.203	38.137	1.00	25.00
2310	N	LEU	254	115.697	58.710	38.105	1.00	66.44
2311	CA	LEU	254	114.271	58.611	38.409	1.00	65.57
2312	C	LEU	254	113.947	59.482	39.616	1.00	67.65
2313	O	LEU	254	112.815	59.931	39.784	1.00	68.72
2314	CB	LEU	254	113.885	57.162	38.698	1.00	61.14
2315	CG	LEU	254	114.124	56.166	37.564	1.00	57.75
2316	CD1	LEU	254	113.718	54.785	38.021	1.00	58.43
2317	CD2	LEU	254	113.343	56.571	36.328	1.00	55.32
2318	H	LEU	254	116.252	57.902	38.125	1.00	25.00
2319	N	ASP	255	114.947	59.661	40.475	1.00	73.64
2320	CA	ASP	255	114.842	60.490	41.670	1.00	78.31
2321	C	ASP	255	113.664	60.123	42.574	1.00	79.28
2322	O	ASP	255	113.079	60.985	43.230	1.00	81.76
2323	CB	ASP	255	114.777	61.971	41.261	1.00	83.27
2324	CG	ASP	255	115.238	62.915	42.364	1.00	87.17
2325	OD1	ASP	255	115.719	62.443	43.420	1.00	86.98
2326	OD2	ASP	255	115.121	64.144	42.165	1.00	87.49
2327	H	ASP	255	115.805	59.226	40.294	1.00	25.00
2328	N	PHE	256	113.357	58.834	42.659	1.00	80.00
2329	CA	PHE	256	112.254	58.378	43.500	1.00	84.32
2330	C	PHE	256	112.504	58.649	44.976	1.00	89.15
2331	O	PHE	256	111.562	58.742	45.759	1.00	87.59
2332	CB	PHE	256	111.987	56.887	43.290	1.00	81.00
2333	CG	PHE	256	111.352	56.566	41.972	1.00	76.86
2334	CD1	PHE	256	110.671	57.544	41.251	1.00	76.59
2335	CD2	PHE	256	111.431	55.283	41.449	1.00	73.54
2336	CE1	PHE	256	110.080	57.247	40.030	1.00	76.03
2337	CE2	PHE	256	110.844	54.976	40.229	1.00	71.61
2338	CZ	PHE	256	110.167	55.958	39.518	1.00	74.95
2339	H	PHE	256	113.874	58.189	42.139	1.00	25.00
2340	N	VAL	257	113.774	53.796	45.344	1.00	97.79
2341	CA	VAL	257	114.160	59.053	46.730	1.00	104.36
2342	C	VAL	257	113.428	60.269	47.303	1.00	105.53
2343	O	VAL	257	112.952	60.239	48.439	1.00	106.91
2344	CB	VAL	257	115.692	59.270	46.854	1.00	107.20
2345	CG1	VAL	257	116.092	59.432	48.316	1.00	107.16
2346	CG2	VAL	257	116.445	58.101	46.220	1.00	106.33
2347	H	VAL	257	114.464	58.732	44.658	1.00	25.00
2348	N	THR	258	113.332	61.329	46.5506	1.00	105.84
2349	CA	THR	258	112.660	62.550	46.935	1.00	104.41
2350	C	THR	258	111.183	62.608	46.531	1.00	104.31
2351	O	THR	258	110.339	63.047	47.314	1.00	104.07
2352	CB	THR	258	113.392	63.805	46.408	1.00	104.30
2353	OG1	THR	258	113.620	63.674	45.000	1.00	104.41
2354	CG2	THR	258	114.729	63.982	47.117	1.00	105.42
2355	H	THR	258	113.711	61.308	45.603	1.00	25.00
2356	HG1	THR	258	114.068	64.458	44.669	1.00	25.00
2357	N	THR	259	110.872	62.161	45.317	1.00	103.41
2358	CA	THR	259	109.497	62.182	44.825	1.00	100.89
2359	C	THR	259	108.599	61.133	45.482	1.00	101.97
2360	O	THR	259	107.414	61.375	45.707	1.00	103.53
2361	CB	THR	259	109.445	62.022	43.289	1.00	97.37
2362	OG1	THR	259	110.219	60.883	42.894	1.00	95.69
2363	CG2	THR	259	109.988	63.267	42.602	1.00	95.50
2364	H	THR	259	111.579	61.811	44.728	1.00	25.00
2365	HG1	THR	259	109.870	60.086	43.290	1.00	25.00
2366	N	LEU	260	109.164	59.969	45.783	1.00	102.18
2367	CA	LEU	260	108.415	58.884	46.412	1.00	103.22
2368	C	LEU	260	109.112	58.431	47.696	1.00	106.86
2369	O	LEU	260	109.742	57.372	47.732	1.00	107.73
2370	CB	LEU	260	108.282	57.700	45.445	1.00	98.81
2371	CG	LEU	260	107.552	57.928	44.119	1.00	94.81
2372	CD1	LEU	260	107.620	56.670	43.269	1.00	89.99
2373	CD2	LEU	260	106.108	58.320	44.380	1.00	92.83
2374	H	LEU	260	110.112	59.844	45.595	1.00	25.00
2375	N	PRO	261	108.963	59.204	48.784	1.00	110.17
2376	CA	PRO	261	109.580	58.889	50.077	1.00	112.52

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2372	C	PRO	261	108.951	57.726	50.855	1.00	114.04
2378	O	PRO	261	108.783	57.813	52.073	1.00	117.31
2379	CB	PRO	261	109.441	60.207	50.836	1.00	113.40
2380	CG	PRO	261	108.124	60.715	50.347	1.00	112.70
2381	CD	PRO	261	108.223	60.477	48.856	1.00	111.17
2382	N	TYR	262	108.599	56.646	50.163	1.00	113.40
2383	CA	TYR	262	108.012	55.479	50.822	1.00	112.08
2384	C	TYR	262	108.608	54.178	50.284	1.00	112.01
2385	O	TYR	262	108.125	53.086	50.582	1.00	110.30
2386	CB	TYR	262	106.477	55.478	50.702	1.00	109.31
2387	CG	TYR	262	105.931	55.286	49.303	1.00	104.93
2388	CD1	TYR	252	105.777	56.369	48.440	1.00	103.18
2389	CD2	TYR	262	105.555	54.021	48.846	1.00	102.84
2390	CE1	TYR	262	105.262	56.201	47.159	1.00	101.09
2391	CE2	TYR	262	105.040	53.842	47.565	1.00	100.35
2392	CZ	TYR	262	104.897	54.938	46.727	1.00	100.07
2393	OH	TYR	262	104.386	54.781	45.459	1.00	97.25
2394	H	TYR	262	103.755	56.615	49.199	1.00	25.00
2395	HH	TYR	262	104.276	53.862	45.236	1.00	25.00
2396	N	ALA	263	109.671	54.310	49.497	1.00	113.11
2397	CA	ALA	263	110.360	53.166	48.913	1.00	114.09
2398	C	ALA	263	111.856	53.343	49.146	1.00	114.75
2399	O	ALA	263	112.375	54.457	49.055	1.00	115.90
2400	CB	ALA	263	110.064	53.077	47.428	1.00	112.96
2401	H	ALA	263	110.034	55.202	49.305	1.00	25.00
2402	N	ARG	264	112.543	52.252	49.467	1.00	113.69
2403	CA	ARG	264	113.979	52.309	49.726	1.00	114.09
2404	C	ARG	264	114.847	51.948	48.526	1.00	109.03
2405	O	ARG	264	114.394	51.280	47.594	1.00	109.80
2406	CB	ARG	264	114.355	51.448	50.945	1.00	116.51
2407	CG	ARG	264	113.434	50.258	51.235	1.00	118.71
2408	CD	ARG	264	113.486	49.190	50.151	1.00	120.73
2409	NE	ARG	264	112.543	48.105	50.418	1.00	118.02
2410	CZ	ARG	264	111.607	47.696	49.565	1.00	115.79
2411	NH1	ARG	264	111.479	48.277	48.380	1.00	114..07
2412	NH2	ARG	264	110.788	46.709	49.904	1.00	113.33
2413	H	ARG	264	112.079	51.393	49.495	1.00	25.00
2414	HE	ARG	264	112.602	47.651	51.284	1.00	25.00
2415	1HH1	ARG	264	112.083	49.029	48.120	1.00	25.00
2416	2HH1	ARG	264	110.766	47.967	47.751	1.00	25.00
2417	1HH2	ARG	264	110.868	46.283	50.807	1.00	25.00
2418	2HH2	ARG	264	110.074	46.408	49.273	1.00	25.00
2419	N	ASP	265	116.089	52.421	48.550	1.00	103.18
2420	CA	ASP	265	117.045	52.152	47.485	1.00	97.60
2421	C	ASP	265	117.480	50.688	47.579	1.00	92.70
2422	O	ASP	265	118.533	50.371	48.138	1.00	96.57
2423	CB	ASP	265	118.255	53.086	47.619	1.00	100.16
2424	CG	ASP	265	1199.317	52.826	46.565	1.00	106.00
2425	OD1	ASP	265	118.992	52.887	45.363	1.00	107.25
2426	OD2	ASP	265	120.479	52.556	46.940	1.00	109.23
2427	H	ASP	265	116.373	52.965	49.310	1.00	25.00
2428	N	ARG	266	116.654	49.799	47.041	1.00	82.19
2429	CA	ARG	266	116.942	48.372	47.073	1.00	73.27
2430	C	ARG	266	117.613	47.910	45.775	1.00	63.23
2431	O	ARG	266	117.711	46.712	45.511	1.00	66.31
2432	CB	ARG	266	115.646	47.585	47.320	1.00	77.54
2433	CG	ARG	266	115.801	46.402	48.274	1.00	83.80
2434	CD	ARG	266	114.480	45.672	48.520	1.00	86.40
2435	NE	ARG	266	114.015	44.911	47.358	1.00	87.97
2436	CZ	ARG	266	114.383	43.661	47.077	1.00	87.83
2437	NH1	ARG	266	115.229	43.014	47.869	1.00	86.43
2438	NH2	ARG	266	113.895	43.049	46.005	1.00	80.67
2439	H	ARG	266	115.816	50.112	46.631	1.00	25.00
2440	HE	ARG	266	113.386	45.348	46.747	1.00	25.00
2441	1HH1	ARG	266	115.600	43.463	48.681	1.00	25.00
2442	2HH1	ARG	266	115.502	42.079	47.647	1.00	25.00
2443	1HH2	ARG	266	113.246	43.525	45.410	1.00	25.00
2444	2HH2	ARG	266	114.170	42.111	45.794	1.00	25.00
2445	N	VAL	267	118.130	48.859	45.000	1.00	54.00
2446	CA	VAL	267	118.778	48.560	43.722	1.00	46.85
2447	C	VAL	267	119.865	47.496	43.784	1.00	44.14

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2448	O	VAL	267	119.911	46.609	42.935	1.00	45.14
2449	CB	VAL	267	119.361	49.827	43.076	1.00	45.45
2450	CG1	VAL	267	119.991	49.499	41.733	1.00	42.99
2451	CG2	VAL	267	118.273	50.848	42.892	1.00	51.05
2452	H	VAL	267	118.072	49.785	45.299	1.00	25.00
2453	N	VAL	268	120.738	47.576	44.781	1.00	40.56
2454	CA	VAL	268	121.813	46.597	44.910	1.00	38.21
2455	C	VAL	268	121.242	45.185	45.125	1.00	35.40
2456	O	VAL	268	121.708	44.220	44.513	1.00	29.56
2457	CB	VAL	268	122.785	46.976	46.046	1.00	40.34
2458	CG1	VAL	268	123.983	46.055	46.040	1.00	41.41
2459	CG2	VAL	268	123.239	48.414	45.880	1.00	43.02
2460	H	VAL	268	120.663	48.303	45.428	1.00	25.00
2461	N	GLU	269	120.202	45.081	45.952	1.00	33.49
2462	CA	GLU	2669	119.553	43.796	46.220	1.00	31.75
2463	C	GLU	269	118.910	43.278	44.938	1.00	31.29
2464	O	GLU	269	119.023	42.095	44.607	1.00	34.74
2465	CB	GLU	269	118.477	43.940	47.300	1.00	30.42
2466	CG	GLU	269	118.998	44.124	48.719	1.00	41.96
2467	CD	GLU	269	119.777	45.418	48.921	1.00	53.70
2468	OE1	GLU	26P	119.387	46.465	48.356	1.00	52.14
2469	OE2	GLU	269	120.785	45.385	49.658	1.00	60.44
2470	H	GLU	269	119.849	45.888	46.369	1.00	25.00
2471	N	CYS	270	118.258	44.179	44.204	1.00	25.87
2472	CA	CYS	270	117.603	43.829	42.948	1.00	31.04
2473	C	CYS	270	118.628	43.330	41.944	1.00	31.66
2474	O	CYS	270	118.352	42.406	41.170	1.00	34.14
2475	CB	CYS	270	116.841	45.029	42.380	1.00	31.00
2476	SG	CYS	270	115.468	45.566	43.429	1.00	41.23
2477	H	CYS	270	118.204	45.102	44.523	1.00	25.00
2478	N	TYR	271	119.817	43.927	41.968	1.00	30.55
2479	CA	TYR	271	120.875	43.506	41.065	1.00	29.41
2480	C	TYR	271	121.365	42.109	41.459	1.00	29.51
2481	O	TYR	271	121.662	41.284	40.592	1.00	30.16
2482	CB	TYR	271	122.048	44.496	41.048	1.00	27.85
2483	CG	TYR	271	123.125	44.061	40.077	1.00	27.35
2484	CD1	TYR	271	123.006	44.327	38.714	1.00	25.72
2485	CD2	TYR	271	124.198	43.279	40.502	1.00	20.62
2486	CE1	TYR	271	123.923	43.813	37.798	1.00	22.98
2487	CE2	TYR	271	125.116	42.762	39.593	1.00	27.42
2488	CZ	TYR	271	124.970	43.030	38.245	1.00	21.79
2489	OH	TYR	271	125.859	42.497	37.343	1.00	23.43
2490	H	TYR	271	119.985	44.662	42.594	1.00	25.00
2491	HH	TYR	271	126.485	41.987	37.843	1.00	25.00
2492	N	PHE	272	121.453	41.845	42.760	1.00	26.47
2493	CA	PHE	272	121.892	40.535	43.220	1.00	28.71
2494	C	PHE	272	120.957	39.486	42.633	1.00	31.32
2495	O	PHE	272	121.408	38.470	42.102	1.00	31.50
2496	CB	PHE	272	121.881	40.442	44.747	1.00	32.54
2497	CG	PHE	272	122.165	39.058	45.264	1.00	34.15
2498	CD1	PHE	272	123.471	38.577	45.323	1.00	32.37
2499	CD2	PHE	272	121.120	38.211	45.638	1.00	34.09
2500	CE11	PHE	272	123.732	37.271	45.739	1.00	35.66
2501	CE2	PHE	272	121.369	36.902	46.055	1.00	34.18
2502	CZ	PHE	272	122.679	36.431	46.105	1.00	36.58
2503	H	PHE	272	121.228	42.541	43.413	1.00	25.00
2504	N	TRP	273	119.656	39.744	42.712	1.00	29.73
2505	CA	TRP	273	118.670	38.817	42.167	1.00	30.60
2506	C	TRP	273	118.924	38.551	40.685	1.00	30.33
2507	O	TRP	273	118.971	37.396	40.250	1.00	32.10
2508	CB	TRP	273	117.255	39.357	42.365	1.00	28.17
2509	CG	TRP	273	116.707	39.092	43.721	1.00	33.41
2510	CD1	TRP	273	117.241	39.478	44.915	1.00	37.71
2511	CD2	TRP	273	115.506	38.381	44.029	1.00	41.82
2512	NE1	TRP	273	116.445	39.053	45.950	1.00	39.11
2513	CE2	TRP	273	115.372	38.378	45.435	1.00	43.90
2514	CE3	TRP	273	114.528	37.747	43.253	1.00	47.13
2515	CZ2	TRP	273	114.296	37.764	46.083	1.00	49.35
2516	CZ3	TRP	273	113.458	37.136	43.898	1.00	53.38
2517	CH2	TRP	273	113.352	37.150	45.300	1.00	53.17
2518	H	TRP	273	119.359	40.569	43.153	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2519	HE1	TRP	273	116.622	39.201	46.903	1.00	25.00
2520	N	ALA	274	119.117	39.617	39.915	1.00	26.20
2521	CA	ALA	274	119.371	39.472	38.489	1.00	25.12
2522	C	ALA	274	120.638	38.657	38.263	1.00	27.03
2523	O	ALA	274	120.686	37.816	37.366	1.00	29.08
2524	CB	ALA	274	119.491	40.832	37.831	1.00	22.68
2525	H	ALA	274	119.0884	40.514	40.313	1.00	25.00
2526	N	LEU	275	121.646	38.886	39.104	1.00	26.74
2527	CA	LEU	275	122.922	38.175	39.011	1.00	23.65
2528	C	LEU	275	122.727	36.689	39.329	1.00	20.19
2529	O	LEU	275	123.432	35.825	38.798	1.00	18.69
2530	CB	LEU	275	123.945	38.802	39.963	1.00	22.77
2531	CG	LEU	275	125.377	38.280	39.867	1.00	22.23
2532	CD1	LEU	275	125.859	38.352	38.427	1.00	20.45
2533	CD2	LEU	275	126.274	39.097	40.779	1.00	24.10
2534	H	LEU	275	121.532	39.552	39.808	1.00	25.00
2535	N	GLY	276	121.765	36.406	40.204	1.00	19.17
2536	CA	GLY	276	121.453	35.035	40.561	1.00	19.61
2537	C	GLY	276	120.811	34.299	39.392	1.00	25.48
2538	O	GLY	276	121.060	33.108	39.199	1.00	28.59
2539	H	GLY	276	121.266	37.137	40.623	1.00	25.00
2540	N	VAL	277	120.000	35.006	38.603	1.00	20.84
2541	CA	VAL	277	119.323	34.415	37.440	1.00	19.19
2542	C	VAL	277	120.304	34.028	36.319	1.00	19.17
2543	O	VAL	277	120.086	33.048	35.606	1.00	21.35
2544	CB	VAL	277	118.201	35.355	36.904	1.00	21.19
2545	CG1	VAL	277	117.560	34.777	35.650	1.00	15.33
2546	CG2	VAL	277	117.138	35.550	37.976	1.00	11.13
2547	H	VAL	277	119.858	35.954	38.810	1.00	25.00
2548	N	TYR	278	121.345	34.834	36.137	1.00	21.16
2549	CA	TYR	278	122.401	34.587	35.150	1.00	24.77
2550	C	TYR	278	123.583	35.532	35.351	1.00	29.35
2551	O	TYR	278	123.405	36.738	35.531	1.00	27.69
2552	CB	TYR	278	121.910	34.611	33.687	1.00	25.96
2553	CG	TYR	278	120.741	35.517	33.341	1.00	26.89
2554	CD1	TYR	278	120.580	36.768	33.937	1.00	25.88
2555	CD2	TYR	278	119.800	35.116	32.388	1.00	27.14
2556	CE1	TYR	278	119.508	37.595	33.594	1.00	29.19
2557	CE2	TYR	278	118.729	35.934	32.037	1.00	31.49
2558	CZ	TYR	278	118.587	37.171	32.643	1.00	31.78
2559	OH	TYR	278	117.522	37.976	32.301	1.00	31.66
2560	H	TYR	278	121.419	35.652	36.684	1.00	25.00
2561	HH	TYR	278	117.022	37.548	31.600	1.00	25.00
2562	N	PHE	279	124.789	34.968	35.332	1.00	31.85
2563	CA	PHE	279	126.017	35.732	35.549	1.00	28.28
2564	C	PHE	279	126.910	35.844	34.318	1.00	28.86
2565	O	PHE	279	127.855	36.636	34.310	1.00	28.24
2566	CB	PHE	279	126.829	35.087	36.678	1.00	24.38
2567	CG	PHE	279	127.334	33.707	36.344	1.00	23.04
2568	CD1	PHE	279	128.563	33.535	35.706	1.00	16.44
2569	CD2	PHE	279	126.557	32.582	36.616	1.00	22.61
2570	CE1	PHE	279	129.005	32.265	35.339	1.00	22.82
2571	CE2	PHE	279	126.989	31.309	36.254	1.00	22.81
2572	CZ	PHE	279	128.214	31.149	35.613	1.00	20.63
2573	H	PHE	279	124.845	34.006	35.181	1.00	25.00
2574	N	GLU	280	126.653	35.010	33.315	1.00	25.83
2575	CA	GLU	280	127.450	34.995	32.093	1.00	25.96
2576	C	GLU	280	127.464	36.347	31.384	1.00	32.09
2577	O	GLU	280	126.461	37.067	31.378	1.00	33.29
2578	CB	GLU	280	126.947	33.909	31.140	1.00	29.64
2579	CG	GLU	280	127.116	32.479	31.652	1.00	31.98
2580	CD	GLU	280	125.873	31.921	32.338	1.00	41.40
2581	OE1	GLU	280	125.089	32.696	32.938	1.00	33.42
2582	OE2	GLU	280	125.681	30.688	32.273	1.00	43.76
2583	H	GLU	280	125.894	34.421	33.402	1.00	25.00
2584	N	PRO	281	128.593	36.687	30.735	1.00	34.75
2585	CA	PRO	281	128.736	37.961	30.018	1.00	32.48
2586	C	PRO	281	127.718	38.182	28.899	1.00	30.11
2587	O	PRO	281	127.273	39.309	28.675	1.00	33.55
2588	CB	PRO	281	130.177	37.901	229.492	1.00	33.45
2589	CG	PRO	281	130.447	36.426	29.366	1.00	34.83

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2590	CD	PRO	281	129.824	35.882	30.625	1.00	32.94
2591	N	GLN	282	127.319	37.106	28.226	1.00	30.38
2592	CA	GLN	282	126.360	37.195	27.134	1.00	31.74
2593	C	GLN	282	124.980	37.704	27.600	1.00	33.53
2594	O	GLN	282	124.194	38.202	26.792	1.00	34.52
2595	CB	GLN	282	126.183	35.829	26.462	1.00	35.52
2596	CG	GLN	282	125.442	34.819	27.323	1.00	47.53
2597	CD	GLN	282	125.543	33.400	26.807	1.00	54.68
2598	OE1	GLN	282	126.378	32.624	27.273	1.00	58.66
2599	NE2	GLN	282	124.675	33.040	25.866	1.00	55.48
2600	H	GLN	282	127.685	36.233	28.468	1.00	25.00
2601	1HE2	GLLN	282	124.740	32.122	25.538	1.00	25.00
2602	2HE2	GLN	282	124.018	33.690	25.551	1.00	25.00
2603	N	TYR	283	124.698	37.577	28.896	1.00	27.81
2604	CA	TYR	283	123.417	38.015	29.447	1.00	26.64
2605	C	TYR	283	123.470	39.392	30.099	1.00	29.80
2606	O	TYR	283	122.615	39.732	30.922	1.00	29.85
2607	CB	TYR	283	122.885	36.982	30.444	1.00	24.82
2608	CG	TYR	283	122.670	35.614	29.840	1.00	26.77
2609	CD1	TYR	283	121.786	35.432	28.775	1.00	28.94
2610	CD2	TYR	283	123.373	34.506	30.313	1.00	26.51
2611	CE1	TYR	283	121.610	34.174	28.192	1.00	32.76
2612	CE2	TYR	283	123.205	33.247	29.740	1.00	28.52
2613	CZ	TYR	283	122.324	33.086	28.680	1.00	30.97
2614	OH	TYR	283	122.164	31.845	28.104	1.00	25.13
2615	H	TYR	283	125.361	37.198	29.509	1.00	25.00
2616	HH	TYR	283	122.723	31.208	28.556	1.00	25.00
2617	N	SER	284	124.449	40.196	29.697	1.00	30.66
2618	CA	SER	284	124.620	41.539	30.239	1.00	33.15
2619	C	SER	284	123.375	42.412	30.040	1.00	32.37
2620	O	SER	284	122.858	42.999	30.999	1.00	32.25
2621	CB	SER	284	125.848	42.201	29.609	1.00	32.60
2622	OG	SER	284	126.037	43.511	30.110	1.00	38.65
2623	H	SER	284	125.090	39.876	29.027	1.00	25.00
2624	HG	SER	284	126.140	43.520	31.058	1.00	25.00
2625	N	GLN	285	122.862	42.477	28.805	1.00	35.28
2626	CA	GLN	285	121.693	43.273	28.505	1.00	36.59
2627	C	GLN	285	120.489	42.735	29.284	1.00	33.06
2628	O	GLN	285	119.713	43.504	29.856	1.00	33.43
2629	CB	GLN	285	121.399	43.255	27.002	1.00	36.57
2630	CG	GLN	285	120.138	44.020	26.611	1.00	48.54
2631	CD	GLN	285	119.829	43.943	25.123	1.00	54.77
2632	OE1	GLN	285	120.079	42.927	24.470	1.00	55.77
2833	NE2	GLN	285	119.280	45.024	24.581	1.00	56.33
2634	H	GLN	285	123.323	41.984	28.086	1.00	25.00
2635	1HE2	GLN	285	119.084	44.982	23.621	1.00	25.00
2636	2HE2	GLN	285	119.099	45.802	25.141	1.00	25.00
2637	N	ALA	286	120.364	41.410	29.324	1.00	32.38
2638	CA	ALA	286	119.272	40.750	30.032	1.00	28.79
2639	C	ALA	286	119.254	41.117	31.512	1.00	26.70
2640	O	ALA	286	118.200	41.438	32.060	1.00	31.71
2641	CB	ALA	286	119.370	39.244	29.859	1.00	30.35
2642	H	ALA	286	121.023	40.859	28.861	1.00	25.00
2643	N	ARG	287	120.422	41.097	32.152	1.00	26.48
2644	CA	ARG	287	120.517	41.442	33.568	1.00	27.31
2645	C	ARG	287	120.056	42.870	33.826	1.00	27.08
2646	O	ARG	287	119.290	43.118	34.760	1.00	28.78
2647	CB	ARG	287	121.946	41.266	34.096	1.00	28.17
2648	OG	ARG	287	122.240	39.891	34.652	1.00	25.50
2649	CD	ARG	287	123.566	39.859	35.396	1.00	24.46
2650	NE	ARG	287	124.703	40.191	34.535	1.00	20.40
2651	CZ	ARG	287	125.252	39.373	33.641	1.00	23.12
2652	NH1	ARG	287	124.781	38.146	33.473	1.00	23.32
2653	NH2	ARG	287	126.268	39.793	32.897	1.00	22.53
2654	H	ARG	287	121.232	40.840	31.670	1.00	25.00
2655	HE	ARG	257	125.093	41.059	34.627	1.00	25.00
2656	1HH1	ARG	287	124.002	37.833	34.014	1.00	25.00
2657	2HH1	ARG	287	125.192	37.542	32.796	1.00	25.00
2658	1HH2	ARG	287	126.623	40.719	33.014	1.00	25.00
2659	2HH2	ARG	287	126.677	39.179	32.225	1.00	25.00
2660	N	VAL	288	120.512	43.802	32.992	1.00	30.28

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2661	CA	VAL	288	120.144	45.208	33.148	1.00	29.94
2662	C	VAL	288	118.628	45.388	33.043	1.00	28.55
2663	O	VAL	288	118.018	46.044	33.890	1.00	35.55
2664	CB	VAL	288	120.874	46.106	32.120	1.00	35.29
2665	CG1	VAL	288	120.536	47.572	32.363	1.00	30.30
2666	CG2	VAL	288	122.378	45.896	32.221	1.00	31.86
2667	H	VAL	288	121.107	43.535	32.256	1.00	25.00
2668	N	MET	289	118.018	44.775	32.031	1.00	27.91
2669	CA	MET	289	116.567	44.856	31.854	1.00	27.36
2670	C	MET	289	115.857	44.248	33.066	1.00	27.49
2671	O	MET	289	114.938	44.845	33.627	1.00	29.43
2672	CB	MET	289	116.136	44.129	30.572	1.00	28.18
2673	CG	MET	289	116.578	44.819	29.282	1.00	28.82
2674	SD	MET	289	116.207	43.882	27.770	1.00	38.33
2675	CE	MET	289	114.526	44.384	27.438	1.00	39.91
2676	H	MET	289	118.554	44.257	31.391	1.00	25.00
2677	N	LEU	290	116.335	43.089	33.511	1.00	25.99
2678	CA	LEU	290	115.743	42.408	34.654	1.00	25.33
2679	C	LEU	290	115.805	43.222	35.949	1.00	26.44
2680	O	LEU	290	114.815	43.289	36.687	1.00	30.04
2681	CB	LEU	290	116.393	41.035	34.843	1.00	25.26
2682	CG	LEU	290	115.880	40.125	35.964	1.00	25.88
2683	CD1	LEU	290	114.357	40.043	35.951	1.00	19.53
2684	CD2	LEU	290	116.499	38.741	35.796	1.00	18.49
2685	H	LEU	290	117.098	42.681	33.057	1.00	25.00
2686	N	VAL	291	116.947	43.857	36.210	1.00	27.54
2687	CA	VAL	291	117.124	44.667	37.421	1.00	28.37
2688	C	VAL	291	116.101	45.799	37.502	1.00	27.52
2689	O	VAL	291	115.487	46.023	38.5550	1.00	27.61
2690	CB	VAL	291	118.544	45.289	37.507	1.00	28.94
2691	CG1	VAL	291	118.706	46.054	38.803	1.00	25.65
2692	CG2	VAL	291	119.592	44.214	37.431	1.00	36.38
2693	H	VAL	291	117.687	43.782	35.573	1.00	25.00
2694	N	LYS	292	115.911	46.502	36.392	1.00	27.46
2695	CA	LYS	292	114.968	47.611	36.345	1.00	28.57
2696	C	LYS	292	113.546	47.158	36.677	1.00	30.77
2697	O	LYS	292	112.834	47.824	37.433	1.00	31.18
2698	CB	LYS	292	115.029	48.285	34.976	1.00	29.35
2699	CG	LYS	292	116.391	48.890	34.676	1.00	29.57
2700	CD	LYS	292	116.463	49.431	33.261	1.00	34.35
2701	CE	LYS	292	117.810	53.079	32.999	1.00	37.92
2702	NZ	LYS	292	117.909	50.619	31.619	1.00	40.64
2703	H	LYS	292	116.413	46.260	35.581	1.00	25.00
2704	1HZ	LYS	292	117.780	49.846	30.936	1.00	25.00
2705	2HZ	LYS	292	117.169	51.334	31.476	1.00	25.00
2706	3HZ	LYS	292	118.844	51.052	31.483	1.00	25.00
2707	N	THR	293	113.146	46.010	36.137	1.00	34.24
2708	CA	THR	293	111.817	45.463	36.395	1.00	27.43
2709	C	THR	293	111.657	45.123	37.872	1.00	31.58
2710	O	THR	293	110.655	45.493	38.491	1.00	28.71
2711	CB	THR	293	111.561	44.214	35.534	1.00	25.43
2712	OG1	THR	293	111.354	44.616	34.175	1.00	30.49
2713	CG2	THR	293	110.348	43.433	36.029	1.00	22.44
2714	H	THR	293	113.756	45.525	35.533	1.00	25.00
2715	HG1	THR	293	110.577	45.180	34.129	1.00	25.00
2716	N	ILE	294	112.647	44.439	38.440	1.00	30.35
2717	CA	ILE	294	112.596	44.064	39.853	1.00	30.45
2718	C	ILE	294	112.481	45.317	40.725	1.00	28.69
2719	O	ILE	294	111.709	45.348	41.685	1.00	30.57
2720	CB	ILE	294	113.837	43.230	40.272	1.00	29.95
2721	CG1	ILE	294	113.948	41.977	39.399	1.00	24.34
2722	CG2	ILE	294	113.733	42.818	41.734	1.00	18.35
2723	CD1	ILE	294	115.165	41.133	39.687	1.00	30.84
2724	H	ILE	294	113.432	44.182	37.906	1.00	25.00
2725	N	SER	295	113.219	46.361	40.359	1.00	32.61
2726	CA	SER	295	113.196	47.623	41.097	1.00	37.07
2727	C	SER	295	111.820	48..276	41.002	1.00	35.65
2728	O	SER	295	111.227	48.673	42.011	1.00	33.09
2729	CB	SER	295	114.248	48.584	40.533	1.00	35.83
2730	OG	SER	295	115.543	48.024	40.608	1.00	42.38
2731	H	SER	295	113.804	46.290	39.575	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2732	HG	SER	295	115.756	47.823	41.523	1.00	25.00
2733	N	MET	296	111.306	48.342	39.779	1.00	34.54
2734	CA	MET	296	110.017	48.951	39.506	1.00	35.02
2735	C	MET	296	108.864	48.263	40.230	1.00	36.33
2736	O	MET	296	108.080	48.919	40.923	1.00	35.61
2737	CB	MET	296	109.768	48.966	37.999	1.00	39.18
2738	CG	MET	296	109.109	50.234	37.507	1.00	49.37
2739	SD	MET	296	109.993	51.708	38.067	1.00	51.57
2740	CE	MET	296	108.888	52.271	39.359	1.00	53.40
2741	H	MET	296	111.819	47.966	39.036	1.00	25.00
2742	N	ILE	297	108.780	46.941	40.103	1.00	37.42
2743	CA	ILE	297	107.709	46.185	40.745	1.00	34.54
2744	C	ILE	297	107.813	46.267	42.267	1.00	36.45
2745	O	ILE	297	106.817	46.101	42.976	1.00	35.56
2746	CB	ILE	297	107.675	44.709	40.265	1.00	36.67
2747	CG1	ILE	297	106.342	44.059	40.648	1.00	30.90
2748	CG2	ILE	297	108.858	43.925	40.821	1.00	34.15
2749	CD1	ILE	297	105.135	44.654	39.935	1.00	28.47
2750	H	ILE	297	109.454	46.468	39.576	1.00	25.00
2751	N	SER	298	109.015	46.559	42.761	1.00	37.95
2752	CA	SER	298	109.250	46.696	44.195	1.00	40.22
2753	C	SER	298	108.531	47.961	44.673	1.00	38.96
2754	O	SER	298	107.934	47.979	45.753	1.00	36.43
2755	CB	SER	298	110.751	46.791	44.481	1.00	43.72
2756	OG	SER	298	111.009	46.764	46.873	1.00	62.08
2757	H	SER	298	109.775	46.674	42.153	1.00	25.00
2758	HG	SER	298	110.573	47.504	46.304	1.00	25.00
2759	N	ILE	299	108.582	49.011	43.857	1.00	39.57
2760	CA	ILE	299	107.912	50.271	44.175	1.00	40.91
2761	C	ILE	299	106.412	49.996	44.293	1.00	40.75
2762	O	ILE	299	105.771	50.378	45.276	1.00	40.26
2763	CB	ILE	299	108.128	51.329	43.060	1.00	37.27
2764	CG1	ILE	299	109.614	51.653	42.908	1.00	37.90
2765	CG2	ILE	299	1077.345	52.592	43.370	1.00	42.54
2766	CD1	ILE	299	110.260	52.146	44.173	1.00	39.79
2767	H	ILE	299	109.091	48.942	43.021	1.00	25.00
2768	N	VAL	300	105.876	49.290	43.301	1.00	34.47
2769	CA	VAL	300	104.462	48.949	43.267	1.00	33.70
2770	C	VAL	300	104.050	48.145	44.497	1.00	38.81
2771	O	VAL	300	103.020	48.431	45.116	1.00	39.02
2772	CB	VAL	300	104.116	48.166	41.990	1.00	35.45
2773	CG1	VAL	300	102.629	47.848	41.951	1.00	37.16
2774	CG2	VAL	300	104.522	48.970	40.762	1.00	29.01
2775	H	VAL	300	106.459	48.994	42.572	1.00	25.00
2776	N	ASP	301	104.868	47.162	44.865	1.00	39.28
2777	CA	ASP	301	104.585	46.327	46.030	1.00	39.76
2778	C	ASP	301	104.477	47.200	47.281	1.00	43.93
2779	O	ASP	301	103.588	47.002	48.113	1.00	43.98
2780	CB	ASP	301	105.684	45.270	46.205	1.00	41.93
2781	CG	ASP	301	105.401	44.299	47.348	1.00	47.18
2782	OD1	ASP	301	104.219	44.006	47.633	1.00	52.50
2783	OD2	ASP	301	106.375	43.817	47.959	1.00	53.58
2784	H	ASP	301	105.672	46.984	44.338	1.00	25.00
2785	N	ASP	302	105.373	48.175	47.401	1.00	48.10
2786	CA	ASP	302	105.371	49.088	48.541	1.00	51.62
2787	C	ASP	302	104.090	49.918	48.560	1.00	50.46
2788	O	ASP	302	103.480	50.114	49.615	1.00	51.17
2789	CB	ASP	302	106.587	50.017	48.487	1.00	55.75
2790	CG	ASP	302	107.904	49.271	48.619	1.00	62.15
2791	OD1	ASP	302	107.922	48.165	49.207	1.00	63.08
2792	OD2	ASP	302	108.928	49.798	48.133	1.00	68.25
2793	H	ASP	302	106.056	48.281	46.704	1.00	25.00
2794	N	THR	303	103.684	50.388	47.383	1.00	50.52
2795	CA	THR	303	102.479	51.192	47.230	1.00	50.05
2796	C	THR	303	101.260	50.472	47.808	1.00	51.84
2797	O	THR	303	100.563	51.013	48.668	1.00	56.07
2798	CB	THR	303	102.222	51.512	45.745	1.00	50.09
2799	OG1	THR	303	103.377	52.153	45.190	1.00	45.79
2800	CG2	THR	303	101.015	52.425	45.593	1.00	50.31
2801	H	THR	303	104.219	50.190	46.581	1.00	25.00
2802	HG1	THR	303	103.480	52.938	45.719	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2803	N	PHE	304	101.025	49.246	47.352	1.00	50.29
2804	CA	PHE	304	99.893	48.450	47.817	1.00	53.29
2805	C	PHE	304	99.997	48.024	49.275	1.00	59.68
2806	O	PHE	304	98.981	47.832	49.940	1.00	62.17
2807	CB	PHE	304	99.744	47.182	46.971	1.00	43.62
2808	CG	PHE	304	99.065	47.398	45.654	1.00	37.53
2809	CD1	PHE	304	99.780	47.857	44.555	1.00	32.17
2810	CD2	PHE	304	97.711	47.113	45.506	1.00	35.92
2811	CE1	PHE	304	99.156	48.029	43.326	1.00	36.26
2812	CE2	PHE	304	97.079	47.280	44.283	1.00	29.26
2813	CZ	PHE	304	97.802	47.739	43.189	1.00	34.73
2814	H	PHE	304	101.636	48.860	46.683	1.00	25.00
2815	N	ASP	305	101.223	47.873	49.765	1.00	69.36
2816	CA	ASP	305	101.450	47.405	51.129	1.00	78.46
2817	C	ASP	305	101.326	48.406	52.279	1.00	80.92
2818	O	ASP	305	100.774	48.064	53.329	1.00	79.13
2819	CB	ASP	305	102.798	46.675	51.210	1.00	84.84
2820	CG	ASP	305	102.851	45.663	52.345	1.00	90.63
2821	OD1	ASP	305	102.142	44.635	52.265	1.00	90.70
2822	OD2	ASP	305	103.610	45.891	53.312	1.00	92.23
2823	H	ASP	305	101.996	48.072	49.197	1.00	25.00
2824	N	ALA	306	101.818	49.631	52.104	1.00	84.70
2825	CA	ALA	306	101.752	50.595	53.201	1.00	89.65
2826	C	ALA	306	101.457	52.057	52.874	1.00	91.11
2827	O	ALA	306	101.606	52.916	53.745	1.00	93.41
2828	CB	ALA	306	103.027	50.500	54.040	1.00	89.50
2829	H	ALA	306	102.229	49.879	51.249	1.00	25.00
2830	N	TYR	307	101.022	52.359	51.655	1.00	90.94
2831	CA	TYR	307	100.743	53.752	51.329	1.00	92.48
2832	C	TYR	307	99.374	54.011	50.701	1.00	90.37
2833	O	TYR	307	98.599	54.824	51.207	1.00	91.55
2834	CB	TYR	307	101.858	54.338	50.453	1.00	98.27
2835	CG	TYR	307	102.031	55.837	50.609	1.00	106.75
2836	CD1	TYR	307	101.301	56.732	49.825	1.00	109.71
2837	CD2	TYR	307	102.918	56.364	51.552	1.00	07.24
2838	CE1	TYR	307	101.447	58.113	49.973	1.00	107.24
2839	CE2	TYR	307	103.072	57.744	51.708	1.00	106.57
2840	CZ	TYR	307	102.332	58.611	50.915	1.00	106.75
2841	OH	TYR	307	102.477	59.971	51.060	1.00	103.97
2842	H	TYR	307	100.876	51.657	50.988	1.00	25.00
2843	HH	TYR	307	101.900	60.427	50.443	1.00	25.00
2844	N	GLY	308	99.079	53.325	49.603	1.00	85.79
2845	CA	GLY	308	97.808	53.522	48.930	1.00	82.54
2846	C	GLY	308	96.583	53.120	49.730	1.00	81.67
2847	O	GLY	308	96.589	52.105	50.428	1.00	80.43
2848	H	GLY	308	99.710	52.666	49.258	1.00	25.00
2849	N	THR	309	95.531	53.928	49.637	1.00	82.42
2850	CA	THR	309	94.282	53.649	50.338	1.00	82.64
2851	C	THR	309	93.397	52.796	49.433	1.00	83.27
2852	O	THR	309	93.592	52.771	48.215	1.00	87.28
2853	CB	THR	309	93.519	54.946	50.696	1.00	80.48
2854	OG1	THR	309	93.166	55.648	49.495	1.00	74.90
2855	CG2	THR	309	94.371	55.844	51.583	1.00	75.37
2856	H	THR	309	95.600	54.729	49.085	1.00	25.00
2857	HG1	THR	309	92.598	55.106	48.954	1.00	25.00
2858	N	VAL	310	92.383	52.172	50.025	1.00	80.18
2859	CA	VAL	310	91.447	51.304	49.309	1.00	73.06
2860	C	VAL	310	91.067	51.822	47.919	1.00	74.05
2861	O	VAL	310	91.209	51.115	46.921	1.00	73.13
2862	CB	VAL	310	90.149	51.103	50.127	1.00	79.21
2863	CG1	VAL	310	89.284	50.020	49.494	1.00	80.28
2864	CG2	VAL	310	90.478	50.760	51.575	1.00	78.07
2865	H	VAL	310	92.275	52.293	50.987	1.00	25.00
2866	N	LYS	311	90.622	53.072	47.859	1.00	73.34
2867	CA	LYS	311	90.210	53.682	46.600	1.00	71.58
2868	C	LYS	311	91.366	53.946	45.639	1.00	67.72
2869	O	LYS	311	91.269	53.642	44.448	1.00	65.13
2870	CB	LYS	311	89.433	54.977	46.866	1.00	79.85
2871	CG	LYS	311	87.977	54.774	47.306	1.00	89.57
2872	CD	LYS	311	87.842	53.976	48.607	1.00	98.38
2873	CE	LYS	311	88.473	54.694	49.795	1.00	102.39

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2874	NZ	LYS	311	87.808	55.997	50.082	1.00	107.12
2875	H	LYS	311	90.572	53.594	48.679	1.00	25.00
2876	1HZ	LYS	311	87.884	56.617	49.250	1.00	25.00
2877	2HZ	LYS	311	86.804	55.833	50.299	1.00	25.00
2878	3HZ	LYS	311	88.268	56.452	50.896	1.00	25.00
2879	N	GLU	312	92.461	54.495	46.162	1.00	64.41
2880	CA	GLU	312	93.634	54.805	45.346	1.00	61.39
2881	C	GLU	312	94.189	53.556	44.667	1.00	61.26
2882	O	GLU	312	94.533	53.585	43.483	1.00	59.48
2883	CB	GLU	312	94.724	55.465	46.194	1.00	63.39
2884	CG	GLU	312	94.348	56.830	46.748	1.00	70.79
2885	CD	GLU	312	95.456	57.456	47.578	1.00	75.21
2886	OE1	GLU	312	95.879	56.840	48.579	1.00	77.19
2887	OE2	GLU	312	95.903	58.570	47.233	1.00	79.86
2888	H	GLU	312	92.482	54.687	47.112	1.00	25.00
2889	N	LEU	313	94.257	52.459	45.418	1.00	57.55
2890	CA	LEU	313	94.765	51.198	44.891	1.00	52.69
2891	C	LEU	313	93.885	50.678	43.762	1.00	52.82
2892	O	LEU	313	94.391	50.281	42.713	1.00	51.15
2893	CB	LEU	313	94.883	50.158	46.005	1.00	48.63
2894	CG	LEU	313	95.886	50.519	47.102	1.00	46.47
2895	CD1	LEU	313	95.941	49.416	48.140	1.00	48.38
2896	CD2	LEU	313	97.259	50.748	46.495	1.00	48.00
2897	H	LEU	313	93.952	52.495	46.346	1.00	25.00
2898	N	GLU	314	92.569	50.724	43.957	1.00	52.92
2899	CA	GLU	314	91.634	50.269	42.933	1.00	54.92
2900	C	GLU	314	91.840	51.087	41.651	1.00	52.05
2901	O	GLU	314	91.801	50.548	40.541	1.00	49.73
2902	CB	GLU	314	90.189	50.400	43.431	1.00	58.82
2903	CG	GLU	314	89.137	49.809	42.488	1.00	68.28
2904	CD	GLU	314	89.281	48.303	42.292	1.00	74.40
2905	OE1	GLU	314	89.097	47.550	43.275	1.00	76.74
2906	OE2	GLU	314	89.568	47.871	41.152	1.00	74.09
2907	H	GLU	314	92.221	51.057	44.810	1.00	25.00
2908	N	ALA	315	92.088	52.383	41.813	1.00	51.92
2909	CA	ALA	315	92.323	53.270	40.678	1.00	54.57
2910	C	ALA	315	93.649	52.920	39.993	1.00	51.51
2911	O	ALA	315	93.762	52.977	38.763	1.00	49.98
2912	CB	ALA	315	92.335	54.722	41.142	1.00	52.19
2913	H	ALA	315	92.103	52.753	42.723	1.00	25.00
2914	N	TYR	316	94.540	52.542	40.796	1.00	49.90
2915	CA	TYR	316	95.960	52.177	40.289	1.00	46.00
2916	C	TYR	316	95.911	50.864	39.506	1.00	42.05
2917	O	TYR	316	96.503	50.756	38.424	1.00	36.96
2918	CB	TYR	316	96.954	52.070	41.445	1.00	48.32
2919	CG	TYR	316	98.405	52.154	41.029	1.00	52.17
2920	CD1	TYR	316	98.975	53.371	40.657	1.00	53.66
2921	CD2	TYR	316	99.218	51.023	41.033	1.00	58.41
2922	CE1	TYR	316	100.320	53.461	40.303	1.00	56.28
2923	CE2	TYR	316	100.566	51.101	40.681	1.00	63.22
2924	CZ	TYR	316	101.110	52.323	40.319	1.00	58.59
2925	OH	TYR	316	102.442	52.405	39.986	1.00	51.77
2926	H	TYR	316	94.483	52.514	41.763	1.00	25.00
2927	HH	TYR	316	102.631	53.311	39.758	1.00	25.00
2928	N	THR	317	95.186	49.881	40.040	1.00	38.98
2929	CA	THR	317	95.044	48.574	39.396	1.00	40.08
2930	C	THR	317	94.391	48.732	38.025	1.00	41.19
2931	O	THR	317	94.755	48.040	37.065	1.00	40.64
2932	CB	THR	317	94.189	47.619	40.245	1.00	39.21
2933	OG1	THR	317	94.658	47.632	41.598	1.00	40.99
2934	CG2	THR	317	94.277	40.198	39.698	1.00	41.75
2935	H	THR	317	94.740	50.022	40.900	1.00	25.00
2936	HG1	THR	317	94.120	47.056	42.134	1.00	25.00
2937	N	ASP	318	93.423	49.641	37.945	1.00	46.22
2938	CA	ASP	318	92.719	49.920	36.700	1.00	44.99
2939	C	ASP	318	93.631	50.595	35.693	1.00	38.74
2940	O	ASP	318	93.695	50.183	34.538	1.00	39.12
2941	CB	ASP	318	91.497	50.799	36.959	1.00	55.80
2942	CG	ASP	318	90.215	50.006	36.977	1.00	64.67
2943	OD1	ASP	318	89.924	49.364	38.010	1.00	73.33
2944	OD2	ASP	318	89.507	50.014	35.948	1.00	72.06

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
2945	H	ASP	318	93.171	50.138	38.755	1.00	25.00
2946	N	ALA	319	94.340	51.628	36.135	1.00	37.74
2947	CA	ALA	319	95.258	52.347	35.260	1.00	40.21
2948	C	ALA	319	96.245	51.360	34.644	1.00	42.98
2947	O	ALA	319	96.528	51.422	33.446	1.00	41.24
2950	CB	ALA	319	95.995	53.426	36.039	1.00	42.19
2951	H	ALA	319	94.240	51.923	37.067	1.00	25.00
2952	N	ILE	320	96.727	50.423	35.462	1.00	41.94
2953	CA	ILE	320	97.670	49.403	35.005	1.00	40.80
2954	C	ILE	320	97.064	48.488	33.934	1.00	37.20
2955	O	ILE	320	97.711	48.200	32.923	1.00	31.26
2956	CB	ILE	320	98.198	48.549	36.191	1.00	40.22
2957	CG1	ILE	320	99.093	49.404	37.091	1.00	38.13
2958	CG2	ILE	320	98.973	47.332	35.680	1.00	36.19
2959	CD1	ILE	320	100.340	49.924	36.392	1.00	35.64
2960	H	ILE	320	96.447	50.429	36.402	1.00	25.00
2961	N	GLN	321	95.830	48.037	34.149	1.00	37.70
2962	CA	GLN	321	95.167	47.161	33.180	1.00	43.79
2963	C	GLN	321	94.959	47.867	31.839	1.00	44.60
2964	O	GLN	321	95.104	47.254	30.777	1.00	43.29
2965	CB	GLN	321	93.818	46.662	33.713	1.00	45.39
2966	CG	GLN	321	93.869	45.997	35.079	1.00	50.49
2967	CD	GLN	321	94.981	44.963	35.182	1.00	52.12
2968	OE1	GLN	321	95.097	44.073	34.341	1.00	53.96
2969	NE2	GLN	321	95.801	45.078	36.220	1.00	49.92
2970	H	GLN	321	95.360	48.301	34.967	1.00	25.00
2971	1HE2	GLN	321	96.511	44.405	36.295	1.00	25.00
2972	2HE2	GLN	321	95.664	45.810	36.855	1.00	25.00
2973	N	ARG	322	94.595	49.148	31.894	1.00	48.28
2974	CA	ARG	322	94.376	49.935	30.683	1.00	48.66
2975	C	ARG	322	95.697	50.181	29.976	1.00	48.74
2976	O	ARG	322	95.756	50.167	28.745	1.00	52.54
2977	CB	ARG	322	93.701	51.272	31.003	1.00	53.96
2978	CG	ARG	322	92.175	51.230	31.029	1.00	62.97
2979	CD	ARG	322	91.642	50.367	32.164	1.00	68.65
29880	NE	ARG	322	90.183	50.288	32.167	1.00	71.23
2981	CZ	ARG	322	89.377	51.274	32.546	1.00	73.12
2982	NH1	ARG	322	89.878	52.432	32.959	1.00	75.57
2983	NH2	ARG	322	88.064	51.101	32.512	1.00	75.20
2984	H	ARG	322	94.477	49.570	32.771	1.00	25.00
2985	HE	ARG	322	89.771	49.449	31.873	1.00	25.00
2986	1HH1	ARG	322	90.868	52.574	32.983	1.00	25.00
2987	2HH1	ARG	322	89.263	53.172	33.235	1.00	25.00
2988	1HH2	ARG	322	87.684	50.229	32.203	1.00	25.00
2989	2HH2	ARG	322	87.455	51.842	32.793	1.00	25.00
2990	N	TRP	323	96.740	50.434	30.765	1.00	48.78
2991	CA	TRP	323	98.086	50.674	30.248	1.00	50.53
2992	C	TRP	323	98.036	51.721	29.139	1.00	51.62
2993	O	TRP	323	98.368	51.442	27.984	1.00	46.60
2994	CB	TRP	323	98.676	49.361	29.719	1.00	45.66
2995	CG	TRP	323	100.171	49.334	29.673	1.00	43.84
2996	CD1	TRP	323	100.972	49.778	28.660	1.00	41.07
2997	CD2	TRP	323	101.045	48.811	30.677	1.00	42.00
2998	NE1	TRP	323	102.292	49.559	28.969	1.00	41.37
2999	CE2	TRP	323	102.367	48.967	30.202	1.00	42.95
3000	CE3	TRP	323	100.841	48.222	31.932	1.00	43.56
3001	CZ2	TRP	323	103.483	48.555	30.939	1.00	41.64
3002	CZ3	TRP	323	101.952	47.812	32.666	1.00	46.00
3003	CH2	TRP	323	103.256	47.982	32.164	1.00	42.99
3004	H	TRP	323	96.604	50.455	31.735	1.00	25.90
3005	HE1	TRP	323	103.052	49.790	28.396	1.00	25.00
3006	N	ASP	324	97.624	52.931	29.503	1.00	59.55
3007	CA	ASP	324	97.500	54.015	28.539	1.00	65.59
3008	C	ASP	324	98.480	55.143	28.844	1.00	64.51
3009	O	ASP	324	99.591	55.176	28.316	1.00	68.35
3010	CB	ASP	324	96.056	54.541	28.552	1.00	70.35
3011	CG	ASP	324	95.713	55.365	27.320	1.00	74.75
3012	OD1	ASP	324	96.439	56.333	27.008	1.00	77.92
3013	OD2	ASP	324	94.698	55.043	26.668	1.00	77.68
3014	H	ASP	324	97.422	53.067	30.447	1.00	25.00
3015	N	ILE	325	98.025	56.067	29.685	1.00	59.63

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3016	CA	ILE	325	98.765	57.248	30.131	1.00	62.22
3017	C	ILE	325	97.699	58.281	30.472	1.00	62.36
3018	O	ILE	325	97.807	58.988	31.467	1.00	57.92
3019	CB	ILE	325	99.752	57.824	29.066	1.00	58.28
3020	CG1	ILE	325	100.656	58.874	29.713	1.00	56.91
3021	CG2	ILE	325	99.004	58.424	27.882	1.00	53.60
3022	CD1	ILE	325	101.760	59.364	28.812	1.00	65.51
3023	H	ILE	325	97.138	55.950	30.059	1.00	25.00
3024	N	ASN	326	96.622	58.287	29.687	1.00	64.69
3025	CA	ASN	326	95.504	59.203	29.902	1.00	68.20
3026	C	ASN	326	94.857	58.860	31.238	1.00	71.30
3027	O	ASN	326	94.171	59.684	31.846	1.00	76.27
3028	CB	ASN	326	94.462	59.058	28.787	1.00	67.58
3029	CG	ASN	326	95.041	59.297	27.406	1.00	69.04
3030	OD1	ASN	326	96.055	59.975	27.225	1.00	68.18
3031	ND2	ASN	326	94.410	58.716	26.395	1.00	67.11
3032	H	ASN	326	96.599	57.685	28.918	1.00	25.00
3033	1HD2	ASN	326	94.783	58.869	25.501	1.00	25.00
3034	2HD2	ASN	326	93.618	58.173	26.568	1.00	25.00
3035	N	GLU	327	95.095	57.631	31.691	1.00	70.98
3036	CA	GLU	327	94.553	57.144	32.952	1.00	69.92
3037	C	GLU	327	95.259	57.798	34.138	1.00	67.58
3038	O	GLU	327	94.751	57.777	35.260	1.00	68.23
3039	CB	GLU	327	94.709	55.622	33.034	1.00	69.72
3040	CG	GLU	327	94.147	54.858	31.838	1.00	66.84
3041	CD	GLU	327	92.650	55.040	31.659	1.00	69.61
3042	OE1	GLU	327	91.899	54.845	32.639	1.00	69.86
3043	OE2	GLU	327	92.225	55.369	30.530	1.00	66.87
3044	H	GLU	327	95.646	57.037	31.159	1.00	25.00
3045	N	ILE	328	96.411	58.407	33.872	1.00	64.07
3046	CA	ILE	328	97.212	59.065	34.901	1.00	63.90
3047	C	ILE	328	96.425	60.142	35.657	1.00	70.44
3048	O	ILE	328	96.624	60.338	36.857	1.00	69.65
3049	CB	ILE	328	98.508	59.669	34.286	1.00	56.23
3050	CG1	ILE	328	99.578	59.844	35.359	1.00	56.00
3051	CG2	ILE	328	98.223	61.007	33.618	1.00	53.09
3052	CD1	ILE	328	100.948	60.162	34.799	1.00	58.67
3053	H	ILE	328	96.744	58.430	32.958	1.00	25.00
3054	N	ASP	329	95.487	60.780	34.961	1.00	75.68
3055	CA	ASP	329	94.659	61.844	35.531	1.00	79.88
3056	C	ASP	329	93.764	61.377	36.677	1.00	79.44
3057	O	ASP	329	93.303	62.188	37.483	1.00	79.71
3058	CB	ASP	329	93.796	62.476	34.435	1.00	85.36
3059	CG	ASP	329	94.608	62.912	33.226	1.00	90.96
3060	OD1	ASP	329	95.719	63.461	33.409	1.00	93.02
3061	OD2	ASP	329	94.133	62.699	32.090	1.00	93.14
3062	H	ASP	329	95.344	60.527	34.026	1.00	25.00
3063	N	ARG	330	93.501	60.074	36.730	1.00	76.85
3064	CA	ARG	330	92.658	59.501	37.775	1.00	75.38
3065	C	ARG	330	93.488	59.059	38.981	1.00	71.57
3066	O	ARG	330	92.935	58.631	39.998	1.00	69.70
3067	CB	ARG	330	91.881	58.300	37.227	1.00	75.33
3068	CG	ARG	330	91.177	58.562	35.905	1.00	78.99
3069	CD	ARG	330	90.383	57.350	35.454	1.00	80.32
3070	NE	ARG	330	39.861	57.517	34.100	1.00	86.31
3071	CZ	ARG	330	88.851	56.816	33.592	1.00	88.51
3072	NH1	ARG	330	88.239	55.894	34.325	1.00	91.01
3073	NH2	ARG	330	88.458	57.030	32.344	1.00	89.50
3074	H	ARG	330	93.891	59.477	36.060	1.00	25.00
3075	HE	ARG	330	90.281	58.188	33.523	1.00	25.00
3076	1HH1	ARG	330	88.533	55.723	35.265	1.00	25.00
3077	2HH1	ARG	330	87.475	55.375	33.942	1.00	25.00
3078	1HH2	ARG	330	88.917	57.720	31.786	1.00	25.00
3079	2HH2	ARG	330	87.692	56.508	31.966	1.00	25.00
3080	N	LEU	331	94.809	59.174	38.867	1.00	67.63
3081	CA	LEU	331	95.723	58.761	39.930	1.00	62.95
3082	C	LEU	331	96.290	59.919	40.735	1.00	60.42
3083	O	LEU	331	96.590	60.974	40.186	1.00	58.28
3084	CB	LEU	331	96.906	57.985	39.338	1.00	58.68
3085	CG	LEU	331	96.664	56.739	38.486	1.00	54.70
3086	CD1	LEU	331	97.992	56.255	37.941	1.00	46.64

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3087	CD2	LEU	331	95.988	55.654	39.304	1.00	48.82
3088	H	LEU	331	95.195	59.574	38.061	1.00	25.00
3089	N	PRO	332	96.426	59.743	42.058	1.00	57.70
3090	CA	PRO	332	96.981	60.814	42.886	1.00	58.87
3091	C	PRO	332	98.455	60.977	42.521	1.00	61.32
3092	O	PRO	332	99.132	59.997	42.207	1.00	63.75
3093	CB	PRO	332	96.800	60.278	44.307	1.00	58.32
3094	CG	PRO	332	96.819	58.793	44.122	1.00	60.80
3095	CD	PRO	332	95.978	58.616	42.892	1.00	59.09
3096	N	ASP	333	98.944	62.210	42.585	1.00	68.56
3097	CA	ASP	333	100.324	62.554	42.237	1.00	71.37
3098	C	ASP	333	101.432	61.520	42.437	1.00	68.42
3099	O	ASP	333	102.188	61.247	41.504	1.00	65.66
3100	CB	ASP	333	100.715	63.879	42.891	1.00	79.84
3101	CG	ASP	333	99.967	65.057	42.298	1.00	86.67
3102	OD1	ASP	333	100.442	65.608	41.283	1.00	91.38
3103	OD2	ASP	333	98.897	65.418	42.834	1.00	90.77
3104	H	ASP	333	98.343	62.928	42.866	1.00	25.00
3105	N	TYR	334	101.538	60.938	43.627	1.00	65.59
3106	CA	TYR	334	1022.588	59.953	43.861	1.00	63.25
3107	C	TYR	334	102.455	58.740	42.938	1.00	60.61
3108	O	TYR	334	103.452	58.243	42.411	1.00	63.00
3109	CB	TYR	334	102.664	59.545	45.341	1.00	65.74
3110	CG	TYR	334	101.539	58.674	45.852	1.00	68.46
3111	CD1	TYR	334	100.343	59.232	46.303	1.00	69.57
3112	CD2	TYR	334	101.690	57.289	45.929	1.00	68.64
3113	CE1	TYR	334	99.326	58.432	46.824	1.00	69.54
3114	CE2	TYR	334	100.682	56.482	46.446	1.00	69.64
3115	CZ	TYR	334	99.504	57.058	46.892	1.00	70.47
3116	OH	TYR	334	98.515	56.257	47.413	1.00	68.60
3117	H	TYR	334	100.910	61.170	44.337	1.00	25.00
3118	HH	TYR	334	97.786	56.812	47.691	1.00	25.00
3119	N	MET	335	101.220	58.311	42.691	1.00	51.84
3120	CA	MET	335	100.977	57.174	41.809	1.00	46.91
3121	C	MET	335	101.236	57.558	40.356	1.00	46.00
3122	O	MET	335	101.540	56.701	39.525	1.00	49.65
3123	CB	MET	335	99.552	56.646	41.969	1.00	41.83
3124	CG	MET	335	99.268	56.054	43.333	1.00	37.39
3125	SD	MET	335	97.625	55.322	43.450	1.00	44.89
3126	CE	MET	335	97.914	54.042	44.666	1.00	45.77
3127	H	MET	335	100.460	58.772	43.094	1.00	25.00
3128	N	LYS	336	101.122	58.848	40.052	1.00	47.61
3129	CA	LYS	336	101.366	59.340	38.699	1.00	48.27
3130	C	LYS	336	102.836	59.143	38.325	1.00	46.89
3131	O	LYS	336	103.161	58.829	37.177	1.00	49.33
3132	CB	LYS	336	101.000	60.824	38.588	1.00	51.58
3133	CG	LYS	336	99.517	61.132	38.743	1.00	54.94
3134	CD	LYS	336	99.233	62.600	38.446	1.00	60.67
3135	CE	LYS	336	97.739	62.882	38.431	1.00	63.81
3136	NZ	LYS	336	97.404	64.287	38.083	1.00	68.16
3137	H	LYS	336	100.869	59.485	40.750	1.00	25.00
3138	1HZ	LYS	336	97.836	64.931	38.776	1.00	25.00
3139	2HZ	LYS	338	97.770	64.503	37.134	1.00	25.00
3140	3HZ	LYS	336	96.371	64.409	38.092	1.00	25.00
3141	N	ILE	337	103.719	59.321	39.303	1.00	44.56
3142	CA	ILE	337	105.154	59.162	39.089	1.00	47.99
3143	C	ILE	337	105.469	57.701	38.782	1.00	50.21
3144	O	ILE	3337	106.153	57.400	37.800	1.00	52.97
3145	CB	ILE	337	105.957	59.595	40.336	1.00	51.57
3146	CG1	ILE	337	105.533	61.001	40.770	1.00	54.20
3147	CG2	ILE	337	107.455	59.569	40.034	1.00	49.66
3148	CD1	ILE	337	106.048	61.406	42.131	1.00	53.35
3149	H	ILE	337	103.390	59.566	40.195	1.00	25.00
3150	N	SER	338	104.951	56.802	39.618	1.00	46.40
3151	CA	SER	338	105.161	55.364	39.458	1.00	41.92
3152	C	SER	338	104.640	54.905	38.098	1.00	39.82
3153	O	SER	338	105.385	54.347	37.286	1.00	36.78
3154	CB	SER	338	104.423	54.598	40.560	1.00	37.35
3155	OG	SER	338	104.502	55.268	41.805	1.00	52.45
3156	H	SER	338	104.411	57.109	40.381	1.00	25.00
3157	HG	SER	338	105.419	55.324	42.084	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3158	N	TYR	339	103.363	55.183	37.848	1.00	39.53
3159	CA	TYR	339	102.697	54.804	36.606	1.00	40.68
3160	C	TYR	339	103.468	55.247	35.362	1.00	39.79
3161	O	TYR	339	103.719	54.444	34.458	1.00	39.78
3162	CB	TYR	339	101.272	55.374	36.586	1.00	39.96
3163	CG	TYR	339	100.388	54.833	35.480	1.00	44.71
3164	CD1	TYR	339	99.948	53.507	35.494	1.00	40.18
3165	CD2	TYR	339	99.992	55.646	34.416	1.00	42.64
3166	CE1	TYR	339	99.136	53.004	34.475	1.00	40.02
3167	CE2	TYR	339	99.180	55.151	33.393	1.00	46.52
3168	CZ	TYR	339	98.758	53.830	33.431	1.00	40.74
3169	OH	TYR	339	97.968	53.3422	32.417	1.00	44.28
3170	H	TYR	339	102.843	55.668	38.522	1.00	25.00
3171	HH	TYR	339	97.819	54.042	31.792	1.00	25.00
3172	N	LYS	340	103.864	58.515	35.324	1.00	42.19
3173	CA	LYS	340	104.599	57.032	34.179	1.00	42.37
3174	C	LYS	340	105.930	56.306	33.992	1.00	40.71
3175	O	LYS	340	106.264	55.885	32.882	1.00	41.93
3176	CB	LYS	340	104.826	58.541	34.306	1.00	48.48
3177	CG	LYS	340	105.461	59.136	33.063	1.00	61.36
3178	CD	LYS	340	105.412	60.647	33.041	1.00	76.14
3179	CE	LYS	340	105.947	61.164	31.713	1.00	85.02
3180	NZ	LYS	340	105.783	62.636	31.566	1.00	94.84
3181	H	LYS	340	103.661	57.115	36.074	1.00	25.00
3182	1HZ	LYS	340	104.774	62.881	31.624	1.00	25.00
3183	2HZ	LYS	340	106.302	63.119	32.327	1.00	25.00
3184	3HZ	LYS	340	106.160	62.937	30.645	1.00	25.00
3185	N	ALA	341	106.668	56.134	35.084	1.00	40.84
3186	CA	ALA	341	107.963	55.455	35.052	1.00	36.82
3187	C	ALA	341	107.837	54.053	34.469	1.00	35.10
3188	O	ALA	341	108.657	53.635	33.650	1.00	34.92
3189	CB	ALA	341	108.548	55.388	36.451	1.00	37.09
3190	H	ALA	341	106.338	56.478	35.942	1.00	25.00
3191	N	ILE	342	106.796	53.338	34.884	1.00	32.81
3192	CA	ILE	342	106.547	51.983	34.409	1.00	31.78
3193	C	ILE	342	106.357	51.982	32.891	1.00	38.13
3194	O	ILE	342	107.061	51.269	32.163	1.00	37.84
3195	CB	ILE	342	105.306	51.377	35.109	1.00	27.44
3196	CG1	ILE	342	105.585	51.219	36.606	1.00	30.45
3197	CG2	ILE	342	104.943	50.031	34.499	1.00	29.34
3198	CD1	ILE	342	104.399	50.759	37.420	1.00	30.40
3199	H	ILE	342	106.179	53.740	35.532	1.00	25.00
3200	N	LEU	343	105.447	52.827	32.414	1.00	44.76
3201	CA	LW	343	105.168	52.920	30.984	1.00	42.79
3202	C	LEU	343	106.428	53.290	30.214	1.00	40.23
3203	O	LEU	343	106.706	52.724	29.153	1.00	39.11
3204	CB	LEU	343	104.061	53.943	30.715	1.00	42.96
3205	CG	LEU	343	102.731	53.704	31.436	1.00	48.89
3206	CD1	LEU	343	101.704	54.723	30.978	1.00	51.34
3207	CD2	LEU	343	102.233	52.302	31.166	1.00	44.17
3208	H	LW	343	104.954	53.403	33.039	1.00	25.00
3209	N	ASP	344	107.202	54.218	30.770	1.00	40.93
3210	CA	ASP	344	108.442	54.660	30.144	1.00	43.89
3211	C	ASP	344	109.443	53.515	30.053	1.00	43.08
3212	O	ASP	344	110.049	53.299	29.001	1.00	38.31
3213	CB	ASP	344	109.056	55.831	30.921	1.00	50.27
3214	CG	ASP	344	108.259	57.124	30.775	1.00	58.66
3215	OD1	ASP	344	107.376	57.206	29.891	1.00	59.02
3216	OD2	ASP	344	108.525	58.070	31.549	1.00	62.70
3217	H	ASP	344	106.928	54.612	31.623	1.00	25.00
3218	N	LEU	345	109.585	52.764	31.144	1.00	40.54
3219	CA	LEU	345	110.511	51.633	31.196	1.00	36.66
3220	C	LEU	345	110.256	50.661	30.048	1.00	36.17
3221	O	LEU	345	111.188	50.256	29.343	1.00	35.58
3222	CB	LEU	345	110.393	50.903	32.540	1.00	38.27
3223	CG	LEU	345	111.284	49.672	32.755	1.00	35.02
3224	CD1	LEU	345	112.750	50.043	32.587	1.00	28.76
3225	CD2	LEU	345	111.030	49.087	34.132	1.00	30.95
3225	H	LEU	345	109.050	52.975	31.934	1.00	25.00
3227	N	TYR	346	108.992	50.304	29.844	1.00	35.43
3228	CA	TYR	346	108.650	49.389	23.768	1.00	32.38

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3229	C	TYR	346	108.906	49.969	27.388	1.00	34.86
3230	O	TYR	346	109.183	49.228	26.448	1.00	36.74
3231	CB	TYR	346	107.227	48.870	28.927	1.00	33.82
3232	CG	TYR	346	107.173	47.798	29.980	1.00	31.79
3233	CD1	TYR	346	107.531	46.487	29.675	1.00	34.43
3234	CD2	TYR	346	106.856	48.107	31.302	1.00	34.30
3235	CE1	TYR	346	107.585	45.507	30.659	1.00	32.57
3236	CE2	TYR	346	106.906	47.137	32.296	1.00	34.14
3237	CZ	TYR	346	107.275	45.839	31.965	1.00	34.31
3238	OH	TYR	346	107.351	44.878	32.938	1.00	32.03
3239	H	TYR	346	108.288	50.665	30.428	1.00	25.00
3240	HH	TYR	346	107.610	44.038	32.582	1.00	25.00
3241	N	LYS	347	108.861	51.295	27.276	1.00	44.24
3242	CA	LYS	347	109.143	51.955	26.004	1.00	44.41
3243	C	LYS	347	110.630	51.792	25.718	1.00	43.81
3244	O	LYS	347	111.030	51.558	24.572	1.00	42.39
3245	CB	LYS	347	108.762	53.437	26.060	1.00	51.50
3246	CG	LYS	347	107.268	53.672	25.945	1.00	55.25
3247	CD	LYS	347	106.759	53.062	24.650	1.00	59.99
3248	CE	LYS	347	105.251	52.978	24.608	1.00	60.17
3249	NZ	LYS	347	104.841	52.152	23.446	1.00	53.42
3250	H	LYS	347	108.627	51.840	28.057	1.00	25.00
3251	1HZ	LYS	347	105.241	51.196	23.537	1.00	25.00
3252	2HZ	LYS	347	103.803	52.090	23.409	1.00	25.00
3253	3HZ	LYS	347	105.190	52.590	22.569	1.00	25.00
3254	N	ASP	348	111.439	51.874	28.771	1.00	45.04
3255	CA	ASP	348	112.884	51.712	26.654	1.00	47.19
3256	C	ASP	348	113.178	50.289	26.211	1.00	44.53
3257	O	ASP	348	113.992	50.074	25.316	1.00	46.94
3258	CB	ASP	348	113.582	51.981	27.991	1.00	55.77
3259	CG	ASP	348	113.469	53.430	28.441	1.00	63.79
3260	OD1	ASP	348	113.017	54.288	27.648	1.00	66.77
3261	OD2	ASP	348	113.840	53.710	29.600	1.00	65.20
3262	H	ASP	348	111.048	52.057	27.652	1.00	25.00
3263	N	TYR	349	112.507	49.321	26.835	1.00	39.87
3264	CA	TYR	349	112.692	47.913	26.491	1.00	40.93
3265	C	TYR	349	112.412	47.704	25.008	1.00	41.26
3266	O	TYR	349	113.189	47.051	24.302	1.00	40.44
3267	CB	TYR	349	111.752	47.015	27.310	1.00	35.88
3268	CG	TYR	349	112.115	46.841	28.773	1.00	33.98
3269	CD1	TYR	349	113.396	47.144	29.250	1.00	29.99
3270	CD2	TYR	349	111.172	46.360	29.680	1.00	27.01
3271	CE1	TYR	349	113.723	45.971	30.596	1.00	27.43
3272	CE2	TYR	349	111.485	43.182	31.021	1.00	32.24
3273	CZ	TYR	349	112.759	46.491	31.476	1.00	34.71
3274	OH	TYR	349	113.045	46.346	32.813	1.00	31.76
3275	H	TYR	349	111.880	49.567	27.549	1.00	25.00
3276	HH	TYR	349	112.295	45.961	33.270	1.00	25.00
3277	N	GLU	350	111.302	48.269	24.541	1.00	44.18
3278	CA	GLU	350	110.911	48.156	23.140	1.00	47.18
3279	C	GLU	350	111.972	48.767	22.235	1.00	45.46
3280	O	GLU	350	112.337	48.175	21.221	1.00	45.14
3281	CB	GLU	350	109.557	48.828	22.903	1.00	46.54
3282	CG	GLU	350	108.396	48.141	23.609	1.00	52.79
3283	CD	GLLU	350	107.078	48.883	23.473	1.00	59.87
3284	OE1	GLU	350	107.070	50.040	23.000	1.00	66.09
3285	OE2	GLU	350	106.037	48.304	23.852	1.00	65.68
3286	H	GLU	350	110.728	48.772	25.158	1.00	25.00
3287	N	LYS	351	112.497	49.923	22.636	1.00	48.01
3288	CA	LYS	351	113.530	50.618	21.871	1.00	51.81
3289	C	LYS	351	114.794	49.758	21.788	1.00	52.11
3290	O	LYS	351	115.311	49.505	20.696	1.00	48.04
3291	CB	LYS	351	113.861	51.973	22.518	1.00	53.86
3292	CG	LYS	351	114.151	53.095	21.520	1.00	60.98
3293	CD	LYS	351	115.235	52.708	20.517	1.00	68.26
3294	CE	LYS	351	115.153	53.551	19.253	1.00	75.67
3295	NZ	LYS	351	115.951	52.975	18.132	1.00	74.32
3296	H	LYS	351	112.180	50.322	23.471	1.00	25.00
3297	1HZ	LYS	351	116.950	52.914	18.410	1.00	25.00
3298	2HZ	LYS	351	115.590	52.025	17.907	1.00	25.00
3299	3HZ	LYS	351	115.855	53.584	17.293	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3300	N	GLU	352	115.275	49.297	22.944	1.00	58.12
3301	CA	GLU	352	116.474	48.461	23.031	1.00	54.04
3302	C	GLU	352	116.409	47.241	22.120	1.00	52.28
3303	O	GLU	352	117.410	46.851	21.514	1.00	52.78
3304	CB	GLU	352	116.688	47.971	24.466	1.00	58.92
3305	CG	GLU	352	117.135	49.023	25.460	1.00	67.31
3306	CD	GLU	352	117.386	48.438	26.842	1.00	71.98
3307	OE1	GLU	352	118.383	47.694	27.004	1.00	69.15
3308	OE2	GLU	352	116.582	48.718	27.760	1.00	65.74
3309	H	GLU	352	114.800	49.527	23.762	1.00	25.00
3310	N	LEU	353	115.235	46.624	22.052	1.00	49.88
3311	CA	LEU	353	115.053	45.435	21.233	1.00	51.47
3312	C	LEU	353	114.701	45.732	19.772	1.00	55.82
3313	O	LEU	353	114.606	44.809	18.955	1.00	56.53
3314	CB	LEU	353	114.009	44.511	21.876	1.00	44.77
3315	CG	LEU	353	114.320	44.017	23.297	1.00	40.31
3316	CD1	LEU	353	113.151	43.224	23.855	1.00	35.62
3317	CD2	LEU	353	115.586	43.172	23.302	1.00	33.71
3318	H	LEU	353	114.478	46.975	22.571	1.00	25.00
3319	N	SER	354	114.538	47.012	19.437	1.00	62.13
3320	CA	SER	354	114.202	47.423	18.071	1.00	66.31
33221	C	SER	354	115.245	46.970	17.058	1.00	64.64
3322	O	SER	354	114.904	46.378	16.035	1.00	66.26
3323	CB	SER	354	114.043	48.945	17.978	1.00	69.09
3324	OG	SER	354	112.959	49.406	18.763	1.00	80.83
3325	H	SER	354	114.623	47.710	20.121	1.00	25.00
3326	HG	SER	354	112.888	50.360	18.684	1.00	25.00
3327	N	SER	355	116.516	47.223	17.359	1.00	65.77
3328	CA	SER	355	117.616	46.850	16.472	1.00	67.77
3329	C	SER	355	117.631	45.364	16.110	1.00	68.81
3330	O	SER	355	118.082	44.990	15.028	1.00	69.36
3331	CB	SER	355	118.956	47.245	17.099	1.00	66.08
3332	OG	SER	355	119.067	46.741	18.419	1.00	68.44
3333	H	SER	355	116.729	47.670	18.209	1.00	25.00
3334	HG	SER	355	119.043	45.780	18.416	1.00	25.00
3335	N	ALA	356	117.150	44.525	17.024	1.00	69.39
3336	CA	ALA	356	117.115	43.082	16.802	1.00	68.66
3337	C	ALA	356	115.741	42.585	16.347	1.00	69.25
3338	O	ALA	356	115.561	41.395	16.084	1.00	71.52
3339	CB	ALA	356	117.549	42.347	18.067	1.00	64.46
3340	H	ALA	356	116.806	44.884	17.867	1.00	25.00
3341	N	GLY	357	114.773	43.493	16.270	1.00	67.77
3342	CA	GLY	357	113.432	43.118	15.854	1.00	62.16
3343	C	GLY	357	112.754	42.202	16.856	1.00	58.02
3344	O	GLY	357	111.969	41.327	16.481	1.00	58.07
3345	H	GLY	357	114.965	44.428	16.477	1.00	25.00
3346	N	ARG	358	113.039	42.416	18.138	1.00	53.28
3347	CA	ARG	358	112.461	41.601	19.204	1.00	50.96
3348	C	ARG	358	111.486	42.359	20.106	1.00	50.55
3349	O	ARG	358	110.885	41.774	20.999	1.00	51.85
3350	CB	ARG	358	113.568	40.953	20.047	1.00	44.69
3351	CG	ARG	358	114.360	39.872	19.314	1.00	43.66
3352	CD	ARG	358	115.389	39.206	20.217	1.00	43.11
3353	NE	ARG	358	114.768	38.503	21.338	1.00	42.40
3354	CZ	ARG	358	114.997	38.783	22.618	1.00	43.84
3355	NH1	ARG	358	115.836	39.754	22.951	1.00	49.95
3356	NH2	ARG	358	114.389	38.089	23.571	1.00	45.03
3357	H	ARG	358	113.664	43.136	18.368	1.00	25.00
3358	HE	ARG	358	114.142	37.776	21.138	1.00	25.00
3359	1HH1	ARG	358	116.301	40.282	22.241	1.00	25.00
3360	2HH1	ARG	358	116.006	39.958	23.915	1.00	25.00
3361	1HH2	ARG	358	113.755	37.355	23.327	1.00	25.00
3362	2HH2	ARG	358	114.562	38.301	24.533	1.00	25.00
3363	N	SER	359	111.270	43.639	19.826	1.00	50.59
3364	CA	SER	359	110.363	44.464	20.625	1.00	47.98
3355	C	SER	359	108.948	43.888	20.767	1.00	48.46
3366	O	SER	359	108.247	44.177	21.737	1.00	46.16
3367	CB	SER	359	110.315	45.879	20.050	1.00	51.38
3368	OG	SER	359	110.450	45.839	18.639	1.00	63.31
3369	H	SER	359	111.730	44.045	19.067	1.00	25.00
3370	HG	SER	359	111.323	45.514	18.419	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3371	N	HIS	360	108.559	43.029	19.8829	1.00	46.52
3372	CA	HIS	360	107.234	42.401	19.837	1.00	47.05
3373	C	HIS	360	106.998	41.398	20.974	1.00	48.80
3374	O	HIS	360	105.893	40.871	21.124	1.00	46.79
3375	CB	HIS	360	106.971	41.713	18.492	1.00	47.13
3376	CG	HIS	360	108.026	40.724	18.100	1.00	47.23
3377	ND1	HIS	360	107.885	39.365	18.289	1.00	50.30
3378	CD2	HIS	360	109.242	40.899	17.532	1.00	49.82
3379	CE1	HIS	360	103.969	38.746	17.855	1.00	47.18
3380	NE2	HIS	360	109.808	39.655	17.391	1.00	46.40
3381	H	HIS	360	109.183	42.837	19.111	1.00	25.00
3382	HD1	HIS	360	107.098	38.919	18.675	1.00	25.00
3383	HE2	HIS	360	110.702	39.494	16.992	1.00	25.00
3384	N	ILE	361	108.042	41.098	21.741	1.00	47.17
3385	CA	ILE	361	107.922	40.152	22.845	1.00	40.37
3386	C	ILE	361	107.657	40.850	24.175	1.00	35.93
3387	O	ILE	361	107.118	40.240	25.103	1.00	41.86
3388	CB	ILE	361	109.187	39.277	22.987	1.00	44.49
3389	CG1	ILE	361	110.392	40.152	23.346	1.00	39.20
3390	CG2	ILE	361	109.421	38.477	21.707	1.00	38.28
3391	CD1	ILE	361	111.680	39.405	23.464	1.00	49.02
3392	H	ILE	361	108.913	41.517	21.574	1.00	25.00
3393	N	VAL	362	108.007	42.131	24.256	1.00	29.83
3394	CA	VAL	362	107.818	42.911	25.478	1.00	28.00
3395	C	VAL	362	106.396	42.815	26.041	1.00	32.52
3396	O	VAL	362	106.209	42.788	27.262	1.00	34.43
3397	CB	VAL	362	108.203	44.401	25.259	1.00	30.93
3398	CG1	VAL	362	107.851	45.233	26.484	1.00	28.70
3399	CG2	VAL	362	109.699	44.524	24.952	1.00	22.99
3400	H	VAL	362	108.395	42.588	23.472	1.00	25.00
3401	N	CYS	363	105.405	42.701	25.160	1.00	29.77
3402	CA	CYS	363	104.011	42.610	25.592	1.00	31.29
3403	C	CYS	363	103.757	41.470	26.581	1.00	29.63
3404	O	CYS	363	102.942	41.610	27.499	1.00	25.93
3405	CB	CYS	363	103.066	42.504	24.387	1.00	33.73
3406	SG	CYS	363	103.387	41.126	23.270	1.00	40.61
3407	H	CYS	363	105.612	42.677	24.204	1.00	25.00
3408	N	HIS	364	104.480	40.362	26.421	1.00	26.78
3409	CA	HIS	364	104.332	39.216	27.315	1.00	24.36
3410	C	HIS	364	104.685	39.599	28.754	1.00	31.26
3411	O	HIS	364	104.029	39.163	29.703	1.00	32.48
3412	CB	HIS	364	105.220	38.064	26.855	1.00	26.25
3413	CG	HIS	364	104.826	37.486	25.531	1.00	29.86
3414	ND1	HIS	364	103.731	36.663	25.372	1.00	39.99
3415	CD2	HIS	364	105.398	37.588	24.308	1.00	32.37
3416	CE1	HIS	364	103.646	36.282	24.110	1.00	36.28
3417	NE2	HIS	364	104.646	36.829	23.444	1.00	32.87
3418	H	HIS	364	105.139	40.332	25.695	1.00	25.00
3419	HD1	HIS	364	103.113	36.392	26.086	1.00	25.00
3420	HE2	HIS	364	104.819	36.718	22.488	1.00	25.00
3421	N	ALA	365	105.711	40.431	28.911	1.00	28.85
3422	CA	ALA	365	106.134	40.880	30.232	1.00	30.11
3423	C	ALA	365	105.075	41.813	30.826	1.00	31.00
3424	O	ALA	365	104.727	41.708	32.005	1.00	31.25
3425	CB	ALA	365	107.482	41.585	30.140	1.00	31.82
3426	H	ALA	365	106.191	40.762	28.123	1.00	25.00
3427	N	ILE	366	104.548	42.708	29.992	1.00	33.54
3428	CA	ILE	366	103.512	43.653	30.417	1.00	33.21
3429	C	ILE	366	102.287	42.889	30.922	1.00	29.56
3430	O	ILE	366	101.743	43.199	31.987	1.00	31.04
3431	CB	ILE	366	103.035	44.582	29.255	1.00	33.17
3432	CG1	ILE	366	104.264	45.455	28.823	1.00	30.87
3433	CG2	ILE	366	101.908	45.453	29.674	1.00	28.96
3434	CD1	ILE	366	103.987	46.289	27.599	1.00	35.02
3435	H	ILE	366	104.869	42.731	29.067	1.00	25.00
3436	N	GLU	367	101.874	41.875	30.167	1.00	28.47
3437	CA	GLU	367	100.726	41.061	30.548	1.00	30.13
3438	C	GLU	367	100.945	40.439	31.929	1.00	30.58
3439	O	GLU	367	100.029	40.407	32.754	1.00	31.55
3440	CB	GLU	367	100.461	39.966	29.507	1.00	38.78
3441	CG	GLU	367	100.228	40.472	28.074	1.00	52.31

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3442	CD	GLU	367	99.180	41.585	27.970	1.00	62.83
3443	OE1	GLU	367	98.144	41.525	28.675	1.00	55.58
3444	OE2	GLU	367	99.395	42.523	27.168	1.00	63.90
3445	H	GLU	367	102.351	41.673	29.337	1.00	25.00
3446	N	ARG	368	102.167	39.985	32.196	1.00	28.25
3447	CA	ARG	368	102.479	39.385	33.487	1.00	21.98
3448	C	ARG	368	102.462	40.420	34.607	1.00	22.36
3449	O	ARG	368	102.080	40.108	35.738	1.00	22.36
3450	CB	ARG	368	103.821	38.661	33.440	1.00	23.96
3451	CG	ARG	368	103.796	37.364	32.642	1.00	17.80
3452	CD	ARG	368	102.812	36.352	33.224	1.00	19.62
3453	NE	ARG	368	103.008	35.034	32.626	1.00	19.60
3454	CZ	ARG	368	102.516	33.897	33.113	1.00	20.41
3455	NH1	ARG	368	101.773	33.898	34.211	1.00	26.21
3456	NH2	ARG	368	102.843	32.743	32.548	1.00	22.02
3457	H	ARG	368	102.868	40.046	31.510	1.00	25.00
3458	HE	ARG	368	103.526	34.993	31.804	1.00	25.00
3459	1HH1	ARG	368	101.580	34.754	34.685	1.00	25.00
3460	2HH1	ARG	368	101.410	33.036	34.566	1.00	25.00
3461	1HH2	ARG	368	103.454	32.730	31.755	1.00	25.00
3462	2HH2	ARG	368	102.476	31.888	32.904	1.00	25.00
3463	N	MET	369	102.849	41.654	34.293	1.00	23.19
3464	CA	MET	369	102.845	42.716	35.295	1.00	20.55
3465	C	MET	369	101.410	43.060	35.657	1.00	20.66
3466	O	MET	369	101.085	43.248	36.833	1.00	24.28
3467	CB	MET	369	103.565	43.966	34.789	1.00	24.43
3468	CG	MET	369	103.575	45.097	35.806	1.00	27.10
3469	SD	MET	369	104.503	46.538	35.283	1.00	33.91
3470	CE	MET	369	105.378	46.942	36.804	1.00	36.11
3471	H	MET	369	103.151	41.852	33.380	1.00	25.00
3472	N	LYS	370	100.550	43.142	34.645	1.00	27.52
3473	CA	LYS	370	99.135	43.441	34.865	1.00	27.03
3474	C	LYS	370	98.572	42.392	35.817	1.00	26.80
3475	O	LYS	370	97.854	42.720	36.766	1.00	31.01
3476	CB	LYS	370	98.361	43.415	33.545	1.00	28.62
3477	CG	LYS	370	98.699	44.546	32.591	1.00	26.77
3478	CD	LYS	370	97.881	44.437	31.318	1.00	32.86
3479	CE	LYS	370	98.174	45.591	30.371	1.00	40.98
3480	NZ	LYS	370	97.397	45.502	29.099	1.00	45.53
3481	H	LYS	370	100.870	43.001	33.729	1.00	25.00
3482	1HZ	LYS	370	96.379	45.511	29.313	1.00	25.00
3483	2HZ	LYS	370	97.630	46.314	28.492	1.00	25.00
3484	3HZ	LYS	370	97.640	44.619	28.607	1.00	25.00
3485	N	GLU	3771	98.959	41.139	35.581	1.00	26.63
3486	CA	GLU	371	98.541	40.006	36.398	1.00	23.16
3487	C	GLU	371	98.981	40.191	37.854	1.00	31.56
3488	O	GLU	371	98.180	40.023	38.782	1.00	33.30
3489	CB	GLU	371	99.125	38.719	35.815	1.00	24.88
3490	CG	GLU	371	98.779	37.449	36.569	1.00	25.01
3491	CD	GLU	371	99.346	36.212	35.892	1.00	38.13
3492	OE1	GLU	371	100.588	36.080	35.815	1.00	34.30
3493	OE2	GLU	371	98.549	35.373	35.425	1.00	44.97
3494	H	GLU	371	99.542	40.972	34.811	1.00	25.00
3495	N	VAL	372	100.243	40.567	38.056	1.00	29.02
3496	CA	VAL	372	100.765	40.789	39.406	1.00	26.07
3497	C	VAL	372	99.952	41.869	40.126	1.00	28.22
3498	O	VAL	372	99.582	41.705	41.293	1.00	27.36
3499	CB	VAL	372	102.261	41.216	39.388	1.00	27.23
3500	CG1	VAL	372	102.738	41.520	40.801	1.00	19.82
3501	CG2	VAL	372	103.124	40.119	38.770	1.00	23.40
3502	H	VAL	372	100.836	40.688	37.283	1.00	25.00
3503	N	VAL	373	99.657	42.964	39.426	1.00	31.06
3504	CA	VAL	373	98.893	44.063	40.018	1.00	32.80
3505	C	VAL	373	97.453	43.670	40.378	1.00	33.82
3506	O	VAL	373	96.952	44.054	41.441	1.00	30.74
3507	CB	VAL	373	98.908	45.314	39.118	1.00	34.89
3508	CG1	VAL	373	98.134	46.454	39.775	1.00	32.71
3509	CG2	VAL	373	100.345	45.741	38.855	1.00	34.17
3510	H	VAL	373	99.960	43.0288	38.495	1.00	25.00
3511	N	ARG	374	96.794	42.900	39.512	1.00	31.81
3512	CA	ARG	374	95.428	42.447	39.789	1.00	29.59

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3513	C	ARG	374	95.422	41.667	41.093	1.00	31.35
3514	O	ARG	374	94.613	41.933	41.989	1.00	36.45
3515	CB	ARG	374	94.910	41.519	38.689	1.00	29.25
3516	CG	ARG	374	94.668	42.166	37.349	1.00	32.69
3517	CD	ARG	374	94.034	41.169	36.396	1.00	33.05
3518	NE	ARG	374	94.840	40.973	35.194	1.00	37.26
3519	CZ	ARG	374	95.399	39.817	34.846	1.00	38.15
3520	NH1	ARG	374	95.247	38.741	35.608	1.00	41.80
3521	NH2	ARG	374	96.114	39.738	33.733	1.00	40.61
3522	H	ARG	374	97.230	42.625	38.677	1.00	25.00
3523	HE	ARG	374	94.974	41.744	34.603	1.00	25.00
3524	1HH1	ARG	374	94.711	38.795	36.448	1.00	25.00
3525	2HH1	ARG	374	95.672	37.878	35.336	1.00	25.00
3526	1HH2	ARG	374	96.232	40.550	33.158	1.00	25.00
3527	2HH2	ARG	374	96.537	38.873	33.467	1.00	25.00
3528	N	ASN	375	96.351	40.721	41.202	1.00	31.47
3529	CA	ASN	375	96.458	39.883	42.388	1.00	28.79
3530	C	ASN	375	96.897	40.652	43.625	1.00	26.40
3531	O	ASN	375	96.561	40.266	44.746	1.00	27.83
3532	CB	ASN	375	97.359	38.683	42.112	1.00	35.49
3533	CG	ASN	375	96.744	37.720	41.111	1.00	32.04
3534	OD1	ASN	375	95.982	38.125	40.237	1.00	33.82
3535	ND2	ASN	375	97.075	36.442	41.231	1.00	34.73
3536	H	ASN	375	96.970	40.566	40.454	1.00	25.00
3537	1HD2	ASN	375	96.671	35.522	40.590	1.00	25.00
3538	2HD2	ASN	375	97.686	36.184	41.941	1.00	25.00
3539	N	TYR	376	97.643	41.736	43.422	1.00	32.41
3540	CA	TYR	376	98.075	42.599	44.526	1.00	36.00
3541	C	TYR	376	96.803	43.220	45.101	1.00	36.51
3542	O	TYR	376	96.585	43.247	46.316	1.00	32.23
3543	CB	TYR	376	98.960	43.739	44.010	1.00	34.19
3544	CG	TYR	376	100.447	43.464	43.979	1.00	41.46
3545	CD1	TYR	376	100.993	42.339	44.601	1.00	40.12
3546	CD2	TYR	376	101.315	44.350	43.336	1.00	41.43
3547	CE1	TYR	376	102.365	42.104	44.580	1.00	38.75
3548	CE2	TYR	376	102.688	44.127	43.310	1.00	37.68
3549	CZ	TYR	376	103.203	43.005	43.932	1.00	41.58
3550	OH	TYR	376	104.560	42.785	43.895	1.00	43.07
3551	H	TYR	376	97.915	41.956	42.506	1.00	25.00
3552	HH	TYR	376	104.761	41.958	44.341	1.00	25.00
3553	N	ASN	377	95.965	43.713	44.194	1.00	37.58
3554	CA	ASN	377	94.704	44.343	44.550	1.00	36.82
3555	C	ASN	377	93.807	43.352	45.285	1.00	35.16
3556	O	ASN	377	93.276	43.658	46.353	1.00	35.66
3557	CB	ASN	377	94.011	44.846	43.287	1.00	38.60
3558	CG	ASN	377	92.858	45.770	43.587	1.00	43.38
3559	OD1	ASN	377	92.949	46.628	44.462	1.00	38.97
3560	ND2	ASN	377	91.774	45.622	42.838	1.00	46.57
3561	H	ASN	377	96.210	43.651	43.245	1.00	25.00
3562	1HD2	ASN	377	91.023	46.218	43.029	1.00	25.00
3563	2HD2	ASN	377	91.765	44.936	42.143	1.00	25.00
3564	N	VAL	378	93.683	42.147	44.735	1.00	32.14
3565	CA	VAL	378	92.857	41.106	45.344	1.00	28.96
3566	C	VAL	378	93.339	40.801	46.766	1.00	33.76
3567	O	VAL	378	92.532	40.647	47.690	1.00	32.35
3568	CB	VAL	378	92.858	39.818	44.490	1.00	30.20
3569	CG1	VAL	378	92.051	38.732	45.169	1.00	28.32
3570	CG2	VAL	378	92.285	40.104	43.105	1.00	26.65
3571	H	VAL	378	94.153	41.951	43.897	1.00	25.00
3572	N	GLU	379	94.657	40.741	46.940	1.00	36.35
3573	CA	GLU	379	95.258	40.478	48.246	1.00	38.43
3574	C	GLU	379	94.875	41.598	49.209	1.00	36.80
3575	O	GLU	379	94.579	41.352	50.383	1.00	37.49
3576	CB	GLU	379	96.780	40.395	48.114	1.00	43.01
3577	CG	GLU	379	97.544	40.416	49.436	1.00	52.96
3578	CD	GLU	379	99.055	40.403	49.250	1.00	61.44
3579	OE1	GLU	379	99.526	40.225	48.107	1.00	70.64
3580	OE2	GLU	379	99.776	40.568	50.255	1.00	66.21
3581	H	GLU	379	95.247	40.882	46.167	1.00	25.00
3582	N	SER	380	94.894	42.827	48.700	1.00	37.49
3583	CA	SER	380	94.531	44.003	49.480	1.00	38.42

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3584	C	SER	380	93.070	43.865	49.906	1.00	37.35
3585	O	SER	380	92.740	44.018	51.085	1.00	38.35
3586	CB	SER	380	94.721	45.264	48.634	1.00	37.87
3587	OG	SER	380	94.344	46.428	49.349	1.00	51.23
3588	H	SER	330	95.167	42.951	47.767	1.00	25.00
3589	HG	SER	380	94.903	46.518	50.127	1.00	25.00
3590	N	THR	381	92.209	43.535	48.945	1.00	36.73
3591	CA	THR	381	90.785	43.349	49.198	1.00	31.31
3592	C	THR	381	90.574	42.286	50.278	1.00	33.52
3593	O	THR	381	89.846	42.514	51.245	1.00	35.95
3594	CB	THR	381	90.043	42.922	47.912	1.00	27.90
3595	OG1	THR	381	90.230	43.914	46.894	1.00	30.65
3596	CG2	THR	381	88.564	42.762	48.174	1.00	30.75
3597	H	THR	381	92.531	43.424	48.030	1.00	25.00
3598	HG1	THR	381	89.901	44.765	47.202	1.00	25.00
3599	N	TRP	382	91.246	41.146	50.137	1.00	31.98
3600	CA	TRP	382	91.124	40.059	51.106	1.00	34.10
3601	C	TRP	382	91.498	40.511	52.513	1.00	37.61
3602	O	TRP	382	90.840	40.145	53.490	1.00	37.71
3603	CB	TRP	382	92.001	38.870	50.701	1.00	29.03
3604	CG	TRP	382	91.465	38.064	49.553	1.00	34.52
3605	CD1	TRP	382	90.298	38.272	48.872	1.00	32.13
3606	CD2	TRP	382	92.073	36.907	48.962	1.00	41.36
3607	NE1	TRP	382	90.141	37.315	47.897	1.00	33.27
3608	CE2	TRP	382	91.215	36.485	47.929	1.00	39.81
3609	CE3	TRP	382	93.262	36.198	49.205	1.00	42.10
3610	CZ2	TRP	382	91.507	35.344	47.138	1.00	41.24
3611	CZ3	TRP	382	93.552	35.082	48.417	1.00	37.35
3612	CH2	TRP	382	92.676	34.669	47.396	1.00	37.45
3613	H	TRP	382	91.841	41.035	49.370	1.00	25.00
3614	HE1	TRP	382	89.384	37.250	47.275	1.00	25.00
3615	N	PHE	383	92.551	41.317	52.601	1.00	42.79
3616	CA	PHE	383	93.040	41.836	53.875	1.00	44.89
3617	C	PHE	383	92.005	42.728	54.561	1.00	45.32
3618	O	PHE	383	91.714	42.557	55.748	1.00	44.05
3619	CB	PHE	383	94.346	42.611	53.657	1.00	45.88
3620	CG	PHE	383	94.818	43.358	54.869	1.00	46.79
3621	CD1	PHE	383	95.254	42.674	55.997	1.00	47.27
3622	CD2	PHE	383	94.800	44.751	54.893	1.00	50.35
3623	CE1	PHE	383	95.665	43.368	57.137	1.00	53.01
3624	CE2	PHE	383	95.208	45.453	56.026	1.00	50.27
3625	CZ	PHE	383	95.641	44.759	57.151	1.00	48.55
3626	H	PHE	383	93.023	41.569	51.778	1.00	25.00
3627	N	ILE	384	91.482	43.677	53.803	1.00	46.83
3628	CA	ILE	384	90.458	44.610	54.306	1.00	46.17
3629	C	ILE	384	89.185	43.894	54.774	1.00	47.27
3630	O	ILE	384	88.608	44.253	55.799	1.00	47.11
3631	CB	ILE	384	90.091	45.646	53.227	1.00	41.64
3632	CG1	ILE	384	91.337	46.434	52.817	1.00	42.54
3633	CG2	ILE	384	89.031	46.597	53.750	1.00	46.00
3634	CD1	ILE	384	91.148	47.270	51.568	1.00	40.69
3635	H	ILE	384	91.753	43.749	52.867	1.00	25.00
3636	N	GLU	385	88.756	42.884	54.022	1.00	45.25
3637	CA	GLU	385	87.554	42.123	54.360	1.00	43.73
3638	C	GLU	385	87.791	41.137	55.495	1.00	46.22
3639	O	GLU	385	36.842	40.636	56.097	1.00	51.43
3640	CB	GLU	385	87.051	41.346	53.142	1.00	42.68
3641	CG	GLU	385	86.657	42.211	51.956	1.00	46.85
3642	CD	GLU	385	86.265	41.397	50.730	1.00	50.00
3643	OE1	GLU	385	86.535	40.175	50.696	1.00	44.05
3644	OE2	GLU	385	85.689	41.988	49.791	1.00	52.88
3645	H	GLU	385	89.262	42.652	53.215	1.00	25.00
3646	N	GLY	386	89.055	40.846	55.777	1.00	45.48
3647	CA	GLY	386	89.371	39.893	56.824	1.00	41.52
3648	C	GLY	386	89.038	38.499	56.328	1.00	42.60
3649	O	GLY	386	88.656	37.625	57.104	1.00	44.94
3650	H	GLY	386	89.784	41.273	55.279	1.00	25.00
3651	N	TYR	387	89.190	38.297	55.023	1.00	42.34
3652	CA	TYR	387	88.897	37.020	54.382	1.00	43.55
3653	C	TYR	387	90.042	36.010	54.474	1.00	45.46
3654	O	TYR	387	91.191	36.329	54.162	1.00	49.16

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3655	CB	TYR	387	88.545	37.254	52.908	1.00	38.26
3656	CG	TYR	387	88.082	36.017	52.162	1.00	36.21
3657	CD1	TYR	387	87.152	35.142	52.727	1.00	36.57
3658	CD2	TYR	387	88.555	35.736	50.880	1.00	31.64
3659	CE1	TYR	387	86.704	34.015	52.035	1.00	32.07
3660	CE2	TYR	387	88.112	34.616	50.178	1.00	32.41
3661	CZ	TYR	387	87.187	33.759	50.763	1.00	34.67
3662	OH	TYR	387	86.749	32.648	50.082	1.00	38.16
3663	H	TYR	387	89.541	39.025	54.474	1.00	25.00
3664	HH	TYR	387	87.147	32.629	49.211	1.00	25.00
3665	N	THR	388	89.706	34.787	54.872	1.00	45.36
3666	CA	THR	388	90.671	33.692	54.986	1.00	43.34
3667	C	THR	388	90.199	32.571	54.048	1.00	41.02
3668	O	THR	388	89.474	31.660	54.459	1.00	45.75
3669	CB	THR	388	90.748	33.161	56.444	1.00	42.74
3670	OG1	THR	388	91.169	34.220	57.314	1.00	43.28
3671	CG2	THR	388	91.741	32.008	56.561	1.00	39.83
3672	H	THR	388	88.782	34.613	55.129	1.00	25.00
3673	HG1	THR	388	91.243	33.885	58.206	1.00	25.00
3674	N	PRO	389	90.575	32.649	52.761	1.00	34.93
3675	CA	PRO	389	90.184	31.645	51.769	1.00	34.82
3676	C	PRO	389	90.846	30.293	51.974	1.00	39.00
3677	O	PRO	389	91.864	30.185	52.658	1.00	44.20
3678	CB	PRO	389	90.654	32.273	50.460	1.00	29.22
3679	CG	PRO	389	91.878	33.003	50.869	1.00	31.21
3680	CD	PRO	389	91.444	33.671	52.151	1.00	33.29
3681	N	PRO	390	90.243	29.231	51.425	1.00	39.35
3682	CA	PRO	390	90.830	27.896	51.566	1.00	38.80
3683	C	PRO	390	92.130	27.894	50.744	1.00	42.47
3684	O	PRO	390	92.264	28.683	49.801	1.00	41.59
3685	CB	PRO	390	89.756	26.991	50.960	1.00	35.31
3686	CG	PRO	390	89.094	27.876	49.944	1.00	39.05
3687	CD	PRO	390	88.968	29.177	50.690	1.00	35.38
3688	N	VAL	391	93.070	27.015	51.085	1.00	42.92
3689	CA	VAL	391	94.367	26.947	50.396	1.00	40.91
3690	C	VAL	391	94.310	27.035	48.869	1.00	40.48
3691	O	VAL	391	95.026	27.832	48.266	1.00	37.26
3692	CB	VAL	391	95.163	25.685	50.800	1.00	42.01
3693	CG1	VAL	391	96.542	25.698	50.149	1.00	37.12
3694	CG2	VAL	391	95.298	25.616	52.307	1.00	37.77
3695	H	VAL	391	92.886	26.404	51.823	1.00	25.00
3696	N	SER	392	93.455	26.228	48.251	1.00	37.92
3697	CA	SER	392	93.316	26.223	46.799	1.00	36.67
3698	C	SER	392	93.065	27.627	46.253	1.00	37.70
3699	O	SER	392	93.699	28.056	45.289	1.00	39.57
3700	CB	SER	392	92.167	25.301	46.399	1.00	41.29
3701	OG	SER	392	91.008	25.599	47.163	1.00	53.55
3702	H	SER	392	92.894	25.625	48.776	1.00	25.00
3703	HG	SER	392	90.720	26.495	46.965	1.00	25.00
3704	N	GLU	393	92.140	28.342	46.883	1.00	35.95
3705	CA	GLU	393	91.806	29.692	46.455	1.00	34.88
3706	C	GLU	393	92.951	30.643	46.783	1.00	31.14
3707	O	GLU	393	93.293	31.516	45.984	1.00	29.96
3708	CB	GLU	393	90.518	30.159	47.130	1.00	35.59
3709	CG	GLU	393	89.956	31.447	46.559	1.00	35.57
3710	CD	GLU	393	88.745	31.951	47.318	1.00	39.64
3711	OE1	GLU	393	88.064	31.141	47.985	1.00	40.88
3712	OE2	GLU	393	88.475	33.167	47.2242	1.00	40.96
3713	H	GLU	393	91.694	27.967	47.669	1.00	25.00
3714	N	TYR	394	93.539	30.476	47.962	1.00	32.04
3715	CA	TYR	394	94.655	31.318	48.371	1.00	29.74
3716	C	TYR	394	95.743	31.287	47.302	1.00	31.70
3717	O	TYR	394	96.180	32.335	46.822	1.00	33.06
3718	CB	TYR	394	95.238	30.844	49.706	1.00	33.01
3719	CG	TYR	394	96.546	31.520	50.059	1.00	42.08
3720	CD1	TYR	394	96.585	32.876	50.392	1.00	45.51
3721	CD2	TYR	394	97.752	30.815	50.021	1.00	35.80
3722	CE1	TYR	394	97.791	33.517	50.675	1.00	45.10
3723	CE2	TYR	394	98.963	31.448	50.299	1.00	36.76
3724	CZ	TYR	394	98.975	32.798	50.627	1.00	42.58
3725	OH	TYR	394	100.164	33.430	50.915	1.00	41.43

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3726	H	TYR	394	93.225	29.778	48.567	1.00	25.00
3727	HH	TYR	394	99.991	34.360	51.082	1.00	25.00
3728	N	LEU	395	96.145	30.082	46.909	1.00	28.83
3729	CA	LEU	395	97.189	29.897	45.910	1.00	26.16
3730	C	LEU	395	96.865	30.472	44.541	1.00	29.12
3731	O	LEU	395	97.737	31.063	43.901	1.00	28.83
3732	CB	LEU	395	97.550	28.415	45.770	1.00	28.06
3733	CG	LEU	395	98.263	27.754	46.951	1.00	27.93
3734	CD1	LEU	395	98.511	26.290	46.636	1.00	28.97
3735	CD2	LEU	395	99.575	28.475	47.245	1.00	24.02
3736	H	LEU	395	95.720	29.293	47.301	1.00	25.00
3737	N	SER	396	95.620	30.324	44.093	1.00	29.97
3738	CA	SER	396	95.239	30.836	42.780	1.00	32.88
3739	C	SER	396	95.535	32.329	42.624	1.00	28.77
3740	O	SER	396	95.715	32.818	41.508	1.00	27.80
3741	CB	SER	396	93.770	30.518	42.465	1.00	39.24
3742	OG	SER	396	92.896	30.992	43.472	1.00	46.99
3743	H	SER	396	94.943	29.866	44.642	1.00	25.00
3744	HG	SER	396	92.971	31.948	43.546	1.00	25.00
3745	N	ASN	397	95.597	33.046	43.745	1.00	25.18
3746	CA	ASN	397	95.907	34.472	43.723	1.00	29.15
3747	C	ASN	397	97.333	34.739	44.226	1.00	27.87
3748	O	ASN	397	98.106	35.459	43.588	1.00	28.50
3749	CB	ASN	397	94.909	35.264	44.577	1.00	29.41
3750	CG	ASN	397	95.146	36.770	44.505	1.00	35.89
3751	OD1	ASN	397	94.831	37.404	43.502	1.00	37.46
3752	ND2	ASN	397	95.715	37.343	45.564	1.00	30.17
3753	H	ASN	397	95.421	32.602	44.603	1.00	25.00
3764	1HD2	ASN	397	95.872	38.310	45.510	1.00	25.00
3755	2HD2	ASN	397	95.953	36.794	46.336	1.00	25.00
3756	N	ALA	398	97.682	34.123	45.351	1.00	26.89
3757	CA	ALA	398	98.986	34.300	45.980	1.00	24.87
3758	C	ALA	398	100.205	33.854	45.178	1.00	28.89
3759	O	ALA	398	101.303	34.358	45.395	1.00	31.67
3760	CB	ALA	398	98.992	33.648	47.337	1.00	24.15
3761	H	ALA	398	97.035	33.533	45.770	1.00	25.00
3762	N	LEU	399	100.039	32.910	44.262	1.00	27.33
3763	CA	LEU	399	101.181	32.484	43.474	1.00	29.45
3764	C	LEU	399	101.755	33.589	42.617	1.00	32.27
3765	O	LEU	399	102.967	33.807	42.603	1.00	34.30
3768	CB	LEU	399	100.823	31.254	42.611	1.00	25.44
3767	CG	LEU	399	100.621	29.949	43.390	1.00	24.86
3768	CD1	LEU	399	100.172	28.853	42.451	1.00	20.68
3769	CD2	LEU	399	101.900	29.549	44.104	1.00	22.68
3770	H	LEU	399	99.159	32.500	44.121	1.00	25.00
3771	N	ALA	400	100.887	34.336	41.943	1.00	29.07
3772	CA	ALA	400	101.343	36.434	41.094	1.00	31.03
3773	C	ALA	400	101.939	36.601	41.882	1.00	29.34
3774	O	ALA	400	102.813	37.303	41.373	1.00	26.86
3775	CB	ALA	400	100.215	35.925	40.192	1.00	32.40
3776	H	ALA	400	99.932	34.143	42.022	1.00	25.00
3777	N	THR	401	101.500	36.796	43.125	1.00	27.66
3778	CA	THR	401	102.024	37.896	43.929	1.00	30.92
3779	C	THR	401	103.505	37.728	44.303	1.00	35.35
3780	O	THR	401	104.118	38.649	44.847	1.00	36.05
3781	CB	THR	401	101.170	38.174	45.194	1.00	27.88
3782	OG1	THR	401	101.106	37.007	46.021	1.00	27.11
3783	CG2	THR	401	99.768	38.593	44.803	1.00	25.60
3784	H	THR	401	100.837	36.193	43.521	1.00	25.00
3785	HG1	THR	401	101.990	36.769	48.324	1.00	25.00
3786	N	THR	402	104.076	36.558	44.016	1.00	30.98
3787	CA	THR	402	105.492	36.310	44.295	1.00	28.76
3788	C	THR	402	106.317	37.040	43.240	1.00	28.41
3789	O	THR	402	107.509	37.248	43.422	1.00	30.86
3790	CB	THR	402	105.861	34.807	44.173	1.00	24.70
3791	OG1	THR	402	105.656	34.372	42.820	1.00	22.39
3792	CG2	THR	402	105.039	33.954	45.117	1.00	21.26
3793	H	THR	402	103.554	35.829	43.612	1.00	25.00
3794	HG1	THR	402	105.851	33.431	42.770	1.00	25.00
3795	N	THR	403	105.656	37.373	42.130	1.00	28.49
3796	CA	THR	403	106.207	38.045	40.946	1.00	25.51

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3797	C	THR	403	107.032	37.101	40.077	1.00	27.25
3798	O	THR	403	107.499	37.495	39.009	1.00	29.50
3799	CB	THR	403	107.060	39.323	41.246	1.00	29.54
3800	OG1	THR	403	108.335	38.954	41.781	1.00	24.64
3801	CG2	THR	403	106.339	40.267	42.203	1.00	26.87
3802	H	THR	403	104.707	37.143	42.086	1.00	25.00
3803	HG1	THR	403	108.248	38.543	42.630	1.00	25.00
3804	N	TYR	404	107.120	35.833	40.474	1.00	25.89
3805	CA	TYR	404	107.914	34.860	39.728	1.00	22.27
3806	C	TYR	404	107.544	34.611	38.272	1.00	24.30
3807	O	TYR	404	108.439	34.511	37.434	1.00	26.21
3808	CB	TYR	404	108.062	33.551	40.509	1.00	30.29
3809	CG	TYR	404	109.278	33.544	41.419	1.00	30.18
3810	CD1	TYR	404	109.800	34.736	41.922	1.00	31.88
3811	CD2	TYR	404	109.925	32.352	41.755	1.00	28.35
3812	CE1	TYR	404	110.937	34.747	42.732	1.00	30.99
3813	CE2	TYR	404	111.065	32.353	42.569	1.00	29.01
3814	CZ	TYR	404	111.563	33.558	43.051	1.00	29.70
3815	OH	TYR	404	112.683	33.593	43.847	1.00	27.42
3816	H	TYR	404	106.644	35.551	41.285	1.00	25.00
3817	HH	TYR	404	113.022	32.697	43.955	1.00	25.00
3818	N	TYR	405	106.253	34.508	37.952	1.00	24.23
3819	CA	TYR	405	105.844	34.306	36.553	1.00	24.60
3820	C	TYR	405	106.361	35.507	35.766	1.00	23.35
3821	O	TYR	405	106.912	35.378	34.672	1.00	23.93
3822	CB	TYR	405	104.317	34.292	36.406	1.00	25.23
3823	CG	TYR	405	103.593	33.163	37.099	1.00	24.35
3824	CD1	TYR	405	103.561	31.879	36.548	1.00	23.45
3825	CD2	TYR	405	102.894	33.390	38.282	1.00	23.55
3826	CE1	TYR	4005	102.846	30.852	37.161	1.00	23.28
3827	CE2	TYR	405	102.179	32.374	38.901	1.00	27.86
3828	CZ	TYR	405	102.155	31.111	38.337	1.00	26.80
3829	OH	TYR	405	101.428	30.121	38.956	1.00	26.06
3830	H	TYR	405	105.577	34.557	38.658	1.00	25.00
3831	HH	TYR	405	101.510	29.308	38.452	1.00	25.00
3832	N	TYR	406	106.160	36.676	36.363	1.00	23.37
3833	CA	TYR	406	106.553	37.964	35.813	1.00	21.93
3834	C	TYR	406	108.072	38.084	35.621	1.00	25.55
3835	O	TYR	406	108.535	38.439	34.538	1.00	24.19
3836	CB	TYR	406	106.021	39.047	36.751	1.00	22.96
3837	CG	TYR	406	106.379	40.468	36.408	1.00	21.90
3838	CD1	TYR	406	106.352	40.926	35.093	1.00	20.58
3839	CD2	TYR	406	106.703	41.375	37.416	1.00	27.70
3840	CE1	TYR	406	106.634	42.252	34.796	1.00	21.17
3841	CE2	TYR	406	106.985	42.700	37.128	1.00	24.51
3842	CZ	TYR	406	106.947	43.131	35.820	1.00	23.02
3843	OH	TYR	406	107.207	44.449	35.541	1.00	28.99
3844	H	TYR	406	105.729	36.670	37.238	1.00	25.00
3845	HH	TYR	406	107.398	44.923	36.351	1.00	25.00
3846	N	LEU	407	108.844	37.750	36.652	1.00	25.38
3847	CA	LEU	407	110.303	37.826	36.574	1.00	23.31
3848	C	LEU	407	110.373	36.825	35.575	1.00	20.18
3849	O	LEU	407	111.803	37.147	34.836	1.00	22.15
3850	CB	LEU	407	110.940	37.620	37.952	1.00	20.82
3851	CG	LEU	407	110.514	38.602	39.048	1.00	25.79
3852	CD1	LEU	407	111.362	38.376	40.287	1.00	24.12
3853	CD2	LEU	407	110.636	40.045	38.562	1.00	15.72
3854	H	LEU	407	108.434	37.445	37.475	1.00	25.00
3855	N	ALA	408	110.299	35.625	35.539	1.00	14.35
3856	CA	ALA	408	110.747	34.591	34.609	1.00	17.38
3857	C	ALA	408	110.520	35.083	33.183	1.00	22.75
3858	O	ALA	408	111.382	34.931	32.318	1.00	25.21
3859	CB	ALA	408	109.991	33.293	34.852	1.00	17.26
3860	H	ALA	408	109.560	35.429	36.149	1.00	25.00
3861	N	THR	409	109.362	35.695	32.949	1.00	23.86
3862	CA	THR	409	109.037	36.228	31.632	1.00	22.93
3863	C	THR	409	110.012	37.353	31.294	1.00	25.61
3864	O	THR	409	110.507	37.443	30.165	1.00	26.75
3865	CB	THR	409	107.598	36.776	31.589	1.00	26.26
3866	OG1	THR	409	106.689	35.765	32.042	1.00	26.48
3867	CG2	THR	409	107.222	37.170	30.173	1.00	18.58

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3868	H	THR	409	108.709	35.780	33.672	1.00	25.00
3869	HG1	THR	409	106.917	35.516	32.932	1.00	25.00
3870	N	THR	410	110.316	38.185	32.287	1.00	26.70
3871	CA	THR	410	111.233	39.299	32.095	1.00	26.67
3872	C	THR	410	112.650	38.835	31.757	1.00	29.09
3873	O	THR	410	113.298	39.411	30.877	1.00	29.16
3874	CB	THR	410	111.281	40.208	33.333	1.00	28.30
3875	OG1	THR	410	109.962	40.684	33.626	1.00	30.05
3876	CG2	THR	410	112.189	41.404	33.082	1.00	28.81
3877	H	THR	410	109.905	38.064	33.169	1.00	25.00
3878	HG1	THR	410	109.991	41.259	34.393	1.00	25.00
3879	N	SER	411	113.105	37.760	32.399	1.00	24.71
3880	CA	SER	411	114.452	37.254	32.155	1.00	24.18
3881	C	SER	411	114.688	36.909	30.687	1.00	25.08
3882	O	SER	411	115.822	36.964	30.204	1.00	27.75
3883	CB	SER	411	114.753	36.048	33.043	1.00	20.40
3884	OG	SER	411	114.010	34.914	32.644	1.00	21.48
3885	H	SER	411	112.534	37.287	33.041	1.00	25.00
3888	HG	SER	411	114.205	34.667	31.738	1.00	25.00
3887	N	TYR	412	113.613	36.573	29.979	1.00	23.79
3888	CA	TYR	412	113.692	36.227	28.562	1.00	24.39
3889	C	TYR	412	113.8774	37.44	27.655	1.00	25.24
3890	O	TYR	412	114.437	37.326	26.570	1.00	27.76
3891	CB	TYR	412	112.419	35.511	28.116	1.00	25.37
3892	CG	TYR	412	112.273	34.072	28.539	1.00	29.38
3893	CD1	TYR	412	113.043	33.531	29.569	1.00	29.32
3894	CD2	TYR	412	111.338	33.248	27.910	1.00	24.28
3895	CE1	TYR	412	112.878	32.199	29.964	1.00	26.36
3896	CE2	TYR	412	111.169	31.927	28.291	1.00	25.08
3897	CZ	TYR	412	111.937	31.408	29.318	1.00	29.45
3898	OH	TYR	412	111.750	30.099	29.693	1.00	27.61
3899	H	TYR	412	112.738	36.552	30.423	1.00	25.00
3900	HH	TYR	412	112.347	29.879	30.418	1.00	25.00
3901	N	LEU	413	113.396	38.604	28.100	1.00	25.11
3902	CA	LEU	413	113.467	39.832	27.304	1.00	27.32
3903	C	LEU	413	114.835	40.149	26.726	1.00	30.49
3904	O	LEU	413	114.957	40.434	25.533	1.00	30.50
3905	CB	LEU	413	112.959	41.039	28.103	1.00	23.58
3906	CG	LEU	413	111.476	41.081	28.478	1.00	31.45
3907	CD1	LEU	413	111.179	42.362	29.242	1.00	31.49
3908	CD2	LEU	413	110.613	40.996	27.231	1.00	30.34
3909	H	LEU	413	112.980	38.636	28.989	1.00	25.00
3910	N	GLY	414	115.859	40.098	27.573	1.00	28.96
3911	CA	GLY	414	117.203	40.404	27.129	1.00	27.47
3912	C	GLY	414	117.990	39.233	26.586	1.00	28.88
3913	O	GLY	414	119.186	39.362	26.340	1.00	34.59
3914	H	GLY	414	115.698	39.833	28.496	1.00	25.00
3915	N	MET	415	117.353	38.079	26.436	1.00	29.79
3916	CA	MET	415	118.043	36.909	25.906	1.00	29.75
3917	C	MET	415	117.861	36.868	24.393	1.00	35.70
3918	O	MET	415	116.795	36.522	23.893	1.00	39.21
3919	CB	MET	415	117.515	35.630	26.554	1.00	22.67
3920	CG	MET	415	117.728	35.581	28.050	1.00	23.60
3921	SD	MET	415	117.062	34.095	28.794	1.00	32.91
3922	CE	MET	415	118.255	32.896	28.242	1.00	24.83
3923	H	MET	415	116.398	38.012	26.652	1.00	25.00
3924	N	LYS	416	118.933	37.181	23.677	1.00	40.25
3925	CA	LYS	416	118.942	37.233	22.218	1.00	43.20
3926	C	LYS	416	118.370	36.031	21.466	1.00	42.08
3927	O	LYS	416	118.037	36.143	20.289	1.00	44.24
3928	CB	LYS	416	120.362	37.539	21.735	1.00	48.69
3929	CG	LYS	416	120.916	38.828	22.333	1.00	60.37
3930	CD	LYS	416	122.427	38.949	22.191	1.00	70.42
3931	CE	LYS	416	122.936	40.173	22.949	1.00	72.06
3932	NZ	LYS	416	124.412	40.319	22.863	1.00	78.00
3933	H	LYS	416	119.749	37.416	24.164	1.00	25.00
3934	1HZ	LYS	416	124.870	39.475	23.262	1.00	25.00
3935	2HZ	LYS	416	124.687	40.423	21.865	1.00	25.00
3938	3HZ	LYS	416	124.709	41.163	23.393	1.00	25.00
3937	N	SER	417	118.239	34.893	22.138	1.00	39.46
3938	CA	SER	417	117.706	33.698	21.491	1.00	36.96

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
3939	C	SER	417	116.247	33.395	21.833	1.00	34.08
3940	O	SER	417	115.637	32.518	21.226	1.00	35.80
3941	CB	SER	417	118.580	32.488	21.823	1.00	39.51
3942	OG	SER	417	119.907	32.675	21.358	1.00	45.86
3943	H	SER	417	118.485	34.856	23.077	1.00	25.00
3944	HG	SER	417	120.288	33.461	21.743	1.00	25.00
3945	N	ALA	418	115.688	34.106	22.806	1.00	30.28
3946	CA	ALA	418	114.303	33.879	23.208	1.00	38.39
3947	C	ALA	418	113.331	34.250	22.087	1.00	40.58
3948	O	ALA	418	113.145	35.427	21.779	1.00	42.57
3949	CB	ALA	418	113.981	34.659	24.484	1.00	32.32
3950	H	ALA	418	116.190	34.823	23.238	1.00	25.00
3951	N	THR	419	112.750	33.232	21.457	1.00	41.43
3952	CA	THR	419	111.799	33.420	220.362	1.00	41.21
3953	C	THR	419	110.357	33.504	20.865	1.00	40.11
3954	O	THR	419	110.077	33.235	22.036	1.00	39.88
3955	CB	THR	419	111.892	32.264	19.338	1.00	39.89
3956	OG1	THR	419	111.666	31.016	20.005	1.00	50.18
3957	CG2	THR	419	113.261	32.238	18.672	1.00	37.82
3958	H	THR	419	112.987	32.335	21.728	1.00	25.00
3959	HG1	THR	419	112.370	30.881	20.644	1.00	25.00
3960	N	GLU	420	109.443	33.848	19.963	1.00	39.64
3961	CA	GLU	420	108.027	33.958	20.292	1.00	39.75
3962	C	GLU	420	107.496	32.650	20.871	1.00	35.49
3963	O	GLU	420	106.718	32.652	21.828	1.00	35.76
3964	CB	GLU	420	107.222	34.321	19.041	1.00	46.65
3965	CG	GLU	420	106.741	35.765	18.980	1.00	56.30
3966	CD	GLU	420	105.668	36.081	20.015	1.00	65.12
3967	OE1	GLU	420	104.685	35.311	20.130	1.00	62.03
3968	OE2	GLU	420	105.804	37.112	20.707	1.00	72.02
3969	H	GLU	420	109.732	34.021	19.047	1.00	25.00
3970	N	GLN	421	107.938	31.537	20.291	1.00	32.71
3971	CA	GLN	421	107.520	30.206	20.722	1.00	36.14
3972	C	GLN	421	107.883	29.959	22.184	1.00	36.63
3973	O	GLN	421	107.105	29.365	22.936	1.00	37.57
3974	CB	GLN	421	108.155	29.133	19.830	1.00	40.03
3975	CG	GLN	421	107.622	29.086	18.398	1.00	53.07
3976	CD	GLN	421	107.819	30.390	17.636	1.00	62.17
3977	OE1	GLN	421	108.877	31.017	17.711	1.00	65.66
3978	NE2	GLN	421	106.788	30.815	16.917	1.00	68.97
3979	H	GLN	421	108.580	31.620	19.555	1.00	25.00
3980	1HE2	GLN	421	106.906	31.650	16.419	1.00	25.00
3981	2HE2	GLN	421	105.963	30.289	16.903	1.00	25.00
3982	N	ASP	422	109.052	30.448	22.589	1.00	34.98
3983	CA	ASP	422	109.521	30.292	23.960	1.00	32.53
3984	C	ASP	422	108.607	31.039	24.924	1.00	30.54
3985	O	ASP	422	108.272	30.525	25.992	1.00	33.81
3986	CB	ASP	422	110.972	30.767	24.085	1.00	28.20
3987	CG	ASP	422	111.929	29.945	23.233	1.00	28.18
3988	OD1	ASP	422	111.755	28.710	23.148	1.00	33.24
3989	OD2	ASP	422	112.855	30.529	22.638	1.00	33.81
3990	H	ASP	422	109.610	30.933	21.946	1.00	25.00
3991	N	PHE	423	108.166	32.229	24.523	1.00	29.33
3992	CA	PHE	423	107.261	33.022	25.348	1.00	28.15
3993	C	PHE	423	105.877	32.373	25.407	1.00	29.51
3994	O	PHE	423	105.205	32.424	26.441	1.00	30.32
3995	CB	PHE	423	107.143	34.448	24.808	1.00	31.32
3996	CG	PHE	423	108.275	35.353	25.214	1.00	27.99
3997	CD1	PHE	423	108.227	36.045	26.421	1.00	26.74
3998	CD2	PHE	423	109.375	35.529	24.387	1.00	26.53
3999	CE1	PHE	423	109.255	36.900	26.794	1.00	21.72
4000	CE2	PHE	423	110.412	36.385	24.753	1.00	23.04
4001	CZ	PHE	423	110.350	37.070	25.958	1.00	23.46
4002	H	PHE	423	108.456	32.575	23.652	1.00	25.00
40003	N	GLU	424	105.450	31.771	24.297	1.00	30.80
4004	CA	GLU	424	104.146	31.107	24.233	1.00	36.62
4005	C	GLU	424	104.128	29.911	25.172	1.00	34.48
4006	O	GLU	424	103.131	29.651	25.343	1.00	34.44
4007	CB	GLU	424	103.823	30.661	22.805	1.00	42.57
4008	CG	GLU	424	103.590	31.813	21.839	1.00	63.38
4009	CD	GLU	424	103.322	31.357	20.414	1.00	70.12

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4010	OE1	GLU	424	103.895	30.329	19.988	1.00	72.19
4011	OE2	GLU	424	102.543	32.039	19.715	1.00	79.30
4012	H	GLU	424	106.023	31.773	23.503	1.00	25.00
4013	N	TRP	425	105.242	29.187	25.221	1.00	32.02
4014	CA	TRP	425	105.367	28.038	26.107	1.00	28.78
4015	C	TRP	425	105.262	28.531	27.553	1.00	33.19
4016	O	TRP	425	104.518	27.974	28.365	1.00	30.47
4017	CB	TRP	425	106.719	27.352	25.881	1.00	29.01
4018	CG	TRP	425	107.077	26.340	26.927	1.00	29.69
4019	CD1	TRP	425	106.621	25.058	27.019	1.00	28.88
4020	CD2	TRP	425	107.970	26.530	28.034	1.00	29.87
4021	NE1	TRP	425	107.171	24.437	28.116	1.00	29.58
4022	CE2	TRP	425	108.003	25.316	28.757	1.00	32.75
4023	CE3	TRP	425	108.742	27.609	28.488	1.00	30.70
4024	CZ2	TRP	425	108.781	25.149	29.912	1.00	27.26
4025	CZ3	TRP	425	109.514	27.444	29.638	1.00	26.04
4026	CH2	TRP	425	109.525	26.222	30.335	1.00	27.12
4027	H	TRP	425	105.993	29.429	24.639	1.00	25.00
4028	HE1	TRP	425	106.983	23.517	28.395	1.00	25.00
4029	N	LEU	426	105.974	29.615	27.848	1.00	31.46
4030	CA	LEU	426	105.994	30.186	29.188	1.00	28.35
4031	C	LEU	426	104.627	30.692	29.650	1.00	31.98
4032	O	LEU	426	104.293	30.585	30.832	1.00	29.19
4033	CB	LEU	426	107.039	31.302	29.268	1.00	21.80
4034	CG	LEU	426	107.525	31.703	30.664	1.00	25.44
4035	CD1	LEU	426	108.240	30.535	31.331	1.00	20.60
4036	CD2	LEU	426	108.454	32.900	30.560	1.00	23.92
4037	H	LEU	426	106.512	30.035	27.141	1.00	25.00
4038	N	SER	427	103.824	31.208	28.720	1.00	33.95
4039	CA	SER	427	102.497	31.722	29.066	1.00	33.39
4049	C	SER	427	101.502	30.647	29.502	1.00	30.91
4041	O	SER	427	100.515	30.951	30.170	1.00	31.38
4042	CB	SER	427	101.917	32.568	27.925	1.00	37.83
4043	OG	SER	427	101.970	31.892	26.683	1.00	46.06
4044	H	SER	427	104.124	31.247	27.790	1.00	25.00
4045	HG	SER	427	102.886	31.692	26.470	1.00	25.00
4046	N	LYS	428	101.780	29.392	29.151	1.00	30.99
4047	CA	LYS	428	100.914	28.271	29.518	1.00	30.38
4048	C	LYS	428	101.124	27.817	30.964	1.00	33.22
4049	O	LYS	428	100.505	26.845	31.410	1.00	34.36
4050	CB	LYS	428	101.166	27.070	28.601	1.00	33.08
4051	CG	LYS	428	100.690	27.213	27.166	1.00	40.80
4052	CD	LYS	428	100.885	25.888	26.433	1.00	48.04
4053	CE	LYS	428	100.314	25.910	25.002	1.00	54.20
4054	NZ	LYS	428	100.438	24.571	24.377	1.00	59.29
4055	H	LYS	428	102.587	29.209	28.628	1.00	25.00
4056	1HZ	LYS	428	99.919	23.866	24.937	1.00	25.00
4057	2HZ	LYS	428	100.037	24.613	23.418	1.00	25.00
4058	3HZ	LYS	428	101.440	24.300	24.323	1.00	25.00
4059	N	ASN	429	101.992	28.618	31.693	1.00	36.19
4060	CA	ASN	429	102.313	28.172	33.081	1.00	31.97
4061	C	ASN	429	102.855	26.740	33.172	1.00	29.89
4062	O	ASN	429	102.272	25.882	33.839	1.00	25.78
4063	CB	ASN	429	101.092	28.334	33.995	1.00	32.22
4064	CG	ASN	429	100.814	29.782	34.358	1.00	36.78
4065	OD1	ASN	429	101.488	30.699	33.894	1.00	40.44
4066	ND2	ASN	429	99.826	29.991	35.215	1.00	41.36
4067	H	ASN	429	102.436	29.294	31.299	1.00	25.00
4068	1HD2	ASN	429	99.643	30.918	35.449	1.00	25.00
4069	2HD2	ASN	429	99.331	29.226	35.566	1.00	25.00
4070	N	PRO	430	103.997	26.472	32.508	1.00	29.30
4071	CA	PRO	430	104.649	25.157	32.492	1.00	25.30
4072	C	PRO	430	104.897	24.669	33.913	1.00	27.01
4073	O	PRO	430	105.218	25.483	34.801	1.00	27.38
4074	CB	PRO	430	105.975	25.447	31.799	1.00	24.23
4075	CG	PRO	430	105.664	26.610	30.932	1.00	30.06
4076	CD	PRO	430	104.835	27.468	31.820	1.00	30.25
4077	N	LYS	431	104.824	23.358	34.108	1.00	25.65
4078	CA	LYS	431	105.020	22.774	35.426	1.00	25.93
4079	C	LYS	431	106.308	23.240	36.107	1.00	24.81
4080	O	LYS	431	106.297	23.570	37.292	1.00	24.36

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4081	CB	LYS	431	105.000	21.252	35.325	1.00	26.70
4082	CG	LYS	431	104.584	20.547	36.604	1.00	40.34
4083	CD	LYS	431	104.361	19.068	36.330	1.00	52.65
4084	CE	LYS	431	103.775	18.345	37.531	1.00	60.92
4085	NZ	LYS	431	103.587	16.892	37.247	1.00	58.59
4086	H	LYS	431	104.6f0	22.777	33.352	1.00	25.00
4087	1HZ	LYS	431	102.939	16.775	36.442	1.00	25.00
4088	2HZ	LYS	431	104.506	16.482	37.018	1.00	25.00
4089	3HZ	LYS	431	103.189	16.424	38.086	1.00	25.00
4090	N	ILE	432	107.401	23.338	35.353	1.00	25.03
4091	CA	ILE	432	108.667	23.774	35.934	1.00	21.64
4092	C	ILE	432	108.561	25.188	36.505	1.00	24.42
4093	O	ILE	432	109.058	25.459	37.602	1.00	25.07
4094	CB	ILS	432	109.847	23.648	34.928	1.00	22.09
4095	CG1	ILE	432	111.179	23.898	35.647	1.00	20.75
4096	CG2	ILE	432	109.662	24.587	33.739	1.00	20.53
4097	CD1	ILE	432	112.403	23.511	34.838	1.00	17.10
4098	H	ILE	432	107.354	23.103	34.410	1.00	25.00
4099	N	LEU	433	107.868	26.070	35.788	1.00	25.32
4100	CA	LEU	433	107.674	27.448	36.240	1.00	23.97
4101	C	LEU	433	106.758	27.446	37.464	1.00	27.11
4102	O	LEU	433	107.051	28.078	38.483	1.00	28.11
4103	CB	LEU	433	107.057	28.298	35.126	1.00	24.53
4104	CG	LEU	433	106.721	29.754	35.473	1.00	28.30
4105	CD1	LEU	433	107.968	30.488	35.945	1.00	23.75
4106	CD2	LEU	433	106.108	30.456	34.265	1.00	27.09
4107	H	LEU	433	107.456	25.788	34.948	1.00	25.00
4108	N	GLU	434	105.667	26.698	37.360	1.00	26.39
4109	CA	GLU	434	104.690	26.566	38.429	1.00	28.21
4110	C	GLU	434	105.393	26.139	39.723	1.00	25.73
4111	O	GLU	434	105.159	26.711	40.790	1.00	25.92
4112	CB	GLU	434	103.656	25.510	38.027	1.00	40.62
4113	CG	GLU	434	102.371	25.510	38.835	1.00	59.16
4114	CD	GLU	434	101.447	26.650	38.457	1.00	69.11
4115	OE1	GLU	434	101.135	26.803	37.255	1.00	76.28
4116	OE2	GLU	434	101.026	27.391	39.366	1.00	78.90
4117	H	GLU	434	105.516	26.206	36.531	1.00	25.00
4118	N	ALA	435	106.272	25.147	39.614	1.00	23.71
4119	CA	ALA	435	107.015	24.632	40.764	1.00	21.25
4120	C	ALA	435	107.915	25.704	41.377	1.00	21.57
4121	O	ALA	435	107.973	25.864	42.599	1.00	21.94
4122	CB	ALA	435	107.838	23.424	40.353	1.00	17.11
4123	H	ALA	435	106.427	24.748	38.737	1.00	25.00
4124	N	SER	436	108.603	26.448	40.519	1.00	20.07
4125	CA	SER	436	109.486	27.510	40.969	1.00	21.72
4126	C	SER	436	108.676	28.531	41.759	1.00	23.51
4127	O	SER	436	109.095	28.979	42.832	1.00	25.11
4128	CB	SER	436	110.147	28.179	39.765	1.00	21.38
4129	OG	SER	436	111.040	29.196	40.173	1.00	36.67
4130	H	SER	436	108.521	26.272	39.556	1.00	25.00
4131	HG	SER	436	110.568	29.867	40.669	1.00	25.00
4132	N	VAL	437	107.501	28.876	41.235	1.00	23.94
4133	CA	VAL	437	106.622	29.846	41.880	1.00	18.07
4134	C	VAL	437	106.134	29.330	43.226	1.00	19.00
4135	O	VAL	437	106.179	30.048	44.227	1.00	24.40
4136	CB	VAL	437	105.410	30.192	40.990	1.00	22.63
4137	CG1	VAL	437	104.498	31.163	41.709	1.00	24.13
4138	CG2	VAL	437	105.879	30.794	39.677	1.00	13.85
4139	H	VAL	437	107.218	28.463	40.391	1.00	25.00
4140	N	ILE	438	105.693	28.076	43.249	1.00	22.97
4141	CA	ILE	438	105.204	27.443	44.472	1.00	25.17
4142	C	ILE	438	106.279	27.478	45.566	1.00	27.56
4143	O	ILE	438	105.996	27.831	46.718	1.00	25.37
4144	CB	ILE	438	104.776	25.975	44.200	1.00	28.36
4145	CG1	ILE	438	103.565	25.952	43.262	1.00	33.63
4146	CG2	ILE	438	104.457	25.255	45.505	1.00	31.72
4147	CD1	ILE	438	103.130	24.569	42.836	1.00	33.54
4148	H	ILE	438	105.697	27.559	42.417	1.00	25.00
4149	N	ILE	439	107.512	27.134	45.196	1.00	27.24
4150	CA	ILE	439	108.635	27.130	46.135	1.00	24.88
4151	C	ILE	439	108.769	28.502	46.787	1.00	20.20

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4152	O	ILE	439	108.842	28.610	48.007	1.00	20.39
4153	CB	ILE	439	109.961	26.739	45.429	1.00	23.09
4154	OG1	ILE	439	109.915	25.264	45.023	1.00	21.73
4155	CG2	ILE	439	111.154	26.939	46.345	1.00	17.14
4156	CD1	ILE	439	110.984	24.859	44.043	1.00	22.40
4157	H	ILE	439	107.670	26.870	44.265	1.00	25.00
4158	N	CYS	440	108.763	29.552	45.974	1.00	21.23
4159	CA	CYS	440	103.873	30.901	46.508	1.00	23.58
4160	C	CYS	440	107.718	31.209	47.458	1.00	27.42
4161	O	CYS	440	107.933	31.707	48.563	1.00	29.41
4162	CB	CYS	440	108.897	31.928	45.376	1.00	26.26
4163	SG	CYS	440	109.015	33.625	45.934	1.00	17.39
4164	H	CYS	440	108.685	29.406	45.006	1.00	25.00
4165	N	ARG	441	106.502	30.869	47.038	1.00	30.12
4166	CA	ARG	441	105.295	31.118	47.825	1.00	28.33
4167	C	ARG	4441	105.280	30.448	49.197	1.00	28.78
4168	O	ARG	441	105.225	31.125	50.223	1.00	28.38
4169	CB	ARG	441	104.056	30.693	47.031	1.00	26.28
4170	CG	ARG	441	102.722	30.927	47.734	1.00	26.09
4171	CD	ARG	441	102.312	32.391	47.725	1.00	32.68
4172	NE	ARG	441	103.001	33.195	48.731	1.00	35.67
4173	CZ	ARG	441	103.243	34.499	48.611	1.00	31.42
4174	NH1	ARG	441	102.861	35.159	47.526	1.00	25.83
4175	NH2	ARG	441	103.851	35.153	49.591	1.00	32.87
4176	H	ARG	441	106.413	30.429	46.165	1.00	25.00
4177	HE	ARG	441	103.307	32.748	49.547	1.00	25.00
4178	1HH1	ARG	441	102.391	34.678	46.792	1.00	25.00
4179	2HH1	ARG	441	103.043	36.138	47.443	1.00	25.00
4180	1HH2	ARG	441	104.133	34.668	50.417	1.00	25.00
4181	2HH2	ARG	441	104.032	36.133	49.498	1.00	25.00
4182	N	VAL	442	105.329	29.120	49.220	1.00	28.03
4183	CA	VAL	442	105.289	28.392	50.484	1.00	29.35
4184	C	VAL	442	106.443	28.708	51.430	1.00	29.48
4185	O	VAL	442	106.248	28.754	52.644	1.00	30.67
4186	CB	VAL	442	105.171	26.884	50.272	1.00	28.34
4187	CG1	VAL	442	103.906	26.546	49.489	1.00	20.42
4188	CG2	VAL	442	106.394	26.322	49.562	1.00	28.17
4189	H	VAL	442	105.405	28.625	46.376	1.00	25.00
4190	N	ILE	443	107.635	28.941	50.885	1.00	32.67
4191	CA	ILE	443	108.788	29.266	51.722	1.00	32.60
4192	C	ILE	443	108.619	30.6722	52.283	1.00	34.90
4193	O	ILE	443	108.866	30.908	53.469	1.00	33.18
4194	CB	ILE	443	110.134	29.150	50.955	1.00	34.36
4195	CG1	ILE	443	110.394	27.689	50.574	1.00	27.67
4196	CG2	ILE	443	111.290	29.649	51.822	1.00	28.68
4197	CD1	ILE	443	110.456	26.745	51.765	1.00	31.24
4198	H	ILE	443	107.746	28.891	49.910	1.00	25.00
4199	N	ASP	444	108.170	31.599	51.441	1.00	33.84
4200	CA	ASP	444	107.954	32.968	51.889	1.00	35.72
4201	C	ASP	444	106.935	32.959	53.023	1.00	38.14
4202	O	ASP	444	107.184	33.520	54.091	1.00	37.60
4203	CB	ASP	444	107.450	33.848	50.744	1.00	39.61
4204	CG	ASP	444	107.110	35.260	51.199	1.00	48.15
4205	OD11	ASP	444	105.972	35.485	51.667	1.00	51.59
4206	OD2	ASP	444	107.980	36.147	51.091	1.00	51.59
4207	H	ASP	444	107.985	31.364	50.507	1.00	25.00
4208	N	ASP	445	105.812	32.279	52.803	1.00	40.33
4209	CA	ASP	445	104.749	32.199	53.803	1.00	39.63
4210	C	ASP	445	105.221	31.599	55.124	1.00	36.43
4211	O	ASP	445	104.826	32.060	56.195	1.00	38.68
4212	CB	ASP	445	103.549	31.415	53.259	1.00	34.74
4213	CG	ASP	445	102.867	32.115	52.087	1.00	37.47
4214	OD1	ASP	445	103.173	33.301	51.818	1.00	32.84
4215	OD2	ASP	445	102.022	31.474	51.429	1.00	34.75
4216	H	ASP	445	105.694	31.823	51.945	1.00	25.00
4217	N	THR	446	106.061	30.574	55.047	1.00	36.21
4218	CA	THR	446	106.586	29.933	56.247	1.00	34.20
4219	C	THR	446	107.469	30.902	57.034	1.00	34.56
4220	O	THR	446	107.396	30.968	58.259	1.00	36.69
4221	CB	THR	446	107.398	28.674	55.890	1.00	29.80
4222	OG1	THR	446	106.545	27.735	55.227	1.00	31.60

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4223	CG2	THR	446	107.970	28.029	57.136	1.00	31.33
4224	H	THR	446	106.322	30.221	54.170	1.00	25.00
4225	HG1	THR	446	107.041	26.946	54.992	1.00	25.00
4226	N	ALA	447	108.266	31.687	56.318	1.00	39.84
4227	CA	ALA	447	109.172	32.644	56.941	1.00	42.07
4228	C	ALA	447	108.495	33.902	57.483	1.00	45.04
4229	O	ALA	447	108.675	34.259	58.647	1.00	48.71
4230	CB	ALA	447	110.2776	33.025	55.959	1.00	36.91
4231	H	ALA	447	108.237	31.624	55.337	1.00	25.00
4232	N	THR	448	107.708	34.565	56.644	1.00	50.59
4233	CA	THR	448	107.036	35.799	57.039	1.00	49.97
4234	C	THR	448	105.729	35.644	57.818	1.00	51.43
4235	O	THR	448	105.100	36.640	58.159	1.00	56.61
4236	CB	THR	448	106.790	36.715	55.811	1.00	47.11
4237	OG1	THR	448	106.095	35.986	54.793	1.00	50.09
4238	CG2	THR	448	108.106	37.214	55.245	1.00	47.36
4239	H	THR	448	107.555	34.230	55.741	1.00	25.00
4240	HG1	THR	448	105.951	36.556	54.034	1.00	25.00
4241	N	TYR	449	105.352	34.415	58.157	1.00	51.91
4242	CA	TYR	449	104.103	34.182	58.881	1.00	53.63
4243	C	TYR	449	103.927	35.020	60.148	1.00	58.13
4244	O	TYR	449	102.939	35.745	60.282	1.00	57.88
4245	CB	TYR	449	103.926	32.696	59.218	1.00	50.75
4246	CG	TYR	449	102.674	32.406	60.025	1.00	55.96
4247	CD1	TYR	449	101.419	32.856	59.596	1.00	60.14
4248	CD2	TYR	449	102.746	31.716	61.235	1.00	56.00
4249	CE1	TYR	449	100.273	32.629	60.353	1.00	55.79
4250	CE2	TYR	449	101.605	31.483	62.000	1.00	57.85
4251	CZ	TYR	449	100.375	31.943	61.554	1.00	60.06
4252	OH	TYR	449	99.250	31.724	62.316	1.00	61.67
4253	H	TYR	449	105.912	33.653	57.905	1.00	25.00
4254	HH	TYR	449	98.487	32.104	61.878	1.00	25.00
4255	N	GLU	450	104.883	34.927	61.067	1.00	64.21
4256	CA	GLU	450	104.810	35.662	62.329	1.00	67.19
4257	C	GLU	450	104.604	37.167	62.173	1.00	68.02
4258	O	GLU	450	103.698	37.742	62.781	1.00	68.60
4259	CB	GLU	450	106.053	35.386	63.178	1.00	73.69
4260	CG	GLU	450	106.228	33.917	63.557	1.00	87.48
4261	CD	GLU	450	104.988	33.311	64.211	1.00	95.20
4262	OE1	GLU	450	104.311	34.009	65.000	1.00	100.27
4263	OE2	GLU	450	104.690	32.129	63.934	1.00	96.38
4264	H	GLU	450	105.651	34.348	60.883	1.00	25.00
4265	N	VAL	451	105.427	37.790	61.336	1.00	69.29
4266	CA	VAL	451	105.351	39.228	61.091	1.00	69.79
4267	C	VAL	451	104.011	39.634	60.479	1.00	71.88
4268	O	VAL	451	103.383	40.594	60.925	1.00	73.87
4269	CB	VAL	451	106.482	39.692	60.149	1.00	68.77
4270	CG1	VAL	451	106.490	41.211	60.036	1.00	67.70
4271	CG2	VAL	451	107.825	39.180	60.647	1.00	74.55
4272	H	VAL	451	106.100	37.263	60.866	1.00	25.00
4273	N	GLU	452	103.572	38.893	59.467	1.00	73.34
4274	CA	GLU	452	102.311	39.191	58.798	1.00	74.52
4275	C	GLU	452	101.096	38.987	59.700	1.00	75.62
4276	O	GLU	452	100.107	39.715	59.575	1.00	75.03
4277	CB	GLU	452	102.176	38.385	57.502	1.00	73.01
4278	CG	GLU	452	103.194	38.774	56.427	1.00	77.67
4279	CD	GLU	452	103.032	38.007	55.118	1.00	81.85
4280	OE1	GLU	452	102.537	36.858	55.137	1.00	80.20
4281	OE2	GLU	452	103.417	38.558	54.061	1.00	82.09
4282	H	GLU	452	104.100	38.124	59.165	1.00	25.00
4283	N	LYS	453	101.173	38.038	60.631	1.00	78.11
4284	CA	LYS	453	100.050	37.799	61.536	1.00	81.43
4285	C	LYS	453	99.887	38.943	62.532	1.00	84.49
4286	O	LYS	453	98.768	39.393	62.783	1.00	88.82
4287	CB	LYS	453	100.176	36.468	62.280	1.00	79.17
4288	CG	LYS	453	98.907	36.134	63.054	1.00	78.09
4289	CD	LYS	453	98.928	34.759	63.674	1.00	79.02
4290	CE	LYS	453	97.583	34.462	64.319	1.00	81.56
4291	NZ	LYS	453	97.525	33.093	64.899	1.00	87.65
4292	H	LYS	453	101.981	37.486	60.701	1.00	25.00
4293	1HZ	LYS	453	98.261	32.991	665.627	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4294	2HZ	LYS	453	96.590	32.937	65.327	1.00	25.00
4295	3HZ	LYS	453	97.682	32.390	64.148	1.00	25.00
4296	N	SER	454	100.996	39.424	63.088	1.00	84.86
4297	CA	SER	454	100.943	40.535	64.037	1.00	83.61
4298	C	SER	454	100.521	41.835	63.338	1.00	83.52
4299	O	SER	454	100.210	42.830	63.991	1.00	82.37
4300	CB	SER	454	102.286	40.703	64.755	1.00	81.64
4301	OG	SER	454	103.363	40.771	63.838	1.00	82.19
4302	H	SER	454	101.863	39.025	62.862	1.00	25.00
4303	HG	SER	454	103.411	39.963	63.320	1.00	25.00
4304	N	ARG	455	100.515	41.813	62.003	1.00	83.63
4305	CA	ARG	455	100.102	42.961	61.197	1.00	86.97
4306	C	ARRG	455	98.616	42.870	60.854	1.00	89.33
4307	O	ARG	455	98.073	43.748	60.183	1.00	89.55
4308	CB	ARG	455	100.892	43.025	59.891	1.00	86.51
4309	CG	ARG	455	102.319	43.493	60.014	1.00	89.64
4310	CD	ARG	455	102.926	43.581	58.632	1.00	98.07
4311	NE	ARG	455	104.296	44.078	58.647	1.00	109.66
4312	CZ	ARG	455	104.976	44.415	57.555	1.00	114.68
4313	NH1	ARG	455	104.411	44.309	56.357	1.00	117.44
4314	NH2	ARG	455	106.220	44.863	57.659	1.00	113.39
4315	H	ARG	455	100.816	41.007	61.542	1.00	25.00
4316	HE	ARG	455	104.745	44.172	59.512	1.00	25.00
4317	1HH1	ARG	455	103.471	43.978	56.270	1.00	25.00
4318	2HH1	ARG	455	104.920	44.568	55.536	1.00	25.00
4319	1HH2	ARG	455	106.646	44.949	58.558	1.00	25.00
4320	2HH2	ARG	455	106.724	45.120	56.834	1.00	25.00
4321	N	GLY	456	97.980	41.773	61.259	1.00	90.67
4322	CA	GLY	456	96.566	41.584	60.989	1.00	90.27
4323	C	GLY	456	96.256	40.876	59.681	1.00	91.84
4324	O	GLY	456	95.087	40.636	59.371	1.00	90.99
4325	H	GLY	456	98.464	41.081	61.752	1.00	25.00
4326	N	GLN	457	97.290	40.528	58.917	1.00	92.16
4327	CA	GLN	457	97.107	39.842	57.638	1.00	90.85
4328	C	GLN	457	96.662	38.395	57.846	1.00	89.74
4329	O	GLN	457	97.442	37.462	57.659	1.00	92.66
4330	CB	GLN	457	98.402	39.868	56.817	1.00	89.90
4331	CG	GLN	457	98.905	41.257	56.457	1.00	95.19
4332	CD	GLN	457	100.145	41.221	55.576	1.00	99.21
4333	OE1	GLN	457	100.325	40.303	54.775	1.00	102.27
4334	NE2	GLN	457	101.002	42.225	55.718	1.00	97.71
4335	H	GLN	457	98.199	40.716	59.228	1.00	25.00
4336	1HE2	GLN	457	101.798	42.200	55.151	1.00	25.00
4337	2HE2	GLN	457	100.809	42.931	56.364	1.00	25.00
4338	N	ILE	458	95.397	38.207	58.209	1.00	88.19
4339	CA	ILE	458	94.859	36.867	58.439	1.00	82.29
4340	C	ILE	458	94.715	36.043	57.159	1.00	75.34
4341	O	ILE	458	94.305	34.887	57.205	1.00	73.69
4342	CB	ILE	458	93.510	36.907	59.199	1.00	85.78
4343	CG1	ILE	458	92.566	37.933	58.562	1.00	86.17
43444	CG2	ILE	458	93.751	37.191	60.681	1.00	85.33
4345	CD1	ILE	458	91.240	38.069	59.277	1.00	89.41
4346	H	ILE	458	94.823	38.995	58.338	1.00	25.00
4347	N	ALA	459	95.077	36.632	56.025	1.00	68.80
4348	CA	ALA	459	95.007	35.936	54.747	1.00	62.63
4349	C	ALA	459	96.368	35.324	54.389	1.00	62.33
4350	O	ALA	459	96.664	35.093	53.216	1.00	62.33
4351	CB	ALA	459	94.549	36.893	53.653	1.00	62.28
4352	H	ALA	459	95.387	37.554	56.036	1.00	25.00
4353	N	THR	460	97.210	35.097	55.396	1.00	59.27
4354	CA	THR	460	98.531	34.513	55.170	1.00	57.11
4355	C	THR	460	98.424	33.034	54.826	1.00	53.62
4356	O	THR	460	97.587	32.319	55.383	1.00	53.81
4357	CB	THR	460	99.453	34.671	56.400	1.00	58.87
4358	OG1	THR	460	98.763	34.257	57.588	1.00	56.81
4359	CG2	THR	460	99.901	36.100	56.541	1.00	60.73
4360	H	THR	460	96.933	35.314	56.305	1.00	25.00
4361	HG1	THR	460	98.004	34.838	57.727	1.00	25.00
4362	N	GLY	461	99.298	32.574	53.937	1.00	44.28
4363	CA	GLY	461	99.289	31.184	53.526	1.00	37.76
4364	C	GLY	461	99.138	30.186	54.652	1.00	39.21

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4365	O	GLY	461	98.265	29.318	54.599	1.00	37.71
4366	H	GLY	461	99.947	33.183	53.532	1.00	25.00
4367	N	ILE	462	99.965	30.320	55.684	1.00	41.07
4368	CA	ILE	462	99.915	29.405	56.821	1.00	43.03
4369	C	ILE	462	98.567	29.461	57.539	1.00	43.30
4370	O	ILE	462	98.063	28.430	57.991	1.00	44.23
4371	CB	ILE	462	101.079	29.658	57.814	1.00	35.94
4372	CG1	ILE	462	102.418	29.419	57.116	1.00	34.23
4373	CG2	ILE	462	100.979	28.720	59.011	1.00	26.77
4374	CD1	ILE	462	102.625	27.987	56.675	1.00	31.75
4375	H	ILE	462	100.618	31.046	55.680	1.00	25.00
4376	N	GLU	463	97.972	30.652	57.602	1.00	47.45
4377	CA	GLU	463	96.673	30.842	58.253	1.00	48.26
4378	C	GLU	463	95.600	30.064	57.495	1.00	43.95
4379	O	GLU	463	94.876	29.250	58.077	1.00	45.29
4380	CB	GLU	463	96.307	32.329	58.291	1.00	55.50
4381	CG	GLU	463	95.120	32.664	59.182	1.00	60.77
4382	CD	GLU	463	95.448	32.555	60.656	1.00	66.36
4383	OE1	GLU	463	96.195	33.419	61.166	1.00	70.77
4384	OE2	GLU	463	94.957	31.605	61.303	1.00	66.97
4385	H	GLU	463	98.403	31.430	57.193	1.00	25.00
4386	N	CYS	464	95.534	30.295	56.186	1.00	38.49
4387	CA	CYS	464	94.575	29.616	55.322	1.00	40.30
4388	C	CYS	464	94.751	28.113	55.451	1.00	40.72
4389	O	CYS	464	93.778	27.364	55.550	1.00	43.89
4390	CB	CYS	464	94.798	30.010	53.860	1.00	33.19
4391	SG	CYS	464	94.721	31.780	53.533	1.00	41.13
4392	H	CYS	464	96.143	30.954	55.789	1.00	25.00
4393	N	CYS	465	96.007	27.682	55.464	1.00	42.83
4394	CA	CYS	465	96.337	26.271	55.557	1.00	45.44
4395	C	CYS	465	95.791	25.654	56.852	1.00	48.27
4396	O	CYS	465	95.165	24.591	56.818	1.00	47.36
4397	CB	CYS	465	97.850	26.074	55.487	1.00	39.55
4398	SG	CYS	465	98.332	24.350	55.349	1.00	40.18
4399	H	CYS	465	96.735	28.334	55.396	1.00	25.00
4400	N	MET	466	96.000	26.340	57.972	1.00	51.35
4401	CA	MET	466	95.531	25.854	59.267	1.00	55.36
4402	C	MET	466	94.019	25.699	59.312	1.00	56.30
4403	O	MET	466	93.512	24.647	59.698	1.00	55.90
4404	CB	MET	466	95.977	26.786	60.391	1.00	52.93
4405	CG	MET	466	97.464	26.797	60.618	1.00	49.91
4406	SD	MET	466	97.890	27.866	61.980	1.00	56.57
4407	CE	MET	466	97.679	29.434	61.228	1.00	45.63
4408	H	MET	466	96.483	27.193	57.936	1.00	25.00
4409	N	ARG	467	93.303	26.744	58.916	1.00	57.72
4410	CA	ARG	467	91.849	26.704	58.921	1.00	60.99
4411	C	ARG	467	91.271	25.700	57.935	1.00	57.48
4412	O	ARG	467	90.406	24.901	58.295	1.00	61.64
4413	CB	ARG	467	91.270	28.089	58.642	1.00	69.59
4414	CG	ARG	467	91.304	29.011	59.839	1.00	84.26
4415	CD	ARG	467	90.397	30.202	59.616	1.00	96.57
4416	NE	ARG	467	90.163	30.938	60.853	1.00	103.82
4417	CZ	ARG	467	89.074	31.660	61.099	1.00	107.61
4418	NH1	ARG	467	88.109	31.749	60.192	1.00	108.04
4419	NH2	ARG	467	88.946	32.284	62.261	1.00	109.38
4420	H	ARG	467	93.769	27.556	58.623	1.00	25.00
4421	HE	ARG	467	90.848	30.890	61.554	1.00	25.00
4422	1HH1	ARG	467	88.194	31.273	59.318	1.00	25.00
4423	2HH1	ARG	467	87.293	32.293	60.390	1.00	25.00
4424	1HH2	ARG	467	89.669	32.209	62.950	1.00	25.00
4425	2HH2	ARG	467	88.130	32.827	62.457	1.00	25.00
4426	N	ASP	468	91.769	25.726	56.704	1.00	52.60
4427	CA	ASP	468	91.287	24.832	55.660	1.00	51.80
4428	C	ASP	468	91.404	23.354	56.032	1.00	52.54
4429	O	ASP	468	90.488	22.574	55.767	1.00	57.49
4430	CB	ASP	468	92.026	25.111	54.346	1.00	49.09
4431	CG	ASP	468	91.328	24.513	53.133	1.00	52.94
4432	OD1	ASP	468	90.127	24.170	53.218	1.00	55.18
4433	OD2	ASP	468	91.983	24.402	52.076	1.00	54.77
4434	H	ASP	468	92.480	26.362	56.496	1.00	25.00
4435	N	TYR	469	92.524	22.973	56.646	1.00	52.44

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4436	CA	TYR	469	92.755	21.581	57.040	1.00	49.37
4437	C	TYR	469	92.458	21.283	58.511	1.00	48.25
4438	O	TYR	469	92.316	20.121	58.894	1.00	46.98
4439	CB	TYR	469	94.200	21.165	56.730	1.00	46.99
4440	CG	TYR	469	94.546	21.129	55.260	1.00	47.76
4441	CD1	TYR	469	94.994	22.273	54.602	1.00	51.80
4442	CD2	TYR	469	94.431	19.947	54.524	1.00	50.13
4443	GE1	TYR	469	95.317	22.246	53.248	1.00	56.40
4444	CE2	TYR	469	94.753	19.908	53.167	1.00	54.09
4445	CZ	TYR	469	95.195	21.063	52.537	1.00	57.04
4446	OH	TYR	469	95.514	21.044	51.198	1.00	62.08
4447	H	TYR	469	93.216	23.642	56.837	1.00	25.00
4448	HH	TYR	469	95.802	21.916	50.922	1.00	25.00
4449	N	GLY	470	92.371	22.328	59.328	1.00	49.37
4450	CA	GLY	470	92.113	22.147	60.746	1.00	51.47
4451	C	GLY	470	93.332	21.551	61.425	1.00	52.90
4452	O	GLY	470	93.247	20.499	62.064	1.00	54.39
4453	H	GLY	470	92.471	23.228	58.968	1.00	25.00
4454	N	ILE	471	94.467	22.238	61.300	1.00	53.10
4455	CA	ILE	471	95.728	21.771	61.874	1.00	48.51
4456	C	ILE	471	96.521	22.877	62.571	1.00	49.16
4457	O	ILE	471	96.230	24.063	62.408	1.00	48.02
4458	CB	ILE	471	96.617	21.131	60.781	1.00	44.19
4459	CG1	ILE	471	96.816	22.116	59.621	1.00	43.37
4460	CG2	ILE	471	95.991	19.829	60.288	1.00	41.20
4461	CD1	ILE	471	97.608	21.558	58.449	1.00	38.24
4462	H	ILE	471	94.452	23.094	60.822	1.00	25.00
4463	N	SER	472	97.517	22.475	63.357	1.00	53.02
4464	CA	SER	472	98.371	23.414	64.085	1.00	57.32
4465	C	SER	472	99.352	24.117	63.146	1.00	60.76
4466	O	SER	472	99.689	23.587	62.084	1.00	61.94
4467	CB	SER	472	99.148	22.672	65.180	1.00	59.87
4468	OG	SER	472	99.873	21.568	64.653	1.00	59.66
4469	H	SER	472	97.697	21.518	63.453	1.00	25.00
4470	HG	SER	472	100.314	21.103	65.376	1.00	25.00
4471	N	THR	473	99.838	25.287	63.557	1.00	61.86
4472	CA	THR	473	100.794	26.053	62.755	1.00	63.28
4473	C	THR	473	101.959	25.160	62.340	1.00	66.44
4474	O	THR	473	102.374	25.158	61.179	1.00	66.96
4475	CB	THR	473	101.366	27.248	63.547	1.00	62.70
4476	OG1	THR	473	100.295	23.083	63.997	1.00	63.68
4477	CG2	THR	473	102.306	28.068	62.677	1.00	63.27
4478	H	THR	473	99.529	25.654	64.404	1.00	25.00
4479	HG1	THR	473	99.682	27.608	64.552	1.00	25.00
4480	N	LYS	474	102.454	24.380	63.296	1.00	65.27
4481	CA	LYS	474	103.568	23.470	63.065	1.00	67.87
4482	C	LYS	474	103.248	22.508	61.922	1.00	65.57
4483	O	LYS	474	104.051	22.325	61.001	1.00	66.11
4484	CB	LYS	474	103.863	22.688	64.349	1.00	71.33
4485	CG	LYS	474	105.150	21.875	64.320	1.00	77.07
4486	CD	LYS	474	105.422	21.234	65.673	1.00	77.42
4487	CE	LYS	474	106.776	20.544	65.698	1.00	78.55
4488	NZ	LYS	474	107.067	19.962	67.037	1.00	75.57
4489	H	LYS	474	102.058	24.422	64.186	1.00	25.00
4490	1HZ	LYS	474	106.336	19.263	67.278	1.00	25.00
4491	2HZ	LYS	474	107.998	19.500	67.020	1.00	25.00
4492	3HZ	LYS	474	107.070	20.720	67.750	1.00	25.00
4493	N	GLU	475	102.047	21.944	61.960	1.00	61.44
4494	CA	GLU	475	101.612	20.998	60.945	1.00	57.77
4495	C	GLU	475	101.378	21.683	59.599	1.00	53.01
4496	O	GLU	475	101.623	21.091	58.545	1.00	55.03
4497	CB	GLU	475	100.352	20.282	61.418	1.00	59.71
4498	CG	GLU	475	100.104	18.950	60.737	1.00	73.81
4499	CD	GLU	475	98.994	18.148	61.399	1.00	84.47
4500	OE1	GLU	475	98.562	18.513	62.518	1.00	88.32
4501	OE2	GLU	475	98.555	17.144	60.797	1.00	88.90
4502	H	GLU	475	101.423	22.181	62.675	1.00	25.00
4503	N	ALA	476	100.931	22.936	59.637	1.00	46.25
4504	CA	ALA	476	100.681	23.703	58.420	1.00	43.91
4505	C	ALA	476	102.003	23.972	57.712	1.00	44.05
4506	O	ALA	476	102.124	23.774	56.501	1.00	42.50

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4507	CB	ALA	476	99.984	25.018	58.749	1.00	34.16
4508	H	ALA	4776	100.761	23.358	60.501	1.00	25.00
4509	N	MET	477	103.000	24.402	58.480	1.00	45.42
4510	CA	MET	477	104.321	24.689	57.932	1.00	46.57
4511	C	MET	477	104.954	23.414	57.395	1.00	46.73
4512	O	MET	477	105.640	23.434	56.369	1.00	48.81
4513	CB	MET	477	105.217	25.331	58.990	1.00	41.20
4514	CG	MET	477	104.699	26.674	59.459	1.00	45.53
4515	SD	MET	477	105.842	27.539	60.529	1.00	50.24
4516	CE	MET	477	105.403	29.229	60.204	1.00	44.87
4517	H	MET	477	102.838	24.531	59.436	1.00	25.00
4518	N	ALA	478	104.689	22.301	58.071	1.00	43.88
4519	CA	ALA	478	105.214	21.012	57.646	1.00	40.24
4520	C	ALA	473	104.608	20.664	56.288	1.00	39.48
4521	O	ALA	478	105.301	20.158	55.404	1.00	42.61
4522	CB	ALA	478	104.887	19.941	58.673	1.00	38.44
4523	H	ALA	473	104.140	22.350	58.883	1.00	25.00
4524	N	LYS	479	103.324	20.969	56.113	1.00	37.41
4525	CA	LYS	479	102.642	20.700	54.850	1.00	36.91
4526	C	LYS	479	103.214	21.598	53.754	1.00	33.62
4527	O	LYS	479	103.408	21.164	52.616	1.00	32.37
4528	CB	LYS	479	101.136	20.931	54.986	1.00	39.38
4529	CG	LYS	479	100.338	20.573	53.736	1.00	46.00
4530	CD	LYS	479	98.850	20.797	53.947	1.00	51.63
4531	CE	LYS	479	98.273	19.858	55.003	1.00	53.61
4532	NZ	LYS	479	98.180	18.451	54.525	1.00	57.01
4533	H	LYS	479	102.820	21.3777	56.852	1.00	25.00
4534	1HZ	LYS	479	99.126	18.106	54.269	1.00	25.00
4535	2HZ	LYS	479	97.776	17.853	55.274	1.00	25.00
4536	3HZ	LYS	479	97.561	18.416	53.688	1.00	25.00
4537	N	PHE	480	103.502	22.845	54.107	1.00	30.92
4538	CA	PHE	480	104.067	23.790	53.157	1.00	31.88
4539	C	PHE	480	105.457	23.356	52.714	1.00	34.12
4540	O	PHE	480	105.812	23.493	51.540	1.00	37.15
4541	CB	PHE	480	104.107	25.198	53.749	1.00	29.35
4542	CG	PHE	480	102.902	26.028	53.408	1.00	37.28
4543	CD1	PHE	480	101.662	25.427	53.190	1.00	37.60
4544	CD2	PHE	480	103.008	27.411	53.283	1.00	36.73
4545	CE1	PHE	480	100.548	26.192	52.850	1.00	36.20
4546	CE22	PHE	480	101.898	28.185	52.942	1.00	38.45
4547	CZ	PHE	480	100.665	27.574	52.726	1.00	36.96
4548	H	PHE	480	103.315	23.138	55.024	1.00	25.00
4549	N	GLN	481	106.238	22.810	53.641	1.00	33.79
4550	CA	GLN	481	107.573	22.352	53.292	1.00	35.43
4551	C	GLN	481	107.453	21.180	52.323	1.00	35.55
4552	O	GLN	481	108.200	21.103	51.347	1.00	35.63
4553	CB	GLN	481	108.368	21.930	54.524	1.00	46.60
4554	CG	GLN	481	109.844	21.688	54.210	1.00	70.92
4555	CD	GLN	481	110.583	20.933	55.302	1.00	83.38
4556	OE1	GLN	481	110.036	20.658	56.371	1.00	93.92
4557	NE2	GLN	481	111.838	20.588	55.032	1.00	88.62
4558	H	GLN	481	105.919	22.723	54.562	1.00	25.00
4559	1HE2	GLN	481	112.316	20.105	55.735	1.00	25.00
4560	2HE2	GLN	481	112.220	20.824	54.166	1.00	25.00
4561	N	ASN	482	106.486	20.297	52.561	1.00	33.51
4562	CA	ASN	482	106.272	19.146	51.682	1.00	36.28
4563	C	ASN	482	105.950	19.606	50.267	1.00	36.07
4564	O	ASN	482	106.380	18.989	49.288	1.00	35.83
4565	CB	ASN	482	105.140	18.252	52.200	1.00	40.65
4566	CG	ASN	482	105.535	17.465	53.436	1.00	54.20
4567	OD1	ASN	482	106.698	17.095	53.607	1.00	57.37
4568	ND2	ASN	482	104.565	17.204	54.307	1.00	59.54
4569	H	ASN	482	105.916	20.415	53.350	1.00	25.00
4570	1HD2	ASN	482	104.821	16.698	55.105	1.00	25.00
4571	2HD2	ASN	482	103.6661	17.519	54.121	1.00	25.00
4572	N	MET	483	105.199	20.698	50.163	1.00	33.64
4573	CA	MET	483	104.831	21.250	48.366	1.00	29.91
4574	C	MET	483	106.080	21.757	48.152	1.00	27.30
4575	O	MET	433	106.240	21.556	46.947	1.00	32.31
4576	CB	MET	483	103.814	22.373	49.036	1.00	29.58
4577	CG	MET	483	102.488	21.916	49.626	1.00	32.65

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4578	SD	MET	483	101.388	23.311	49.943	1.00	37.42
4579	CE	MET	483	100.988	23.770	48.275	1.00	33.87
4580	H	MET	483	104.879	21.134	50.982	1.00	25.00
4581	N	ALA	484	106.979	22.385	48.903	1.00	24.24
4582	CA	ALA	484	108.226	22.895	48.339	1.00	25.37
4583	C	ALA	484	109.086	21.724	47.845	1.00	27.23
4584	O	ALA	484	109.696	21.792	46.772	1.00	26.13
4585	CB	ALA	484	108.979	23.703	49.385	1.00	20.73
4586	H	ALA	484	106.799	22.516	49.859	1.00	25.00
4587	N	GLU	485	109.103	20.642	48.622	1.00	27.25
4588	CA	GLU	485	109.864	19.437	48.289	1.00	29.59
4589	C	GLU	485	109.317	18.807	47.015	1.00	26.53
4590	O	GLU	485	110.070	18.386	46.139	1.00	32.01
4591	CB	GLU	485	109.792	18.425	49.437	1.00	39.77
4592	CG	GLU	485	110.327	18.942	50.779	1.00	61.11
4593	CD	GLU	485	110.170	17.953	51.934	1.00	69.27
4594	OE1	GLU	485	109.663	16.830	51.716	1.00	73.83
4595	OE2	GLU	485	110.561	18.302	53.073	1.00	69.26
4596	H	GLU	485	108.574	20.683	49.449	1.00	25.00
4597	N	THR	488	107.997	18.755	46.917	1.00	26.56
4598	CA	THR	488	107.323	18.207	45.749	1.00	26.51
4599	C	THR	488	107.673	19.050	44.520	1.00	24.78
4600	O	THR	486	107.961	18.514	43.437	1.00	24.00
4601	CB	THR	486	105.790	18.211	45.973	1.00	30.57
4602	OG1	THR	486	105.463	17.277	47.010	1.00	30.11
4603	CG2	THR	486	105.034	17.855	44.694	1.00	27.79
4604	H	THR	488	107.446	19.085	47.660	1.00	25.00
4605	HG1	THR	486	105.755	16.396	46.782	1.00	25.00
4606	N	ALA	487	107.672	20.367	44.712	1.00	20.69
4607	CA	ALA	487	107.980	21.319	43.651	1.00	19.32
4608	C	ALA	487	109.409	21.127	43.141	1.00	18.49
4609	O	ALA	487	109.654	21.149	41.929	1.00	15.86
4610	CB	ALA	487	107.768	22.750	44.152	1.00	15.08
4611	H	ALA	487	107.454	20.716	45.604	1.00	25.00
4612	N	TRP	488	110.349	20.909	44.058	1.00	20.11
4613	CA	TRP	488	111.736	20.695	43.661	1.00	19.04
4614	C	TRP	488	111.856	19.461	42.781	1.00	20.42
4615	O	TRP	488	112.555	19.486	41.768	1.00	23.27
4616	CB	TRP	488	112.656	20.590	44.879	1.00	19.13
4617	CG	TRP	488	113.256	21.905	45.262	1.00	20.79
4618	CD1	TRP	488	113.017	22.619	46.402	1.00	19.35
4619	CD2	TRP	488	114.173	22.689	44.481	1.00	18.53
4620	NE1	TRP	488	113.723	23.801	46.376	1.00	21.34
4621	CE2	TRP	488	114.441	23.869	45.210	1.00	17.70
4622	CE3	TRP	488	114.793	22.507	43.237	1.00	18.03
4623	CZ2	TRP	488	115.305	24.863	44.736	1.00	16.71
4624	CZ3	TRP	488	115.654	23.499	42.765	1.00	15.24
4625	CH2	TRP	488	115.899	24.659	43.515	1.00	14.14
4626	H	TRP	488	110.109	20.905	45.009	1.00	25.00
4627	HE1	TRP	488	113.699	24.482	47.075	1.00	25.00
4628	N	LYS	489	111.136	18.399	43.138	1.00	21.51
4629	CA	LYS	489	111.162	17.175	42.345	1.00	17.89
4630	C	LYS	489	110.604	17.476	40.961	1.00	19.66
4631	O	LYS	489	111.091	16.947	39.960	1.00	22.89
4632	CB	LYS	489	110.351	16.069	43.019	1.00	17.77
4633	CG	LYS	489	110.922	15.624	44.344	1.00	15.98
4634	CD	LYS	489	110.074	14.540	44.972	1.00	22.31
4635	CE	LYS	489	110.525	14.254	46.392	1.00	24.45
4636	NZ	LYS	489	109.694	13.199	47.029	1.00	26.46
4637	H	LYS	489	110.589	18.443	43.952	1.00	25.00
4638	1HZ	LYS	489	108.703	13.510	47.052	1.00	25.00
4639	2HZ	LYS	489	109.772	12.320	46.482	1.00	25.00
4640	3HZ	LYS	489	110.028	13.037	47.997	1.00	25.00
4641	N	ASP	490	109.590	18.338	40.906	1.00	20.77
4642	CA	ASP	490	108.991	18.721	39.630	1.00	21.97
4643	C	ASP	490	110.008	19.479	38.786	1.00	24.19
4644	O	ASP	490	110.098	19.264	37.575	1.00	21.17
4645	CB	ASP	490	101.739	19.585	39.837	1.00	26.18
4646	CG	ASP	490	106.561	18.799	40.395	1.00	29.44
4647	OD1	ASSP	490	106.524	17.562	40.236	1.00	35.64
4648	OD2	ASP	490	105.657	19.425	40.982	1.00	29.87

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4649	H	ASP	490	109.245	18.731	41.736	1.00	25.00
4650	N	ILE	491	110.776	20.362	39.419	1.00	20.68
4651	CA	ILE	491	111.789	21.120	38.692	1.00	20.37
4652	C	ILE	491	112.810	20.146	38.115	1.00	19.25
4653	O	ILE	491	113.158	20.221	36.934	1.00	20.39
4654	CB	ILE	491	112.508	22.153	39.595	1.00	22.00
4655	CG1	ILE	491	111.540	23.278	39.975	1.00	21.39
4656	CG2	ILE	491	113.737	22.716	38.877	1.00	21.00
4657	CD1	ILE	491	112.159	24.376	40.803	1.00	22.99
4658	H	ILE	491	110.657	20.508	40.379	1.00	25.00
4659	N	ASN	492	113.239	19.198	38.943	1.00	19.07
4660	CA	ASN	492	114.216	18.196	38.529	1.00	18.67
4661	C	ASN	492	113.700	17.404	37.332	1.00	20.34
4662	O	ASN	492	114.446	17.133	36.393	1.00	20.40
4663	CB	ASN	492	114.567	17.271	39.699	1.00	16.62
4664	CG	ASN	492	115.269	18.007	40.839	1.00	18.56
4665	OD1	ASN	492	115.924	19.035	40.625	1.00	15.51
4666	ND2	ASN	492	115.140	17.484	42.050	1.00	15.73
4667	H	ASN	492	112.899	19.181	39.862	1.00	25.00
4668	1HD2	ASN	492	115.583	17.939	42.793	1.00	25.00
4669	2HD2	ASN	492	114.613	16.661	42.164	1.00	25.00
4670	N	GLU	493	112.412	17.073	37.341	1.00	21.12
4671	CA	GLU	493	111.816	16.341	36.225	1.00	22.19
4672	C	GLU	493	111.736	17.225	34.985	1.00	24.12
4673	O	GLU	493	111.958	16.755	33.869	1.00	26.10
4674	CB	GLU	493	110.416	15.850	36.578	1.00	19.71
4675	CG	GLU	493	110.394	14.831	37.690	1.00	30.24
4676	CD	GLU	493	109.056	14.143	37.849	1.00	25.61
4677	OE1	GLU	493	108.111	14.460	37.100	1.00	36.10
4678	OE2	GLU	493	108.953	13.268	38.728	1.00	35.77
4679	H	GLU	493	111.859	17.328	38.111	1.00	25.00
4680	N	GLY	494	111.423	18.504	35.194	1.00	24.81
4681	CA	GLY	494	111.311	19.451	34.096	1.00	18.06
4682	C	GLY	494	112.614	19.686	33.352	1.00	25.75
4683	O	GLY	494	112.605	20.176	32.217	1.00	25.47
4684	H	GLY	494	111.263	18.819	36.107	1.00	25.00
46885	N	LEU	495	113.735	19.350	33.986	1.00	24.09
4686	CA	LEU	495	115.047	19.523	33.367	1.00	23.57
4687	C	LEU	495	115.465	18.331	32.503	1.00	23.66
4688	O	LEU	495	116.385	18.445	31.700	1.00	25.21
4689	CB	LEU	495	116.111	19.781	34.439	1.00	21.29
4690	CG	LEU	495	115.968	21.063	35.270	1.00	24.69
4691	CD1	LEU	495	116.913	21.024	36.459	1.00	15.49
4692	CD2	LEU	495	116.230	22.287	34.409	1.00	21.41
4693	H	LEU	495	113.681	18.985	34.893	1.00	25.00
4694	N	LEU	496	114.781	17.200	32.651	1.00	22.59
4695	CA	LEU	496	115.118	15.996	31.889	1.00	20.47
4696	C	LEU	496	114.749	16.049	30.409	1.00	24.46
4697	O	LEU	496	113.692	16.556	30.033	1.00	22.73
4698	CB	LEU	496	114.504	14.758	32.548	1.00	20.18
4699	CG	LEU	496	115.016	14.454	33.959	1.00	23.38
4700	CD1	LEU	496	114.276	13.265	34.524	1.00	21.31
4701	CD2	LEU	496	116.523	14.187	33.938	1.00	20.33
4702	H	LEU	496	114.020	17.172	33.267	1.00	25.00
4703	N	ARG	497	115.642	15.530	29.573	1.00	26.43
4704	CA	ARG	497	115.443	15.501	28.128	1.00	31.12
4705	C	ARG	497	114.347	14.498	27.766	1.00	32.68
4706	O	ARG	497	114.217	13.457	28.411	1.00	27.55
4707	CB	ARG	497	116.757	15.124	27.431	1.00	30.06
4708	CG	ARG	497	117.863	16.155	27.626	1.00	38.94
4709	CD	ARG	497	119.217	15.505	27.851	1.00	37.77
4710	NE	ARG	497	120.087	15.584	26.683	1.00	50.61
4711	CZ	ARG	497	121.282	16.173	26.676	1.00	51.72
4712	NH1	ARG	497	121.754	16.744	27.777	1.00	46.52
4713	NH2	ARG	497	122.023	16.166	25.575	1.00	51.65
4714	H	ARG	497	116.457	15.140	29.946	1.00	25.00
4715	HE	ARG	497	119.773	15.180	25.847	1.00	25.00
4716	1HH1	ARG	497	121.213	16.733	28.615	1.00	25.00
4717	2HH1	ARG	497	122.653	17.183	27.766	1.00	25.00
4718	1HH2	ARG	497	121.685	15.718	24.748	1.00	25.00
4719	2HH2	ARG	497	122.920	16.608	25.576	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4720	N	PRO	498	113.542	14.798	26.731	1.00	34.46
4721	CA	PRO	498	113.595	16.005	25.897	1.00	31.05
4722	C	PRO	498	112.886	17.179	26.568	1.00	32.44
4723	O	PRO	498	111.757	17.040	27.043	1.00	32.35
4724	CB	PRO	498	112.831	15.587	24.635	1.00	30.63
4725	CG	PRO	498	112.768	14.079	24.707	1.00	38.95
4726	CD	PRO	498	112.593	13.830	26.162	1.00	34.35
4727	N	THR	499	113.544	18.332	26.612	1.00	33.10
4728	CA	THR	499	112.940	19.513	27.218	1.00	30.18
4729	C	THR	499	112.075	20.223	26.170	1.00	31.00
4730	O	THR	499	112.389	20.172	24.974	1.00	33.56
4731	CB	THR	499	114.016	20.474	27.795	1.00	25.39
4732	OG1	THR	499	115.004	20.752	26.798	1.00	24.84
4733	CG2	THR	499	114.703	19.843	28.996	1.00	22.98
4734	H	THR	499	114.435	18.421	26.223	1.00	25.00
4735	HG1	THR	499	115.646	21.357	27.117	1.00	25.00
4736	N	PRO	500	110.963	20.844	26.600	1.00	31.06
4737	CA	PRO	500	110.053	21.558	25.692	1.00	32.31
4738	C	PRO	500	110.705	22.740	24.967	1.00	34.94
4739	O	PRO	500	110.328	23.075	23.843	1.00	39.31
4740	CB	PRO	500	108.916	21.994	26.620	1.00	29.71
4741	CG	PRO	500	109.576	22.086	27.968	1.00	28.06
4742	CD	PRO	500	110.460	20.876	27.984	1.00	23.70
4743	N	VAL	501	111.642	23.398	25.641	1.00	32.94
4744	CA	VAL	501	112.390	24.523	25.078	1.00	33.22
4745	C	VAL	501	113.858	24.257	25.421	1.00	33.52
4746	O	VAL	501	114.154	23.347	26.204	1.00	33.00
4747	CB	VAL	501	111.959	25.887	25.686	1.00	29.14
4748	CG1	VAL	501	110.515	26.198	25.330	1.00	26.33
4749	CG2	VAL	501	112.153	25.887	27.195	1.00	24.60
4750	H	VAL	501	111.875	23.112	26.546	1.00	25.00
4751	N	SER	502	114.775	25.026	24.844	1.00	30.56
4752	CA	SER	502	116.194	24.832	25.128	1.00	33.20
4753	C	SER	502	116.485	25.025	26.611	1.00	32.05
4754	O	SER	502	115.869	25.869	27.265	1.00	34.57
4755	CB	SER	502	117.039	25.807	24.316	1.00	35.54
4756	OG	SER	502	116.837	25.601	22.934	1.00	56.52
4757	H	SER	502	114.502	25.729	24.224	1.00	25.00
4758	HG	SER	502	117.098	24.709	22.686	1.00	25.00
4759	N	THR	503	117.443	24.260	27.126	1.00	29.15
4760	CA	THR	503	117.836	24.333	28.530	1.00	33.23
4761	C	THR	503	118.166	25.771	28.927	1.00	31.90
4762	O	THR	503	117.977	26.177	30.078	1.00	32.13
4763	CB	THR	503	119.058	23.443	28.797	1.00	38.70
4764	CG1	THR	503	118.767	22.110	28.366	1.00	51.69
4765	CG2	THR	503	119.395	23.420	30.278	1.00	40.66
4766	H	THR	503	117.884	23.611	26.547	1.00	25.00
4767	HG1	THR	503	118.560	22.075	27.436	1.00	25.00
4768	N	GLU	504	118.637	26.542	27.956	1.00	27.88
4769	CA	GLU	504	118.982	27.935	28.184	1.00	31.30
4770	C	GLU	504	117.801	28.706	28.789	1.00	31.46
4771	O	GLU	504	117.987	29.643	29.568	1.00	29.72
4772	CB	GLU	504	119.396	28.578	26.863	1.00	32.18
4773	CG	GLU	504	119.754	30.042	26.997	1.00	44.47
4774	CD	GLU	504	120.045	30.714	25.672	1.00	47.35
4775	OE1	GLU	504	119.634	30.183	24.618	1.00	49.18
4776	OE2	GLU	504	120.683	31.788	25.691	1.00	48.31
4777	H	GLU	504	118.771	26.169	27.067	1.00	25.00
4778	N	PHE	505	118.588	28.274	28.464	1.00	27.10
4779	CA	PHE	505	115.390	28.936	28.957	1.00	23.02
4780	C	PHE	505	114.809	28.314	30.218	1.00	24.14
4781	O	PHE	505	113.888	28.869	30.818	1.00	22.77
4782	CB	PHE	505	114.356	29.036	27.335	1.00	28.22
4783	CG	PHE	505	114.888	29.711	26.602	1.00	28.58
4784	CD1	PHE	505	115.307	31.039	26.651	1.00	28.23
4785	CD2	PHE	505	115.048	29.001	25.417	1.00	28.81
4786	CE1	PHE	505	115.884	31.646	25.539	1.00	25.11
4787	CE2	PHE	505	116.623	29.597	24.300	1.00	28.43
4788	CZ	PHE	505	116.043	30.922	24.362	1.00	29.72
4789	H	PHE	505	116.489	27.504	27.881	1.00	25.00
4790	N	LEU	506	115.367	27.182	30.641	1.00	21.53

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4791	CA	LEU	506	114.915	26.516	31.862	1.00	20.00
4792	C	LEU	506	115.763	26.980	33.054	1.00	20.28
4793	O	LEU	506	115.270	27.120	34.176	1.00	21.38
4794	CB	LEU	506	115.033	24.995	31.732	1.00	17.84
4795	CG	LEU	506	114.265	24.277	30.621	1.00	23.70
4796	CD1	LEU	506	114.409	22.781	30.832	1.00	19.27
4797	CD2	LEU	506	112.797	24.671	30.645	1.00	20.22
4798	H	LEU	506	116.092	26.791	30.120	1.00	25.00
4799	N	THR	507	117.040	27.237	32.796	1.00	24.00
4800	CA	THR	507	117.968	27.666	33.837	1.00	21.87
4801	C	THR	507	117.508	28.894	34.634	1.00	21.92
4802	O	THR	507	117.636	28.913	35.858	1.00	25.77
4803	CB	THR	507	119.382	27.870	33.260	1.00	22.57
4804	OG1	THR	507	119.728	26.728	32.465	1.00	23.76
4805	CG2	THR	507	120.400	28.014	34.381	1.00	20.42
4806	H	THR	507	117.372	27.127	31.883	1.00	25.00
4807	HG1	THR	507	119.106	26.624	31.739	1.00	25.00
4808	N	PRO	508	116.960	29.928	33.963	1.00	17.26
4809	CA	PRO	508	116.503	31.114	34.698	1.00	18.03
4810	C	PRO	508	115.423	30.774	35.735	1.00	19.69
4811	O	PRO	508	1155.417	31.309	36.847	1.00	22.29
4812	CB	PRO	508	115.943	31.999	33.583	1.00	18.28
4813	CG	PRO	508	116.841	31.690	32.444	1.00	16.25
4814	CD	PRO	508	116.909	30.177	32.510	1.00	14.75
4815	N	ILE	509	114.528	29.864	35.362	1.00	21.35
4816	CA	ILE	509	113.435	29.420	36.230	1.00	22.73
4817	C	ILE	509	114.024	28.653	37.412	1.00	19.96
4818	O	ILE	509	113.627	28.854	38.561	1.00	22.40
4819	CB	ILE	509	112.450	28.523	35.441	1.00	18.26
4820	CG1	ILE	509	111.867	29.317	34.267	1.00	20.40
4821	CG2	ILE	509	111.360	27.998	36.351	1.00	12.67
4822	CD1	ILE	509	111.082	28.486	33.280	1.00	22.89
4823	H	ILE	509	114.597	29.488	34.470	1.00	25.00
4824	N	LEU	510	114.989	27.788	37.114	1.00	21.34
4825	CA	LEU	510	115.684	27.003	38.130	1.00	19.45
4826	C	LEU	510	116.420	27.956	39.075	1.00	18.03
4827	O	LEU	510	116.372	27.799	40.300	1.00	23.54
4828	CB	LEU	510	116.693	26.064	37.454	1.00	18.99
4829	CG	LEU	510	117.747	25.351	38.309	1.00	17.88
4830	CD1	LEU	510	117.092	24.447	39.347	1.00	13.70
4831	CD2	LEU	510	118.660	24.548	37.401	1.00	12.82
4832	H	LEU	510	115.234	27.670	36.174	1.00	25.00
4833	N	ASN	511	117.070	28.966	38.502	1.00	16.84
4834	CA	ASN	511	117.816	29.940	39.293	1.00	18.52
4835	C	ASN	511	116.918	30.774	40.185	1.00	19.49
4836	O	ASN	511	117.299	31.111	41.307	1.00	21.10
4837	CB	ASN	511	118.704	30.806	38.400	1.00	14.99
4838	CG	ASN	511	119.926	30.046	37.903	1.00	19.61
4839	OD1	ASN	511	120.276	29.004	38.456	1.00	22.94
4840	ND2	ASN	511	120.562	30.543	36.849	1.00	17.54
4841	H	ASN	511	117.040	29.059	37.540	1.00	25.00
4842	1HD2	ASN	511	121.341	30.052	36.532	1.00	25.00
4843	2HD2	ASN	511	120.230	31.364	36.438	1.00	25.00
4844	N	LEU	512	115.705	31.061	39.719	1.00	18.46
4845	CA	LEU	512	114.751	31.814	40.527	1.00	15.00
4846	C	LEU	512	114.415	31.007	41.778	1.00	16.15
4847	O	LEU	512	114.304	31.561	42.872	1.00	24.00
4848	CB	LEU	512	113.484	32.114	39.727	1.00	17.19
4849	CG	LEU	5112	113.569	33.341	38.818	1.00	16.79
4850	CD1	LEU	512	112.331	33.430	37.943	1.00	22.39
4851	CD2	LEU	512	113.702	34.591	39.672	1.00	14.37
4852	H	LEU	512	115.450	30.773	38.817	1.00	25.00
4853	N	ALA	513	114.279	29.692	41.624	1.00	19.31
4854	CA	ALA	513	113.979	28.814	42.760	1.00	18.01
4855	C	ALA	513	115.178	28.789	43.710	1.00	18.19
4856	O	ALA	513	115.017	28.802	44.933	1.00	16.94
4857	CB	ALA	513	113.654	27.403	42.274	1.00	12.64
4858	H	ALA	513	114.362	29.302	40.726	1.00	25.00
4859	N	ARG	514	116.381	28.767	43.140	1.00	19.70
4860	CA	ARG	514	117.609	28.763	43.934	1.00	18.80
4861	C	ARG	514	117.696	30.031	44.784	1.00	17.46

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4862	O	ARG	514	118.041	29.978	45.967	1.00	21.48
4863	CB	ARG	514	118.832	28.638	43.024	1.00	13.68
4864	CG	ARG	514	118.981	27.255	42.404	1.00	14.32
4865	CD	ARG	514	120.084	27.218	41.354	1.00	17.33
4866	NE	ARG	514	120.490	25.848	41.066	1.00	16.97
4867	CZ	ARG	514	121.107	25.453	39.958	1.00	19.03
4868	NH1	ARG	514	121.398	26.320	38.998	1.00	15.08
4869	NH2	ARG	514	121.450	24.180	39.821	1.00	15.36
4870	H	ARG	514	116.440	28.744	42.160	1.00	25.00
4871	HE	ARG	514	120.282	25.180	41.738	1.00	25.00
4872	1HH1	ARG	514	121.159	27.283	39.100	1.00	25.00
4873	2HH1	ARG	514	121.862	26.006	38.170	1.00	25.00
4874	1HH2	ARG	514	121.245	23.5244	40.547	1.00	25.00
4875	2HH2	ARG	514	121.913	23.875	38.988	1.00	25.00
4876	N	ILE	515	117.330	31.164	44.196	1.00	20.52
4877	CA	ILE	515	117.352	32.438	44.911	1.00	22.89
4878	C	ILE	515	116.489	32.357	46.169	1.00	25.55
4879	O	ILE	515	116.851	32.914	47.206	1.00	28.26
4880	CB	ILE	515	116.863	33.591	44.018	1.00	18.86
4881	CG1	ILE	515	117.857	33.824	42.883	1.00	18.35
4882	CG2	ILE	515	116.695	34.855	44.832	1.00	23.30
4883	CD1	ILE	515	117.408	34.863	41.885	1.00	19.17
4884	H	ILE	515	117.045	31.141	43.257	1.00	25.00
4885	N	VAL	516	115.372	31.637	46.082	1.00	27.24
4886	CA	VAL	516	114.467	31.463	47.220	1.00	26.85
4887	C	VAL	516	115.229	30.838	48.378	1.00	30.63
4888	O	VAL	516	115.219	31.354	49.496	1.00	28.87
4889	CB	VAL	516	113.280	30.512	46.881	1.00	28.84
4890	CG1	VAL	516	112.433	30.248	48.122	1.00	23.42
4891	CG2	VAL	516	112.423	31.096	45.776	1.00	22.08
4892	H	VAL	516	115.144	31.219	45.225	1.00	25.00
4893	N	GLU	517	115.910	29.736	48.085	1.00	35.61
4894	CA	GLU	517	116.680	28.997	49.081	1.00	41.24
4895	C	GLU	517	117.696	29.890	49.796	1.00	42.08
4896	O	GLU	517	117.872	29.789	51.009	1.00	46.37
4897	CB	GLU	517	117.385	27.802	48.424	1.00	41.58
4898	CG	GLU	517	116.496	26.950	47.503	1.00	52.96
4899	CD	GLU	517	115.344	26.242	48.223	1.00	59.58
4900	OE1	GLU	517	115.593	25.557	49.236	1.00	60.41
4901	OE2	GLU	517	114.187	26.352	47.762	1.00	63.04
4902	H	GLU	517	115.899	29.407	47.161	1.00	25.00
4903	N	VAL	518	118.314	30.799	49.050	1.00	40.18
4904	CA	VAL	518	119.310	31.714	49.600	1.00	42.32
4905	C	VAL	518	118.704	32.885	50.386	1.00	47.45
4906	O	VAL	518	119.269	33.326	51.389	1.00	48.49
4907	CB	VAL	518	120.219	32.251	48.474	1.00	41.14
4908	CG1	VAL	518	121.133	33.350	48.986	1.00	39.83
4909	CG2	VAL	518	121.034	31.108	47.896	1.00	45.30
4910	H	VAL	518	118.097	30.844	48.095	1.00	25.00
4911	N	THR	519	117.563	33.387	49.923	1.00	45.49
4912	CA	THR	519	116.899	34.505	50.577	1.00	44.49
4913	C	THR	519	116.183	34.117	51.884	1.00	44.03
4914	O	THR	519	115.983	34.964	52.754	1.00	41.48
4915	CB	THR	519	115.868	35.165	49.622	1.00	45.40
4916	OG1	THR	519	116.518	35.516	48.394	1.00	47.45
4917	CG2	THR	519	115.283	36.424	50.240	1.00	50.81
4918	H	THR	519	117.161	32.996	49.123	1.00	25.00
4919	HG1	THR	519	116.872	34.719	47.980	1.00	25.00
4920	N	TYR	520	115.827	32.843	52.034	1.00	49.74
4921	CA	TYR	520	115.130	32.385	53.240	1.00	54.71
4922	C	TYR	520	115.783	31.213	53.984	1.00	60.58
4923	O	TYR	520	115.129	30.191	54.209	1.00	65.16
4924	CB	TYR	520	113.686	31.988	52.905	1.00	52.58
4925	CG	TYR	520	112.886	33.018	52.142	1.00	53.27
4926	CD1	TYR	520	112.885	33.027	50.748	1.00	54.77
4927	CD2	TYR	520	112.105	33.962	52.809	1.00	50.10
4928	CE1	TYR	520	112.127	33.946	50.032	1.00	57.50
4929	CE2	TYR	520	111.340	34.889	52.102	1.00	54.19
4930	CZ	TYR	520	111.357	34.873	50.713	1.00	56.86
4931	OH	TYR	520	110.604	35.777	49.999	1.00	58.70
4932	H	TYR	520	116.029	32.189	51.330	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
4933	HH	TYR	520	110.726	35.626	49.057	1.00	25.00
4934	N	ILE	521	117.056	31.340	54.350	1.00	67.35
4935	CA	ILE	521	117.729	30.269	55.091	1.00	74.89
4936	C	ILE	521	117.425	30.428	56.583	1.00	75.44
4937	O	ILE	521	117.194	29.397	57.255	1.00	76.20
4938	CB	ILE	521	119.276	30.258	54.856	1.00	75.70
4939	CG1	ILE	521	119.586	29.919	53.394	1.00	76.18
4940	CG2	ILE	521	119.953	29.222	55.766	1.00	77.50
4941	CD1	ILE	521	121.064	29.755	53.080	1.00	71.61
4942	H	ILE	521	117.546	32.156	54.145	1.00	25.00
4943	N	VAL	533	120.428	39.967	55.248	1.00	55.02
4944	CA	VAL	533	120.478	38.584	54.683	1.00	57.02
4945	C	VAL	533	121.277	38.505	53.373	1.00	55.80
4946	O	VAL	533	122.075	37.588	53.181	1.00	56.73
4947	CB	VAL	533	119.048	37.995	54.485	1.00	56.30
4948	CG1	VAL	533	118.225	38.868	53.539	1.00	56.90
4949	CG2	VAL	533	119.125	36.552	53.986	1.00	50.74
4950	1H	VAL	533	119.970	40.608	54.578	1.00	25.00
4951	2H	VAL	533	119.880	39.938	56.132	1.00	25.00
4952	3H	VAL	533	121.396	40.274	55.462	1.00	25.00
4953	N	LEU	534	121.095	39.483	52.491	1.00	49.61
4954	CA	LEU	534	121.812	39.490	51.218	1.00	48.50
4955	C	LEU	534	123.194	40.138	51.300	1.00	47.52
4956	O	LEU	534	124.075	39.830	50.496	1.00	44.98
4957	CB	LEU	534	120.983	40.190	50.137	1.00	48.86
4958	CG	LEU	534	119.659	39.533	49.744	1.00	50.00
4959	CD1	LEU	534	119.054	40.290	48.567	1.00	46.00
4960	CD2	LEU	534	119.888	38.066	49.384	1.00	42.36
4961	H	LEU	534	120.456	40.200	52.652	1.00	25.00
4962	N	LYS	535	123.382	40.993	52.303	1.00	45.93
4963	CA	LYS	535	124.633	41.722	52.510	1.00	45.11
4964	C	LYS	535	125.921	40.923	52.284	1.00	43.08
4965	O	LYS	535	126.729	41.288	51.428	1.00	42.36
4966	CB	LYS	535	124.651	42.385	53.895	1.00	46.19
4967	CG	LYS	535	125.855	43.288	54.130	1.00	54.44
4968	CD	LYS	535	125.868	43.868	55.536	1.00	57.76
4969	CE	LYS	535	127.075	44.774	55.747	1.00	61.61
4970	NZ	LYS	535	127.099	45.378	57.111	1.00	62.66
4971	H	LYS	535	122.651	41.156	52.915	1.00	25.00
4972	1HZ	LYS	535	127.134	44.621	57.824	1.00	25.00
4973	2HZ	LYS	535	127.936	45.986	57.207	1.00	25.00
4974	3HZ	LYS	535	126.239	45.946	57.252	1.00	25.00
4975	N	PRO	536	126.115	39.809	53.019	1.00	39.15
4976	CA	PRO	536	127.337	39.020	52.829	1.00	37.51
4977	C	PRO	536	127.564	38.579	51.386	1.00	33.92
4978	O	PRO	536	128.684	38.644	50.877	1.00	33.28
4979	CB	PRO	536	127.128	37.827	53.770	1.00	38.16
4980	CG	PRO	536	125.638	37.724	53.893	1.00	42.17
4981	CD	PRO	536	125.233	39.164	54.008	1.00	38.53
4982	N	HIS	537	126.488	38.181	50.714	1.00	33.98
4983	CA	HIS	537	126.575	37.730	49.327	1.00	34.56
4984	C	HIS	537	126.929	38.877	48.390	1.00	34.75
4985	O	HIS	537	127.742	38.714	47.479	1.00	29.05
4986	CB	HIS	537	125.264	37.071	48.900	1.00	34.41
4987	CG	HIS	537	124.917	35.855	49.703	1.00	41.27
4988	ND1	HIS	537	123.749	35.746	50.426	1.00	43.98
4989	CD2	HIS	537	125.601	34.705	49.917	1.00	37.03
4990	CE1	HIS	537	123.726	34.584	51.053	1.00	40.28
4991	NE2	HIS	537	124.838	33.933	50.760	1.00	39.05
4992	H	HIS	537	125.616	38.225	51.154	1.00	25.00
4993	HD1	HIS	537	123.030	36.418	50.483	1.00	25.00
4994	HE2	HIS	537	125.072	33.038	51.088	1.00	25.00
4995	N	ILE	538	126.333	40.040	48.634	1.00	34.95
4996	CA	ILE	538	126.596	41.225	47.829	1.00	35.08
4997	C	ILE	538	128.063	41.612	47.969	1.00	36.46
4998	O	ILE	538	128.703	41.999	46.990	1.00	38.58
4999	CB	ILE	538	125.701	42.406	48.263	1.00	35.99
5000	CG1	ILE	538	124.230	42.072	47.983	1.00	37.36
5001	CG2	ILE	538	126.124	43.681	47.542	1.00	34.76
5002	CD1	ILE	538	123.248	43.112	48.460	1.00	36.39
5003	H	ILE	538	125.708	40.113	49.385	1.00	25.00

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
5004	N	ILE	539	128.588	41.491	49.185	1.00	34.70
5005	CA	ILE	539	129.979	41.807	49.473	1.00	33.68
5006	C	ILE	539	130.912	40.828	48.769	1.00	34.74
5007	O	ILE	539	131.868	41.239	48.093	1.00	30.49
5008	CB	ILE	539	130.253	41.761	51.004	1.00	35.37
5009	CG1	ILE	539	129.559	42.939	51.686	1.00	33.35
5010	CG2	ILE	539	131.749	41.790	51.285	1.00	32.80
5011	CD1	ILE	539	129.684	42.933	53.189	1.00	34.58
5012	H	ILE	539	127.999	41.207	49.913	1.00	25.00
5013	N	ASN	540	130.603	39.538	48.864	1.00	33.09
5014	CA	ASN	540	131.440	38.505	48.263	1.00	33.80
5015	C	ASN	540	131.355	38.498	46.749	1.00	34.25
5016	O	ASN	540	132.298	38.166	46.065	1.00	33.46
5017	CB	ASN	540	131.047	37.127	48.775	1.00	33.03
5018	CG	ASN	540	131.463	36.902	50.198	1.00	39.77
5019	OD1	ASN	540	130.776	36.219	50.965	1.00	45.10
5020	ND2	ASN	540	132.581	37.502	50.579	1.00	36.91
5021	H	ASN	540	129.781	39.280	49.311	1.00	25.00
5022	1HD2	ASN	540	132.850	37.386	51.503	1.00	25.00
5023	2HD2	ASN	540	133.079	38.025	49.919	1.00	25.00
5024	N	LEU	541	130.185	38.821	46.253	1.00	30.66
5025	CA	LEU	541	129.997	38.848	44.821	1.00	31.93
5026	C	LEU	541	130.262	40.166	44.110	1.00	33.86
5027	O	LEU	541	130.805	40.129	42.977	1.00	30.07
5028	CB	LEU	541	128.600	38.308	44.486	1.00	34.62
5029	CG	LEU	541	128.194	36.907	44.990	1.00	35.64
5030	CD1	LEU	541	126.882	36.542	44.345	1.00	31.26
5031	CD2	LEU	541	129.256	35.866	44.669	1.00	29.53
5032	H	LEU	541	129.518	38.998	46.982	1.00	25.00
5033	N	LEU	542	129.910	41.305	44.706	1.00	35.33
5034	CA	LEU	542	130.075	42.581	44.033	1.00	39.16
5035	C	LEU	542	131.084	43.566	44.635	1.00	42.69
5036	O	LEU	542	131.361	44.614	44.055	1.00	45.28
5037	CB	LEU	542	128.721	43.258	43.921	1.00	37.88
5038	CG	LEU	542	127.685	42.494	43.105	1.00	37.82
5039	CD1	LEU	542	126.275	42.902	43.505	1.00	37.78
5040	CD2	LEU	542	127.947	42.728	41.619	1.00	33.54
5041	H	LEU	542	129.525	41.317	45.569	1.00	25.00
5042	N	VAL	543	131.590	43.264	45.822	1.00	40.06
5043	CA	VAL	543	132.536	44.167	46.483	1.00	39.32
5044	C	VAL	543	133.930	43.601	46.457	1.00	40.35
5045	O	VAL	543	134.834	44.117	45.766	1.00	36.40
5046	CB	VAL	543	132.112	44.458	47.351	1.00	38.67
5047	CG1	VAL	543	133.154	45.323	48.643	1.00	41.60
5048	CG2	VAL	543	130.762	45.137	47.966	1.00	33.55
5049	H	VAL	543	131.348	42.421	46.245	1.00	25.00
5050	N	ASP	544	134.175	42.518	47.191	1.00	39.19
5051	CA	ASP	544	135.485	41.887	47.274	1.00	37.12
5052	C	ASP	544	135.802	40.970	46.112	1.00	38.65
5053	O	ASP	544	134.991	40.124	45.739	1.00	42.40
5054	CB	ASP	544	135.609	41.070	48.566	1.00	37.00
5055	CG	ASP	544	135.384	41.894	49.812	1.00	42.35
5056	OD1	ASP	544	135.659	43.114	49.803	1.00	49.35
5057	OD2	ASP	544	134.933	41.304	50.813	1.00	50.35
5058	H	ASP	544	133.427	42.119	47.665	1.00	25.00
5059	N	SER	545	136.984	41.153	45.543	1.00	36.71
5060	CA	SER	545	137.444	40.303	44.464	1.00	39.73
5061	C	SER	545	138.200	39.158	45.142	1.00	38.96
5062	O	SER	545	138.585	39.269	46.310	1.00	40.93
5063	CB	SER	545	138.379	41.084	43.540	1.00	43.38
5064	OG	SER	545	139.362	41.790	44.280	1.00	51.44
5065	H	SER	545	137.544	41.896	45.832	1.00	25.00
5066	HG	SER	545	139.870	41.166	44.808	1.00	25.00
5067	N	ILE	546	138.377	38.046	44.442	1.00	36.92
5068	CA	ILE	546	139.109	36.920	45.011	1.00	40.59
5069	C	ILE	546	140.602	37.261	44.954	1.00	45.93
5070	O	ILE	546	141.117	37.620	43.889	1.00	46.41
5071	CB	ILE	546	138.839	35.612	44.226	1.00	36.34
5072	CG1	ILE	546	137.346	35.288	44.264	1.00	34.10
5073	CG2	ILE	546	139.629	34.456	44.829	1.00	31.04
5074	CD1	ILE	546	136.979	34.011	43.525	1.00	36.46

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
5075	H	ILE	546	138.009	37.990	43.533	1.00	25.00
5076	N	LYS	547	141.282	37.201	46.009	1.00	52.49
5077	CA	LYS	547	142.706	37.502	46.134	1.00	58.52
5078	C	LYS	547	143.483	36.450	45.353	1.00	60.95
5079	O	LYS	547	143.488	35.273	45.713	1.00	60.42
5080	CB	LYS	547	143.217	37.599	47.572	1.00	59.36
5081	CG	LYS	547	144.684	38.023	47.659	1.00	68.28
5082	CD	LYS	547	145.065	38.553	49.037	1.00	72.08
5083	CE	LYS	547	146.486	39.105	49.029	1.00	74.86
5084	NZ	LYS	547	146.796	39.880	50.265	1.00	78.47
5085	H	LYS	547	140.806	36.948	46.910	1.00	25.00
5086	1HZ	LYS	547	146.680	39.273	51.099	1.00	25.00
5087	2HZ	LYS	547	147.770	40.240	50.222	1.00	25.00
5088	3HZ	LYS	547	146.139	40.685	50.334	1.00	25.00
5089	N	ILE	548	144.086	36.890	44.254	1.00	67.72
5090	CA	ILE	548	144.868	36.018	43.381	1.00	76.79
5091	C	ILE	548	146.198	35.622	44.025	1.00	83.68
5092	O	ILE	548	146.583	34.440	43.897	1.00	86.24
5093	CB	ILE	548	145.120	36.678	41.986	1.00	75.68
5094	CG1	ILE	548	145.604	38.125	42.152	1.00	78.47
5095	CG2	ILE	548	143.855	36.623	41.137	1.00	68.49
5096	CD1	ILE	548	145.930	38.827	40.831	1.00	78.93
5097	OXT	ILE	548	146.823	36.492	44.672	1.00	92.78
5098	H	ILE	548	144.032	37.836	44.045	1.00	25.00
5099	ILE	548						
5100	MG	MG	851	104.185	36.235	53.030	1.00	61.83
5101	MG	MG	852	102.138	43.657	49.009	1.00	62.23
5102	O	HOH	601	107.742	22.057	32.406	1.00	15.11
5103	O	HOH	602	122.540	22.695	37.531	1.00	32.44
5104	O	HOH	603	127.188	14.109	43.835	1.00	23.85
5105	O	HOH	604	123.257	32.177	37.651	1.00	25.21
5106	O	HOH	605	131.975	36.814	38.945	1.00	20.08
5107	O	HOH	606	130.320	38.579	40.729	1.00	28.69
5108	O	HOH	607	124.735	33.181	39.810	1.00	19.46
5109	O	HOH	608	119.958	22.714	50.725	1.00	24.82
5110	O	HOH	609	125.172	22.654	40.253	1.00	21.47
5111	O	HOH	610	106.047	21.994	29.826	1.00	26.03
5112	O	HOH	611	123.659	29.782	47.444	1.00	22.10
5113	O	HOH	612	129.924	22.165	49.955	1.00	20.33
5114	O	HOH	613	117.254	16.672	36.732	1.00	18.88
5115	O	HOH	614	131.911	22.935	48.204	1.00	23.59
5116	O	HOH	615	123.421	30.030	35.911	1.00	23.89
5117	O	HOH	616	128.952	30.316	38.829	1.00	22.41
5118	O	HOH	617	98.347	33.326	40.948	1.00	28.07
5119	O	HOH	618	126.062	19.250	36.922	1.00	29.11
5120	O	HOH	619	133.788	33.099	36.415	1.00	20.10
5121	O	HOH	620	127.252	22.013	48.848	1.00	24.10
5122	O	HOH	621	123.122	19.043	45.472	1.00	19.68
5123	O	HOH	622	124.636	25.767	41.845	1.00	42.37
5124	O	HOH	623	138.021	26.937	54.497	1.00	33.32
5125	O	HOH	624	130.604	16.213	44.273	1.00	25.46
5126	O	HOH	625	119.735	17.425	55.175	1.00	23.51
5127	O	HOH	626	109.560	43.332	32.386	1.00	27.79
5128	O	HOH	627	104.016	36.817	39.018	1.00	24.34
5129	O	HOH	628	134.051	35.256	29.604	1.00	37.22
5130	O	HOH	629	107.947	18.792	36.023	1.00	35.84
5131	O	HOH	630	129.821	19.576	48.096	1.00	29.63
5132	O	HOH	631	104.550	21.758	41.675	1.00	38.10
5133	O	HOH	632	111.970	10.709	47.161	1.00	23.86
5134	O	HOH	633	125.976	29.448	50.341	1.00	26.42
5135	O	HOH	634	97.143	36.787	48.102	1.00	35.12
5136	O	HOH	635	121.582	36.805	25.111	1.00	35.51
5137	O	HOH	636	113.756	26.801	22.571	1.00	30.58
5138	O	HOH	637	124.698	19.485	28.803	1.00	29.60
5139	O	HOH	638	130.563	25.567	43.476	1.00	29..93
5140	O	HOH	639	121.706	39.646	27.124	1.00	32.61
5141	O	HOH	640	104.749	34.099	30.683	1.00	28.14
5142	O	HOH	641	111.751	8.174	35.080	1.00	34.23
5143	O	HOH	642	120.339	31.400	41.487	1.00	52.69
5144	O	HOH	643	95.163	26.623	43.384	1.00	36.83
5145	O	HOH	644	137.113	41.980	40.124	1.00	30.35

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
5146	O	HOH	645	116.126	11.318	49.986	1.00	25.34
5147	O	HOH	646	110.165	35.328	17.495	1.00	37.81
5148	O	HOH	647	118.054	20.287	30.749	1.00	33.12
5149	O	HOH	648	115.899	40.354	30.351	1.00	29.82
5150	O	HOH	649	113.524	64.000	32.295	1.00	30.14
5151	O	HOH	650	127.950	27.982	37.184	1.00	28.39
5152	O	HOH	651	108.770	18.109	30.127	1.00	36.94
5153	O	HOH	652	112.843	23.036	50.160	1.00	41.87
5154	O	HOH	653	132.804	32.747	50.167	1.00	34.56
5155	O	HOH	654	99.278	32.670	36.214	1.00	31.88
5156	O	HOH	655	93.100	36.093	41.777	1.00	39.13
5157	O	HOH	656	114.575	17.087	50.058	1.00	29.96
5158	O	HOH	657	134.890	18.651	45.599	1.00	29.79
5159	O	HOH	658	134.764	16.354	47.235	1.00	41.87
5160	O	HOH	659	138.146	19.452	46.210	1.00	40.62
5161	O	HOH	660	113.498	7.243	37.601	1.00	44.14
5162	O	HOH	661	118.735	25.324	49.539	1.00	32.46
5163	O	HOH	662	121.072	19.323	57.037	1.00	28.13
5164	O	HOH	663	120.647	52.139	31.726	1.00	31.21
5165	O	HOH	664	125.201	27.805	35.886	1.00	35.41
5166	O	HOH	665	103.040	17.910	41.249	1.00	34.74
5167	O	HOH	666	92.281	23.719	49.317	1.00	36.36
5168	O	HOH	667	120.731	30.312	30.736	1.00	40.91
5169	O	HOH	668	111.010	16.805	31.260	1.00	37.18
5170	O	HOH	669	98.374	30.892	39.496	1.00	39.09
5171	O	HOH	670	142.913	20.086	59.043	1.00	40.89
5172	O	HOH	671	120.070	4.238	32.203	1.00	32.10
5173	O	HOH	672	116.885	14.360	38.230	1.00	19.20
5174	O	HOH	673	135.198	31.364	38.159	1.00	21.99
5175	O	HOH	674	130.652	23.815	45.653	1.00	22.37
5176	O	HOH	675	116.184	18.170	25.042	1.00	33.65
5177	O	HOH	676	102.763	37.505	36.535	1.00	29.50
5178	O	HOH	677	113.482	17.709	47.318	1.00	24.10
5179	O	HOH	678	128.292	24.082	47.295	1.00	27.62
5180	O	HOH	679	128.934	20.011	39.747	1.00	26.34
5181	O	HOH	680	129.840	32.556	48.799	1.00	34.07
5182	O	HOH	681	115.123	17.894	45.342	1.00	23.02
5183	O	HOH	682	134.875	11.928	61.810	1.00	24.68
5184	O	HOH	683	140.837	17.873	38.782	1.00	33.65
5185	O	HOH	684	135.724	8.315	55.152	1.00	37.93
5186	O	HOH	685	131.660	25.765	56.520	1.00	36.71
5187	O	HOH	686	148.447	27.966	42.675	1.00	38.11
5188	O	HOH	687	110.190	10.176	45.195	1.00	35.74
5189	O	HOH	688	109.091	17.883	25.410	1.00	38.94
5190	O	HOH	6889	104.860	34.526	28.030	1.00	38.81
5191	O	HOH	690	102.070	36.177	27.889	1.00	35.60
5192	O	HOH	691	118.113	11.174	28.782	1.00	38.94
5193	O	HOH	692	131.635	20.640	62.725	1.00	33.60
5194	O	HOH	693	136.344	35.530	31.124	1.00	36.08
5195	O	HOH	694	120.257	31.406	33.335	1.00	31.14
5196	O	HOH	695	102.005	32.616	56.124	1.00	33.30
5197	O	HOH	696	124.575	21.994	35.468	1.00	36.59
5198	O	HOH	697	101.923	20.169	46.398	1.00	40.37
5199	O	HOH	698	129.243	49.171	40.765	1.00	49.17
5200	O	HOH	699	139.196	35.578	48.616	1.00	31.26
5201	O	HOH	700	134.064	15.022	43.146	1.00	40.48
5202	O	HOH	701	128.514	31.051	51.675	1.00	39.32
5203	O	HOH	702	112.958	10.222	36.694	1.00	47.07
5204	O	HOH	703	109.649	15.841	28.459	1.00	35.43
5205	O	HOH	704	140.094	42.685	39.958	1.00	41.31
5206	O	HOH	705	86.608	31.749	55.350	1.00	36.82
5207	O	HOH	706	128.605	34.147	28.351	1.00	35.79
5208	O	HOH	707	87.075	34.369	56.433	1.00	42.04
5209	O	HOH	708	89.030	34.345	44.620	1.00	40.07
5210	O	HOH	709	104.535	51.407	27.998	1.00	39.44
5211	O	HOH	710	120.125	34.187	24.397	1.00	63.74
5212	O	HOH	711	100.184	37.778	52.580	1.00	43.18
5213	O	HOH	712	109.218	37.444	46.111	1.00	37.68
5214	O	HOH	713	139.550	20.401	60.539	1.00	40.82
5215	O	HOH	714	140.612	17.7933	52.684	1.00	42.33
5216	O	HOH	715	120.330	21.170	32.392	1.00	31.20

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
5217	O	HOH	716	100.372	35.917	30.033	1.00	43.22
5218	O	HOH	717	120.163	23.899	33.930	1.00	33.67
5219	O	HOH	718	146.383	28.556	40.921	1.00	38.01
5220	O	HOH	719	109.966	20.788	31.041	1.00	38.62
5221	O	HOH	720	105.493	40.925	45.887	1.00	35.53
5222	O	HOH	721	119.171	27.937	23.152	1.00	55.39
5223	O	HOH	722	124.424	41.390	25.938	1.00	43.52
5224	O	HOH	723	102.779	17.993	48.134	1.00	38.38
5225	O	HOH	724	112.387	75.685	33.453	1.00	48.35
5226	O	HOH	725	151.082	25.140	44.349	1.00	35.50
5227	O	HOH	726	127.089	21.203	29.049	1.00	45.21
5228	O	HOH	727	133.178	5.551	47.734	1.00	39.38
5229	O	HOH	728	151.127	34.628	33.927	1.00	42.02
5230	O	HOH	729	150.405	22.240	44.559	1.00	38.43
5231	O	HOH	730	131.660	2.107	47.933	1.00	37.78
5232	O	HOH	731	135.465	8.584	52.047	1.00	40.15
5233	O	HOH	732	147.814	29.664	45.229	1.00	44.50
5234	O	HOH	733	140.989	33.094	47.707	1.00	43.19
5235	O	HOH	734	103.951	49.441	25.596	1.00	38.72
5236	O	HOH	735	86.471	53.747	29.731	1.00	43.56
5237	O	HOH	736	134.470	31.168	25.546	1.00	52.39
5238	O	HOH	737	122.918	25.464	36.469	1.00	42.39
5239	O	HOH	738	99.309	33.456	31.178	1.00	48.32
5240	O	HOH	739	91.548	47.290	47.278	1.00	45.43
5241	O	HOH	740	92.024	43.380	40.690	1.00	42.02
5242	O	HOH	741	149.190	38.195	52.530	1.00	47.74
5243	O	HOH	742	153.088	41.575	36.804	1.00	46.51
5244	O	HOH	743	138.714	31.651	53.657	1.00	43.64
5245	O	HOH	744	143.900	19.054	51.722	1.00	40.32
5246	O	HOH	745	138.795	15.536	49.608	1.00	43.79
5247	O	HOH	746	124.711	−3.430	56.077	1.00	44.40
5248	O	HOH	747	145.969	30.921	42.825	1.00	39.08
5249	O	HOH	748	134.979	10.249	59.470	1.00	35.78
5250	O	HOH	749	133.932	40.151	29.911	1.00	41.40
5251	O	HOH	750	114.521	21.309	22.697	1.00	33.72
5252	O	HOH	751	129.614	38.180	25.426	1.00	39.89
5253	O	HOH	752	111.644	313.087	29.735	1.00	45.90
5254	O	HOH	753	104.216	21.388	44.848	1.00	33.35
5255	O	HOH	754	110.986	12.520	49.459	1.00	49.32
5256	O	HOH	755	139.600	40.725	48.728	1.00	46.07
5257	O	HOH	756	113.295	9.448	29.832	1.00	35.78
5258	O	HOH	757	127.101	23.382	34.156	1.00	48.02
5259	O	HOH	758	127.933	18.490	63.251	1.00	46.33
5260	O	HOH	759	130.420	26.867	25.702	1.00	40.40
5261	O	HOH	760	122.231	3.237	35.918	1.00	44.61
5262	O	HOH	761	128.310	26.484	40.968	1.00	32.14
5263	O	HOH	762	88.443	24.530	48.586	1.00	57.07
5264	O	HOH	763	103.542	23.739	25.080	1.00	45.05
5265	O	HOH	764	116.278	57.331	34.559	1.00	42.40
5266	O	HOH	765	120.787	5.886	61.156	1.00	43.73
5267	O	HOH	766	142.631	40.352	42.775	1.00	65.94
5268	O	HOH	767	124.244	13.057	63.666	1.00	43.68
5269	O	HOH	768	101.830	22.900	29.735	1.00	36.47
5270	O	HOH	769	137.190	5.022	37.071	1.00	50.65
5271	O	HOH	770	135.078	34.403	50.639	1.00	51.53
5272	O	HOH	771	103.266	58.719	26.225	1.00	46.58
5273	O	HOH	772	144.319	16.861	24.565	1.00	53.32
5274	O	HOH	773	127.856	47.718	31.019	1.00	45.45
5275	O	HOH	774	95.530	18.110	49.546	1.00	52.47
5276	O	HOH	775	148.435	20.165	43.831	1.00	49.25
5277	O	HOH	776	118.026	13.535	59.021	1.00	48.41
5278	O	HOH	777	110.119	43.903	16.201	1.00	37.10
5279	O	HOH	778	110.457	61.356	39.879	1.00	44.66
5280	O	HOH	779	105.313	56.879	27.692	1.00	51.08
5281	O	HOH	780	106.267	19.656	28.049	1.00	45.55
5282	O	HOH	781	122.226	20.789	29.638	1.00	45.73
5283	O	HOH	782	107.680	19.165	33.248	1.00	35.37
5284	O	HOH	783	141.434	30.527	58.190	1.00	56.49
5285	O	HOH	784	121.953	27.180	30.544	1.00	43.22
5286	O	HOH	785	116.050	27.492	52.913	1.00	59.86
5287	O	HOH	786	115.271	11.494	53.629	1.00	47.46

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
5288	O	HOH	787	136.166	43.700	43.430	1.00	44.89
5289	O	HOH	788	123.135	5.923	32.296	1.00	61.24
5290	O	HOH	789	148.342	38.089	38.232	1.00	41.22
5291	O	HOH	790	112.195	39.980	44.065	1.00	44.26
5292	O	HOH	791	108.340	50.773	20.100	1.00	62.55
5293	O	HOH	792	126.140	29.670	29.775	1.00	38.87
5294	O	HOH	793	122.347	26.176	27.904	1.00	47.43
5295	O	HOH	794	105.375	13.283	37.860	1.00	40.63
5296	O	HOH	795	146.608	19.061	33.529	1.00	50.53
5297	O	HOH	796	112.240	28.192	56.028	1.00	54.08
5298	O	HOH	797	106.519	16.717	37.160	1.00	39.17
5299	O	HOH	798	122.257	-2.147	57.632	1.00	59.87
5300	O	HOH	799	105.969	47.469	20.174	1.00	42.44
5301	O	HOH	800	124.201	23.387	29.951	1.00	51.85
5302	O	HOH	801	104.010	26.139	23.199	1.00	57.02
5303	O	HOH	802	106.547	37.540	47.839	1.00	46.00
5304	O	HOH	803	126.083	27.795	33.246	1.00	45.66
5305	O	HOH	804	93.229	25.530	63.301	1.00	50.45
5306	O	HOH	805	126.637	14.627	66.291	1.00	54.63
5307	O	HOH	806	117.649	48.031	30.248	1.00	44.41
5308	O	HOH	807	112.889	34.483	46.820	1.00	41.77
5309	O	HOH	808	143.749	8.474	39.051	1.00	58.35
5310	O	HOH	809	117.223	16.467	56.527	1.00	54.55
5311	O	HOH	810	136.640	48.794	42.640	1.00	59.70
5312	O	HOH	811	130.573	47.631	52.219	1.00	43.65
5313	O	HOH	812	119.790	22.620	53.732	1.00	49.88
5314	O	HOH	813	105.220	9.911	43.334	1.00	53.82
5315	O	HOH	814	94.459	22.230	65.891	1.00	53.43
5316	O	HOH	815	145.893	33.119	447.904	1.00	50.15
5317	O	HOH	816	137.540	19.003	49.581	1.00	32.04
5318	O	HOH	817	127.395	18.676	22.177	1.00	58.02
5319	O	HOH	818	135.930	19.361	20.695	1.00	61.65
5320	O	HOH	819	122.368	-4.865	43.028	1.00	43.72
5321	O	HOH	820	117.352	52.131	24.538	1.00	49.67
5322	O	HOH	821	129.874	51.577	33.814	1.00	58.12
5323	O	HOH	822	129.360	28.179	34.594	1.00	43.67
5324	O	HOH	823	97.243	40.051	31.308	1.00	40.94
5325	O	HOH	824	119.361	23.189	24.691	1.00	55.59
5326	O	HOH	825	105.947	8.433	39.961	1.00	47.78
5327	O	HOH	826	124.177	-6.929	48.285	1.00	50.47
5328	O	HOH	827	143.743	41.219	49.977	1.00	54.42
5329	O	HOH	828	117.815	15.765	23.926	1.00	47.10
5330	O	HOH	829	106.852	11.509	45.366	1.00	59.91
5331	O	HOH	830	114.340	49.442	45.031	1.00	54.21
5332	O	HOH	831	107.212	10.319	38.018	1.00	47.91
5333	O	HOH	832	89.843	54.539	37.711	1.00	55.79
5334	O	HOH	833	115.120	21.415	49.941	1.00	40.64
5335	O	HOH	834	119.324	14.942	62.472	1.00	63.27
5336	O	HOH	835	149.479	14.241	50.723	1.00	65.18
5337	O	HOH	836	99.208	46.311	26.331	1.00	59.48
5338	O	HOH	837	146.479	34.108	25.046	1.00	49.79
5339	O	HOH	838	117.731	49.616	19.065	1.00	60.65
5340	O	HOH	839	115.539	6.301	34.276	1.00	51.97

TABLE 11-continued

Structural Coordinates of Tobacco 5-Epi-Aristolochene Synthase In the Absence of Bound Substrate

Atom Type	Atom	Residue	Residue #	X	Y	Z	OCC	B-factor
5341	O	HOH	840	97.213	27.831	34.233	1.00	45.30
5342	O	HOH	841	89.788	22.728	43.919	1.00	61.79
5343	O	HOH	842	147.830	32.323	40.885	1.00	46.95
5344	O	HOH	843	132.462	17.381	68.762	1.00	50.53
5345	O	HOH	844	140.816	13.261	39.613	1.00	50.48
5346	O	HOH	845	131.788	48.689	43.107	1.00	55.44
5347	O	HOH	846	106.451	38.430	52.704	1.00	44.59
5348	O	HOH	847	112.522	3.225	51.067	1.00	62.24
5349	O	HOH	848	116.588	33.059	17.286	1.00	51.54
5350	O	HOH	849	121.984	13.530	21.831	1.00	59.69
5351	O	HOH	850	121.351	34.646	19.580	1.00	63.69
5352	O	HOH	853	119.444	26.300	52.657	1.00	48.12
5353	O	HOH	854	119.223	18.972	28.280	1.00	43.53
5354	O	HOH	855	109.476	29.077	61.498	1.00	46.95
5355	O	HOH	856	96.378	36.846	50.773	1.00	37.88
5356	O	HOH	857	96.918	48.467	51.605	1.00	69.73
5357	O	HOH	858	97.861	35.983	32.096	1.00	48.71
5358	O	HOH	859	105.582	44.217	22.626	1.00	52.96
5359	O	HOH	860	111.207	54.577	33.852	1.00	44.86
5360	O	HOH	861	106.475	45.773	50.620	1.00	52.70
5361	O	HOH	862	136.750	45.222	40.123	1.00	53.92
5362	O	HOH	863	134.438	43.600	31.414	1.00	51.51
5363	O	HOH	864	147.130	24.676	49.884	1.00	42.49
5364	O	HOH	865	126.425	22.757	59.405	1.00	54.25
5365	O	HOH	866	135.514	7.098	48.245	1.00	59.13
5366	O	HOH	867	114.942	1.622	48.125	1.00	56.08
5367	O	HOH	868	119.740	-4.108	46.312	1.00	51.35
5368	O	HOH	869	134.478	8.308	29.219	1.00	53.23
5369	O	HOH	870	127.297	14.232	21.009	1.00	54.19
5370	O	HOH	871	134.315	17.294	22.547	1.00	59.58
5371	O	HOH	872	130.159	26.543	36.441	1.00	34.46
5372	O	HOH	873	136.207	18.694	43.344	1.00	35.20
5373	O	HOH	874	134.779	10.368	41.428	1.00	45.81
5374	O	HOH	875	137.054	3.899	33.453	1.00	51.47
5375	O	HOH	876	145.762	17.318	28.638	1.00	52.42
5376	O	HOH	877	146.344	20.944	29.342	1.00	47.62

TABLE 12

```
Score = 167 bits (419), Expect = 5e-41
Identities = 88/270 (32%), Poslitives = 152/270 (55%), Gaps = 5/270 (1%)

Query:   1 DRVVECYFWALGVYFEPQYSQARVMLVKTISMISIVDDTFDAYGTVKELEAYTDAIQRWD  60
           DR+VECYFW  G+    Q++ AR+M+ K   ++I+++DD +D YGT++ELE +TD I+RWD
Sbjct: 316 DRLVECYFWNTGIIEPRQHASARIMMGKVNALITVIDDIYDVYGTLEELEQFTDLIRRWD 375

Query:  61 INEIDRLPDYMKISYKAILDLYKDYEKELSSAGRSHIVCHAIERMKEVVRNYNVESTWFI 120
           IN ID+LPDYM++ + A+ +   D   ++      +++ +  +   ++   Y VE+WF
Sbjct: 376 INSIDQLPDYMQLCFLALNNFVDDTSYDVMKEKGVNVIPYLRQSWVDLADKYMVEARWFY 435
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TABLE 12-continued

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Query: 121 EGYMPPVSEYLSNALATTTYYYLATTSYLGM-KSATEQDFEWLSKNPKILEASVIICRVI 179
           G+ P + EYL N+  + +   + T  +  +  S T++  + L K   ++  S  + R+
Sbjct: 436 GGHKPSLEEYLENSWQSISGPCMLTHIFFRVTDSFTKETVDSLYKYHDLVRWSSFVLRLA 495

Query: 180 DDTATYEVEKSRGQIATGIECCMRDYGISTKEAMAKFQNMAETAWKDIN-EGLLRPTPVS 238
           DD  T   E SRG +   ++C M DY  S  EA    + +    WK +N E + + +P
Sbjct: 496 DDLGTSVEEVSRGDVPKSLQCYMSDYNASEAEARKHVKWLIAEVWKKMNAERVSKDSPFG 555

Query: 239 TEFLTPILNLARIVEVTYIHNLDGY--THP                                266
           +F+   ++L R+ ++ Y HN DG+   HP
Sbjct: 556 KDFIGCAVDLGRMAQLMY-HNGDGHGTQHP                                584
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TABLE 13

```
Score =  116 bits (289), Expect = 1e-25
Identities = 77/270 (28%), Positives = 126/270 (46%), Gaps = 6/270 (2%)

Query:   3 VAEVYFSSATFEP-EYSATRIAFTKIGCLQVLFDDMADIFATLDELKSFTEGVKRWDTSL   61
           V   +++   FEP ++   R     I  L  + DD+ D++ TLDEL+ FT+  KRWDT
Sbjct: 318 VESFFWAVGMFEPHQHGYQRKMAATIIVLATVIDDIYDVYGTLDELELFTDTFKRWDTES  377

Query:  62 LHEIPECMQTCFKVWFKLMEEVNNDVVKVQGRDMLAHIRKPWELYFNCYVQEREWLEAGY  121
           +  +P  MQ C+      + +   D++K  G   L ++RK        Y  E +W  +GY
Sbjct: 378 ITRLPYYMQLCYWGVHNYISDAAYDILKEHGFFCLQYLRKSVVDLVEAYFHEAKWYHSGY  437

Query: 122 IPTFEEYLKTYAISVGLGPCTLQPILLMGELVKDD--VVEKVHYPSNMFELVSLSWRLTN  179
           P+ +EYL    ISV   P  + P          D  V++ ++   ++  L  +  RL +
Sbjct: 438 TPSLDEYLNIAKISVA-SPAIISPTYFTFANASHDTAVIDSLYQYHDILCLAGIILRLPD  496

Query: 180 DTKTYQAEKARGQQASGIACYMKDNPGATEEDAIKHICRVVDRALKEASFEYFKPSNDIP  239
           D  T   E ARG     I CYMK+   A+EE+A++H+  ++  A K+ +          P
Sbjct: 497 DLGTSYFELARGDVPKTIQCYMKET-NASEEEAVEHVKFLIREAWKDMN-TAIAAGYPFP  554

Query: 240 MGCKSFIFNLRLCVQIFYKFIDGYGIANEE                                269
           G  +   N+    Q  Y   DG+G+ + +
Sbjct: 555 DGMVAGAANIGRVAQFIYLHGDGFGVQHSK                                584
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TABLE 14

```
Score = 120 bits (299), Expect = 6e-27
Identities = 70/272 (25%), Positives = 137/272 (49%), Gaps = 3/272 (1%)

Query:   2 RVVECYFWALGVYFEPQYSQARVMLVKTISMISIVDDTFDAYGTVKELEAYTDAIQRWDI   61
           R VE Y W +   FEP++S++R+   KT  + +++DD +D + T+ E++  T+ ++RWD+
Sbjct: 296 RHVEYYSWVVMCIFEPEFSESRIAFAKTAILCTVLDDLYDTHATLHEIKIMTEGVRRWDL  355

Query:  62 NEIDRLPDYMKISYKAILDLYKDYEKELSSAGRSHIVCHAIERMKEVVRNYNVESTWFIE  121
           +  D LPDY+KI+++   +   +  E+       +     +  K  + +Y  E+ W
Sbjct: 356 SLTDDLPDYIKIAFQFFFNTVNELIVEIVKRQGRDMTTIVKDCWKRYIESYLQEAEWIAT  415

Query: 122 GYMPPVSEYLSNALATTTYYYLATTSYLGM-KSATEQDFEWLSKNPKILEASVIICRVID  180
           G++P  +EY+ N +A++    L     L + K   +E +    KIL+   +  R+ D
Sbjct: 416 GHIPTFNEYIKNGMASSGMCILNLNPLLLLDKLLPDNILEQIHSPSKILDLLELTGRIAD  475

Query: 181 DTATYEVEKSRGQIATGIECCMRDYGISTKE-AMAKFQNMAETAWKDINEGLLRPTPVST  239
           D   +E EK RG++A+ ++C M++   ST E A+   + +   + ++ N   ++   V
Sbjct: 476 DLKDFEDEKERGEMASSLQCYMKENPESTVENALNHIKGILNRSLEEFNWEFMKQDSVPM  535

Query: 240 EFLTPILNLARIVEVTYIHNLDGYTHPEKVLK                              271
                N+ R ++  Y +  DG    +K +K
Sbjct: 536 CCKKFTFNIGRGLQFIYKYR-DGLYISDKEVK                              566
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TABLE 15

```
Score = 221 bits (557), Expect = 4e-57
Identities = 120/263 (42%), Positives = 178/283 (62%), Gaps = 6/283 (2%)

Query:   5 EFYFWMAAAISEPEFSGSRVAFTKIAILMTMLDDLYDTHGTLDQLKIFTEGVRRWDVSLV   64
           E YF  A+ I EPEFS  R  +TK +    +LDDLYD HG+LD LK+FTE V+RWD+SLV
Sbjct: 589 EIYFSPASFIFEPEFSKCREVYTKTSNFTVILDDLYDAHGSLDDLKLFTESVKRWDLSLV  648
```

TABLE 15-continued

```
Query:  65 EGLPDFMKIAFEFWLKTSNELIAEAVKAQGQDMAAYIRKNAWERYLEAYLQDAEWIATGH  124
           + +P  MKI F  +  T N++  E  + QG+D+  YI +N W+  LEAY ++AEW    +
Sbjct: 649 DQMPQQMKICFVGFYNTFNDIAKEGRERQGRDVLGYI-QNVWKVQLEAYTKEAEWSEAKY  707

Query: 125 VPTFDEYLNNGTPNTGMCVLNLIPLLLMGEHLPIDILEQIFLPSRFHHLIELASRLVDDA  184
           VP+F+EY+ N + +  +  + LI  L  GE L  ++L +I   SRF  L+ L  RLV+D
Sbjct: 708 VPSFNEYIENASVSIALGTVVLISALFTGEVLTDEVLSKIDRESRFLQLMGLTGRLVNDT  767

Query: 185 RDFQAEKDHGDL-SCIECYLKDHPESTVEDALNHVNGLLGNCLLEMNWKFLKKQDSVPLS  243
           + +QAE+  G++ S I+CY+KDHP+ + E+AL HV  ++ N L E+N +F+   + +P
Sbjct: 768 KTYQAERGQGEVASAIQCYMKDHPKISEEEALQHVYSVMENALEELNREFV--NNKIPDI  825

Query: 244 CKKYSFHVLARSIQFMYNQGDGFSISNKV-IKDQVQKVLIVPV                    285
            K+  F   AR +Q  Y QGDG ++S+ + IK+ V+  L  PV
Sbjct: 826 YKRLVFET-ARIMQLFYMQGDGLTLSHDMEIKEHVKNCLFQPV                    867
```

SEQUENCE LISTING

<160> NUMBER OF SEQ ID NOS: 58

<210> SEQ ID NO 1
<211> LENGTH: 1671
<212> TYPE: DNA
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (25)...(1668)

<400> SEQUENCE: 1

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atggtccatc atcatcatca tcat atg gcc tca gca gca gtt gca aac tat        51
                          Met Ala Ser Ala Ala Val Ala Asn Tyr
                           1               5

gaa gaa gag att gtt cgc ccc gtc gcc gac ttc tcc cct agt ttg tgg       99
Glu Glu Glu Ile Val Arg Pro Val Ala Asp Phe Ser Pro Ser Leu Trp
 10                  15                  20                  25

ggt gat cag ttc ctt tca ttc tcc att aaa aat cag gtt gca gaa aag      147
Gly Asp Gln Phe Leu Ser Phe Ser Ile Lys Asn Gln Val Ala Glu Lys
                 30                  35                  40

tat gct caa gag att gaa gca ttg aag gaa caa acg agg aat atg ctg      195
Tyr Ala Gln Glu Ile Glu Ala Leu Lys Glu Gln Thr Arg Asn Met Leu
             45                  50                  55

tta gca act gga atg aaa ttg gct gat aca ctg aat ttg ata gac act      243
Leu Ala Thr Gly Met Lys Leu Ala Asp Thr Leu Asn Leu Ile Asp Thr
         60                  65                  70

att gaa cgc ctt ggc ata tcc tac cac ttt gag aaa gaa att gat gat      291
Ile Glu Arg Leu Gly Ile Ser Tyr His Phe Glu Lys Glu Ile Asp Asp
     75                  80                  85

att ttg gat cag att tac aac caa aac tca aac tgc aac gat ttg tgc      339
Ile Leu Asp Gln Ile Tyr Asn Gln Asn Ser Asn Cys Asn Asp Leu Cys
 90                  95                 100                 105

act tct gca ctt caa ttt cga ttg ctc agg caa cat ggt ttc aac atc      387
Thr Ser Ala Leu Gln Phe Arg Leu Leu Arg Gln His Gly Phe Asn Ile
                110                 115                 120

tct cct gaa att ttc agc aaa ttc caa gac gaa aat ggc aaa ttc aag      435
Ser Pro Glu Ile Phe Ser Lys Phe Gln Asp Glu Asn Gly Lys Phe Lys
            125                 130                 135

gaa tct ctt gct agt gat gtc tta gga tta ttg aac ttg tat gaa gct      483
Glu Ser Leu Ala Ser Asp Val Leu Gly Leu Leu Asn Leu Tyr Glu Ala
        140                 145                 150

tca cat gta agg act cat gct gac gat atc tta gaa gac gca ctt gct      531
Ser His Val Arg Thr His Ala Asp Asp Ile Leu Glu Asp Ala Leu Ala
    155                 160                 165
```

-continued

```
ttc tcc act atc cat ctt gaa tct gca gct cca cat ttg aaa tct cca      579
Phe Ser Thr Ile His Leu Glu Ser Ala Ala Pro His Leu Lys Ser Pro
170                 175                 180                 185

ctt agg gag caa gtg aca cat gcc ctt gag caa tgt ttg cac aag ggt      627
Leu Arg Glu Gln Val Thr His Ala Leu Glu Gln Cys Leu His Lys Gly
                190                 195                 200

gtt cct aga gtc gag acc cga ttc ttc atc tca tca atc tat gac aag      675
Val Pro Arg Val Glu Thr Arg Phe Phe Ile Ser Ser Ile Tyr Asp Lys
            205                 210                 215

gaa caa tcg aag aat aat gtg tta ctt cga ttt gcc aaa ttg gat ttc      723
Glu Gln Ser Lys Asn Asn Val Leu Leu Arg Phe Ala Lys Leu Asp Phe
        220                 225                 230

aac ttg ctc cag atg ttg cac aaa caa gaa ctt gct caa gta tca agg      771
Asn Leu Leu Gln Met Leu His Lys Gln Glu Leu Ala Gln Val Ser Arg
    235                 240                 245

tgg tgg aaa gat ttg gat ttt gta aca aca ctt cca tat gct aga gat      819
Trp Trp Lys Asp Leu Asp Phe Val Thr Thr Leu Pro Tyr Ala Arg Asp
250                 255                 260                 265

cga gta gtt gaa tgc tac ttt tgg gca tta gga gtt tat ttt gag cct      867
Arg Val Val Glu Cys Tyr Phe Trp Ala Leu Gly Val Tyr Phe Glu Pro
                270                 275                 280

caa tac tct caa gct cgc gtc atg ctc gtt aag acc ata tca atg att      915
Gln Tyr Ser Gln Ala Arg Val Met Leu Val Lys Thr Ile Ser Met Ile
            285                 290                 295

tcg att gtc gat gac acc ttt gat gct tac ggt aca gtt aaa gaa ctt      963
Ser Ile Val Asp Asp Thr Phe Asp Ala Tyr Gly Thr Val Lys Glu Leu
        300                 305                 310

gag gca tac aca gat gcc ata caa aga tgg gat atc aac gaa att gat     1011
Glu Ala Tyr Thr Asp Ala Ile Gln Arg Trp Asp Ile Asn Glu Ile Asp
    315                 320                 325

cgg ctt cct gat tac atg aaa atc agt tac aaa gct att cta gat ctc     1059
Arg Leu Pro Asp Tyr Met Lys Ile Ser Tyr Lys Ala Ile Leu Asp Leu
330                 335                 340                 345

tac aag gat tat gaa aag gaa ttg tct agt gcc gga aga tct cat att     1107
Tyr Lys Asp Tyr Glu Lys Glu Leu Ser Ser Ala Gly Arg Ser His Ile
                350                 355                 360

gtc tgc cat gca ata gaa aga atg aaa gaa gta gta aga aat tat aat     1155
Val Cys His Ala Ile Glu Arg Met Lys Glu Val Val Arg Asn Tyr Asn
            365                 370                 375

gtc gag tca aca tgg ttt att gaa gga tat acg cca cct gtt tct gaa     1203
Val Glu Ser Thr Trp Phe Ile Glu Gly Tyr Thr Pro Pro Val Ser Glu
        380                 385                 390

tac cta agc aat gca cta gca act acc aca tat tac tac ctc gcg aca     1251
Tyr Leu Ser Asn Ala Leu Ala Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr
    395                 400                 405

aca tcg tat ttg ggc atg aag tct gcc acg gag caa gat ttt gag tgg     1299
Thr Ser Tyr Leu Gly Met Lys Ser Ala Thr Glu Gln Asp Phe Glu Trp
410                 415                 420                 425

ttg tca aag aat cca aaa att ctt gaa gct agt gta att ata tgt cga     1347
Leu Ser Lys Asn Pro Lys Ile Leu Glu Ala Ser Val Ile Ile Cys Arg
                430                 435                 440

gtt atc gat gac aca gcc acg tac gag gtt gag aaa agc agg gga caa     1395
Val Ile Asp Asp Thr Ala Thr Tyr Glu Val Glu Lys Ser Arg Gly Gln
            445                 450                 455

att gca act gga att gag tgc tgc atg aga gat tat ggt ata tca aca     1443
Ile Ala Thr Gly Ile Glu Cys Cys Met Arg Asp Tyr Gly Ile Ser Thr
        460                 465                 470

aaa gag gca atg gct aaa ttt caa aat atg gct gag aca gca tgg aaa     1491
Lys Glu Ala Met Ala Lys Phe Gln Asn Met Ala Glu Thr Ala Trp Lys
    475                 480                 485
```

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```
gat att aat gaa gga ctt ctt agg ccc act ccc gtc tct aca gaa ttt     1539
Asp Ile Asn Glu Gly Leu Leu Arg Pro Thr Pro Val Ser Thr Glu Phe
490                 495                 500                 505

tta act cct att ctc aat ctt gct cgt att gtt gag gtt aca tat ata     1587
Leu Thr Pro Ile Leu Asn Leu Ala Arg Ile Val Glu Val Thr Tyr Ile
                510                 515                 520

cac aat cta gat gga tac act cat ccg gag aaa gtc tta aaa cct cac     1635
His Asn Leu Asp Gly Tyr Thr His Pro Glu Lys Val Leu Lys Pro His
            525                 530                 535

att att aac cta ctt gtg gac tcc atc aaa att tga                     1671
Ile Ile Asn Leu Leu Val Asp Ser Ile Lys Ile
        540                 545


<210> SEQ ID NO 2
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Nicotiana tabacum

<400> SEQUENCE: 2

Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20                  25                  30

Ser Ile Lys Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
        35                  40                  45

Leu Lys Glu Gln Thr Arg Asn Met Leu Leu Ala Thr Gly Met Lys Leu
    50                  55                  60

Ala Asp Thr Leu Asn Leu Ile Asp Thr Ile Glu Arg Leu Gly Ile Ser
65                  70                  75                  80

Tyr His Phe Glu Lys Glu Ile Asp Asp Ile Leu Asp Gln Ile Tyr Asn
                85                  90                  95

Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285
```

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```
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

Glu Gly Tyr Thr Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

Ser Ile Lys Ile
545
```

<210> SEQ ID NO 3
<211> LENGTH: 1644
<212> TYPE: DNA
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1)...(1644)

<400> SEQUENCE: 3

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atg gcc tca gca gca gtt gca aac tat gaa gaa gag att gtt cgc ccc       48
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc       96
Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
             20                  25                  30

tcc att gat aat cag gtt gcg gaa aag tat gct caa gag att gaa gca      144
Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
         35                  40                  45

ttg aag gaa caa acg agg agt atg ctg tta gca acc gga agg aaa ttg      192
Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
     50                  55                  60
```

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```
gcc gat aca ttg aat ttg att gac att att gaa cgc ctt ggt ata tcc      240
Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65                  70                  75                  80

tac cac ttt gag aaa gaa att gat gag att ttg gat cag att tac aac      288
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                 85                  90                  95

caa aac tca aac tgc aat gat ttg tgc acc tct gca ctt caa ttt cga      336
Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

ttg ctc agg caa cac ggt ttc aac atc tct cct gaa att ttc agc aaa      384
Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

ttc caa gat gaa aat ggc aaa ttc aag gag tct ctt gct agt gat gtc      432
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

tta gga tta tta aac ttg tat gaa gct tca cat gta agg act cat gct      480
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

gac gat atc tta gaa gac gca ctt gct ttc tcc act atc cat ctt gaa      528
Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat      576
Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

gcc ctt gag caa tgt ttg cac aag ggt gtt cct aga gtc gag acc cga      624
Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg      672
Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac      720
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt      768
Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt      816
Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

gag gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc      864
Glu Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt      912
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata      960
Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa     1008
Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa     1056
Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga     1104
Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att     1152
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380
```

-continued

```
gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca     1200
Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

act acc aca tat tac tac ctc gcg aca aca tcg tat ttg ggc atg aag     1248
Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att     1296
Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg     1344
Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc     1392
Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt     1440
Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt     1488
Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt     1536
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga tac act     1584
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac     1632
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

tcc atc aaa att                                                    1644
Ser Ile Lys Ile
545
```

<210> SEQ ID NO 4
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Nicotiana tabacum

<400> SEQUENCE: 4

```
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20                  25                  30

Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
        35                  40                  45

Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
    50                  55                  60

Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
65                  70                  75                  80

Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                85                  90                  95

Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140
```

-continued

```
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

Glu Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

Ser Ile Lys Ile
545
```

-continued

<210> SEQ ID NO 5
<211> LENGTH: 1644
<212> TYPE: DNA
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1)...(1644)

<400> SEQUENCE: 5

```
atg gcc tca gca gca gtt gca aac tat gaa gaa gag att gtt cgc ccc       48
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc       96
Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20                  25                  30

tcc att gat aat cag gtt gcg gaa aag tat gct caa gag att gaa gca      144
Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
         35                  40                  45

ttg aag gaa caa acg agg agt atg ctg tta gca acc gga agg aaa ttg      192
Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
     50                  55                  60

gcc gat aca ttg aat ttg att gac att att gaa cgc ctt ggt ata tcc      240
Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65                  70                  75                  80

tac cac ttt gag aaa gaa att gat gag att ttg gat cag att tac aac      288
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                85                  90                  95

caa aac tca aac tgc aat gat ttg tgc acc tct gca ctt caa ttt cga      336
Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

ttg ctc agg caa cac ggt ttc aac atc tct cct gaa att ttc agc aaa      384
Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

ttc caa gat gaa aat ggc aaa ttc aag gag tct ctt gct agt gat gtc      432
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

tta gga tta tta aac ttg tat gaa gct tca cat gta agg act cat gct      480
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

gac gat atc tta gaa gac gca ctt gct ttc tcc act atc cat ctt gaa      528
Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat      576
Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

gcc ctt gag caa tgt ttg cac aag ggt gtt cct aga gtc gag acc cga      624
Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg      672
Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac      720
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt      768
Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt      816
Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270
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tgg gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc      864
Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt      912
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata      960
Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa     1008
Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa     1056
Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga     1104
Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att     1152
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca     1200
Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

act acc aca tat tac tac ctc gcg aca aca tcg tat ttg ggc atg aag     1248
Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att     1296
Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg     1344
Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc     1392
Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt     1440
Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt     1488
Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt     1536
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

gct cgt att gtt gag gtt aca ttc ata cac aat cta gat gga tac act     1584
Ala Arg Ile Val Glu Val Thr Phe Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac     1632
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

tcc atc aaa att                                                    1644
Ser Ile Lys Ile
545
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<210> SEQ ID NO 6
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Nicotiana tabacum

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<400> SEQUENCE: 6

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Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20                  25                  30

Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
        35                  40                  45

Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
    50                  55                  60

Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
65                  70                  75                  80

Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                85                  90                  95

Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415
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Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

Ala Arg Ile Val Glu Val Thr Phe Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

Ser Ile Lys Ile
545


<210> SEQ ID NO 7
<211> LENGTH: 1644
<212> TYPE: DNA
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1)...(1644)

<400> SEQUENCE: 7

atg gcc tca gca gca gtt gca aac tat gaa gaa gag att gtt cgc ccc       48
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc       96
Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
             20                  25                  30

tcc att gat aat cag gtt gcg gaa aag tat gct caa gag att gaa gca      144
Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
         35                  40                  45

ttg aag gaa caa acg agg agt atg ctg tta gca acc gga agg aaa ttg      192
Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
     50                  55                  60

gcc gat aca ttg aat ttg att gac att att gaa cgc ctt ggt ata tcc      240
Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65                  70                  75                  80

tac cac ttt gag aaa gaa att gat gag att ttg gat cag att tac aac      288
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                 85                  90                  95

caa aac tca aac tgc aat gat ttg tgc acc tct gca ctt caa ttt cga      336
Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

ttg ctc agg caa cac ggt ttc aac atc tct cct gaa att ttc agc aaa      384
Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

ttc caa gat gaa aat ggc aaa ttc aag gag tct ctt gct agt gat gtc      432
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

tta gga tta tta aac ttg tat gaa gct tca cat gta agg act cat gct      480
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160
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gac gat atc tta gaa gac gca ctt gct ttc tcc act atc cat ctt gaa      528
Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat      576
Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

gcc ctt gag caa tgt ttg cac aag ggt gtt cct aga gtc gag acc cga      624
Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg      672
Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac      720
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt      768
Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt      816
Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

tgg gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc      864
Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt      912
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata      960
Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa     1008
Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa     1056
Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga     1104
Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att     1152
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca     1200
Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

act acc aca tat tac tac ctc gcg aca aca tcg tat ttg ggc atg aag     1248
Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att     1296
Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg     1344
Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc     1392
Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt     1440
Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480
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caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt     1488
Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt     1536
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga ttc act     1584
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Phe Thr
        515                 520                 525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac     1632
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

tcc atc aaa att                                                    1644
Ser Ile Lys Ile
545


<210> SEQ ID NO 8
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Nicotiana tabacum

<400> SEQUENCE: 8

Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20                  25                  30

Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
        35                  40                  45

Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
    50                  55                  60

Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
65                  70                  75                  80

Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                85                  90                  95

Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270
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Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Phe Thr
        515                 520                 525

His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

Ser Ile Lys Ile
545
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<210> SEQ ID NO 9
<211> LENGTH: 1644
<212> TYPE: DNA
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1)...(1644)

<400> SEQUENCE: 9

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atg gcc tca gca gca gtt gca aac tat gaa gaa gag att gtt cgc ccc       48
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc       96
Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
             20                  25                  30

tcc att gat aat cag gtt gcg gaa aag tat gct caa gag att gaa gca      144
Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
         35                  40                  45
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```
ttg aag gaa caa acg agg agt atg ctg tta gca acc gga agg aaa ttg      192
Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
     50                  55                  60

gcc gat aca ttg aat ttg att gac att att gaa cgc ctt ggt ata tcc      240
Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65                  70                  75                  80

tac cac ttt gag aaa gaa att gat gag att ttg gat cag att tac aac      288
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                 85                  90                  95

caa aac tca aac tgc aat gat ttg tgc acc tct gca ctt caa ttt cga      336
Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

ttg ctc agg caa cac ggt ttc aac atc tct cct gaa att ttc agc aaa      384
Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

ttc caa gat gaa aat ggc aaa ttc aag gag tct ctt gct agt gat gtc      432
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

tta gga tta tta aac ttg tat gaa gct tca cat gta agg act cat gct      480
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

gac gat atc tta gaa gac gca ctt gct ttc tcc act atc cat ctt gaa      528
Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat      576
Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

gcc ctt gag caa tgt ttg cac aag ggt gtt cct aga gtc gag acc cga      624
Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg      672
Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac      720
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt      768
Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt      816
Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

tcg gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc      864
Ser Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt      912
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata      960
Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa     1008
Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa     1056
Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga     1104
Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365
```

-continued

```
atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att     1152
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca     1200
Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

act acc aca tat tac tac ctc gcg aca aca tcg tat ttg ggc atg aag     1248
Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att     1296
Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

ctt gaa gct agt gta att ata tgg cga gtt atc gat gac aca gcc acg     1344
Leu Glu Ala Ser Val Ile Ile Trp Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc     1392
Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt     1440
Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt     1488
Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt     1536
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga tac act     1584
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac     1632
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

tcc atc aaa att                                                    1644
Ser Ile Lys Ile
545
```

<210> SEQ ID NO 10
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Nicotiana tabacum

<400> SEQUENCE: 10

```
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20                  25                  30

Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
        35                  40                  45

Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
    50                  55                  60

Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
65                  70                  75                  80

Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                85                  90                  95

Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125
```

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```
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240

Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

Ser Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

Thr Thr Thr Tyr Tyr Tyr Leu Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

Leu Glu Ala Ser Val Ile Ile Trp Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525
```

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```
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

Ser Ile Lys Ile
545


<210> SEQ ID NO 11
<211> LENGTH: 1644
<212> TYPE: DNA
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1)...(1644)
<221> NAME/KEY: misc_feature
<222> LOCATION: (1)...(1644)
<223> OTHER INFORMATION: n = A,T,C or G

<400> SEQUENCE: 11

atg gcc tca gca gca gtt gca aac tat gaa gaa gag att gtt cgc ccc       48
Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1               5                  10                  15

gtc gcc gac ttc tcc cct agt ctc tgg ggt gat cag ttc ctt tca ttc       96
Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
             20                  25                  30

tcc att gat aat cag gtt gcg gaa aag tat gct caa gag att gaa gca      144
Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
         35                  40                  45

ttg aag gaa caa acg agg agt atg ctg tta gca acc gga agg aaa ttg      192
Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
     50                  55                  60

gcc gat aca ttg aat ttg att gac att att gaa cgc ctt ggt ata tcc      240
Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
 65                  70                  75                  80

tac cac ttt gag aaa gaa att gat gag att ttg gat cag att tac aac      288
Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                 85                  90                  95

caa aac tca aac tgc aat gat ttg tgc acc tct gca ctt caa ttt cga      336
Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100                 105                 110

ttg ctc agg caa cac ggt ttc aac atc tct cct gaa att ttc agc aaa      384
Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115                 120                 125

ttc caa gat gaa aat ggc aaa ttc aag gag tct ctt gct agt gat gtc      432
Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130                 135                 140

tta gga tta tta aac ttg tat gaa gct tca cat gta agg act cat gct      480
Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145                 150                 155                 160

gac gat atc tta gaa gac gca ctt gct ttc tcc act atc cat ctt gaa      528
Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165                 170                 175

tct gca gct cca cat ttg aaa tct cca ctt agg gag caa gtg aca cat      576
Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180                 185                 190

gcc ctt gag caa tgt ttg cac aag ggt gtt cct aga gtc gag acc cga      624
Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195                 200                 205

ttc ttc atc tca tca atc tat gac aag gaa caa tcg aag aat aat gtg      672
Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210                 215                 220

tta ctt cga ttt gcc aaa ttg gat ttc aac ttg ctc cag atg ttg cac      720
Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225                 230                 235                 240
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aaa caa gaa ctt gct caa gta tca agg tgg tgg aaa gat ttg gat ttt      768
Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245                 250                 255

gta aca aca ctt cca tat gct aga gat cga gta gtt gaa tgc tac ttt      816
Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260                 265                 270

tgg gca tta gga gtt tat ttt gag cct caa tac tct caa gct cgc gtc      864
Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275                 280                 285

atg ctc gtt aag acc ata tca atg att tcg att gtc gat gac acc ttt      912
Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290                 295                 300

gat gct tac ggt aca gtt aaa gaa ctt gag gca tac aca gat gcc ata      960
Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305                 310                 315                 320

caa aga tgg gat atc aac gaa att gat cgg ctt cct gat tac atg aaa     1008
Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325                 330                 335

atc agt tat aaa gct att cta gat ctc tac aag gat tat gaa aag gaa     1056
Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340                 345                 350

ttg tct agt gcc gga aga tct cat att gtc tgc cat gca ata gaa aga     1104
Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355                 360                 365

atg aaa gaa gta gta aga aat tat aat gtc gag tca aca tgg ttt att     1152
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

gaa gga tat atg cca cct gtt tct gaa tac cta agc aat gca cta gca     1200
Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

act acc aca tat tac nns nns gcg aca aca tcg tat ttg ggc atg aag     1248
Thr Thr Thr Tyr Tyr Xaa Xaa Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

tct gcc acg gag caa gat ttt gag tgg ttg tca aag aat cca aaa att     1296
Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

ctt gaa gct agt gta att ata tgt cga gtt atc gat gac aca gcc acg     1344
Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

tac gag gtt gag aaa agc agg gga caa att gca act gga att gag tgc     1392
Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

tgc atg aga gat tat ggt ata tca aca aaa gag gca atg gct aaa ttt     1440
Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

caa aat atg gct gag aca gca tgg aaa gat att aat gaa gga ctt ctt     1488
Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

agg ccc act ccc gtc tct aca gaa ttt tta act cct att ctc aat ctt     1536
Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

gct cgt att gtt gag gtt aca tat ata cac aat cta gat gga tac act     1584
Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

cat ccg gag aaa gtc tta aaa cct cac att att aac cta ctt gtg gac     1632
His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

tcc atc aaa att                                                    1644
Ser Ile Lys Ile
545
```

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<210> SEQ ID NO 12
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Nicotiana tabacum
<220> FEATURE:
<221> NAME/KEY: VARIANT
<222> LOCATION: (1)...(548)
<223> OTHER INFORMATION: Xaa = Any Amino Acid

<400> SEQUENCE: 12

Met Ala Ser Ala Ala Val Ala Asn Tyr Glu Glu Glu Ile Val Arg Pro
 1   5   10   15

Val Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Gln Phe Leu Ser Phe
            20   25   30

Ser Ile Asp Asn Gln Val Ala Glu Lys Tyr Ala Gln Glu Ile Glu Ala
        35   40   45

Leu Lys Glu Gln Thr Arg Ser Met Leu Leu Ala Thr Gly Arg Lys Leu
    50   55   60

Ala Asp Thr Leu Asn Leu Ile Asp Ile Ile Glu Arg Leu Gly Ile Ser
65   70   75   80

Tyr His Phe Glu Lys Glu Ile Asp Glu Ile Leu Asp Gln Ile Tyr Asn
                85   90   95

Gln Asn Ser Asn Cys Asn Asp Leu Cys Thr Ser Ala Leu Gln Phe Arg
            100   105   110

Leu Leu Arg Gln His Gly Phe Asn Ile Ser Pro Glu Ile Phe Ser Lys
        115   120   125

Phe Gln Asp Glu Asn Gly Lys Phe Lys Glu Ser Leu Ala Ser Asp Val
    130   135   140

Leu Gly Leu Leu Asn Leu Tyr Glu Ala Ser His Val Arg Thr His Ala
145   150   155   160

Asp Asp Ile Leu Glu Asp Ala Leu Ala Phe Ser Thr Ile His Leu Glu
                165   170   175

Ser Ala Ala Pro His Leu Lys Ser Pro Leu Arg Glu Gln Val Thr His
            180   185   190

Ala Leu Glu Gln Cys Leu His Lys Gly Val Pro Arg Val Glu Thr Arg
        195   200   205

Phe Phe Ile Ser Ser Ile Tyr Asp Lys Glu Gln Ser Lys Asn Asn Val
    210   215   220

Leu Leu Arg Phe Ala Lys Leu Asp Phe Asn Leu Leu Gln Met Leu His
225   230   235   240

Lys Gln Glu Leu Ala Gln Val Ser Arg Trp Trp Lys Asp Leu Asp Phe
                245   250   255

Val Thr Thr Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Cys Tyr Phe
            260   265   270

Trp Ala Leu Gly Val Tyr Phe Glu Pro Gln Tyr Ser Gln Ala Arg Val
        275   280   285

Met Leu Val Lys Thr Ile Ser Met Ile Ser Ile Val Asp Asp Thr Phe
    290   295   300

Asp Ala Tyr Gly Thr Val Lys Glu Leu Glu Ala Tyr Thr Asp Ala Ile
305   310   315   320

Gln Arg Trp Asp Ile Asn Glu Ile Asp Arg Leu Pro Asp Tyr Met Lys
                325   330   335

Ile Ser Tyr Lys Ala Ile Leu Asp Leu Tyr Lys Asp Tyr Glu Lys Glu
            340   345   350

Leu Ser Ser Ala Gly Arg Ser His Ile Val Cys His Ala Ile Glu Arg
        355   360   365

-continued

```
Met Lys Glu Val Val Arg Asn Tyr Asn Val Glu Ser Thr Trp Phe Ile
    370                 375                 380

Glu Gly Tyr Met Pro Pro Val Ser Glu Tyr Leu Ser Asn Ala Leu Ala
385                 390                 395                 400

Thr Thr Thr Tyr Tyr Xaa Xaa Ala Thr Thr Ser Tyr Leu Gly Met Lys
                405                 410                 415

Ser Ala Thr Glu Gln Asp Phe Glu Trp Leu Ser Lys Asn Pro Lys Ile
            420                 425                 430

Leu Glu Ala Ser Val Ile Ile Cys Arg Val Ile Asp Asp Thr Ala Thr
        435                 440                 445

Tyr Glu Val Glu Lys Ser Arg Gly Gln Ile Ala Thr Gly Ile Glu Cys
    450                 455                 460

Cys Met Arg Asp Tyr Gly Ile Ser Thr Lys Glu Ala Met Ala Lys Phe
465                 470                 475                 480

Gln Asn Met Ala Glu Thr Ala Trp Lys Asp Ile Asn Glu Gly Leu Leu
                485                 490                 495

Arg Pro Thr Pro Val Ser Thr Glu Phe Leu Thr Pro Ile Leu Asn Leu
            500                 505                 510

Ala Arg Ile Val Glu Val Thr Tyr Ile His Asn Leu Asp Gly Tyr Thr
        515                 520                 525

His Pro Glu Lys Val Leu Lys Pro His Ile Ile Asn Leu Leu Val Asp
    530                 535                 540

Ser Ile Lys Ile
545
```

<210> SEQ ID NO 13
<211> LENGTH: 33
<212> TYPE: DNA
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: primer for mutagenesis

<400> SEQUENCE: 13

```
gttgaatgct acttttcggc attaggagtt tat                                33
```

<210> SEQ ID NO 14
<211> LENGTH: 33
<212> TYPE: DNA
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: primer for mutagenesis

<400> SEQUENCE: 14

```
ataaactcct aatgccgaaa agtagcattc aac                                33
```

<210> SEQ ID NO 15
<211> LENGTH: 33
<212> TYPE: DNA
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: primer for mutagenesis

<400> SEQUENCE: 15

```
gctagtgtaa ttatatggcg agttatcgat gac                                33
```

<210> SEQ ID NO 16
<211> LENGTH: 33
<212> TYPE: DNA
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: primer for mutagenesis

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<400> SEQUENCE: 16

gtcatcgata actcgccata taattacact agc 33

<210> SEQ ID NO 17
<211> LENGTH: 54
<212> TYPE: DNA
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: primer for mutagenesis
<221> NAME/KEY: misc_feature
<222> LOCATION: (1)...(54)
<223> OTHER INFORMATION: n = A,T,C or G

<400> SEQUENCE: 17

gcactagcaa ctaccacata ttacnnsnns gcgacaacat cgtatttggg catg 54

<210> SEQ ID NO 18
<211> LENGTH: 54
<212> TYPE: DNA
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: primer for mutagenesis
<221> NAME/KEY: misc_feature
<222> LOCATION: (1)...(54)
<223> OTHER INFORMATION: n = A,T,C or G

<400> SEQUENCE: 18

catgcccaaa tacgatgttg tcgcsnnsnn gtaatatgtg gtagttgcta gtgc 54

<210> SEQ ID NO 19
<211> LENGTH: 2018
<212> TYPE: DNA
<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (6)...(1889)
<223> OTHER INFORMATION: pinene synthase

<400> SEQUENCE: 19

```
cagca atg gct cta gtt tct acc gca ccg ttg gct tcc aaa tca tgc ctg     50
      Met Ala Leu Val Ser Thr Ala Pro Leu Ala Ser Lys Ser Cys Leu
       1               5                  10                  15

cac aaa tcg ttg atc agt tct acc cat gag ctt aag gct ctc tct aga       98
His Lys Ser Leu Ile Ser Ser Thr His Glu Leu Lys Ala Leu Ser Arg
                 20                  25                  30

aca att cca gct cta gga atg agt agg cga ggg aaa tct atc act cct      146
Thr Ile Pro Ala Leu Gly Met Ser Arg Arg Gly Lys Ser Ile Thr Pro
             35                  40                  45

tcc atc agc atg agc tct acc acc gtt gta acc gat gat ggt gta cga      194
Ser Ile Ser Met Ser Ser Thr Thr Val Val Thr Asp Asp Gly Val Arg
         50                  55                  60

aga cgc atg ggc gat ttc cat tcc aac ctc tgg gac gat gat gtc ata      242
Arg Arg Met Gly Asp Phe His Ser Asn Leu Trp Asp Asp Asp Val Ile
     65                  70                  75

cag tct tta cca acg gct tat gag gaa aaa tcg tac ctg gag cgt gct      290
Gln Ser Leu Pro Thr Ala Tyr Glu Glu Lys Ser Tyr Leu Glu Arg Ala
 80                  85                  90                  95

gag aaa ctg atc ggg gaa gta aag aac atg ttc aat tcg atg tca tta      338
Glu Lys Leu Ile Gly Glu Val Lys Asn Met Phe Asn Ser Met Ser Leu
                100                 105                 110

gaa gat gga gag tta atg agt ccg ctc aat gat ctc att caa cgc ctt      386
Glu Asp Gly Glu Leu Met Ser Pro Leu Asn Asp Leu Ile Gln Arg Leu
            115                 120                 125
```

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```
tgg att gtc gac agc ctt gaa cgt ttg ggg atc cat aga cat ttc aaa      434
Trp Ile Val Asp Ser Leu Glu Arg Leu Gly Ile His Arg His Phe Lys
        130                 135                 140

gat gag ata aaa tcg gcg ctt gat tat gtt tac agt tat tgg ggc gaa      482
Asp Glu Ile Lys Ser Ala Leu Asp Tyr Val Tyr Ser Tyr Trp Gly Glu
    145                 150                 155

aat ggc atc gga tgc ggg agg gag agt gtt gtt act gat ctg aac tca      530
Asn Gly Ile Gly Cys Gly Arg Glu Ser Val Val Thr Asp Leu Asn Ser
160                 165                 170                 175

act gcg ttg ggg ctt cga acc cta cga cta cac gga tac ccg gtg tct      578
Thr Ala Leu Gly Leu Arg Thr Leu Arg Leu His Gly Tyr Pro Val Ser
                180                 185                 190

tca gat gtt ttc aaa gct ttc aaa ggc caa aat ggg cag ttt tcc tgc      626
Ser Asp Val Phe Lys Ala Phe Lys Gly Gln Asn Gly Gln Phe Ser Cys
            195                 200                 205

tct gaa aat att cag aca gat gaa gag atc aga ggc gtt ctg aat tta      674
Ser Glu Asn Ile Gln Thr Asp Glu Glu Ile Arg Gly Val Leu Asn Leu
        210                 215                 220

ttc cgg gcc tcc ctc att gcc ttt cca ggg gag aaa att atg gat gag      722
Phe Arg Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Ile Met Asp Glu
    225                 230                 235

gct gaa atc ttc tct acc aaa tat tta aaa gaa gcc ctg caa aag att      770
Ala Glu Ile Phe Ser Thr Lys Tyr Leu Lys Glu Ala Leu Gln Lys Ile
240                 245                 250                 255

ccg gtc tcc agt ctt tcg cga gag atc ggg gac gtt ttg gaa tat ggt      818
Pro Val Ser Ser Leu Ser Arg Glu Ile Gly Asp Val Leu Glu Tyr Gly
                260                 265                 270

tgg cac aca tat ttg ccg cga ttg gaa gca agg aat tac atc caa gtc      866
Trp His Thr Tyr Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Gln Val
            275                 280                 285

ttt gga cag gac act gag aac acg aag tca tat gtg aag agc aaa aaa      914
Phe Gly Gln Asp Thr Glu Asn Thr Lys Ser Tyr Val Lys Ser Lys Lys
        290                 295                 300

ctt tta gaa ctc gca aaa ttg gag ttc aac atc ttt caa tcc tta caa      962
Leu Leu Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Gln Ser Leu Gln
    305                 310                 315

aag agg gag tta gaa agt ctg gtc aga tgg tgg aaa gaa tcg ggt ttt     1010
Lys Arg Glu Leu Glu Ser Leu Val Arg Trp Trp Lys Glu Ser Gly Phe
320                 325                 330                 335

cct gag atg acc ttc tgc cga cat cgt cac gtg gaa tac tac act ttg     1058
Pro Glu Met Thr Phe Cys Arg His Arg His Val Glu Tyr Tyr Thr Leu
                340                 345                 350

gct tcc tgc att gcg ttc gag cct caa cat tct gga ttc aga ctc ggc     1106
Ala Ser Cys Ile Ala Phe Glu Pro Gln His Ser Gly Phe Arg Leu Gly
            355                 360                 365

ttt gcc aag acg tgt cat ctt atc acg gtt ctt gac gat atg tac gac     1154
Phe Ala Lys Thr Cys His Leu Ile Thr Val Leu Asp Asp Met Tyr Asp
        370                 375                 380

acc ttc ggc aca gta gac gag ctg gaa ctc ttc aca gcg aca atg aag     1202
Thr Phe Gly Thr Val Asp Glu Leu Glu Leu Phe Thr Ala Thr Met Lys
    385                 390                 395

aga tgg gat ccg tcc tcg ata gat tgc ctt cca gaa tat atg aaa gga     1250
Arg Trp Asp Pro Ser Ser Ile Asp Cys Leu Pro Glu Tyr Met Lys Gly
400                 405                 410                 415

gtg tac ata gcg gtt tac gac acc gta aat gaa atg gct cga gag gca     1298
Val Tyr Ile Ala Val Tyr Asp Thr Val Asn Glu Met Ala Arg Glu Ala
                420                 425                 430

gag gag gct caa ggc cga gat acg ctc aca tat gct cgg gaa gct tgg     1346
Glu Glu Ala Gln Gly Arg Asp Thr Leu Thr Tyr Ala Arg Glu Ala Trp
            435                 440                 445
```

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```
gag gct tat att gat tcg tat atg caa gaa gca agg tgg atc gcc act     1394
Glu Ala Tyr Ile Asp Ser Tyr Met Gln Glu Ala Arg Trp Ile Ala Thr
        450                 455                 460

ggt tac ctg ccc tcc ttt gat gag tac tac gag aat ggg aaa gtt agc     1442
Gly Tyr Leu Pro Ser Phe Asp Glu Tyr Tyr Glu Asn Gly Lys Val Ser
    465                 470                 475

tgt ggt cat cgc ata tcc gca ttg caa ccc att ctg aca atg gac atc     1490
Cys Gly His Arg Ile Ser Ala Leu Gln Pro Ile Leu Thr Met Asp Ile
480                 485                 490                 495

ccc ttt cct gat cat atc ctc aag gaa gtt gac ttc cca tca aag ctt     1538
Pro Phe Pro Asp His Ile Leu Lys Glu Val Asp Phe Pro Ser Lys Leu
                500                 505                 510

aac gac ttg gca tgt gcc atc ctt cga tta cga ggt gat acg cgg tgc     1586
Asn Asp Leu Ala Cys Ala Ile Leu Arg Leu Arg Gly Asp Thr Arg Cys
            515                 520                 525

tac aag gcg gac agg gct cgt gga gaa gaa gct tcc tct ata tca tgt     1634
Tyr Lys Ala Asp Arg Ala Arg Gly Glu Glu Ala Ser Ser Ile Ser Cys
        530                 535                 540

tat atg aaa gac aat cct gga gta tca gag gaa gat gct ctc gat cat     1682
Tyr Met Lys Asp Asn Pro Gly Val Ser Glu Glu Asp Ala Leu Asp His
    545                 550                 555

atc aac gcc atg atc agt gac gta atc aaa gga tta aat tgg gaa ctt     1730
Ile Asn Ala Met Ile Ser Asp Val Ile Lys Gly Leu Asn Trp Glu Leu
560                 565                 570                 575

ctc aaa cca gac atc aat gtt ccc atc tcg gcg aag aaa cat gct ttt     1778
Leu Lys Pro Asp Ile Asn Val Pro Ile Ser Ala Lys Lys His Ala Phe
                580                 585                 590

gac atc gcc aga gct ttc cat tac ggc tac aaa tac cga gac ggc tac     1826
Asp Ile Ala Arg Ala Phe His Tyr Gly Tyr Lys Tyr Arg Asp Gly Tyr
            595                 600                 605

agc gtt gcc aac gtt gaa acg aag agt ttg gtc acg aga acc ctc ctt     1874
Ser Val Ala Asn Val Glu Thr Lys Ser Leu Val Thr Arg Thr Leu Leu
        610                 615                 620

gaa tct gtg cct ttg tag caacagctca aatctatgcc ctatgctatg           1922
Glu Ser Val Pro Leu
    625

tcgggttaaa atatatgtgg aaggtagccg ttggatgtag aggataagtt tgttataatt   1982

taataaagtt gtaatttaaa aaaaaaaaaa aaaaaa                             2018


<210> SEQ ID NO 20
<211> LENGTH: 628
<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 20

Met Ala Leu Val Ser Thr Ala Pro Leu Ala Ser Lys Ser Cys Leu His
 1               5                  10                  15

Lys Ser Leu Ile Ser Ser Thr His Glu Leu Lys Ala Leu Ser Arg Thr
            20                  25                  30

Ile Pro Ala Leu Gly Met Ser Arg Arg Gly Lys Ser Ile Thr Pro Ser
        35                  40                  45

Ile Ser Met Ser Ser Thr Thr Val Val Thr Asp Asp Gly Val Arg Arg
    50                  55                  60

Arg Met Gly Asp Phe His Ser Asn Leu Trp Asp Asp Asp Val Ile Gln
65                  70                  75                  80

Ser Leu Pro Thr Ala Tyr Glu Glu Lys Ser Tyr Leu Glu Arg Ala Glu
                85                  90                  95
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Lys Leu Ile Gly Glu Val Lys Asn Met Phe Asn Ser Met Ser Leu Glu
            100                 105                 110

Asp Gly Glu Leu Met Ser Pro Leu Asn Asp Leu Ile Gln Arg Leu Trp
        115                 120                 125

Ile Val Asp Ser Leu Glu Arg Leu Gly Ile His Arg His Phe Lys Asp
    130                 135                 140

Glu Ile Lys Ser Ala Leu Asp Tyr Val Tyr Ser Tyr Trp Gly Glu Asn
145                 150                 155                 160

Gly Ile Gly Cys Gly Arg Glu Ser Val Val Thr Asp Leu Asn Ser Thr
                165                 170                 175

Ala Leu Gly Leu Arg Thr Leu Arg Leu His Gly Tyr Pro Val Ser Ser
            180                 185                 190

Asp Val Phe Lys Ala Phe Lys Gly Gln Asn Gly Gln Phe Ser Cys Ser
        195                 200                 205

Glu Asn Ile Gln Thr Asp Glu Glu Ile Arg Gly Val Leu Asn Leu Phe
    210                 215                 220

Arg Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Ile Met Asp Glu Ala
225                 230                 235                 240

Glu Ile Phe Ser Thr Lys Tyr Leu Lys Glu Ala Leu Gln Lys Ile Pro
                245                 250                 255

Val Ser Ser Leu Ser Arg Glu Ile Gly Asp Val Leu Glu Tyr Gly Trp
            260                 265                 270

His Thr Tyr Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Gln Val Phe
        275                 280                 285

Gly Gln Asp Thr Glu Asn Thr Lys Ser Tyr Val Lys Ser Lys Lys Leu
    290                 295                 300

Leu Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Gln Ser Leu Gln Lys
305                 310                 315                 320

Arg Glu Leu Glu Ser Leu Val Arg Trp Trp Lys Glu Ser Gly Phe Pro
                325                 330                 335

Glu Met Thr Phe Cys Arg His Arg His Val Glu Tyr Tyr Thr Leu Ala
            340                 345                 350

Ser Cys Ile Ala Phe Glu Pro Gln His Ser Gly Phe Arg Leu Gly Phe
        355                 360                 365

Ala Lys Thr Cys His Leu Ile Thr Val Leu Asp Asp Met Tyr Asp Thr
    370                 375                 380

Phe Gly Thr Val Asp Glu Leu Glu Leu Phe Thr Ala Thr Met Lys Arg
385                 390                 395                 400

Trp Asp Pro Ser Ser Ile Asp Cys Leu Pro Glu Tyr Met Lys Gly Val
                405                 410                 415

Tyr Ile Ala Val Tyr Asp Thr Val Asn Glu Met Ala Arg Glu Ala Glu
            420                 425                 430

Glu Ala Gln Gly Arg Asp Thr Leu Thr Tyr Ala Arg Glu Ala Trp Glu
        435                 440                 445

Ala Tyr Ile Asp Ser Tyr Met Gln Glu Ala Arg Trp Ile Ala Thr Gly
    450                 455                 460

Tyr Leu Pro Ser Phe Asp Glu Tyr Tyr Glu Asn Gly Lys Val Ser Cys
465                 470                 475                 480

Gly His Arg Ile Ser Ala Leu Gln Pro Ile Leu Thr Met Asp Ile Pro
                485                 490                 495

Phe Pro Asp His Ile Leu Lys Glu Val Asp Phe Pro Ser Lys Leu Asn
            500                 505                 510
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Asp Leu Ala Cys Ala Ile Leu Arg Leu Arg Gly Asp Thr Arg Cys Tyr
        515                 520                 525

Lys Ala Asp Arg Ala Arg Gly Glu Glu Ala Ser Ser Ile Ser Cys Tyr
    530                 535                 540

Met Lys Asp Asn Pro Gly Val Ser Glu Glu Asp Ala Leu Asp His Ile
545                 550                 555                 560

Asn Ala Met Ile Ser Asp Val Ile Lys Gly Leu Asn Trp Glu Leu Leu
                565                 570                 575

Lys Pro Asp Ile Asn Val Pro Ile Ser Ala Lys Lys His Ala Phe Asp
            580                 585                 590

Ile Ala Arg Ala Phe His Tyr Gly Tyr Lys Tyr Arg Asp Gly Tyr Ser
        595                 600                 605

Val Ala Asn Val Glu Thr Lys Ser Leu Val Thr Arg Thr Leu Leu Glu
    610                 615                 620

Ser Val Pro Leu
625


<210> SEQ ID NO 21
<211> LENGTH: 2170
<212> TYPE: DNA
<213> ORGANISM: Mentha spicata
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (29)...(1825)
<223> OTHER INFORMATION: 4S-limonene synthase

<400> SEQUENCE: 21

agagagagag aggaaggaaa gattaatc atg gct ctc aaa gtg tta agt gtt        52
                            Met Ala Leu Lys Val Leu Ser Val
                             1               5

gca act caa atg gcg att cct agc aac cta acg aca tgt ctt caa ccc      100
Ala Thr Gln Met Ala Ile Pro Ser Asn Leu Thr Thr Cys Leu Gln Pro
     10                  15                  20

tca cac ttc aaa tct tct cca aaa ctg tta tct agc act aac agt agt      148
Ser His Phe Lys Ser Ser Pro Lys Leu Leu Ser Ser Thr Asn Ser Ser
 25                  30                  35                  40

agt cgg tct cgc ctc cgt gtg tat tgc tcc tcc tcg caa ctc act act      196
Ser Arg Ser Arg Leu Arg Val Tyr Cys Ser Ser Ser Gln Leu Thr Thr
                 45                  50                  55

gaa aga cga tcc gga aac tac aac cct tct cgt tgg gat gtc aac ttc      244
Glu Arg Arg Ser Gly Asn Tyr Asn Pro Ser Arg Trp Asp Val Asn Phe
             60                  65                  70

atc caa tcg ctt ctc agt gac tat aag gag gac aaa cac gtg att agg      292
Ile Gln Ser Leu Leu Ser Asp Tyr Lys Glu Asp Lys His Val Ile Arg
         75                  80                  85

gct tct gag ctg gtc act ttg gtg aag atg gaa ctg gag aaa gaa acg      340
Ala Ser Glu Leu Val Thr Leu Val Lys Met Glu Leu Glu Lys Glu Thr
     90                  95                  100

gat caa att cga caa ctt gag ttg atc gat gac ttg cag agg atg ggg      388
Asp Gln Ile Arg Gln Leu Glu Leu Ile Asp Asp Leu Gln Arg Met Gly
105                 110                 115                 120

ctg tcc gat cat ttc caa aat gag ttc aaa gaa atc ttg tcc tct ata      436
Leu Ser Asp His Phe Gln Asn Glu Phe Lys Glu Ile Leu Ser Ser Ile
                125                 130                 135

tat ctc gac cat cac tat tac aag aac cct ttt cca aaa gaa gaa agg      484
Tyr Leu Asp His His Tyr Tyr Lys Asn Pro Phe Pro Lys Glu Glu Arg
            140                 145                 150

gat ctc tac tcc aca tct ctt gca ttt agg ctc ctc aga gaa cat ggt      532
Asp Leu Tyr Ser Thr Ser Leu Ala Phe Arg Leu Leu Arg Glu His Gly
        155                 160                 165
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ttt caa gtc gca caa gag gta ttc gat agt ttc aag aac gag gag ggt      580
Phe Gln Val Ala Gln Glu Val Phe Asp Ser Phe Lys Asn Glu Glu Gly
    170                 175                 180

gag ttc aaa gaa agc ctt agc gac gac acc aga gga ttg ttg caa ctg      628
Glu Phe Lys Glu Ser Leu Ser Asp Asp Thr Arg Gly Leu Leu Gln Leu
185                 190                 195                 200

tat gaa gct tcc ttt ctg ttg acg gaa ggc gaa acc acg ctc gag tca      676
Tyr Glu Ala Ser Phe Leu Leu Thr Glu Gly Glu Thr Thr Leu Glu Ser
                205                 210                 215

gcg agg gaa ttc gcc acc aaa ttt ttg gag gaa aaa gtg aac gag ggt      724
Ala Arg Glu Phe Ala Thr Lys Phe Leu Glu Glu Lys Val Asn Glu Gly
            220                 225                 230

ggt gtt gat ggc gac ctt tta aca aga atc gca tat tct ttg gac atc      772
Gly Val Asp Gly Asp Leu Leu Thr Arg Ile Ala Tyr Ser Leu Asp Ile
        235                 240                 245

cct ctt cat tgg agg att aaa agg cca aat gca cct gtg tgg atc gaa      820
Pro Leu His Trp Arg Ile Lys Arg Pro Asn Ala Pro Val Trp Ile Glu
    250                 255                 260

tgg tat agg aag agg ccc gac atg aat cca gta gtg ttg gag ctt gcc      868
Trp Tyr Arg Lys Arg Pro Asp Met Asn Pro Val Val Leu Glu Leu Ala
265                 270                 275                 280

ata ctc gac tta aat att gtt caa gca caa ttt caa gaa gag ctc aaa      916
Ile Leu Asp Leu Asn Ile Val Gln Ala Gln Phe Gln Glu Glu Leu Lys
                285                 290                 295

gaa tcc ttc agg tgg tgg aga aat act ggg ttt gtt gag aag ctg ccc      964
Glu Ser Phe Arg Trp Trp Arg Asn Thr Gly Phe Val Glu Lys Leu Pro
            300                 305                 310

ttc gca agg gat aga ctg gtg gaa tgc tac ttt tgg aat act ggg atc     1012
Phe Ala Arg Asp Arg Leu Val Glu Cys Tyr Phe Trp Asn Thr Gly Ile
        315                 320                 325

atc gag cca cgt cag cat gca agt gca agg ata atg atg ggc aaa gtc     1060
Ile Glu Pro Arg Gln His Ala Ser Ala Arg Ile Met Met Gly Lys Val
    330                 335                 340

aac gct ctg att acg gtg atc gat gat att tat gat gtc tat ggc acc     1108
Asn Ala Leu Ile Thr Val Ile Asp Asp Ile Tyr Asp Val Tyr Gly Thr
345                 350                 355                 360

tta gaa gaa ctc gaa caa ttc act gac ctc att cga aga tgg gat ata     1156
Leu Glu Glu Leu Glu Gln Phe Thr Asp Leu Ile Arg Arg Trp Asp Ile
                365                 370                 375

aac tca atc gac caa ctt ccc gat tac atg caa ctg tgc ttt ctt gca     1204
Asn Ser Ile Asp Gln Leu Pro Asp Tyr Met Gln Leu Cys Phe Leu Ala
            380                 385                 390

ctc aac aac ttc gtc gat gat aca tcg tac gat gtt atg aag gag aaa     1252
Leu Asn Asn Phe Val Asp Asp Thr Ser Tyr Asp Val Met Lys Glu Lys
        395                 400                 405

ggc gtc aac gtt ata ccc tac ctg cgg caa tcg tgg gtt gat ttg gcg     1300
Gly Val Asn Val Ile Pro Tyr Leu Arg Gln Ser Trp Val Asp Leu Ala
    410                 415                 420

gat aag tat atg gta gag gca cgg tgg ttc tac ggc ggg cac aaa cca     1348
Asp Lys Tyr Met Val Glu Ala Arg Trp Phe Tyr Gly Gly His Lys Pro
425                 430                 435                 440

agt ttg gaa gag tat ttg gag aac tca tgg cag tcg ata agt ggg ccc     1396
Ser Leu Glu Glu Tyr Leu Glu Asn Ser Trp Gln Ser Ile Ser Gly Pro
                445                 450                 455

tgt atg tta acg cac ata ttc ttc cga gta aca gat tcg ttc aca aag     1444
Cys Met Leu Thr His Ile Phe Phe Arg Val Thr Asp Ser Phe Thr Lys
            460                 465                 470

gag acc gtc gac agt ttg tac aaa tac cac gat tta gtt cgt tgg tca     1492
Glu Thr Val Asp Ser Leu Tyr Lys Tyr His Asp Leu Val Arg Trp Ser
        475                 480                 485
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tcc ttc gtt ctg cgg ctt gct gat gat ttg gga acc tcg gtg gaa gag     1540
Ser Phe Val Leu Arg Leu Ala Asp Asp Leu Gly Thr Ser Val Glu Glu
    490                 495                 500

gtg agc aga ggg gat gtg ccg aaa tca ctt cag tgc tac atg agt gac     1588
Val Ser Arg Gly Asp Val Pro Lys Ser Leu Gln Cys Tyr Met Ser Asp
505                 510                 515                 520

tac aat gca tcg gag gcg gag gcg cgg aag cac gtg aaa tgg ctg ata     1636
Tyr Asn Ala Ser Glu Ala Glu Ala Arg Lys His Val Lys Trp Leu Ile
                525                 530                 535

gcg gag gtg tgg aag aag atg aat gcg gag agg gtg tcg aag gat tct     1684
Ala Glu Val Trp Lys Lys Met Asn Ala Glu Arg Val Ser Lys Asp Ser
            540                 545                 550

cca ttc ggc aaa gat ttt ata gga tgt gca gtt gat tta gga agg atg     1732
Pro Phe Gly Lys Asp Phe Ile Gly Cys Ala Val Asp Leu Gly Arg Met
        555                 560                 565

gcg cag ttg atg tac cat aat gga gat ggg cac ggc aca caa cac cct     1780
Ala Gln Leu Met Tyr His Asn Gly Asp Gly His Gly Thr Gln His Pro
    570                 575                 580

att ata cat caa caa atg acc aga acc tta ttc gag ccc ttt gca tga     1828
Ile Ile His Gln Gln Met Thr Arg Thr Leu Phe Glu Pro Phe Ala
585                 590                 595

gagatgatga cgagccatcg tttacttact taaattctac caaagttttt cgaaggcata   1888

gttcgtaatt tttcaagcac caataaataa ggagaatcgg ctcaaacaaa cgtggcattt   1948

gccaccacgt gagcacaagg gagagtctgt cgtcgtttat ggatgaacta ttcaatttttt   2008

atgcatgtaa taattaagtt caagttcaag agccttctgc atatttaact atgtatttga   2068

atttatcgag tgtgattttc tgtctttggc aacatatatt tttgtcatat gtggcatctt   2128

attatgatat catacagtgt ttatggatga tatgatacta tc                     2170


<210> SEQ ID NO 22
<211> LENGTH: 599
<212> TYPE: PRT
<213> ORGANISM: Mentha spicata

<400> SEQUENCE: 22

Met Ala Leu Lys Val Leu Ser Val Ala Thr Gln Met Ala Ile Pro Ser
 1               5                  10                  15

Asn Leu Thr Thr Cys Leu Gln Pro Ser His Phe Lys Ser Ser Pro Lys
            20                  25                  30

Leu Leu Ser Ser Thr Asn Ser Ser Ser Arg Ser Arg Leu Arg Val Tyr
        35                  40                  45

Cys Ser Ser Ser Gln Leu Thr Thr Glu Arg Arg Ser Gly Asn Tyr Asn
    50                  55                  60

Pro Ser Arg Trp Asp Val Asn Phe Ile Gln Ser Leu Leu Ser Asp Tyr
65                  70                  75                  80

Lys Glu Asp Lys His Val Ile Arg Ala Ser Glu Leu Val Thr Leu Val
                85                  90                  95

Lys Met Glu Leu Glu Lys Glu Thr Asp Gln Ile Arg Gln Leu Glu Leu
            100                 105                 110

Ile Asp Asp Leu Gln Arg Met Gly Leu Ser Asp His Phe Gln Asn Glu
        115                 120                 125

Phe Lys Glu Ile Leu Ser Ser Ile Tyr Leu Asp His His Tyr Tyr Lys
    130                 135                 140

Asn Pro Phe Pro Lys Glu Glu Arg Asp Leu Tyr Ser Thr Ser Leu Ala
145                 150                 155                 160
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Phe Arg Leu Leu Arg Glu His Gly Phe Gln Val Ala Gln Glu Val Phe
                165                 170                 175

Asp Ser Phe Lys Asn Glu Glu Gly Glu Phe Lys Glu Ser Leu Ser Asp
            180                 185                 190

Asp Thr Arg Gly Leu Leu Gln Leu Tyr Glu Ala Ser Phe Leu Leu Thr
        195                 200                 205

Glu Gly Glu Thr Thr Leu Glu Ser Ala Arg Glu Phe Ala Thr Lys Phe
    210                 215                 220

Leu Glu Glu Lys Val Asn Glu Gly Gly Val Asp Gly Asp Leu Leu Thr
225                 230                 235                 240

Arg Ile Ala Tyr Ser Leu Asp Ile Pro Leu His Trp Arg Ile Lys Arg
                245                 250                 255

Pro Asn Ala Pro Val Trp Ile Glu Trp Tyr Arg Lys Arg Pro Asp Met
            260                 265                 270

Asn Pro Val Val Leu Glu Leu Ala Ile Leu Asp Leu Asn Ile Val Gln
        275                 280                 285

Ala Gln Phe Gln Glu Glu Leu Lys Glu Ser Phe Arg Trp Trp Arg Asn
    290                 295                 300

Thr Gly Phe Val Glu Lys Leu Pro Phe Ala Arg Asp Arg Leu Val Glu
305                 310                 315                 320

Cys Tyr Phe Trp Asn Thr Gly Ile Ile Glu Pro Arg Gln His Ala Ser
                325                 330                 335

Ala Arg Ile Met Met Gly Lys Val Asn Ala Leu Ile Thr Val Ile Asp
            340                 345                 350

Asp Ile Tyr Asp Val Tyr Gly Thr Leu Glu Glu Leu Glu Gln Phe Thr
        355                 360                 365

Asp Leu Ile Arg Arg Trp Asp Ile Asn Ser Ile Asp Gln Leu Pro Asp
    370                 375                 380

Tyr Met Gln Leu Cys Phe Leu Ala Leu Asn Asn Phe Val Asp Asp Thr
385                 390                 395                 400

Ser Tyr Asp Val Met Lys Glu Lys Gly Val Asn Val Ile Pro Tyr Leu
                405                 410                 415

Arg Gln Ser Trp Val Asp Leu Ala Asp Lys Tyr Met Val Glu Ala Arg
            420                 425                 430

Trp Phe Tyr Gly Gly His Lys Pro Ser Leu Glu Glu Tyr Leu Glu Asn
        435                 440                 445

Ser Trp Gln Ser Ile Ser Gly Pro Cys Met Leu Thr His Ile Phe Phe
    450                 455                 460

Arg Val Thr Asp Ser Phe Thr Lys Glu Thr Val Asp Ser Leu Tyr Lys
465                 470                 475                 480

Tyr His Asp Leu Val Arg Trp Ser Ser Phe Val Leu Arg Leu Ala Asp
                485                 490                 495

Asp Leu Gly Thr Ser Val Glu Glu Val Ser Arg Gly Asp Val Pro Lys
            500                 505                 510

Ser Leu Gln Cys Tyr Met Ser Asp Tyr Asn Ala Ser Glu Ala Glu Ala
        515                 520                 525

Arg Lys His Val Lys Trp Leu Ile Ala Glu Val Trp Lys Lys Met Asn
    530                 535                 540

Ala Glu Arg Val Ser Lys Asp Ser Pro Phe Gly Lys Asp Phe Ile Gly
545                 550                 555                 560

Cys Ala Val Asp Leu Gly Arg Met Ala Gln Leu Met Tyr His Asn Gly
                565                 570                 575
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Asp Gly His Gly Thr Gln His Pro Ile Ile His Gln Gln Met Thr Arg
            580                 585                 590

Thr Leu Phe Glu Pro Phe Ala
        595
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<210> SEQ ID NO 23
<211> LENGTH: 1967
<212> TYPE: DNA
<213> ORGANISM: Salvia officinalis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (13)...(1785)
<223> OTHER INFORMATION: 1,8-cineole synthase

<400> SEQUENCE: 23

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gatcaccaca ag atg tcg agt ctt ata atg caa gtt gtt att cct aag cca     51
              Met Ser Ser Leu Ile Met Gln Val Val Ile Pro Lys Pro
               1               5                  10

gcc aaa att ttt cac aat aac tta ttc agc gtg att tca aaa cga cat       99
Ala Lys Ile Phe His Asn Asn Leu Phe Ser Val Ile Ser Lys Arg His
     15                  20                  25

cgt ttc agt act aca atc acc act cgt ggt ggc agg tgg gca cat tgc      147
Arg Phe Ser Thr Thr Ile Thr Thr Arg Gly Gly Arg Trp Ala His Cys
 30                  35                  40                  45

tca cta caa atg ggt aat gag atc caa act gga cga cga act gga ggc      195
Ser Leu Gln Met Gly Asn Glu Ile Gln Thr Gly Arg Arg Thr Gly Gly
                 50                  55                  60

tac cag cct acc ctt tgg gat ttc agc acc att caa ttg ttc gac tct      243
Tyr Gln Pro Thr Leu Trp Asp Phe Ser Thr Ile Gln Leu Phe Asp Ser
             65                  70                  75

gag tat aag gaa gag aag cac ttg atg agg gcc gca ggt atg ata gcc      291
Glu Tyr Lys Glu Glu Lys His Leu Met Arg Ala Ala Gly Met Ile Ala
         80                  85                  90

caa gtg aat atg ttg ttg cag gaa gaa gta gat tcg att caa cgg ttg      339
Gln Val Asn Met Leu Leu Gln Glu Glu Val Asp Ser Ile Gln Arg Leu
     95                  100                 105

gag ttg att gat gac cta cga agg ctg ggt ata tct tgc cat ttt gac      387
Glu Leu Ile Asp Asp Leu Arg Arg Leu Gly Ile Ser Cys His Phe Asp
110                 115                 120                 125

cgc gag atc gtt gaa ata tta aac tca aaa tat tat acc aac aat gag      435
Arg Glu Ile Val Glu Ile Leu Asn Ser Lys Tyr Tyr Thr Asn Asn Glu
                130                 135                 140

ata gat gaa agt gat cta tac tca aca gcc ctt aga ttc aag ctc cta      483
Ile Asp Glu Ser Asp Leu Tyr Ser Thr Ala Leu Arg Phe Lys Leu Leu
            145                 150                 155

aga caa tac gat ttt agc gtc tct caa gag gta ttt gat tgt ttc aag      531
Arg Gln Tyr Asp Phe Ser Val Ser Gln Glu Val Phe Asp Cys Phe Lys
        160                 165                 170

aat gac aag ggt act gat ttc aag cca agc cta gtc gat gat act aga      579
Asn Asp Lys Gly Thr Asp Phe Lys Pro Ser Leu Val Asp Asp Thr Arg
    175                 180                 185

gga ttg tta caa ttg tac gaa gct tcg ttt tta tca gca caa ggc gaa      627
Gly Leu Leu Gln Leu Tyr Glu Ala Ser Phe Leu Ser Ala Gln Gly Glu
190                 195                 200                 205

gaa acc cta cat ctt gcc aga gat ttt gct act aaa ttt ctg cat aaa      675
Glu Thr Leu His Leu Ala Arg Asp Phe Ala Thr Lys Phe Leu His Lys
                210                 215                 220

aga gta cta gtt gat aaa gac att aat ctc tta tca tca att gaa cgt      723
Arg Val Leu Val Asp Lys Asp Ile Asn Leu Leu Ser Ser Ile Glu Arg
            225                 230                 235
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gcg ttg gag ttg cct act cat tgg agg gtt caa atg ccc aac gca aga      771
Ala Leu Glu Leu Pro Thr His Trp Arg Val Gln Met Pro Asn Ala Arg
        240                 245                 250

tcc ttc att gat gct tat aag agg aga ccc gac atg aat ccg act gtg      819
Ser Phe Ile Asp Ala Tyr Lys Arg Arg Pro Asp Met Asn Pro Thr Val
    255                 260                 265

cta gaa cta gct aaa ttg gac ttc aat atg gtt caa gca caa ttt caa      867
Leu Glu Leu Ala Lys Leu Asp Phe Asn Met Val Gln Ala Gln Phe Gln
270                 275                 280                 285

caa gag ctc aaa gag gcc tct agg tgg tgg aat agt acg ggt ctt gtc      915
Gln Glu Leu Lys Glu Ala Ser Arg Trp Trp Asn Ser Thr Gly Leu Val
                290                 295                 300

cac gag ctt ccc ttt gtg aga gat agg att gtg gaa tgc tac tac tgg      963
His Glu Leu Pro Phe Val Arg Asp Arg Ile Val Glu Cys Tyr Tyr Trp
            305                 310                 315

acg aca gga gtg gtt gag cgt cgt gaa cat gga tac gag agg ata atg     1011
Thr Thr Gly Val Val Glu Arg Arg Glu His Gly Tyr Glu Arg Ile Met
        320                 325                 330

ctc acc aaa ata aat gct ctt gtt aca aca ata gac gat gtc ttt gat     1059
Leu Thr Lys Ile Asn Ala Leu Val Thr Thr Ile Asp Asp Val Phe Asp
    335                 340                 345

att tat ggt acg ctt gaa gag cta caa cta ttc aca act gct att caa     1107
Ile Tyr Gly Thr Leu Glu Glu Leu Gln Leu Phe Thr Thr Ala Ile Gln
350                 355                 360                 365

aga tgg gat att gaa tca atg aag caa ctc cct cct tac atg caa ata     1155
Arg Trp Asp Ile Glu Ser Met Lys Gln Leu Pro Pro Tyr Met Gln Ile
                370                 375                 380

tgt tat ctt gct ctc ttc aac ttt gtg aat gag atg gct tat gat act     1203
Cys Tyr Leu Ala Leu Phe Asn Phe Val Asn Glu Met Ala Tyr Asp Thr
            385                 390                 395

ctt agg gat aaa ggt ttc aac tcc acc cca tat cta cga aaa gcg tgg     1251
Leu Arg Asp Lys Gly Phe Asn Ser Thr Pro Tyr Leu Arg Lys Ala Trp
        400                 405                 410

gtt gat ttg gtt gag tca tat cta ata gag gca aag tgg tac tac atg     1299
Val Asp Leu Val Glu Ser Tyr Leu Ile Glu Ala Lys Trp Tyr Tyr Met
    415                 420                 425

gga cat aaa cct agt ttg gaa gaa tat atg aag aat agt tgg ata tca     1347
Gly His Lys Pro Ser Leu Glu Glu Tyr Met Lys Asn Ser Trp Ile Ser
430                 435                 440                 445

atc gga ggc atc ccc att cta tct cat cta ttt ttc cgg cta aca gat     1395
Ile Gly Gly Ile Pro Ile Leu Ser His Leu Phe Phe Arg Leu Thr Asp
                450                 455                 460

tcg att gag gaa gag gat gct gag agt atg cat aaa tac cat gat att     1443
Ser Ile Glu Glu Glu Asp Ala Glu Ser Met His Lys Tyr His Asp Ile
            465                 470                 475

gtt cgt gca tcg tgt act att cta agg ctt gct gat gat atg gga aca     1491
Val Arg Ala Ser Cys Thr Ile Leu Arg Leu Ala Asp Asp Met Gly Thr
        480                 485                 490

tcg ctg gat gag gtg gag aga ggc gac gtg ccc aaa tca gtt cag tgc     1539
Ser Leu Asp Glu Val Glu Arg Gly Asp Val Pro Lys Ser Val Gln Cys
    495                 500                 505

tac atg aat gag aag aat gct tcg gaa gaa gaa gcg cga gag cat gtg     1587
Tyr Met Asn Glu Lys Asn Ala Ser Glu Glu Glu Ala Arg Glu His Val
510                 515                 520                 525

cga tca ctc ata gac caa aca tgg aag atg atg aac aag gaa atg atg     1635
Arg Ser Leu Ile Asp Gln Thr Trp Lys Met Met Asn Lys Glu Met Met
                530                 535                 540

acg tca tca ttt tcc aaa tat ttt gta caa gtt tct gct aat ctt gca     1683
Thr Ser Ser Phe Ser Lys Tyr Phe Val Gln Val Ser Ala Asn Leu Ala
            545                 550                 555
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aga atg gcg caa tgg ata tac cag cat gaa tct gat gga ttt ggc atg     1731
Arg Met Ala Gln Trp Ile Tyr Gln His Glu Ser Asp Gly Phe Gly Met
        560                 565                 570

caa cat tca ttg gtg aac aaa atg ctc aga ggg ttg ttg ttc gac cgc     1779
Gln His Ser Leu Val Asn Lys Met Leu Arg Gly Leu Leu Phe Asp Arg
    575                 580                 585

tat gag taa ctaatcttcg cccgggttcc aaatgaatca atctgttgtg             1828
Tyr Glu
590

ttgctgttcc acctgatatc aataataatt agacaaatgt ttctgtacgg gtggcccaac   1888

cgtcaggccc atttcgctca tgttcataat aaataataaa actgttaatc aataacaaaa   1948

aaaaaaaaaa aaaaaaaaa                                               1967


<210> SEQ ID NO 24
<211> LENGTH: 591
<212> TYPE: PRT
<213> ORGANISM: Salvia officinalis

<400> SEQUENCE: 24

Met Ser Ser Leu Ile Met Gln Val Val Ile Pro Lys Pro Ala Lys Ile
 1               5                  10                  15

Phe His Asn Asn Leu Phe Ser Val Ile Ser Lys Arg His Arg Phe Ser
            20                  25                  30

Thr Thr Ile Thr Thr Arg Gly Gly Arg Trp Ala His Cys Ser Leu Gln
        35                  40                  45

Met Gly Asn Glu Ile Gln Thr Gly Arg Arg Thr Gly Gly Tyr Gln Pro
    50                  55                  60

Thr Leu Trp Asp Phe Ser Thr Ile Gln Leu Phe Asp Ser Glu Tyr Lys
65                  70                  75                  80

Glu Glu Lys His Leu Met Arg Ala Ala Gly Met Ile Ala Gln Val Asn
                85                  90                  95

Met Leu Leu Gln Glu Glu Val Asp Ser Ile Gln Arg Leu Glu Leu Ile
            100                 105                 110

Asp Asp Leu Arg Arg Leu Gly Ile Ser Cys His Phe Asp Arg Glu Ile
        115                 120                 125

Val Glu Ile Leu Asn Ser Lys Tyr Tyr Thr Asn Asn Glu Ile Asp Glu
    130                 135                 140

Ser Asp Leu Tyr Ser Thr Ala Leu Arg Phe Lys Leu Leu Arg Gln Tyr
145                 150                 155                 160

Asp Phe Ser Val Ser Gln Glu Val Phe Asp Cys Phe Lys Asn Asp Lys
                165                 170                 175

Gly Thr Asp Phe Lys Pro Ser Leu Val Asp Asp Thr Arg Gly Leu Leu
            180                 185                 190

Gln Leu Tyr Glu Ala Ser Phe Leu Ser Ala Gln Gly Glu Glu Thr Leu
        195                 200                 205

His Leu Ala Arg Asp Phe Ala Thr Lys Phe Leu His Lys Arg Val Leu
    210                 215                 220

Val Asp Lys Asp Ile Asn Leu Leu Ser Ser Ile Glu Arg Ala Leu Glu
225                 230                 235                 240

Leu Pro Thr His Trp Arg Val Gln Met Pro Asn Ala Arg Ser Phe Ile
                245                 250                 255

Asp Ala Tyr Lys Arg Arg Pro Asp Met Asn Pro Thr Val Leu Glu Leu
            260                 265                 270

Ala Lys Leu Asp Phe Asn Met Val Gln Ala Gln Phe Gln Gln Glu Leu
        275                 280                 285
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Lys Glu Ala Ser Arg Trp Trp Asn Ser Thr Gly Leu Val His Glu Leu
    290                 295                 300

Pro Phe Val Arg Asp Arg Ile Val Glu Cys Tyr Tyr Trp Thr Thr Gly
305                 310                 315                 320

Val Val Glu Arg Arg Glu His Gly Tyr Glu Arg Ile Met Leu Thr Lys
                325                 330                 335

Ile Asn Ala Leu Val Thr Thr Ile Asp Asp Val Phe Asp Ile Tyr Gly
            340                 345                 350

Thr Leu Glu Glu Leu Gln Leu Phe Thr Thr Ala Ile Gln Arg Trp Asp
        355                 360                 365

Ile Glu Ser Met Lys Gln Leu Pro Pro Tyr Met Gln Ile Cys Tyr Leu
    370                 375                 380

Ala Leu Phe Asn Phe Val Asn Glu Met Ala Tyr Asp Thr Leu Arg Asp
385                 390                 395                 400

Lys Gly Phe Asn Ser Thr Pro Tyr Leu Arg Lys Ala Trp Val Asp Leu
                405                 410                 415

Val Glu Ser Tyr Leu Ile Glu Ala Lys Trp Tyr Tyr Met Gly His Lys
            420                 425                 430

Pro Ser Leu Glu Glu Tyr Met Lys Asn Ser Trp Ile Ser Ile Gly Gly
        435                 440                 445

Ile Pro Ile Leu Ser His Leu Phe Phe Arg Leu Thr Asp Ser Ile Glu
    450                 455                 460

Glu Glu Asp Ala Glu Ser Met His Lys Tyr His Asp Ile Val Arg Ala
465                 470                 475                 480

Ser Cys Thr Ile Leu Arg Leu Ala Asp Asp Met Gly Thr Ser Leu Asp
                485                 490                 495

Glu Val Glu Arg Gly Asp Val Pro Lys Ser Val Gln Cys Tyr Met Asn
            500                 505                 510

Glu Lys Asn Ala Ser Glu Glu Glu Ala Arg Glu His Val Arg Ser Leu
        515                 520                 525

Ile Asp Gln Thr Trp Lys Met Met Asn Lys Glu Met Met Thr Ser Ser
    530                 535                 540

Phe Ser Lys Tyr Phe Val Gln Val Ser Ala Asn Leu Ala Arg Met Ala
545                 550                 555                 560

Gln Trp Ile Tyr Gln His Glu Ser Asp Gly Phe Gly Met Gln His Ser
                565                 570                 575

Leu Val Asn Lys Met Leu Arg Gly Leu Leu Phe Asp Arg Tyr Glu
            580                 585                 590


<210> SEQ ID NO 25
<211> LENGTH: 2024
<212> TYPE: DNA
<213> ORGANISM: Salvia officinalis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (11)...(1804)
<223> OTHER INFORMATION: (+)-bornyl diphosphate synthase

<400> SEQUENCE: 25

gatcacaaaa atg tct atc att agc atg aac gta tcg atc ctt agc aag       49
           Met Ser Ile Ile Ser Met Asn Val Ser Ile Leu Ser Lys
             1               5                   10

cca cta aat tgc ctc cac aac ttg gag agg aga cct tca aaa gcc ttg       97
Pro Leu Asn Cys Leu His Asn Leu Glu Arg Arg Pro Ser Lys Ala Leu
     15                  20                  25
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ctt gtc cct tgc act gca ccc acc gct cgc ctc cgg gca tct tgc tcc      145
Leu Val Pro Cys Thr Ala Pro Thr Ala Arg Leu Arg Ala Ser Cys Ser
 30                  35                  40                  45

tca aaa cta caa gaa gct cat caa atc cga cga tct gga aac tac caa      193
Ser Lys Leu Gln Glu Ala His Gln Ile Arg Arg Ser Gly Asn Tyr Gln
                 50                  55                  60

cct gcc ctt tgg gat tcc aat tac att cag tct ctc aat act cca tat      241
Pro Ala Leu Trp Asp Ser Asn Tyr Ile Gln Ser Leu Asn Thr Pro Tyr
             65                  70                  75

acg gag gag agg cac ttg gat aga aaa gca gag ctg att gtg caa gtg      289
Thr Glu Glu Arg His Leu Asp Arg Lys Ala Glu Leu Ile Val Gln Val
         80                  85                  90

agg ata ctg cta aag gaa aaa atg gag cct gtt caa caa ttg gag ttg      337
Arg Ile Leu Leu Lys Glu Lys Met Glu Pro Val Gln Gln Leu Glu Leu
     95                 100                 105

att cat gac ttg aaa tat ttg ggg ctc tcg gat ttt ttt caa gat gag      385
Ile His Asp Leu Lys Tyr Leu Gly Leu Ser Asp Phe Phe Gln Asp Glu
110                 115                 120                 125

att aag gag atc tta ggt gtt ata tac aat gag cac aaa tgc ttt cac      433
Ile Lys Glu Ile Leu Gly Val Ile Tyr Asn Glu His Lys Cys Phe His
                130                 135                 140

aat aat gaa gta gag aaa atg gat ttg tat ttc aca gct ctt gga ttc      481
Asn Asn Glu Val Glu Lys Met Asp Leu Tyr Phe Thr Ala Leu Gly Phe
            145                 150                 155

aga ctc ctc aga caa cat ggt ttt aat att tcc caa gat gta ttt aat      529
Arg Leu Leu Arg Gln His Gly Phe Asn Ile Ser Gln Asp Val Phe Asn
        160                 165                 170

tgt ttc aag aac gag aag ggt att gat ttc aag gca agc ctt gct caa      577
Cys Phe Lys Asn Glu Lys Gly Ile Asp Phe Lys Ala Ser Leu Ala Gln
    175                 180                 185

gat acg aag gga atg tta caa ctg tat gaa gcg tct ttc ctt ttg aga      625
Asp Thr Lys Gly Met Leu Gln Leu Tyr Glu Ala Ser Phe Leu Leu Arg
190                 195                 200                 205

aaa ggt gaa gat aca ttg gag ctt gca aga gaa ttt gcc aca aaa tgt      673
Lys Gly Glu Asp Thr Leu Glu Leu Ala Arg Glu Phe Ala Thr Lys Cys
                210                 215                 220

ctg cag aaa aaa ctt gat gaa ggt ggt aat gaa att gat gag aat cta      721
Leu Gln Lys Lys Leu Asp Glu Gly Gly Asn Glu Ile Asp Glu Asn Leu
            225                 230                 235

tta ttg tgg att cgc cac tct ttg gat ctt cct ctc cac tgg agg att      769
Leu Leu Trp Ile Arg His Ser Leu Asp Leu Pro Leu His Trp Arg Ile
        240                 245                 250

caa agt gta gag gca aga tgg ttc ata gat gct tat gcg aga agg cca      817
Gln Ser Val Glu Ala Arg Trp Phe Ile Asp Ala Tyr Ala Arg Arg Pro
    255                 260                 265

gac atg aat cca ctt att ttc gag ctt gcc aaa ctc aac ttc aat att      865
Asp Met Asn Pro Leu Ile Phe Glu Leu Ala Lys Leu Asn Phe Asn Ile
270                 275                 280                 285

att caa gca aca cat caa caa gaa ctg aaa gat ctc tcg agg tgg tgg      913
Ile Gln Ala Thr His Gln Gln Glu Leu Lys Asp Leu Ser Arg Trp Trp
                290                 295                 300

agt aga tta tgc ttc cct gaa aag ctc cca ttt gtg agg gat agg ctc      961
Ser Arg Leu Cys Phe Pro Glu Lys Leu Pro Phe Val Arg Asp Arg Leu
            305                 310                 315

gtt gaa tcc ttc ttt tgg gcg gtt ggg atg ttt gag cca cat caa cat     1009
Val Glu Ser Phe Phe Trp Ala Val Gly Met Phe Glu Pro His Gln His
        320                 325                 330

gga tat cag aga aaa atg gcc gcc aca att att gtt tta gca aca gtt     1057
Gly Tyr Gln Arg Lys Met Ala Ala Thr Ile Ile Val Leu Ala Thr Val
    335                 340                 345
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ata gat gat att tac gat gtg tat ggt aca cta gat gaa cta gaa cta     1105
Ile Asp Asp Ile Tyr Asp Val Tyr Gly Thr Leu Asp Glu Leu Glu Leu
350                 355                 360                 365

ttt aca gac acg ttt aag aga tgg gat act gaa tca ata acc cga ctt     1153
Phe Thr Asp Thr Phe Lys Arg Trp Asp Thr Glu Ser Ile Thr Arg Leu
                370                 375                 380

cct tat tac atg caa tta tgt tat tgg ggt gtc cac aac tat att tcc     1201
Pro Tyr Tyr Met Gln Leu Cys Tyr Trp Gly Val His Asn Tyr Ile Ser
            385                 390                 395

gat gca gca tat gat att ctc aaa gaa cat ggt ttc ttt tgt ctc caa     1249
Asp Ala Ala Tyr Asp Ile Leu Lys Glu His Gly Phe Phe Cys Leu Gln
        400                 405                 410

tat ctc cgg aaa tcg gtg gta gat ttg gtt gaa gca tat ttt cac gag     1297
Tyr Leu Arg Lys Ser Val Val Asp Leu Val Glu Ala Tyr Phe His Glu
    415                 420                 425

gca aag tgg tac cac agc ggt tat aca cca agc ctg gat gaa tat ctc     1345
Ala Lys Trp Tyr His Ser Gly Tyr Thr Pro Ser Leu Asp Glu Tyr Leu
430                 435                 440                 445

aac atc gcc aag att tca gtg gcg tct cct gca ata ata tcc cca acc     1393
Asn Ile Ala Lys Ile Ser Val Ala Ser Pro Ala Ile Ile Ser Pro Thr
                450                 455                 460

tat ttc aca ttc gca aac gcg tct cat gac aca gca gtc atc gac agc     1441
Tyr Phe Thr Phe Ala Asn Ala Ser His Asp Thr Ala Val Ile Asp Ser
            465                 470                 475

ttg tac caa tat cat gac ata ctt tgc cta gca gga att att ttg agg     1489
Leu Tyr Gln Tyr His Asp Ile Leu Cys Leu Ala Gly Ile Ile Leu Arg
        480                 485                 490

ctt ccc gac gat ctt ggg aca tca tat ttt gag ctg gcg aga ggc gac     1537
Leu Pro Asp Asp Leu Gly Thr Ser Tyr Phe Glu Leu Ala Arg Gly Asp
    495                 500                 505

gtg ccg aaa aca atc cag tgc tac atg aag gaa aca aat gct agt gag     1585
Val Pro Lys Thr Ile Gln Cys Tyr Met Lys Glu Thr Asn Ala Ser Glu
510                 515                 520                 525

gag gag gcg gtg gag cac gtg aag ttt ctg ata agg gag gcg tgg aag     1633
Glu Glu Ala Val Glu His Val Lys Phe Leu Ile Arg Glu Ala Trp Lys
                530                 535                 540

gat atg aac acg gcc ata gca gcc ggt tat ccg ttt ccg gat ggt atg     1681
Asp Met Asn Thr Ala Ile Ala Ala Gly Tyr Pro Phe Pro Asp Gly Met
            545                 550                 555

gtg gcg ggc gca gct aat att ggg cgc gtg gcg cag ttt att tat ctc     1729
Val Ala Gly Ala Ala Asn Ile Gly Arg Val Ala Gln Phe Ile Tyr Leu
        560                 565                 570

cac gga gat ggg ttt ggc gtg caa cac tcg aaa acg tac gag cat atc     1777
His Gly Asp Gly Phe Gly Val Gln His Ser Lys Thr Tyr Glu His Ile
    575                 580                 585

gcc ggc cta ctg ttc gag cct tat gca tga acaaatggga gactgcttga       1827
Ala Gly Leu Leu Phe Glu Pro Tyr Ala
590                 595

tatatattaa tttggcacac caataattgc atgttatata tgttggaaaa taagtgtctg   1887

gttgagatgt catgtggtgt attatctaaa taattcaagg ttgccttgtt tatgtagccg   1947

gtggtgcaac tacctcccat tcaaatcaat taaatctaaa cagtcgagtc aagctcgagc   2007

tcgaggaaaa aaaaaaa                                                  2024


<210> SEQ ID NO 26
<211> LENGTH: 598
<212> TYPE: PRT
<213> ORGANISM: Salvia officinalis
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<400> SEQUENCE: 26

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Met Ser Ile Ile Ser Met Asn Val Ser Ile Leu Ser Lys Pro Leu Asn
 1               5                  10                  15

Cys Leu His Asn Leu Glu Arg Arg Pro Ser Lys Ala Leu Leu Val Pro
            20                  25                  30

Cys Thr Ala Pro Thr Ala Arg Leu Arg Ala Ser Cys Ser Ser Lys Leu
        35                  40                  45

Gln Glu Ala His Gln Ile Arg Arg Ser Gly Asn Tyr Gln Pro Ala Leu
    50                  55                  60

Trp Asp Ser Asn Tyr Ile Gln Ser Leu Asn Thr Pro Tyr Thr Glu Glu
65                  70                  75                  80

Arg His Leu Asp Arg Lys Ala Glu Leu Ile Val Gln Val Arg Ile Leu
                85                  90                  95

Leu Lys Glu Lys Met Glu Pro Val Gln Gln Leu Glu Leu Ile His Asp
            100                 105                 110

Leu Lys Tyr Leu Gly Leu Ser Asp Phe Phe Gln Asp Glu Ile Lys Glu
        115                 120                 125

Ile Leu Gly Val Ile Tyr Asn Glu His Lys Cys Phe His Asn Asn Glu
    130                 135                 140

Val Glu Lys Met Asp Leu Tyr Phe Thr Ala Leu Gly Phe Arg Leu Leu
145                 150                 155                 160

Arg Gln His Gly Phe Asn Ile Ser Gln Asp Val Phe Asn Cys Phe Lys
                165                 170                 175

Asn Glu Lys Gly Ile Asp Phe Lys Ala Ser Leu Ala Gln Asp Thr Lys
            180                 185                 190

Gly Met Leu Gln Leu Tyr Glu Ala Ser Phe Leu Leu Arg Lys Gly Glu
        195                 200                 205

Asp Thr Leu Glu Leu Ala Arg Glu Phe Ala Thr Lys Cys Leu Gln Lys
    210                 215                 220

Lys Leu Asp Glu Gly Gly Asn Glu Ile Asp Glu Asn Leu Leu Leu Trp
225                 230                 235                 240

Ile Arg His Ser Leu Asp Leu Pro Leu His Trp Arg Ile Gln Ser Val
                245                 250                 255

Glu Ala Arg Trp Phe Ile Asp Ala Tyr Ala Arg Arg Pro Asp Met Asn
            260                 265                 270

Pro Leu Ile Phe Glu Leu Ala Lys Leu Asn Phe Asn Ile Ile Gln Ala
        275                 280                 285

Thr His Gln Gln Glu Leu Lys Asp Leu Ser Arg Trp Trp Ser Arg Leu
    290                 295                 300

Cys Phe Pro Glu Lys Leu Pro Phe Val Arg Asp Arg Leu Val Glu Ser
305                 310                 315                 320

Phe Phe Trp Ala Val Gly Met Phe Glu Pro His Gln His Gly Tyr Gln
                325                 330                 335

Arg Lys Met Ala Ala Thr Ile Ile Val Leu Ala Thr Val Ile Asp Asp
            340                 345                 350

Ile Tyr Asp Val Tyr Gly Thr Leu Asp Glu Leu Glu Leu Phe Thr Asp
        355                 360                 365

Thr Phe Lys Arg Trp Asp Thr Glu Ser Ile Thr Arg Leu Pro Tyr Tyr
    370                 375                 380

Met Gln Leu Cys Tyr Trp Gly Val His Asn Tyr Ile Ser Asp Ala Ala
385                 390                 395                 400

Tyr Asp Ile Leu Lys Glu His Gly Phe Phe Cys Leu Gln Tyr Leu Arg
                405                 410                 415
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Lys Ser Val Val Asp Leu Val Glu Ala Tyr Phe His Glu Ala Lys Trp
            420                 425                 430

Tyr His Ser Gly Tyr Thr Pro Ser Leu Asp Glu Tyr Leu Asn Ile Ala
        435                 440                 445

Lys Ile Ser Val Ala Ser Pro Ala Ile Ile Ser Pro Thr Tyr Phe Thr
    450                 455                 460

Phe Ala Asn Ala Ser His Asp Thr Ala Val Ile Asp Ser Leu Tyr Gln
465                 470                 475                 480

Tyr His Asp Ile Leu Cys Leu Ala Gly Ile Ile Leu Arg Leu Pro Asp
                485                 490                 495

Asp Leu Gly Thr Ser Tyr Phe Glu Leu Ala Arg Gly Asp Val Pro Lys
            500                 505                 510

Thr Ile Gln Cys Tyr Met Lys Glu Thr Asn Ala Ser Glu Glu Glu Ala
        515                 520                 525

Val Glu His Val Lys Phe Leu Ile Arg Glu Ala Trp Lys Asp Met Asn
    530                 535                 540

Thr Ala Ile Ala Ala Gly Tyr Pro Phe Pro Asp Gly Met Val Ala Gly
545                 550                 555                 560

Ala Ala Asn Ile Gly Arg Val Ala Gln Phe Ile Tyr Leu His Gly Asp
                565                 570                 575

Gly Phe Gly Val Gln His Ser Lys Thr Tyr Glu His Ile Ala Gly Leu
            580                 585                 590

Leu Phe Glu Pro Tyr Ala
        595


<210> SEQ ID NO 27
<211> LENGTH: 1959
<212> TYPE: DNA
<213> ORGANISM: Mentha x piperita
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (71)...(1720)
<223> OTHER INFORMATION: (E)-B-farnesene synthase

<400> SEQUENCE: 27

aaactctgca atttcatata taacatcata aaatcagaga gagagacaga gagtttgttg     60

tagtgaaaaa atg gct aca aac ggc gtc gta att agt tgc tta agg gaa       109
           Met Ala Thr Asn Gly Val Val Ile Ser Cys Leu Arg Glu
             1               5                   10

gta agg cca cct atg acg aag cat gcg cca agc atg tgg act gat acc      157
Val Arg Pro Pro Met Thr Lys His Ala Pro Ser Met Trp Thr Asp Thr
     15                  20                  25

ttt tct aac ttt tct ctt gac gat aag gaa caa caa aag tgc tca gaa      205
Phe Ser Asn Phe Ser Leu Asp Asp Lys Glu Gln Gln Lys Cys Ser Glu
 30                  35                  40                  45

acc atc gaa gca ctt aag caa gaa gca aga ggc atg ctt atg gct gca      253
Thr Ile Glu Ala Leu Lys Gln Glu Ala Arg Gly Met Leu Met Ala Ala
                 50                  55                  60

acc act cct ctc caa caa atg aca cta atc gac act ctc gag cgt ttg      301
Thr Thr Pro Leu Gln Gln Met Thr Leu Ile Asp Thr Leu Glu Arg Leu
             65                  70                  75

gga ttg tct ttc cat ttt gag acg gag atc gaa tac aaa atc gaa cta      349
Gly Leu Ser Phe His Phe Glu Thr Glu Ile Glu Tyr Lys Ile Glu Leu
         80                  85                  90

atc aac gct gca gaa gac gac ggc ttt gat ttg ttc gct act gct ctt      397
Ile Asn Ala Ala Glu Asp Asp Gly Phe Asp Leu Phe Ala Thr Ala Leu
     95                  100                 105
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cgt ttc cgt ttg ctc aga caa cat caa cgc cac gtt tct tgt gat gtt      445
Arg Phe Arg Leu Leu Arg Gln His Gln Arg His Val Ser Cys Asp Val
110                 115                 120                 125

ttc gac aag ttc atc gac aaa gat ggc aag ttc gaa gaa tcc ctt agc      493
Phe Asp Lys Phe Ile Asp Lys Asp Gly Lys Phe Glu Glu Ser Leu Ser
                130                 135                 140

aat aat gtt gaa ggc cta tta agc ttg tat gaa gca gct cat gtt ggg      541
Asn Asn Val Glu Gly Leu Leu Ser Leu Tyr Glu Ala Ala His Val Gly
            145                 150                 155

ttt cgc gaa gaa aga ata tta caa gag gct gta aat ttt acg agg cat      589
Phe Arg Glu Glu Arg Ile Leu Gln Glu Ala Val Asn Phe Thr Arg His
        160                 165                 170

cac ttg gaa gga gca gag tta gat cag tct cca tta ttg att aga gag      637
His Leu Glu Gly Ala Glu Leu Asp Gln Ser Pro Leu Leu Ile Arg Glu
    175                 180                 185

aaa gtg aag cga gct ttg gag cac cct ctt cat agg gat ttc ccc att      685
Lys Val Lys Arg Ala Leu Glu His Pro Leu His Arg Asp Phe Pro Ile
190                 195                 200                 205

gtc tat gca cgc ctt ttc atc tcc att tac gaa aag gat gac tct aga      733
Val Tyr Ala Arg Leu Phe Ile Ser Ile Tyr Glu Lys Asp Asp Ser Arg
                210                 215                 220

gat gaa tta ctt ctc aag cta tcc aaa gtc aac ttc aaa ttc atg cag      781
Asp Glu Leu Leu Leu Lys Leu Ser Lys Val Asn Phe Lys Phe Met Gln
            225                 230                 235

aat ttg tat aag gaa gag ctc tcc caa ctc tcc agg tgg tgg aac aca      829
Asn Leu Tyr Lys Glu Glu Leu Ser Gln Leu Ser Arg Trp Trp Asn Thr
        240                 245                 250

tgg aat ctg aaa tca aaa tta cca tat gca aga gat cga gtc gtg gag      877
Trp Asn Leu Lys Ser Lys Leu Pro Tyr Ala Arg Asp Arg Val Val Glu
    255                 260                 265

gct tat gtt tgg gga gta ggt tac cat tac gaa ccc caa tac tca tat      925
Ala Tyr Val Trp Gly Val Gly Tyr His Tyr Glu Pro Gln Tyr Ser Tyr
270                 275                 280                 285

gtt cga atg gga ctt gcc aaa ggc gta cta att tgt gga atc atg gac      973
Val Arg Met Gly Leu Ala Lys Gly Val Leu Ile Cys Gly Ile Met Asp
                290                 295                 300

gat aca tat gat aat tat gct aca ctc aat gaa gct caa ctt ttt act     1021
Asp Thr Tyr Asp Asn Tyr Ala Thr Leu Asn Glu Ala Gln Leu Phe Thr
            305                 310                 315

caa gtc tta gac aag tgg gat aga gat gaa gct gaa cga ctc cca gaa     1069
Gln Val Leu Asp Lys Trp Asp Arg Asp Glu Ala Glu Arg Leu Pro Glu
        320                 325                 330

tac atg aaa atc gtt tat cga ttt att ttg agt ata tat gaa aat tat     1117
Tyr Met Lys Ile Val Tyr Arg Phe Ile Leu Ser Ile Tyr Glu Asn Tyr
    335                 340                 345

gaa cgt gat gca gcg aaa ctt gga aaa agc ttt gca gct cct tat ttt     1165
Glu Arg Asp Ala Ala Lys Leu Gly Lys Ser Phe Ala Ala Pro Tyr Phe
350                 355                 360                 365

aag gaa acc gtg aaa caa ctg gca agg gca ttt aat gag gag cag aag     1213
Lys Glu Thr Val Lys Gln Leu Ala Arg Ala Phe Asn Glu Glu Gln Lys
                370                 375                 380

tgg gtt atg gaa agg cag cta ccg tca ttc caa gac tac gta aag aat     1261
Trp Val Met Glu Arg Gln Leu Pro Ser Phe Gln Asp Tyr Val Lys Asn
            385                 390                 395

tca gag aaa acc agc tgc att tat acc atg ttt gct tct atc atc cca     1309
Ser Glu Lys Thr Ser Cys Ile Tyr Thr Met Phe Ala Ser Ile Ile Pro
        400                 405                 410

ggc ttg aaa tct gtt acc caa gaa acc att gat tgg atc aag agt gaa     1357
Gly Leu Lys Ser Val Thr Gln Glu Thr Ile Asp Trp Ile Lys Ser Glu
    415                 420                 425
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ccc acg ctc gca aca tcg acc gct atg atc ggt cgg tat tgg aat gac     1405
Pro Thr Leu Ala Thr Ser Thr Ala Met Ile Gly Arg Tyr Trp Asn Asp
430                 435                 440                 445

acc agc tct cag ctc cgt gaa agc aaa gga ggg gaa atg ctg act gcg     1453
Thr Ser Ser Gln Leu Arg Glu Ser Lys Gly Gly Glu Met Leu Thr Ala
                450                 455                 460

ttg gat ttc cac atg aaa gaa tat ggt ctg acg aag gaa gag gcg gca     1501
Leu Asp Phe His Met Lys Glu Tyr Gly Leu Thr Lys Glu Glu Ala Ala
            465                 470                 475

tct aag ttt gaa gga ttg gtt gag gaa aca tgg aag gat ata aac aag     1549
Ser Lys Phe Glu Gly Leu Val Glu Glu Thr Trp Lys Asp Ile Asn Lys
        480                 485                 490

gaa ttc ata gcc aca act aat tat aat gtg ggt aga gaa att gcc atc     1597
Glu Phe Ile Ala Thr Thr Asn Tyr Asn Val Gly Arg Glu Ile Ala Ile
    495                 500                 505

aca ttc ctc aac tac gct cgg ata tgt gaa gcc agt tac agc aaa act     1645
Thr Phe Leu Asn Tyr Ala Arg Ile Cys Glu Ala Ser Tyr Ser Lys Thr
510                 515                 520                 525

gac gga gac gct tat tca gat cct aat gtt gcc aag gca aat gtc gtt     1693
Asp Gly Asp Ala Tyr Ser Asp Pro Asn Val Ala Lys Ala Asn Val Val
                530                 535                 540

gct ctc ttt gtt gat gcc ata gtc ttt tga tttgcataat caaagaccct      1743
Ala Leu Phe Val Asp Ala Ile Val Phe
            545                 550

ataattataa ttatatgtgt ttaagaaact aataagcttg ctttatgtat agttgtcaat   1803

tgaataataa tgtattaatt agtagagtta agaagttata aagaataaag aggagctggt   1863

agacgtaaac aagaaataat gtgtcaaaat aacttcaact ttttcaagaa taaagaattg   1923

gaagagacca atatatacaa aaaaaaaaaa aaaaaa                             1959


<210> SEQ ID NO 28
<211> LENGTH: 550
<212> TYPE: PRT
<213> ORGANISM: Mentha x piperita

<400> SEQUENCE: 28

Met Ala Thr Asn Gly Val Val Ile Ser Cys Leu Arg Glu Val Arg Pro
 1               5                  10                  15

Pro Met Thr Lys His Ala Pro Ser Met Trp Thr Asp Thr Phe Ser Asn
            20                  25                  30

Phe Ser Leu Asp Asp Lys Glu Gln Gln Lys Cys Ser Glu Thr Ile Glu
        35                  40                  45

Ala Leu Lys Gln Glu Ala Arg Gly Met Leu Met Ala Ala Thr Thr Pro
    50                  55                  60

Leu Gln Gln Met Thr Leu Ile Asp Thr Leu Glu Arg Leu Gly Leu Ser
65                  70                  75                  80

Phe His Phe Glu Thr Glu Ile Glu Tyr Lys Ile Glu Leu Ile Asn Ala
                85                  90                  95

Ala Glu Asp Asp Gly Phe Asp Leu Phe Ala Thr Ala Leu Arg Phe Arg
            100                 105                 110

Leu Leu Arg Gln His Gln Arg His Val Ser Cys Asp Val Phe Asp Lys
        115                 120                 125

Phe Ile Asp Lys Asp Gly Lys Phe Glu Glu Ser Leu Ser Asn Asn Val
    130                 135                 140

Glu Gly Leu Leu Ser Leu Tyr Glu Ala Ala His Val Gly Phe Arg Glu
145                 150                 155                 160
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Glu Arg Ile Leu Gln Glu Ala Val Asn Phe Thr Arg His His Leu Glu
                165                 170                 175

Gly Ala Glu Leu Asp Gln Ser Pro Leu Leu Ile Arg Glu Lys Val Lys
            180                 185                 190

Arg Ala Leu Glu His Pro Leu His Arg Asp Phe Pro Ile Val Tyr Ala
        195                 200                 205

Arg Leu Phe Ile Ser Ile Tyr Glu Lys Asp Asp Ser Arg Asp Glu Leu
    210                 215                 220

Leu Leu Lys Leu Ser Lys Val Asn Phe Lys Phe Met Gln Asn Leu Tyr
225                 230                 235                 240

Lys Glu Glu Leu Ser Gln Leu Ser Arg Trp Trp Asn Thr Trp Asn Leu
                245                 250                 255

Lys Ser Lys Leu Pro Tyr Ala Arg Asp Arg Val Val Glu Ala Tyr Val
            260                 265                 270

Trp Gly Val Gly Tyr His Tyr Glu Pro Gln Tyr Ser Tyr Val Arg Met
        275                 280                 285

Gly Leu Ala Lys Gly Val Leu Ile Cys Gly Ile Met Asp Asp Thr Tyr
    290                 295                 300

Asp Asn Tyr Ala Thr Leu Asn Glu Ala Gln Leu Phe Thr Gln Val Leu
305                 310                 315                 320

Asp Lys Trp Asp Arg Asp Glu Ala Glu Arg Leu Pro Glu Tyr Met Lys
                325                 330                 335

Ile Val Tyr Arg Phe Ile Leu Ser Ile Tyr Glu Asn Tyr Glu Arg Asp
            340                 345                 350

Ala Ala Lys Leu Gly Lys Ser Phe Ala Ala Pro Tyr Phe Lys Glu Thr
        355                 360                 365

Val Lys Gln Leu Ala Arg Ala Phe Asn Glu Glu Gln Lys Trp Val Met
    370                 375                 380

Glu Arg Gln Leu Pro Ser Phe Gln Asp Tyr Val Lys Asn Ser Glu Lys
385                 390                 395                 400

Thr Ser Cys Ile Tyr Thr Met Phe Ala Ser Ile Ile Pro Gly Leu Lys
                405                 410                 415

Ser Val Thr Gln Glu Thr Ile Asp Trp Ile Lys Ser Glu Pro Thr Leu
            420                 425                 430

Ala Thr Ser Thr Ala Met Ile Gly Arg Tyr Trp Asn Asp Thr Ser Ser
        435                 440                 445

Gln Leu Arg Glu Ser Lys Gly Gly Glu Met Leu Thr Ala Leu Asp Phe
    450                 455                 460

His Met Lys Glu Tyr Gly Leu Thr Lys Glu Glu Ala Ala Ser Lys Phe
465                 470                 475                 480

Glu Gly Leu Val Glu Glu Thr Trp Lys Asp Ile Asn Lys Glu Phe Ile
                485                 490                 495

Ala Thr Thr Asn Tyr Asn Val Gly Arg Glu Ile Ala Ile Thr Phe Leu
            500                 505                 510

Asn Tyr Ala Arg Ile Cys Glu Ala Ser Tyr Ser Lys Thr Asp Gly Asp
        515                 520                 525

Ala Tyr Ser Asp Pro Asn Val Ala Lys Ala Asn Val Val Ala Leu Phe
    530                 535                 540

Val Asp Ala Ile Val Phe
545                 550
```

<210> SEQ ID NO 29
<211> LENGTH: 2196
<212> TYPE: DNA

-continued

<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (69)...(1949)
<223> OTHER INFORMATION: myrcene synthase

<400> SEQUENCE: 29

tgccggcacg aggttatctt gagcttcctc catataggcc aacacatatc atatcaaagg 60

gagcaaga atg gct ctg gtt tct atc tca ccg ttg gct tcg aaa tct tgc 110
Met Ala Leu Val Ser Ile Ser Pro Leu Ala Ser Lys Ser Cys
1 5 10

ctg cgc aag tcg ttg atc agt tca att cat gaa cat aag cct ccc tat 158
Leu Arg Lys Ser Leu Ile Ser Ser Ile His Glu His Lys Pro Pro Tyr
15 20 25 30

aga aca atc cca aat ctt gga atg cgt agg cga ggg aaa tct gtc acg 206
Arg Thr Ile Pro Asn Leu Gly Met Arg Arg Arg Gly Lys Ser Val Thr
35 40 45

cct tcc atg agc atc agt ttg gcc acc gct gca cct gat gat ggt gta 254
Pro Ser Met Ser Ile Ser Leu Ala Thr Ala Ala Pro Asp Asp Gly Val
50 55 60

caa aga cgc ata ggt gac tac cat tcc aat atc tgg gac gat gat ttc 302
Gln Arg Arg Ile Gly Asp Tyr His Ser Asn Ile Trp Asp Asp Asp Phe
65 70 75

ata cag tct cta tca acg cct tat ggg gaa ccc tct tac cag gaa cgt 350
Ile Gln Ser Leu Ser Thr Pro Tyr Gly Glu Pro Ser Tyr Gln Glu Arg
80 85 90

gct gag aga tta att gtg gag gta aag aag ata ttc aat tca atg tac 398
Ala Glu Arg Leu Ile Val Glu Val Lys Lys Ile Phe Asn Ser Met Tyr
95 100 105 110

ctg gat gat gga aga tta atg agt tcc ttt aat gat ctc atg caa cgc 446
Leu Asp Asp Gly Arg Leu Met Ser Ser Phe Asn Asp Leu Met Gln Arg
115 120 125

ctt tgg ata gtc gat agc gtt gaa cgt ttg ggg ata gct aga cat ttc 494
Leu Trp Ile Val Asp Ser Val Glu Arg Leu Gly Ile Ala Arg His Phe
130 135 140

aag aac gag ata aca tca gct ctg gat tat gtt ttc cgt tac tgg gag 542
Lys Asn Glu Ile Thr Ser Ala Leu Asp Tyr Val Phe Arg Tyr Trp Glu
145 150 155

gaa aac ggc att gga tgt ggg aga gac agt att gtt act gat ctc aac 590
Glu Asn Gly Ile Gly Cys Gly Arg Asp Ser Ile Val Thr Asp Leu Asn
160 165 170

tca act gcg ttg ggg ttt cga act ctt cga tta cac ggg tac act gta 638
Ser Thr Ala Leu Gly Phe Arg Thr Leu Arg Leu His Gly Tyr Thr Val
175 180 185 190

tct cca gag gtt tta aaa gct ttt caa gat caa aat gga cag ttt gta 686
Ser Pro Glu Val Leu Lys Ala Phe Gln Asp Gln Asn Gly Gln Phe Val
195 200 205

tgc tcc ccc ggt cag aca gag ggt gag atc aga agc gtt ctt aac tta 734
Cys Ser Pro Gly Gln Thr Glu Gly Glu Ile Arg Ser Val Leu Asn Leu
210 215 220

tat cgg gct tcc ctc att gcc ttc cct ggt gag aaa gtt atg gaa gaa 782
Tyr Arg Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Val Met Glu Glu
225 230 235

gct gaa atc ttc tcc aca aga tat ttg aaa gaa gct cta caa aag att 830
Ala Glu Ile Phe Ser Thr Arg Tyr Leu Lys Glu Ala Leu Gln Lys Ile
240 245 250

cca gtc tcc gct ctt tca caa gag ata aag ttt gtt atg gaa tat ggc 878
Pro Val Ser Ala Leu Ser Gln Glu Ile Lys Phe Val Met Glu Tyr Gly
255 260 265 270

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tgg cac aca aat ttg cca aga ttg gaa gca aga aat tac ata gac aca      926
Trp His Thr Asn Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Asp Thr
                275                 280                 285

ctt gag aaa gac acc agt gca tgg ctc aat aaa aat gct ggg aag aag      974
Leu Glu Lys Asp Thr Ser Ala Trp Leu Asn Lys Asn Ala Gly Lys Lys
            290                 295                 300

ctt tta gaa ctt gca aaa ttg gag ttc aat ata ttt aac tcc tta caa     1022
Leu Leu Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Asn Ser Leu Gln
        305                 310                 315

caa aag gaa tta caa tat ctt ttg aga tgg tgg aaa gag tcg gat ttg     1070
Gln Lys Glu Leu Gln Tyr Leu Leu Arg Trp Trp Lys Glu Ser Asp Leu
    320                 325                 330

cct aaa ttg aca ttt gct cgg cat cgt cat gtg gaa ttc tac act ttg     1118
Pro Lys Leu Thr Phe Ala Arg His Arg His Val Glu Phe Tyr Thr Leu
335                 340                 345                 350

gcc tct tgt att gcc att gac cca aaa cat tct gca ttc aga cta ggc     1166
Ala Ser Cys Ile Ala Ile Asp Pro Lys His Ser Ala Phe Arg Leu Gly
                355                 360                 365

ttc gcc aaa atg tgt cat ctt gtc aca gtt ttg gac gat att tac gac     1214
Phe Ala Lys Met Cys His Leu Val Thr Val Leu Asp Asp Ile Tyr Asp
            370                 375                 380

act ttt gga acg att gac gag ctt gaa ctc ttc aca tct gca att aag     1262
Thr Phe Gly Thr Ile Asp Glu Leu Glu Leu Phe Thr Ser Ala Ile Lys
        385                 390                 395

aga tgg aat tca tca gag ata gaa cac ctt cca gaa tat atg aaa tgt     1310
Arg Trp Asn Ser Ser Glu Ile Glu His Leu Pro Glu Tyr Met Lys Cys
    400                 405                 410

gtg tac atg gtc gtg ttt gaa act gta aat gaa ctg aca cga gag gcg     1358
Val Tyr Met Val Val Phe Glu Thr Val Asn Glu Leu Thr Arg Glu Ala
415                 420                 425                 430

gag aag act caa ggg aga aac act ctc aac tat gtt cga aag gct tgg     1406
Glu Lys Thr Gln Gly Arg Asn Thr Leu Asn Tyr Val Arg Lys Ala Trp
                435                 440                 445

gag gct tat ttt gat tca tat atg gaa gaa gca aaa tgg atc tct aat     1454
Glu Ala Tyr Phe Asp Ser Tyr Met Glu Glu Ala Lys Trp Ile Ser Asn
            450                 455                 460

ggt tat ctg cca atg ttt gaa gag tac cat gag aat ggg aaa gtg agc     1502
Gly Tyr Leu Pro Met Phe Glu Glu Tyr His Glu Asn Gly Lys Val Ser
        465                 470                 475

tct gca tat cgc gta gca aca ttg caa ccc atc ctc act ttg aat gca     1550
Ser Ala Tyr Arg Val Ala Thr Leu Gln Pro Ile Leu Thr Leu Asn Ala
    480                 485                 490

tgg ctt cct gat tac atc ttg aag gga att gat ttt cca tcc agg ttc     1598
Trp Leu Pro Asp Tyr Ile Leu Lys Gly Ile Asp Phe Pro Ser Arg Phe
495                 500                 505                 510

aat gat ttg gca tcg tcc ttc ctt cgg cta cga ggt gac aca cgc tgc     1646
Asn Asp Leu Ala Ser Ser Phe Leu Arg Leu Arg Gly Asp Thr Arg Cys
                515                 520                 525

tac aag gcc gat agg gat cgt ggt gaa gaa gct tcg tgt ata tca tgt     1694
Tyr Lys Ala Asp Arg Asp Arg Gly Glu Glu Ala Ser Cys Ile Ser Cys
            530                 535                 540

tat atg aaa gac aat cct gga tca acc gaa gaa gat gcc ctc aat cat     1742
Tyr Met Lys Asp Asn Pro Gly Ser Thr Glu Glu Asp Ala Leu Asn His
        545                 550                 555

atc aat gcc atg gtc aat gac ata atc aaa gaa tta aat tgg gaa ctt     1790
Ile Asn Ala Met Val Asn Asp Ile Ile Lys Glu Leu Asn Trp Glu Leu
    560                 565                 570

cta aga tcc aac gac aat att cca atg ctg gcc aag aaa cat gct ttt     1838
Leu Arg Ser Asn Asp Asn Ile Pro Met Leu Ala Lys Lys His Ala Phe
575                 580                 585                 590
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gac ata aca aga gct ctc cac cat ctc tac ata tat cga gat ggc ttt     1886
Asp Ile Thr Arg Ala Leu His His Leu Tyr Ile Tyr Arg Asp Gly Phe
                595                 600                 605

agt gtt gcc aac aag gaa aca aaa aaa ttg gtt atg gaa aca ctc ctt     1934
Ser Val Ala Asn Lys Glu Thr Lys Lys Leu Val Met Glu Thr Leu Leu
            610                 615                 620

gaa tct atg ctt ttt taa ctataaccat atccataata ataagctcat            1982
Glu Ser Met Leu Phe
        625

aatgctaaat tattggcctt atgacatagt ttatgtatgt acttgtgtga attcaatcat   2042

atcgtgtggg tatgattaaa aagctagagc ttactaggtt agtaacatgg tgataaaagt   2102

tataaaatgt gagttataga gatacccatg ttgaataatg aattacaaaa agagaaattt   2162

atgtagaata agattggaag cttttcaatt gttt                               2196


<210> SEQ ID NO 30
<211> LENGTH: 627
<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 30

Met Ala Leu Val Ser Ile Ser Pro Leu Ala Ser Lys Ser Cys Leu Arg
 1               5                  10                  15

Lys Ser Leu Ile Ser Ser Ile His Glu His Lys Pro Pro Tyr Arg Thr
            20                  25                  30

Ile Pro Asn Leu Gly Met Arg Arg Arg Gly Lys Ser Val Thr Pro Ser
        35                  40                  45

Met Ser Ile Ser Leu Ala Thr Ala Ala Pro Asp Asp Gly Val Gln Arg
    50                  55                  60

Arg Ile Gly Asp Tyr His Ser Asn Ile Trp Asp Asp Asp Phe Ile Gln
65                  70                  75                  80

Ser Leu Ser Thr Pro Tyr Gly Glu Pro Ser Tyr Gln Glu Arg Ala Glu
                85                  90                  95

Arg Leu Ile Val Glu Val Lys Lys Ile Phe Asn Ser Met Tyr Leu Asp
            100                 105                 110

Asp Gly Arg Leu Met Ser Ser Phe Asn Asp Leu Met Gln Arg Leu Trp
        115                 120                 125

Ile Val Asp Ser Val Glu Arg Leu Gly Ile Ala Arg His Phe Lys Asn
    130                 135                 140

Glu Ile Thr Ser Ala Leu Asp Tyr Val Phe Arg Tyr Trp Glu Glu Asn
145                 150                 155                 160

Gly Ile Gly Cys Gly Arg Asp Ser Ile Val Thr Asp Leu Asn Ser Thr
                165                 170                 175

Ala Leu Gly Phe Arg Thr Leu Arg Leu His Gly Tyr Thr Val Ser Pro
            180                 185                 190

Glu Val Leu Lys Ala Phe Gln Asp Gln Asn Gly Gln Phe Val Cys Ser
        195                 200                 205

Pro Gly Gln Thr Glu Gly Glu Ile Arg Ser Val Leu Asn Leu Tyr Arg
    210                 215                 220

Ala Ser Leu Ile Ala Phe Pro Gly Glu Lys Val Met Glu Glu Ala Glu
225                 230                 235                 240

Ile Phe Ser Thr Arg Tyr Leu Lys Glu Ala Leu Gln Lys Ile Pro Val
                245                 250                 255

Ser Ala Leu Ser Gln Glu Ile Lys Phe Val Met Glu Tyr Gly Trp His
            260                 265                 270
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Thr Asn Leu Pro Arg Leu Glu Ala Arg Asn Tyr Ile Asp Thr Leu Glu
        275                 280                 285

Lys Asp Thr Ser Ala Trp Leu Asn Lys Asn Ala Gly Lys Lys Leu Leu
    290                 295                 300

Glu Leu Ala Lys Leu Glu Phe Asn Ile Phe Asn Ser Leu Gln Gln Lys
305                 310                 315                 320

Glu Leu Gln Tyr Leu Leu Arg Trp Trp Lys Glu Ser Asp Leu Pro Lys
                325                 330                 335

Leu Thr Phe Ala Arg His Arg His Val Glu Phe Tyr Thr Leu Ala Ser
            340                 345                 350

Cys Ile Ala Ile Asp Pro Lys His Ser Ala Phe Arg Leu Gly Phe Ala
        355                 360                 365

Lys Met Cys His Leu Val Thr Val Leu Asp Asp Ile Tyr Asp Thr Phe
    370                 375                 380

Gly Thr Ile Asp Glu Leu Glu Leu Phe Thr Ser Ala Ile Lys Arg Trp
385                 390                 395                 400

Asn Ser Ser Glu Ile Glu His Leu Pro Glu Tyr Met Lys Cys Val Tyr
                405                 410                 415

Met Val Val Phe Glu Thr Val Asn Glu Leu Thr Arg Glu Ala Glu Lys
            420                 425                 430

Thr Gln Gly Arg Asn Thr Leu Asn Tyr Val Arg Lys Ala Trp Glu Ala
        435                 440                 445

Tyr Phe Asp Ser Tyr Met Glu Glu Ala Lys Trp Ile Ser Asn Gly Tyr
    450                 455                 460

Leu Pro Met Phe Glu Glu Tyr His Glu Asn Gly Lys Val Ser Ser Ala
465                 470                 475                 480

Tyr Arg Val Ala Thr Leu Gln Pro Ile Leu Thr Leu Asn Ala Trp Leu
                485                 490                 495

Pro Asp Tyr Ile Leu Lys Gly Ile Asp Phe Pro Ser Arg Phe Asn Asp
            500                 505                 510

Leu Ala Ser Ser Phe Leu Arg Leu Arg Gly Asp Thr Arg Cys Tyr Lys
        515                 520                 525

Ala Asp Arg Asp Arg Gly Glu Glu Ala Ser Cys Ile Ser Cys Tyr Met
    530                 535                 540

Lys Asp Asn Pro Gly Ser Thr Glu Glu Asp Ala Leu Asn His Ile Asn
545                 550                 555                 560

Ala Met Val Asn Asp Ile Ile Lys Glu Leu Asn Trp Glu Leu Leu Arg
                565                 570                 575

Ser Asn Asp Asn Ile Pro Met Leu Ala Lys Lys His Ala Phe Asp Ile
            580                 585                 590

Thr Arg Ala Leu His His Leu Tyr Ile Tyr Arg Asp Gly Phe Ser Val
        595                 600                 605

Ala Asn Lys Glu Thr Lys Lys Leu Val Met Glu Thr Leu Leu Glu Ser
    610                 615                 620

Met Leu Phe
625
```

<210> SEQ ID NO 31
<211> LENGTH: 1944
<212> TYPE: DNA
<213> ORGANISM: Solanum tuberosum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (57)...(1724)
<223> OTHER INFORMATION: vetispiradiene synthase

-continued

<400> SEQUENCE: 31

```
gaaagaaaga aaattctctc tgtttttttcc acaagcaaag agtacacaca ctagaa atg     59
                                                                  Met
                                                                   1

acc cca gct gct gta gta atg agt aac tac gga gag gag gag att gtt      107
Thr Pro Ala Ala Val Val Met Ser Asn Tyr Gly Glu Glu Glu Ile Val
            5                  10                  15

cgc ccc ata gct gac ttc tct cca agt ctt tgg ggt gat cgt ttt cat      155
Arg Pro Ile Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Arg Phe His
         20                  25                  30

tca ttc tcc ctc gac aat cag att gct gga aaa tat gct caa gag atc      203
Ser Phe Ser Leu Asp Asn Gln Ile Ala Gly Lys Tyr Ala Gln Glu Ile
     35                  40                  45

gaa act ttg aag gaa caa tca aga att ata tta tct gca tct tct cga      251
Glu Thr Leu Lys Glu Gln Ser Arg Ile Ile Leu Ser Ala Ser Ser Arg
 50                  55                  60                  65

aga aca ttg gct gag aaa ttg gat ctg ata gac att gtt gag cgc ctt      299
Arg Thr Leu Ala Glu Lys Leu Asp Leu Ile Asp Ile Val Glu Arg Leu
                70                  75                  80

ggc att gct tat cat ttt gaa aaa caa ata gat gat atg ttg gat caa      347
Gly Ile Ala Tyr His Phe Glu Lys Gln Ile Asp Asp Met Leu Asp Gln
            85                  90                  95

ttt tac aaa gca gat cct aac ttt gag gct cac gag tac aat gat tta      395
Phe Tyr Lys Ala Asp Pro Asn Phe Glu Ala His Glu Tyr Asn Asp Leu
        100                 105                 110

caa act tta tcc gtt caa ttt cga cta ttg aga caa cat ggt tac aat      443
Gln Thr Leu Ser Val Gln Phe Arg Leu Leu Arg Gln His Gly Tyr Asn
    115                 120                 125

atc tcc cca aaa ctt ttt att aga ttc caa gat gca aaa ggc aaa ttt      491
Ile Ser Pro Lys Leu Phe Ile Arg Phe Gln Asp Ala Lys Gly Lys Phe
130                 135                 140                 145

aaa gaa tct ctt tgt aac gac atc aag ggt ctt ttg aac tta tac gaa      539
Lys Glu Ser Leu Cys Asn Asp Ile Lys Gly Leu Leu Asn Leu Tyr Glu
                150                 155                 160

gcc tcg cat gta agg act cat gga gaa gat att ttg gaa gag gca ctt      587
Ala Ser His Val Arg Thr His Gly Glu Asp Ile Leu Glu Glu Ala Leu
            165                 170                 175

gct ttc tct act gct cat ctt gaa tct gca gct cca cat ttg aag tca      635
Ala Phe Ser Thr Ala His Leu Glu Ser Ala Ala Pro His Leu Lys Ser
        180                 185                 190

cct ctg agt aag caa gtg aca cat gcc ctt gag caa tct ctc cat aag      683
Pro Leu Ser Lys Gln Val Thr His Ala Leu Glu Gln Ser Leu His Lys
    195                 200                 205

agc att cca aga gtt gag aca cgc tac ttc atc tct atc tac gaa gag      731
Ser Ile Pro Arg Val Glu Thr Arg Tyr Phe Ile Ser Ile Tyr Glu Glu
210                 215                 220                 225

gag gaa cag aag aat gat gtg ttg ctt caa ttt gca aaa ctg gac ttc      779
Glu Glu Gln Lys Asn Asp Val Leu Leu Gln Phe Ala Lys Leu Asp Phe
                230                 235                 240

aac tta ctt cag atg ttg cac aaa caa gaa ctt agt gaa gta tca agg      827
Asn Leu Leu Gln Met Leu His Lys Gln Glu Leu Ser Glu Val Ser Arg
            245                 250                 255

tgg tgg aaa gat ttg gat ttt gtg aca aca ctt cca tat gct agg gat      875
Trp Trp Lys Asp Leu Asp Phe Val Thr Thr Leu Pro Tyr Ala Arg Asp
        260                 265                 270

aga gca gtg gaa tgc tac ttt tgg acg atg ggg gtg tat gct gaa cct      923
Arg Ala Val Glu Cys Tyr Phe Trp Thr Met Gly Val Tyr Ala Glu Pro
    275                 280                 285
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caa tac tct cag gct cgt gtc atg ctt gct aag act ata gca atg att      971
Gln Tyr Ser Gln Ala Arg Val Met Leu Ala Lys Thr Ile Ala Met Ile
290                 295                 300                 305

tct ata gta gat gac aca ttc gat gct tat ggc att gtc aaa gaa ctt     1019
Ser Ile Val Asp Asp Thr Phe Asp Ala Tyr Gly Ile Val Lys Glu Leu
                310                 315                 320

gag atc tac acc gat gcc ata cag agg tgg gat att agc caa att gat     1067
Glu Ile Tyr Thr Asp Ala Ile Gln Arg Trp Asp Ile Ser Gln Ile Asp
            325                 330                 335

cgg ctc cct gat tac atg aaa atc agt tac aaa gca ctt tta gat ctc     1115
Arg Leu Pro Asp Tyr Met Lys Ile Ser Tyr Lys Ala Leu Leu Asp Leu
        340                 345                 350

tac aat gat tat gaa atg gag ttg tcc aag gat ggt aga tct gat gtt     1163
Tyr Asn Asp Tyr Glu Met Glu Leu Ser Lys Asp Gly Arg Ser Asp Val
    355                 360                 365

gtt cac tac gcg aaa gaa aga atg aaa gaa atc gtg aga aac tat ttt     1211
Val His Tyr Ala Lys Glu Arg Met Lys Glu Ile Val Arg Asn Tyr Phe
370                 375                 380                 385

gtg gaa gca aaa tgg ttc att gaa gga tat atg ccg cca gtc tct gag     1259
Val Glu Ala Lys Trp Phe Ile Glu Gly Tyr Met Pro Pro Val Ser Glu
                390                 395                 400

tat ctt agc aat gca tta gct acc agc act tat tac ttg ctt acg act     1307
Tyr Leu Ser Asn Ala Leu Ala Thr Ser Thr Tyr Tyr Leu Leu Thr Thr
            405                 410                 415

aca tct tat ttg ggc atg aag tct gct aac aag caa gat ttt gaa tgg     1355
Thr Ser Tyr Leu Gly Met Lys Ser Ala Asn Lys Gln Asp Phe Glu Trp
        420                 425                 430

ttg gcc aag aac cct aaa att ctt gag gct aat gtg acg tta tgc cga     1403
Leu Ala Lys Asn Pro Lys Ile Leu Glu Ala Asn Val Thr Leu Cys Arg
    435                 440                 445

gtc ata gat gac ata gcc acc tat gag gtt gag aag ggt aga ggt cag     1451
Val Ile Asp Asp Ile Ala Thr Tyr Glu Val Glu Lys Gly Arg Gly Gln
450                 455                 460                 465

att gcc act gga att gaa tgt tac atg aga gat tat ggt gta tcc aca     1499
Ile Ala Thr Gly Ile Glu Cys Tyr Met Arg Asp Tyr Gly Val Ser Thr
                470                 475                 480

gaa aag gcc atg gaa aaa ttc caa gaa atg gct gag aca gca tgg aag     1547
Glu Lys Ala Met Glu Lys Phe Gln Glu Met Ala Glu Thr Ala Trp Lys
            485                 490                 495

gat gta aat gaa gga atc ctt cga cca act ccc gtc tct aca gag att     1595
Asp Val Asn Glu Gly Ile Leu Arg Pro Thr Pro Val Ser Thr Glu Ile
        500                 505                 510

ctc act cgc att ctc aat ctt gct cgc att atc gat gtt act tat aag     1643
Leu Thr Arg Ile Leu Asn Leu Ala Arg Ile Ile Asp Val Thr Tyr Lys
    515                 520                 525

cac aat caa gat gga tac act cat ccg gaa aaa gta cta aaa cct cat     1691
His Asn Gln Asp Gly Tyr Thr His Pro Glu Lys Val Leu Lys Pro His
530                 535                 540                 545

att att gcg ttg ttg gtg gac tct att gaa att taa atcatcgatt          1737
Ile Ile Ala Leu Leu Val Asp Ser Ile Glu Ile
                550                 555

gttttgtaca tctgggagca cttgcttccc atcccctaaa attataagta tttgattgat   1797

gccttgttgg tatctatgct gctaggcgct agctaagata ggagttgctg gagatacatg   1857

ttatagtgca gtgcagttaa ttccttaatt ttttttgta tcattattga cattttaaat   1917

atatatatat atatcactgc tttttat                                      1944
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<210> SEQ ID NO 32
<211> LENGTH: 556

-continued

<212> TYPE: PRT
<213> ORGANISM: Solanum tuberosum

<400> SEQUENCE: 32

Met Thr Pro Ala Ala Val Val Met Ser Asn Tyr Gly Glu Glu Glu Ile
 1   5   10   15

Val Arg Pro Ile Ala Asp Phe Ser Pro Ser Leu Trp Gly Asp Arg Phe
            20   25   30

His Ser Phe Ser Leu Asp Asn Gln Ile Ala Gly Lys Tyr Ala Gln Glu
        35   40   45

Ile Glu Thr Leu Lys Glu Gln Ser Arg Ile Ile Leu Ser Ala Ser Ser
    50   55   60

Arg Arg Thr Leu Ala Glu Lys Leu Asp Leu Ile Asp Ile Val Glu Arg
65   70   75   80

Leu Gly Ile Ala Tyr His Phe Glu Lys Gln Ile Asp Asp Met Leu Asp
                85   90   95

Gln Phe Tyr Lys Ala Asp Pro Asn Phe Glu Ala His Glu Tyr Asn Asp
            100   105   110

Leu Gln Thr Leu Ser Val Gln Phe Arg Leu Leu Arg Gln His Gly Tyr
        115   120   125

Asn Ile Ser Pro Lys Leu Phe Ile Arg Phe Gln Asp Ala Lys Gly Lys
    130   135   140

Phe Lys Glu Ser Leu Cys Asn Asp Ile Lys Gly Leu Leu Asn Leu Tyr
145   150   155   160

Glu Ala Ser His Val Arg Thr His Gly Glu Asp Ile Leu Glu Glu Ala
                165   170   175

Leu Ala Phe Ser Thr Ala His Leu Glu Ser Ala Ala Pro His Leu Lys
            180   185   190

Ser Pro Leu Ser Lys Gln Val Thr His Ala Leu Glu Gln Ser Leu His
        195   200   205

Lys Ser Ile Pro Arg Val Glu Thr Arg Tyr Phe Ile Ser Ile Tyr Glu
    210   215   220

Glu Glu Glu Gln Lys Asn Asp Val Leu Leu Gln Phe Ala Lys Leu Asp
225   230   235   240

Phe Asn Leu Leu Gln Met Leu His Lys Gln Glu Leu Ser Glu Val Ser
                245   250   255

Arg Trp Trp Lys Asp Leu Asp Phe Val Thr Thr Leu Pro Tyr Ala Arg
            260   265   270

Asp Arg Ala Val Glu Cys Tyr Phe Trp Thr Met Gly Val Tyr Ala Glu
        275   280   285

Pro Gln Tyr Ser Gln Ala Arg Val Met Leu Ala Lys Thr Ile Ala Met
    290   295   300

Ile Ser Ile Val Asp Asp Thr Phe Asp Ala Tyr Gly Ile Val Lys Glu
305   310   315   320

Leu Glu Ile Tyr Thr Asp Ala Ile Gln Arg Trp Asp Ile Ser Gln Ile
                325   330   335

Asp Arg Leu Pro Asp Tyr Met Lys Ile Ser Tyr Lys Ala Leu Leu Asp
            340   345   350

Leu Tyr Asn Asp Tyr Glu Met Glu Leu Ser Lys Asp Gly Arg Ser Asp
        355   360   365

Val Val His Tyr Ala Lys Glu Arg Met Lys Glu Ile Val Arg Asn Tyr
    370   375   380

Phe Val Glu Ala Lys Trp Phe Ile Glu Gly Tyr Met Pro Pro Val Ser
385   390   395   400

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Glu Tyr Leu Ser Asn Ala Leu Ala Thr Ser Thr Tyr Tyr Leu Leu Thr
                405                 410                 415

Thr Thr Ser Tyr Leu Gly Met Lys Ser Ala Asn Lys Gln Asp Phe Glu
            420                 425                 430

Trp Leu Ala Lys Asn Pro Lys Ile Leu Glu Ala Asn Val Thr Leu Cys
        435                 440                 445

Arg Val Ile Asp Asp Ile Ala Thr Tyr Glu Val Glu Lys Gly Arg Gly
    450                 455                 460

Gln Ile Ala Thr Gly Ile Glu Cys Tyr Met Arg Asp Tyr Gly Val Ser
465                 470                 475                 480

Thr Glu Lys Ala Met Glu Lys Phe Gln Glu Met Ala Glu Thr Ala Trp
                485                 490                 495

Lys Asp Val Asn Glu Gly Ile Leu Arg Pro Thr Pro Val Ser Thr Glu
            500                 505                 510

Ile Leu Thr Arg Ile Leu Asn Leu Ala Arg Ile Ile Asp Val Thr Tyr
        515                 520                 525

Lys His Asn Gln Asp Gly Tyr Thr His Pro Glu Lys Val Leu Lys Pro
    530                 535                 540

His Ile Ile Ala Leu Leu Val Asp Ser Ile Glu Ile
545                 550                 555


<210> SEQ ID NO 33
<211> LENGTH: 3950
<212> TYPE: DNA
<213> ORGANISM: Gossypium arboreum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1457)...(1579)
<223> OTHER INFORMATION: cadinene synthase
<221> NAME/KEY: CDS
<222> LOCATION: (1670)...(1939)
<221> NAME/KEY: CDS
<222> LOCATION: (2092)...(2466)
<221> NAME/KEY: CDS
<222> LOCATION: (2559)...(2774)
<221> NAME/KEY: CDS
<222> LOCATION: (2963)...(3103)
<221> NAME/KEY: CDS
<222> LOCATION: (3206)...(3454)
<221> NAME/KEY: CDS
<222> LOCATION: (3596)...(3886)

<400> SEQUENCE: 33

aatttaactt ttattaattt aaaatttaaa gatttcaaag gggttctaaa atggaaattt     60

ttcgatttta agggaattgt gccagcccct agtttcgccc ttgtttgtag tgctttattt    120

taaaaaagta aatataatag aatatgtata tatatatata tataaaccaa agtgaaagat    180

gaaaatttat ataaatgatc gctgcaagct tcaagctcac aataatatga ttctttacca    240

tcaagaaaca ttggtgcttt atacagagaa aagaaaaact ttggtcctcc tcgtagctaa    300

tattttaaca atttaatttt tatataataa atttttaaca attatttcat atttttaaa     360

tatattcatg ttgaatgtag cagtatatag ttatattagt tatgctcata aattttggat    420

gcattagatt ttccttatgt aatttgataa caatgattat tattttact tctaacaaat     480

aattaaatat ttttttgttg attcgataaa tatcattatt ttttaaatga tttaaaatat    540

aaaaataata atagattcga ccgaacgctc accctattga gtgagtatat caattattag    600

aatttaatta aaaaaggaaa ccaaatatag ccggcttaat tttgtttaat attaatttat    660

gtgtggaaat tcacttaaaa acagagtcca tggctgctaa catattatat attaaaccat    720

ttcctattaa taaatttatg aacgagagtt acatccttct aaattcattt tacttagagg    780
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cggagtataa tattttatgt agtagttatt cttttactat ataaataaat aaataaaatt    840

ttaatcgcct gtgtattatg attgattcag ctgaatcaaa gttggaataa tattttaatt    900

tgggatccca attaattgag attggtttga ttttgggttg taaatatttt ttattaattt    960

tagataaatt attggaagtt ggagtcaaaa ttgaccgtct cagctaatta tacaaataat   1020

aataatatag agaaatgggt atattgctca acactcacat ttactacgtc agcaatagtc   1080

agacagactg ctaagtaaac aatgtacact caattcgagt caaacaaatc ctttatccca   1140

agattctaaa ataatgtgtt tgaggcacca attttgaagg atagaaagtg gaaacaaaca   1200

aaaggatatt aaaaaacaag gaaatttctc actgtatttg catatttttc tccttccagt   1260

ataattaaaa tacgtgcaat ttacgttgta ctttgttgac tcctatctta tacctataaa   1320

tacatgcaac aattgcacac atcgtctcat ccaaaacctg tgttttaaac actaaacagt   1380

aagcaaaggc agcaaattaa tctttgaatt atttgcttcc aaaaccctac acttttcctt   1440

caacacatcc tagaaa atg gct tca caa gct tct caa gtt ctt gct tca ccc   1492
                  Met Ala Ser Gln Ala Ser Gln Val Leu Ala Ser Pro
                   1               5                  10

cat ccc gcc att tca tcc gaa aat cga ccc aag gct gat ttt cat ccc     1540
His Pro Ala Ile Ser Ser Glu Asn Arg Pro Lys Ala Asp Phe His Pro
         15                  20                  25

ggt att tgg ggt gat atg ttc atc atc tgt cct gat acg gtaatctata      1589
Gly Ile Trp Gly Asp Met Phe Ile Ile Cys Pro Asp Thr
     30                  35                  40

atttttttct tactttctct tttatcgatt tttaagtttt ttggagattt catggaaaag   1649

cattatacgt acttgagcag gat atc gat gct gca act gaa tta caa tat gaa   1702
                     Asp Ile Asp Ala Ala Thr Glu Leu Gln Tyr Glu
                                 45                  50

gaa tta aaa gca caa gtg agg aag atg att atg gaa cct gtt gat gat     1750
Glu Leu Lys Ala Gln Val Arg Lys Met Ile Met Glu Pro Val Asp Asp
         55                  60                  65

tca aac caa aag ttg ccc ttc att gat gct gtt caa aga tta ggt gtg     1798
Ser Asn Gln Lys Leu Pro Phe Ile Asp Ala Val Gln Arg Leu Gly Val
     70                  75                  80

agt tat cat ttt gag aaa gag att gaa gat gaa cta gag aat att tac     1846
Ser Tyr His Phe Glu Lys Glu Ile Glu Asp Glu Leu Glu Asn Ile Tyr
 85                  90                  95                  100

cgt gac acc aac aac aat gat gcg gac acc gat ctc tac act aca gct     1894
Arg Asp Thr Asn Asn Asn Asp Ala Asp Thr Asp Leu Tyr Thr Thr Ala
                105                 110                 115

ctt cga ttc cgg tta ctt aga gag cat ggc ttc gat att tct tgt         1939
Leu Arg Phe Arg Leu Leu Arg Glu His Gly Phe Asp Ile Ser Cys
            120                 125                 130

ggtaattaag tcttaaactt tcataactct tcttatccat ttatcaatta atattatcaa   1999

actttacatt aataatcatc tgtacaatac ttcaatatat atatatttat tgatgaaact   2059

aatgtttgat gatgattttg ggtgcttgac ca gat gca ttc aac aag ttc aaa     2112
                                  Asp Ala Phe Asn Lys Phe Lys
                                              135

gat gag gca ggg aac ttc aag gca tca ttg aca agt gat gtg caa ggg     2160
Asp Glu Ala Gly Asn Phe Lys Ala Ser Leu Thr Ser Asp Val Gln Gly
    140                 145                 150

ttg ttg gaa ctt tat gaa gct tcc tat atg agg gtc cat ggg gaa gat     2208
Leu Leu Glu Leu Tyr Glu Ala Ser Tyr Met Arg Val His Gly Glu Asp
155                 160                 165                 170

ata ctt gat gaa gcc att tct ttc acc act gct caa ctt aca ctt gct     2256
Ile Leu Asp Glu Ala Ile Ser Phe Thr Thr Ala Gln Leu Thr Leu Ala
                175                 180                 185
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cta cca act tta cac cat cct tta tcg gaa cag gtc ggc cat gcc tta     2304
Leu Pro Thr Leu His His Pro Leu Ser Glu Gln Val Gly His Ala Leu
            190                 195                 200

aag cag tct atc cga agg ggc ttg cca agg gtt gag gcc cgg aat ttc     2352
Lys Gln Ser Ile Arg Arg Gly Leu Pro Arg Val Glu Ala Arg Asn Phe
        205                 210                 215

att tcg ata tac caa gat tta gaa tcc cat aac aaa tcg ttg ctt caa     2400
Ile Ser Ile Tyr Gln Asp Leu Glu Ser His Asn Lys Ser Leu Leu Gln
    220                 225                 230

ttt gca aag att gat ttc aac ttg ttg cag ctt ttg cat agg aaa gag     2448
Phe Ala Lys Ile Asp Phe Asn Leu Leu Gln Leu Leu His Arg Lys Glu
235                 240                 245                 250

cta agt gag atc tgc agg taagtgtttg gagatcttta aagctatgaa            2496
Leu Ser Glu Ile Cys Arg
                255

gtctaatact atttcaattg atcacacgac tgttgctgac attttatgat gctttttta   2556

gg tgg tgg aaa gat tta gac ttt aca aga aaa cta cca ttt gca aga      2603
   Trp Trp Lys Asp Leu Asp Phe Thr Arg Lys Leu Pro Phe Ala Arg
               260                 265                 270

gat aga gtg gtt gaa ggc tat ttt tgg ata atg gga gtt tac ttt gaa     2651
Asp Arg Val Val Glu Gly Tyr Phe Trp Ile Met Gly Val Tyr Phe Glu
            275                 280                 285

ccc caa tac tct ctt ggt aga aag atg ttg aca aaa gtc ata gca atg     2699
Pro Gln Tyr Ser Leu Gly Arg Lys Met Leu Thr Lys Val Ile Ala Met
        290                 295                 300

gct tcc att gtt gat gat act tat gat tca tat gca acc tat gat gaa     2747
Ala Ser Ile Val Asp Asp Thr Tyr Asp Ser Tyr Ala Thr Tyr Asp Glu
    305                 310                 315

ctc att ccc tat aca aat gca att gaa ggtgagattt tttttccttt           2794
Leu Ile Pro Tyr Thr Asn Ala Ile Glu
320                 325

cctccaaaaa aaaaaaaagt ttttgagatc ccccaagaat aggggaaaat atatgttttt   2854

aaacgttagg atattcactc caacttgcag ttgctcatat tttaatggtg atagtatgaa   2914

ctaaccaggc taagttttag attcaaatta accctgaaat tgtgtttt agg tgg gat    2971
                                                    Arg Trp Asp
                                                        330

att aaa tgc atg aac caa ctc ccg aat tac atg aaa ata agc tac aag     3019
Ile Lys Cys Met Asn Gln Leu Pro Asn Tyr Met Lys Ile Ser Tyr Lys
            335                 340                 345

gca cta tta gat gtt tat gaa gaa atg gaa cag ctg ttg gca aat caa     3067
Ala Leu Leu Asp Val Tyr Glu Glu Met Glu Gln Leu Leu Ala Asn Gln
        350                 355                 360

ggg aga cag tac cga gtt gag tat gcg aaa aag gcg gtatgtaatg          3113
Gly Arg Gln Tyr Arg Val Glu Tyr Ala Lys Lys Ala
    365                 370                 375

atacaatagt atgatatgct ttaatcataa acgtataaaa tttgaaaatt acattagcaa   3173
tttgcttact tttttatgcc tttaatcctc ag atg ata cgt ctt gtt caa gct     3226
                                  Met Ile Arg Leu Val Gln Ala
                                                    380

tac ctt ttg gag gcc aaa tgg act cat caa aat tat aaa cca acc ttt     3274
Tyr Leu Leu Glu Ala Lys Trp Thr His Gln Asn Tyr Lys Pro Thr Phe
        385                 390                 395

gag gaa ttt aga gat aat gca ttg cca acc tct ggc tat gcc atg ctt     3322
Glu Glu Phe Arg Asp Asn Ala Leu Pro Thr Ser Gly Tyr Ala Met Leu
    400                 405                 410

gct ata acg gcg ttt gtc ggc atg ggc gaa gtt ata acc cct gag acc     3370
Ala Ile Thr Ala Phe Val Gly Met Gly Glu Val Ile Thr Pro Glu Thr
415                 420                 425                 430
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ttc aaa tgg gcc gcc agt gac ccc aag atc att aag gct tcc acc att     3418
Phe Lys Trp Ala Ala Ser Asp Pro Lys Ile Ile Lys Ala Ser Thr Ile
                435                 440                 445

att tgc agg ttc atg gac gat att gct gaa cat aag gtatactata          3464
Ile Cys Arg Phe Met Asp Asp Ile Ala Glu His Lys
            450                 455

tattcatatt caagaattct aaaaatcgat tatggtatat atatgcactt aaatctatat   3524

catagaattg taaggcttct agggtttgca tttgctaagt taattaatat acatggttca   3584

tatgggtgca g ttc aac cat agg aga gaa gac gat tgc tca gcg atc gaa     3634
             Phe Asn His Arg Arg Glu Asp Asp Cys Ser Ala Ile Glu
                 460                 465                 470

tgt tac atg aaa caa tat ggg gtg aca gcg cag gaa gca tac aat gaa     3682
Cys Tyr Met Lys Gln Tyr Gly Val Thr Ala Gln Glu Ala Tyr Asn Glu
            475                 480                 485

ttc aac aaa cac att gag agt tca tgg aaa gat gta aat gaa gag ttc     3730
Phe Asn Lys His Ile Glu Ser Ser Trp Lys Asp Val Asn Glu Glu Phe
        490                 495                 500

ttg aaa ccg aca gaa atg ccg aca ccc gtt ctt tgt cgt agc ctc aac     3778
Leu Lys Pro Thr Glu Met Pro Thr Pro Val Leu Cys Arg Ser Leu Asn
    505                 510                 515

ctt gct agg gtt atg gat gta ctt tac aga gaa ggt gac ggt tat aca     3826
Leu Ala Arg Val Met Asp Val Leu Tyr Arg Glu Gly Asp Gly Tyr Thr
520                 525                 530                 535

cat gtt ggg aaa gct gct aaa ggt ggg atc act tca tta ttg att gat     3874
His Val Gly Lys Ala Ala Lys Gly Gly Ile Thr Ser Leu Leu Ile Asp
                540                 545                 550

cca ata caa att tga aattcaacat tggcttaaga tttactatga gataaaatta     3929
Pro Ile Gln Ile
            555

ataaggtttg tacaatgaag g                                             3950


<210> SEQ ID NO 34
<211> LENGTH: 41
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 34

Met Ala Ser Gln Ala Ser Gln Val Leu Ala Ser Pro His Pro Ala Ile
 1               5                  10                  15

Ser Ser Glu Asn Arg Pro Lys Ala Asp Phe His Pro Gly Ile Trp Gly
            20                  25                  30

Asp Met Phe Ile Ile Cys Pro Asp Thr
        35                  40


<210> SEQ ID NO 35
<211> LENGTH: 90
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 35

Asp Ile Asp Ala Ala Thr Glu Leu Gln Tyr Glu Glu Leu Lys Ala Gln
 1               5                  10                  15

Val Arg Lys Met Ile Met Glu Pro Val Asp Asp Ser Asn Gln Lys Leu
            20                  25                  30

Pro Phe Ile Asp Ala Val Gln Arg Leu Gly Val Ser Tyr His Phe Glu
        35                  40                  45

Lys Glu Ile Glu Asp Glu Leu Glu Asn Ile Tyr Arg Asp Thr Asn Asn
    50                  55                  60
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Asn Asp Ala Asp Thr Asp Leu Tyr Thr Thr Ala Leu Arg Phe Arg Leu
65                  70                  75                  80

Leu Arg Glu His Gly Phe Asp Ile Ser Cys
                85                  90


<210> SEQ ID NO 36
<211> LENGTH: 125
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 36

Asp Ala Phe Asn Lys Phe Lys Asp Glu Ala Gly Asn Phe Lys Ala Ser
 1               5                  10                  15

Leu Thr Ser Asp Val Gln Gly Leu Leu Glu Leu Tyr Glu Ala Ser Tyr
            20                  25                  30

Met Arg Val His Gly Glu Asp Ile Leu Asp Glu Ala Ile Ser Phe Thr
        35                  40                  45

Thr Ala Gln Leu Thr Leu Ala Leu Pro Thr Leu His His Pro Leu Ser
    50                  55                  60

Glu Gln Val Gly His Ala Leu Lys Gln Ser Ile Arg Arg Gly Leu Pro
65                  70                  75                  80

Arg Val Glu Ala Arg Asn Phe Ile Ser Ile Tyr Gln Asp Leu Glu Ser
                85                  90                  95

His Asn Lys Ser Leu Leu Gln Phe Ala Lys Ile Asp Phe Asn Leu Leu
            100                 105                 110

Gln Leu Leu His Arg Lys Glu Leu Ser Glu Ile Cys Arg
        115                 120                 125


<210> SEQ ID NO 37
<211> LENGTH: 72
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 37

Trp Trp Lys Asp Leu Asp Phe Thr Arg Lys Leu Pro Phe Ala Arg Asp
 1               5                  10                  15

Arg Val Val Glu Gly Tyr Phe Trp Ile Met Gly Val Tyr Phe Glu Pro
            20                  25                  30

Gln Tyr Ser Leu Gly Arg Lys Met Leu Thr Lys Val Ile Ala Met Ala
        35                  40                  45

Ser Ile Val Asp Asp Thr Tyr Asp Ser Tyr Ala Thr Tyr Asp Glu Leu
    50                  55                  60

Ile Pro Tyr Thr Asn Ala Ile Glu
65                  70


<210> SEQ ID NO 38
<211> LENGTH: 47
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 38

Arg Trp Asp Ile Lys Cys Met Asn Gln Leu Pro Asn Tyr Met Lys Ile
 1               5                  10                  15

Ser Tyr Lys Ala Leu Leu Asp Val Tyr Glu Glu Met Glu Gln Leu Leu
            20                  25                  30

Ala Asn Gln Gly Arg Gln Tyr Arg Val Glu Tyr Ala Lys Lys Ala
        35                  40                  45
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<210> SEQ ID NO 39
<211> LENGTH: 83
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 39

Met Ile Arg Leu Val Gln Ala Tyr Leu Leu Glu Ala Lys Trp Thr His
 1   5   10   15

Gln Asn Tyr Lys Pro Thr Phe Glu Glu Phe Arg Asp Asn Ala Leu Pro
            20   25   30

Thr Ser Gly Tyr Ala Met Leu Ala Ile Thr Ala Phe Val Gly Met Gly
        35   40   45

Glu Val Ile Thr Pro Glu Thr Phe Lys Trp Ala Ala Ser Asp Pro Lys
    50   55   60

Ile Ile Lys Ala Ser Thr Ile Ile Cys Arg Phe Met Asp Asp Ile Ala
65   70   75   80

Glu His Lys

<210> SEQ ID NO 40
<211> LENGTH: 97
<212> TYPE: PRT
<213> ORGANISM: Gossypium arboreum

<400> SEQUENCE: 40

Phe Asn His Arg Arg Glu Asp Asp Cys Ser Ala Ile Glu Cys Tyr Met
 1   5   10   15

Lys Gln Tyr Gly Val Thr Ala Gln Glu Ala Tyr Asn Glu Phe Asn Lys
            20   25   30

His Ile Glu Ser Ser Trp Lys Asp Val Asn Glu Glu Phe Leu Lys Pro
        35   40   45

Thr Glu Met Pro Thr Pro Val Leu Cys Arg Ser Leu Asn Leu Ala Arg
    50   55   60

Val Met Asp Val Leu Tyr Arg Glu Gly Asp Gly Tyr Thr His Val Gly
65   70   75   80

Lys Ala Ala Lys Gly Gly Ile Thr Ser Leu Leu Ile Asp Pro Ile Gln
                85   90   95

Ile

<210> SEQ ID NO 41
<211> LENGTH: 1994
<212> TYPE: DNA
<213> ORGANISM: Ricinus communis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (67)...(1869)
<223> OTHER INFORMATION: casbene synthase

<400> SEQUENCE: 41

actcagcagc cgcctctcct accccaatta gcacagaaga tttggtggtt cctctccttg   60

tgaaac atg gca ttg cca tca gct gct atg caa tcc aac cct gaa aag   108
       Met Ala Leu Pro Ser Ala Ala Met Gln Ser Asn Pro Glu Lys
        1   5   10

ctt aac tta ttt cac aga ttg tca agc tta ccc acc act agc ttg gaa   156
Leu Asn Leu Phe His Arg Leu Ser Ser Leu Pro Thr Thr Ser Leu Glu
 15   20   25   30

tat ggc aat aat cgc ttc cct ttc ttt tcc tca tct gcc aag tca cac   204
Tyr Gly Asn Asn Arg Phe Pro Phe Phe Ser Ser Ser Ala Lys Ser His
                35   40   45

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ttt aaa aaa cca act caa gca tgt tta tcc tca aca acc cac caa gaa      252
Phe Lys Lys Pro Thr Gln Ala Cys Leu Ser Ser Thr Thr His Gln Glu
             50                  55                  60

gtt cgt cca tta gca tac ttt cct cct act gtc tgg ggc aat cgc ttt      300
Val Arg Pro Leu Ala Tyr Phe Pro Pro Thr Val Trp Gly Asn Arg Phe
         65                  70                  75

gct tcc ttg acc ttc aat cca tcg gaa ttt gaa tcg tat gat gaa cgg      348
Ala Ser Leu Thr Phe Asn Pro Ser Glu Phe Glu Ser Tyr Asp Glu Arg
     80                  85                  90

gta att gtg ctg aag aaa aaa gtt aag gac ata tta att tca tct aca      396
Val Ile Val Leu Lys Lys Lys Val Lys Asp Ile Leu Ile Ser Ser Thr
 95                 100                 105                 110

agt gat tca gtg gag acc gtt att tta atc gac tta tta tgt cgg ctt      444
Ser Asp Ser Val Glu Thr Val Ile Leu Ile Asp Leu Leu Cys Arg Leu
                115                 120                 125

ggc gta tca tat cac ttt gaa aat gat att gaa gag cta cta agt aaa      492
Gly Val Ser Tyr His Phe Glu Asn Asp Ile Glu Glu Leu Leu Ser Lys
            130                 135                 140

atc ttc aac tcc cag cct gac ctt gtc gat gaa aaa gaa tgt gat ctc      540
Ile Phe Asn Ser Gln Pro Asp Leu Val Asp Glu Lys Glu Cys Asp Leu
        145                 150                 155

tac act gcg gca att gta ttc cga gtt ttc aga cag cat ggt ttt aaa      588
Tyr Thr Ala Ala Ile Val Phe Arg Val Phe Arg Gln His Gly Phe Lys
    160                 165                 170

atg tct tcg gat gtg ttt agc aaa ttc aag gac agt gat ggt aag ttc      636
Met Ser Ser Asp Val Phe Ser Lys Phe Lys Asp Ser Asp Gly Lys Phe
175                 180                 185                 190

aag gaa tcc cta cgg ggt gat gct aag ggt atg ctc agc ctt ttt gaa      684
Lys Glu Ser Leu Arg Gly Asp Ala Lys Gly Met Leu Ser Leu Phe Glu
                195                 200                 205

gct tcc cat cta agt gtg cat gga gaa gac att ctt gaa gaa gcc ttt      732
Ala Ser His Leu Ser Val His Gly Glu Asp Ile Leu Glu Glu Ala Phe
            210                 215                 220

gct ttc acc aag gat tac tta cag tcc tct gca gtt gag tta ttc cct      780
Ala Phe Thr Lys Asp Tyr Leu Gln Ser Ser Ala Val Glu Leu Phe Pro
        225                 230                 235

aat ctc aaa agg cat ata acg aac gcc cta gag cag cct ttc cac agt      828
Asn Leu Lys Arg His Ile Thr Asn Ala Leu Glu Gln Pro Phe His Ser
    240                 245                 250

ggc gtg ccg agg cta gag gcc agg aaa ttc atc gat cta tac gaa gct      876
Gly Val Pro Arg Leu Glu Ala Arg Lys Phe Ile Asp Leu Tyr Glu Ala
255                 260                 265                 270

gat att gaa tgc cgg aat gaa act ctg ctc gag ttt gca aag ttg gat      924
Asp Ile Glu Cys Arg Asn Glu Thr Leu Leu Glu Phe Ala Lys Leu Asp
                275                 280                 285

tat aat aga gtt cag tta ttg cac caa caa gag ctg tgc cag ttc tca      972
Tyr Asn Arg Val Gln Leu Leu His Gln Gln Glu Leu Cys Gln Phe Ser
            290                 295                 300

aag tgg tgg aaa gac ctg aat ctt gct tcg gat att cct tat gca aga     1020
Lys Trp Trp Lys Asp Leu Asn Leu Ala Ser Asp Ile Pro Tyr Ala Arg
        305                 310                 315

gac aga atg gca gag att ttc ttt tgg gca gtc gcg atg tac ttt gag     1068
Asp Arg Met Ala Glu Ile Phe Phe Trp Ala Val Ala Met Tyr Phe Glu
    320                 325                 330

cct gac tat gca cac acc cga atg att att gcg aag gtt gta ttg ctt     1116
Pro Asp Tyr Ala His Thr Arg Met Ile Ile Ala Lys Val Val Leu Leu
335                 340                 345                 350

ata tca cta ata gat gat aca att gat gcg tat gca aca atg gag gaa     1164
Ile Ser Leu Ile Asp Asp Thr Ile Asp Ala Tyr Ala Thr Met Glu Glu
                355                 360                 365
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act cat att ctt gct gaa gca gtc gca agg tgg gac atg agc tgc ctc     1212
Thr His Ile Leu Ala Glu Ala Val Ala Arg Trp Asp Met Ser Cys Leu
            370                 375                 380

gag aag ctg cca gat tac atg aaa gtt att tat aaa cta ttg cta aac     1260
Glu Lys Leu Pro Asp Tyr Met Lys Val Ile Tyr Lys Leu Leu Leu Asn
        385                 390                 395

acc ttc tct gaa ttc gag aaa gaa ttg acg gcg gaa ggc aag tcc tac     1308
Thr Phe Ser Glu Phe Glu Lys Glu Leu Thr Ala Glu Gly Lys Ser Tyr
    400                 405                 410

agc gtc aaa tac gga agg gaa gcg ttt caa gaa cta gtg aga ggt tac     1356
Ser Val Lys Tyr Gly Arg Glu Ala Phe Gln Glu Leu Val Arg Gly Tyr
415                 420                 425                 430

tac ctg gag gct gta tgg cgc gac gag ggt aaa ata cca tcg ttc gat     1404
Tyr Leu Glu Ala Val Trp Arg Asp Glu Gly Lys Ile Pro Ser Phe Asp
                435                 440                 445

gac tac ttg tat aat gga tcc atg acc acc gga ttg cct ctc gtc tca     1452
Asp Tyr Leu Tyr Asn Gly Ser Met Thr Thr Gly Leu Pro Leu Val Ser
            450                 455                 460

aca gct tct ttc atg gga gtt caa gaa att aca ggt ctc aac gaa ttc     1500
Thr Ala Ser Phe Met Gly Val Gln Glu Ile Thr Gly Leu Asn Glu Phe
        465                 470                 475

caa tgg ctg gaa act aat ccc aaa tta agt tat gct tcc ggt gca ttc     1548
Gln Trp Leu Glu Thr Asn Pro Lys Leu Ser Tyr Ala Ser Gly Ala Phe
    480                 485                 490

atc cga ctt gtc aac gac tta act tct cat gtg act gaa caa caa aga     1596
Ile Arg Leu Val Asn Asp Leu Thr Ser His Val Thr Glu Gln Gln Arg
495                 500                 505                 510

gga cac gtt gca tct tgc atc gac tgc tat atg aac caa cat gga gtt     1644
Gly His Val Ala Ser Cys Ile Asp Cys Tyr Met Asn Gln His Gly Val
                515                 520                 525

tcc aaa gac gaa gca gtc aaa ata ctt caa aaa atg gct aca gat tgt     1692
Ser Lys Asp Glu Ala Val Lys Ile Leu Gln Lys Met Ala Thr Asp Cys
            530                 535                 540

tgg aaa gaa att aat gaa gaa tgt atg agg cag agt caa gtg tca gtg     1740
Trp Lys Glu Ile Asn Glu Glu Cys Met Arg Gln Ser Gln Val Ser Val
        545                 550                 555

ggt cac cta atg aga ata gtt aat ctg gca cgt ctt acg gat gtg agt     1788
Gly His Leu Met Arg Ile Val Asn Leu Ala Arg Leu Thr Asp Val Ser
    560                 565                 570

tac aag tat gga gac ggt tac act gat tcc cag caa ttg aaa caa ttt     1836
Tyr Lys Tyr Gly Asp Gly Tyr Thr Asp Ser Gln Gln Leu Lys Gln Phe
575                 580                 585                 590

gtt aag gga ttg ttc gtt gat cca att tct att tgaactcaat aattccttt    1889
Val Lys Gly Leu Phe Val Asp Pro Ile Ser Ile
                595                 600

ttcattttgt acttcaataa gttataaatg acccgtgcac tagcggtggt gattattgta   1949

tttaaattgc cttttaaatt aatatatgaa tcaagaattt tatag                   1994


<210> SEQ ID NO 42
<211> LENGTH: 601
<212> TYPE: PRT
<213> ORGANISM: Ricinus communis

<400> SEQUENCE: 42

Met Ala Leu Pro Ser Ala Ala Met Gln Ser Asn Pro Glu Lys Leu Asn
 1               5                  10                  15

Leu Phe His Arg Leu Ser Ser Leu Pro Thr Thr Ser Leu Glu Tyr Gly
            20                  25                  30
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Asn Asn Arg Phe Pro Phe Phe Ser Ser Ser Ala Lys Ser His Phe Lys
        35                  40                  45

Lys Pro Thr Gln Ala Cys Leu Ser Ser Thr Thr His Gln Glu Val Arg
    50                  55                  60

Pro Leu Ala Tyr Phe Pro Pro Thr Val Trp Gly Asn Arg Phe Ala Ser
65                  70                  75                  80

Leu Thr Phe Asn Pro Ser Glu Phe Glu Ser Tyr Asp Glu Arg Val Ile
                85                  90                  95

Val Leu Lys Lys Lys Val Lys Asp Ile Leu Ile Ser Ser Thr Ser Asp
            100                 105                 110

Ser Val Glu Thr Val Ile Leu Ile Asp Leu Leu Cys Arg Leu Gly Val
        115                 120                 125

Ser Tyr His Phe Glu Asn Asp Ile Glu Glu Leu Leu Ser Lys Ile Phe
    130                 135                 140

Asn Ser Gln Pro Asp Leu Val Asp Glu Lys Glu Cys Asp Leu Tyr Thr
145                 150                 155                 160

Ala Ala Ile Val Phe Arg Val Phe Arg Gln His Gly Phe Lys Met Ser
                165                 170                 175

Ser Asp Val Phe Ser Lys Phe Lys Asp Ser Asp Gly Lys Phe Lys Glu
            180                 185                 190

Ser Leu Arg Gly Asp Ala Lys Gly Met Leu Ser Leu Phe Glu Ala Ser
        195                 200                 205

His Leu Ser Val His Gly Glu Asp Ile Leu Glu Glu Ala Phe Ala Phe
    210                 215                 220

Thr Lys Asp Tyr Leu Gln Ser Ser Ala Val Glu Leu Phe Pro Asn Leu
225                 230                 235                 240

Lys Arg His Ile Thr Asn Ala Leu Glu Gln Pro Phe His Ser Gly Val
                245                 250                 255

Pro Arg Leu Glu Ala Arg Lys Phe Ile Asp Leu Tyr Glu Ala Asp Ile
            260                 265                 270

Glu Cys Arg Asn Glu Thr Leu Leu Glu Phe Ala Lys Leu Asp Tyr Asn
        275                 280                 285

Arg Val Gln Leu Leu His Gln Gln Glu Leu Cys Gln Phe Ser Lys Trp
    290                 295                 300

Trp Lys Asp Leu Asn Leu Ala Ser Asp Ile Pro Tyr Ala Arg Asp Arg
305                 310                 315                 320

Met Ala Glu Ile Phe Phe Trp Ala Val Ala Met Tyr Phe Glu Pro Asp
                325                 330                 335

Tyr Ala His Thr Arg Met Ile Ile Ala Lys Val Val Leu Leu Ile Ser
            340                 345                 350

Leu Ile Asp Asp Thr Ile Asp Ala Tyr Ala Thr Met Glu Glu Thr His
        355                 360                 365

Ile Leu Ala Glu Ala Val Ala Arg Trp Asp Met Ser Cys Leu Glu Lys
    370                 375                 380

Leu Pro Asp Tyr Met Lys Val Ile Tyr Lys Leu Leu Leu Asn Thr Phe
385                 390                 395                 400

Ser Glu Phe Glu Lys Glu Leu Thr Ala Glu Gly Lys Ser Tyr Ser Val
                405                 410                 415

Lys Tyr Gly Arg Glu Ala Phe Gln Glu Leu Val Arg Gly Tyr Tyr Leu
            420                 425                 430

Glu Ala Val Trp Arg Asp Glu Gly Lys Ile Pro Ser Phe Asp Asp Tyr
        435                 440                 445
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Leu Tyr Asn Gly Ser Met Thr Thr Gly Leu Pro Leu Val Ser Thr Ala
    450                 455                 460

Ser Phe Met Gly Val Gln Glu Ile Thr Gly Leu Asn Glu Phe Gln Trp
465                 470                 475                 480

Leu Glu Thr Asn Pro Lys Leu Ser Tyr Ala Ser Gly Ala Phe Ile Arg
                485                 490                 495

Leu Val Asn Asp Leu Thr Ser His Val Thr Glu Gln Gln Arg Gly His
            500                 505                 510

Val Ala Ser Cys Ile Asp Cys Tyr Met Asn Gln His Gly Val Ser Lys
        515                 520                 525

Asp Glu Ala Val Lys Ile Leu Gln Lys Met Ala Thr Asp Cys Trp Lys
    530                 535                 540

Glu Ile Asn Glu Glu Cys Met Arg Gln Ser Gln Val Ser Val Gly His
545                 550                 555                 560

Leu Met Arg Ile Val Asn Leu Ala Arg Leu Thr Asp Val Ser Tyr Lys
                565                 570                 575

Tyr Gly Asp Gly Tyr Thr Asp Ser Gln Gln Leu Lys Gln Phe Val Lys
            580                 585                 590

Gly Leu Phe Val Asp Pro Ile Ser Ile
        595                 600


<210> SEQ ID NO 43
<211> LENGTH: 2700
<212> TYPE: DNA
<213> ORGANISM: Taxus brevifolia
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (22)...(2607)
<223> OTHER INFORMATION: taxadiene synthase

<400> SEQUENCE: 43

ttcccctgcc tctctggaga a atg gct cag ctc tca ttt aat gca gcg ctg       51
                       Met Ala Gln Leu Ser Phe Asn Ala Ala Leu
                        1               5                   10

aag atg aac gca ttg ggg aac aag gca atc cac gat cca acg aat tgc       99
Lys Met Asn Ala Leu Gly Asn Lys Ala Ile His Asp Pro Thr Asn Cys
                15                  20                  25

aga gcc aaa tct gag cgc caa atg atg tgg gtt tgc tcc aga tca ggg      147
Arg Ala Lys Ser Glu Arg Gln Met Met Trp Val Cys Ser Arg Ser Gly
            30                  35                  40

cga acc aga gta aaa atg tcg aga gga agt ggt ggt cct ggt cct gtc      195
Arg Thr Arg Val Lys Met Ser Arg Gly Ser Gly Gly Pro Gly Pro Val
        45                  50                  55

gta atg atg agc agc agc act ggc act agc aag gtg gtt tcc gag act      243
Val Met Met Ser Ser Ser Thr Gly Thr Ser Lys Val Val Ser Glu Thr
    60                  65                  70

tcc agt acc att gtg gat gat atc cct cga ctc tcc gcc aat tat cat      291
Ser Ser Thr Ile Val Asp Asp Ile Pro Arg Leu Ser Ala Asn Tyr His
75                  80                  85                  90

ggc gat ctg tgg cac cac aat gtt ata caa act ctg gag aca ccg ttt      339
Gly Asp Leu Trp His His Asn Val Ile Gln Thr Leu Glu Thr Pro Phe
                95                  100                 105

cgt gag agt tct act tac caa gaa cgg gca gat gag ctg gtt gtg aaa      387
Arg Glu Ser Ser Thr Tyr Gln Glu Arg Ala Asp Glu Leu Val Val Lys
            110                 115                 120

att aaa gat atg ttc aat gcg ctc gga gac gga gat atc agt ccg tct      435
Ile Lys Asp Met Phe Asn Ala Leu Gly Asp Gly Asp Ile Ser Pro Ser
        125                 130                 135
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gca tac gac act gcg tgg gtg gcg agg ctg gcg acc att tcc tct gat      483
Ala Tyr Asp Thr Ala Trp Val Ala Arg Leu Ala Thr Ile Ser Ser Asp
    140                 145                 150

gga tct gag aag cca cgg ttt cct cag gcc ctc aac tgg gtt ttc aac      531
Gly Ser Glu Lys Pro Arg Phe Pro Gln Ala Leu Asn Trp Val Phe Asn
155                 160                 165                 170

aac cag ctc cag gat gga tcg tgg ggt atc gaa tcg cac ttt agt tta      579
Asn Gln Leu Gln Asp Gly Ser Trp Gly Ile Glu Ser His Phe Ser Leu
                175                 180                 185

tgc gat cga ttg ctt aac acg acc aat tct gtt atc gcc ctc tcg gtt      627
Cys Asp Arg Leu Leu Asn Thr Thr Asn Ser Val Ile Ala Leu Ser Val
            190                 195                 200

tgg aaa aca ggg cac agc caa gta caa caa ggt gct gag ttt att gca      675
Trp Lys Thr Gly His Ser Gln Val Gln Gln Gly Ala Glu Phe Ile Ala
        205                 210                 215

gag aat cta aga tta ctc aat gag gaa gat gag ttg tcc ccg gat ttc      723
Glu Asn Leu Arg Leu Leu Asn Glu Glu Asp Glu Leu Ser Pro Asp Phe
    220                 225                 230

caa ata atc ttt cct gct ctg ctg caa aag gca aaa gcg ttg ggg atc      771
Gln Ile Ile Phe Pro Ala Leu Leu Gln Lys Ala Lys Ala Leu Gly Ile
235                 240                 245                 250

aat ctt cct tac gat ctt cca ttt atc aaa tat ttg tcg aca aca cgg      819
Asn Leu Pro Tyr Asp Leu Pro Phe Ile Lys Tyr Leu Ser Thr Thr Arg
                255                 260                 265

gaa gcc agg ctt aca gat gtt tct gcg gca gca gac aat att cca gcc      867
Glu Ala Arg Leu Thr Asp Val Ser Ala Ala Ala Asp Asn Ile Pro Ala
            270                 275                 280

aac atg ttg aat gcg ttg gaa ggt ctc gag gaa gtt att gac tgg aac      915
Asn Met Leu Asn Ala Leu Glu Gly Leu Glu Glu Val Ile Asp Trp Asn
        285                 290                 295

aag att atg agg ttt caa agt aaa gat gga tct ttc ctg agc tcc cct      963
Lys Ile Met Arg Phe Gln Ser Lys Asp Gly Ser Phe Leu Ser Ser Pro
    300                 305                 310

gcc tcc act gcc tgt gta ctg atg aat aca ggg gac gaa aaa tgt ttc     1011
Ala Ser Thr Ala Cys Val Leu Met Asn Thr Gly Asp Glu Lys Cys Phe
315                 320                 325                 330

act ttt ctc aac aat ctg ctc gac aaa ttc ggc ggc tgc gtg ccc tgt     1059
Thr Phe Leu Asn Asn Leu Leu Asp Lys Phe Gly Gly Cys Val Pro Cys
                335                 340                 345

atg tat tcc atc gat ctg ctg gaa cgc ctt tcg ctg gtt gat aac att     1107
Met Tyr Ser Ile Asp Leu Leu Glu Arg Leu Ser Leu Val Asp Asn Ile
            350                 355                 360

gag cat ctc gga atc ggt cgc cat ttc aaa caa gaa atc aaa gga gct     1155
Glu His Leu Gly Ile Gly Arg His Phe Lys Gln Glu Ile Lys Gly Ala
        365                 370                 375

ctt gat tat gtc tac aga cat tgg agt gaa agg ggc atc ggt tgg ggc     1203
Leu Asp Tyr Val Tyr Arg His Trp Ser Glu Arg Gly Ile Gly Trp Gly
    380                 385                 390

aga gac agc ctt gtt cca gat ctc aac acc aca gcc ctc ggc ctg cga     1251
Arg Asp Ser Leu Val Pro Asp Leu Asn Thr Thr Ala Leu Gly Leu Arg
395                 400                 405                 410

act ctt cgc atg cac gga tac aat gtt tct tca gac gtt ttg aat aat     1299
Thr Leu Arg Met His Gly Tyr Asn Val Ser Ser Asp Val Leu Asn Asn
                415                 420                 425

ttc aaa gat gaa aac ggg cgg ttc ttc tcc tct gcg ggc caa acc cat     1347
Phe Lys Asp Glu Asn Gly Arg Phe Phe Ser Ser Ala Gly Gln Thr His
            430                 435                 440

gtc gaa ttg aga agc gtg gtg aat ctt ttc aga gct tcc gac ctt gca     1395
Val Glu Leu Arg Ser Val Val Asn Leu Phe Arg Ala Ser Asp Leu Ala
        445                 450                 455
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ttt cct gac gaa aga gct atg gac gat gct aga aaa ttt gca gaa cca     1443
Phe Pro Asp Glu Arg Ala Met Asp Asp Ala Arg Lys Phe Ala Glu Pro
    460                 465                 470

tat ctt aga gag gca ctt gca acg aaa atc tca acc aat aca aaa cta     1491
Tyr Leu Arg Glu Ala Leu Ala Thr Lys Ile Ser Thr Asn Thr Lys Leu
475                 480                 485                 490

ttc aaa gag att gag tac gtg gtg gag tac cct tgg cac atg agt atc     1539
Phe Lys Glu Ile Glu Tyr Val Val Glu Tyr Pro Trp His Met Ser Ile
                495                 500                 505

cca cgc tta gaa gcc aga agt tat att gat tca tat gac gac aat tat     1587
Pro Arg Leu Glu Ala Arg Ser Tyr Ile Asp Ser Tyr Asp Asp Asn Tyr
            510                 515                 520

gta tgg cag agg aag act cta tat aga atg cca tct ttg agt aat tca     1635
Val Trp Gln Arg Lys Thr Leu Tyr Arg Met Pro Ser Leu Ser Asn Ser
        525                 530                 535

aaa tgt tta gaa ttg gca aaa ttg gac ttc aat atc gta caa tct ttg     1683
Lys Cys Leu Glu Leu Ala Lys Leu Asp Phe Asn Ile Val Gln Ser Leu
    540                 545                 550

cat caa gag gag ttg aag ctt cta aca aga tgg tgg aag gaa tcc ggc     1731
His Gln Glu Glu Leu Lys Leu Leu Thr Arg Trp Trp Lys Glu Ser Gly
555                 560                 565                 570

atg gca gat ata aat ttc act cga cac cga gtg gcg gag gtt tat ttt     1779
Met Ala Asp Ile Asn Phe Thr Arg His Arg Val Ala Glu Val Tyr Phe
                575                 580                 585

tca tca gct aca ttt gaa ccc gaa tat tct gcc act aga att gcc ttc     1827
Ser Ser Ala Thr Phe Glu Pro Glu Tyr Ser Ala Thr Arg Ile Ala Phe
            590                 595                 600

aca aaa att ggt tgt tta caa gtc ctt ttt gat gat atg gct gac atc     1875
Thr Lys Ile Gly Cys Leu Gln Val Leu Phe Asp Asp Met Ala Asp Ile
        605                 610                 615

ttt gca aca cta gat gaa ttg aaa agt ttc act gag gga gta aag aga     1923
Phe Ala Thr Leu Asp Glu Leu Lys Ser Phe Thr Glu Gly Val Lys Arg
    620                 625                 630

tgg gat aca tct ttg cta cat gag att cca gag tgt atg caa act tgc     1971
Trp Asp Thr Ser Leu Leu His Glu Ile Pro Glu Cys Met Gln Thr Cys
635                 640                 645                 650

ttt aaa gtt tgg ttc aaa tta atg gaa gaa gta aat aat gat gtg gtt     2019
Phe Lys Val Trp Phe Lys Leu Met Glu Glu Val Asn Asn Asp Val Val
                655                 660                 665

aag gta caa gga cgt gac atg ctc gct cac ata aga aaa ccc tgg gag     2067
Lys Val Gln Gly Arg Asp Met Leu Ala His Ile Arg Lys Pro Trp Glu
            670                 675                 680

ttg tac ttc aat tgt tat gta caa gaa agg gag tgg ctt gaa gcc ggg     2115
Leu Tyr Phe Asn Cys Tyr Val Gln Glu Arg Glu Trp Leu Glu Ala Gly
        685                 690                 695

tat ata cca act ttt gaa gag tac tta aag act tat gct ata tca gta     2163
Tyr Ile Pro Thr Phe Glu Glu Tyr Leu Lys Thr Tyr Ala Ile Ser Val
    700                 705                 710

ggc ctt gga ccg tgt acc cta caa cca ata cta cta atg ggt gag ctt     2211
Gly Leu Gly Pro Cys Thr Leu Gln Pro Ile Leu Leu Met Gly Glu Leu
715                 720                 725                 730

gtg aaa gat gat gtt gtt gag aaa gtg cac tat ccc tca aat atg ttt     2259
Val Lys Asp Asp Val Val Glu Lys Val His Tyr Pro Ser Asn Met Phe
                735                 740                 745

gag ctt gta tcc ttg agc tgg cga cta aca aac gac acc aaa aca tat     2307
Glu Leu Val Ser Leu Ser Trp Arg Leu Thr Asn Asp Thr Lys Thr Tyr
            750                 755                 760

cag gct gaa aag gct cga gga caa caa gcc tca ggc ata gca tgc tat     2355
Gln Ala Glu Lys Ala Arg Gly Gln Gln Ala Ser Gly Ile Ala Cys Tyr
        765                 770                 775
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atg aag gat aat cca gga gca act gag gaa gat gcc att aag cac ata     2403
Met Lys Asp Asn Pro Gly Ala Thr Glu Glu Asp Ala Ile Lys His Ile
    780                 785                 790

tgt cgt gtt gtt gat cgg gcc ttg aaa gaa gca agc ttt gaa tat ttc     2451
Cys Arg Val Val Asp Arg Ala Leu Lys Glu Ala Ser Phe Glu Tyr Phe
795                 800                 805                 810

aaa cca tcc aat gat atc cca atg ggt tgc aag tcc ttt att ttt aac     2499
Lys Pro Ser Asn Asp Ile Pro Met Gly Cys Lys Ser Phe Ile Phe Asn
                815                 820                 825

ctt aga ttg tgt gtc caa atc ttt tac aag ttt ata gat ggg tac gga     2547
Leu Arg Leu Cys Val Gln Ile Phe Tyr Lys Phe Ile Asp Gly Tyr Gly
            830                 835                 840

atc gcc aat gag gag att aag gac tat ata aga aaa gtt tat att gat     2595
Ile Ala Asn Glu Glu Ile Lys Asp Tyr Ile Arg Lys Val Tyr Ile Asp
        845                 850                 855

cca att caa gta tga tatatcatgt aaaacctctt tttcatgata aattgactta     2650
Pro Ile Gln Val
    860

ttattgtatt ggcaaaaaaa aaaaaaaaaa aaaaaaaaaa aaaaaaaaaa             2700


<210> SEQ ID NO 44
<211> LENGTH: 862
<212> TYPE: PRT
<213> ORGANISM: Taxus brevifolia

<400> SEQUENCE: 44

Met Ala Gln Leu Ser Phe Asn Ala Ala Leu Lys Met Asn Ala Leu Gly
 1               5                  10                  15

Asn Lys Ala Ile His Asp Pro Thr Asn Cys Arg Ala Lys Ser Glu Arg
            20                  25                  30

Gln Met Met Trp Val Cys Ser Arg Ser Gly Arg Thr Arg Val Lys Met
        35                  40                  45

Ser Arg Gly Ser Gly Gly Pro Gly Pro Val Val Met Met Ser Ser Ser
    50                  55                  60

Thr Gly Thr Ser Lys Val Val Ser Glu Thr Ser Ser Thr Ile Val Asp
65                  70                  75                  80

Asp Ile Pro Arg Leu Ser Ala Asn Tyr His Gly Asp Leu Trp His His
                85                  90                  95

Asn Val Ile Gln Thr Leu Glu Thr Pro Phe Arg Glu Ser Ser Thr Tyr
            100                 105                 110

Gln Glu Arg Ala Asp Glu Leu Val Val Lys Ile Lys Asp Met Phe Asn
        115                 120                 125

Ala Leu Gly Asp Gly Asp Ile Ser Pro Ser Ala Tyr Asp Thr Ala Trp
    130                 135                 140

Val Ala Arg Leu Ala Thr Ile Ser Ser Asp Gly Ser Glu Lys Pro Arg
145                 150                 155                 160

Phe Pro Gln Ala Leu Asn Trp Val Phe Asn Asn Gln Leu Gln Asp Gly
                165                 170                 175

Ser Trp Gly Ile Glu Ser His Phe Ser Leu Cys Asp Arg Leu Leu Asn
            180                 185                 190

Thr Thr Asn Ser Val Ile Ala Leu Ser Val Trp Lys Thr Gly His Ser
        195                 200                 205

Gln Val Gln Gln Gly Ala Glu Phe Ile Ala Glu Asn Leu Arg Leu Leu
    210                 215                 220

Asn Glu Glu Asp Glu Leu Ser Pro Asp Phe Gln Ile Ile Phe Pro Ala
225                 230                 235                 240
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Leu Leu Gln Lys Ala Lys Ala Leu Gly Ile Asn Leu Pro Tyr Asp Leu
                245                 250                 255

Pro Phe Ile Lys Tyr Leu Ser Thr Thr Arg Glu Ala Arg Leu Thr Asp
            260                 265                 270

Val Ser Ala Ala Ala Asp Asn Ile Pro Ala Asn Met Leu Asn Ala Leu
        275                 280                 285

Glu Gly Leu Glu Glu Val Ile Asp Trp Asn Lys Ile Met Arg Phe Gln
    290                 295                 300

Ser Lys Asp Gly Ser Phe Leu Ser Ser Pro Ala Ser Thr Ala Cys Val
305                 310                 315                 320

Leu Met Asn Thr Gly Asp Glu Lys Cys Phe Thr Phe Leu Asn Asn Leu
                325                 330                 335

Leu Asp Lys Phe Gly Gly Cys Val Pro Cys Met Tyr Ser Ile Asp Leu
            340                 345                 350

Leu Glu Arg Leu Ser Leu Val Asp Asn Ile Glu His Leu Gly Ile Gly
        355                 360                 365

Arg His Phe Lys Gln Glu Ile Lys Gly Ala Leu Asp Tyr Val Tyr Arg
    370                 375                 380

His Trp Ser Glu Arg Gly Ile Gly Trp Gly Arg Asp Ser Leu Val Pro
385                 390                 395                 400

Asp Leu Asn Thr Thr Ala Leu Gly Leu Arg Thr Leu Arg Met His Gly
                405                 410                 415

Tyr Asn Val Ser Ser Asp Val Leu Asn Asn Phe Lys Asp Glu Asn Gly
            420                 425                 430

Arg Phe Phe Ser Ser Ala Gly Gln Thr His Val Glu Leu Arg Ser Val
        435                 440                 445

Val Asn Leu Phe Arg Ala Ser Asp Leu Ala Phe Pro Asp Glu Arg Ala
    450                 455                 460

Met Asp Asp Ala Arg Lys Phe Ala Glu Pro Tyr Leu Arg Glu Ala Leu
465                 470                 475                 480

Ala Thr Lys Ile Ser Thr Asn Thr Lys Leu Phe Lys Glu Ile Glu Tyr
                485                 490                 495

Val Val Glu Tyr Pro Trp His Met Ser Ile Pro Arg Leu Glu Ala Arg
            500                 505                 510

Ser Tyr Ile Asp Ser Tyr Asp Asp Asn Tyr Val Trp Gln Arg Lys Thr
        515                 520                 525

Leu Tyr Arg Met Pro Ser Leu Ser Asn Ser Lys Cys Leu Glu Leu Ala
    530                 535                 540

Lys Leu Asp Phe Asn Ile Val Gln Ser Leu His Gln Glu Glu Leu Lys
545                 550                 555                 560

Leu Leu Thr Arg Trp Trp Lys Glu Ser Gly Met Ala Asp Ile Asn Phe
                565                 570                 575

Thr Arg His Arg Val Ala Glu Val Tyr Phe Ser Ser Ala Thr Phe Glu
            580                 585                 590

Pro Glu Tyr Ser Ala Thr Arg Ile Ala Phe Thr Lys Ile Gly Cys Leu
        595                 600                 605

Gln Val Leu Phe Asp Asp Met Ala Asp Ile Phe Ala Thr Leu Asp Glu
    610                 615                 620

Leu Lys Ser Phe Thr Glu Gly Val Lys Arg Trp Asp Thr Ser Leu Leu
625                 630                 635                 640

His Glu Ile Pro Glu Cys Met Gln Thr Cys Phe Lys Val Trp Phe Lys
                645                 650                 655
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Leu Met Glu Glu Val Asn Asn Asp Val Val Lys Val Gln Gly Arg Asp
            660                 665                 670

Met Leu Ala His Ile Arg Lys Pro Trp Glu Leu Tyr Phe Asn Cys Tyr
        675                 680                 685

Val Gln Glu Arg Glu Trp Leu Glu Ala Gly Tyr Ile Pro Thr Phe Glu
    690                 695                 700

Glu Tyr Leu Lys Thr Tyr Ala Ile Ser Val Gly Leu Gly Pro Cys Thr
705                 710                 715                 720

Leu Gln Pro Ile Leu Leu Met Gly Glu Leu Val Lys Asp Asp Val Val
                725                 730                 735

Glu Lys Val His Tyr Pro Ser Asn Met Phe Glu Leu Val Ser Leu Ser
            740                 745                 750

Trp Arg Leu Thr Asn Asp Thr Lys Thr Tyr Gln Ala Glu Lys Ala Arg
        755                 760                 765

Gly Gln Gln Ala Ser Gly Ile Ala Cys Tyr Met Lys Asp Asn Pro Gly
    770                 775                 780

Ala Thr Glu Glu Asp Ala Ile Lys His Ile Cys Arg Val Val Asp Arg
785                 790                 795                 800

Ala Leu Lys Glu Ala Ser Phe Glu Tyr Phe Lys Pro Ser Asn Asp Ile
                805                 810                 815

Pro Met Gly Cys Lys Ser Phe Ile Phe Asn Leu Arg Leu Cys Val Gln
            820                 825                 830

Ile Phe Tyr Lys Phe Ile Asp Gly Tyr Gly Ile Ala Asn Glu Glu Ile
        835                 840                 845

Lys Asp Tyr Ile Arg Lys Val Tyr Ile Asp Pro Ile Gln Val
    850                 855                 860


<210> SEQ ID NO 45
<211> LENGTH: 2424
<212> TYPE: DNA
<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (2)...(2347)
<223> OTHER INFORMATION: E-alpha-bisabolene synthase

<400> SEQUENCE: 45

g ggt tat gat ctt gtg cat tct ctt aaa tca cct tat att gat tct agt     49
  Gly Tyr Asp Leu Val His Ser Leu Lys Ser Pro Tyr Ile Asp Ser Ser
   1               5                  10                  15

tac aga gaa cgc gcg gag gtc ctt gtt agc gag att aaa gtg atg ctt       97
Tyr Arg Glu Arg Ala Glu Val Leu Val Ser Glu Ile Lys Val Met Leu
             20                  25                  30

aat cca gct att aca gga gat gga gaa tca atg att act cca tct gct      145
Asn Pro Ala Ile Thr Gly Asp Gly Glu Ser Met Ile Thr Pro Ser Ala
         35                  40                  45

tat gac aca gca tgg gta gcg agg gtg ccc gcc att gat ggc tct gct      193
Tyr Asp Thr Ala Trp Val Ala Arg Val Pro Ala Ile Asp Gly Ser Ala
     50                  55                  60

cgc ccg caa ttt ccc caa aca gtt gac tgg att ttg aaa aac cag tta      241
Arg Pro Gln Phe Pro Gln Thr Val Asp Trp Ile Leu Lys Asn Gln Leu
 65                  70                  75                  80

aaa gat ggt tca tgg gga att cag tcc cac ttt ctg ctg tcc gac cgt      289
Lys Asp Gly Ser Trp Gly Ile Gln Ser His Phe Leu Leu Ser Asp Arg
                 85                  90                  95

ctt ctt gcc act ctt tct tgt gtt ctt gtg ctc ctt aaa tgg aac gtt      337
Leu Leu Ala Thr Leu Ser Cys Val Leu Val Leu Leu Lys Trp Asn Val
            100                 105                 110
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ggg gat ctg caa gta gag cag gga att gaa ttc ata aag agc aat ctg      385
Gly Asp Leu Gln Val Glu Gln Gly Ile Glu Phe Ile Lys Ser Asn Leu
        115                 120                 125

gaa cta gta aag gat gaa acc gat caa gat agc ttg gta aca gac ttt      433
Glu Leu Val Lys Asp Glu Thr Asp Gln Asp Ser Leu Val Thr Asp Phe
    130                 135                 140

gag atc ata ttt cct tct ctg tta aga gaa gct caa tct ctg cgc ctc      481
Glu Ile Ile Phe Pro Ser Leu Leu Arg Glu Ala Gln Ser Leu Arg Leu
145                 150                 155                 160

gga ctt ccc tac gac ctg cct tat ata cat ctg ttg cag act aaa cgg      529
Gly Leu Pro Tyr Asp Leu Pro Tyr Ile His Leu Leu Gln Thr Lys Arg
                165                 170                 175

cag gaa aga tta gca aaa ctt tca agg gag gaa att tat gcg gtt ccg      577
Gln Glu Arg Leu Ala Lys Leu Ser Arg Glu Glu Ile Tyr Ala Val Pro
            180                 185                 190

tcg cca ttg ttg tat tct tta gag gga ata caa gat ata gtt gaa tgg      625
Ser Pro Leu Leu Tyr Ser Leu Glu Gly Ile Gln Asp Ile Val Glu Trp
        195                 200                 205

gaa cga ata atg gaa gtt caa agt cag gat ggg tct ttc tta agc tca      673
Glu Arg Ile Met Glu Val Gln Ser Gln Asp Gly Ser Phe Leu Ser Ser
    210                 215                 220

cct gct tct act gcc tgc gtt ttc atg cac aca gga gac gcg aaa tgc      721
Pro Ala Ser Thr Ala Cys Val Phe Met His Thr Gly Asp Ala Lys Cys
225                 230                 235                 240

ctt gaa ttc ttg aac agt gtg atg atc aag ttt gga aat ttt gtt ccc      769
Leu Glu Phe Leu Asn Ser Val Met Ile Lys Phe Gly Asn Phe Val Pro
                245                 250                 255

tgc ctg tat cct gtg gat ctg ctg gaa cgc ctg ttg atc gta gat aat      817
Cys Leu Tyr Pro Val Asp Leu Leu Glu Arg Leu Leu Ile Val Asp Asn
            260                 265                 270

att gta cgc ctt gga atc tat aga cac ttt gaa aag gaa atc aag gaa      865
Ile Val Arg Leu Gly Ile Tyr Arg His Phe Glu Lys Glu Ile Lys Glu
        275                 280                 285

gct ctt gat tat gtt tac agg cat tgg aac gaa aga gga att ggg tgg      913
Ala Leu Asp Tyr Val Tyr Arg His Trp Asn Glu Arg Gly Ile Gly Trp
    290                 295                 300

ggc aga cta aat ccc ata gca gat ctt gag acc act gct ttg gga ttt      961
Gly Arg Leu Asn Pro Ile Ala Asp Leu Glu Thr Thr Ala Leu Gly Phe
305                 310                 315                 320

cga ttg ctt cgg ctg cat agg tac aat gta tct cca gcc att ttt gac     1009
Arg Leu Leu Arg Leu His Arg Tyr Asn Val Ser Pro Ala Ile Phe Asp
                325                 330                 335

aac ttc aaa gat gcc aat ggg aaa ttc att tgc tcg acc ggt caa ttc     1057
Asn Phe Lys Asp Ala Asn Gly Lys Phe Ile Cys Ser Thr Gly Gln Phe
            340                 345                 350

aac aaa gat gta gca agc atg ctg aat ctt tat aga gct tcc cag ctc     1105
Asn Lys Asp Val Ala Ser Met Leu Asn Leu Tyr Arg Ala Ser Gln Leu
        355                 360                 365

gca ttt ccc gga gaa aac att ctt gat gaa gct aaa agc ttc gct act     1153
Ala Phe Pro Gly Glu Asn Ile Leu Asp Glu Ala Lys Ser Phe Ala Thr
    370                 375                 380

aaa tat ttg aga gaa gct ctt gag aaa agt gag act tcc agt gca tgg     1201
Lys Tyr Leu Arg Glu Ala Leu Glu Lys Ser Glu Thr Ser Ser Ala Trp
385                 390                 395                 400

aac aac aaa caa aac ctg agc caa gag atc aaa tac gcg ctg aag act     1249
Asn Asn Lys Gln Asn Leu Ser Gln Glu Ile Lys Tyr Ala Leu Lys Thr
                405                 410                 415

tct tgg cat gcc agt gtt ccg aga gtg gaa gca aag aga tac tgt caa     1297
Ser Trp His Ala Ser Val Pro Arg Val Glu Ala Lys Arg Tyr Cys Gln
            420                 425                 430
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gtg tat cgc cca gat tat gca cgc ata gca aaa tgc gtt tac aag cta     1345
Val Tyr Arg Pro Asp Tyr Ala Arg Ile Ala Lys Cys Val Tyr Lys Leu
        435                 440                 445

ccc tac gtg aac aat gaa aag ttt tta gag ctg gga aaa tta gat ttc     1393
Pro Tyr Val Asn Asn Glu Lys Phe Leu Glu Leu Gly Lys Leu Asp Phe
    450                 455                 460

aac att atc cag tcc atc cac caa gaa gaa atg aag aat gtt acc agc     1441
Asn Ile Ile Gln Ser Ile His Gln Glu Glu Met Lys Asn Val Thr Ser
465                 470                 475                 480

tgg ttt aga gat tcg ggg ttg cca cta ttc acc ttc gct cgg gag agg     1489
Trp Phe Arg Asp Ser Gly Leu Pro Leu Phe Thr Phe Ala Arg Glu Arg
                485                 490                 495

ccg ctg gaa ttc tac ttc tta gta gcg gcg ggg acc tat gaa ccc cag     1537
Pro Leu Glu Phe Tyr Phe Leu Val Ala Ala Gly Thr Tyr Glu Pro Gln
            500                 505                 510

tat gcc aaa tgc agg ttc ctc ttt aca aaa gtg gca tgc ttg cag act     1585
Tyr Ala Lys Cys Arg Phe Leu Phe Thr Lys Val Ala Cys Leu Gln Thr
        515                 520                 525

gtt ctg gac gat atg tat gac act tat gga acc cta gat gaa ttg aag     1633
Val Leu Asp Asp Met Tyr Asp Thr Tyr Gly Thr Leu Asp Glu Leu Lys
    530                 535                 540

cta ttc act gag gct gtg aga aga tgg gac ctc tcc ttt aca gaa aac     1681
Leu Phe Thr Glu Ala Val Arg Arg Trp Asp Leu Ser Phe Thr Glu Asn
545                 550                 555                 560

ctt cca gac tat atg aaa cta tgt tac caa atc tat tat gac ata gtt     1729
Leu Pro Asp Tyr Met Lys Leu Cys Tyr Gln Ile Tyr Tyr Asp Ile Val
                565                 570                 575

cac gag gtg gct tgg gag gca gag aag gaa cag ggg cgt gaa ttg gtc     1777
His Glu Val Ala Trp Glu Ala Glu Lys Glu Gln Gly Arg Glu Leu Val
            580                 585                 590

agc ttt ttc aga aag gga tgg gag gat tat ctt ctg ggt tat tat gaa     1825
Ser Phe Phe Arg Lys Gly Trp Glu Asp Tyr Leu Leu Gly Tyr Tyr Glu
        595                 600                 605

gaa gct gaa tgg tta gct gct gag tat gtg cct acc ttg gac gag tac     1873
Glu Ala Glu Trp Leu Ala Ala Glu Tyr Val Pro Thr Leu Asp Glu Tyr
    610                 615                 620

ata aag aat gga atc aca tct atc ggc caa cgt ata ctt ctg ttg agt     1921
Ile Lys Asn Gly Ile Thr Ser Ile Gly Gln Arg Ile Leu Leu Leu Ser
625                 630                 635                 640

gga gtg ttg ata atg gat ggg caa ctc ctt tcg caa gag gca tta gag     1969
Gly Val Leu Ile Met Asp Gly Gln Leu Leu Ser Gln Glu Ala Leu Glu
                645                 650                 655

aaa gta gat tat cca gga aga cgt gtt ctc aca gag ctg aat agc ctc     2017
Lys Val Asp Tyr Pro Gly Arg Arg Val Leu Thr Glu Leu Asn Ser Leu
            660                 665                 670

att tcc cgc ctg gcg gat gac acg aag aca tat aaa gct gag aag gct     2065
Ile Ser Arg Leu Ala Asp Asp Thr Lys Thr Tyr Lys Ala Glu Lys Ala
        675                 680                 685

cgt gga gaa ttg gcg tcc agc att gaa tgt tac atg aaa gac cat cct     2113
Arg Gly Glu Leu Ala Ser Ser Ile Glu Cys Tyr Met Lys Asp His Pro
    690                 695                 700

gaa tgt aca gag gaa gag gct ctc gat cac atc tat agc att ctg gag     2161
Glu Cys Thr Glu Glu Glu Ala Leu Asp His Ile Tyr Ser Ile Leu Glu
705                 710                 715                 720

ccg gcg gtg aag gaa ctg aca aga gag ttt ctg aag ccc gac gac gtc     2209
Pro Ala Val Lys Glu Leu Thr Arg Glu Phe Leu Lys Pro Asp Asp Val
                725                 730                 735

cca ttc gcc tgc aag aag atg ctt ttc gag gag aca aga gtg acg atg     2257
Pro Phe Ala Cys Lys Lys Met Leu Phe Glu Glu Thr Arg Val Thr Met
            740                 745                 750
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gtg ata ttc aag gat gga gat gga ttc ggt gtt tcc aaa tta gaa gtc     2305
Val Ile Phe Lys Asp Gly Asp Gly Phe Gly Val Ser Lys Leu Glu Val
        755                 760                 765

aaa gat cat atc aaa gag tgt ctc att gaa ccg ctg cca ctg taa         2350
Lys Asp His Ile Lys Glu Cys Leu Ile Glu Pro Leu Pro Leu
    770                 775                 780

tcaaaatagt tgcaataata attgaaataa tgtcaactat gtttcacaaa aaaaaaaaaa   2410

aaaaaaaaaa aaaa                                                    2424


<210> SEQ ID NO 46
<211> LENGTH: 782
<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 46

Gly Tyr Asp Leu Val His Ser Leu Lys Ser Pro Tyr Ile Asp Ser Ser
 1               5                  10                  15

Tyr Arg Glu Arg Ala Glu Val Leu Val Ser Glu Ile Lys Val Met Leu
            20                  25                  30

Asn Pro Ala Ile Thr Gly Asp Gly Glu Ser Met Ile Thr Pro Ser Ala
        35                  40                  45

Tyr Asp Thr Ala Trp Val Ala Arg Val Pro Ala Ile Asp Gly Ser Ala
    50                  55                  60

Arg Pro Gln Phe Pro Gln Thr Val Asp Trp Ile Leu Lys Asn Gln Leu
65                  70                  75                  80

Lys Asp Gly Ser Trp Gly Ile Gln Ser His Phe Leu Leu Ser Asp Arg
                85                  90                  95

Leu Leu Ala Thr Leu Ser Cys Val Leu Val Leu Leu Lys Trp Asn Val
            100                 105                 110

Gly Asp Leu Gln Val Glu Gln Gly Ile Glu Phe Ile Lys Ser Asn Leu
        115                 120                 125

Glu Leu Val Lys Asp Glu Thr Asp Gln Asp Ser Leu Val Thr Asp Phe
    130                 135                 140

Glu Ile Ile Phe Pro Ser Leu Leu Arg Glu Ala Gln Ser Leu Arg Leu
145                 150                 155                 160

Gly Leu Pro Tyr Asp Leu Pro Tyr Ile His Leu Leu Gln Thr Lys Arg
                165                 170                 175

Gln Glu Arg Leu Ala Lys Leu Ser Arg Glu Glu Ile Tyr Ala Val Pro
            180                 185                 190

Ser Pro Leu Leu Tyr Ser Leu Glu Gly Ile Gln Asp Ile Val Glu Trp
        195                 200                 205

Glu Arg Ile Met Glu Val Gln Ser Gln Asp Gly Ser Phe Leu Ser Ser
    210                 215                 220

Pro Ala Ser Thr Ala Cys Val Phe Met His Thr Gly Asp Ala Lys Cys
225                 230                 235                 240

Leu Glu Phe Leu Asn Ser Val Met Ile Lys Phe Gly Asn Phe Val Pro
                245                 250                 255

Cys Leu Tyr Pro Val Asp Leu Leu Glu Arg Leu Leu Ile Val Asp Asn
            260                 265                 270

Ile Val Arg Leu Gly Ile Tyr Arg His Phe Glu Lys Glu Ile Lys Glu
        275                 280                 285

Ala Leu Asp Tyr Val Tyr Arg His Trp Asn Glu Arg Gly Ile Gly Trp
    290                 295                 300

Gly Arg Leu Asn Pro Ile Ala Asp Leu Glu Thr Thr Ala Leu Gly Phe
305                 310                 315                 320
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Arg Leu Leu Arg Leu His Arg Tyr Asn Val Ser Pro Ala Ile Phe Asp
                325                 330                 335

Asn Phe Lys Asp Ala Asn Gly Lys Phe Ile Cys Ser Thr Gly Gln Phe
            340                 345                 350

Asn Lys Asp Val Ala Ser Met Leu Asn Leu Tyr Arg Ala Ser Gln Leu
        355                 360                 365

Ala Phe Pro Gly Glu Asn Ile Leu Asp Glu Ala Lys Ser Phe Ala Thr
    370                 375                 380

Lys Tyr Leu Arg Glu Ala Leu Glu Lys Ser Glu Thr Ser Ser Ala Trp
385                 390                 395                 400

Asn Asn Lys Gln Asn Leu Ser Gln Glu Ile Lys Tyr Ala Leu Lys Thr
                405                 410                 415

Ser Trp His Ala Ser Val Pro Arg Val Glu Ala Lys Arg Tyr Cys Gln
            420                 425                 430

Val Tyr Arg Pro Asp Tyr Ala Arg Ile Ala Lys Cys Val Tyr Lys Leu
        435                 440                 445

Pro Tyr Val Asn Asn Glu Lys Phe Leu Glu Leu Gly Lys Leu Asp Phe
    450                 455                 460

Asn Ile Ile Gln Ser Ile His Gln Glu Glu Met Lys Asn Val Thr Ser
465                 470                 475                 480

Trp Phe Arg Asp Ser Gly Leu Pro Leu Phe Thr Phe Ala Arg Glu Arg
                485                 490                 495

Pro Leu Glu Phe Tyr Phe Leu Val Ala Ala Gly Thr Tyr Glu Pro Gln
            500                 505                 510

Tyr Ala Lys Cys Arg Phe Leu Phe Thr Lys Val Ala Cys Leu Gln Thr
        515                 520                 525

Val Leu Asp Asp Met Tyr Asp Thr Tyr Gly Thr Leu Asp Glu Leu Lys
    530                 535                 540

Leu Phe Thr Glu Ala Val Arg Arg Trp Asp Leu Ser Phe Thr Glu Asn
545                 550                 555                 560

Leu Pro Asp Tyr Met Lys Leu Cys Tyr Gln Ile Tyr Tyr Asp Ile Val
                565                 570                 575

His Glu Val Ala Trp Glu Ala Glu Lys Glu Gln Gly Arg Glu Leu Val
            580                 585                 590

Ser Phe Phe Arg Lys Gly Trp Glu Asp Tyr Leu Leu Gly Tyr Tyr Glu
        595                 600                 605

Glu Ala Glu Trp Leu Ala Ala Glu Tyr Val Pro Thr Leu Asp Glu Tyr
    610                 615                 620

Ile Lys Asn Gly Ile Thr Ser Ile Gly Gln Arg Ile Leu Leu Leu Ser
625                 630                 635                 640

Gly Val Leu Ile Met Asp Gly Gln Leu Leu Ser Gln Glu Ala Leu Glu
                645                 650                 655

Lys Val Asp Tyr Pro Gly Arg Arg Val Leu Thr Glu Leu Asn Ser Leu
            660                 665                 670

Ile Ser Arg Leu Ala Asp Asp Thr Lys Thr Tyr Lys Ala Glu Lys Ala
        675                 680                 685

Arg Gly Glu Leu Ala Ser Ser Ile Glu Cys Tyr Met Lys Asp His Pro
    690                 695                 700

Glu Cys Thr Glu Glu Glu Ala Leu Asp His Ile Tyr Ser Ile Leu Glu
705                 710                 715                 720

Pro Ala Val Lys Glu Leu Thr Arg Glu Phe Leu Lys Pro Asp Asp Val
                725                 730                 735
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```
Pro Phe Ala Cys Lys Lys Met Leu Phe Glu Glu Thr Arg Val Thr Met
            740                 745                 750

Val Ile Phe Lys Asp Gly Asp Gly Phe Gly Val Ser Lys Leu Glu Val
        755                 760                 765

Lys Asp His Ile Lys Glu Cys Leu Ile Glu Pro Leu Pro Leu
    770                 775                 780
```

<210> SEQ ID NO 47
<211> LENGTH: 1865
<212> TYPE: DNA
<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (1)...(1743)
<223> OTHER INFORMATION: d-selinene synthase

<400> SEQUENCE: 47

```
atg gct gag att tct gaa tct tcc atc cct cga cgc aca ggg aat cat       48
Met Ala Glu Ile Ser Glu Ser Ser Ile Pro Arg Arg Thr Gly Asn His
 1               5                  10                  15

cac gga aat gtg tgg gac gat gac ctc ata cac tct ctc aac tcg ccc       96
His Gly Asn Val Trp Asp Asp Asp Leu Ile His Ser Leu Asn Ser Pro
             20                  25                  30

tat ggg gca cct gca tat tat gag ctc ctt caa aag ctt att cag gag      144
Tyr Gly Ala Pro Ala Tyr Tyr Glu Leu Leu Gln Lys Leu Ile Gln Glu
         35                  40                  45

atc aag cat tta ctt ttg act gaa atg gaa atg gat gat ggc gat cat      192
Ile Lys His Leu Leu Leu Thr Glu Met Glu Met Asp Asp Gly Asp His
     50                  55                  60

gat tta atc aaa cgt ctt cag atc gtt gac act ttg gaa tgc ctg gga      240
Asp Leu Ile Lys Arg Leu Gln Ile Val Asp Thr Leu Glu Cys Leu Gly
 65                  70                  75                  80

atc gat aga cat ttt gaa cac gaa ata caa aca gct gct tta gat tac      288
Ile Asp Arg His Phe Glu His Glu Ile Gln Thr Ala Ala Leu Asp Tyr
                 85                  90                  95

gtt tac aga tgg tgg aac gaa aaa ggt atc ggg gag gga tca aga gat      336
Val Tyr Arg Trp Trp Asn Glu Lys Gly Ile Gly Glu Gly Ser Arg Asp
            100                 105                 110

tcc ttc agc aaa gat ctg aac gct acg gct tta gga ttt cgc gct ctc      384
Ser Phe Ser Lys Asp Leu Asn Ala Thr Ala Leu Gly Phe Arg Ala Leu
        115                 120                 125

cga ctg cat cga tat aac gta tcg tca ggt gtg ttg aag aat ttc aag      432
Arg Leu His Arg Tyr Asn Val Ser Ser Gly Val Leu Lys Asn Phe Lys
    130                 135                 140

gat gaa aac ggg aag ttc ttc tgc aac ttt act ggt gaa gaa gga aga      480
Asp Glu Asn Gly Lys Phe Phe Cys Asn Phe Thr Gly Glu Glu Gly Arg
145                 150                 155                 160

gga gat aaa caa gtg aga agc atg ttg tcg tta ctt cga gct tca gag      528
Gly Asp Lys Gln Val Arg Ser Met Leu Ser Leu Leu Arg Ala Ser Glu
                165                 170                 175

att tcg ttt ccc gga gaa aaa gtg atg gaa gag gcc aag gca ttc aca      576
Ile Ser Phe Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr
            180                 185                 190

aga gaa tat cta aac caa gtt tta gct gga cac ggg gat gtg act gac      624
Arg Glu Tyr Leu Asn Gln Val Leu Ala Gly His Gly Asp Val Thr Asp
        195                 200                 205

gtg gat caa agc ctt ttg aga gag gtg aag tac gca ttg gag ttt cca      672
Val Asp Gln Ser Leu Leu Arg Glu Val Lys Tyr Ala Leu Glu Phe Pro
    210                 215                 220
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tgg cat tgc agt gtg ccg aga tgg gag gca agg agc ttt ctc gaa ata      720
Trp His Cys Ser Val Pro Arg Trp Glu Ala Arg Ser Phe Leu Glu Ile
225                 230                 235                 240

tat gga cac aac cat tcg tgg ctc aag tcg aat atc aac caa aaa atg      768
Tyr Gly His Asn His Ser Trp Leu Lys Ser Asn Ile Asn Gln Lys Met
                245                 250                 255

ttg aag tta gcc aaa ttg gac ttc aat att ctg caa tgc aaa cat cac      816
Leu Lys Leu Ala Lys Leu Asp Phe Asn Ile Leu Gln Cys Lys His His
            260                 265                 270

aag gag ata cag ttt att aca agg tgg tgg aga gac tcg ggt ata tcg      864
Lys Glu Ile Gln Phe Ile Thr Arg Trp Trp Arg Asp Ser Gly Ile Ser
        275                 280                 285

cag ctg aat ttc tat cga aag cga cac gtg gaa tat tat tct tgg gtt      912
Gln Leu Asn Phe Tyr Arg Lys Arg His Val Glu Tyr Tyr Ser Trp Val
    290                 295                 300

gtt atg tgc att ttt gag cca gag ttc tct gaa agt aga att gcc ttc      960
Val Met Cys Ile Phe Glu Pro Glu Phe Ser Glu Ser Arg Ile Ala Phe
305                 310                 315                 320

gcc aaa act gct atc ctg tgt act gtt cta gat gac ctc tat gat acg     1008
Ala Lys Thr Ala Ile Leu Cys Thr Val Leu Asp Asp Leu Tyr Asp Thr
                325                 330                 335

cac gca aca ttg cat gaa atc aaa atc atg aca gag gga gtg aga cga     1056
His Ala Thr Leu His Glu Ile Lys Ile Met Thr Glu Gly Val Arg Arg
            340                 345                 350

tgg gat ctt tcg ttg aca gat gac ctc cca gac tac att aaa att gca     1104
Trp Asp Leu Ser Leu Thr Asp Asp Leu Pro Asp Tyr Ile Lys Ile Ala
        355                 360                 365

ttc cag ttc ttc ttc aat aca gtg aat gaa ttg ata gtt gaa atc gtg     1152
Phe Gln Phe Phe Phe Asn Thr Val Asn Glu Leu Ile Val Glu Ile Val
    370                 375                 380

aaa cgg caa ggg cgg gat atg aca acc ata gtt aaa gat tgc tgg aag     1200
Lys Arg Gln Gly Arg Asp Met Thr Thr Ile Val Lys Asp Cys Trp Lys
385                 390                 395                 400

cga tac att gag tct tat ctg caa gaa gcg gaa tgg ata gca act gga     1248
Arg Tyr Ile Glu Ser Tyr Leu Gln Glu Ala Glu Trp Ile Ala Thr Gly
                405                 410                 415

cat att ccc act ttt aac gaa tac ata aag aac ggc atg gct agc tca     1296
His Ile Pro Thr Phe Asn Glu Tyr Ile Lys Asn Gly Met Ala Ser Ser
            420                 425                 430

ggg atg tgt att cta aat ttg aat cca ctt ctc ttg ttg gat aaa ctt     1344
Gly Met Cys Ile Leu Asn Leu Asn Pro Leu Leu Leu Leu Asp Lys Leu
        435                 440                 445

ctc ccc gac aac att ctg gag caa ata cat tct cca tcc aag atc ctg     1392
Leu Pro Asp Asn Ile Leu Glu Gln Ile His Ser Pro Ser Lys Ile Leu
    450                 455                 460

gac ctc tta gaa ttg acg ggc aga atc gcc gat gac tta aaa gat ttc     1440
Asp Leu Leu Glu Leu Thr Gly Arg Ile Ala Asp Asp Leu Lys Asp Phe
465                 470                 475                 480

gag gac gag aag gaa cgc ggg gag atg gct tca tct tta cag tgt tat     1488
Glu Asp Glu Lys Glu Arg Gly Glu Met Ala Ser Ser Leu Gln Cys Tyr
                485                 490                 495

atg aaa gaa aat cct gaa tct aca gtg gaa aat gct tta aat cac ata     1536
Met Lys Glu Asn Pro Glu Ser Thr Val Glu Asn Ala Leu Asn His Ile
            500                 505                 510

aaa ggc atc ctt aat cgt tcc ctt gag gaa ttt aat tgg gag ttt atg     1584
Lys Gly Ile Leu Asn Arg Ser Leu Glu Glu Phe Asn Trp Glu Phe Met
        515                 520                 525

aag cag gat agt gtc cca atg tgt tgc aag aaa ttc act ttc aat ata     1632
Lys Gln Asp Ser Val Pro Met Cys Cys Lys Lys Phe Thr Phe Asn Ile
    530                 535                 540
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ggt cga gga ctt caa ttc atc tac aaa tac aga gac ggc tta tac att     1680
Gly Arg Gly Leu Gln Phe Ile Tyr Lys Tyr Arg Asp Gly Leu Tyr Ile
545                 550                 555                 560

tct gac aag gaa gta aag gac cag ata ttc aaa att cta gtc cac caa     1728
Ser Asp Lys Glu Val Lys Asp Gln Ile Phe Lys Ile Leu Val His Gln
                565                 570                 575

gtt cca atg gag gaa tag tgatggtctt ggttgtagtt gtctattatg           1776
Val Pro Met Glu Glu
            580

gtatattgca ttgacattta tgcttaaagg tgtttcttaa acgtttaggg cggaccgtta   1836

aataagttgg caataattaa tatctcgag                                    1865


<210> SEQ ID NO 48
<211> LENGTH: 581
<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 48

Met Ala Glu Ile Ser Glu Ser Ser Ile Pro Arg Arg Thr Gly Asn His
 1               5                  10                  15

His Gly Asn Val Trp Asp Asp Asp Leu Ile His Ser Leu Asn Ser Pro
            20                  25                  30

Tyr Gly Ala Pro Ala Tyr Tyr Glu Leu Leu Gln Lys Leu Ile Gln Glu
        35                  40                  45

Ile Lys His Leu Leu Leu Thr Glu Met Glu Met Asp Asp Gly Asp His
    50                  55                  60

Asp Leu Ile Lys Arg Leu Gln Ile Val Asp Thr Leu Glu Cys Leu Gly
65                  70                  75                  80

Ile Asp Arg His Phe Glu His Glu Ile Gln Thr Ala Ala Leu Asp Tyr
                85                  90                  95

Val Tyr Arg Trp Trp Asn Glu Lys Gly Ile Gly Glu Gly Ser Arg Asp
            100                 105                 110

Ser Phe Ser Lys Asp Leu Asn Ala Thr Ala Leu Gly Phe Arg Ala Leu
        115                 120                 125

Arg Leu His Arg Tyr Asn Val Ser Ser Gly Val Leu Lys Asn Phe Lys
    130                 135                 140

Asp Glu Asn Gly Lys Phe Phe Cys Asn Phe Thr Gly Glu Glu Gly Arg
145                 150                 155                 160

Gly Asp Lys Gln Val Arg Ser Met Leu Ser Leu Leu Arg Ala Ser Glu
                165                 170                 175

Ile Ser Phe Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr
            180                 185                 190

Arg Glu Tyr Leu Asn Gln Val Leu Ala Gly His Gly Asp Val Thr Asp
        195                 200                 205

Val Asp Gln Ser Leu Leu Arg Glu Val Lys Tyr Ala Leu Glu Phe Pro
    210                 215                 220

Trp His Cys Ser Val Pro Arg Trp Glu Ala Arg Ser Phe Leu Glu Ile
225                 230                 235                 240

Tyr Gly His Asn His Ser Trp Leu Lys Ser Asn Ile Asn Gln Lys Met
                245                 250                 255

Leu Lys Leu Ala Lys Leu Asp Phe Asn Ile Leu Gln Cys Lys His His
            260                 265                 270

Lys Glu Ile Gln Phe Ile Thr Arg Trp Trp Arg Asp Ser Gly Ile Ser
        275                 280                 285
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Gln Leu Asn Phe Tyr Arg Lys Arg His Val Glu Tyr Tyr Ser Trp Val
    290                 295                 300

Val Met Cys Ile Phe Glu Pro Glu Phe Ser Glu Ser Arg Ile Ala Phe
305                 310                 315                 320

Ala Lys Thr Ala Ile Leu Cys Thr Val Leu Asp Asp Leu Tyr Asp Thr
                325                 330                 335

His Ala Thr Leu His Glu Ile Lys Ile Met Thr Glu Gly Val Arg Arg
            340                 345                 350

Trp Asp Leu Ser Leu Thr Asp Asp Leu Pro Asp Tyr Ile Lys Ile Ala
        355                 360                 365

Phe Gln Phe Phe Phe Asn Thr Val Asn Glu Leu Ile Val Glu Ile Val
    370                 375                 380

Lys Arg Gln Gly Arg Asp Met Thr Thr Ile Val Lys Asp Cys Trp Lys
385                 390                 395                 400

Arg Tyr Ile Glu Ser Tyr Leu Gln Glu Ala Glu Trp Ile Ala Thr Gly
                405                 410                 415

His Ile Pro Thr Phe Asn Glu Tyr Ile Lys Asn Gly Met Ala Ser Ser
            420                 425                 430

Gly Met Cys Ile Leu Asn Leu Asn Pro Leu Leu Leu Leu Asp Lys Leu
        435                 440                 445

Leu Pro Asp Asn Ile Leu Glu Gln Ile His Ser Pro Ser Lys Ile Leu
    450                 455                 460

Asp Leu Leu Glu Leu Thr Gly Arg Ile Ala Asp Asp Leu Lys Asp Phe
465                 470                 475                 480

Glu Asp Glu Lys Glu Arg Gly Glu Met Ala Ser Ser Leu Gln Cys Tyr
                485                 490                 495

Met Lys Glu Asn Pro Glu Ser Thr Val Glu Asn Ala Leu Asn His Ile
            500                 505                 510

Lys Gly Ile Leu Asn Arg Ser Leu Glu Glu Phe Asn Trp Glu Phe Met
        515                 520                 525

Lys Gln Asp Ser Val Pro Met Cys Cys Lys Lys Phe Thr Phe Asn Ile
    530                 535                 540

Gly Arg Gly Leu Gln Phe Ile Tyr Lys Tyr Arg Asp Gly Leu Tyr Ile
545                 550                 555                 560

Ser Asp Lys Glu Val Lys Asp Gln Ile Phe Lys Ile Leu Val His Gln
                565                 570                 575

Val Pro Met Glu Glu
            580


<210> SEQ ID NO 49
<211> LENGTH: 1785
<212> TYPE: DNA
<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (4)...(1782)
<223> OTHER INFORMATION: gamma-humulene synthase

<400> SEQUENCE: 49

tcc atg gct cag att tct gaa tct gta tca ccc tct acc gat ttg aag       48
    Met Ala Gln Ile Ser Glu Ser Val Ser Pro Ser Thr Asp Leu Lys
     1               5                  10                  15

agc acc gaa tct tcc att acc tct aat cga cat gga aat atg tgg gag       96
Ser Thr Glu Ser Ser Ile Thr Ser Asn Arg His Gly Asn Met Trp Glu
                20                  25                  30
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gac gat cgc ata cag tct ctc aac tca cct tat ggg gca cct gca tat      144
Asp Asp Arg Ile Gln Ser Leu Asn Ser Pro Tyr Gly Ala Pro Ala Tyr
             35                  40                  45

caa gaa cgc agc gaa aag ctt att gaa gag atc aaa ctt tta ttt ttg      192
Gln Glu Arg Ser Glu Lys Leu Ile Glu Glu Ile Lys Leu Leu Phe Leu
         50                  55                  60

agt gac atg gac gat agc tgc aat gat agc gat cgt gat tta atc aaa      240
Ser Asp Met Asp Asp Ser Cys Asn Asp Ser Asp Arg Asp Leu Ile Lys
     65                  70                  75

cgt ctt gag atc gtt gat act gtc gag tgt ctg gga att gat cga cat      288
Arg Leu Glu Ile Val Asp Thr Val Glu Cys Leu Gly Ile Asp Arg His
 80                  85                  90                  95

ttt caa cct gag ata aaa tta gct ctg gat tac gtt tac aga tgt tgg      336
Phe Gln Pro Glu Ile Lys Leu Ala Leu Asp Tyr Val Tyr Arg Cys Trp
                100                 105                 110

aac gaa aga ggc atc gga gag gga tca aga gat tcc ctc aag aaa gat      384
Asn Glu Arg Gly Ile Gly Glu Gly Ser Arg Asp Ser Leu Lys Lys Asp
            115                 120                 125

ctg aac gct aca gct ttg gga ttc cgg gct ctc cga ctc cat cga tat      432
Leu Asn Ala Thr Ala Leu Gly Phe Arg Ala Leu Arg Leu His Arg Tyr
        130                 135                 140

aac gta tcc tca ggt gtc ttg gag aat ttc aga gat gat aac ggg cag      480
Asn Val Ser Ser Gly Val Leu Glu Asn Phe Arg Asp Asp Asn Gly Gln
    145                 150                 155

ttc ttc tgc ggt tct aca gtt gaa gaa gaa gga gca gaa gca tat aat      528
Phe Phe Cys Gly Ser Thr Val Glu Glu Glu Gly Ala Glu Ala Tyr Asn
160                 165                 170                 175

aaa cac gta aga tgc atg ctg tca tta tcg cga gct tca aac att tta      576
Lys His Val Arg Cys Met Leu Ser Leu Ser Arg Ala Ser Asn Ile Leu
                180                 185                 190

ttt ccg ggc gaa aaa gtg atg gaa gag gcg aag gca ttc aca aca aat      624
Phe Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr Thr Asn
            195                 200                 205

tat cta aag aaa gtt tta gca gga cgg gag gct acc cac gtc gat gaa      672
Tyr Leu Lys Lys Val Leu Ala Gly Arg Glu Ala Thr His Val Asp Glu
        210                 215                 220

agc ctt ttg gga gag gtg aag tac gca ttg gag ttt cca tgg cat tgc      720
Ser Leu Leu Gly Glu Val Lys Tyr Ala Leu Glu Phe Pro Trp His Cys
    225                 230                 235

agt gtg cag aga tgg gag gca agg agc ttt atc gaa ata ttt gga caa      768
Ser Val Gln Arg Trp Glu Ala Arg Ser Phe Ile Glu Ile Phe Gly Gln
240                 245                 250                 255

att gat tca gag ctt aag tcg aat ttg agc aaa aaa atg tta gag ttg      816
Ile Asp Ser Glu Leu Lys Ser Asn Leu Ser Lys Lys Met Leu Glu Leu
                260                 265                 270

gcg aaa ttg gac ttc aat att ctg caa tgc aca cat cag aaa gaa ctg      864
Ala Lys Leu Asp Phe Asn Ile Leu Gln Cys Thr His Gln Lys Glu Leu
            275                 280                 285

cag att atc tca agg tgg ttc gca gac tca agt ata gca tcc ctg aat      912
Gln Ile Ile Ser Arg Trp Phe Ala Asp Ser Ser Ile Ala Ser Leu Asn
        290                 295                 300

ttc tat cgg aaa tgt tac gtc gaa ttt tac ttt tgg atg gct gca gcc      960
Phe Tyr Arg Lys Cys Tyr Val Glu Phe Tyr Phe Trp Met Ala Ala Ala
    305                 310                 315

atc tcc gag ccg gag ttt tct gga agc aga gtt gcc ttc aca aaa att     1008
Ile Ser Glu Pro Glu Phe Ser Gly Ser Arg Val Ala Phe Thr Lys Ile
320                 325                 330                 335

gct ata ctg atg aca atg cta gat gac ctg tac gat act cac gga acc     1056
Ala Ile Leu Met Thr Met Leu Asp Asp Leu Tyr Asp Thr His Gly Thr
                340                 345                 350
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ttg gac caa ctc aaa atc ttt aca gag gga gtg aga cga tgg gat gtt     1104
Leu Asp Gln Leu Lys Ile Phe Thr Glu Gly Val Arg Arg Trp Asp Val
            355                 360                 365

tcg ttg gta gag ggc ctc cca gac ttc atg aaa att gca ttc gag ttc     1152
Ser Leu Val Glu Gly Leu Pro Asp Phe Met Lys Ile Ala Phe Glu Phe
        370                 375                 380

tgg tta aag aca tct aat gaa ttg att gct gaa gct gtt aaa gcg caa     1200
Trp Leu Lys Thr Ser Asn Glu Leu Ile Ala Glu Ala Val Lys Ala Gln
    385                 390                 395

ggg caa gat atg gcg gcc tac ata aga aaa aat gca tgg gag cga tac     1248
Gly Gln Asp Met Ala Ala Tyr Ile Arg Lys Asn Ala Trp Glu Arg Tyr
400                 405                 410                 415

ctt gaa gct tat ctg caa gat gcg gaa tgg ata gcc act gga cat gtc     1296
Leu Glu Ala Tyr Leu Gln Asp Ala Glu Trp Ile Ala Thr Gly His Val
                420                 425                 430

ccc acc ttt gat gag tac ttg aat aat ggc aca cca aac act ggg atg     1344
Pro Thr Phe Asp Glu Tyr Leu Asn Asn Gly Thr Pro Asn Thr Gly Met
            435                 440                 445

tgt gta ttg aat ttg att ccg ctt ctg tta atg ggt gaa cat tta cca     1392
Cys Val Leu Asn Leu Ile Pro Leu Leu Leu Met Gly Glu His Leu Pro
        450                 455                 460

atc gac att ctg gag caa ata ttc ttg ccc tcc agg ttc cac cat ctc     1440
Ile Asp Ile Leu Glu Gln Ile Phe Leu Pro Ser Arg Phe His His Leu
    465                 470                 475

att gaa ttg gct tcc agg ctc gtc gat gac gcg aga gat ttc cag gcg     1488
Ile Glu Leu Ala Ser Arg Leu Val Asp Asp Ala Arg Asp Phe Gln Ala
480                 485                 490                 495

gag aag gat cat ggg gat tta tcg tgt att gag tgt tat tta aaa gat     1536
Glu Lys Asp His Gly Asp Leu Ser Cys Ile Glu Cys Tyr Leu Lys Asp
                500                 505                 510

cat cct gag tct aca gta gaa gat gct tta aat cat gtt aat ggc ctc     1584
His Pro Glu Ser Thr Val Glu Asp Ala Leu Asn His Val Asn Gly Leu
            515                 520                 525

ctt ggc aat tgc ctt ctg gaa atg aat tgg aag ttc tta aag aag cag     1632
Leu Gly Asn Cys Leu Leu Glu Met Asn Trp Lys Phe Leu Lys Lys Gln
        530                 535                 540

gac agt gtg cca ctc tcg tgt aag aag tac agc ttc cat gta ttg gca     1680
Asp Ser Val Pro Leu Ser Cys Lys Lys Tyr Ser Phe His Val Leu Ala
    545                 550                 555

cga agc atc caa ttc atg tac aat caa ggc gat ggc ttc tcc att tcg     1728
Arg Ser Ile Gln Phe Met Tyr Asn Gln Gly Asp Gly Phe Ser Ile Ser
560                 565                 570                 575

aac aaa gtg atc aag gat caa gtg cag aaa gtt ctt att gtc ccc gtg     1776
Asn Lys Val Ile Lys Asp Gln Val Gln Lys Val Leu Ile Val Pro Val
                580                 585                 590

cct att tga                                                        1785
Pro Ile
```

<210> SEQ ID NO 50
<211> LENGTH: 593
<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 50

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Met Ala Gln Ile Ser Glu Ser Val Ser Pro Ser Thr Asp Leu Lys Ser
 1               5                  10                  15

Thr Glu Ser Ser Ile Thr Ser Asn Arg His Gly Asn Met Trp Glu Asp
            20                  25                  30

Asp Arg Ile Gln Ser Leu Asn Ser Pro Tyr Gly Ala Pro Ala Tyr Gln
        35                  40                  45
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Glu Arg Ser Glu Lys Leu Ile Glu Glu Ile Lys Leu Leu Phe Leu Ser
    50                  55                  60

Asp Met Asp Asp Ser Cys Asn Asp Ser Asp Arg Asp Leu Ile Lys Arg
65                  70                  75                  80

Leu Glu Ile Val Asp Thr Val Glu Cys Leu Gly Ile Asp Arg His Phe
                85                  90                  95

Gln Pro Glu Ile Lys Leu Ala Leu Asp Tyr Val Tyr Arg Cys Trp Asn
            100                 105                 110

Glu Arg Gly Ile Gly Glu Gly Ser Arg Asp Ser Leu Lys Lys Asp Leu
        115                 120                 125

Asn Ala Thr Ala Leu Gly Phe Arg Ala Leu Arg Leu His Arg Tyr Asn
    130                 135                 140

Val Ser Ser Gly Val Leu Glu Asn Phe Arg Asp Asp Asn Gly Gln Phe
145                 150                 155                 160

Phe Cys Gly Ser Thr Val Glu Glu Glu Gly Ala Glu Ala Tyr Asn Lys
                165                 170                 175

His Val Arg Cys Met Leu Ser Leu Ser Arg Ala Ser Asn Ile Leu Phe
            180                 185                 190

Pro Gly Glu Lys Val Met Glu Glu Ala Lys Ala Phe Thr Thr Asn Tyr
        195                 200                 205

Leu Lys Lys Val Leu Ala Gly Arg Glu Ala Thr His Val Asp Glu Ser
    210                 215                 220

Leu Leu Gly Glu Val Lys Tyr Ala Leu Glu Phe Pro Trp His Cys Ser
225                 230                 235                 240

Val Gln Arg Trp Glu Ala Arg Ser Phe Ile Glu Ile Phe Gly Gln Ile
                245                 250                 255

Asp Ser Glu Leu Lys Ser Asn Leu Ser Lys Lys Met Leu Glu Leu Ala
            260                 265                 270

Lys Leu Asp Phe Asn Ile Leu Gln Cys Thr His Gln Lys Glu Leu Gln
        275                 280                 285

Ile Ile Ser Arg Trp Phe Ala Asp Ser Ser Ile Ala Ser Leu Asn Phe
    290                 295                 300

Tyr Arg Lys Cys Tyr Val Glu Phe Tyr Phe Trp Met Ala Ala Ala Ile
305                 310                 315                 320

Ser Glu Pro Glu Phe Ser Gly Ser Arg Val Ala Phe Thr Lys Ile Ala
                325                 330                 335

Ile Leu Met Thr Met Leu Asp Asp Leu Tyr Asp Thr His Gly Thr Leu
            340                 345                 350

Asp Gln Leu Lys Ile Phe Thr Glu Gly Val Arg Arg Trp Asp Val Ser
        355                 360                 365

Leu Val Glu Gly Leu Pro Asp Phe Met Lys Ile Ala Phe Glu Phe Trp
    370                 375                 380

Leu Lys Thr Ser Asn Glu Leu Ile Ala Glu Ala Val Lys Ala Gln Gly
385                 390                 395                 400

Gln Asp Met Ala Ala Tyr Ile Arg Lys Asn Ala Trp Glu Arg Tyr Leu
                405                 410                 415

Glu Ala Tyr Leu Gln Asp Ala Glu Trp Ile Ala Thr Gly His Val Pro
            420                 425                 430

Thr Phe Asp Glu Tyr Leu Asn Asn Gly Thr Pro Asn Thr Gly Met Cys
        435                 440                 445

Val Leu Asn Leu Ile Pro Leu Leu Leu Met Gly Glu His Leu Pro Ile
    450                 455                 460
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Asp Ile Leu Glu Gln Ile Phe Leu Pro Ser Arg Phe His His Leu Ile
465                 470                 475                 480

Glu Leu Ala Ser Arg Leu Val Asp Asp Ala Arg Asp Phe Gln Ala Glu
                485                 490                 495

Lys Asp His Gly Asp Leu Ser Cys Ile Glu Cys Tyr Leu Lys Asp His
            500                 505                 510

Pro Glu Ser Thr Val Glu Asp Ala Leu Asn His Val Asn Gly Leu Leu
        515                 520                 525

Gly Asn Cys Leu Leu Glu Met Asn Trp Lys Phe Leu Lys Lys Gln Asp
    530                 535                 540

Ser Val Pro Leu Ser Cys Lys Lys Tyr Ser Phe His Val Leu Ala Arg
545                 550                 555                 560

Ser Ile Gln Phe Met Tyr Asn Gln Gly Asp Gly Phe Ser Ile Ser Asn
                565                 570                 575

Lys Val Ile Lys Asp Gln Val Gln Lys Val Leu Ile Val Pro Val Pro
            580                 585                 590

Ile


<210> SEQ ID NO 51
<211> LENGTH: 2024
<212> TYPE: DNA
<213> ORGANISM: Lycopersicon esculentum
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (32)...(1675)
<223> OTHER INFORMATION: VFNT germacrene C synthase

<400> SEQUENCE: 51

aaaaaaagcc aaaccttaga acaaacaagc a atg gct gct tct tct gct gat        52
                                  Met Ala Ala Ser Ser Ala Asp
                                   1               5

aag tgt cgc ccc ttg gct aat ttt cac cca tct gtt tgg gga tat cat      100
Lys Cys Arg Pro Leu Ala Asn Phe His Pro Ser Val Trp Gly Tyr His
         10                  15                  20

ttc ctt tct tat act cat gaa att act aat caa gaa aaa gtt gaa gtt      148
Phe Leu Ser Tyr Thr His Glu Ile Thr Asn Gln Glu Lys Val Glu Val
     25                  30                  35

gat gag tac aaa gag aca att aga aaa atg ctg gtg gaa act tgc gac      196
Asp Glu Tyr Lys Glu Thr Ile Arg Lys Met Leu Val Glu Thr Cys Asp
 40                  45                  50                  55

aat agc act caa aag ctt gtg ttg ata gac gcg atg caa cga ttg gga      244
Asn Ser Thr Gln Lys Leu Val Leu Ile Asp Ala Met Gln Arg Leu Gly
                 60                  65                  70

gtg gct tat cat ttc gat aat gaa att gaa aca tcc att caa aac att      292
Val Ala Tyr His Phe Asp Asn Glu Ile Glu Thr Ser Ile Gln Asn Ile
             75                  80                  85

ttt gat gca tcg tcc aaa cag aat gat aat gac aac aac ctt tac gtt      340
Phe Asp Ala Ser Ser Lys Gln Asn Asp Asn Asp Asn Asn Leu Tyr Val
         90                  95                 100

gtg tct ctt cgt ttt cga ctt gtg agg caa caa ggc cat tac atg tct      388
Val Ser Leu Arg Phe Arg Leu Val Arg Gln Gln Gly His Tyr Met Ser
    105                 110                 115

tca gat gtg ttc aag caa ttc acc aac caa gat ggg aaa ttc aag gaa      436
Ser Asp Val Phe Lys Gln Phe Thr Asn Gln Asp Gly Lys Phe Lys Glu
120                 125                 130                 135

aca ctt act aat gat gtc caa gga tta ttg agt ttg tat gaa gca tca      484
Thr Leu Thr Asn Asp Val Gln Gly Leu Leu Ser Leu Tyr Glu Ala Ser
                140                 145                 150
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cat ctg aga gtg cgt aat gag gag att ctt gaa gaa gct ctt aca ttt      532
His Leu Arg Val Arg Asn Glu Glu Ile Leu Glu Glu Ala Leu Thr Phe
            155                 160                 165

acc acc act cat ctc gag tct att gtc tcc aac ttg agc aat aat aat      580
Thr Thr Thr His Leu Glu Ser Ile Val Ser Asn Leu Ser Asn Asn Asn
        170                 175                 180

aac tct ctt aag gtt gaa gtt ggt gaa gcc tta act cag cct att cgc      628
Asn Ser Leu Lys Val Glu Val Gly Glu Ala Leu Thr Gln Pro Ile Arg
    185                 190                 195

atg act tta cca agg atg gga gct aga aaa tac ata tcc att tac gaa      676
Met Thr Leu Pro Arg Met Gly Ala Arg Lys Tyr Ile Ser Ile Tyr Glu
200                 205                 210                 215

aac aat gat gca cac cac cat ttg ctt ttg aaa ttt gct aaa ttg gat      724
Asn Asn Asp Ala His His His Leu Leu Leu Lys Phe Ala Lys Leu Asp
                220                 225                 230

ttt aac atg ctg caa aag ttt cac caa aga gag ctt agt gat ctt aca      772
Phe Asn Met Leu Gln Lys Phe His Gln Arg Glu Leu Ser Asp Leu Thr
            235                 240                 245

agg tgg tgg aaa gat ttg gat ttt gca aat aaa tat cca tat gca aga      820
Arg Trp Trp Lys Asp Leu Asp Phe Ala Asn Lys Tyr Pro Tyr Ala Arg
        250                 255                 260

gac agg ttg gtt gag tgt tac ttc tgg ata tta gga gtg tat ttt gag      868
Asp Arg Leu Val Glu Cys Tyr Phe Trp Ile Leu Gly Val Tyr Phe Glu
    265                 270                 275

cca aaa tat agt cgt gcg aga aaa atg atg aca aaa gta ctc aac ctg      916
Pro Lys Tyr Ser Arg Ala Arg Lys Met Met Thr Lys Val Leu Asn Leu
280                 285                 290                 295

acc tcc att att gac gac act ttt gat gct tat gca acc ttt gac gaa      964
Thr Ser Ile Ile Asp Asp Thr Phe Asp Ala Tyr Ala Thr Phe Asp Glu
                300                 305                 310

ctt gtg act ttc aat gat gca atc cag aga tgg gat gct aat gca att     1012
Leu Val Thr Phe Asn Asp Ala Ile Gln Arg Trp Asp Ala Asn Ala Ile
            315                 320                 325

gat tca ata caa cca tat atg aga cct gct tat caa gct ctt cta gac     1060
Asp Ser Ile Gln Pro Tyr Met Arg Pro Ala Tyr Gln Ala Leu Leu Asp
        330                 335                 340

att tac agt gaa atg gaa caa gtg ttg tcc aaa gaa ggt aaa ctg gac     1108
Ile Tyr Ser Glu Met Glu Gln Val Leu Ser Lys Glu Gly Lys Leu Asp
    345                 350                 355

cgt gta tac tat gca aaa aat gag atg aaa aag ttg gtg aga gcc tat     1156
Arg Val Tyr Tyr Ala Lys Asn Glu Met Lys Lys Leu Val Arg Ala Tyr
360                 365                 370                 375

ttt aag gaa acc caa tgg ttg aat gat tgt gac cat att cca aaa tat     1204
Phe Lys Glu Thr Gln Trp Leu Asn Asp Cys Asp His Ile Pro Lys Tyr
                380                 385                 390

gag gaa caa gtg gag aat gca atc gta agt gct ggc tat atg atg ata     1252
Glu Glu Gln Val Glu Asn Ala Ile Val Ser Ala Gly Tyr Met Met Ile
            395                 400                 405

tca aca act tgc ttg gtc ggt ata gaa gaa ttt ata tcc cac gag act     1300
Ser Thr Thr Cys Leu Val Gly Ile Glu Glu Phe Ile Ser His Glu Thr
        410                 415                 420

ttt gaa tgg ttg atg aat gag tct gtg att gtt cga gct tcc gca ttg     1348
Phe Glu Trp Leu Met Asn Glu Ser Val Ile Val Arg Ala Ser Ala Leu
    425                 430                 435

att gcc aga gca atg aac gat att gtt gga cat gaa gat gaa caa gaa     1396
Ile Ala Arg Ala Met Asn Asp Ile Val Gly His Glu Asp Glu Gln Glu
440                 445                 450                 455

aga gga cat gta gct tca ctt att gaa tgt tac atg aaa gat tat gga     1444
Arg Gly His Val Ala Ser Leu Ile Glu Cys Tyr Met Lys Asp Tyr Gly
                460                 465                 470
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gct tca aag caa gag act tac att aag ttc ctg aaa gag gtc acc aat     1492
Ala Ser Lys Gln Glu Thr Tyr Ile Lys Phe Leu Lys Glu Val Thr Asn
            475                 480                 485

gca tgg aag gac ata aac aaa caa ttc tcc cgt cca act gaa gta cca     1540
Ala Trp Lys Asp Ile Asn Lys Gln Phe Ser Arg Pro Thr Glu Val Pro
        490                 495                 500

atg ttt gtc ctt gaa cga gtt cta aat ttg aca cgt gtg gct gac acg     1588
Met Phe Val Leu Glu Arg Val Leu Asn Leu Thr Arg Val Ala Asp Thr
    505                 510                 515

tta tat aag gag aaa gat aca tat tca acc gcc aaa gga aaa ctt aaa     1636
Leu Tyr Lys Glu Lys Asp Thr Tyr Ser Thr Ala Lys Gly Lys Leu Lys
520                 525                 530                 535

aac atg att aat cca ata cta att gaa tct gtc aaa ata taa             1678
Asn Met Ile Asn Pro Ile Leu Ile Glu Ser Val Lys Ile
                540                 545

atataatgct gaaattgcac cttcatcatc caactattca cagcaaaata aggcatataa   1738

taaattgaag actcacaaca tatgagttgt taattcctgg gatgtttgaa ataaacaata   1798

attgttttta tttaatttgc taagccaaag tgaaatatac aacacttgag ttgtattaaa   1858

tcatgtttta tctcatttcc agcttgtgag tttggattat tatattgtta attatcatca   1918

ctttataatg tactgtaatc gtattgtatt tgtattgtag tgttgtcata ataaaatttg   1978

aataaaatat atttttgttt caattccaaa aaaaaaaaaa aaaaaa                  2024


<210> SEQ ID NO 52
<211> LENGTH: 548
<212> TYPE: PRT
<213> ORGANISM: Lycopersicon esculentum

<400> SEQUENCE: 52

Met Ala Ala Ser Ser Ala Asp Lys Cys Arg Pro Leu Ala Asn Phe His
 1               5                  10                  15

Pro Ser Val Trp Gly Tyr His Phe Leu Ser Tyr Thr His Glu Ile Thr
            20                  25                  30

Asn Gln Glu Lys Val Glu Val Asp Glu Tyr Lys Glu Thr Ile Arg Lys
        35                  40                  45

Met Leu Val Glu Thr Cys Asp Asn Ser Thr Gln Lys Leu Val Leu Ile
    50                  55                  60

Asp Ala Met Gln Arg Leu Gly Val Ala Tyr His Phe Asp Asn Glu Ile
65                  70                  75                  80

Glu Thr Ser Ile Gln Asn Ile Phe Asp Ala Ser Ser Lys Gln Asn Asp
                85                  90                  95

Asn Asp Asn Asn Leu Tyr Val Val Ser Leu Arg Phe Arg Leu Val Arg
            100                 105                 110

Gln Gln Gly His Tyr Met Ser Ser Asp Val Phe Lys Gln Phe Thr Asn
        115                 120                 125

Gln Asp Gly Lys Phe Lys Glu Thr Leu Thr Asn Asp Val Gln Gly Leu
    130                 135                 140

Leu Ser Leu Tyr Glu Ala Ser His Leu Arg Val Arg Asn Glu Glu Ile
145                 150                 155                 160

Leu Glu Glu Ala Leu Thr Phe Thr Thr Thr His Leu Glu Ser Ile Val
                165                 170                 175

Ser Asn Leu Ser Asn Asn Asn Asn Ser Leu Lys Val Glu Val Gly Glu
            180                 185                 190

Ala Leu Thr Gln Pro Ile Arg Met Thr Leu Pro Arg Met Gly Ala Arg
        195                 200                 205
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Lys Tyr Ile Ser Ile Tyr Glu Asn Asn Asp Ala His His His Leu Leu
    210                 215                 220

Leu Lys Phe Ala Lys Leu Asp Phe Asn Met Leu Gln Lys Phe His Gln
225                 230                 235                 240

Arg Glu Leu Ser Asp Leu Thr Arg Trp Trp Lys Asp Leu Asp Phe Ala
                245                 250                 255

Asn Lys Tyr Pro Tyr Ala Arg Asp Arg Leu Val Glu Cys Tyr Phe Trp
            260                 265                 270

Ile Leu Gly Val Tyr Phe Glu Pro Lys Tyr Ser Arg Ala Arg Lys Met
        275                 280                 285

Met Thr Lys Val Leu Asn Leu Thr Ser Ile Ile Asp Asp Thr Phe Asp
    290                 295                 300

Ala Tyr Ala Thr Phe Asp Glu Leu Val Thr Phe Asn Asp Ala Ile Gln
305                 310                 315                 320

Arg Trp Asp Ala Asn Ala Ile Asp Ser Ile Gln Pro Tyr Met Arg Pro
                325                 330                 335

Ala Tyr Gln Ala Leu Leu Asp Ile Tyr Ser Glu Met Glu Gln Val Leu
            340                 345                 350

Ser Lys Glu Gly Lys Leu Asp Arg Val Tyr Tyr Ala Lys Asn Glu Met
        355                 360                 365

Lys Lys Leu Val Arg Ala Tyr Phe Lys Glu Thr Gln Trp Leu Asn Asp
    370                 375                 380

Cys Asp His Ile Pro Lys Tyr Glu Glu Gln Val Glu Asn Ala Ile Val
385                 390                 395                 400

Ser Ala Gly Tyr Met Met Ile Ser Thr Thr Cys Leu Val Gly Ile Glu
                405                 410                 415

Glu Phe Ile Ser His Glu Thr Phe Glu Trp Leu Met Asn Glu Ser Val
            420                 425                 430

Ile Val Arg Ala Ser Ala Leu Ile Ala Arg Ala Met Asn Asp Ile Val
        435                 440                 445

Gly His Glu Asp Glu Gln Glu Arg Gly His Val Ala Ser Leu Ile Glu
    450                 455                 460

Cys Tyr Met Lys Asp Tyr Gly Ala Ser Lys Gln Glu Thr Tyr Ile Lys
465                 470                 475                 480

Phe Leu Lys Glu Val Thr Asn Ala Trp Lys Asp Ile Asn Lys Gln Phe
                485                 490                 495

Ser Arg Pro Thr Glu Val Pro Met Phe Val Leu Glu Arg Val Leu Asn
            500                 505                 510

Leu Thr Arg Val Ala Asp Thr Leu Tyr Lys Glu Lys Asp Thr Tyr Ser
        515                 520                 525

Thr Ala Lys Gly Lys Leu Lys Asn Met Ile Asn Pro Ile Leu Ile Glu
    530                 535                 540

Ser Val Lys Ile
545
```

<210> SEQ ID NO 53
<211> LENGTH: 1912
<212> TYPE: DNA
<213> ORGANISM: Salvia officinalis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (26)...(1795)
<223> OTHER INFORMATION: (+)-sabinene syntase

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<400> SEQUENCE: 53

```
agcaatatta caactaacaa taaaa atg tct tcc att agc ata aac ata gct       52
                           Met Ser Ser Ile Ser Ile Asn Ile Ala
                            1               5

atg cca ctg aat tcc ctc cac aac ttt gag agg aaa cct tca aaa gca      100
Met Pro Leu Asn Ser Leu His Asn Phe Glu Arg Lys Pro Ser Lys Ala
 10                  15                  20                  25

tgg tct acc tct tgc act gca ccc gca gct cgc ctc cgg gca tct tcc      148
Trp Ser Thr Ser Cys Thr Ala Pro Ala Ala Arg Leu Arg Ala Ser Ser
                 30                  35                  40

tcc tta caa caa gaa aaa cct cac caa atc cga cgc tct ggg gat tac      196
Ser Leu Gln Gln Glu Lys Pro His Gln Ile Arg Arg Ser Gly Asp Tyr
             45                  50                  55

caa ccc tct ctt tgg gat ttc aat tac ata cag tct ctc aac act ccg      244
Gln Pro Ser Leu Trp Asp Phe Asn Tyr Ile Gln Ser Leu Asn Thr Pro
         60                  65                  70

tat aag gag cag aga cac ttt aat agg caa gca gag ttg att atg caa      292
Tyr Lys Glu Gln Arg His Phe Asn Arg Gln Ala Glu Leu Ile Met Gln
     75                  80                  85

gtg agg atg ttg ctc aag gta aag atg gag gca att caa cag ttg gag      340
Val Arg Met Leu Leu Lys Val Lys Met Glu Ala Ile Gln Gln Leu Glu
 90                  95                 100                 105

ttg att gat gac ttg caa tac ctg gga ctg tct tat ttc ttt caa gat      388
Leu Ile Asp Asp Leu Gln Tyr Leu Gly Leu Ser Tyr Phe Phe Gln Asp
                110                 115                 120

gag att aaa caa atc tta agt tct ata cac aat gag ccc aga tat ttc      436
Glu Ile Lys Gln Ile Leu Ser Ser Ile His Asn Glu Pro Arg Tyr Phe
            125                 130                 135

cac aat aat gat ttg tat ttc aca gct ctt gga ttc aga atc ctc aga      484
His Asn Asn Asp Leu Tyr Phe Thr Ala Leu Gly Phe Arg Ile Leu Arg
        140                 145                 150

caa cat ggt ttt aat gtt tcc gaa gat gta ttt gat tgt ttc aaa att      532
Gln His Gly Phe Asn Val Ser Glu Asp Val Phe Asp Cys Phe Lys Ile
    155                 160                 165

gag aag tgc agt gat ttc aat gca aac ctt gct caa gat acg aag gga      580
Glu Lys Cys Ser Asp Phe Asn Ala Asn Leu Ala Gln Asp Thr Lys Gly
170                 175                 180                 185

atg tta caa ctt tat gaa gca tct ttc ctt ttg aga gaa ggt gaa gat      628
Met Leu Gln Leu Tyr Glu Ala Ser Phe Leu Leu Arg Glu Gly Glu Asp
                190                 195                 200

aca ttg gag cta gca aga cga ttt tcc acc aga tct cta cga gaa aaa      676
Thr Leu Glu Leu Ala Arg Arg Phe Ser Thr Arg Ser Leu Arg Glu Lys
            205                 210                 215

ttt gat gaa ggt ggt gat gaa att gat gaa gat cta tca tcg tgg att      724
Phe Asp Glu Gly Gly Asp Glu Ile Asp Glu Asp Leu Ser Ser Trp Ile
        220                 225                 230

cgc cat tcc ttg gat ctt cct ctt cat tgg agg gtc caa gga tta gag      772
Arg His Ser Leu Asp Leu Pro Leu His Trp Arg Val Gln Gly Leu Glu
    235                 240                 245

gca aga tgg ttc tta gat gct tat gcg agg agg ccg gac atg aat cca      820
Ala Arg Trp Phe Leu Asp Ala Tyr Ala Arg Arg Pro Asp Met Asn Pro
250                 255                 260                 265

ctt att ttc aaa ctc gcc aaa ctc aac ttc aat att gtt cag gca aca      868
Leu Ile Phe Lys Leu Ala Lys Leu Asn Phe Asn Ile Val Gln Ala Thr
                270                 275                 280

tat caa gaa gaa ctg aaa gat atc tca agg tgg tgg aat agt tcg tgc      916
Tyr Gln Glu Glu Leu Lys Asp Ile Ser Arg Trp Trp Asn Ser Ser Cys
            285                 290                 295
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ctt gct gag aaa ctc cca ttt gtg aga gat agg att gtg gaa tgc ttc      964
Leu Ala Glu Lys Leu Pro Phe Val Arg Asp Arg Ile Val Glu Cys Phe
        300                 305                 310

ttt tgg gcc atc gcg gct ttt gag cct cac caa tat agt tat cag aga     1012
Phe Trp Ala Ile Ala Ala Phe Glu Pro His Gln Tyr Ser Tyr Gln Arg
    315                 320                 325

aaa atg gcc gcc gtt att att act ttc ata aca att atc gat gat gtt     1060
Lys Met Ala Ala Val Ile Ile Thr Phe Ile Thr Ile Ile Asp Asp Val
330                 335                 340                 345

tat gat gtg tat gga aca ata gaa gaa cta gaa cta tta aca gat atg     1108
Tyr Asp Val Tyr Gly Thr Ile Glu Glu Leu Glu Leu Leu Thr Asp Met
                350                 355                 360

att cgc aga tgg gat aat aaa tca ata agc caa ctt cca tat tat atg     1156
Ile Arg Arg Trp Asp Asn Lys Ser Ile Ser Gln Leu Pro Tyr Tyr Met
            365                 370                 375

caa gtg tgc tat ttg gca cta tac aac ttc gtt tct gag cgg gct tac     1204
Gln Val Cys Tyr Leu Ala Leu Tyr Asn Phe Val Ser Glu Arg Ala Tyr
        380                 385                 390

gat att cta aaa gat caa cat ttc aac agc atc cca tat tta cag aga     1252
Asp Ile Leu Lys Asp Gln His Phe Asn Ser Ile Pro Tyr Leu Gln Arg
    395                 400                 405

tcg tgg gta agt ttg gtt gaa gga tat ctt aag gag gca tac tgg tac     1300
Ser Trp Val Ser Leu Val Glu Gly Tyr Leu Lys Glu Ala Tyr Trp Tyr
410                 415                 420                 425

tac aat ggc tat aaa cca agc ttg gaa gaa tat ctc aac aac gcc aag     1348
Tyr Asn Gly Tyr Lys Pro Ser Leu Glu Glu Tyr Leu Asn Asn Ala Lys
                430                 435                 440

att tca ata tcg gct cct aca atc ata tcc cag ctt tat ttt aca tta     1396
Ile Ser Ile Ser Ala Pro Thr Ile Ile Ser Gln Leu Tyr Phe Thr Leu
            445                 450                 455

gca aac tcg att gat gaa aca gct atc gag agc ttg tac caa tat cat     1444
Ala Asn Ser Ile Asp Glu Thr Ala Ile Glu Ser Leu Tyr Gln Tyr His
        460                 465                 470

aac ata ctt tac cta tca gga acc ata tta agg ctt gct gac gat ctt     1492
Asn Ile Leu Tyr Leu Ser Gly Thr Ile Leu Arg Leu Ala Asp Asp Leu
    475                 480                 485

ggg aca tca caa cat gag ctg gag aga gga gac gta ccg aaa gca atc     1540
Gly Thr Ser Gln His Glu Leu Glu Arg Gly Asp Val Pro Lys Ala Ile
490                 495                 500                 505

cag tgc tac atg aat gac aca aat gct tcg gag aga gag gcg gtg gaa     1588
Gln Cys Tyr Met Asn Asp Thr Asn Ala Ser Glu Arg Glu Ala Val Glu
                510                 515                 520

cac gtg aag ttt ctg ata agg gag gcg tgg aag gag atg aac acg gtc     1636
His Val Lys Phe Leu Ile Arg Glu Ala Trp Lys Glu Met Asn Thr Val
            525                 530                 535

aca aca gcc agc gat tgt ccg ttt acg gat gat ttg gtt gcg gcc gca     1684
Thr Thr Ala Ser Asp Cys Pro Phe Thr Asp Asp Leu Val Ala Ala Ala
        540                 545                 550

gct aat ctt gca agg gcg gct cag ttt ata tat ctc gac ggg gat ggg     1732
Ala Asn Leu Ala Arg Ala Ala Gln Phe Ile Tyr Leu Asp Gly Asp Gly
    555                 560                 565

cat ggc gtg caa cac tca gaa ata cat caa cag atg gga ggc ctg cta     1780
His Gly Val Gln His Ser Glu Ile His Gln Gln Met Gly Gly Leu Leu
570                 575                 580                 585

ttc cag cct tat gtc tga ataaatcgaa aatccaacct actatgtatc            1828
Phe Gln Pro Tyr Val
                590

cctcgataat atattcttgg ggttaacatg tttaattaaa gttctaattd aaagagctga   1888

atcgatcctc aaaaaaaaaa aaaa                                          1912
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<210> SEQ ID NO 54
<211> LENGTH: 590
<212> TYPE: PRT
<213> ORGANISM: Salvia officinalis

<400> SEQUENCE: 54

Met Ser Ser Ile Ser Ile Asn Ile Ala Met Pro Leu Asn Ser Leu His
 1   5   10   15

Asn Phe Glu Arg Lys Pro Ser Lys Ala Trp Ser Thr Ser Cys Thr Ala
            20   25   30

Pro Ala Ala Arg Leu Arg Ala Ser Ser Ser Leu Gln Gln Glu Lys Pro
        35   40   45

His Gln Ile Arg Arg Ser Gly Asp Tyr Gln Pro Ser Leu Trp Asp Phe
    50   55   60

Asn Tyr Ile Gln Ser Leu Asn Thr Pro Tyr Lys Glu Gln Arg His Phe
65   70   75   80

Asn Arg Gln Ala Glu Leu Ile Met Gln Val Arg Met Leu Leu Lys Val
                85   90   95

Lys Met Glu Ala Ile Gln Gln Leu Glu Leu Ile Asp Asp Leu Gln Tyr
            100   105   110

Leu Gly Leu Ser Tyr Phe Phe Gln Asp Glu Ile Lys Gln Ile Leu Ser
        115   120   125

Ser Ile His Asn Glu Pro Arg Tyr Phe His Asn Asn Asp Leu Tyr Phe
    130   135   140

Thr Ala Leu Gly Phe Arg Ile Leu Arg Gln His Gly Phe Asn Val Ser
145   150   155   160

Glu Asp Val Phe Asp Cys Phe Lys Ile Glu Lys Cys Ser Asp Phe Asn
                165   170   175

Ala Asn Leu Ala Gln Asp Thr Lys Gly Met Leu Gln Leu Tyr Glu Ala
            180   185   190

Ser Phe Leu Leu Arg Glu Gly Glu Asp Thr Leu Glu Leu Ala Arg Arg
        195   200   205

Phe Ser Thr Arg Ser Leu Arg Glu Lys Phe Asp Glu Gly Gly Asp Glu
    210   215   220

Ile Asp Glu Asp Leu Ser Ser Trp Ile Arg His Ser Leu Asp Leu Pro
225   230   235   240

Leu His Trp Arg Val Gln Gly Leu Glu Ala Arg Trp Phe Leu Asp Ala
                245   250   255

Tyr Ala Arg Arg Pro Asp Met Asn Pro Leu Ile Phe Lys Leu Ala Lys
            260   265   270

Leu Asn Phe Asn Ile Val Gln Ala Thr Tyr Gln Glu Glu Leu Lys Asp
        275   280   285

Ile Ser Arg Trp Trp Asn Ser Ser Cys Leu Ala Glu Lys Leu Pro Phe
    290   295   300

Val Arg Asp Arg Ile Val Glu Cys Phe Phe Trp Ala Ile Ala Ala Phe
305   310   315   320

Glu Pro His Gln Tyr Ser Tyr Gln Arg Lys Met Ala Ala Val Ile Ile
                325   330   335

Thr Phe Ile Thr Ile Ile Asp Asp Val Tyr Asp Val Tyr Gly Thr Ile
            340   345   350

Glu Glu Leu Glu Leu Leu Thr Asp Met Ile Arg Arg Trp Asp Asn Lys
        355   360   365

Ser Ile Ser Gln Leu Pro Tyr Tyr Met Gln Val Cys Tyr Leu Ala Leu
    370   375   380

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Tyr Asn Phe Val Ser Glu Arg Ala Tyr Asp Ile Leu Lys Asp Gln His
385                 390                 395                 400

Phe Asn Ser Ile Pro Tyr Leu Gln Arg Ser Trp Val Ser Leu Val Glu
                405                 410                 415

Gly Tyr Leu Lys Glu Ala Tyr Trp Tyr Tyr Asn Gly Tyr Lys Pro Ser
            420                 425                 430

Leu Glu Glu Tyr Leu Asn Asn Ala Lys Ile Ser Ile Ser Ala Pro Thr
        435                 440                 445

Ile Ile Ser Gln Leu Tyr Phe Thr Leu Ala Asn Ser Ile Asp Glu Thr
    450                 455                 460

Ala Ile Glu Ser Leu Tyr Gln Tyr His Asn Ile Leu Tyr Leu Ser Gly
465                 470                 475                 480

Thr Ile Leu Arg Leu Ala Asp Asp Leu Gly Thr Ser Gln His Glu Leu

                485                 490                 495
Glu Arg Gly Asp Val Pro Lys Ala Ile Gln Cys Tyr Met Asn Asp Thr

            500                 505                 510
Asn Ala Ser Glu Arg Glu Ala Val Glu His Val Lys Phe Leu Ile Arg
        515                 520                 525

Glu Ala Trp Lys Glu Met Asn Thr Val Thr Thr Ala Ser Asp Cys Pro
    530                 535                 540

Phe Thr Asp Asp Leu Val Ala Ala Ala Ala Asn Leu Ala Arg Ala Ala
545                 550                 555                 560

Gln Phe Ile Tyr Leu Asp Gly Asp Gly His Gly Val Gln His Ser Glu
                565                 570                 575

Ile His Gln Gln Met Gly Gly Leu Leu Phe Gln Pro Tyr Val
            580                 585                 590


<210> SEQ ID NO 55
<211> LENGTH: 2861
<212> TYPE: DNA
<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (3)...(2606)
<223> OTHER INFORMATION: abietadiene synthase

<400> SEQUENCE: 55

ag atg gcc atg cct tcc tct tca ttg tca tca cag att ccc act gct        47
   Met Ala Met Pro Ser Ser Ser Leu Ser Ser Gln Ile Pro Thr Ala
    1               5                  10                  15

gct cat cat cta act gct aac gca caa tcc att ccg cat ttc tcc acg       95
Ala His His Leu Thr Ala Asn Ala Gln Ser Ile Pro His Phe Ser Thr
                20                  25                  30

acg ctg aat gct gga agc agt gct agc aaa cgg aga agc ttg tac cta      143
Thr Leu Asn Ala Gly Ser Ser Ala Ser Lys Arg Arg Ser Leu Tyr Leu
            35                  40                  45

cga tgg ggt aaa ggt tca aac aag atc att gcc tgt gtt gga gaa ggt      191
Arg Trp Gly Lys Gly Ser Asn Lys Ile Ile Ala Cys Val Gly Glu Gly
        50                  55                  60

ggt gca acc tct gtt cct tat cag tct gct gaa aag aat gat tcg ctt      239
Gly Ala Thr Ser Val Pro Tyr Gln Ser Ala Glu Lys Asn Asp Ser Leu
    65                  70                  75

tct tct tct aca ttg gtg aaa cga gaa ttt cct cca gga ttt tgg aag      287
Ser Ser Ser Thr Leu Val Lys Arg Glu Phe Pro Pro Gly Phe Trp Lys
80                  85                  90                  95

gat gat ctt atc gat tct cta acg tca tct cac aag gtt gca gca tca      335
Asp Asp Leu Ile Asp Ser Leu Thr Ser Ser His Lys Val Ala Ala Ser
                100                 105                 110
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gac gag aag cgt atc gag aca tta ata tcc gag att aag aat atg ttt      383
Asp Glu Lys Arg Ile Glu Thr Leu Ile Ser Glu Ile Lys Asn Met Phe
            115                 120                 125

aga tgt atg ggc tat ggc gaa acg aat ccc tct gca tat gac act gct      431
Arg Cys Met Gly Tyr Gly Glu Thr Asn Pro Ser Ala Tyr Asp Thr Ala
        130                 135                 140

tgg gta gca agg att cca gca gtt gat ggc tct gac aac cct cac ttt      479
Trp Val Ala Arg Ile Pro Ala Val Asp Gly Ser Asp Asn Pro His Phe
    145                 150                 155

cct gag acg gtt gaa tgg att ctt caa aat cag ttg aaa gat ggg tct      527
Pro Glu Thr Val Glu Trp Ile Leu Gln Asn Gln Leu Lys Asp Gly Ser
160                 165                 170                 175

tgg ggt gaa gga ttc tac ttc ttg gca tat gac aga ata ctg gct aca      575
Trp Gly Glu Gly Phe Tyr Phe Leu Ala Tyr Asp Arg Ile Leu Ala Thr
                180                 185                 190

ctt gca tgt att att acc ctt acc ctc tgg cgt act ggg gag aca caa      623
Leu Ala Cys Ile Ile Thr Leu Thr Leu Trp Arg Thr Gly Glu Thr Gln
            195                 200                 205

gta cag aaa ggt att gaa ttc ttc agg aca caa gct gga aag atg gaa      671
Val Gln Lys Gly Ile Glu Phe Phe Arg Thr Gln Ala Gly Lys Met Glu
        210                 215                 220

gat gaa gct gat agt cat agg cca agt gga ttt gaa ata gta ttt cct      719
Asp Glu Ala Asp Ser His Arg Pro Ser Gly Phe Glu Ile Val Phe Pro
    225                 230                 235

gca atg cta aag gaa gct aaa atc tta ggc ttg gat ctg cct tac gat      767
Ala Met Leu Lys Glu Ala Lys Ile Leu Gly Leu Asp Leu Pro Tyr Asp
240                 245                 250                 255

ttg cca ttc ctg aaa caa atc atc gaa aag cgg gag gct aag ctt aaa      815
Leu Pro Phe Leu Lys Gln Ile Ile Glu Lys Arg Glu Ala Lys Leu Lys
                260                 265                 270

agg att ccc act gat gtt ctc tat gcc ctt cca aca acg tta ttg tat      863
Arg Ile Pro Thr Asp Val Leu Tyr Ala Leu Pro Thr Thr Leu Leu Tyr
            275                 280                 285

tct ttg gaa ggt tta caa gaa ata gta gac tgg cag aaa ata atg aaa      911
Ser Leu Glu Gly Leu Gln Glu Ile Val Asp Trp Gln Lys Ile Met Lys
        290                 295                 300

ctt caa tcc aag gat gga tca ttt ctc agc tct ccg gca tct aca gcg      959
Leu Gln Ser Lys Asp Gly Ser Phe Leu Ser Ser Pro Ala Ser Thr Ala
    305                 310                 315

gct gta ttc atg cgt aca ggg aac aaa aag tgc ttg gat ttc ttg aac     1007
Ala Val Phe Met Arg Thr Gly Asn Lys Lys Cys Leu Asp Phe Leu Asn
320                 325                 330                 335

ttt gtc ttg aag aaa ttc gga aac cat gtg cct tgt cac tat ccg ctt     1055
Phe Val Leu Lys Lys Phe Gly Asn His Val Pro Cys His Tyr Pro Leu
                340                 345                 350

gat cta ttt gaa cgt ttg tgg gcg gtt gat aca gtt gag cgg cta ggt     1103
Asp Leu Phe Glu Arg Leu Trp Ala Val Asp Thr Val Glu Arg Leu Gly
            355                 360                 365

atc gat cgt cat ttc aaa gag gag atc aag gaa gca ttg gat tat gtt     1151
Ile Asp Arg His Phe Lys Glu Glu Ile Lys Glu Ala Leu Asp Tyr Val
        370                 375                 380

tac agc cat tgg gac gaa aga ggc att gga tgg gcg aga gag aat cct     1199
Tyr Ser His Trp Asp Glu Arg Gly Ile Gly Trp Ala Arg Glu Asn Pro
    385                 390                 395

gtt cct gat att gat gat aca gcc atg ggc ctt cga atc ttg aga tta     1247
Val Pro Asp Ile Asp Asp Thr Ala Met Gly Leu Arg Ile Leu Arg Leu
400                 405                 410                 415

cat gga tac aat gta tcc tca gat gtt tta aaa aca ttt aga gat gag     1295
His Gly Tyr Asn Val Ser Ser Asp Val Leu Lys Thr Phe Arg Asp Glu
                420                 425                 430
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aat ggg gag ttc ttt tgc ttc ttg ggt caa aca cag aga gga gtt aca     1343
Asn Gly Glu Phe Phe Cys Phe Leu Gly Gln Thr Gln Arg Gly Val Thr
            435                 440                 445

gac atg tta aac gtc aat cgt tgt tca cat gtt tca ttt ccg gga gaa     1391
Asp Met Leu Asn Val Asn Arg Cys Ser His Val Ser Phe Pro Gly Glu
        450                 455                 460

acg atc atg gaa gaa gca aaa ctc tgt acc gaa agg tat ctg agg aat     1439
Thr Ile Met Glu Glu Ala Lys Leu Cys Thr Glu Arg Tyr Leu Arg Asn
    465                 470                 475

gct ctg gaa aat gtg gat gcc ttt gac aaa tgg gct ttt aaa aag aat     1487
Ala Leu Glu Asn Val Asp Ala Phe Asp Lys Trp Ala Phe Lys Lys Asn
480                 485                 490                 495

att cgg gga gag gta gag tat gca ctc aaa tat ccc tgg cat aag agt     1535
Ile Arg Gly Glu Val Glu Tyr Ala Leu Lys Tyr Pro Trp His Lys Ser
                500                 505                 510

atg cca agg ttg gag gct aga agc tat att gaa aac tat ggg cca gat     1583
Met Pro Arg Leu Glu Ala Arg Ser Tyr Ile Glu Asn Tyr Gly Pro Asp
            515                 520                 525

gat gtg tgg ctt gga aaa act gta tat atg atg cca tac att tcg aat     1631
Asp Val Trp Leu Gly Lys Thr Val Tyr Met Met Pro Tyr Ile Ser Asn
        530                 535                 540

gaa aag tat tta gaa cta gcg aaa ctg gac ttc aat aag gtg cag tct     1679
Glu Lys Tyr Leu Glu Leu Ala Lys Leu Asp Phe Asn Lys Val Gln Ser
    545                 550                 555

ata cac caa aca gag ctt caa gat ctt cga agg tgg tgg aaa tca tcc     1727
Ile His Gln Thr Glu Leu Gln Asp Leu Arg Arg Trp Trp Lys Ser Ser
560                 565                 570                 575

ggt ttc acg gat ctg aat ttc act cgt gag cgt gtg acg gaa ata tat     1775
Gly Phe Thr Asp Leu Asn Phe Thr Arg Glu Arg Val Thr Glu Ile Tyr
                580                 585                 590

ttc tca ccg gca tcc ttt atc ttt gag ccc gag ttt tct aag tgc aga     1823
Phe Ser Pro Ala Ser Phe Ile Phe Glu Pro Glu Phe Ser Lys Cys Arg
            595                 600                 605

gag gtt tat aca aaa act tcc aat ttc act gtt att tta gat gat ctt     1871
Glu Val Tyr Thr Lys Thr Ser Asn Phe Thr Val Ile Leu Asp Asp Leu
        610                 615                 620

tat gac gcc cat gga tct tta gac gat ctt aag ttg ttc aca gaa tca     1919
Tyr Asp Ala His Gly Ser Leu Asp Asp Leu Lys Leu Phe Thr Glu Ser
    625                 630                 635

gtc aaa aga tgg gat cta tca cta gtg gac caa atg cca caa caa atg     1967
Val Lys Arg Trp Asp Leu Ser Leu Val Asp Gln Met Pro Gln Gln Met
640                 645                 650                 655

aaa ata tgt ttt gtg ggt ttc tac aat act ttt aat gat ata gca aaa     2015
Lys Ile Cys Phe Val Gly Phe Tyr Asn Thr Phe Asn Asp Ile Ala Lys
                660                 665                 670

gaa gga cgt gag agg caa ggg cgc gat gtg cta ggc tac att caa aat     2063
Glu Gly Arg Glu Arg Gln Gly Arg Asp Val Leu Gly Tyr Ile Gln Asn
            675                 680                 685

gtt tgg aaa gtc caa ctt gaa gct tac acg aaa gaa gca gaa tgg tct     2111
Val Trp Lys Val Gln Leu Glu Ala Tyr Thr Lys Glu Ala Glu Trp Ser
        690                 695                 700

gaa gct aaa tat gtg cca tcc ttc aat gaa tac ata gag aat gcg agt     2159
Glu Ala Lys Tyr Val Pro Ser Phe Asn Glu Tyr Ile Glu Asn Ala Ser
    705                 710                 715

gtg tca ata gca ttg gga aca gtc gtt ctc att agt gct ctt ttc act     2207
Val Ser Ile Ala Leu Gly Thr Val Val Leu Ile Ser Ala Leu Phe Thr
720                 725                 730                 735

ggg gag gtt ctt aca gat gaa gta ctc tcc aaa att gat cgc gaa tct     2255
Gly Glu Val Leu Thr Asp Glu Val Leu Ser Lys Ile Asp Arg Glu Ser
                740                 745                 750
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aga ttt ctt caa ctc atg ggc tta aca ggg cgt ttg gtg aat gac acc     2303
Arg Phe Leu Gln Leu Met Gly Leu Thr Gly Arg Leu Val Asn Asp Thr
            755                 760                 765

aaa act tat cag gca gag aga ggt caa ggt gag gtg gct tct gcc ata     2351
Lys Thr Tyr Gln Ala Glu Arg Gly Gln Gly Glu Val Ala Ser Ala Ile
        770                 775                 780

caa tgt tat atg aag gac cat cct aaa atc tct gaa gaa gaa gct cta     2399
Gln Cys Tyr Met Lys Asp His Pro Lys Ile Ser Glu Glu Glu Ala Leu
    785                 790                 795

caa cat gtc tat agt gtc atg gaa aat gcc ctc gaa gag ttg aat agg     2447
Gln His Val Tyr Ser Val Met Glu Asn Ala Leu Glu Glu Leu Asn Arg
800                 805                 810                 815

gag ttt gtg aat aac aaa ata ccg gat att tac aaa aga ctg gtt ttt     2495
Glu Phe Val Asn Asn Lys Ile Pro Asp Ile Tyr Lys Arg Leu Val Phe
                820                 825                 830

gaa act gca aga ata atg caa ctc ttt tat atg caa ggg gat ggt ttg     2543
Glu Thr Ala Arg Ile Met Gln Leu Phe Tyr Met Gln Gly Asp Gly Leu
            835                 840                 845

aca cta tca cat gat atg gaa att aaa gag cat gtc aaa aat tgc ctc     2591
Thr Leu Ser His Asp Met Glu Ile Lys Glu His Val Lys Asn Cys Leu
        850                 855                 860

ttc caa cca gtt gcc tag attaaattat tcagttaaag gccctcatgg           2639
Phe Gln Pro Val Ala
    865

tattgtgtta acattataat aacagatgct caaaagcttt gagcggtatt tgttaaggct   2699

atctttgttt gtttgtttgt ttactgccaa ccaaaaagcg ttcctaaacc tttgaagaca   2759

tttccatcca agagatggag tctacatttt atttatgaga ttgaattatt tcaagagaat   2819

atactacata tatttaaaag taaaaaaaaa aaaaaaaaaa aa                      2861


<210> SEQ ID NO 56
<211> LENGTH: 868
<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 56

Met Ala Met Pro Ser Ser Ser Leu Ser Ser Gln Ile Pro Thr Ala Ala
 1               5                  10                  15

His His Leu Thr Ala Asn Ala Gln Ser Ile Pro His Phe Ser Thr Thr
            20                  25                  30

Leu Asn Ala Gly Ser Ser Ala Ser Lys Arg Arg Ser Leu Tyr Leu Arg
        35                  40                  45

Trp Gly Lys Gly Ser Asn Lys Ile Ile Ala Cys Val Gly Glu Gly Gly
    50                  55                  60

Ala Thr Ser Val Pro Tyr Gln Ser Ala Glu Lys Asn Asp Ser Leu Ser
65                  70                  75                  80

Ser Ser Thr Leu Val Lys Arg Glu Phe Pro Pro Gly Phe Trp Lys Asp
                85                  90                  95

Asp Leu Ile Asp Ser Leu Thr Ser Ser His Lys Val Ala Ala Ser Asp
            100                 105                 110

Glu Lys Arg Ile Glu Thr Leu Ile Ser Glu Ile Lys Asn Met Phe Arg
        115                 120                 125

Cys Met Gly Tyr Gly Glu Thr Asn Pro Ser Ala Tyr Asp Thr Ala Trp
    130                 135                 140

Val Ala Arg Ile Pro Ala Val Asp Gly Ser Asp Asn Pro His Phe Pro
145                 150                 155                 160
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Glu Thr Val Glu Trp Ile Leu Gln Asn Gln Leu Lys Asp Gly Ser Trp
                165                 170                 175

Gly Glu Gly Phe Tyr Phe Leu Ala Tyr Asp Arg Ile Leu Ala Thr Leu
            180                 185                 190

Ala Cys Ile Ile Thr Leu Thr Leu Trp Arg Thr Gly Glu Thr Gln Val
        195                 200                 205

Gln Lys Gly Ile Glu Phe Phe Arg Thr Gln Ala Gly Lys Met Glu Asp
    210                 215                 220

Glu Ala Asp Ser His Arg Pro Ser Gly Phe Glu Ile Val Phe Pro Ala
225                 230                 235                 240

Met Leu Lys Glu Ala Lys Ile Leu Gly Leu Asp Leu Pro Tyr Asp Leu
                245                 250                 255

Pro Phe Leu Lys Gln Ile Ile Glu Lys Arg Glu Ala Lys Leu Lys Arg
            260                 265                 270

Ile Pro Thr Asp Val Leu Tyr Ala Leu Pro Thr Thr Leu Leu Tyr Ser
        275                 280                 285

Leu Glu Gly Leu Gln Glu Ile Val Asp Trp Gln Lys Ile Met Lys Leu
    290                 295                 300

Gln Ser Lys Asp Gly Ser Phe Leu Ser Ser Pro Ala Ser Thr Ala Ala
305                 310                 315                 320

Val Phe Met Arg Thr Gly Asn Lys Lys Cys Leu Asp Phe Leu Asn Phe
                325                 330                 335

Val Leu Lys Lys Phe Gly Asn His Val Pro Cys His Tyr Pro Leu Asp
            340                 345                 350

Leu Phe Glu Arg Leu Trp Ala Val Asp Thr Val Glu Arg Leu Gly Ile
        355                 360                 365

Asp Arg His Phe Lys Glu Glu Ile Lys Glu Ala Leu Asp Tyr Val Tyr
    370                 375                 380

Ser His Trp Asp Glu Arg Gly Ile Gly Trp Ala Arg Glu Asn Pro Val
385                 390                 395                 400

Pro Asp Ile Asp Asp Thr Ala Met Gly Leu Arg Ile Leu Arg Leu His
                405                 410                 415

Gly Tyr Asn Val Ser Ser Asp Val Leu Lys Thr Phe Arg Asp Glu Asn
            420                 425                 430

Gly Glu Phe Phe Cys Phe Leu Gly Gln Thr Gln Arg Gly Val Thr Asp
        435                 440                 445

Met Leu Asn Val Asn Arg Cys Ser His Val Ser Phe Pro Gly Glu Thr
    450                 455                 460

Ile Met Glu Glu Ala Lys Leu Cys Thr Glu Arg Tyr Leu Arg Asn Ala
465                 470                 475                 480

Leu Glu Asn Val Asp Ala Phe Asp Lys Trp Ala Phe Lys Lys Asn Ile
                485                 490                 495

Arg Gly Glu Val Glu Tyr Ala Leu Lys Tyr Pro Trp His Lys Ser Met
            500                 505                 510

Pro Arg Leu Glu Ala Arg Ser Tyr Ile Glu Asn Tyr Gly Pro Asp Asp
        515                 520                 525

Val Trp Leu Gly Lys Thr Val Tyr Met Met Pro Tyr Ile Ser Asn Glu
    530                 535                 540

Lys Tyr Leu Glu Leu Ala Lys Leu Asp Phe Asn Lys Val Gln Ser Ile
545                 550                 555                 560

His Gln Thr Glu Leu Gln Asp Leu Arg Arg Trp Trp Lys Ser Ser Gly
                565                 570                 575
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Phe Thr Asp Leu Asn Phe Thr Arg Glu Arg Val Thr Glu Ile Tyr Phe
            580                 585                 590

Ser Pro Ala Ser Phe Ile Phe Glu Pro Glu Phe Ser Lys Cys Arg Glu
        595                 600                 605

Val Tyr Thr Lys Thr Ser Asn Phe Thr Val Ile Leu Asp Asp Leu Tyr
    610                 615                 620

Asp Ala His Gly Ser Leu Asp Asp Leu Lys Leu Phe Thr Glu Ser Val
625                 630                 635                 640

Lys Arg Trp Asp Leu Ser Leu Val Asp Gln Met Pro Gln Gln Met Lys
                645                 650                 655

Ile Cys Phe Val Gly Phe Tyr Asn Thr Phe Asn Asp Ile Ala Lys Glu
            660                 665                 670

Gly Arg Glu Arg Gln Gly Arg Asp Val Leu Gly Tyr Ile Gln Asn Val
        675                 680                 685

Trp Lys Val Gln Leu Glu Ala Tyr Thr Lys Glu Ala Glu Trp Ser Glu
    690                 695                 700

Ala Lys Tyr Val Pro Ser Phe Asn Glu Tyr Ile Glu Asn Ala Ser Val
705                 710                 715                 720

Ser Ile Ala Leu Gly Thr Val Val Leu Ile Ser Ala Leu Phe Thr Gly
                725                 730                 735

Glu Val Leu Thr Asp Glu Val Leu Ser Lys Ile Asp Arg Glu Ser Arg
            740                 745                 750

Phe Leu Gln Leu Met Gly Leu Thr Gly Arg Leu Val Asn Asp Thr Lys
        755                 760                 765

Thr Tyr Gln Ala Glu Arg Gly Gln Gly Glu Val Ala Ser Ala Ile Gln
    770                 775                 780

Cys Tyr Met Lys Asp His Pro Lys Ile Ser Glu Glu Glu Ala Leu Gln
785                 790                 795                 800

His Val Tyr Ser Val Met Glu Asn Ala Leu Glu Glu Leu Asn Arg Glu
                805                 810                 815

Phe Val Asn Asn Lys Ile Pro Asp Ile Tyr Lys Arg Leu Val Phe Glu
            820                 825                 830

Thr Ala Arg Ile Met Gln Leu Phe Tyr Met Gln Gly Asp Gly Leu Thr
        835                 840                 845

Leu Ser His Asp Met Glu Ile Lys Glu His Val Lys Asn Cys Leu Phe
    850                 855                 860

Gln Pro Val Ala
865
```

<210> SEQ ID NO 57
<211> LENGTH: 2089
<212> TYPE: DNA
<213> ORGANISM: Abies grandis
<220> FEATURE:
<221> NAME/KEY: CDS
<222> LOCATION: (73)...(1983)
<223> OTHER INFORMATION: (-)-4S-limonene synthase

<400> SEQUENCE: 57

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tgccgtttaa tcggtttaaa gaagctacca tagttcggtt taaagaagct accatagttt     60

aggcaggaat cc atg gct ctc ctt tct atc gta tct ttg cag gtt ccc aaa    111
              Met Ala Leu Leu Ser Ile Val Ser Leu Gln Val Pro Lys
               1               5                  10

tcc tgc ggg ctg aaa tcg ttg atc agt tcc agc aat gtg cag aag gct      159
Ser Cys Gly Leu Lys Ser Leu Ile Ser Ser Ser Asn Val Gln Lys Ala
     15                  20                  25
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ctc tgt atc tct aca gca gtc cca aca ctc aga atg cgt agg cga cag      207
Leu Cys Ile Ser Thr Ala Val Pro Thr Leu Arg Met Arg Arg Arg Gln
 30                  35                  40                  45

aaa gct ctg gtc atc aac atg aaa ttg acc act gta tcc cat cgt gat      255
Lys Ala Leu Val Ile Asn Met Lys Leu Thr Thr Val Ser His Arg Asp
                 50                  55                  60

gat aat ggt ggt ggt gta ctg caa aga cgc ata gcc gat cat cat ccc      303
Asp Asn Gly Gly Gly Val Leu Gln Arg Arg Ile Ala Asp His His Pro
             65                  70                  75

aac ctg tgg gaa gat gat ttc ata caa tca ttg tcc tca cct tat ggg      351
Asn Leu Trp Glu Asp Asp Phe Ile Gln Ser Leu Ser Ser Pro Tyr Gly
         80                  85                  90

gga tct tcg tac agt gaa cgt gct gag aca gtc gtt gag gaa gta aaa      399
Gly Ser Ser Tyr Ser Glu Arg Ala Glu Thr Val Val Glu Glu Val Lys
     95                 100                 105

gag atg ttc aat tca ata cca aat aat aga gaa tta ttt ggt tcc caa      447
Glu Met Phe Asn Ser Ile Pro Asn Asn Arg Glu Leu Phe Gly Ser Gln
110                 115                 120                 125

aat gat ctc ctt aca cgc ctt tgg atg gtg gat agc att gaa cgt ctg      495
Asn Asp Leu Leu Thr Arg Leu Trp Met Val Asp Ser Ile Glu Arg Leu
                130                 135                 140

ggg ata gat aga cat ttc caa aat gag ata aga gta gcc ctc gat tat      543
Gly Ile Asp Arg His Phe Gln Asn Glu Ile Arg Val Ala Leu Asp Tyr
            145                 150                 155

gtt tac agt tat tgg aag gaa aag gaa ggc att ggg tgt ggc aga gat      591
Val Tyr Ser Tyr Trp Lys Glu Lys Glu Gly Ile Gly Cys Gly Arg Asp
        160                 165                 170

tct act ttt cct gat ctc aac tcg act gcc ttg gcg ctt cga act ctt      639
Ser Thr Phe Pro Asp Leu Asn Ser Thr Ala Leu Ala Leu Arg Thr Leu
    175                 180                 185

cga ctg cac gga tac aat gtg tct tca gat gtg ctg gaa tac ttc aaa      687
Arg Leu His Gly Tyr Asn Val Ser Ser Asp Val Leu Glu Tyr Phe Lys
190                 195                 200                 205

gat gaa aag ggg cat ttt gcc tgc cct gca atc cta acc gag gga cag      735
Asp Glu Lys Gly His Phe Ala Cys Pro Ala Ile Leu Thr Glu Gly Gln
                210                 215                 220

atc act aga agt gtt cta aat tta tat cgg gct tcc ctg gtc gcc ttt      783
Ile Thr Arg Ser Val Leu Asn Leu Tyr Arg Ala Ser Leu Val Ala Phe
            225                 230                 235

ccc ggg gag aaa gtt atg gaa gag gct gaa atc ttc tcg gca tct tat      831
Pro Gly Glu Lys Val Met Glu Glu Ala Glu Ile Phe Ser Ala Ser Tyr
        240                 245                 250

ttg aaa aaa gtc tta caa aag att ccg gtc tcc aat ctt tca gga gag      879
Leu Lys Lys Val Leu Gln Lys Ile Pro Val Ser Asn Leu Ser Gly Glu
    255                 260                 265

ata gaa tat gtt ttg gaa tat ggt tgg cac acg aat ttg ccg aga ttg      927
Ile Glu Tyr Val Leu Glu Tyr Gly Trp His Thr Asn Leu Pro Arg Leu
270                 275                 280                 285

gaa gca aga aat tat atc gag gtc tac gag cag agc ggc tat gaa agc      975
Glu Ala Arg Asn Tyr Ile Glu Val Tyr Glu Gln Ser Gly Tyr Glu Ser
                290                 295                 300

tta aac gag atg cca tat atg aac atg aag aag ctt tta caa ctt gca     1023
Leu Asn Glu Met Pro Tyr Met Asn Met Lys Lys Leu Leu Gln Leu Ala
            305                 310                 315

aaa ttg gag ttc aat atc ttt cac tct ttg caa cta aga gag tta caa     1071
Lys Leu Glu Phe Asn Ile Phe His Ser Leu Gln Leu Arg Glu Leu Gln
        320                 325                 330

tct atc tcc aga tgg tgg aaa gaa tca ggt tcg tct caa ctg act ttt     1119
Ser Ile Ser Arg Trp Trp Lys Glu Ser Gly Ser Ser Gln Leu Thr Phe
    335                 340                 345
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aca cgg cat cgt cac gtg gaa tac tac act atg gca tct tgc att tct     1167
Thr Arg His Arg His Val Glu Tyr Tyr Thr Met Ala Ser Cys Ile Ser
350                 355                 360                 365

atg ttg cca aaa cat tca gct ttc aga atg gag ttt gtc aaa gtg tgt     1215
Met Leu Pro Lys His Ser Ala Phe Arg Met Glu Phe Val Lys Val Cys
                370                 375                 380

cat ctt gta aca gtt ctc gat gat ata tat gac act ttt gga aca atg     1263
His Leu Val Thr Val Leu Asp Asp Ile Tyr Asp Thr Phe Gly Thr Met
            385                 390                 395

aac gaa ctc caa ctt ttt acg gat gca att aag aga tgg gat ttg tca     1311
Asn Glu Leu Gln Leu Phe Thr Asp Ala Ile Lys Arg Trp Asp Leu Ser
        400                 405                 410

acg aca agg tgg ctt cca gaa tat atg aaa gga gtg tac atg gac ttg     1359
Thr Thr Arg Trp Leu Pro Glu Tyr Met Lys Gly Val Tyr Met Asp Leu
    415                 420                 425

tat caa tgc att aat gaa atg gtg gaa gag gct gag aag act caa ggc     1407
Tyr Gln Cys Ile Asn Glu Met Val Glu Glu Ala Glu Lys Thr Gln Gly
430                 435                 440                 445

cga gat atg ctc aac tat att caa aat gct tgg gaa gcc cta ttt gat     1455
Arg Asp Met Leu Asn Tyr Ile Gln Asn Ala Trp Glu Ala Leu Phe Asp
                450                 455                 460

acc ttt atg caa gaa gca aag tgg atc tcc agc agt tat ctc cca acg     1503
Thr Phe Met Gln Glu Ala Lys Trp Ile Ser Ser Ser Tyr Leu Pro Thr
            465                 470                 475

ttt gag gag tac ttg aag aat gca aaa gtt agt tct ggt tct cgc ata     1551
Phe Glu Glu Tyr Leu Lys Asn Ala Lys Val Ser Ser Gly Ser Arg Ile
        480                 485                 490

gcc aca tta caa ccc att ctc act ttg gat gta cca ctt cct gat tac     1599
Ala Thr Leu Gln Pro Ile Leu Thr Leu Asp Val Pro Leu Pro Asp Tyr
    495                 500                 505

ata ctg caa gaa att gat tat cca tcc aga ttc aat gag tta gct tcg     1647
Ile Leu Gln Glu Ile Asp Tyr Pro Ser Arg Phe Asn Glu Leu Ala Ser
510                 515                 520                 525

tcc atc ctt cga cta cga ggt gac acg cgc tgc tac aag gcg gat agg     1695
Ser Ile Leu Arg Leu Arg Gly Asp Thr Arg Cys Tyr Lys Ala Asp Arg
                530                 535                 540

gcc cgt gga gaa gaa gct tca gct ata tcg tgt tat atg aaa gac cat     1743
Ala Arg Gly Glu Glu Ala Ser Ala Ile Ser Cys Tyr Met Lys Asp His
            545                 550                 555

cct gga tca ata gag gaa gat gct ctc aat cat atc aac gcc atg atc     1791
Pro Gly Ser Ile Glu Glu Asp Ala Leu Asn His Ile Asn Ala Met Ile
        560                 565                 570

agt gat gca atc aga gaa tta aat tgg gag ctt ctc aga ccg gat agc     1839
Ser Asp Ala Ile Arg Glu Leu Asn Trp Glu Leu Leu Arg Pro Asp Ser
    575                 580                 585

aaa agt ccc atc tct tcc aag aaa cat gct ttt gac atc acc aga gct     1887
Lys Ser Pro Ile Ser Ser Lys Lys His Ala Phe Asp Ile Thr Arg Ala
590                 595                 600                 605

ttc cat cat gtc tac aaa tat cga gat ggt tac act gtt tcc aac aac     1935
Phe His His Val Tyr Lys Tyr Arg Asp Gly Tyr Thr Val Ser Asn Asn
                610                 615                 620

gaa aca aag aat ttg gtg atg aaa acc gtt ctt gaa cct ctc gct ttg     1983
Glu Thr Lys Asn Leu Val Met Lys Thr Val Leu Glu Pro Leu Ala Leu
            625                 630                 635

taa aaacatatag aatgcattaa aatgtgggaa gtctataatc tagactattc          2036

tctatctttc ataatgtaga tctggatgtg tattgaactc taaaaaaaaa aaa          2089
```

<210> SEQ ID NO 58
<211> LENGTH: 637

-continued

<212> TYPE: PRT
<213> ORGANISM: Abies grandis

<400> SEQUENCE: 58

Met Ala Leu Leu Ser Ile Val Ser Leu Gln Val Pro Lys Ser Cys Gly
 1   5   10   15

Leu Lys Ser Leu Ile Ser Ser Ser Asn Val Gln Lys Ala Leu Cys Ile
            20   25   30

Ser Thr Ala Val Pro Thr Leu Arg Met Arg Arg Arg Gln Lys Ala Leu
        35   40   45

Val Ile Asn Met Lys Leu Thr Thr Val Ser His Arg Asp Asp Asn Gly
    50   55   60

Gly Gly Val Leu Gln Arg Arg Ile Ala Asp His His Pro Asn Leu Trp
65   70   75   80

Glu Asp Asp Phe Ile Gln Ser Leu Ser Ser Pro Tyr Gly Gly Ser Ser
                85   90   95

Tyr Ser Glu Arg Ala Glu Thr Val Val Glu Glu Val Lys Glu Met Phe
            100   105   110

Asn Ser Ile Pro Asn Asn Arg Glu Leu Phe Gly Ser Gln Asn Asp Leu
        115   120   125

Leu Thr Arg Leu Trp Met Val Asp Ser Ile Glu Arg Leu Gly Ile Asp
    130   135   140

Arg His Phe Gln Asn Glu Ile Arg Val Ala Leu Asp Tyr Val Tyr Ser
145   150   155   160

Tyr Trp Lys Glu Lys Glu Gly Ile Gly Cys Gly Arg Asp Ser Thr Phe
                165   170   175

Pro Asp Leu Asn Ser Thr Ala Leu Ala Leu Arg Thr Leu Arg Leu His
            180   185   190

Gly Tyr Asn Val Ser Ser Asp Val Leu Glu Tyr Phe Lys Asp Glu Lys
        195   200   205

Gly His Phe Ala Cys Pro Ala Ile Leu Thr Glu Gly Gln Ile Thr Arg
    210   215   220

Ser Val Leu Asn Leu Tyr Arg Ala Ser Leu Val Ala Phe Pro Gly Glu
225   230   235   240

Lys Val Met Glu Glu Ala Glu Ile Phe Ser Ala Ser Tyr Leu Lys Lys
                245   250   255

Val Leu Gln Lys Ile Pro Val Ser Asn Leu Ser Gly Glu Ile Glu Tyr
            260   265   270

Val Leu Glu Tyr Gly Trp His Thr Asn Leu Pro Arg Leu Glu Ala Arg
        275   280   285

Asn Tyr Ile Glu Val Tyr Glu Gln Ser Gly Tyr Glu Ser Leu Asn Glu
    290   295   300

Met Pro Tyr Met Asn Met Lys Lys Leu Leu Gln Leu Ala Lys Leu Glu
305   310   315   320

Phe Asn Ile Phe His Ser Leu Gln Leu Arg Glu Leu Gln Ser Ile Ser
                325   330   335

Arg Trp Trp Lys Glu Ser Gly Ser Ser Gln Leu Thr Phe Thr Arg His
            340   345   350

Arg His Val Glu Tyr Tyr Thr Met Ala Ser Cys Ile Ser Met Leu Pro
        355   360   365

Lys His Ser Ala Phe Arg Met Glu Phe Val Lys Val Cys His Leu Val
    370   375   380

Thr Val Leu Asp Asp Ile Tyr Asp Thr Phe Gly Thr Met Asn Glu Leu
385   390   395   400

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Gln Leu Phe Thr Asp Ala Ile Lys Arg Trp Asp Leu Ser Thr Thr Arg
                405                 410                 415

Trp Leu Pro Glu Tyr Met Lys Gly Val Tyr Met Asp Leu Tyr Gln Cys
            420                 425                 430

Ile Asn Glu Met Val Glu Glu Ala Glu Lys Thr Gln Gly Arg Asp Met
        435                 440                 445

Leu Asn Tyr Ile Gln Asn Ala Trp Glu Ala Leu Phe Asp Thr Phe Met
    450                 455                 460

Gln Glu Ala Lys Trp Ile Ser Ser Ser Tyr Leu Pro Thr Phe Glu Glu
465                 470                 475                 480

Tyr Leu Lys Asn Ala Lys Val Ser Ser Gly Ser Arg Ile Ala Thr Leu
                485                 490                 495

Gln Pro Ile Leu Thr Leu Asp Val Pro Leu Pro Asp Tyr Ile Leu Gln
            500                 505                 510

Glu Ile Asp Tyr Pro Ser Arg Phe Asn Glu Leu Ala Ser Ser Ile Leu
        515                 520                 525

Arg Leu Arg Gly Asp Thr Arg Cys Tyr Lys Ala Asp Arg Ala Arg Gly
    530                 535                 540

Glu Glu Ala Ser Ala Ile Ser Cys Tyr Met Lys Asp His Pro Gly Ser
545                 550                 555                 560

Ile Glu Glu Asp Ala Leu Asn His Ile Asn Ala Met Ile Ser Asp Ala
                565                 570                 575

Ile Arg Glu Leu Asn Trp Glu Leu Leu Arg Pro Asp Ser Lys Ser Pro
            580                 585                 590

Ile Ser Ser Lys Lys His Ala Phe Asp Ile Thr Arg Ala Phe His His
        595                 600                 605

Val Tyr Lys Tyr Arg Asp Gly Tyr Thr Val Ser Asn Asn Glu Thr Lys
    610                 615                 620

Asn Leu Val Met Lys Thr Val Leu Glu Pro Leu Ala Leu
625                 630                 635
```

We claim the following:

1. An isolated synthase having a region with 40% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2, wherein one or more amino acid residues of said synthase that align with amino acids at positions 270, 273, 294, 297, 298, 376, 401, 402, 403, 404, 407, 440, 444, 516, 519, 520, 525, 527, and 528 of SEQ ID NO:2 are residues other than the following ordered arrangements of residues:

Ordered Arrangement of R-Groups at α-carbons 1–19									
1	2	3	4	5	6	7	8	9	10
C	W	I	I	S	Y	T	T	T	Y
C	W	I	I	S	Y	T	S	T	Y
G	W	I	A	S	Y	T	C	G	Y
G	W	I	A	S	Y	T	S	G	Y
C	W	L	T	S	Y	S	A	G	Y
G	W	L	L	S	Y	S	T	V	H
C	W	L	T	S	Y	S	A	G	Y
L	W	I	T	T	Y	S	V	G	N
P	W	I	V	D	Y	S	T	A	G
A	W	V	C	G	F	T	S	C	I
N	F	F	L	G	A	E	I	T	A
C	W	N	I	T	Y	S	I	S	G
S	W	V	L	T	Y	S	S	S	Y
N	F	F	L	V	N	A	T	L	A

-continued

Ordered Arrangement of R-Groups at α-carbons 1–19									
C	W	N	I	T	Y	I	S	G	P
C	W	N	V	T	Y	I	G	G	I
C	Y	L	L	T	F	A	V	T	M
C	W	I	I	T	Y	S	I	S	A
S	W	F	I	V	F	S	S	S	V
S	W	I	A	T	Y	S	V	A	S
N	W	N	L	T	Y	S	I	S	S
F	L	A	Q	T	Y	S	I	G	Q
I	S	S	T	V	Y	S	I	A	L
Y	L	C	I	T	Y	S	C	G	H
G	S	F	I	T	F	S	S	S	V
Y	W	A	C	T	Y	S	S	G	M
A	A	N	L	T	N	A	L	T	S
F	L	C	V	T	Y	S	S	A	Y
F	W	A	M	T	Y	N	T	G	M
Y	M	C	V	T	F	V	S	S	G
V	S	G	Q	V	Y	S	V	G	L
C	S	G	T	T	M	F	A	L	G
C	S	G	T	T	M	S	F	A	L
C	A	G	T	T	M	S	F	A	L
I	W	V	I	S	Y	T	T	G	L
Y	W	A	C	T	Y	S	S	G	M
C	W	I	I	S	Y	T	S	T	Y
C	W	I	I	S	Y	T	T	T	Y
C	W	N	I	T	Y	S	I	S	G
F	A	A	Q	T	Y	S	I	G	Q

-continued

Ordered Arrangement of R-Groups at α-carbons 1–19								
F	A	I	A	T	Y	S	V	A	S
11	12	13	14	15	16	17	18	19	
L	C	D	V	T	Y	D	Y	T	
L	C	D	I	T	Y	D	Y	T	
L	C	D	M	L	Y	D	Y	T	
L	C	D	M	L	Y	D	Y	T	
I	A	N	A	L	Y	D	Y	T	
L	G	D	A	V	Y	D	Y	T	
I	A	N	A	L	Y	D	Y	S	
L	F	D	V	L	Y	D	F	T	
L	S	D	A	C	Y	D	Y	T	
M	G	N	C	S	Y	D	Y	S	
T	G	N	I	T	Y	E	F	T	
M	L	D	A	M	Y	D	H	Q	
L	G	G	V	L	Y	D	F	T	
L	G	N	L	S	Y	E	F	T	
L	L	D	A	M	Y	D	H	G	
L	L	D	A	I	Y	D	F	G	
T	G	N	I	T	Y	D	Y	T	
I	L	D	A	I	Y	D	D	G	
I	L	N	V	I	Y	D	H	G	
I	L	D	A	I	Y	D	F	G	
I	F	N	S	M	Y	D	H	G	
L	S	D	T	I	F	D	F	G	
V	G	N	M	F	Y	D	L	T	
S	L	G	F	G	Y	D	Y	S	
I	L	N	A	V	Y	D	H	G	
L	G	D	L	I	Y	D	L	Y	
T	C	M	L	L	Y	D	Y	N	
V	L	G	L	L	Y	D	F	S	
L	S	D	I	M	Y	D	F	S	
I	L	G	F	V	Y	D	Y	T	
C	W	N	V	F	Y	D	Y	G	
V	G	N	L	F	Y	D	F	T	
I	G	N	L	F	Y	D	F	T	
I	G	N	V	F	Y	D	Y	T	
V	I	N	T	S	Y	D	Y	T	
L	G	D	L	I	Y	D	L	Y	
L	C	D	V	T	Y	D	Y	T	

-continued

Ordered Arrangement of R-Groups at α-carbons 1–19								
L	C	D	I	T	Y	D	Y	T
M	L	D	A	M	Y	D	H	G
L	S	D	T	I	F	D	F	G
I	L	D	A	I	Y	D	F	G.

2. The synthase of claim **1**, wherein said synthase has 50% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2.

3. The synthase of claim **1**, wherein said synthase has 60% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2.

4. The synthase of claim **1**, wherein said synthase catalyses the formation of a terpenoid product from a monoterpene substrate.

5. The synthase of claim **1**, wherein said synthase catalyses the formation of a terpenoid product from a sesquiterpene substrate.

6. The synthase of claim **1**, wherein said synthase catalyses the formation of a terpenoid product from a diterpene substrate.

7. The synthase of claim **4**, wherein said product is a cyclic terpenoid hydrocarbon.

8. The synthase of claim **5**, wherein said product is a cyclic terpenoid hydrocarbon.

9. The synthase of claim **6**, wherein said product is a cyclic terpenoid hydrocarbon.

10. The synthase of claim **1**, wherein said synthase has 70% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2.

11. The synthase of claim **1**, wherein said synthase has 80% or greater sequence identity to residues 265 to 535 of SEQ ID NO:2.

* * * * *