Effect on the Conformation of a Terminally Blocked, (*E*) β,γ-Unsaturated δ-Amino Acid Residue Induced by Carbon Methylation

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SUPPORTING INFORMATION

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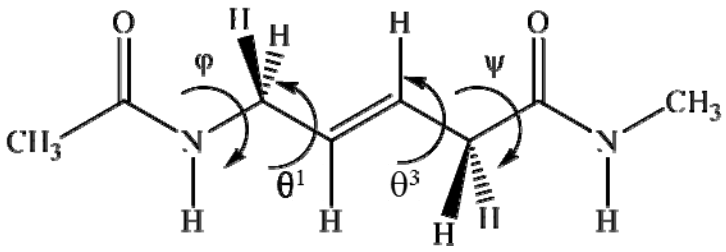
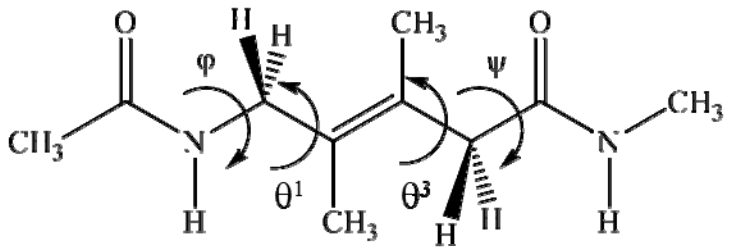
Table S1. Values obtained for the torsion angles (in degrees) of compound **A** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



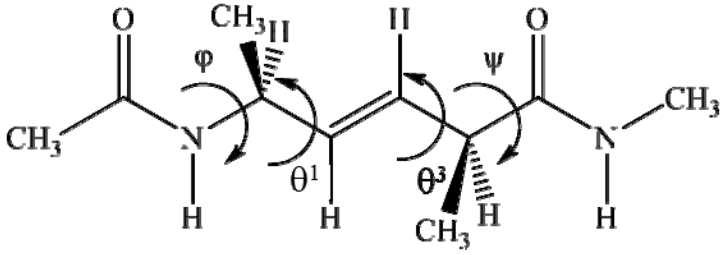
ΔG (kcal/mol)	d(N-H···O) (Å)	<N-H···O (º)	φ (º)	θ^1 (º)	θ^3 (º)	ψ (º)	Population (T=298 K)
0.0	2.17	155.5	-69.0	-6.0	-104.0	13.7	50.0
0.1	2.08	160.6	-66.1	116.0	105.0	-11.0	41.2
1.5	-	-	121.6	122.9	-111.0	25.4	3.8
1.6	-	-	97.8	119.8	-132.4	132.1	3.4
2.4	-	-	99.3	124.9	112.8	-26.5	0.8
2.7	-	-	99.1	120.2	130.5	-139.7	0.6
3.3	-	-	85.6	-110.9	111. 9	-20.3	0.2
3.8	-	-	81.5	-103.9	117.2	66.7	0.0
4.3	-	-	130.3	123.3	-106.2	-95.7	0.0

Table S2. Values obtained for the torsion angles (in degrees) of compound **B** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



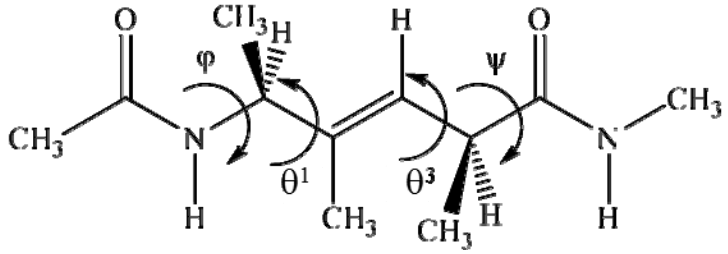
ΔG (kcal/mol)	d(N-H···O) (Å)	<N-H···O (º)	φ (º)	θ^1 (º)	θ^3 (º)	ψ (º)	Population (T=298 K)
0.0	2.07	157.7	61.6	-124.3	-95.2	14.1	93.4
1.8	2.11	152.3	51.3	56.2	91.0	-27.7	2.4
2.9	2.10	140.1	-106.8	-109.9	98.1	-96.6	0.8
3.3			-105.2	-101.6	-93.1	24.8	0.4
3.3			-85.9	108.9	-87.1	12.4	0.4
3.6			-104.9	-123.0	95.5	-21.7	0.2
3.7			-164.8	-81.9	-89.9	-159.6	0.2
4.6			-87.1	109.9	-84.7	-95.7	0.0
4.8			117.3	110.9	-92.5	-118.5	0.0

Table S3. Values obtained for the torsion angles (in degrees) of compound **C** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



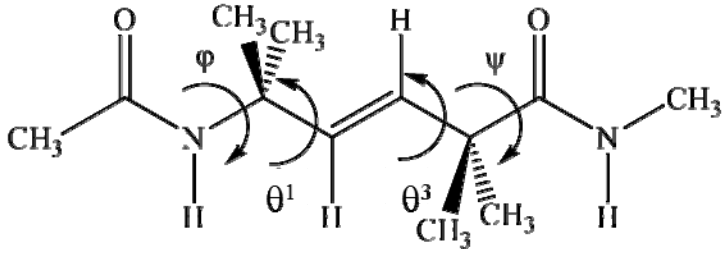
ΔG (kcal/mol)	d(N-H···O) (Å)	<N-H···O (º)	φ (º)	θ^1 (º)	θ^3 (º)	ψ (º)	Population (T=298 K)
0.0	2.07	159.6	-65.7	115.3	105.6	-12.1	76.9
1.0	2.16	154.2	-68.5	-5.6	-110.4	17.1	13.8
1.9	2.10	155.2	63.0	13.3	103.2	-15.3	3.1
2.2	-	-	-93.3	-125.7	111.4	-33.4	1.8
2.3	-	-	-145.1	-126.5	109.9	-29.3	1.5
2.4	2.06	156.7	59.4	-127.5	-107.7	25.4	1.3
2.8	-	-	-148.4	12.3	121.6	-116.1	0.7
3.8	-	-	-87.4	1.3	-9. 8	-82.1	0.1
3.8	-	-	-149.4	-124.5	-115.2	-92.7	0.1
3.8	-	-	-81. 8	103. 5	-119.4	25.1	0.1
3.9	-	-	-148.8	-130.5	-122.0	23.1	0.1
3.9	-	-	-160.7	118.0	-3.7	-97.0	0.1
4.1	-	-	-150.8	-127.2	-9.9	-93.5	0.1
4.2	-	-	-160.9	121.0	-116.1	26.7	0.1
4.3	-	-	-160.5	113.2	119.8	-108.5	0.1
4.4	-	-	-75.2	100.4	-12.9	-96.2	0.0
5.0	-	-	62.5	123.4	-116.0	32.7	0.0
5.3	-	-	-160.8	107.7	95.1	107.7	0.0
5.5	-	-	62.6	-130.3	116.5	-28.9	0.0
5.9	-	-	61.4	127.0	5.5	-80.2	0.0
6.0	-	-	71.2	1.2	-118.9	28.5	0.0
6.2	-	-	61.6	-134.7	125.0	-111.0	0.0
6.7	-	-	70.7	-1.6	-21.4	-92.9	0.0

Table S4. Values obtained for the torsion angles (in degrees) of compound **D** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



ΔG (kcal/mol)	d(N-H···O) (Å)	<N-H···O (º)	φ (º)	θ^1 (º)	θ^3 (º)	ψ (º)	Population (T=298 K)
0.0	2.07	154.0	-57.9	131.3	89.4	-13.5	98.6
2.8	2.12	151.6	52.8	55.4	93.2	-28.7	0.8
3.4	2.14	162.5	-60.1	-31.9	-51.1	-31.5	0.3
3.8	2.09	158.1	65.3	10.3	94.4	-4.3	0.1
4.3			54.7	-132.1	-49.7	-32.8	0.1
4.9			-103.1	-119.1	106.0	-85.5	0.0
4.9			-63.7	-30.3	149.5	-133.3	0.0
5.5			-79.5	105.6	-49.1	-41.1	0.0
5.7			-101.9	-123.1	-49.8	-37.2	0.0
6.2			61.6	-135.2	101.9	-21.0	0.0
6.5			-158.6	107.53	86.31	100.2	0.0
7.0			-162.37	106.5	109.7	-98.6	0.0
7.3			-159.5	110.2	-49.1	-41.2	0.0
7.4			57.5	-135.1	149.0	-133.2	0.0
7.7			84.3	129.2	-52.0	-34.0	0.0
7.9			83.1	116. 8	99.7	-90.7	0.0
8.0			-160.9	-34.2	-49.2	-37.6	0.0
9.4			74.2	0.6	-55.8	-36.3	0.0

Table S5. Values obtained for the torsion angles (in degrees) of compound **E** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



ΔG (kcal/mol)	d(N-H···O) (Å)	<N-H···O (º)	φ (º)	θ^1 (º)	θ^3 (º)	ψ (º)	Population (T=298 K)
0.0	2.04	155.7	58.1	-125.8	-107.4	23.8	74.2
0.6	2.05	157.3	-61.5	-14.0	-109.9	15.8	25.4
3.9	-	-	-176.7	-126.1	112.5	-28.7	0.3
4.2	-	-	-59.4	-125.2	113.1	-32.4	0.1
4.4	-	-	-63.3	-13.3	115. 8	-28.5	0.0
4.4	-	-	-59.8	-119.7	-113.8	32.4	0.0
4.5	-	-	61.1	-126.0	116.3	-27.7	0.0
4.7	-	-	58.9	122. 9	-126.6	117.4	0.0
4.8	-	-	177.4	-25.5	113.3	-29.7	0.0
4.9	-	-	-176.5	-126.5	-117.8	23.7	0.0
5.2	-	-	-178.5	19.2	115.1	-33.7	0.0
5.6	-	-	-176.4	-122.2	-1.0	99.0	0.0
5.7	-	-	-176.5	-117.8	-104.3	-103.2	0.0
5.8	-	-	58.3	120.4	127.7	-117.9	0.0
5.9	-	-	-179.3	21.0	126.8	-124.9	0.0
6.0	-	-	-61.3	-13.3	130.7	-122.3	0.0
6.1	-	-	-178.7	16.8	-131.2	120.2	0.0
6.4	-	-	60.5	-130.7	128.7	-120.3	0.0
6.5	-	-	65.6	7.4	-32.4	-45.9	0.0
6.7	-	-	-177.4	19.4	-29.3	-51.5	0.0
6.7	-	-	-176.8	-124.0	-8.6	-96.8	0.0
6.9	-	-	61.7	-111.5	22.5	56.6	0.0
7.0	-	-	179.2	-19.1	-19.9	-58.8	0.0

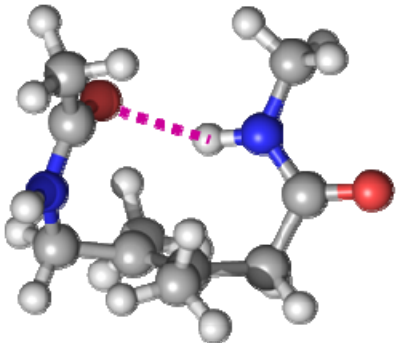


Figure S1. Minimum energy structure of compound **B** destabilized by 1.8 kcal/mol with respect to the global minimum (Table S2). Despite the high ΔG value, this structure presents a C_{10} H-bonded ring.

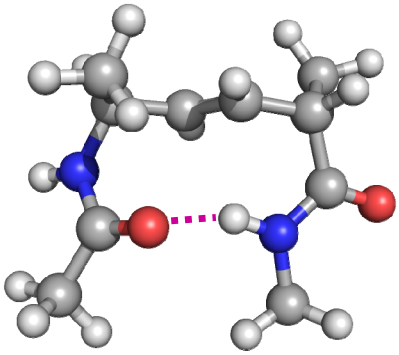


Figure S2. Minimum energy structure of compound **C** destabilized by 2.4 kcal/mol with respect to the global minimum (Table S3). Despite the high ΔG value, this structure presents a C_{10} H-bonded ring.

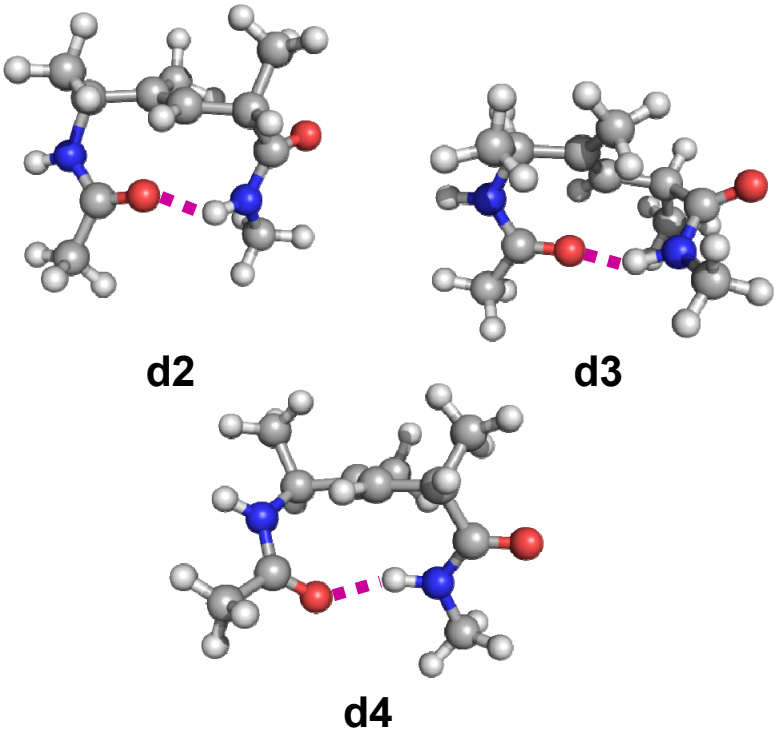


Figure S3. Minimum energy structures of compound **D** destabilized by 2.8 (**d2**), 3.4 (**d3**) and 3.8 (**d4**) kcal/mol with respect to the global minimum (Table S4). Despite the high ΔG values, each structure presents a C_{10} H-bonded ring.

Table S6. Crystal data and structure refinement parameters for Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**)

Identification code	mc309B2	
Empirical formula	$C_{13}H_{24}N_2O_3$	
Formula weight	256.34	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 54.6587(11) Å	α= 90°.
	b = 5.86885(11) Å	β= 99.241(2)°.
	c = 29.3845(4) Å	γ = 90°.
Volume	9303.7(3) $Å^3$	
Z	24	
Density (calculated)	1.098 Mg/m^3	
Absorption coefficient	0.630 mm^{-1}	
F(000)	3360	
Crystal size	0.10 × 0.10 × 0.02 mm^3	
Theta range for data collection	3.047 to 72.173°.	
Index ranges	$-66 \le h \le 62$, $-5 \le k \le 7$, $-36 \le l \le 34$	
Reflections collected	32059	
Independent reflections	9073 [R(int) = 0.0244]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.78404	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9073 / 405 / 502	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R_1 = 0.0548, wR_2 = 0.1502	
R indices (all data)	R_1 = 0.0821, wR_2 = 0.1660	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.299 and -0.173 e.$Å^{-3}$	
CCDC deposition no.	1948908	

Table S7. Crystal data and structure refinement parameters for Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**)

Identification code	mc92p2	
Empirical formula	$C_{17}H_{32}N_2O_3$	
Formula weight	312.44	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	*a* = 5.990(2) Å	α= 88.95(5)°.
	b = 8.937(2) Å	β= 87.04(8)°.
	c = 17.928(3) Å	γ = 80.67(7)°.
Volume	945.7(5) $Å^3$	
Z	2	
Density (calculated)	1.097 Mg/m^3	
Absorption coefficient	0.594 mm^{-1}	
F(000)	344	
Crystal size	0.55 × 0.35 × 0.10 mm^3	
Theta range for data collection	4.940 to 60.001°.	
Index ranges	$-6 \le h \le 6, -10 \le k \le 10, 0 \le l \le 20$	
Reflections collected	2793	
Independent reflections	2793 [R(int) = 0.000]	
Completeness to theta = 60.001°	99.9 %	
Absorption correction	none	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	2793 / 0 / 200	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R_1 = 0.0692, wR_2 = 0.1924	
R indices (all data)	R_1 = 0.0736, wR_2 = 0.2017	
Extinction coefficient	0.026(4)	
Largest diff. peak and hole	0.612 and -0.336 e.$Å^{-3}$	
CCDC deposition no.	1948909	

Table S8. Crystal data and structure refinement parameters for Azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**)

Identification code	mc310	
Empirical formula	$C_{13}H_{23}N_5O_2$	
Formula weight	281.36	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.1653(3) Å	α= 107.580(3)°.
	b = 9.4255(3) Å	β= 91.726(3)°.
	c = 10.5148(3) Å	γ = 106.465(3)°.
Volume	823.73(5) $Å^3$	
Z	2	
Density (calculated)	1.134 Mg/m^3	
Absorption coefficient	0.645 mm^{-1}	
F(000)	304	
Crystal size	0.50 × 0.40 × 0.20 mm^3	
Theta range for data collection	4.447 to 72.814°.	
Index ranges	$-11 \le h \le 11$, $-11 \le k \le 11$, $-13 \le l \le 10$	
Reflections collected	13055	
Independent reflections	3269 [R(int) = 0.0168]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.80313	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3269 / 44 / 203	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R_1 = 0.0523, wR_2 = 0.1533	
R indices (all data)	R_1 = 0.0550, wR_2 = 0.1567	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.303 and -0.217 $e.Å^{-3}$	
CCDC deposition no.	1952416	

Table S9. Backbone torsion angles (°) for the three independent molecules in the X-ray diffraction structure of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**)

Molecule	ω^N	ϕ	θ^1	θ^2	θ^3	ψ	ω^C
1	174.7(2)	141.8(2)	119.8(3)	178.5(2)	-121.2(3)	-123.2(2)	179.3(2)
2	174.96(19)	140.2(2)	125.6(2)	178.7(2)	-117.9(3)	-142.2(2)	-178.4(2)
3	-167.41(16)	87.9(2)	127.4(2)	-178.39(18)	-107.4(2)	-138.7(2)	-178.8(2)

Table S10. Intermolecular H-bond parameters [Å and °] in the X-ray diffraction structure of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N_1-H0_1...O0_3#1	0.86	2.13	2.982(2)	170.5
NT_1-HT_1...O_3#2	0.86	2.13	2.967(2)	163.1
N_2-H0_2...O0_1	0.86	2.12	2.9545(19)	163.7
NT_2-HT_2...O_1	0.86	2.07	2.905(2)	164.7
N_3-H0_3...O0_2	0.86	2.20	2.9459(19)	145.1
NT_3-HT_3...O_2	0.86	2.05	2.898(2)	169.9

Symmetry transformations used to generate equivalent atoms:

#1 x, -y+1, z-1/2 #2 x, -y, z-1/2

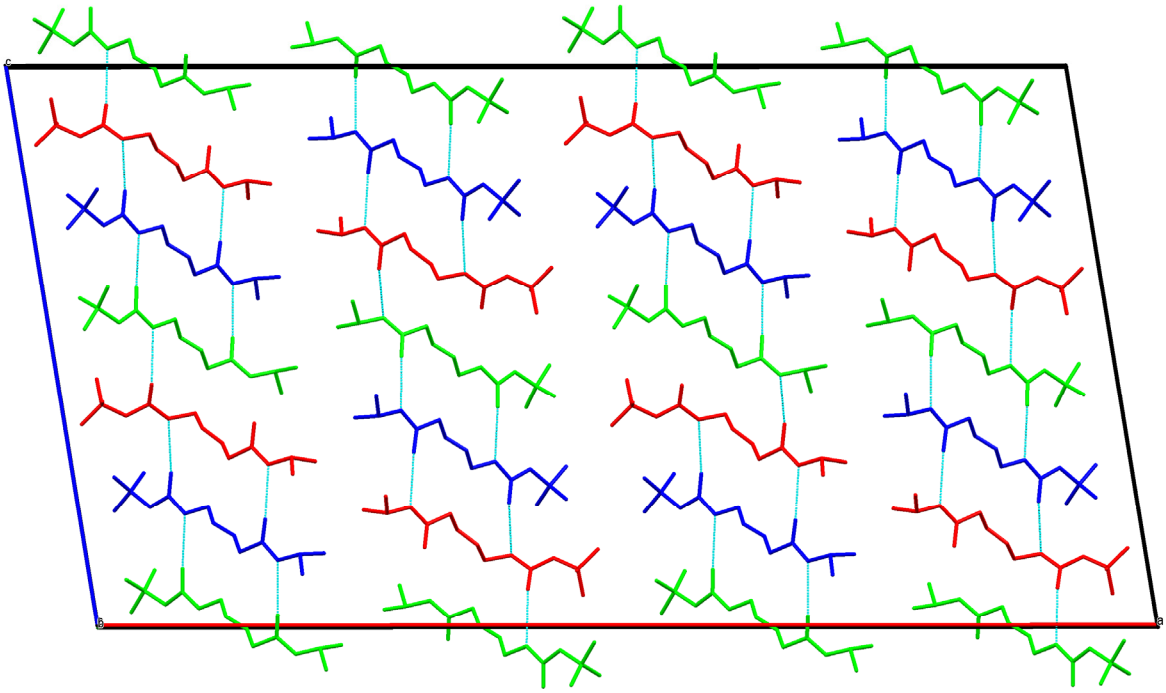


Figure S4. Packing mode of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**) as viewed nearly down the *b* direction. Each of the three independent molecules is shown in a different color. Intermolecular H-bonds are indicated by dashed lines.

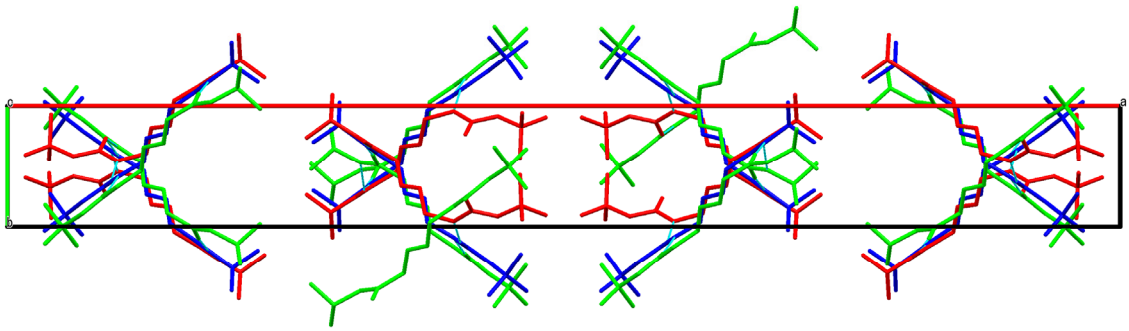


Figure S5. Packing mode of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**) as viewed down the *c* direction. Each of the three independent molecules is shown in a different color.

Table S11. Backbone torsion angles (°) in the X-ray diffraction structure of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**)

ω^N	ϕ	θ^1	θ^2	θ^3	ψ	ω^C
178.29(18)	60.4(3)	8.9(4)	-175.3(2)	98.7(3)	-3.3(3)	-177.9(2)

Table S12. Intra- and interermolecular H-bond parameters [Å and °] in the X-ray diffraction structure of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
NT-HT...O0	0.86	2.30	3.120(3)	160.6
N1-H1...O1#1	0.86	2.14	2.988(3)	166.9

Symmetry transformations used to generate equivalent atoms:

#1 *x*, *y*-1, *z*

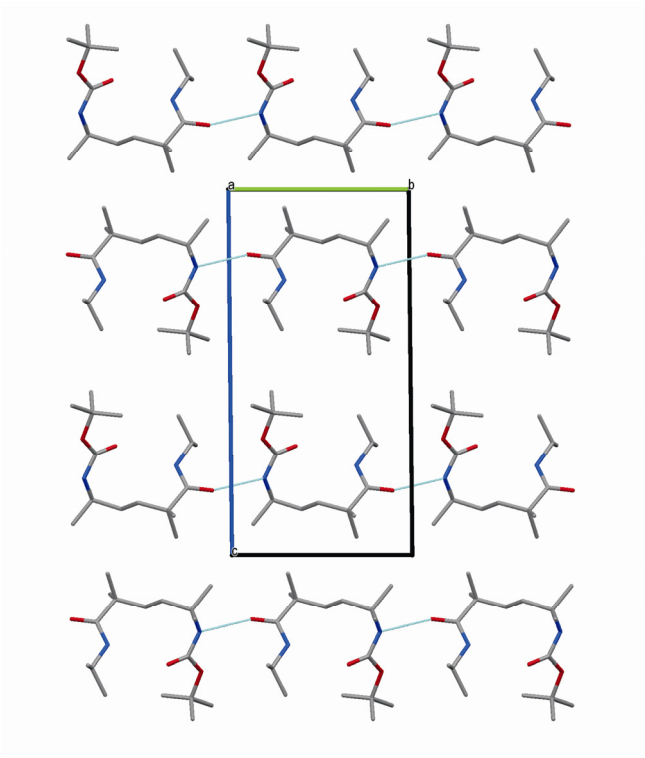


Figure S6. Packing mode of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**) as viewed down the *a* direction. Intermolecular H-bonds are represented by dashed lines.

Table S13. Backbone torsion angles (°) in the X-ray diffraction structure of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**)

ω^N	ϕ	θ^1	θ^2	θ^3	ψ	ω^C
176.09(14)	50.7(2)	-130.52(15)	177.94(12)	-110.48(15)	32.42(17)	177.21(14)

Table S14. Intra- and interermolecular H-bond parameters [Å and °] in the X-ray diffraction structure of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
NT-HT...O0	0.86	2.25	3.0641(15)	158.7
N1-H1...O1#1	0.86	2.05	2.8694(15)	159.3

Symmetry transformations used to generate equivalent atoms:

#1 *x*, *y*-1, *z*

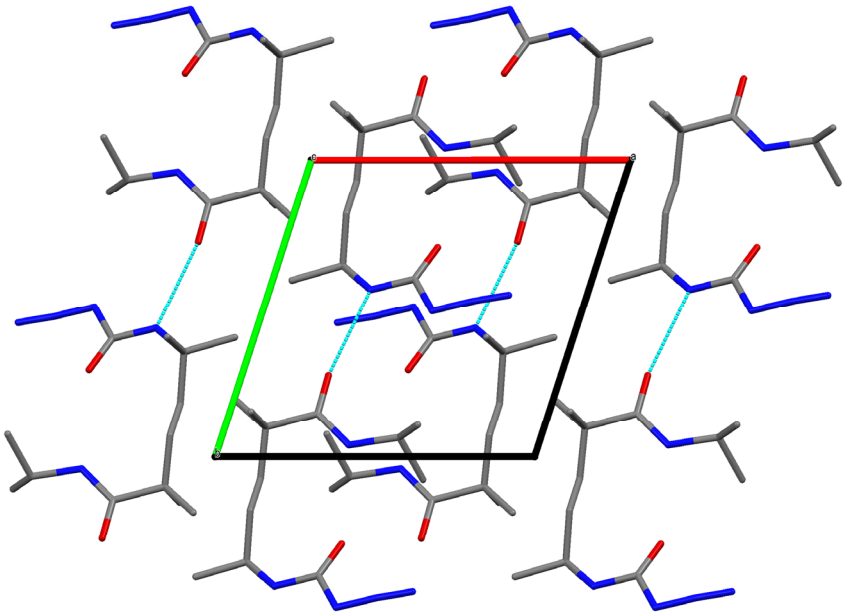


Figure S7. Packing mode of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**) as viewed down the *c* direction. Intermolecular H-bonds are represented by dashed lines.

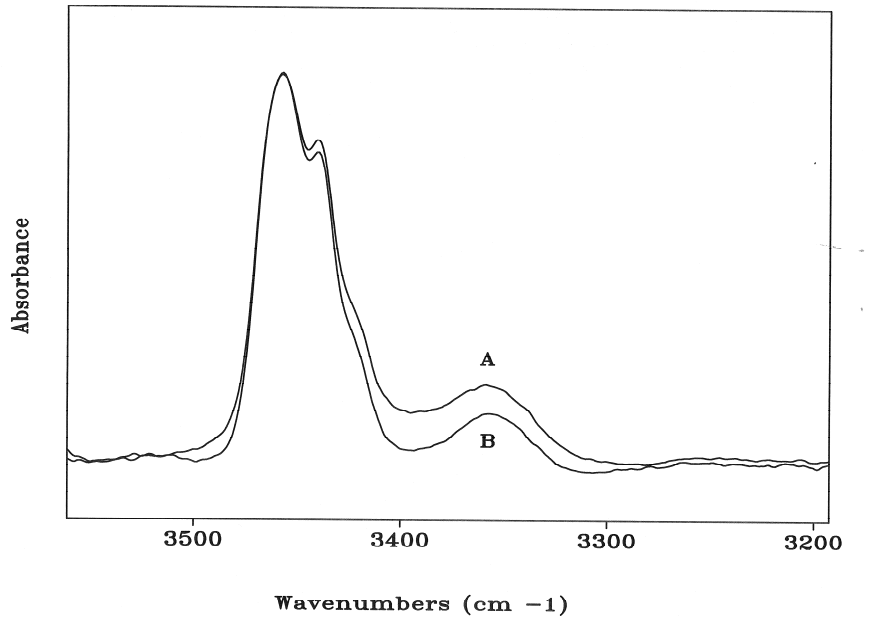


Figure S8. FT-IR absorption spectra in $CDCl_3$ solution of compound (Boc)**A 6** in the 3500-3200 cm^{-1} wavenumber (N-H stretching) region in $CDCl_3$ solution at the concentrations of 1.0 mM (**A**) and 0.1 mM (**B**).

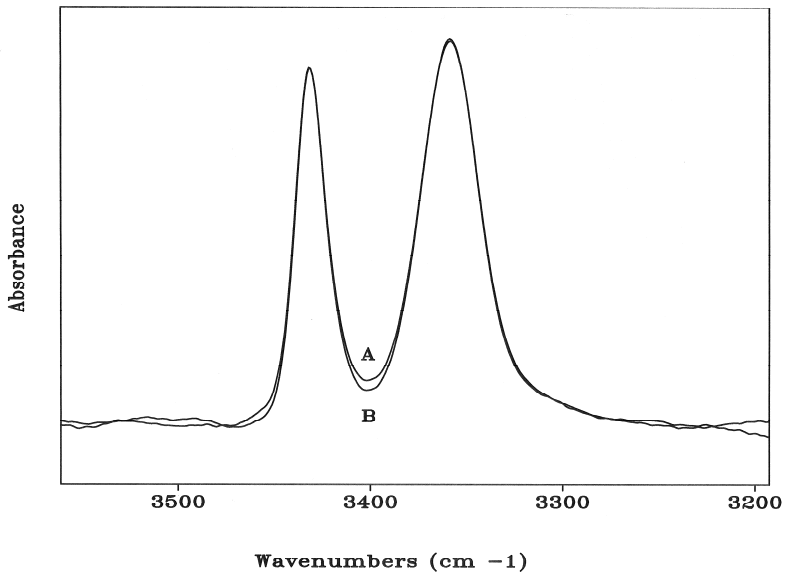
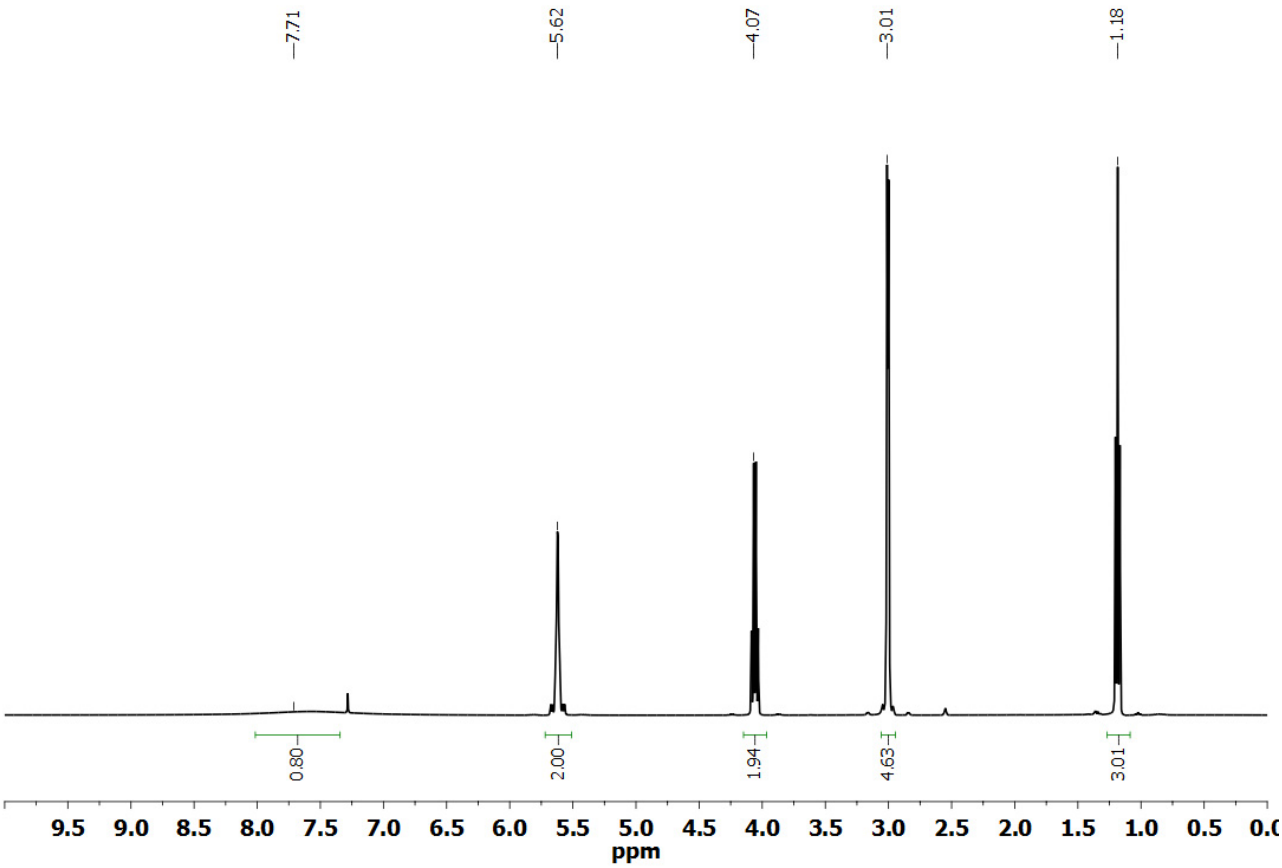
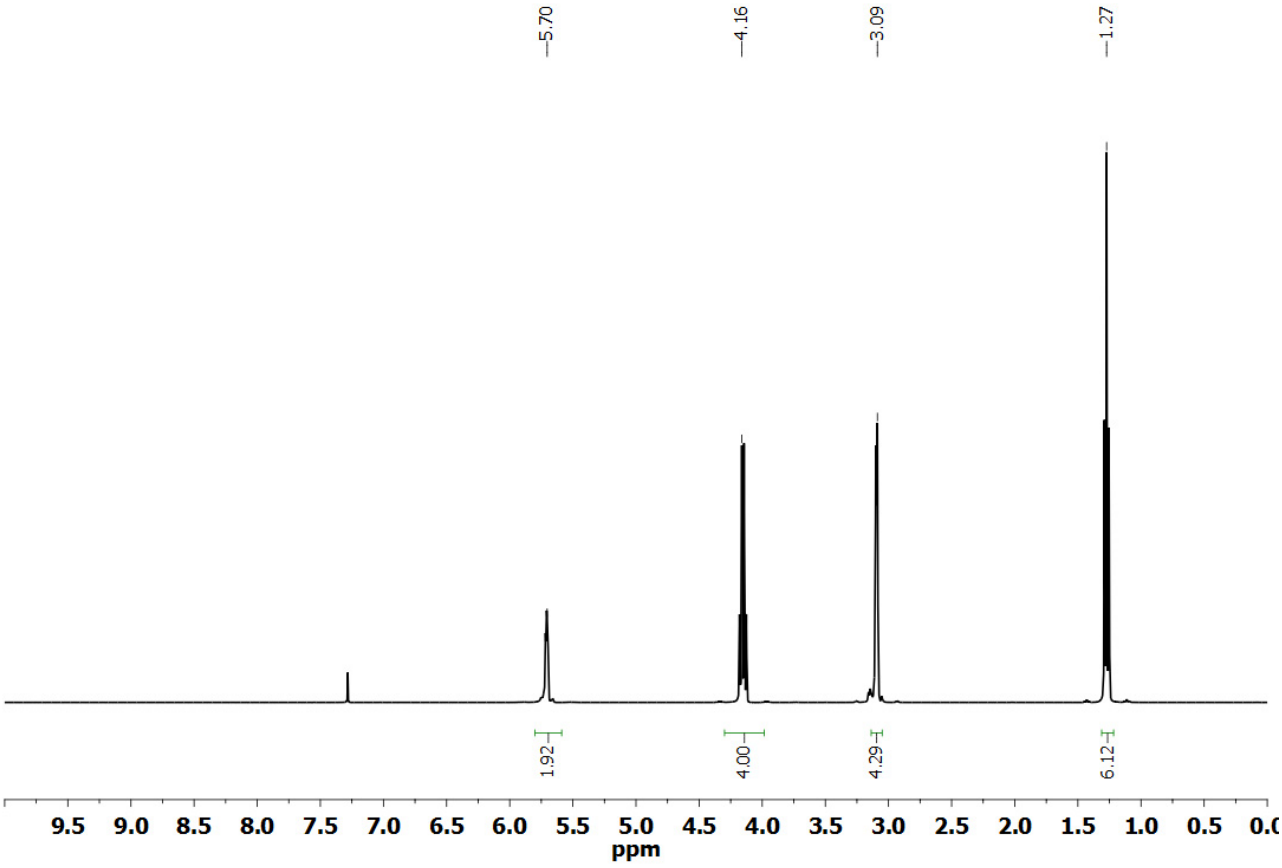


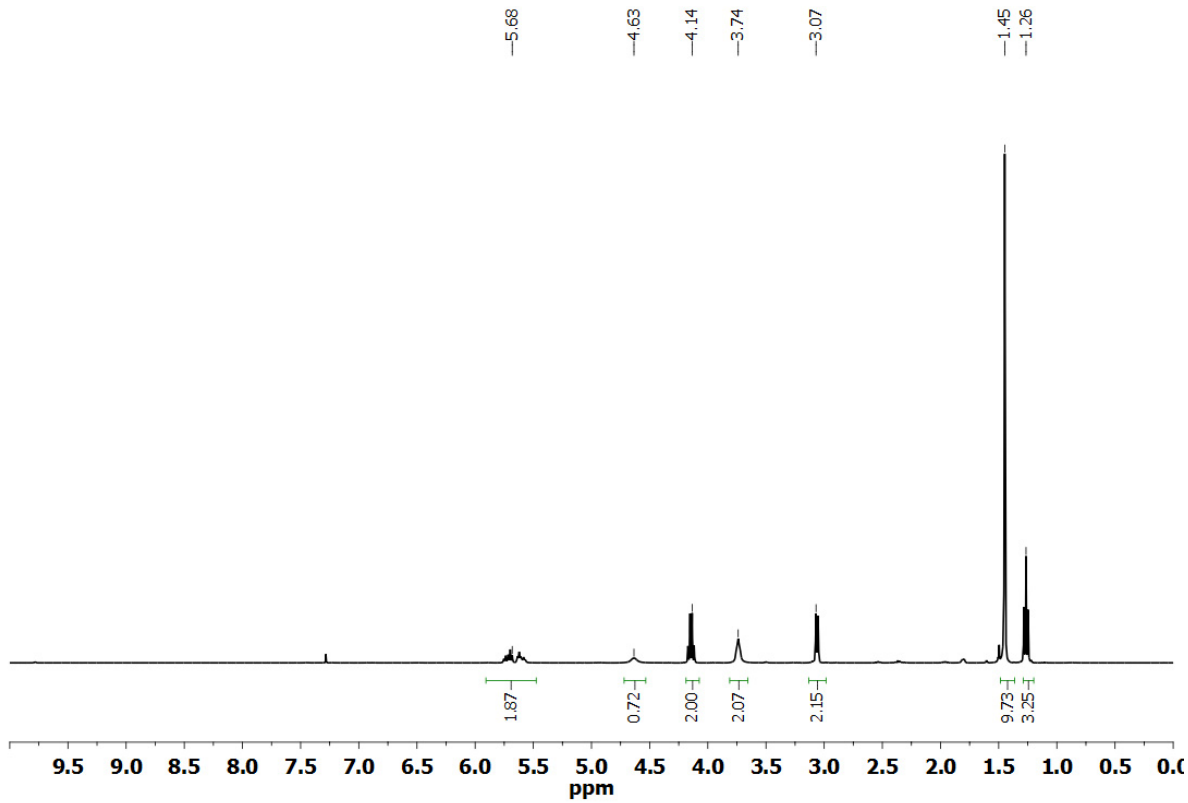
Figure S9. FT-IR absorption spectra in $CDCl_3$ solution (1.0 mM concentration) of compound (Boc)**E 10** in the 3500-3200 cm^{-1} wavenumber (N-H stretching) region in $CDCl_3$ solution at the concentrations of 1.0 mM (**A**) and 0.1 mM (**B**).



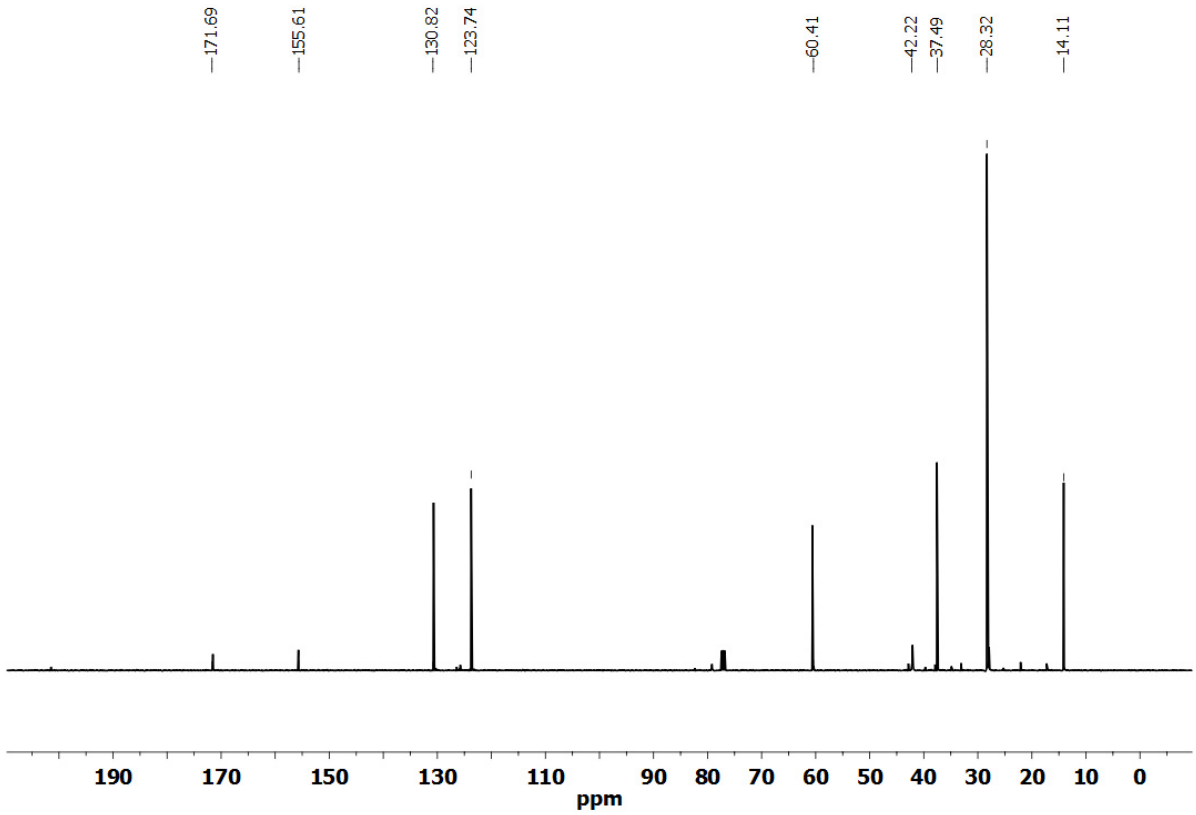
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2**.



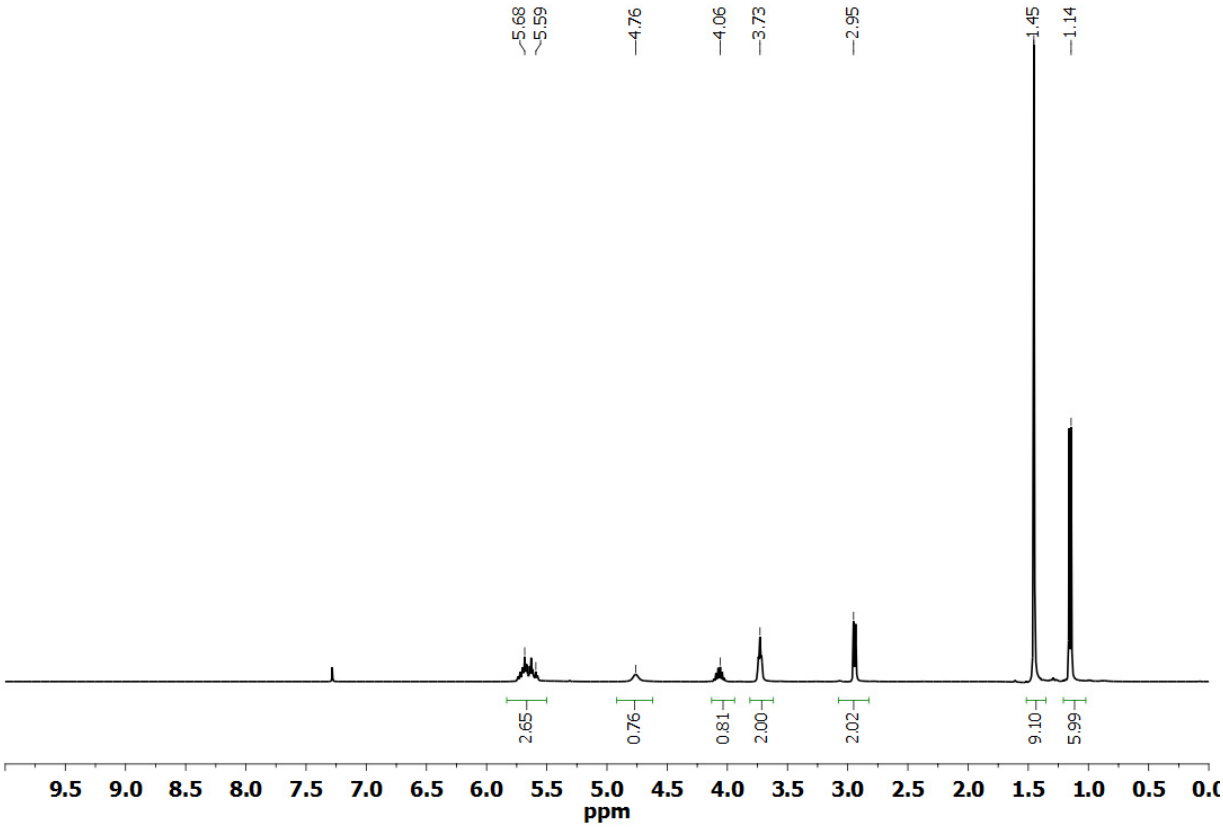
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3**.



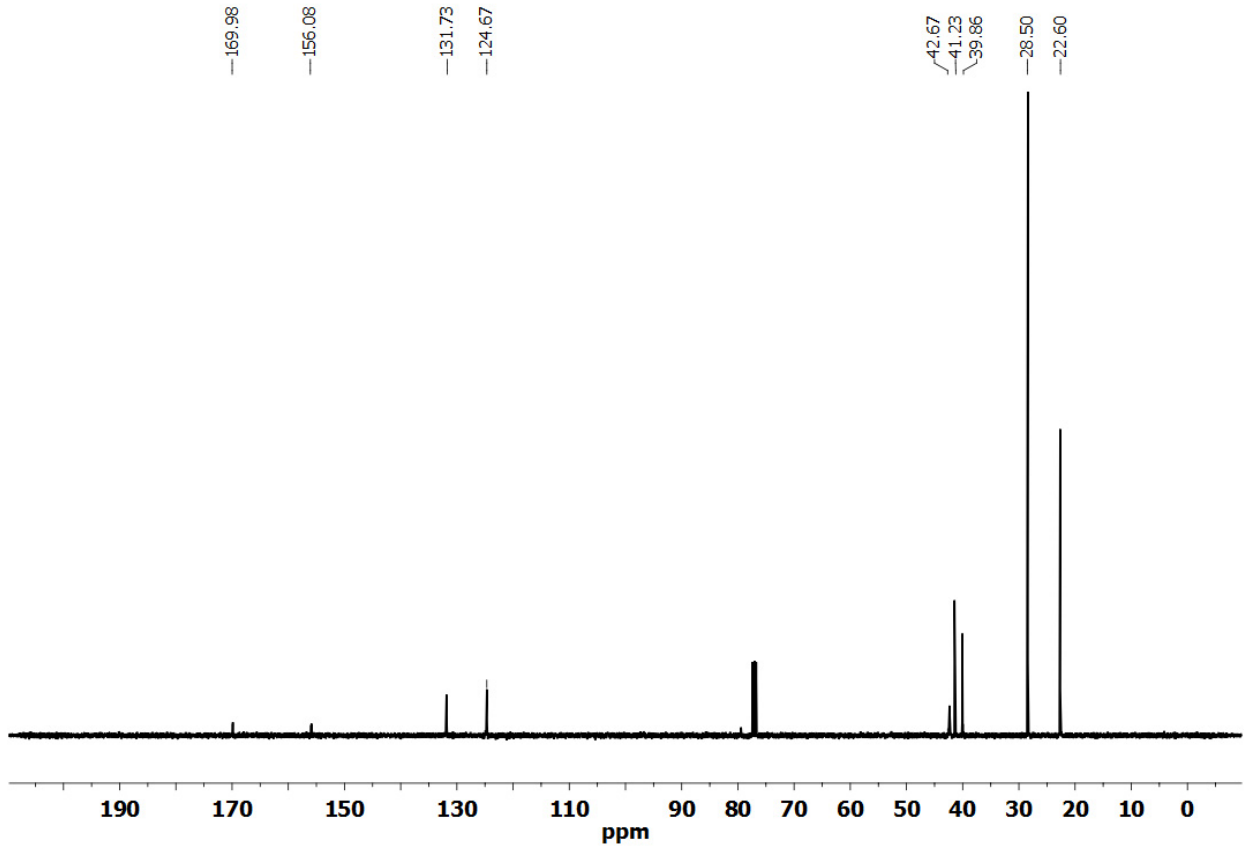
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4**.



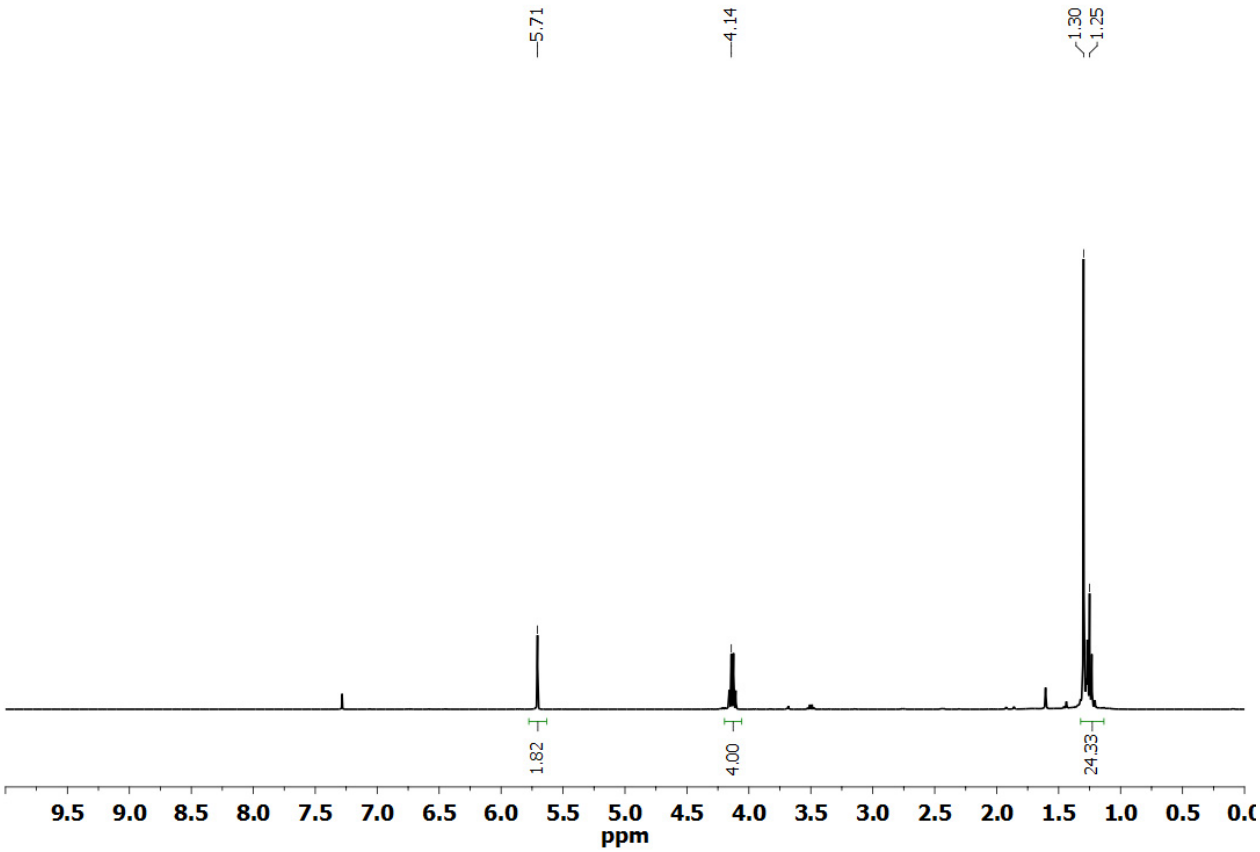
^{13}C NMR (101 MHz, $CDCl_3$) of compound **4**.



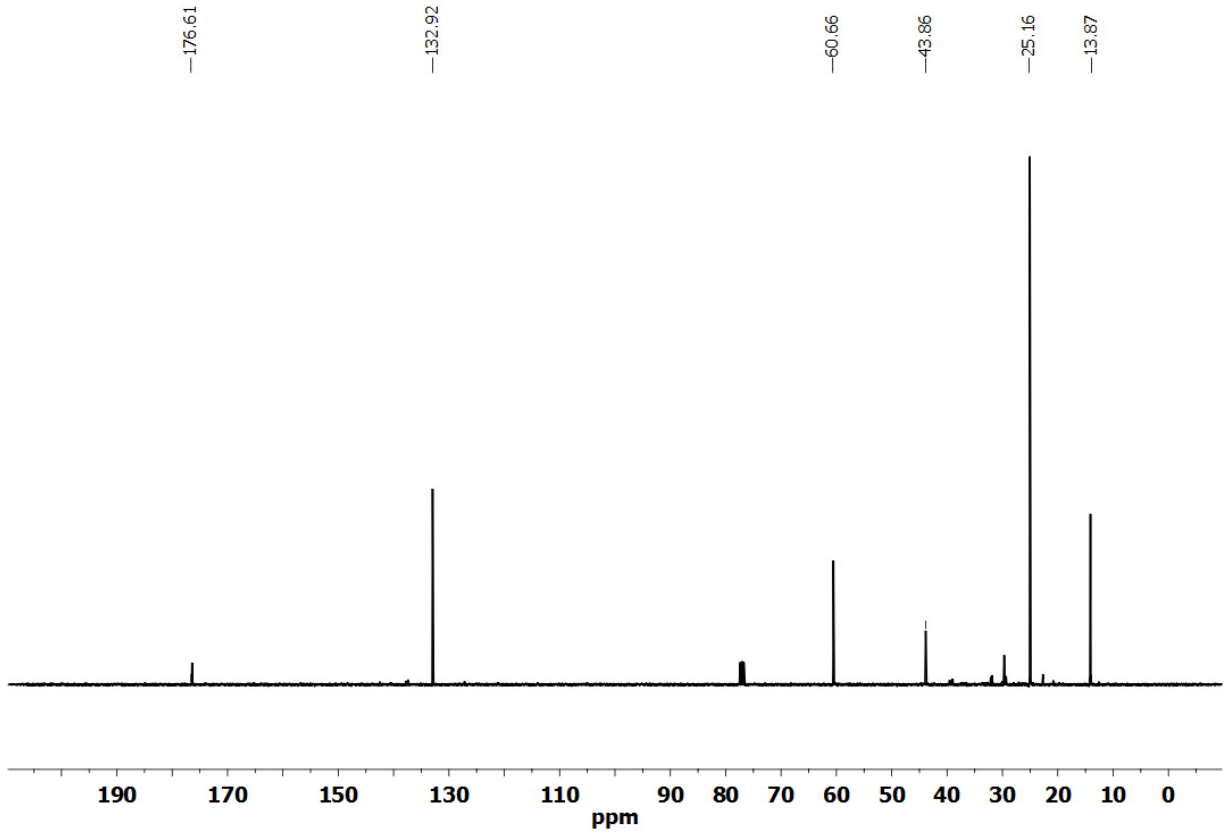
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6**.



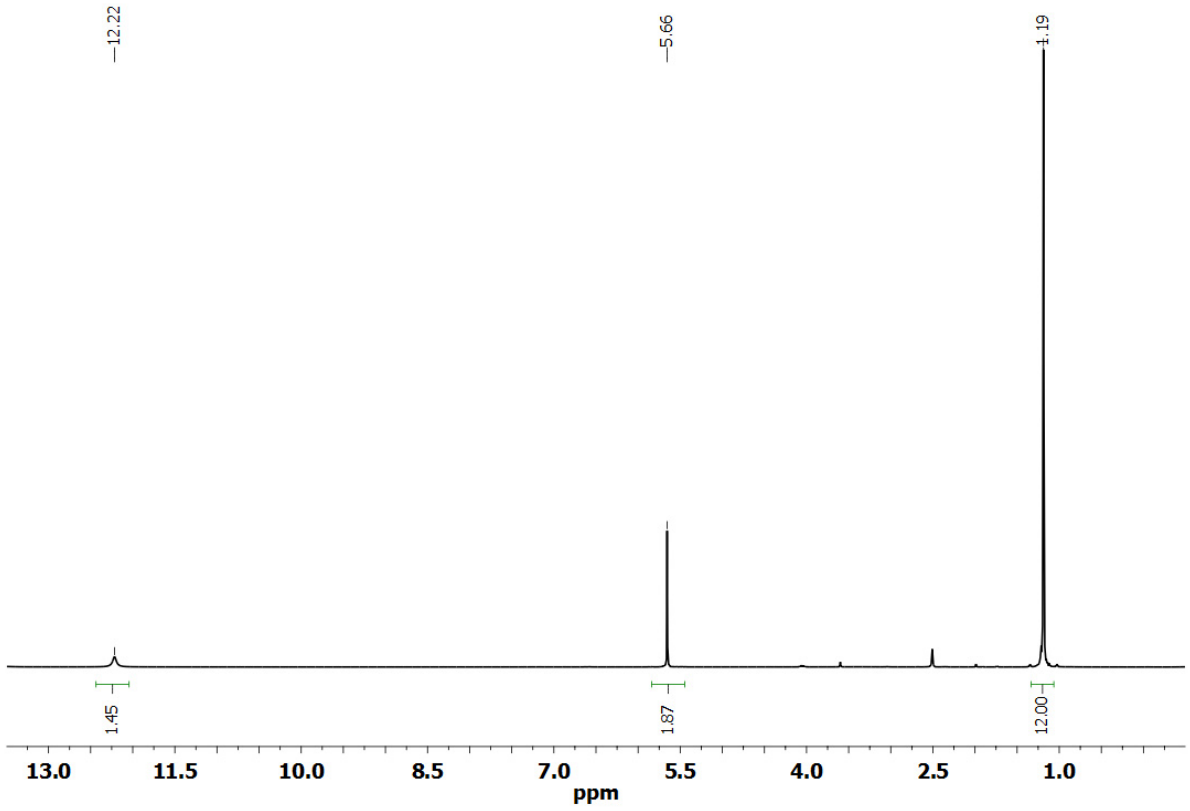
^{13}C NMR (101 MHz, $CDCl_3$) of compound **6**.



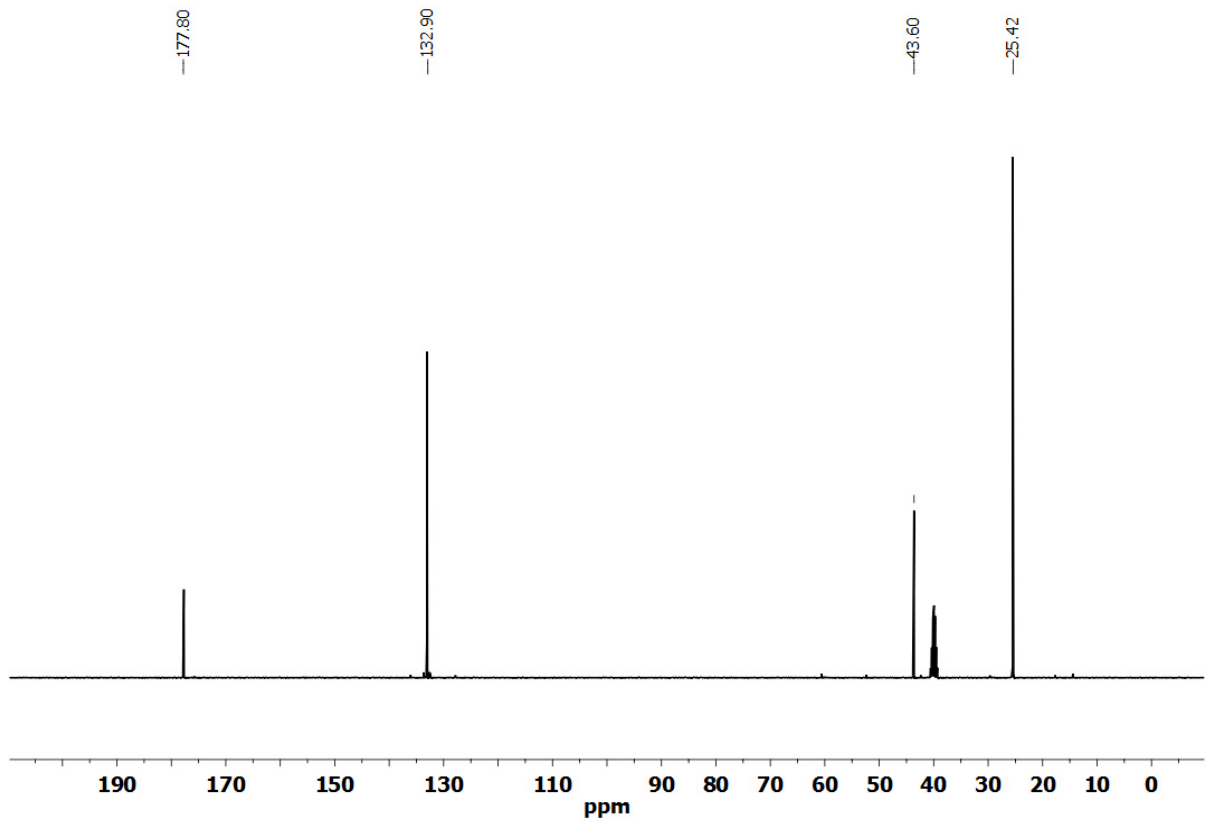
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7**.



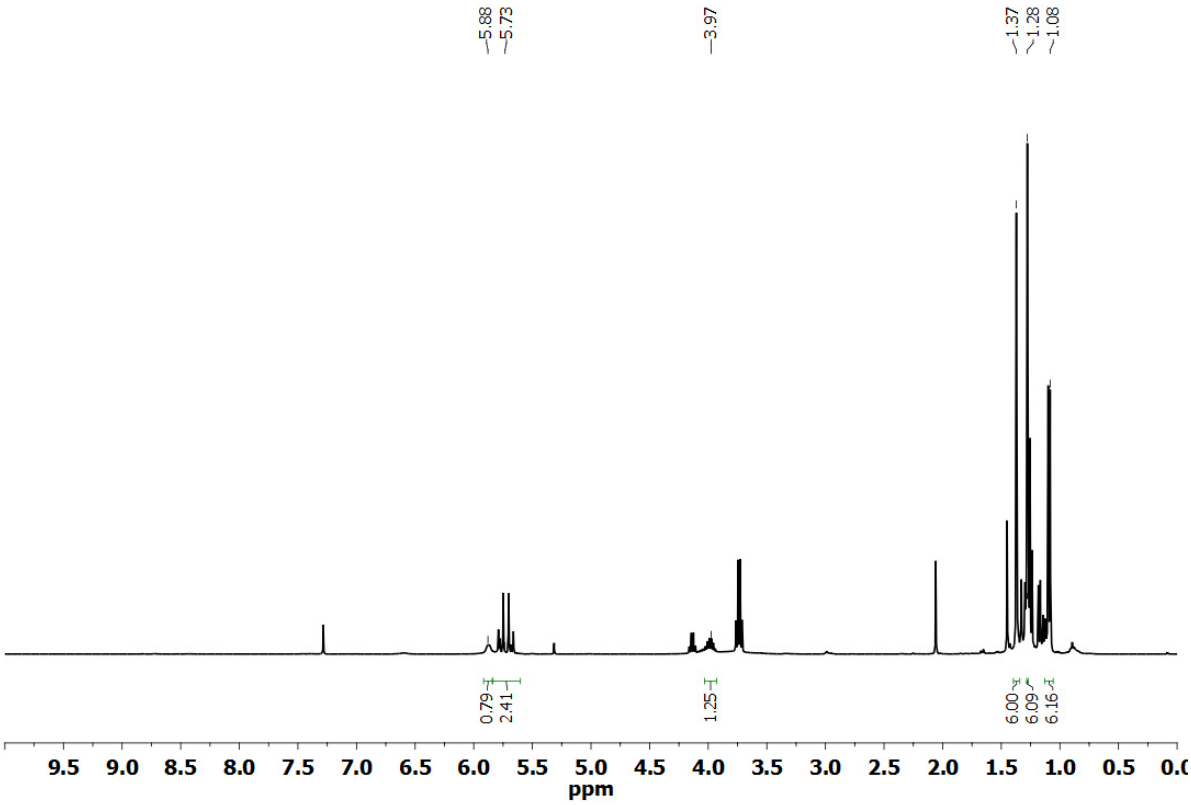
^{13}C NMR (101 MHz, $CDCl_3$) of compound **7**.



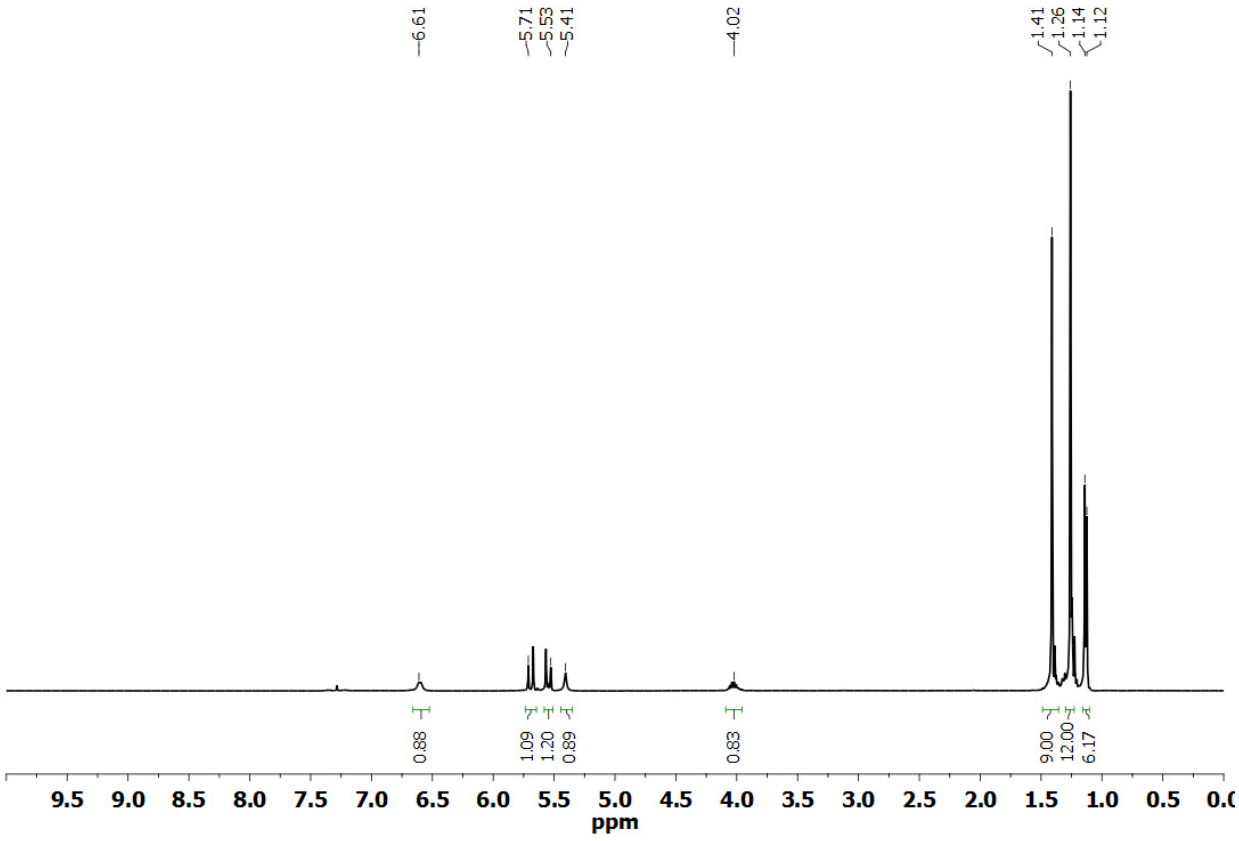
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8**.



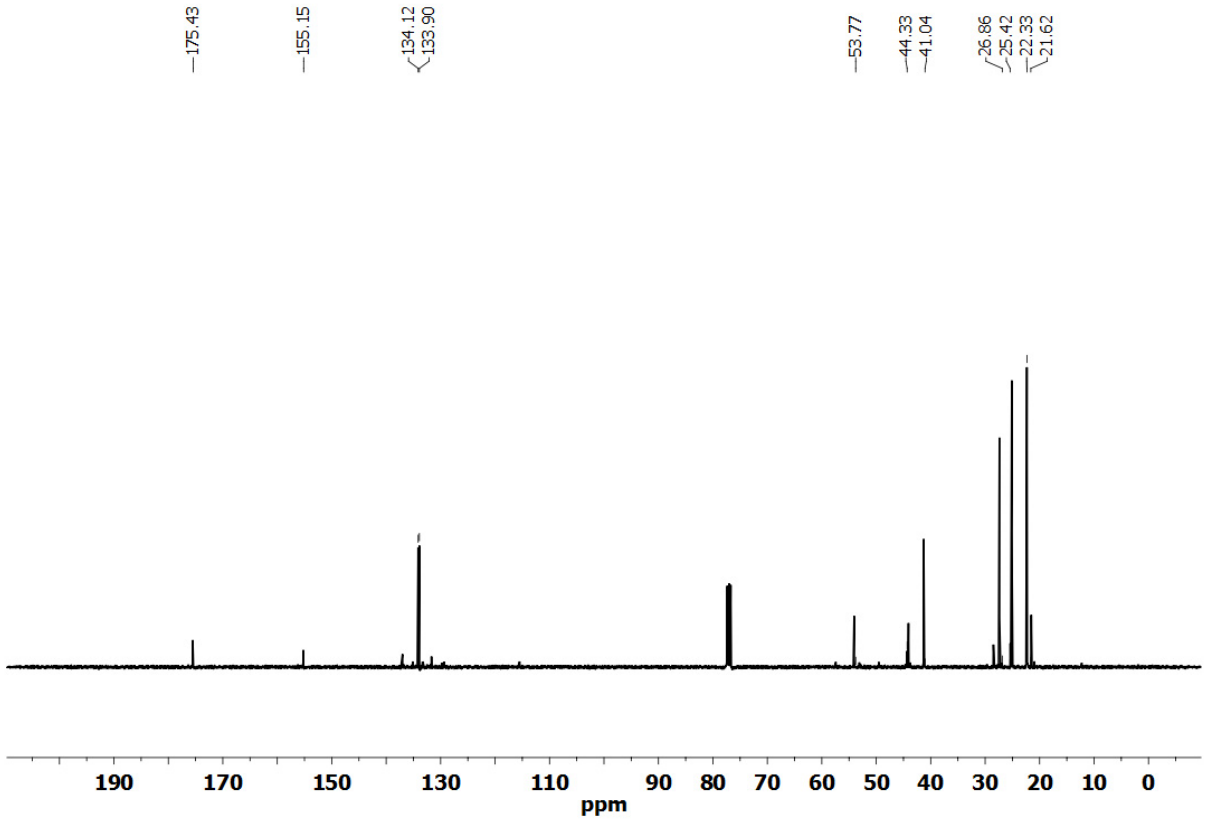
^{13}C NMR (101 MHz, $CDCl_3$) of compound **8**.



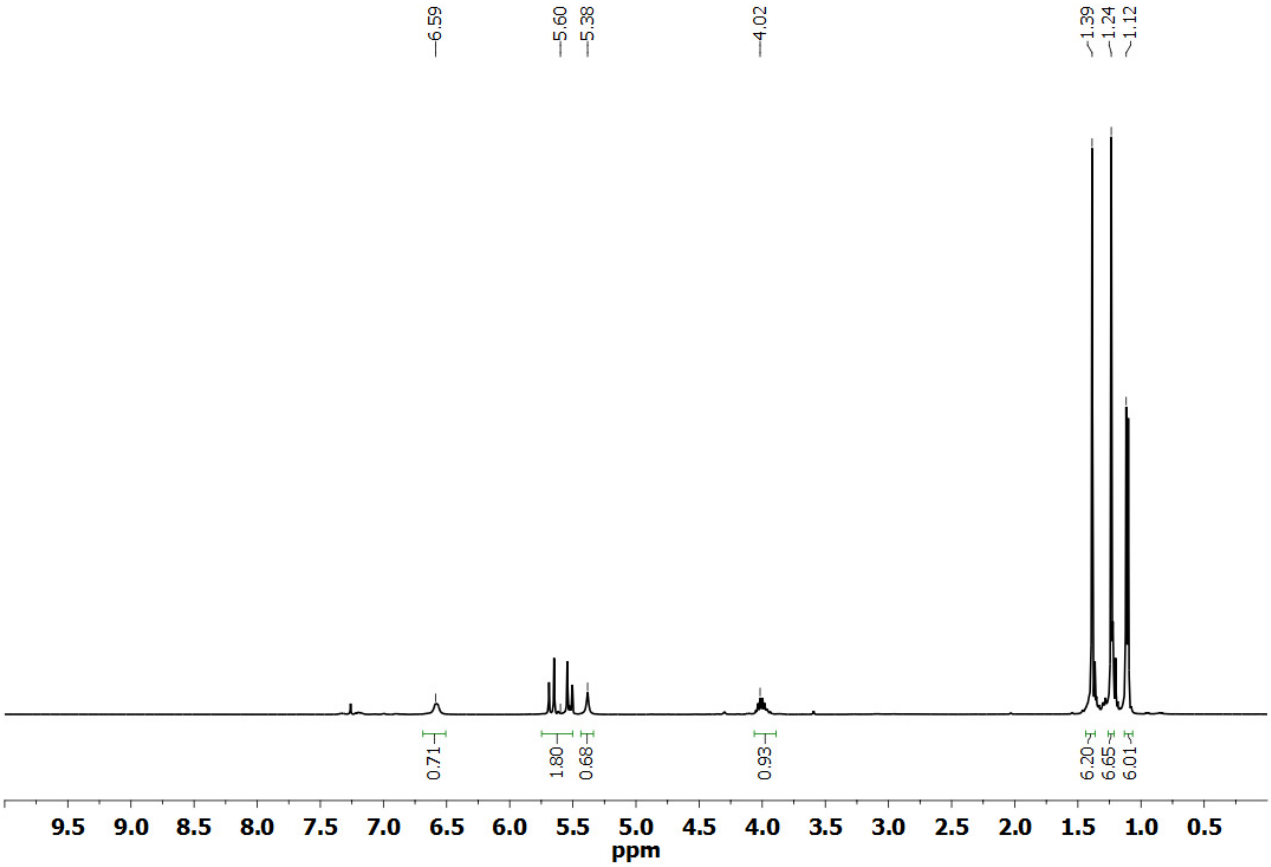
^{1}H NMR (400 MHz, $CDCl_3$) of compound **9**.



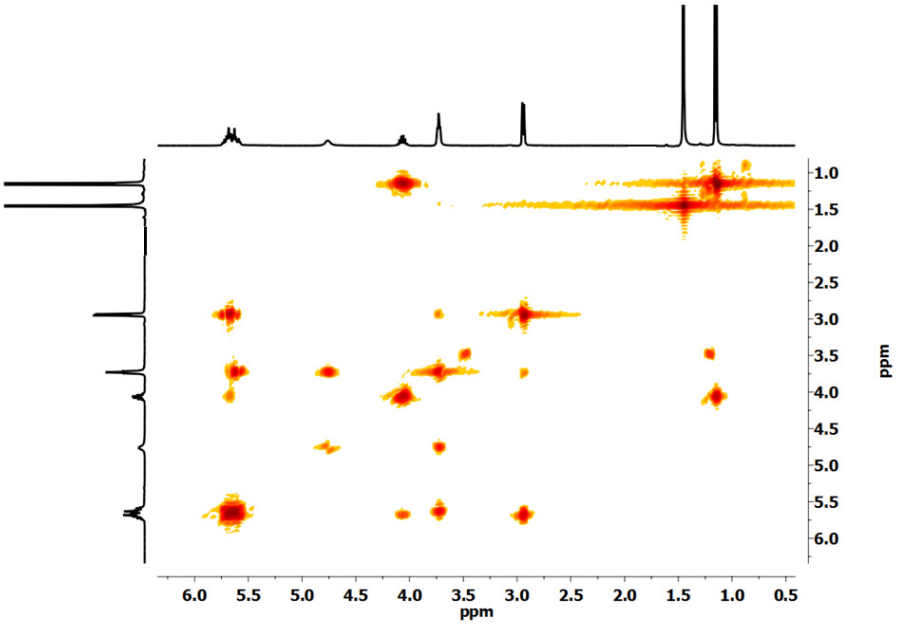
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10**.



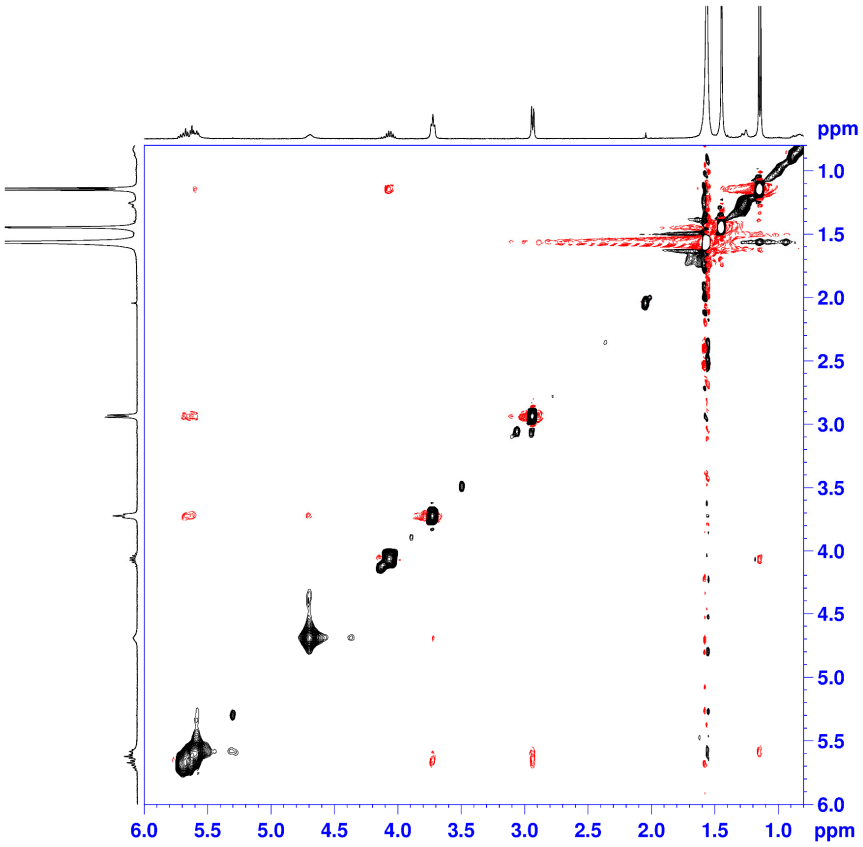
^{13}C NMR (101 MHz, $CDCl_3$) of compound **10**.



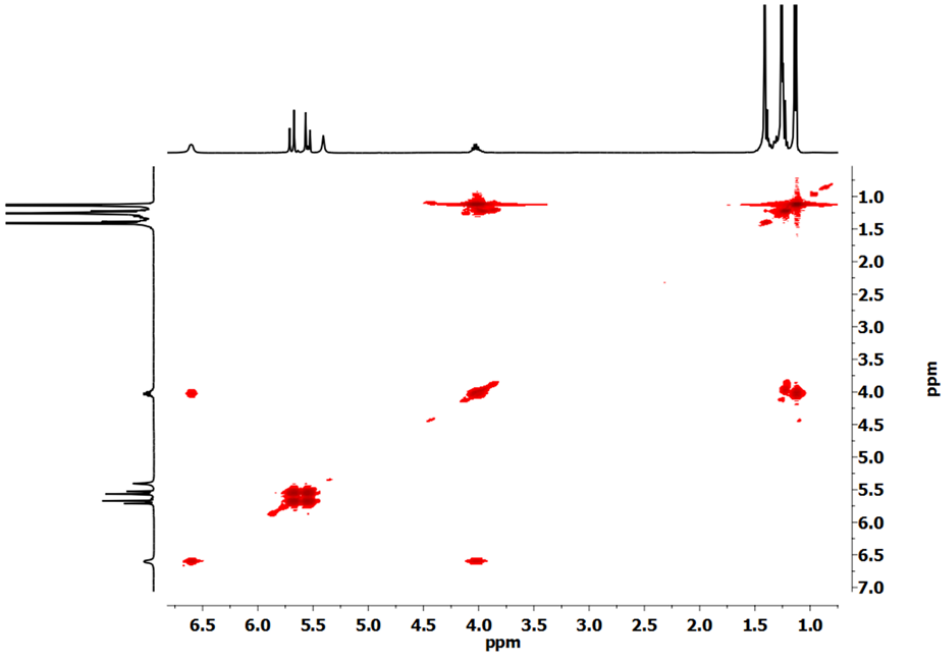
^{1}H NMR (400 MHz, $CDCl_3$) of compound **11**.



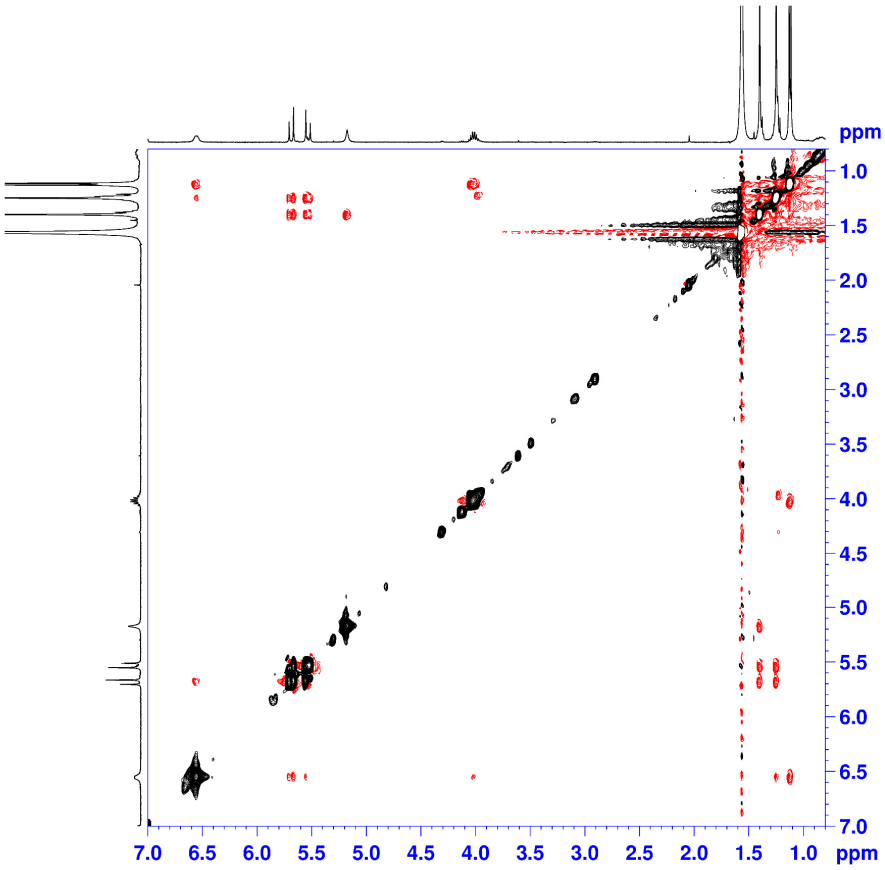
2D-COSY NMR (400 MHz, $CDCl_3$) of compound **6**.



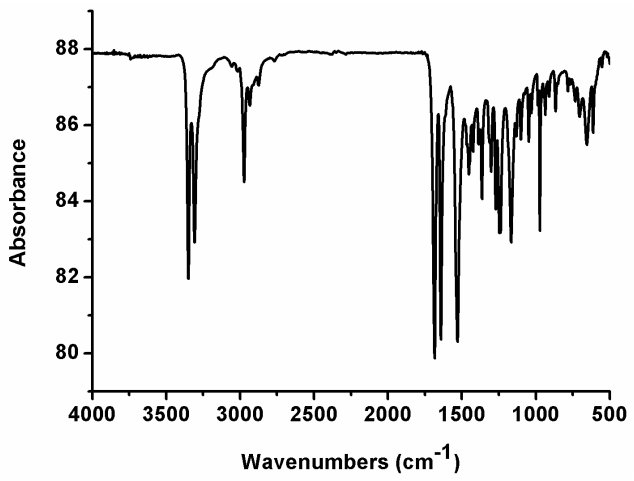
2D-NOESY NMR (400 MHz, $CDCl_3$) of compound **6**.



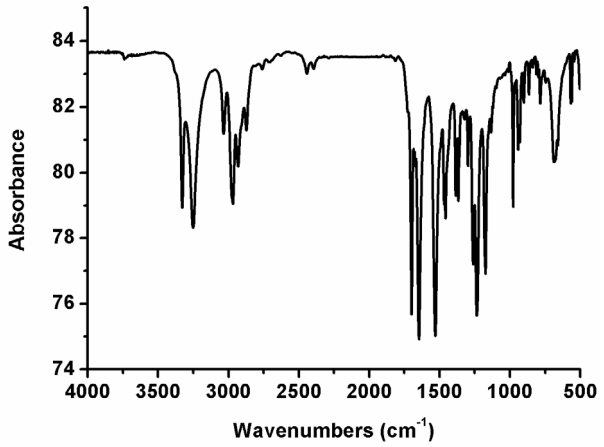
2D-COSY NMR (400 MHz, $CDCl_3$) of compound **10**.



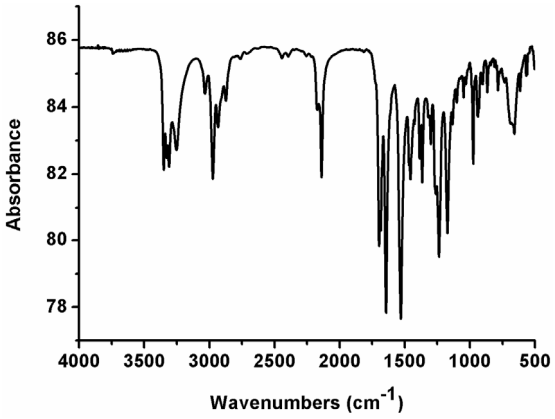
2D-NOESY NMR (400 MHz, $CDCl_3$) of compound **10**.



FT-IR (KBr) spectrum of compound **6**.



FT-IR (KBr) spectrum of compound **10**.



FT-IR (KBr) spectrum of compound **11**.

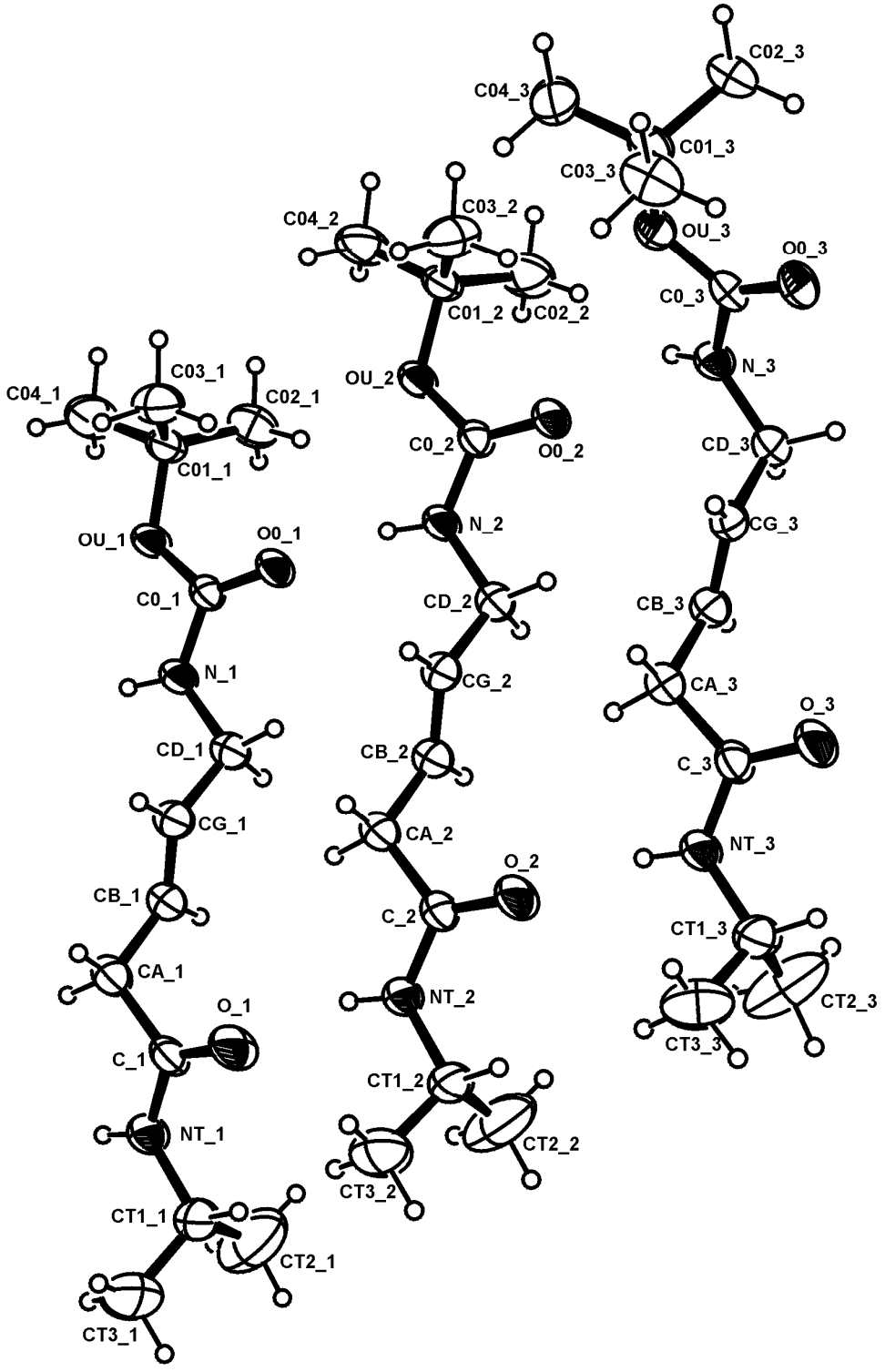


Figure S10 – ORTEP drawing of the X-Ray diffraction structure of Boc-5-aminopent-3-(*E*)-enoyl-NH*i*Pr (**6**). Anisotropic displacement ellipsoids for the non-H atoms are drawn at the 30% probability level.

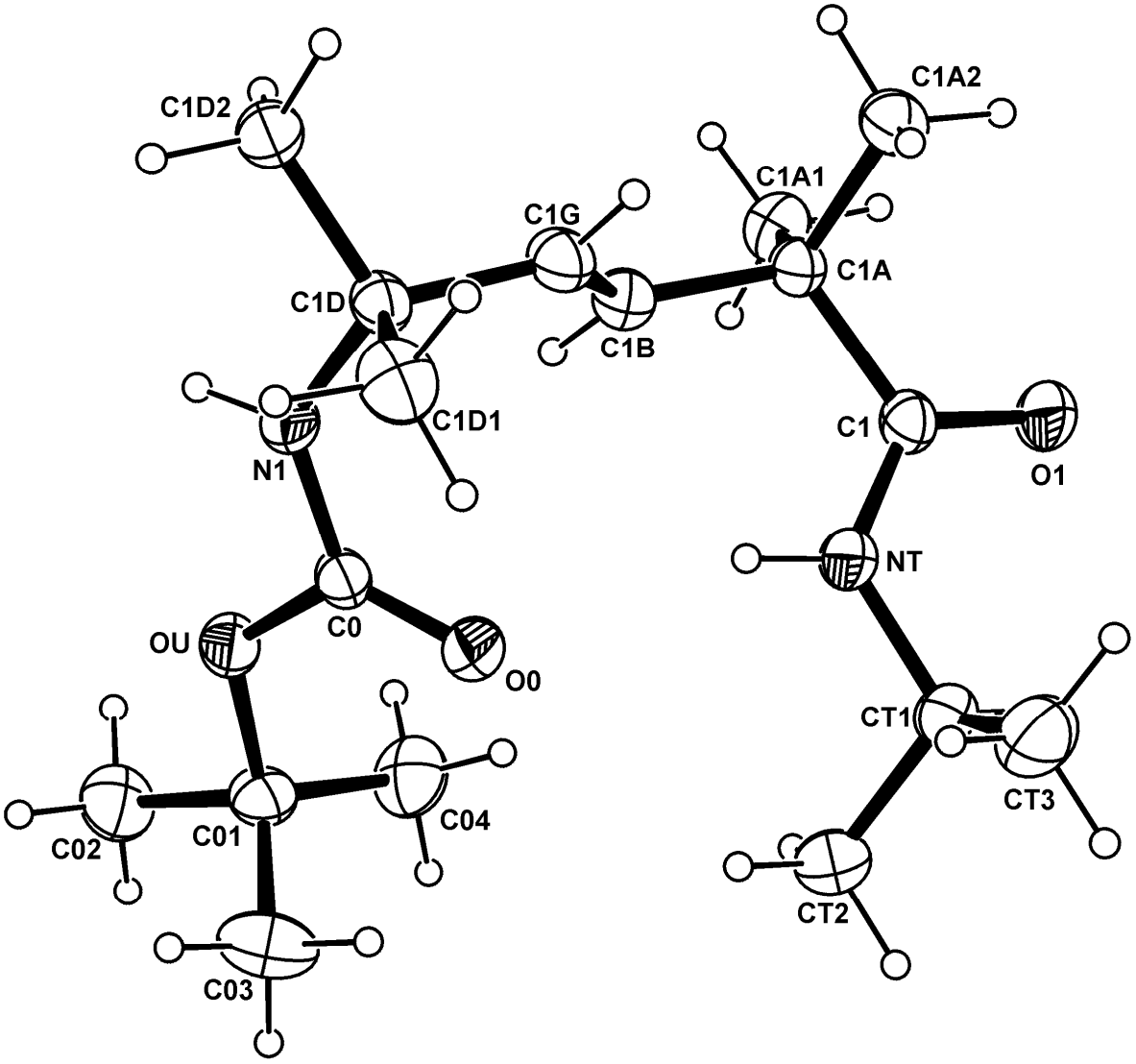


Figure S11 – ORTEP drawing of the X-Ray diffraction structure of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**). Anisotropic displacement ellipsoids for the non-H atoms are drawn at the 30% probability level.

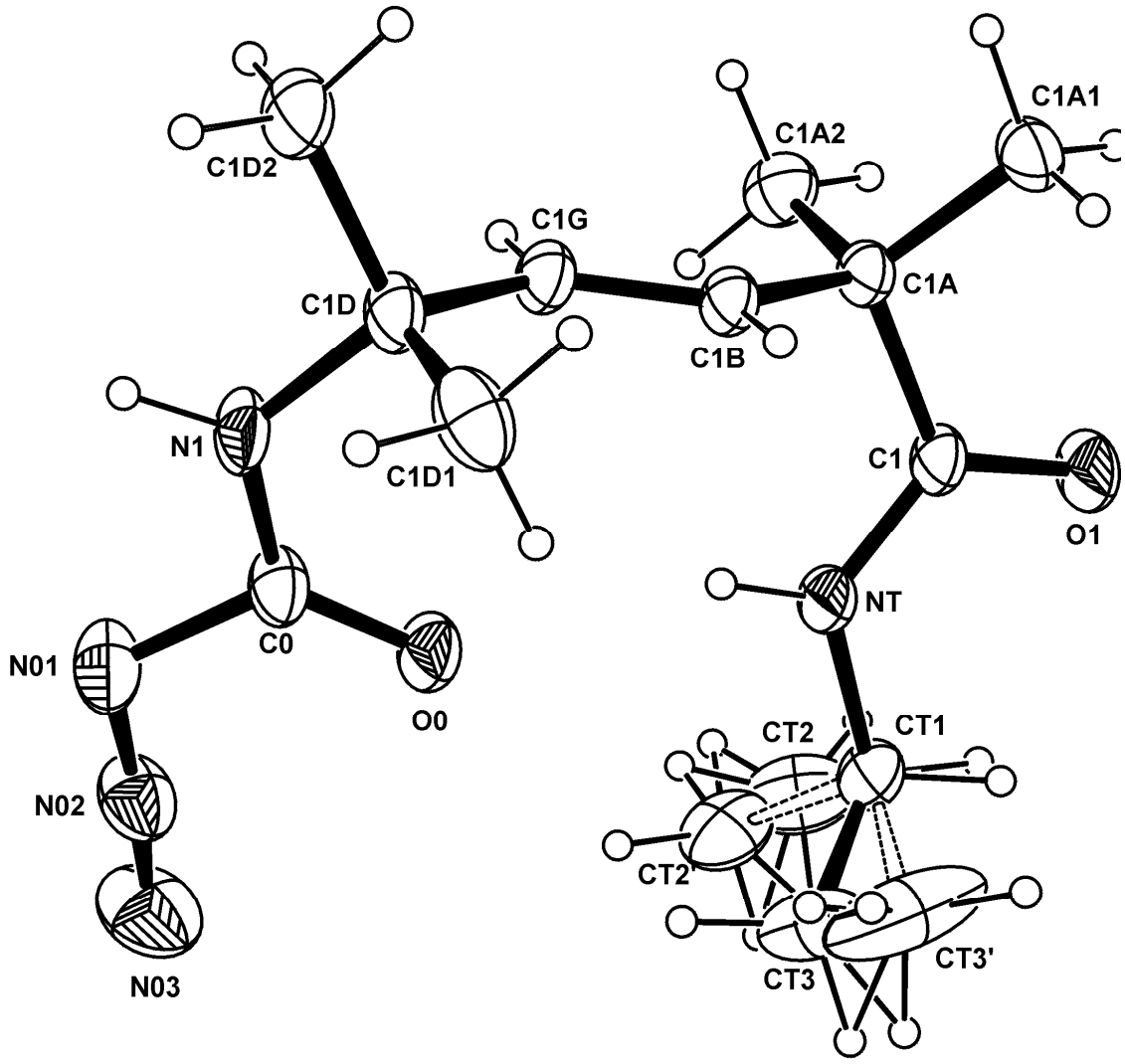


Figure S12 – ORTEP drawing of the X-Ray diffraction structure of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**). Anisotropic displacement ellipsoids for the non-H atoms are drawn at the 30% probability level. The second position for the methyl groups of the disordered C-terminal isopropyl group (atoms CT2′ and CT3′) is highlighted by dashed bonds.

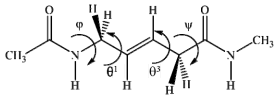
Coordinates files

Per each studied compound several conformational minima were generated. This file contains a list of all minimal energy structures in pdb format per each studied compound (i.e. named *A*, *B*, *C*, *D* and *E*, *see below*).

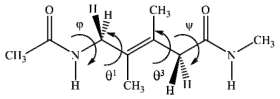
In the first row of each coordinates set, the name of the compound and the energy ranking position in the corresponding Table S*n* is included (being 1 the absolute minimum and the subsequent less stable conformers listed as n > 1).

All used energy components to characterize each studied structure are included as well, as part of following rows of the header.

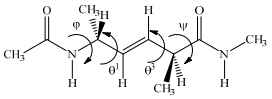
Compound A **Table S1**



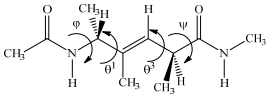
Compound B **Table S2**



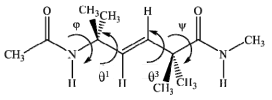
Compound C **Table S3**



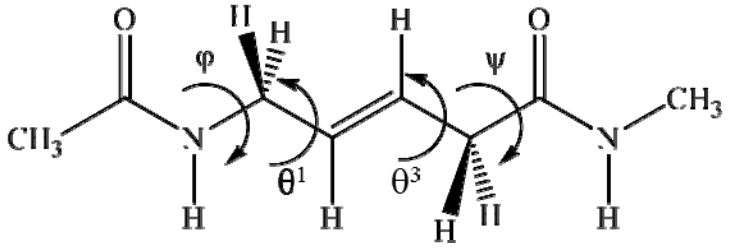
Compound D **Table S4**



Compound E **Table S5**



COMPOUND A



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REMARK   Sum of electronic and thermal Energies=    -572.980690
REMARK   Sum of electronic and thermal Enthalpies=  -572.979746
REMARK   Sum of electronic and thermal Free Energies=  -573.036492
REMARK   0 Virtual frequencies used

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ATOM      3  H   RES     1       2.038   2.109   1.706
ATOM      4  H   RES     1       3.592   1.250   1.663
ATOM      5  C   RES     1       2.189   0.784   0.048
ATOM      6  O   RES     1       1.364   1.169  -0.779
ATOM      7  N   RES     1       2.581  -0.520   0.117
ATOM      8  H   RES     1       3.214  -0.808   0.846
ATOM      9  C   RES     1       2.025  -1.520  -0.774
ATOM     10  H   RES     1       2.655  -2.415  -0.712
ATOM     11  H   RES     1       2.121  -1.147  -1.802
ATOM     12  C   RES     1       0.582  -1.843  -0.528
ATOM     13  H   RES     1       0.109  -2.451  -1.301
ATOM     14  C   RES     1      -0.157  -1.380   0.482
ATOM     15  H   RES     1       0.324  -0.753   1.236
ATOM     16  C   RES     1      -1.635  -1.515   0.585
ATOM     17  H   RES     1      -2.009  -2.283  -0.101
ATOM     18  H   RES     1      -1.956  -1.818   1.588
ATOM     19  C   RES     1      -2.411  -0.230   0.271
ATOM     20  O   RES     1      -3.602  -0.125   0.549
ATOM     21  N   RES     1      -1.699   0.757  -0.329
ATOM     22  H   RES     1      -0.726   0.613  -0.574
ATOM     23  C   RES     1      -2.317   2.008  -0.697
ATOM     24  H   RES     1      -2.848   1.939  -1.653
ATOM     25  H   RES     1      -3.044   2.292   0.067
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REMARK   Sum of electronic and thermal Energies=    -572.980617
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REMARK   Sum of electronic and thermal Free Energies=  -573.036310
REMARK   0 Virtual frequencies used

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ATOM      4  H   RES     1       2.600   2.360  -1.234
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ATOM      6  O   RES     1       1.350   0.974   0.744
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ATOM      8  H   RES     1       3.488  -0.786  -0.773
ATOM      9  C   RES     1       1.912  -1.729   0.324
ATOM     10  H   RES     1       1.816  -1.625   1.411
ATOM     11  H   RES     1       2.502  -2.631   0.129
ATOM     12  C   RES     1       0.553  -1.802  -0.295
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ATOM     14  C   RES     1      -0.576  -1.651   0.403
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ATOM     17  H   RES     1      -1.944  -1.848  -1.230
ATOM     18  H   RES     1      -2.668  -2.155   0.336
ATOM     19  C   RES     1      -2.517  -0.107  -0.156
ATOM     20  O   RES     1      -3.696   0.096  -0.430
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REMARK   Sum of electronic and thermal Energies=    -572.975651
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REMARK   Sum of electronic and thermal Free Energies=  -573.034083
REMARK   0 Virtual frequencies used

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ATOM      4  H   RES     1       4.890  -1.645  -0.060
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ATOM      6  O   RES     1       3.836   1.470  -0.406
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ATOM      9  C   RES     1       1.497   0.337   0.678
ATOM     10  H   RES     1       1.670   1.370   0.354
ATOM     11  H   RES     1       1.296   0.360   1.758
ATOM     12  C   RES     1       0.347  -0.278  -0.048
ATOM     13  H   RES     1       0.449  -0.350  -1.133
ATOM     14  C   RES     1      -0.761  -0.743   0.543
ATOM     15  H   RES     1      -0.840  -0.671   1.630
ATOM     16  C   RES     1      -1.927  -1.340  -0.171
ATOM     17  H   RES     1      -1.677  -1.517  -1.224
ATOM     18  H   RES     1      -2.192  -2.315   0.250
ATOM     19  C   RES     1      -3.220  -0.524  -0.159
ATOM     20  O   RES     1      -4.312  -1.056  -0.310
ATOM     21  N   RES     1      -3.055   0.819  -0.001
ATOM     22  H   RES     1      -2.114   1.176   0.078
ATOM     23  C   RES     1      -4.161   1.744  -0.037
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ATOM     25  H   RES     1      -5.079   1.157  -0.074
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REMARK   0 Virtual frequencies used

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ATOM      2  C   RES     1      -5.064  -0.115   0.805
ATOM      3  H   RES     1      -5.973  -0.083   0.200
ATOM      4  H   RES     1      -4.965  -1.114   1.236
ATOM      5  C   RES     1      -3.895   0.305  -0.050
ATOM      6  O   RES     1      -3.845   1.404  -0.592
ATOM      7  N   RES     1      -2.910  -0.632  -0.196
ATOM      8  H   RES     1      -2.942  -1.464   0.372
ATOM      9  C   RES     1      -1.683  -0.349  -0.925
ATOM     10  H   RES     1      -1.930   0.477  -1.599
ATOM     11  H   RES     1      -1.416  -1.218  -1.537
ATOM     12  C   RES     1      -0.551   0.024  -0.023
ATOM     13  H   RES     1      -0.712   0.909   0.596
ATOM     14  C   RES     1       0.597  -0.653   0.059
ATOM     15  H   RES     1       0.757  -1.533  -0.565
ATOM     16  C   RES     1       1.742  -0.287   0.946
ATOM     17  H   RES     1       1.561   0.678   1.434
ATOM     18  H   RES     1       1.845  -1.033   1.746
ATOM     19  C   RES     1       3.062  -0.312   0.191
ATOM     20  O   RES     1       3.385  -1.265  -0.508
ATOM     21  N   RES     1       3.853   0.784   0.371
ATOM     22  H   RES     1       3.503   1.544   0.932
ATOM     23  C   RES     1       5.144   0.923  -0.262
ATOM     24  H   RES     1       5.338   0.003  -0.813
ATOM     25  H   RES     1       5.157   1.763  -0.964
ATOM     26  H   RES     1       5.936   1.068   0.479
TER
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REMARK  Compound A structure 05
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -572.988527
REMARK   Sum of electronic and thermal Energies=    -572.974228
REMARK   Sum of electronic and thermal Enthalpies=  -572.973284
REMARK   Sum of electronic and thermal Free Energies=  -573.032592
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.161   1.582  -0.016
ATOM      2  C   RES     1      -4.122   1.630  -0.348
ATOM      3  H   RES     1      -3.613   2.428   0.199
ATOM      4  H   RES     1      -4.140   1.885  -1.410
ATOM      5  C   RES     1      -3.492   0.271  -0.180
ATOM      6  O   RES     1      -3.945  -0.732  -0.718
ATOM      7  N   RES     1      -2.385   0.234   0.626
ATOM      8  H   RES     1      -2.009   1.100   0.980
ATOM      9  C   RES     1      -1.635  -0.991   0.849
ATOM     10  H   RES     1      -2.327  -1.805   0.603
ATOM     11  H   RES     1      -1.380  -1.076   1.911
ATOM     12  C   RES     1      -0.407  -1.084   0.003
ATOM     13  H   RES     1      -0.569  -1.017  -1.076
ATOM     14  C   RES     1       0.831  -1.263   0.478
ATOM     15  H   RES     1       0.969  -1.328   1.561
ATOM     16  C   RES     1       2.062  -1.388  -0.357
ATOM     17  H   RES     1       2.614  -2.301  -0.111
ATOM     18  H   RES     1       1.794  -1.470  -1.417
ATOM     19  C   RES     1       3.075  -0.250  -0.245
ATOM     20  O   RES     1       4.262  -0.417  -0.493
ATOM     21  N   RES     1       2.547   0.955   0.115
ATOM     22  H   RES     1       1.550   1.006   0.266
ATOM     23  C   RES     1       3.341   2.156   0.195
ATOM     24  H   RES     1       4.379   1.875   0.017
ATOM     25  H   RES     1       3.041   2.889  -0.561
ATOM     26  H   RES     1       3.262   2.619   1.184
TER
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REMARK  Compound A structure 06
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -572.988426
REMARK   Sum of electronic and thermal Energies=    -572.974151
REMARK   Sum of electronic and thermal Enthalpies=  -572.973206
REMARK   Sum of electronic and thermal Free Energies=  -573.032239
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.342   1.606   0.535
ATOM      2  C   RES     1      -4.300   1.756   0.245
ATOM      3  H   RES     1      -3.790   2.306   1.040
ATOM      4  H   RES     1      -4.307   2.367  -0.661
ATOM      5  C   RES     1      -3.683   0.417  -0.069
ATOM      6  O   RES     1      -4.141  -0.326  -0.931
ATOM      7  N   RES     1      -2.593   0.082   0.685
ATOM      8  H   RES     1      -2.190   0.776   1.297
ATOM      9  C   RES     1      -1.843  -1.142   0.455
ATOM     10  H   RES     1      -2.531  -1.810  -0.073
ATOM     11  H   RES     1      -1.594  -1.602   1.418
ATOM     12  C   RES     1      -0.604  -0.910  -0.349
ATOM     13  H   RES     1      -0.758  -0.485  -1.343
ATOM     14  C   RES     1       0.630  -1.185   0.079
ATOM     15  H   RES     1       0.780  -1.594   1.079
ATOM     16  C   RES     1       1.873  -0.971  -0.718
ATOM     17  H   RES     1       2.322  -1.943  -0.970
ATOM     18  H   RES     1       1.643  -0.479  -1.670
ATOM     19  C   RES     1       2.933  -0.216   0.070
ATOM     20  O   RES     1       3.158  -0.454   1.251
ATOM     21  N   RES     1       3.622   0.720  -0.646
ATOM     22  H   RES     1       3.370   0.874  -1.609
ATOM     23  C   RES     1       4.689   1.504  -0.071
ATOM     24  H   RES     1       4.451   2.572  -0.080
ATOM     25  H   RES     1       4.810   1.180   0.963
ATOM     26  H   RES     1       5.632   1.348  -0.605
TER
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REMARK  Compound A structure 07
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -572.987842
REMARK   Sum of electronic and thermal Energies=    -572.973553
REMARK   Sum of electronic and thermal Enthalpies=  -572.972609
REMARK   Sum of electronic and thermal Free Energies=  -573.031235
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.538  -0.491   0.557
ATOM      2  C   RES     1      -4.773  -0.657  -0.203
ATOM      3  H   RES     1      -5.106  -0.210  -1.143
ATOM      4  H   RES     1      -4.686  -1.737  -0.338
ATOM      5  C   RES     1      -3.457  -0.119   0.299
ATOM      6  O   RES     1      -2.967  -0.468   1.365
ATOM      7  N   RES     1      -2.853   0.806  -0.511
ATOM      8  H   RES     1      -3.249   1.000  -1.417
ATOM      9  C   RES     1      -1.533   1.330  -0.190
ATOM     10  H   RES     1      -1.478   1.402   0.900
ATOM     11  H   RES     1      -1.466   2.344  -0.600
ATOM     12  C   RES     1      -0.422   0.464  -0.702
ATOM     13  H   RES     1      -0.314   0.393  -1.788
ATOM     14  C   RES     1       0.393  -0.248   0.082
ATOM     15  H   RES     1       0.252  -0.189   1.164
ATOM     16  C   RES     1       1.488  -1.135  -0.407
ATOM     17  H   RES     1       1.396  -2.140   0.018
ATOM     18  H   RES     1       1.421  -1.259  -1.495
ATOM     19  C   RES     1       2.918  -0.691  -0.109
ATOM     20  O   RES     1       3.855  -1.479  -0.154
ATOM     21  N   RES     1       3.067   0.634   0.174
ATOM     22  H   RES     1       2.244   1.218   0.158
ATOM     23  C   RES     1       4.356   1.231   0.427
ATOM     24  H   RES     1       4.625   1.954  -0.350
ATOM     25  H   RES     1       4.376   1.734   1.398
ATOM     26  H   RES     1       5.094   0.428   0.427
TER
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REMARK  Compound A structure 08
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -572.986046
REMARK   Sum of electronic and thermal Energies=    -572.971526
REMARK   Sum of electronic and thermal Enthalpies=  -572.970582
REMARK   Sum of electronic and thermal Free Energies=  -573.030504
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.216   1.352  -0.436
ATOM      2  C   RES     1       4.602   0.523  -0.794
ATOM      3  H   RES     1       5.177  -0.404  -0.719
ATOM      4  H   RES     1       4.387   0.716  -1.847
ATOM      5  C   RES     1       3.306   0.503  -0.024
ATOM      6  O   RES     1       2.603   1.499   0.103
ATOM      7  N   RES     1       2.971  -0.699   0.535
ATOM      8  H   RES     1       3.529  -1.511   0.323
ATOM      9  C   RES     1       1.684  -0.879   1.198
ATOM     10  H   RES     1       1.483   0.043   1.751
ATOM     11  H   RES     1       1.795  -1.689   1.926
ATOM     12  C   RES     1       0.566  -1.154   0.241
ATOM     13  H   RES     1       0.529  -2.146  -0.215
ATOM     14  C   RES     1      -0.344  -0.239  -0.103
ATOM     15  H   RES     1      -0.267   0.751   0.350
ATOM     16  C   RES     1      -1.459  -0.468  -1.071
ATOM     17  H   RES     1      -1.384   0.252  -1.899
ATOM     18  H   RES     1      -1.401  -1.472  -1.498
ATOM     19  C   RES     1      -2.839  -0.335  -0.435
ATOM     20  O   RES     1      -3.599  -1.286  -0.306
ATOM     21  N   RES     1      -3.149   0.929  -0.019
ATOM     22  H   RES     1      -2.468   1.661  -0.150
ATOM     23  C   RES     1      -4.388   1.247   0.648
ATOM     24  H   RES     1      -4.948   2.015   0.105
ATOM     25  H   RES     1      -4.983   0.334   0.681
ATOM     26  H   RES     1      -4.217   1.595   1.672
TER
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REMARK  Compound A structure 09
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -572.985956
REMARK   Sum of electronic and thermal Energies=    -572.971669
REMARK   Sum of electronic and thermal Enthalpies=  -572.970725
REMARK   Sum of electronic and thermal Free Energies=  -573.029642
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.569  -0.393   1.203
ATOM      2  C   RES     1      -5.146  -0.654   0.231
ATOM      3  H   RES     1      -5.923  -0.471  -0.514
ATOM      4  H   RES     1      -4.898  -1.719   0.227
ATOM      5  C   RES     1      -3.972   0.251  -0.049
ATOM      6  O   RES     1      -4.073   1.472  -0.039
ATOM      7  N   RES     1      -2.793  -0.390  -0.316
ATOM      8  H   RES     1      -2.769  -1.398  -0.315
ATOM      9  C   RES     1      -1.561   0.324  -0.603
ATOM     10  H   RES     1      -1.780   1.376  -0.388
ATOM     11  H   RES     1      -1.314   0.258  -1.672
ATOM     12  C   RES     1      -0.423  -0.175   0.221
ATOM     13  H   RES     1      -0.557  -0.139   1.304
ATOM     14  C   RES     1       0.723  -0.640  -0.284
ATOM     15  H   RES     1       0.851  -0.660  -1.369
ATOM     16  C   RES     1       1.892  -1.083   0.538
ATOM     17  H   RES     1       1.600  -1.173   1.587
ATOM     18  H   RES     1       2.246  -2.066   0.200
ATOM     19  C   RES     1       3.025  -0.063   0.478
ATOM     20  O   RES     1       3.039   0.934   1.187
ATOM     21  N   RES     1       3.989  -0.333  -0.452
ATOM     22  H   RES     1       3.927  -1.189  -0.979
ATOM     23  C   RES     1       5.111   0.546  -0.682
ATOM     24  H   RES     1       6.059   0.069  -0.414
ATOM     25  H   RES     1       5.158   0.864  -1.728
ATOM     26  H   RES     1       4.969   1.424  -0.051
TER
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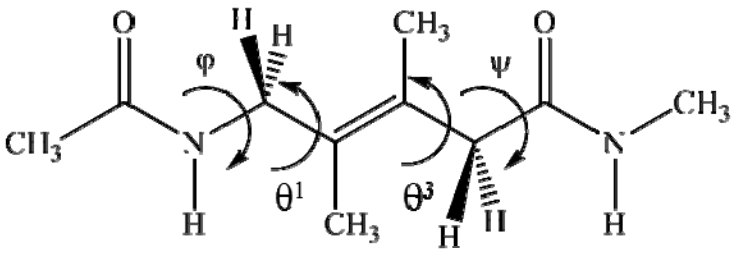
COMPOUND B



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REMARK  Compound B structure 01
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.566852
REMARK   Sum of electronic and thermal Energies=    -651.549664
REMARK   Sum of electronic and thermal Enthalpies=  -651.548720
REMARK   Sum of electronic and thermal Free Energies=  -651.612528
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       2.859   2.528  -1.042
ATOM      2  C   RES     1       3.356   1.899  -0.299
ATOM      3  H   RES     1       3.635   2.549   0.532
ATOM      4  H   RES     1       4.262   1.481  -0.744
ATOM      5  C   RES     1       2.380   0.862   0.192
ATOM      6  O   RES     1       1.350   1.171   0.793
ATOM      7  N   RES     1       2.701  -0.431  -0.071
ATOM      8  H   RES     1       3.543  -0.630  -0.586
ATOM      9  C   RES     1       1.821  -1.538   0.308
ATOM     10  H   RES     1       1.722  -1.548   1.397
ATOM     11  H   RES     1       2.347  -2.456   0.020
ATOM     12  C   RES     1       0.477  -1.463  -0.367
ATOM     13  C   RES     1       0.546  -1.310  -1.857
ATOM     14  H   RES     1       1.380  -1.886  -2.276
ATOM     15  H   RES     1       0.717  -0.263  -2.144
ATOM     16  H   RES     1      -0.364  -1.632  -2.365
ATOM     17  C   RES     1      -0.667  -1.457   0.347
ATOM     18  C   RES     1      -0.679  -1.507   1.855
ATOM     19  H   RES     1      -1.691  -1.358   2.240
ATOM     20  H   RES     1      -0.049  -0.721   2.288
ATOM     21  H   RES     1      -0.324  -2.466   2.248
ATOM     22  C   RES     1      -2.010  -1.243  -0.283
ATOM     23  H   RES     1      -2.041  -1.547  -1.334
ATOM     24  H   RES     1      -2.782  -1.835   0.220
ATOM     25  C   RES     1      -2.513   0.205  -0.248
ATOM     26  O   RES     1      -3.682   0.476  -0.509
ATOM     27  N   RES     1      -1.592   1.149   0.063
ATOM     28  H   RES     1      -0.636   0.894   0.287
ATOM     29  C   RES     1      -1.962   2.544   0.124
ATOM     30  H   RES     1      -2.332   2.897  -0.844
ATOM     31  H   RES     1      -2.759   2.707   0.856
ATOM     32  H   RES     1      -1.086   3.125   0.410
TER
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REMARK  Compound B structure 02
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.565562
REMARK   Sum of electronic and thermal Energies=    -651.548817
REMARK   Sum of electronic and thermal Enthalpies=  -651.547873
REMARK   Sum of electronic and thermal Free Energies=  -651.609718
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       1.472   2.649  -1.228
ATOM      2  C   RES     1       2.397   2.255  -0.794
ATOM      3  H   RES     1       2.817   3.042  -0.167
ATOM      4  H   RES     1       3.093   2.031  -1.606
ATOM      5  C   RES     1       2.050   1.066   0.063
ATOM      6  O   RES     1       1.410   1.180   1.109
ATOM      7  N   RES     1       2.453  -0.144  -0.403
ATOM      8  H   RES     1       2.925  -0.189  -1.292
ATOM      9  C   RES     1       2.062  -1.393   0.248
ATOM     10  H   RES     1       2.587  -1.464   1.209
ATOM     11  H   RES     1       2.446  -2.204  -0.381
ATOM     12  C   RES     1       0.571  -1.530   0.490
ATOM     13  C   RES     1       0.208  -1.706   1.931
ATOM     14  H   RES     1       0.504  -0.817   2.502
ATOM     15  H   RES     1       0.750  -2.554   2.368
ATOM     16  H   RES     1      -0.857  -1.876   2.099
ATOM     17  C   RES     1      -0.315  -1.434  -0.524
ATOM     18  C   RES     1       0.104  -1.248  -1.954
ATOM     19  H   RES     1       1.131  -1.567  -2.148
ATOM     20  H   RES     1       0.021  -0.197  -2.264
ATOM     21  H   RES     1      -0.551  -1.817  -2.622
ATOM     22  C   RES     1      -1.801  -1.365  -0.314
ATOM     23  H   RES     1      -2.338  -1.822  -1.150
ATOM     24  H   RES     1      -2.120  -1.910   0.580
ATOM     25  C   RES     1      -2.375   0.050  -0.180
ATOM     26  O   RES     1      -3.539   0.298  -0.483
ATOM     27  N   RES     1      -1.526   0.988   0.311
ATOM     28  H   RES     1      -0.596   0.727   0.621
ATOM     29  C   RES     1      -1.976   2.335   0.569
ATOM     30  H   RES     1      -2.646   2.384   1.436
ATOM     31  H   RES     1      -1.106   2.965   0.760
ATOM     32  H   RES     1      -2.528   2.716  -0.293
TER
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REMARK  Compound B structure 03
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.559594
REMARK   Sum of electronic and thermal Energies=    -651.542202
REMARK   Sum of electronic and thermal Enthalpies=  -651.541258
REMARK   Sum of electronic and thermal Free Energies=  -651.608228
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.830   0.042  -0.003
ATOM      2  C   RES     1      -4.955   0.048   0.651
ATOM      3  H   RES     1      -5.133  -0.699   1.427
ATOM      4  H   RES     1      -4.874   1.033   1.119
ATOM      5  C   RES     1      -3.743  -0.353  -0.151
ATOM      6  O   RES     1      -3.672  -1.434  -0.727
ATOM      7  N   RES     1      -2.739   0.574  -0.197
ATOM      8  H   RES     1      -2.824   1.412   0.357
ATOM      9  C   RES     1      -1.487   0.348  -0.906
ATOM     10  H   RES     1      -1.305   1.184  -1.584
ATOM     11  H   RES     1      -1.665  -0.541  -1.521
ATOM     12  C   RES     1      -0.333   0.102   0.033
ATOM     13  C   RES     1      -0.432  -1.232   0.714
ATOM     14  H   RES     1      -0.161  -2.043   0.025
ATOM     15  H   RES     1      -1.466  -1.437   1.013
ATOM     16  H   RES     1       0.191  -1.325   1.606
ATOM     17  C   RES     1       0.671   0.987   0.217
ATOM     18  C   RES     1       0.795   2.315  -0.468
ATOM     19  H   RES     1       0.798   3.123   0.274
ATOM     20  H   RES     1       0.005   2.527  -1.189
ATOM     21  H   RES     1       1.759   2.383  -0.985
ATOM     22  C   RES     1       1.847   0.699   1.123
ATOM     23  H   RES     1       2.170   1.623   1.614
ATOM     24  H   RES     1       1.598  -0.023   1.905
ATOM     25  C   RES     1       3.029   0.211   0.296
ATOM     26  O   RES     1       3.776   0.980  -0.298
ATOM     27  N   RES     1       3.160  -1.147   0.240
ATOM     28  H   RES     1       2.468  -1.714   0.705
ATOM     29  C   RES     1       4.149  -1.798  -0.585
ATOM     30  H   RES     1       4.819  -1.025  -0.964
ATOM     31  H   RES     1       4.730  -2.521  -0.007
ATOM     32  H   RES     1       3.692  -2.312  -1.437
TER
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REMARK  Compound B structure 04
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.560502
REMARK   Sum of electronic and thermal Energies=    -651.543359
REMARK   Sum of electronic and thermal Enthalpies=  -651.542414
REMARK   Sum of electronic and thermal Free Energies=  -651.607198
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.850   1.610  -0.911
ATOM      2  C   RES     1      -3.801   1.754  -0.645
ATOM      3  H   RES     1      -3.768   2.554   0.098
ATOM      4  H   RES     1      -3.253   2.074  -1.536
ATOM      5  C   RES     1      -3.277   0.484  -0.024
ATOM      6  O   RES     1      -3.757   0.012   1.000
ATOM      7  N   RES     1      -2.234  -0.105  -0.686
ATOM      8  H   RES     1      -1.864   0.338  -1.513
ATOM      9  C   RES     1      -1.620  -1.350  -0.239
ATOM     10  H   RES     1      -1.572  -2.046  -1.080
ATOM     11  H   RES     1      -2.318  -1.768   0.493
ATOM     12  C   RES     1      -0.275  -1.130   0.406
ATOM     13  C   RES     1      -0.383  -0.591   1.802
ATOM     14  H   RES     1      -0.846  -1.326   2.472
ATOM     15  H   RES     1      -1.050   0.279   1.825
ATOM     16  H   RES     1       0.572  -0.288   2.236
ATOM     17  C   RES     1       0.894  -1.359  -0.233
ATOM     18  C   RES     1       1.010  -1.814  -1.658
ATOM     19  H   RES     1       1.680  -1.144  -2.212
ATOM     20  H   RES     1       0.062  -1.850  -2.199
ATOM     21  H   RES     1       1.466  -2.809  -1.718
ATOM     22  C   RES     1       2.234  -1.131   0.415
ATOM     23  H   RES     1       2.195  -1.277   1.500
ATOM     24  H   RES     1       2.963  -1.860   0.047
ATOM     25  C   RES     1       2.881   0.236   0.192
ATOM     26  O   RES     1       4.092   0.395   0.292
ATOM     27  N   RES     1       2.015   1.251  -0.091
ATOM     28  H   RES     1       1.029   1.033  -0.122
ATOM     29  C   RES     1       2.449   2.617  -0.250
ATOM     30  H   RES     1       2.076   3.256   0.557
ATOM     31  H   RES     1       3.540   2.621  -0.223
ATOM     32  H   RES     1       2.116   3.030  -1.207
TER
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REMARK  Compound B structure 05
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.560446
REMARK   Sum of electronic and thermal Energies=    -651.543158
REMARK   Sum of electronic and thermal Enthalpies=  -651.542213
REMARK   Sum of electronic and thermal Free Energies=  -651.607388
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.585  -0.413   0.116
ATOM      2  C   RES     1      -4.760  -0.012   0.708
ATOM      3  H   RES     1      -4.708  -0.605   1.625
ATOM      4  H   RES     1      -4.985   1.024   0.973
ATOM      5  C   RES     1      -3.474  -0.185  -0.060
ATOM      6  O   RES     1      -3.111  -1.271  -0.497
ATOM      7  N   RES     1      -2.740   0.953  -0.248
ATOM      8  H   RES     1      -3.057   1.818   0.159
ATOM      9  C   RES     1      -1.445   0.911  -0.918
ATOM     10  H   RES     1      -1.289   1.896  -1.376
ATOM     11  H   RES     1      -1.531   0.184  -1.726
ATOM     12  C   RES     1      -0.305   0.594   0.018
ATOM     13  C   RES     1       0.001   1.719   0.964
ATOM     14  H   RES     1      -0.886   1.989   1.553
ATOM     15  H   RES     1       0.291   2.624   0.414
ATOM     16  H   RES     1       0.804   1.500   1.668
ATOM     17  C   RES     1       0.360  -0.583   0.011
ATOM     18  C   RES     1       0.081  -1.720  -0.924
ATOM     19  H   RES     1      -0.722  -1.536  -1.636
ATOM     20  H   RES     1      -0.211  -2.607  -0.351
ATOM     21  H   RES     1       0.991  -1.995  -1.474
ATOM     22  C   RES     1       1.495  -0.866   0.963
ATOM     23  H   RES     1       1.330  -0.420   1.948
ATOM     24  H   RES     1       1.568  -1.943   1.147
ATOM     25  C   RES     1       2.900  -0.436   0.542
ATOM     26  O   RES     1       3.888  -0.818   1.159
ATOM     27  N   RES     1       2.968   0.397  -0.534
ATOM     28  H   RES     1       2.100   0.676  -0.968
ATOM     29  C   RES     1       4.218   0.908  -1.039
ATOM     30  H   RES     1       4.304   1.990  -0.892
ATOM     31  H   RES     1       5.021   0.416  -0.488
ATOM     32  H   RES     1       4.332   0.689  -2.105
TER
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REMARK  Compound B structure 06
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.560747
REMARK   Sum of electronic and thermal Energies=    -651.543715
REMARK   Sum of electronic and thermal Enthalpies=  -651.542771
REMARK   Sum of electronic and thermal Free Energies=  -651.606743
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.988  -0.624   1.619
ATOM      2  C   RES     1      -4.916   0.008   0.731
ATOM      3  H   RES     1      -4.917   1.055   1.042
ATOM      4  H   RES     1      -5.809  -0.183   0.132
ATOM      5  C   RES     1      -3.700  -0.397  -0.061
ATOM      6  O   RES     1      -3.564  -1.528  -0.515
ATOM      7  N   RES     1      -2.766   0.586  -0.241
ATOM      8  H   RES     1      -2.898   1.474   0.219
ATOM      9  C   RES     1      -1.510   0.356  -0.941
ATOM     10  H   RES     1      -1.380   1.131  -1.700
ATOM     11  H   RES     1      -1.650  -0.598  -1.462
ATOM     12  C   RES     1      -0.345   0.266   0.008
ATOM     13  C   RES     1      -0.517  -0.796   1.064
ATOM     14  H   RES     1      -1.228  -1.558   0.730
ATOM     15  H   RES     1      -0.916  -0.385   2.000
ATOM     16  H   RES     1       0.422  -1.299   1.312
ATOM     17  C   RES     1       0.748   1.059  -0.056
ATOM     18  C   RES     1       0.999   2.110  -1.097
ATOM     19  H   RES     1       0.224   2.187  -1.860
ATOM     20  H   RES     1       1.948   1.915  -1.614
ATOM     21  H   RES     1       1.112   3.096  -0.631
ATOM     22  C   RES     1       1.871   0.931   0.938
ATOM     23  H   RES     1       2.295   1.915   1.161
ATOM     24  H   RES     1       1.521   0.537   1.898
ATOM     25  C   RES     1       3.065   0.064   0.533
ATOM     26  O   RES     1       4.153   0.184   1.084
ATOM     27  N   RES     1       2.816  -0.853  -0.442
ATOM     28  H   RES     1       1.883  -0.889  -0.829
ATOM     29  C   RES     1       3.816  -1.784  -0.906
ATOM     30  H   RES     1       3.544  -2.818  -0.670
ATOM     31  H   RES     1       3.966  -1.699  -1.986
ATOM     32  H   RES     1       4.750  -1.541  -0.397
TER
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REMARK  Compound B structure 07
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.559519
REMARK   Sum of electronic and thermal Energies=    -651.542174
REMARK   Sum of electronic and thermal Enthalpies=  -651.541230
REMARK   Sum of electronic and thermal Free Energies=  -651.606709
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.152   2.564  -0.826
ATOM      2  C   RES     1       3.577   2.250   0.047
ATOM      3  H   RES     1       2.626   2.789   0.056
ATOM      4  H   RES     1       4.154   2.537   0.929
ATOM      5  C   RES     1       3.428   0.749   0.022
ATOM      6  O   RES     1       4.393  -0.009   0.003
ATOM      7  N   RES     1       2.148   0.284   0.021
ATOM      8  H   RES     1       1.363   0.920   0.041
ATOM      9  C   RES     1       1.856  -1.145  -0.014
ATOM     10  H   RES     1       2.114  -1.604   0.949
ATOM     11  H   RES     1       2.523  -1.604  -0.753
ATOM     12  C   RES     1       0.409  -1.335  -0.381
ATOM     13  C   RES     1       0.178  -1.472  -1.854
ATOM     14  H   RES     1       0.614  -0.615  -2.383
ATOM     15  H   RES     1      -0.873  -1.523  -2.141
ATOM     16  H   RES     1       0.681  -2.363  -2.249
ATOM     17  C   RES     1      -0.564  -1.232   0.544
ATOM     18  C   RES     1      -0.316  -0.967   1.998
ATOM     19  H   RES     1      -0.722   0.015   2.276
ATOM     20  H   RES     1       0.739  -0.970   2.275
ATOM     21  H   RES     1      -0.833  -1.703   2.627
ATOM     22  C   RES     1      -2.019  -1.195   0.179
ATOM     23  H   RES     1      -2.232  -1.763  -0.733
ATOM     24  H   RES     1      -2.628  -1.656   0.970
ATOM     25  C   RES     1      -2.497   0.239  -0.054
ATOM     26  O   RES     1      -1.731   1.158  -0.325
ATOM     27  N   RES     1      -3.847   0.405   0.044
ATOM     28  H   RES     1      -4.414  -0.399   0.266
ATOM     29  C   RES     1      -4.501   1.667  -0.211
ATOM     30  H   RES     1      -3.721   2.405  -0.401
ATOM     31  H   RES     1      -5.155   1.613  -1.087
ATOM     32  H   RES     1      -5.092   1.989   0.651
TER
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REMARK  Compound B structure 08
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.558345
REMARK   Sum of electronic and thermal Energies=    -651.541047
REMARK   Sum of electronic and thermal Enthalpies=  -651.540103
REMARK   Sum of electronic and thermal Free Energies=  -651.605328
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.612  -0.671  -0.216
ATOM      2  C   RES     1       4.830  -0.042  -0.647
ATOM      3  H   RES     1       4.777  -0.284  -1.711
ATOM      4  H   RES     1       5.121   1.006  -0.539
ATOM      5  C   RES     1       3.512  -0.383   0.000
ATOM      6  O   RES     1       3.060  -1.525   0.001
ATOM      7  N   RES     1       2.861   0.656   0.599
ATOM      8  H   RES     1       3.246   1.584   0.524
ATOM      9  C   RES     1       1.541   0.480   1.196
ATOM     10  H   RES     1       1.450   1.219   2.002
ATOM     11  H   RES     1       1.535  -0.508   1.656
ATOM     12  C   RES     1       0.411   0.668   0.212
ATOM     13  C   RES     1       0.230   2.096  -0.201
ATOM     14  H   RES     1       1.183   2.536  -0.526
ATOM     15  H   RES     1      -0.124   2.698   0.646
ATOM     16  H   RES     1      -0.500   2.240  -0.997
ATOM     17  C   RES     1      -0.360  -0.351  -0.220
ATOM     18  C   RES     1      -0.214  -1.781   0.206
ATOM     19  H   RES     1      -1.084  -2.106   0.795
ATOM     20  H   RES     1       0.689  -1.982   0.780
ATOM     21  H   RES     1      -0.172  -2.433  -0.674
ATOM     22  C   RES     1      -1.514  -0.124  -1.175
ATOM     23  H   RES     1      -1.301   0.675  -1.887
ATOM     24  H   RES     1      -1.687  -1.039  -1.755
ATOM     25  C   RES     1      -2.775   0.279  -0.425
ATOM     26  O   RES     1      -2.986   1.434  -0.074
ATOM     27  N   RES     1      -3.630  -0.751  -0.146
ATOM     28  H   RES     1      -3.391  -1.675  -0.469
ATOM     29  C   RES     1      -4.844  -0.568   0.612
ATOM     30  H   RES     1      -4.922   0.494   0.848
ATOM     31  H   RES     1      -5.724  -0.869   0.036
ATOM     32  H   RES     1      -4.823  -1.137   1.547
TER
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REMARK  Compound B structure 09
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.557408
REMARK   Sum of electronic and thermal Energies=    -651.540157
REMARK   Sum of electronic and thermal Enthalpies=  -651.539213
REMARK   Sum of electronic and thermal Free Energies=  -651.605070
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.366  -0.564   1.352
ATOM      2  C   RES     1       5.072   0.283   0.728
ATOM      3  H   RES     1       5.939   0.543   0.117
ATOM      4  H   RES     1       4.829   1.131   1.373
ATOM      5  C   RES     1       3.945  -0.145  -0.179
ATOM      6  O   RES     1       4.058  -1.084  -0.959
ATOM      7  N   RES     1       2.798   0.592  -0.069
ATOM      8  H   RES     1       2.748   1.315   0.632
ATOM      9  C   RES     1       1.592   0.304  -0.833
ATOM     10  H   RES     1       1.856  -0.544  -1.475
ATOM     11  H   RES     1       1.366   1.146  -1.493
ATOM     12  C   RES     1       0.438  -0.063   0.062
ATOM     13  C   RES     1       0.605  -1.409   0.701
ATOM     14  H   RES     1       0.048  -1.527   1.633
ATOM     15  H   RES     1       1.661  -1.609   0.910
ATOM     16  H   RES     1       0.255  -2.197   0.024
ATOM     17  C   RES     1      -0.641   0.729   0.232
ATOM     18  C   RES     1      -0.861   2.053  -0.440
ATOM     19  H   RES     1      -1.726   2.008  -1.115
ATOM     20  H   RES     1      -0.012   2.406  -1.026
ATOM     21  H   RES     1      -1.094   2.829   0.301
ATOM     22  C   RES     1      -1.818   0.308   1.075
ATOM     23  H   RES     1      -1.525  -0.411   1.845
ATOM     24  H   RES     1      -2.235   1.182   1.594
ATOM     25  C   RES     1      -2.888  -0.376   0.233
ATOM     26  O   RES     1      -2.663  -1.407  -0.388
ATOM     27  N   RES     1      -4.101   0.253   0.216
ATOM     28  H   RES     1      -4.222   1.082   0.775
ATOM     29  C   RES     1      -5.234  -0.270  -0.509
ATOM     30  H   RES     1      -6.016  -0.635   0.166
ATOM     31  H   RES     1      -5.664   0.488  -1.169
ATOM     32  H   RES     1      -4.877  -1.106  -1.113
TER
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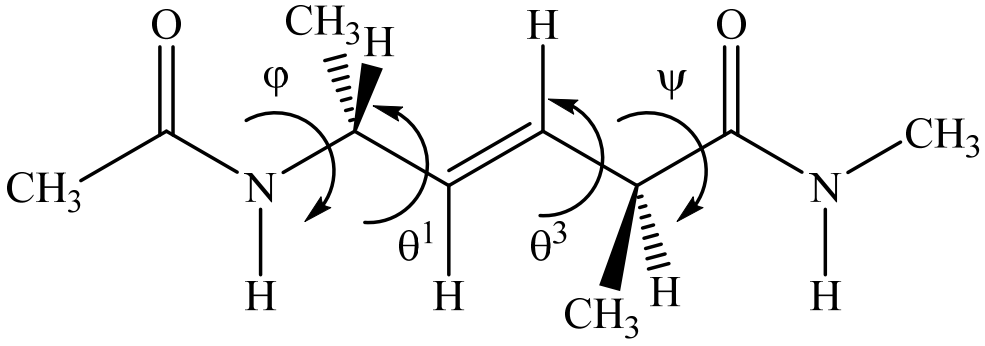
COMPOUND C



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REMARK  Compound C structure 01
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.563040
REMARK   Sum of electronic and thermal Energies=    -651.546084
REMARK   Sum of electronic and thermal Enthalpies=  -651.545140
REMARK   Sum of electronic and thermal Free Energies=  -651.608291
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       9.578  -7.725  -7.655
ATOM      2  C   RES     1      10.237  -6.715  -9.377
ATOM      3  H   RES     1      10.750  -7.596  -9.773
ATOM      4  H   RES     1       9.241  -6.554  -9.796
ATOM      5  H   RES     1      10.773  -5.796  -9.646
ATOM      6  H   RES     1       8.835  -2.552  -7.786
ATOM      7  C   RES     1       9.028  -3.275  -6.990
ATOM      8  H   RES     1       8.074  -3.619  -6.585
ATOM      9  H   RES     1       9.574  -2.747  -6.204
ATOM     10  C   RES     1       9.898  -4.380  -7.533
ATOM     11  O   RES     1      10.987  -4.150  -8.060
ATOM     12  N   RES     1       9.403  -5.641  -7.410
ATOM     13  H   RES     1       8.516  -5.776  -6.949
ATOM     14  C   RES     1      10.140  -6.830  -7.859
ATOM     15  C   RES     1      11.491  -6.886  -7.208
ATOM     16  H   RES     1      11.499  -6.959  -6.117
ATOM     17  C   RES     1      12.639  -6.789  -7.882
ATOM     18  H   RES     1      12.590  -6.690  -8.970
ATOM     19  C   RES     1      14.000  -6.702  -7.277
ATOM     20  H   RES     1      14.684  -7.321  -7.858
ATOM     21  C   RES     1      14.600  -5.284  -7.357
ATOM     22  O   RES     1      15.783  -5.085  -7.091
ATOM     23  N   RES     1      13.752  -4.289  -7.710
ATOM     24  H   RES     1      12.778  -4.481  -7.919
ATOM     25  C   RES     1      14.214  -2.923  -7.789
ATOM     26  H   RES     1      14.481  -2.532  -6.801
ATOM     27  H   RES     1      15.104  -2.853  -8.420
ATOM     28  H   RES     1      13.419  -2.309  -8.214
ATOM     29  C   RES     1      13.889  -7.114  -5.813
ATOM     30  H   RES     1      14.569  -7.953  -5.626
ATOM     31  H   RES     1      12.877  -7.484  -5.624
ATOM     32  H   RES     1      14.158  -6.256  -5.195
TER
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REMARK  Compound C structure 02
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.561816
REMARK   Sum of electronic and thermal Energies=    -651.545003
REMARK   Sum of electronic and thermal Enthalpies=  -651.544059
REMARK   Sum of electronic and thermal Free Energies=  -651.606675
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      18.289  10.480   8.527
ATOM      2  C   RES     1      18.511   9.589   9.116
ATOM      3  H   RES     1      17.629   9.318   9.702
ATOM      4  H   RES     1      19.319   9.854   9.803
ATOM      5  C   RES     1      18.995   8.498   8.197
ATOM      6  O   RES     1      19.902   8.681   7.386
ATOM      7  N   RES     1      18.379   7.291   8.328
ATOM      8  H   RES     1      17.673   7.172   9.039
ATOM      9  C   RES     1      18.765   6.133   7.531
ATOM     10  H   RES     1      18.092   5.274   7.657
ATOM     11  C   RES     1      20.191   5.707   7.753
ATOM     12  H   RES     1      20.544   4.948   7.053
ATOM     13  C   RES     1      21.029   6.221   8.655
ATOM     14  H   RES     1      20.651   6.991   9.331
ATOM     15  C   RES     1      22.495   5.950   8.760
ATOM     16  H   RES     1      22.835   5.101   8.185
ATOM     17  C   RES     1      23.344   7.178   8.375
ATOM     18  O   RES     1      24.570   7.136   8.435
ATOM     19  N   RES     1      22.660   8.270   7.949
ATOM     20  H   RES     1      21.648   8.250   7.887
ATOM     21  C   RES     1      23.346   9.465   7.519
ATOM     22  H   RES     1      23.663   9.402   6.471
ATOM     23  H   RES     1      22.679  10.321   7.635
ATOM     24  H   RES     1      24.241   9.608   8.129
ATOM     26  C   RES     1      18.607   6.717   6.129
ATOM     27  H   RES     1      19.103   7.688   6.036
ATOM     28  H   RES     1      19.133   6.005   5.489
ATOM     29  H   RES     1      17.586   6.807   5.744
ATOM     30  C   RES     1      22.813   5.699  10.225
ATOM     31  H   RES     1      23.608   4.946  10.243
ATOM     32  H   RES     1      21.902   5.241  10.622
ATOM     33  H   RES     1      23.112   6.514  10.886
TER
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REMARK  Compound C structure 03
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.560331
REMARK   Sum of electronic and thermal Energies=    -651.543472
REMARK   Sum of electronic and thermal Enthalpies=  -651.542528
REMARK   Sum of electronic and thermal Free Energies=  -651.605270
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       1.856  -2.108   2.296
ATOM      2  C   RES     1       2.693  -1.717   1.711
ATOM      3  H   RES     1       3.356  -1.159   2.377
ATOM      4  H   RES     1       3.233  -2.578   1.313
ATOM      5  C   RES     1       2.146  -0.907   0.563
ATOM      6  O   RES     1       1.433  -1.416  -0.302
ATOM      7  N   RES     1       2.481   0.413   0.564
ATOM      8  H   RES     1       3.070   0.751   1.308
ATOM      9  C   RES     1       2.072   1.366  -0.471
ATOM     10  H   RES     1       2.523   2.321  -0.166
ATOM     11  C   RES     1       2.653   0.997  -1.835
ATOM     12  H   RES     1       3.742   0.918  -1.784
ATOM     13  H   RES     1       2.401   1.767  -2.570
ATOM     14  H   RES     1       2.249   0.044  -2.181
ATOM     15  C   RES     1       0.580   1.546  -0.542
ATOM     16  H   RES     1       0.227   2.033  -1.454
ATOM     17  C   RES     1      -0.317   1.144   0.360
ATOM     18  H   RES     1       0.030   0.644   1.269
ATOM     19  C   RES     1      -1.798   1.225   0.188
ATOM     20  H   RES     1      -2.014   1.859  -0.685
ATOM     21  C   RES     1      -2.499   1.818   1.405
ATOM     22  H   RES     1      -2.268   1.240   2.307
ATOM     23  H   RES     1      -2.182   2.851   1.576
ATOM     24  H   RES     1      -3.581   1.791   1.264
ATOM     25  C   RES     1      -2.438  -0.137  -0.154
ATOM     26  O   RES     1      -3.653  -0.304  -0.077
ATOM     27  N   RES     1      -1.589  -1.110  -0.562
ATOM     28  H   RES     1      -0.590  -0.942  -0.598
ATOM     29  C   RES     1      -2.079  -2.419  -0.926
ATOM     30  H   RES     1      -2.757  -2.801  -0.158
ATOM     31  H   RES     1      -1.228  -3.094  -1.029
ATOM     32  H   RES     1      -2.633  -2.393  -1.871
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REMARK  Compound C structure 04
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.556939
REMARK   Sum of electronic and thermal Energies=    -651.539714
REMARK   Sum of electronic and thermal Enthalpies=  -651.538770
REMARK   Sum of electronic and thermal Free Energies=  -651.604785
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.789  -0.112  -0.766
ATOM      2  C   RES     1      -4.853  -0.649  -0.936
ATOM      3  H   RES     1      -4.881  -1.590  -0.381
ATOM      4  H   RES     1      -4.802  -0.869  -2.004
ATOM      5  C   RES     1      -3.700   0.248  -0.564
ATOM      6  O   RES     1      -3.544   1.355  -1.069
ATOM      7  N   RES     1      -2.853  -0.249   0.389
ATOM      8  H   RES     1      -2.949  -1.214   0.671
ATOM      9  C   RES     1      -1.636   0.455   0.793
ATOM     10  H   RES     1      -1.829   1.497   0.507
ATOM     11  C   RES     1      -1.452   0.365   2.297
ATOM     12  H   RES     1      -2.334   0.754   2.811
ATOM     13  H   RES     1      -0.584   0.945   2.622
ATOM     14  H   RES     1      -1.296  -0.670   2.622
ATOM     15  C   RES     1      -0.472  -0.046  -0.017
ATOM     16  H   RES     1      -0.628  -0.010  -1.098
ATOM     17  C   RES     1       0.681  -0.530   0.458
ATOM     18  H   RES     1       0.845  -0.575   1.538
ATOM     19  C   RES     1       1.810  -1.044  -0.384
ATOM     20  H   RES     1       1.485  -1.023  -1.436
ATOM     21  C   RES     1       2.179  -2.476  -0.013
ATOM     22  H   RES     1       2.472  -2.541   1.040
ATOM     23  H   RES     1       1.331  -3.146  -0.173
ATOM     24  H   RES     1       3.028  -2.818  -0.607
ATOM     25  C   RES     1       3.062  -0.150  -0.336
ATOM     26  O   RES     1       4.193  -0.608  -0.446
ATOM     27  N   RES     1       2.808   1.182  -0.205
ATOM     28  H   RES     1       1.844   1.475  -0.140
ATOM     29  C   RES     1       3.850   2.179  -0.238
ATOM     30  H   RES     1       4.807   1.656  -0.250
ATOM     31  H   RES     1       3.808   2.823   0.646
ATOM     32  H   RES     1       3.782   2.806  -1.133
TER
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REMARK  Compound C structure 05
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.557536
REMARK   Sum of electronic and thermal Energies=    -651.540350
REMARK   Sum of electronic and thermal Enthalpies=  -651.539406
REMARK   Sum of electronic and thermal Free Energies=  -651.604573
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.481  -0.462  -1.685
ATOM      2  C   RES     1      -5.057  -0.770  -0.727
ATOM      3  H   RES     1      -5.858  -0.700   0.013
ATOM      4  H   RES     1      -4.734  -1.811  -0.800
ATOM      5  C   RES     1      -3.956   0.188  -0.349
ATOM      6  O   RES     1      -4.139   1.398  -0.267
ATOM      7  N   RES     1      -2.735  -0.380  -0.116
ATOM      8  H   RES     1      -2.645  -1.385  -0.113
ATOM      9  C   RES     1      -1.589   0.415   0.323
ATOM     10  H   RES     1      -1.776   1.409  -0.107
ATOM     11  C   RES     1      -1.555   0.556   1.837
ATOM     12  H   RES     1      -2.496   0.985   2.189
ATOM     13  H   RES     1      -0.742   1.216   2.155
ATOM     14  H   RES     1      -1.413  -0.414   2.325
ATOM     15  C   RES     1      -0.345  -0.154  -0.289
ATOM     16  H   RES     1      -0.378  -0.269  -1.375
ATOM     17  C   RES     1       0.763  -0.526   0.363
ATOM     18  H   RES     1       0.806  -0.426   1.451
ATOM     19  C   RES     1       1.993  -1.084  -0.283
ATOM     20  H   RES     1       1.780  -1.225  -1.354
ATOM     21  C   RES     1       2.386  -2.429   0.318
ATOM     22  H   RES     1       2.566  -2.335   1.394
ATOM     23  H   RES     1       1.592  -3.165   0.170
ATOM     24  H   RES     1       3.308  -2.795  -0.136
ATOM     25  C   RES     1       3.198  -0.126  -0.248
ATOM     26  O   RES     1       4.352  -0.539  -0.260
ATOM     27  N   RES     1       2.883   1.199  -0.246
ATOM     28  H   RES     1       1.907   1.454  -0.256
ATOM     29  C   RES     1       3.887   2.234  -0.306
ATOM     30  H   RES     1       4.861   1.756  -0.198
ATOM     31  H   RES     1       3.753   2.959   0.502
ATOM     32  H   RES     1       3.862   2.767  -1.263
TER
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REMARK  Compound C structure 06
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.560267
REMARK   Sum of electronic and thermal Energies=    -651.543637
REMARK   Sum of electronic and thermal Enthalpies=  -651.542693
REMARK   Sum of electronic and thermal Free Energies=  -651.604461
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -2.667  -9.643  -8.259
ATOM      2  C   RES     1      -2.155 -10.164 -10.231
ATOM      3  H   RES     1      -1.968 -11.210  -9.972
ATOM      4  H   RES     1      -3.145  -9.979 -10.653
ATOM      5  H   RES     1      -1.477  -9.831 -11.028
ATOM      6  H   RES     1      -2.303  -5.777 -11.730
ATOM      7  C   RES     1      -2.020  -5.865 -10.679
ATOM      8  H   RES     1      -2.850  -5.520 -10.059
ATOM      9  H   RES     1      -1.164  -5.203 -10.522
ATOM     10  C   RES     1      -1.597  -7.286 -10.403
ATOM     11  O   RES     1      -0.702  -7.834 -11.046
ATOM     12  N   RES     1      -2.269  -7.922  -9.406
ATOM     13  H   RES     1      -2.978  -7.419  -8.894
ATOM     14  C   RES     1      -1.957  -9.297  -8.991
ATOM     15  C   RES     1      -0.556  -9.379  -8.460
ATOM     16  H   RES     1      -0.350  -8.809  -7.550
ATOM     17  C   RES     1       0.425 -10.047  -9.069
ATOM     18  H   RES     1       0.187 -10.584  -9.992
ATOM     19  C   RES     1       1.861 -10.051  -8.661
ATOM     20  H   RES     1       2.431 -10.826  -9.152
ATOM     21  C   RES     1       2.549  -8.690  -8.885
ATOM     22  O   RES     1       3.697  -8.493  -8.494
ATOM     23  N   RES     1       1.815  -7.737  -9.509
ATOM     24  H   RES     1       0.867  -7.926  -9.817
ATOM     25  C   RES     1       2.364  -6.422  -9.742
ATOM     26  H   RES     1       2.522  -5.881  -8.803
ATOM     27  H   RES     1       3.331  -6.492 -10.247
ATOM     28  H   RES     1       1.669  -5.859 -10.367
ATOM     29  C   RES     1       1.966 -10.435  -7.192
ATOM     30  H   RES     1       2.922 -10.942  -7.019
ATOM     31  H   RES     1       1.127 -11.083  -6.920
ATOM     32  H   RES     1       1.974  -9.527  -6.585
TER
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REMARK  Compound C structure 07
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.556076
REMARK   Sum of electronic and thermal Energies=    -651.538761
REMARK   Sum of electronic and thermal Enthalpies=  -651.537816
REMARK   Sum of electronic and thermal Free Energies=  -651.603832
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.100   2.702  -0.208
ATOM      2  C   RES     1      -3.737   1.961  -0.922
ATOM      3  H   RES     1      -4.537   1.801  -1.649
ATOM      4  H   RES     1      -2.865   2.366  -1.441
ATOM      5  C   RES     1      -3.470   0.668  -0.193
ATOM      6  O   RES     1      -4.322   0.117   0.496
ATOM      7  N   RES     1      -2.212   0.158  -0.345
ATOM      8  H   RES     1      -1.578   0.591  -1.000
ATOM      9  C   RES     1      -1.835  -1.126   0.222
ATOM     10  H   RES     1      -2.456  -1.231   1.122
ATOM     11  C   RES     1      -2.187  -2.278  -0.718
ATOM     12  H   RES     1      -3.256  -2.267  -0.941
ATOM     13  H   RES     1      -1.943  -3.242  -0.261
ATOM     14  H   RES     1      -1.631  -2.200  -1.659
ATOM     15  C   RES     1      -0.387  -1.153   0.610
ATOM     16  H   RES     1       0.001  -2.148   0.839
ATOM     17  C   RES     1       0.438  -0.106   0.694
ATOM     18  H   RES     1       0.077   0.902   0.482
ATOM     19  C   RES     1       1.883  -0.185   1.087
ATOM     20  H   RES     1       2.147  -1.239   1.253
ATOM     21  C   RES     1       2.153   0.613   2.364
ATOM     22  H   RES     1       1.907   1.666   2.204
ATOM     23  H   RES     1       1.544   0.235   3.190
ATOM     24  H   RES     1       3.206   0.556   2.655
ATOM     25  C   RES     1       2.727   0.390  -0.050
ATOM     26  O   RES     1       2.637   1.567  -0.385
ATOM     27  N   RES     1       3.569  -0.496  -0.654
ATOM     28  H   RES     1       3.565  -1.453  -0.338
ATOM     29  C   RES     1       4.418  -0.131  -1.763
ATOM     30  H   RES     1       4.293   0.939  -1.933
ATOM     31  H   RES     1       4.139  -0.667  -2.676
ATOM     32  H   RES     1       5.469  -0.335  -1.542
TER
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REMARK  Compound C structure 08
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.555343
REMARK   Sum of electronic and thermal Energies=    -651.538026
REMARK   Sum of electronic and thermal Enthalpies=  -651.537082
REMARK   Sum of electronic and thermal Free Energies=  -651.602276
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.835  -1.835  -1.615
ATOM      2  C   RES     1      -4.156  -1.096  -0.877
ATOM      3  H   RES     1      -5.069  -0.638  -1.262
ATOM      4  H   RES     1      -4.387  -1.612   0.059
ATOM      5  C   RES     1      -3.091  -0.036  -0.748
ATOM      6  O   RES     1      -2.742   0.659  -1.696
ATOM      7  N   RES     1      -2.548   0.102   0.499
ATOM      8  H   RES     1      -2.816  -0.543   1.228
ATOM      9  C   RES     1      -1.474   1.041   0.775
ATOM     10  H   RES     1      -1.624   1.861   0.059
ATOM     11  C   RES     1      -1.606   1.582   2.193
ATOM     12  H   RES     1      -2.571   2.075   2.336
ATOM     13  H   RES     1      -0.816   2.306   2.405
ATOM     14  H   RES     1      -1.512   0.777   2.931
ATOM     15  C   RES     1      -0.103   0.469   0.531
ATOM     16  H   RES     1       0.717   1.156   0.749
ATOM     17  C   RES     1       0.167  -0.758   0.082
ATOM     18  H   RES     1      -0.662  -1.438  -0.125
ATOM     19  C   RES     1       1.538  -1.335  -0.165
ATOM     20  H   RES     1       1.544  -1.729  -1.193
ATOM     21  C   RES     1       1.833  -2.485   0.792
ATOM     22  H   RES     1       1.910  -2.109   1.815
ATOM     23  H   RES     1       1.039  -3.236   0.751
ATOM     24  H   RES     1       2.780  -2.972   0.545
ATOM     25  C   RES     1       2.612  -0.256  -0.065
ATOM     26  O   RES     1       3.270  -0.062   0.952
ATOM     27  N   RES     1       2.768   0.489  -1.199
ATOM     28  H   RES     1       2.090   0.368  -1.936
ATOM     29  C   RES     1       3.605   1.666  -1.225
ATOM     30  H   RES     1       4.354   1.560  -0.440
ATOM     31  H   RES     1       3.034   2.583  -1.033
ATOM     32  H   RES     1       4.105   1.758  -2.191
TER
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REMARK  Compound C structure 09
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.555571
REMARK   Sum of electronic and thermal Energies=    -651.538508
REMARK   Sum of electronic and thermal Enthalpies=  -651.537564
REMARK   Sum of electronic and thermal Free Energies=  -651.602269
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.996   1.502   1.600
ATOM      2  C   RES     1      -4.401   0.598   1.746
ATOM      3  H   RES     1      -3.659   0.788   2.526
ATOM      4  H   RES     1      -5.084  -0.181   2.090
ATOM      5  C   RES     1      -3.806   0.181   0.425
ATOM      6  O   RES     1      -4.501  -0.129  -0.538
ATOM      7  N   RES     1      -2.442   0.162   0.372
ATOM      8  H   RES     1      -1.904   0.484   1.163
ATOM      9  C   RES     1      -1.724  -0.171  -0.859
ATOM     10  H   RES     1      -2.365  -0.911  -1.358
ATOM     11  C   RES     1      -1.604   1.038  -1.774
ATOM     12  H   RES     1      -2.599   1.434  -1.988
ATOM     13  H   RES     1      -1.135   0.767  -2.725
ATOM     14  H   RES     1      -1.007   1.831  -1.311
ATOM     15  C   RES     1      -0.429  -0.824  -0.482
ATOM     16  H   RES     1      -0.532  -1.692   0.170
ATOM     17  C   RES     1       0.788  -0.426  -0.862
ATOM     18  H   RES     1       0.883   0.452  -1.503
ATOM     19  C   RES     1       2.088  -1.065  -0.453
ATOM     20  H   RES     1       2.664  -1.259  -1.372
ATOM     21  C   RES     1       1.936  -2.362   0.322
ATOM     22  H   RES     1       1.444  -2.176   1.280
ATOM     23  H   RES     1       1.348  -3.089  -0.244
ATOM     24  H   RES     1       2.912  -2.803   0.537
ATOM     25  C   RES     1       2.868  -0.042   0.384
ATOM     26  O   RES     1       2.692   0.084   1.590
ATOM     27  N   RES     1       3.737   0.733  -0.327
ATOM     28  H   RES     1       3.853   0.547  -1.311
ATOM     29  C   RES     1       4.522   1.782   0.281
ATOM     30  H   RES     1       4.243   1.827   1.334
ATOM     31  H   RES     1       4.320   2.752  -0.184
ATOM     32  H   RES     1       5.594   1.573   0.209
TER
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REMARK  Compound C structure 10
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.555434
REMARK   Sum of electronic and thermal Energies=    -651.538244
REMARK   Sum of electronic and thermal Enthalpies=  -651.537300
REMARK   Sum of electronic and thermal Free Energies=  -651.602264
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.236   1.296  -1.000
ATOM      2  C   RES     1       4.530   1.291  -0.168
ATOM      3  H   RES     1       5.029   0.896   0.721
ATOM      4  H   RES     1       4.252   2.331   0.021
ATOM      5  C   RES     1       3.298   0.521  -0.571
ATOM      6  O   RES     1       2.693   0.751  -1.613
ATOM      7  N   RES     1       2.905  -0.461   0.297
ATOM      8  H   RES     1       3.373  -0.546   1.187
ATOM      9  C   RES     1       1.653  -1.193   0.100
ATOM     10  H   RES     1       1.544  -1.291  -0.985
ATOM     11  C   RES     1       1.763  -2.563   0.747
ATOM     12  H   RES     1       2.611  -3.123   0.344
ATOM     13  H   RES     1       0.854  -3.145   0.576
ATOM     14  H   RES     1       1.894  -2.479   1.833
ATOM     15  C   RES     1       0.487  -0.404   0.629
ATOM     16  H   RES     1       0.394  -0.363   1.718
ATOM     17  C   RES     1      -0.374   0.264  -0.146
ATOM     18  H   RES     1      -0.222   0.221  -1.226
ATOM     19  C   RES     1      -1.529   1.097   0.321
ATOM     20  H   RES     1      -1.427   2.093  -0.131
ATOM     21  C   RES     1      -1.611   1.272   1.836
ATOM     22  H   RES     1      -1.750   0.309   2.341
ATOM     23  H   RES     1      -0.697   1.728   2.227
ATOM     24  H   RES     1      -2.457   1.912   2.094
ATOM     25  C   RES     1      -2.895   0.608  -0.178
ATOM     26  O   RES     1      -3.858   1.364  -0.239
ATOM     27  N   RES     1      -2.967  -0.717  -0.487
ATOM     28  H   RES     1      -2.127  -1.271  -0.399
ATOM     29  C   RES     1      -4.190  -1.350  -0.917
ATOM     30  H   RES     1      -4.961  -0.579  -0.954
ATOM     31  H   RES     1      -4.505  -2.131  -0.218
ATOM     32  H   RES     1      -4.083  -1.791  -1.913
TER
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REMARK  Compound C structure 11
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.555700
REMARK   Sum of electronic and thermal Energies=    -651.538720
REMARK   Sum of electronic and thermal Enthalpies=  -651.537776
REMARK   Sum of electronic and thermal Free Energies=  -651.602088
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.019  -0.827  -2.006
ATOM      2  C   RES     1      -4.392  -1.319  -1.259
ATOM      3  H   RES     1      -5.050  -1.953  -0.659
ATOM      4  H   RES     1      -3.663  -1.952  -1.770
ATOM      5  C   RES     1      -3.776  -0.269  -0.369
ATOM      6  O   RES     1      -4.449   0.559   0.234
ATOM      7  N   RES     1      -2.411  -0.295  -0.285
ATOM      8  H   RES     1      -1.901  -1.040  -0.734
ATOM      9  C   RES     1      -1.680   0.621   0.591
ATOM     10  H   RES     1      -2.283   1.540   0.583
ATOM     11  C   RES     1      -1.634   0.104   2.021
ATOM     12  H   RES     1      -2.650  -0.081   2.375
ATOM     13  H   RES     1      -1.170   0.834   2.691
ATOM     14  H   RES     1      -1.067  -0.831   2.090
ATOM     15  C   RES     1      -0.347   0.918  -0.027
ATOM     16  H   RES     1      -0.392   1.239  -1.069
ATOM     17  C   RES     1       0.839   0.850   0.590
ATOM     18  H   RES     1       0.868   0.538   1.636
ATOM     19  C   RES     1       2.171   1.187  -0.012
ATOM     20  H   RES     1       2.638   1.955   0.620
ATOM     21  C   RES     1       2.107   1.728  -1.437
ATOM     22  H   RES     1       1.676   0.991  -2.124
ATOM     23  H   RES     1       1.494   2.632  -1.488
ATOM     24  H   RES     1       3.112   1.969  -1.789
ATOM     25  C   RES     1       3.182   0.032   0.019
ATOM     26  O   RES     1       4.386   0.241  -0.074
ATOM     27  N   RES     1       2.647  -1.219   0.107
ATOM     28  H   RES     1       1.642  -1.303   0.153
ATOM     29  C   RES     1       3.458  -2.412   0.085
ATOM     30  H   RES     1       3.270  -3.011  -0.812
ATOM     31  H   RES     1       3.274  -3.033   0.967
ATOM     32  H   RES     1       4.502  -2.098   0.083
TER
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REMARK  Compound C structure 12
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.554623
REMARK   Sum of electronic and thermal Energies=    -651.537266
REMARK   Sum of electronic and thermal Enthalpies=  -651.536321
REMARK   Sum of electronic and thermal Free Energies=  -651.602059
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.846  -1.524   1.431
ATOM      2  C   RES     1      -4.362  -0.559   1.598
ATOM      3  H   RES     1      -5.153   0.161   1.820
ATOM      4  H   RES     1      -3.705  -0.639   2.468
ATOM      5  C   RES     1      -3.655  -0.137   0.334
ATOM      6  O   RES     1      -4.248   0.011  -0.731
ATOM      7  N   RES     1      -2.314   0.077   0.451
ATOM      8  H   RES     1      -1.848  -0.138   1.320
ATOM      9  C   RES     1      -1.491   0.431  -0.710
ATOM     10  H   RES     1      -1.824  -0.204  -1.542
ATOM     11  C   RES     1      -1.706   1.892  -1.096
ATOM     12  H   RES     1      -2.764   2.075  -1.294
ATOM     13  H   RES     1      -1.135   2.138  -1.996
ATOM     14  H   RES     1      -1.378   2.557  -0.290
ATOM     15  C   RES     1      -0.057   0.143  -0.394
ATOM     16  H   RES     1       0.374   0.715   0.432
ATOM     17  C   RES     1       0.697  -0.739  -1.054
ATOM     18  H   RES     1       0.241  -1.311  -1.866
ATOM     19  C   RES     1       2.140  -1.071  -0.783
ATOM     20  H   RES     1       2.704  -0.885  -1.711
ATOM     21  C   RES     1       2.294  -2.546  -0.417
ATOM     22  H   RES     1       1.817  -2.739   0.547
ATOM     23  H   RES     1       1.829  -3.184  -1.174
ATOM     24  H   RES     1       3.348  -2.826  -0.334
ATOM     25  C   RES     1       2.706  -0.188   0.324
ATOM     26  O   RES     1       2.526  -0.432   1.512
ATOM     27  N   RES     1       3.400   0.903  -0.112
ATOM     28  H   RES     1       3.451   1.072  -1.104
ATOM     29  C   RES     1       3.918   1.904   0.790
ATOM     30  H   RES     1       3.863   1.498   1.801
ATOM     31  H   RES     1       3.330   2.829   0.754
ATOM     32  H   RES     1       4.959   2.139   0.555
TER
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REMARK  Compound C structure 13
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.554694
REMARK   Sum of electronic and thermal Energies=    -651.537411
REMARK   Sum of electronic and thermal Enthalpies=  -651.536467
REMARK   Sum of electronic and thermal Free Energies=  -651.601829
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.092  -1.513  -0.892
ATOM      2  C   RES     1       4.190  -1.805  -0.349
ATOM      3  H   RES     1       3.549  -2.387  -1.016
ATOM      4  H   RES     1       4.509  -2.441   0.479
ATOM      5  C   RES     1       3.530  -0.569   0.210
ATOM      6  O   RES     1       4.090   0.165   1.017
ATOM      7  N   RES     1       2.263  -0.325  -0.237
ATOM      8  H   RES     1       1.869  -0.906  -0.961
ATOM      9  C   RES     1       1.523   0.873   0.165
ATOM     10  H   RES     1       1.837   1.051   1.204
ATOM     11  C   RES     1       1.936   2.081  -0.662
ATOM     12  H   RES     1       3.016   2.222  -0.587
ATOM     13  H   RES     1       1.450   2.991  -0.299
ATOM     14  H   RES     1       1.673   1.950  -1.717
ATOM     15  C   RES     1       0.059   0.557   0.155
ATOM     16  H   RES     1      -0.228  -0.312   0.750
ATOM     17  C   RES     1      -0.884   1.254  -0.486
ATOM     18  H   RES     1      -0.599   2.138  -1.059
ATOM     19  C   RES     1      -2.366   0.984  -0.461
ATOM     20  H   RES     1      -2.713   0.947  -1.506
ATOM     21  C   RES     1      -3.106   2.115   0.251
ATOM     22  H   RES     1      -2.839   2.117   1.310
ATOM     23  H   RES     1      -2.842   3.084  -0.181
ATOM     24  H   RES     1      -4.190   1.989   0.176
ATOM     25  C   RES     1      -2.674  -0.353   0.204
ATOM     26  O   RES     1      -2.792  -0.473   1.418
ATOM     27  N   RES     1      -2.779  -1.408  -0.657
ATOM     28  H   RES     1      -2.634  -1.240  -1.640
ATOM     29  C   RES     1      -2.979  -2.764  -0.204
ATOM     30  H   RES     1      -3.174  -2.724   0.868
ATOM     31  H   RES     1      -2.093  -3.385  -0.376
ATOM     32  H   RES     1      -3.835  -3.225  -0.705
TER
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REMARK  Compound C structure 14
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.555207
REMARK   Sum of electronic and thermal Energies=    -651.538010
REMARK   Sum of electronic and thermal Enthalpies=  -651.537066
REMARK   Sum of electronic and thermal Free Energies=  -651.601663
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.864   0.545   0.377
ATOM      2  C   RES     1       5.034   1.000  -0.169
ATOM      3  H   RES     1       4.739   1.919   0.344
ATOM      4  H   RES     1       5.409   1.255  -1.163
ATOM      5  C   RES     1       3.923  -0.010  -0.305
ATOM      6  O   RES     1       4.084  -1.096  -0.854
ATOM      7  N   RES     1       2.721   0.357   0.228
ATOM      8  H   RES     1       2.603   1.292   0.588
ATOM      9  C   RES     1       1.539  -0.499   0.106
ATOM     10  H   RES     1       1.531  -0.888  -0.921
ATOM     11  C   RES     1       1.625  -1.679   1.071
ATOM     12  H   RES     1       2.543  -2.244   0.893
ATOM     13  H   RES     1       0.773  -2.352   0.931
ATOM     14  H   RES     1       1.619  -1.333   2.110
ATOM     15  C   RES     1       0.307   0.317   0.347
ATOM     16  H   RES     1       0.229   0.775   1.337
ATOM     17  C   RES     1      -0.686   0.467  -0.536
ATOM     18  H   RES     1      -0.577  -0.012  -1.513
ATOM     19  C   RES     1      -1.968   1.212  -0.322
ATOM     20  H   RES     1      -2.103   1.902  -1.165
ATOM     21  C   RES     1      -2.023   2.024   0.969
ATOM     22  H   RES     1      -1.948   1.379   1.851
ATOM     23  H   RES     1      -1.206   2.750   1.012
ATOM     24  H   RES     1      -2.969   2.565   1.029
ATOM     25  C   RES     1      -3.216   0.317  -0.380
ATOM     26  O   RES     1      -4.315   0.780  -0.663
ATOM     27  N   RES     1      -3.017  -0.989  -0.047
ATOM     28  H   RES     1      -2.082  -1.278   0.203
ATOM     29  C   RES     1      -4.095  -1.945   0.026
ATOM     30  H   RES     1      -4.260  -2.289   1.052
ATOM     31  H   RES     1      -3.894  -2.815  -0.608
ATOM     32  H   RES     1      -5.000  -1.450  -0.327
TER
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REMARK  Compound C structure 15
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.554103
REMARK   Sum of electronic and thermal Energies=    -651.536733
REMARK   Sum of electronic and thermal Enthalpies=  -651.535789
REMARK   Sum of electronic and thermal Free Energies=  -651.601448
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.018  -2.187  -0.418
ATOM      2  C   RES     1       3.980  -2.220  -0.082
ATOM      3  H   RES     1       3.376  -2.709  -0.851
ATOM      4  H   RES     1       3.957  -2.830   0.824
ATOM      5  C   RES     1       3.525  -0.822   0.257
ATOM      6  O   RES     1       4.122  -0.115   1.063
ATOM      7  N   RES     1       2.407  -0.390  -0.396
ATOM      8  H   RES     1       1.874  -1.049  -0.943
ATOM      9  C   RES     1       1.788   0.902  -0.075
ATOM     10  H   RES     1       1.798   0.997   1.019
ATOM     11  C   RES     1       2.595   2.049  -0.673
ATOM     12  H   RES     1       3.627   2.010  -0.319
ATOM     13  H   RES     1       2.163   3.011  -0.382
ATOM     14  H   RES     1       2.597   1.990  -1.767
ATOM     15  C   RES     1       0.373   0.907  -0.566
ATOM     16  H   RES     1       0.244   0.915  -1.654
ATOM     17  C   RES     1      -0.705   0.944   0.220
ATOM     18  H   RES     1      -0.583   0.944   1.306
ATOM     19  C   RES     1      -2.123   0.996  -0.266
ATOM     20  H   RES     1      -2.115   0.986  -1.366
ATOM     21  C   RES     1      -2.830   2.258   0.229
ATOM     22  H   RES     1      -2.870   2.255   1.321
ATOM     23  H   RES     1      -2.297   3.153  -0.101
ATOM     24  H   RES     1      -3.858   2.308  -0.143
ATOM     25  C   RES     1      -2.863  -0.237   0.255
ATOM     26  O   RES     1      -3.144  -0.367   1.441
ATOM     27  N   RES     1      -3.160  -1.173  -0.691
ATOM     28  H   RES     1      -2.901  -0.989  -1.647
ATOM     29  C   RES     1      -3.833  -2.411  -0.376
ATOM     30  H   RES     1      -4.004  -2.425   0.700
ATOM     31  H   RES     1      -3.223  -3.278  -0.649
ATOM     32  H   RES     1      -4.798  -2.484  -0.887
TER
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REMARK  Compound C structure 16
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.554408
REMARK   Sum of electronic and thermal Energies=    -651.537223
REMARK   Sum of electronic and thermal Enthalpies=  -651.536279
REMARK   Sum of electronic and thermal Free Energies=  -651.601288
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.818   1.407   0.904
ATOM      2  C   RES     1       3.889   1.006   1.313
ATOM      3  H   RES     1       4.126   0.265   2.082
ATOM      4  H   RES     1       3.359   1.838   1.785
ATOM      5  C   RES     1       3.043   0.466   0.188
ATOM      6  O   RES     1       2.841   1.099  -0.843
ATOM      7  N   RES     1       2.524  -0.784   0.387
ATOM      8  H   RES     1       2.600  -1.198   1.305
ATOM      9  C   RES     1       1.528  -1.341  -0.534
ATOM     10  H   RES     1       1.875  -1.070  -1.538
ATOM     11  C   RES     1       1.490  -2.851  -0.378
ATOM     12  H   RES     1       2.474  -3.294  -0.553
ATOM     13  H   RES     1       0.782  -3.291  -1.085
ATOM     14  H   RES     1       1.161  -3.134   0.629
ATOM     15  C   RES     1       0.189  -0.700  -0.298
ATOM     16  H   RES     1      -0.349  -1.018   0.599
ATOM     17  C   RES     1      -0.296   0.278  -1.066
ATOM     18  H   RES     1       0.302   0.609  -1.917
ATOM     19  C   RES     1      -1.554   1.070  -0.827
ATOM     20  H   RES     1      -2.123   1.093  -1.770
ATOM     21  C   RES     1      -1.196   2.507  -0.445
ATOM     22  H   RES     1      -0.712   2.513   0.535
ATOM     23  H   RES     1      -0.507   2.941  -1.174
ATOM     24  H   RES     1      -2.088   3.138  -0.388
ATOM     25  C   RES     1      -2.417   0.428   0.251
ATOM     26  O   RES     1      -2.218   0.602   1.448
ATOM     27  N   RES     1      -3.413  -0.379  -0.221
ATOM     28  H   RES     1      -3.476  -0.528  -1.216
ATOM     29  C   RES     1      -4.266  -1.149   0.651
ATOM     30  H   RES     1      -4.126  -0.771   1.665
ATOM     31  H   RES     1      -4.008  -2.215   0.640
ATOM     32  H   RES     1      -5.316  -1.038   0.370
TER
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REMARK  Compound C structure 17
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.553968
REMARK   Sum of electronic and thermal Energies=    -651.536871
REMARK   Sum of electronic and thermal Enthalpies=  -651.535927
REMARK   Sum of electronic and thermal Free Energies=  -651.600310
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.624   0.460   0.502
ATOM      2  C   RES     1       4.818   0.928  -0.066
ATOM      3  H   RES     1       4.756   1.967   0.266
ATOM      4  H   RES     1       5.079   0.911  -1.127
ATOM      5  C   RES     1       3.520   0.231   0.263
ATOM      6  O   RES     1       3.106   0.138   1.414
ATOM      7  N   RES     1       2.852  -0.295  -0.806
ATOM      8  H   RES     1       3.191  -0.080  -1.730
ATOM      9  C   RES     1       1.536  -0.943  -0.704
ATOM     10  H   RES     1       1.283  -1.241  -1.730
ATOM     11  C   RES     1       1.599  -2.199   0.162
ATOM     12  H   RES     1       2.383  -2.875  -0.192
ATOM     13  H   RES     1       0.643  -2.728   0.118
ATOM     14  H   RES     1       1.810  -1.940   1.201
ATOM     15  C   RES     1       0.486   0.017  -0.222
ATOM     16  H   RES     1       0.687   0.480   0.744
ATOM     17  C   RES     1      -0.638   0.283  -0.896
ATOM     18  H   RES     1      -0.794  -0.213  -1.860
ATOM     19  C   RES     1      -1.748   1.190  -0.456
ATOM     20  H   RES     1      -1.968   1.887  -1.275
ATOM     21  C   RES     1      -1.432   2.006   0.795
ATOM     22  H   RES     1      -1.256   1.360   1.661
ATOM     23  H   RES     1      -0.536   2.616   0.648
ATOM     24  H   RES     1      -2.267   2.668   1.033
ATOM     25  C   RES     1      -3.077   0.455  -0.232
ATOM     26  O   RES     1      -4.156   1.012  -0.404
ATOM     27  N   RES     1      -2.960  -0.825   0.223
ATOM     28  H   RES     1      -2.030  -1.195   0.358
ATOM     29  C   RES     1      -4.102  -1.628   0.584
ATOM     30  H   RES     1      -4.105  -1.867   1.653
ATOM     31  H   RES     1      -4.126  -2.564   0.016
ATOM     32  H   RES     1      -4.996  -1.049   0.351
TER
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REMARK  Compound C structure 18
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.552926
REMARK   Sum of electronic and thermal Energies=    -651.535731
REMARK   Sum of electronic and thermal Enthalpies=  -651.534787
REMARK   Sum of electronic and thermal Free Energies=  -651.599868
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.895   2.102   0.746
ATOM      2  C   RES     1       3.881   2.150   0.341
ATOM      3  H   RES     1       3.213   2.540   1.113
ATOM      4  H   RES     1       3.906   2.853  -0.494
ATOM      5  C   RES     1       3.494   0.787  -0.175
ATOM      6  O   RES     1       4.131   0.213  -1.053
ATOM      7  N   RES     1       2.394   0.227   0.407
ATOM      8  H   RES     1       1.816   0.790   1.013
ATOM      9  C   RES     1       1.842  -1.047  -0.072
ATOM     10  H   RES     1       1.856  -1.011  -1.170
ATOM     11  C   RES     1       2.702  -2.218   0.391
ATOM     12  H   RES     1       3.729  -2.093   0.042
ATOM     13  H   RES     1       2.311  -3.159  -0.006
ATOM     14  H   RES     1       2.707  -2.283   1.484
ATOM     15  C   RES     1       0.432  -1.157   0.415
ATOM     16  H   RES     1       0.304  -1.317   1.489
ATOM     17  C   RES     1      -0.652  -1.038  -0.353
ATOM     18  H   RES     1      -0.532  -0.865  -1.426
ATOM     19  C   RES     1      -2.063  -1.063   0.161
ATOM     20  H   RES     1      -2.045  -1.479   1.176
ATOM     21  C   RES     1      -2.969  -1.918  -0.717
ATOM     22  H   RES     1      -2.943  -1.596  -1.766
ATOM     23  H   RES     1      -2.635  -2.959  -0.706
ATOM     24  H   RES     1      -4.009  -1.901  -0.376
ATOM     25  C   RES     1      -2.512   0.391   0.373
ATOM     26  O   RES     1      -2.041   1.064   1.283
ATOM     27  N   RES     1      -3.419   0.881  -0.518
ATOM     28  H   RES     1      -3.790   0.268  -1.226
ATOM     29  C   RES     1      -3.918   2.235  -0.449
ATOM     30  H   RES     1      -3.389   2.739   0.360
ATOM     31  H   RES     1      -4.991   2.257  -0.237
ATOM     32  H   RES     1      -3.733   2.772  -1.385
TER
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REMARK  Compound C structure 19
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.553124
REMARK   Sum of electronic and thermal Energies=    -651.536008
REMARK   Sum of electronic and thermal Enthalpies=  -651.535064
REMARK   Sum of electronic and thermal Free Energies=  -651.599447
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.468  -0.849   0.080
ATOM      2  C   RES     1      -4.758  -0.690  -0.735
ATOM      3  H   RES     1      -4.682  -1.634  -1.279
ATOM      4  H   RES     1      -5.160   0.073  -1.408
ATOM      5  C   RES     1      -3.407  -0.353  -0.152
ATOM      6  O   RES     1      -2.812  -1.118   0.598
ATOM      7  N   RES     1      -2.897   0.861  -0.522
ATOM      8  H   RES     1      -3.456   1.459  -1.109
ATOM      9  C   RES     1      -1.605   1.372  -0.042
ATOM     10  H   RES     1      -1.488   2.333  -0.565
ATOM     11  C   RES     1      -1.626   1.643   1.455
ATOM     12  H   RES     1      -2.450   2.315   1.707
ATOM     13  H   RES     1      -0.693   2.117   1.776
ATOM     14  H   RES     1      -1.755   0.712   2.011
ATOM     15  C   RES     1      -0.490   0.471  -0.499
ATOM     16  H   RES     1      -0.524   0.206  -1.559
ATOM     17  C   RES     1       0.482  -0.040   0.260
ATOM     18  H   RES     1       0.503   0.180   1.330
ATOM     19  C   RES     1       1.530  -0.993  -0.226
ATOM     20  H   RES     1       1.350  -1.179  -1.296
ATOM     21  C   RES     1       1.443  -2.323   0.517
ATOM     22  H   RES     1       1.602  -2.178   1.590
ATOM     23  H   RES     1       0.456  -2.772   0.381
ATOM     24  H   RES     1       2.214  -3.009   0.161
ATOM     25  C   RES     1       2.961  -0.443  -0.157
ATOM     26  O   RES     1       3.937  -1.176  -0.045
ATOM     27  N   RES     1       3.062   0.912  -0.277
ATOM     28  H   RES     1       2.208   1.442  -0.369
ATOM     29  C   RES     1       4.332   1.596  -0.310
ATOM     30  H   RES     1       5.110   0.851  -0.138
ATOM     31  H   RES     1       4.392   2.361   0.470
ATOM     32  H   RES     1       4.509   2.071  -1.281
TER
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REMARK  Compound C structure 20
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.552282
REMARK   Sum of electronic and thermal Energies=    -651.535106
REMARK   Sum of electronic and thermal Enthalpies=  -651.534162
REMARK   Sum of electronic and thermal Free Energies=  -651.598853
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.489  -1.597  -1.301
ATOM      2  C   RES     1      -3.653  -0.995  -1.665
ATOM      3  H   RES     1      -3.070  -1.631  -2.335
ATOM      4  H   RES     1      -4.047  -0.151  -2.236
ATOM      5  C   RES     1      -2.787  -0.599  -0.495
ATOM      6  O   RES     1      -2.357  -1.424   0.305
ATOM      7  N   RES     1      -2.526   0.739  -0.388
ATOM      8  H   RES     1      -2.781   1.327  -1.166
ATOM      9  C   RES     1      -1.584   1.301   0.592
ATOM     10  H   RES     1      -1.580   2.382   0.402
ATOM     11  C   RES     1      -2.064   1.068   2.022
ATOM     12  H   RES     1      -3.086   1.436   2.150
ATOM     13  H   RES     1      -1.413   1.600   2.721
ATOM     14  H   RES     1      -2.047   0.004   2.266
ATOM     15  C   RES     1      -0.197   0.773   0.361
ATOM     16  H   RES     1      -0.120  -0.314   0.328
ATOM     17  C   RES     1       0.880   1.549   0.214
ATOM     18  H   RES     1       0.754   2.635   0.251
ATOM     19  C   RES     1       2.298   1.096  -0.030
ATOM     20  H   RES     1       2.889   1.353   0.865
ATOM     21  C   RES     1       2.899   1.824  -1.227
ATOM     22  H   RES     1       2.366   1.550  -2.139
ATOM     23  H   RES     1       2.835   2.908  -1.092
ATOM     24  H   RES     1       3.949   1.555  -1.366
ATOM     25  C   RES     1       2.369  -0.416  -0.231
ATOM     26  O   RES     1       2.433  -0.933  -1.340
ATOM     27  N   RES     1       2.345  -1.143   0.925
ATOM     28  H   RES     1       2.136  -0.650   1.780
ATOM     29  C   RES     1       2.168  -2.578   0.911
ATOM     30  H   RES     1       2.557  -2.952  -0.036
ATOM     31  H   RES     1       1.110  -2.862   0.983
ATOM     32  H   RES     1       2.718  -3.038   1.735
TER
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REMARK  Compound C structure 21
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.552223
REMARK   Sum of electronic and thermal Energies=    -651.535062
REMARK   Sum of electronic and thermal Enthalpies=  -651.534118
REMARK   Sum of electronic and thermal Free Energies=  -651.598740
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -2.736   2.792  -1.414
ATOM      2  C   RES     1      -3.294   2.293  -0.619
ATOM      3  H   RES     1      -3.219   2.891   0.293
ATOM      4  H   RES     1      -4.339   2.264  -0.935
ATOM      5  C   RES     1      -2.786   0.877  -0.478
ATOM      6  O   RES     1      -2.787   0.090  -1.415
ATOM      7  N   RES     1      -2.322   0.551   0.768
ATOM      8  H   RES     1      -2.356   1.259   1.484
ATOM      9  C   RES     1      -1.821  -0.769   1.146
ATOM     10  H   RES     1      -1.678  -0.711   2.235
ATOM     11  C   RES     1      -2.846  -1.874   0.888
ATOM     12  H   RES     1      -3.795  -1.641   1.379
ATOM     13  H   RES     1      -2.479  -2.824   1.288
ATOM     14  H   RES     1      -3.024  -1.991  -0.182
ATOM     15  C   RES     1      -0.488  -1.109   0.535
ATOM     16  H   RES     1      -0.136  -2.113   0.778
ATOM     17  C   RES     1       0.245  -0.330  -0.264
ATOM     18  H   RES     1      -0.137   0.660  -0.516
ATOM     19  C   RES     1       1.560  -0.689  -0.889
ATOM     20  H   RES     1       1.477  -0.516  -1.970
ATOM     21  C   RES     1       1.992  -2.138  -0.677
ATOM     22  H   RES     1       2.130  -2.363   0.387
ATOM     23  H   RES     1       1.244  -2.830  -1.074
ATOM     24  H   RES     1       2.940  -2.325  -1.185
ATOM     25  C   RES     1       2.717   0.223  -0.459
ATOM     26  O   RES     1       3.699   0.395  -1.172
ATOM     27  N   RES     1       2.591   0.774   0.782
ATOM     28  H   RES     1       1.763   0.551   1.314
ATOM     29  C   RES     1       3.627   1.579   1.382
ATOM     30  H   RES     1       4.105   1.067   2.224
ATOM     31  H   RES     1       3.230   2.536   1.733
ATOM     32  H   RES     1       4.382   1.766   0.617
TER
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REMARK  Compound C structure 22
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.551920
REMARK   Sum of electronic and thermal Energies=    -651.534787
REMARK   Sum of electronic and thermal Enthalpies=  -651.533843
REMARK   Sum of electronic and thermal Free Energies=  -651.598478
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.519  -0.887  -0.091
ATOM      2  C   RES     1      -4.799  -0.666  -0.882
ATOM      3  H   RES     1      -4.709  -1.567  -1.492
ATOM      4  H   RES     1      -5.197   0.142  -1.503
ATOM      5  C   RES     1      -3.459  -0.362  -0.256
ATOM      6  O   RES     1      -2.863  -1.181   0.436
ATOM      7  N   RES     1      -2.960   0.882  -0.521
ATOM      8  H   RES     1      -3.530   1.523  -1.049
ATOM      9  C   RES     1      -1.691   1.381   0.029
ATOM     10  H   RES     1      -1.571   2.371  -0.435
ATOM     11  C   RES     1      -1.765   1.563   1.538
ATOM     12  H   RES     1      -2.608   2.205   1.803
ATOM     13  H   RES     1      -0.851   2.030   1.917
ATOM     14  H   RES     1      -1.894   0.597   2.030
ATOM     15  C   RES     1      -0.548   0.523  -0.439
ATOM     16  H   RES     1      -0.575   0.268  -1.501
ATOM     17  C   RES     1       0.447   0.056   0.315
ATOM     18  H   RES     1       0.486   0.271   1.384
ATOM     19  C   RES     1       1.538  -0.841  -0.188
ATOM     20  H   RES     1       1.424  -0.955  -1.276
ATOM     21  C   RES     1       1.446  -2.215   0.479
ATOM     22  H   RES     1       1.602  -2.115   1.556
ATOM     23  H   RES     1       0.459  -2.653   0.310
ATOM     24  H   RES     1       2.208  -2.898   0.091
ATOM     25  C   RES     1       2.892  -0.208   0.126
ATOM     26  O   RES     1       3.305  -0.097   1.275
ATOM     27  N   RES     1       3.590   0.233  -0.962
ATOM     28  H   RES     1       3.173   0.128  -1.873
ATOM     29  C   RES     1       4.866   0.896  -0.850
ATOM     30  H   RES     1       5.145   0.888   0.204
ATOM     31  H   RES     1       4.812   1.935  -1.191
ATOM     32  H   RES     1       5.638   0.376  -1.425
TER
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REMARK  Compound C structure 23
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -651.550456
REMARK   Sum of electronic and thermal Energies=    -651.533131
REMARK   Sum of electronic and thermal Enthalpies=  -651.532187
REMARK   Sum of electronic and thermal Free Energies=  -651.597687
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.944  -1.946  -1.353
ATOM      2  C   RES     1      -4.180  -0.904  -1.126
ATOM      3  H   RES     1      -4.316  -0.360  -2.064
ATOM      4  H   RES     1      -5.127  -0.905  -0.581
ATOM      5  C   RES     1      -3.102  -0.340  -0.229
ATOM      6  O   RES     1      -2.832  -0.844   0.855
ATOM      7  N   RES     1      -2.460   0.762  -0.723
ATOM      8  H   RES     1      -2.731   1.093  -1.634
ATOM      9  C   RES     1      -1.409   1.501  -0.024
ATOM     10  H   RES     1      -1.234   2.390  -0.648
ATOM     11  C   RES     1      -1.871   1.997   1.347
ATOM     12  H   RES     1      -2.781   2.597   1.253
ATOM     13  H   RES     1      -1.094   2.620   1.799
ATOM     14  H   RES     1      -2.072   1.155   2.011
ATOM     15  C   RES     1      -0.105   0.761   0.080
ATOM     16  H   RES     1       0.677   1.309   0.610
ATOM     17  C   RES     1       0.148  -0.469  -0.366
ATOM     18  H   RES     1      -0.650  -1.034  -0.850
ATOM     19  C   RES     1       1.431  -1.236  -0.170
ATOM     20  H   RES     1       1.649  -1.770  -1.108
ATOM     21  C   RES     1       1.260  -2.266   0.946
ATOM     22  H   RES     1       1.140  -1.749   1.901
ATOM     23  H   RES     1       0.370  -2.878   0.773
ATOM     24  H   RES     1       2.130  -2.924   1.020
ATOM     25  C   RES     1       2.596  -0.301   0.132
ATOM     26  O   RES     1       2.858   0.090   1.265
ATOM     27  N   RES     1       3.309   0.089  -0.966
ATOM     28  H   RES     1       2.997  -0.223  -1.872
ATOM     29  C   RES     1       4.378   1.055  -0.893
ATOM     30  H   RES     1       4.600   1.216   0.162
ATOM     31  H   RES     1       4.093   2.014  -1.340
ATOM     32  H   RES     1       5.277   0.687  -1.395
TER
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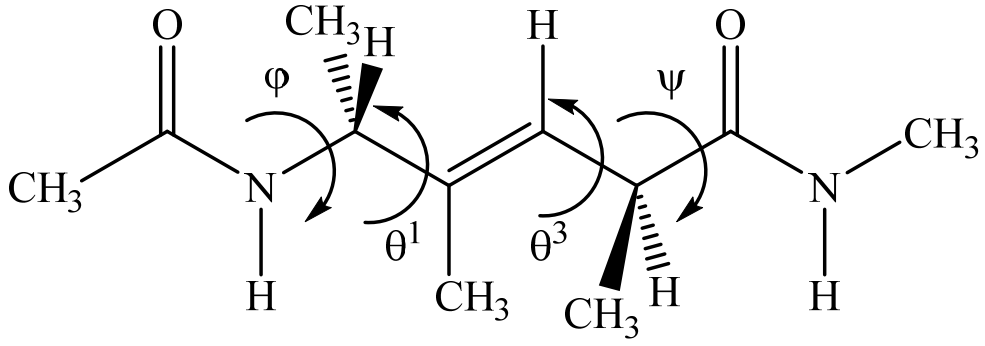
COMPOUND D



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REMARK  Compound D structure 01
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.850519
REMARK   Sum of electronic and thermal Energies=    -690.831929
REMARK   Sum of electronic and thermal Enthalpies=  -690.830985
REMARK   Sum of electronic and thermal Free Energies=  -690.898529
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      24.700   2.565   5.823
ATOM      2  C   RES     1      24.177   2.185   4.942
ATOM      3  H   RES     1      23.786   3.052   4.407
ATOM      4  H   RES     1      23.341   1.564   5.272
ATOM      5  C   RES     1      25.164   1.466   4.060
ATOM      6  O   RES     1      26.134   2.046   3.568
ATOM      7  N   RES     1      24.922   0.143   3.855
ATOM      8  H   RES     1      24.107  -0.270   4.281
ATOM      9  C   RES     1      25.775  -0.715   3.026
ATOM     10  H   RES     1      25.601  -1.767   3.282
ATOM     11  C   RES     1      27.243  -0.402   3.228
ATOM     12  C   RES     1      27.705  -0.260   4.643
ATOM     13  H   RES     1      27.889  -1.233   5.113
ATOM     14  H   RES     1      26.944   0.242   5.254
ATOM     15  H   RES     1      28.620   0.331   4.724
ATOM     16  C   RES     1      28.026  -0.225   2.153
ATOM     17  H   RES     1      27.550  -0.295   1.170
ATOM     18  C   RES     1      29.466   0.171   2.136
ATOM     19  H   RES     1      29.798   0.500   1.152
ATOM     20  C   RES     1      29.816   1.248   3.185
ATOM     21  O   RES     1      30.986   1.484   3.477
ATOM     22  N   RES     1      28.776   1.878   3.779
ATOM     23  H   RES     1      27.819   1.698   3.493
ATOM     24  C   RES     1      29.012   2.884   4.788
ATOM     25  H   RES     1      29.574   2.468   5.630
ATOM     26  H   RES     1      29.595   3.719   4.387
ATOM     27  H   RES     1      28.049   3.254   5.142
ATOM     29  C   RES     1      25.437  -0.488   1.623
ATOM     30  H   RES     1      24.414  -0.874   1.644
ATOM     31  H   RES     1      25.406   0.535   1.246
ATOM     32  H   RES     1      26.015  -1.089   0.908
ATOM     33  C   RES     1      30.295  -1.094   2.407
ATOM     34  H   RES     1      29.696  -1.968   2.688
ATOM     35  H   RES     1      30.764  -0.726   3.328
ATOM     36  H   RES     1      31.101  -1.435   1.753
TER
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REMARK  Compound D structure 02
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.845900
REMARK   Sum of electronic and thermal Energies=    -690.827615
REMARK   Sum of electronic and thermal Enthalpies=  -690.826671
REMARK   Sum of electronic and thermal Free Energies=  -690.892524
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      20.614  -1.737  -1.337
ATOM      2  C   RES     1      20.546  -1.626  -0.251
ATOM      3  H   RES     1      19.534  -1.303   0.002
ATOM      4  H   RES     1      21.254  -0.849   0.038
ATOM      5  C   RES     1      20.952  -2.930   0.385
ATOM      6  O   RES     1      22.106  -3.360   0.306
ATOM      7  N   RES     1      19.967  -3.623   1.012
ATOM      8  H   RES     1      19.046  -3.219   1.062
ATOM      9  C   RES     1      20.191  -4.941   1.632
ATOM     10  C   RES     1      21.581  -5.014   2.273
ATOM     11  C   RES     1      21.682  -4.787   3.747
ATOM     12  H   RES     1      21.545  -5.713   4.317
ATOM     13  H   RES     1      20.904  -4.090   4.079
ATOM     14  H   RES     1      22.648  -4.366   4.032
ATOM     15  C   RES     1      22.635  -5.230   1.469
ATOM     16  H   RES     1      22.434  -5.345   0.400
ATOM     17  C   RES     1      24.089  -5.237   1.824
ATOM     18  H   RES     1      24.721  -5.401   0.955
ATOM     19  C   RES     1      24.536  -3.956   2.561
ATOM     20  O   RES     1      25.176  -4.005   3.610
ATOM     21  N   RES     1      24.148  -2.785   2.000
ATOM     22  H   RES     1      23.607  -2.780   1.144
ATOM     23  C   RES     1      24.431  -1.521   2.637
ATOM     24  H   RES     1      25.473  -1.493   2.967
ATOM     25  H   RES     1      24.250  -0.718   1.920
ATOM     26  H   RES     1      23.802  -1.357   3.519
ATOM     28  H   RES     1      19.397  -5.096   2.374
ATOM     29  C   RES     1      20.099  -5.990   0.554
ATOM     30  H   RES     1      20.322  -6.962   1.003
ATOM     31  H   RES     1      19.180  -6.094  -0.028
ATOM     32  H   RES     1      20.912  -5.734  -0.128
ATOM     33  C   RES     1      24.359  -6.448   2.719
ATOM     34  H   RES     1      25.273  -6.943   2.371
ATOM     35  H   RES     1      23.534  -7.150   2.553
ATOM     36  H   RES     1      24.455  -6.298   3.795
TER
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REMARK  Compound D structure 03
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.846859
REMARK   Sum of electronic and thermal Energies=    -690.828829
REMARK   Sum of electronic and thermal Enthalpies=  -690.827885
REMARK   Sum of electronic and thermal Free Energies=  -690.892021
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -2.036  16.465  -8.597
ATOM      2  C   RES     1      -1.859  15.387  -8.565
ATOM      3  H   RES     1      -2.073  15.000  -9.564
ATOM      4  H   RES     1      -2.556  14.938  -7.853
ATOM      5  C   RES     1      -0.410  15.140  -8.241
ATOM      6  O   RES     1       0.499  15.521  -8.980
ATOM      7  N   RES     1      -0.162  14.483  -7.075
ATOM      8  H   RES     1      -0.935  14.181  -6.504
ATOM      9  C   RES     1       1.197  14.168  -6.644
ATOM     10  H   RES     1       1.289  14.393  -5.582
ATOM     11  C   RES     1       2.254  14.955  -7.400
ATOM     12  C   RES     1       3.490  14.166  -7.692
ATOM     13  H   RES     1       3.425  13.736  -8.699
ATOM     14  H   RES     1       3.598  13.321  -6.998
ATOM     15  H   RES     1       4.407  14.755  -7.641
ATOM     16  C   RES     1       2.033  16.211  -7.811
ATOM     17  H   RES     1       1.068  16.657  -7.565
ATOM     18  C   RES     1       2.968  17.036  -8.656
ATOM     19  C   RES     1       2.181  18.189  -9.259
ATOM     20  H   RES     1       1.736  18.783  -8.455
ATOM     21  H   RES     1       1.363  17.785  -9.860
ATOM     22  H   RES     1       2.860  18.840  -9.812
ATOM     23  C   RES     1       3.645  16.239  -9.787
ATOM     24  O   RES     1       4.840  16.368 -10.043
ATOM     25  N   RES     1       2.827  15.441 -10.522
ATOM     26  H   RES     1       1.901  15.216 -10.175
ATOM     27  C   RES     1       3.371  14.600 -11.561
ATOM     28  H   RES     1       3.958  15.195 -12.263
ATOM     29  H   RES     1       4.033  13.826 -11.153
ATOM     30  H   RES     1       2.548  14.119 -12.090
ATOM     32  C   RES     1       1.434  12.694  -6.860
ATOM     33  H   RES     1       0.570  12.060  -6.631
ATOM     34  H   RES     1       1.727  12.497  -7.895
ATOM     35  H   RES     1       2.272  12.396  -6.221
ATOM     36  H   RES     1       3.709  17.589  -8.082
TER
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REMARK  Compound D structure 04
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.845165
REMARK   Sum of electronic and thermal Energies=    -690.827151
REMARK   Sum of electronic and thermal Enthalpies=  -690.826207
REMARK   Sum of electronic and thermal Free Energies=  -690.891357
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       1.574   2.494   2.759
ATOM      2  C   RES     1       2.403   2.312   2.070
ATOM      3  H   RES     1       3.229   1.866   2.629
ATOM      4  H   RES     1       2.716   3.284   1.685
ATOM      5  C   RES     1       1.906   1.466   0.926
ATOM      6  O   RES     1       1.074   1.891   0.123
ATOM      7  N   RES     1       2.415   0.206   0.861
ATOM      8  H   RES     1       3.066  -0.080   1.574
ATOM      9  C   RES     1       2.059  -0.767  -0.173
ATOM     10  H   RES     1       2.509  -0.486  -1.128
ATOM     11  C   RES     1       0.562  -1.023  -0.274
ATOM     12  C   RES     1       0.107  -1.514  -1.614
ATOM     13  H   RES     1       0.892  -1.399  -2.371
ATOM     14  H   RES     1      -0.760  -0.948  -1.976
ATOM     15  H   RES     1      -0.180  -2.567  -1.593
ATOM     16  C   RES     1      -0.269  -0.812   0.758
ATOM     17  H   RES     1       0.161  -0.448   1.693
ATOM     18  C   RES     1      -1.760  -0.901   0.755
ATOM     19  C   RES     1      -2.153  -2.267   0.217
ATOM     20  H   RES     1      -1.430  -3.007   0.548
ATOM     21  H   RES     1      -2.237  -2.225  -0.873
ATOM     22  H   RES     1      -3.123  -2.550   0.631
ATOM     23  C   RES     1      -2.437   0.175  -0.120
ATOM     24  O   RES     1      -3.631   0.086  -0.403
ATOM     25  N   RES     1      -1.657   1.196  -0.545
ATOM     26  H   RES     1      -0.680   1.250  -0.276
ATOM     27  C   RES     1      -2.201   2.260  -1.355
ATOM     28  H   RES     1      -3.207   2.510  -1.007
ATOM     29  H   RES     1      -1.554   3.135  -1.273
ATOM     30  H   RES     1      -2.278   1.974  -2.410
ATOM     32  C   RES     1       2.780  -2.080   0.100
ATOM     33  H   RES     1       3.584  -1.972   0.834
ATOM     34  H   RES     1       1.999  -2.729   0.501
ATOM     35  H   RES     1       3.208  -2.551  -0.791
ATOM     36  H   RES     1      -2.170  -0.852   1.762
TER
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REMARK  Compound D structure 05
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.845956
REMARK   Sum of electronic and thermal Energies=    -690.828142
REMARK   Sum of electronic and thermal Enthalpies=  -690.827198
REMARK   Sum of electronic and thermal Free Energies=  -690.890930
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       3.035  -2.574   0.927
ATOM      2  C   RES     1       3.543  -1.739   0.437
ATOM      3  H   RES     1       4.272  -1.317   1.132
ATOM      4  H   RES     1       4.069  -2.150  -0.426
ATOM      5  C   RES     1       2.504  -0.755  -0.040
ATOM      6  O   RES     1       1.662  -1.067  -0.883
ATOM      7  N   RES     1       2.549   0.474   0.541
ATOM      8  H   RES     1       3.282   0.657   1.206
ATOM      9  C   RES     1       1.624   1.576   0.215
ATOM     10  H   RES     1       1.819   2.322   1.000
ATOM     11  C   RES     1       1.979   2.190  -1.129
ATOM     12  H   RES     1       3.031   2.485  -1.142
ATOM     13  H   RES     1       1.378   3.082  -1.327
ATOM     14  H   RES     1       1.814   1.473  -1.938
ATOM     15  C   RES     1       0.186   1.127   0.380
ATOM     16  C   RES     1      -0.094   0.396   1.659
ATOM     17  H   RES     1       0.310  -0.624   1.630
ATOM     18  H   RES     1       0.384   0.898   2.509
ATOM     19  H   RES     1      -1.160   0.312   1.876
ATOM     20  C   RES     1      -0.742   1.358  -0.560
ATOM     21  H   RES     1      -0.441   1.883  -1.464
ATOM     22  C   RES     1      -2.177   0.899  -0.509
ATOM     23  H   RES     1      -2.579   0.992  -1.528
ATOM     24  C   RES     1      -3.055   1.761   0.396
ATOM     25  H   RES     1      -2.696   1.750   1.429
ATOM     26  H   RES     1      -3.053   2.800   0.054
ATOM     27  H   RES     1      -4.080   1.386   0.399
ATOM     28  C   RES     1      -2.347  -0.594  -0.177
ATOM     29  O   RES     1      -3.345  -1.017   0.402
ATOM     30  N   RES     1      -1.360  -1.407  -0.639
ATOM     31  H   RES     1      -0.478  -0.997  -0.927
ATOM     32  C   RES     1      -1.363  -2.820  -0.348
ATOM     33  H   RES     1      -2.395  -3.173  -0.313
ATOM     34  H   RES     1      -0.897  -3.042   0.622
ATOM     35  H   RES     1      -0.815  -3.355  -1.126
TER
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REMARK  Compound D structure 06
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.842324
REMARK   Sum of electronic and thermal Energies=    -690.823884
REMARK   Sum of electronic and thermal Enthalpies=  -690.822940
REMARK   Sum of electronic and thermal Free Energies=  -690.890171
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.070  -0.088  -1.797
ATOM      2  C   RES     1       4.947   0.307  -0.786
ATOM      3  H   RES     1       5.849   0.044  -0.230
ATOM      4  H   RES     1       4.870   1.396  -0.839
ATOM      5  C   RES     1       3.761  -0.363  -0.138
ATOM      6  O   RES     1       3.705  -1.578   0.020
ATOM      7  N   RES     1       2.759   0.478   0.256
ATOM      8  H   RES     1       2.837   1.464   0.057
ATOM      9  C   RES     1       1.530   0.014   0.903
ATOM     10  H   RES     1       1.748  -1.033   1.154
ATOM     11  C   RES     1       1.301   0.795   2.184
ATOM     12  H   RES     1       2.163   0.685   2.846
ATOM     13  H   RES     1       0.414   0.437   2.713
ATOM     14  H   RES     1       1.161   1.865   1.989
ATOM     15  C   RES     1       0.380   0.015  -0.090
ATOM     16  C   RES     1       0.593  -0.904  -1.253
ATOM     17  H   RES     1       1.554  -0.708  -1.740
ATOM     18  H   RES     1       0.645  -1.948  -0.919
ATOM     19  H   RES     1      -0.186  -0.825  -2.014
ATOM     20  C   RES     1      -0.717   0.766   0.099
ATOM     21  H   RES     1      -0.781   1.384   0.995
ATOM     22  C   RES     1      -1.940   0.848  -0.771
ATOM     23  H   RES     1      -1.747   0.351  -1.730
ATOM     24  C   RES     1      -2.345   2.295  -1.023
ATOM     25  H   RES     1      -2.596   2.785  -0.079
ATOM     26  H   RES     1      -1.530   2.846  -1.502
ATOM     27  H   RES     1      -3.228   2.353  -1.664
ATOM     28  C   RES     1      -3.076   0.099  -0.062
ATOM     29  O   RES     1      -3.880   0.661   0.672
ATOM     30  N   RES     1      -3.095  -1.245  -0.299
ATOM     31  H   RES     1      -2.346  -1.642  -0.846
ATOM     32  C   RES     1      -4.002  -2.137   0.383
ATOM     33  H   RES     1      -4.761  -1.523   0.869
ATOM     34  H   RES     1      -3.493  -2.732   1.150
ATOM     35  H   RES     1      -4.489  -2.815  -0.324
TER
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REMARK  Compound D structure 07
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.841331
REMARK   Sum of electronic and thermal Energies=    -690.822699
REMARK   Sum of electronic and thermal Enthalpies=  -690.821755
REMARK   Sum of electronic and thermal Free Energies=  -690.889586
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.676   3.082  -0.034
ATOM      2  C   RES     1      -2.892   2.537  -0.560
ATOM      3  H   RES     1      -3.098   2.549  -1.634
ATOM      4  H   RES     1      -1.950   3.068  -0.388
ATOM      5  C   RES     1      -2.771   1.149   0.014
ATOM      6  O   RES     1      -2.881   0.914   1.213
ATOM      7  N   RES     1      -2.504   0.158  -0.891
ATOM      8  H   RES     1      -2.277   0.415  -1.841
ATOM      9  C   RES     1      -2.123  -1.166  -0.425
ATOM     10  H   RES     1      -2.904  -1.474   0.283
ATOM     11  C   RES     1      -2.105  -2.132  -1.602
ATOM     12  H   RES     1      -3.086  -2.195  -2.082
ATOM     13  H   RES     1      -1.823  -3.135  -1.273
ATOM     14  H   RES     1      -1.367  -1.816  -2.348
ATOM     15  C   RES     1      -0.805  -1.176   0.336
ATOM     16  C   RES     1      -0.738  -2.209   1.413
ATOM     17  H   RES     1      -1.416  -1.935   2.231
ATOM     18  H   RES     1      -1.069  -3.191   1.052
ATOM     19  H   RES     1       0.262  -2.331   1.836
ATOM     20  C   RES     1       0.162  -0.295   0.053
ATOM     21  H   RES     1      -0.013   0.457  -0.717
ATOM     22  C   RES     1       1.459  -0.116   0.780
ATOM     23  H   RES     1       1.779  -1.061   1.240
ATOM     24  C   RES     1       1.292   0.933   1.891
ATOM     25  H   RES     1       0.971   1.885   1.458
ATOM     26  H   RES     1       0.524   0.612   2.600
ATOM     27  H   RES     1       2.228   1.102   2.434
ATOM     28  C   RES     1       2.536   0.368  -0.186
ATOM     29  O   RES     1       2.346   1.305  -0.954
ATOM     30  N   RES     1       3.727  -0.292  -0.101
ATOM     31  H   RES     1       3.804  -1.061   0.546
ATOM     32  C   RES     1       4.874   0.061  -0.903
ATOM     33  H   RES     1       4.581   0.895  -1.541
ATOM     34  H   RES     1       5.192  -0.773  -1.536
ATOM     35  H   RES     1       5.719   0.373  -0.280
TER
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REMARK  Compound D structure 08
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.841206
REMARK   Sum of electronic and thermal Energies=    -690.822763
REMARK   Sum of electronic and thermal Enthalpies=  -690.821819
REMARK   Sum of electronic and thermal Free Energies=  -690.888678
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.161   1.910   1.153
ATOM      2  C   RES     1       4.413   0.928   0.746
ATOM      3  H   RES     1       5.307   1.057   0.132
ATOM      4  H   RES     1       4.647   0.255   1.575
ATOM      5  C   RES     1       3.278   0.453  -0.126
ATOM      6  O   RES     1       2.941   1.046  -1.145
ATOM      7  N   RES     1       2.655  -0.691   0.289
ATOM      8  H   RES     1       2.939  -1.121   1.157
ATOM      9  C   RES     1       1.486  -1.224  -0.413
ATOM     10  H   RES     1       1.672  -1.035  -1.476
ATOM     11  C   RES     1       1.393  -2.720  -0.161
ATOM     12  H   RES     1       2.289  -3.234  -0.521
ATOM     13  H   RES     1       0.526  -3.144  -0.675
ATOM     14  H   RES     1       1.280  -2.944   0.906
ATOM     15  C   RES     1       0.232  -0.470  -0.018
ATOM     16  C   RES     1      -0.298  -0.735   1.359
ATOM     17  H   RES     1      -0.777  -1.721   1.426
ATOM     18  H   RES     1       0.514  -0.733   2.096
ATOM     19  H   RES     1      -1.034   0.004   1.684
ATOM     20  C   RES     1      -0.309   0.404  -0.882
ATOM     21  H   RES     1       0.206   0.542  -1.833
ATOM     22  C   RES     1      -1.492   1.303  -0.621
ATOM     23  H   RES     1      -1.839   1.674  -1.596
ATOM     24  C   RES     1      -1.097   2.517   0.217
ATOM     25  H   RES     1      -0.758   2.211   1.211
ATOM     26  H   RES     1      -0.279   3.058  -0.265
ATOM     27  H   RES     1      -1.947   3.189   0.352
ATOM     28  C   RES     1      -2.717   0.604  -0.019
ATOM     29  O   RES     1      -3.429   1.132   0.829
ATOM     30  N   RES     1      -2.995  -0.622  -0.552
ATOM     31  H   RES     1      -2.290  -1.044  -1.139
ATOM     32  C   RES     1      -4.088  -1.435  -0.077
ATOM     33  H   RES     1      -4.787  -0.781   0.445
ATOM     34  H   RES     1      -3.753  -2.209   0.625
ATOM     35  H   RES     1      -4.602  -1.918  -0.912
TER
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REMARK  Compound D structure 09
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.841437
REMARK   Sum of electronic and thermal Energies=    -690.823143
REMARK   Sum of electronic and thermal Enthalpies=  -690.822199
REMARK   Sum of electronic and thermal Free Energies=  -690.888621
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       3.705  -2.641   0.532
ATOM      2  C   RES     1       3.967  -1.804  -0.119
ATOM      3  H   RES     1       5.043  -1.650  -0.022
ATOM      4  H   RES     1       3.740  -2.079  -1.153
ATOM      5  C   RES     1       3.248  -0.568   0.359
ATOM      6  O   RES     1       3.438  -0.095   1.475
ATOM      7  N   RES     1       2.371  -0.019  -0.533
ATOM      8  H   RES     1       2.244  -0.461  -1.432
ATOM      9  C   RES     1       1.585   1.184  -0.247
ATOM     10  H   RES     1       2.050   1.586   0.663
ATOM     11  C   RES     1       1.752   2.186  -1.374
ATOM     12  H   RES     1       2.811   2.410  -1.520
ATOM     13  H   RES     1       1.233   3.121  -1.151
ATOM     14  H   RES     1       1.354   1.805  -2.322
ATOM     15  C   RES     1       0.159   0.810   0.108
ATOM     16  C   RES     1       0.048  -0.124   1.276
ATOM     17  H   RES     1       0.362  -1.140   1.003
ATOM     18  H   RES     1       0.720   0.189   2.082
ATOM     19  H   RES     1      -0.965  -0.193   1.678
ATOM     20  C   RES     1      -0.899   1.292  -0.567
ATOM     21  H   RES     1      -0.716   1.984  -1.388
ATOM     22  C   RES     1      -2.353   1.035  -0.249
ATOM     23  H   RES     1      -2.935   1.340  -1.132
ATOM     24  C   RES     1      -2.838   1.878   0.929
ATOM     25  H   RES     1      -2.285   1.631   1.839
ATOM     26  H   RES     1      -2.689   2.941   0.724
ATOM     27  H   RES     1      -3.896   1.693   1.124
ATOM     28  C   RES     1      -2.732  -0.438  -0.045
ATOM     29  O   RES     1      -3.602  -0.787   0.746
ATOM     30  N   RES     1      -2.091  -1.321  -0.865
ATOM     31  H   RES     1      -1.279  -0.982  -1.361
ATOM     32  C   RES     1      -2.286  -2.745  -0.742
ATOM     33  H   RES     1      -1.545  -3.208  -0.077
ATOM     34  H   RES     1      -2.229  -3.225  -1.722
ATOM     35  H   RES     1      -3.274  -2.915  -0.315
TER
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REMARK  Compound D structure 10
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.839553
REMARK   Sum of electronic and thermal Energies=    -690.820953
REMARK   Sum of electronic and thermal Enthalpies=  -690.820008
REMARK   Sum of electronic and thermal Free Energies=  -690.888270
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.776  -1.093  -1.579
ATOM      2  C   RES     1      -4.792  -0.391  -0.742
ATOM      3  H   RES     1      -5.177   0.569  -1.096
ATOM      4  H   RES     1      -5.484  -0.797  -0.001
ATOM      5  C   RES     1      -3.411  -0.320  -0.137
ATOM      6  O   RES     1      -2.838  -1.311   0.301
ATOM      7  N   RES     1      -2.839   0.921  -0.128
ATOM      8  H   RES     1      -3.383   1.703  -0.453
ATOM      9  C   RES     1      -1.521   1.195   0.467
ATOM     10  H   RES     1      -1.342   2.255   0.223
ATOM     11  C   RES     1      -1.565   1.056   1.980
ATOM     12  H   RES     1      -2.379   1.660   2.388
ATOM     13  H   RES     1      -0.632   1.400   2.436
ATOM     14  H   RES     1      -1.730   0.014   2.264
ATOM     15  C   RES     1      -0.433   0.404  -0.237
ATOM     16  C   RES     1      -0.510   0.443  -1.734
ATOM     17  H   RES     1      -1.287  -0.237  -2.103
ATOM     18  H   RES     1      -0.782   1.444  -2.090
ATOM     19  H   RES     1       0.431   0.165  -2.213
ATOM     20  C   RES     1       0.522  -0.250   0.442
ATOM     21  H   RES     1       0.482  -0.240   1.531
ATOM     22  C   RES     1       1.639  -1.074  -0.127
ATOM     23  H   RES     1       1.429  -1.291  -1.184
ATOM     24  C   RES     1       1.757  -2.408   0.604
ATOM     25  H   RES     1       1.952  -2.250   1.670
ATOM     26  H   RES     1       0.830  -2.979   0.513
ATOM     27  H   RES     1       2.586  -2.991   0.198
ATOM     28  C   RES     1       3.009  -0.376  -0.154
ATOM     29  O   RES     1       4.053  -1.010  -0.264
ATOM     30  N   RES     1       2.971   0.985  -0.096
ATOM     31  H   RES     1       2.068   1.421   0.020
ATOM     32  C   RES     1       4.159   1.800  -0.154
ATOM     33  H   RES     1       5.016   1.128  -0.217
ATOM     34  H   RES     1       4.261   2.420   0.743
ATOM     35  H   RES     1       4.157   2.453  -1.033
TER
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REMARK  Compound D structure 11
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.839966
REMARK   Sum of electronic and thermal Energies=    -690.821378
REMARK   Sum of electronic and thermal Enthalpies=  -690.820434
REMARK   Sum of electronic and thermal Free Energies=  -690.887910
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.704  -2.398   0.547
ATOM      2  C   RES     1      -3.652  -2.403   0.253
ATOM      3  H   RES     1      -3.046  -2.685   1.118
ATOM      4  H   RES     1      -3.541  -3.167  -0.520
ATOM      5  C   RES     1      -3.299  -1.058  -0.332
ATOM      6  O   RES     1      -3.896  -0.585  -1.295
ATOM      7  N   RES     1      -2.280  -0.395   0.286
ATOM      8  H   RES     1      -1.731  -0.882   0.980
ATOM      9  C   RES     1      -1.755   0.869  -0.249
ATOM     10  H   RES     1      -1.707   0.751  -1.340
ATOM     11  C   RES     1      -2.703   2.020   0.066
ATOM     12  H   RES     1      -3.680   1.828  -0.380
ATOM     13  H   RES     1      -2.314   2.959  -0.341
ATOM     14  H   RES     1      -2.833   2.141   1.146
ATOM     15  C   RES     1      -0.360   1.080   0.290
ATOM     16  C   RES     1      -0.250   1.445   1.740
ATOM     17  H   RES     1      -0.526   2.494   1.904
ATOM     18  H   RES     1      -0.945   0.855   2.349
ATOM     19  H   RES     1       0.751   1.271   2.137
ATOM     20  C   RES     1       0.691   0.929  -0.530
ATOM     21  H   RES     1       0.495   0.648  -1.567
ATOM     22  C   RES     1       2.147   1.071  -0.169
ATOM     23  H   RES     1       2.241   1.747   0.688
ATOM     24  C   RES     1       2.944   1.649  -1.334
ATOM     25  H   RES     1       2.802   1.069  -2.254
ATOM     26  H   RES     1       2.607   2.664  -1.557
ATOM     27  H   RES     1       4.016   1.693  -1.117
ATOM     28  C   RES     1       2.643  -0.277   0.366
ATOM     29  O   RES     1       2.380  -0.635   1.510
ATOM     30  N   RES     1       3.344  -1.053  -0.508
ATOM     31  H   RES     1       3.533  -0.699  -1.432
ATOM     32  C   RES     1       3.828  -2.369  -0.161
ATOM     33  H   RES     1       3.548  -2.558   0.876
ATOM     34  H   RES     1       4.917  -2.428  -0.250
ATOM     35  H   RES     1       3.379  -3.139  -0.796
TER
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REMARK  Compound D structure 12
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.839101
REMARK   Sum of electronic and thermal Energies=    -690.820450
REMARK   Sum of electronic and thermal Enthalpies=  -690.819506
REMARK   Sum of electronic and thermal Free Energies=  -690.887452
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.706  -2.433   0.286
ATOM      2  C   RES     1      -3.684  -2.378  -0.093
ATOM      3  H   RES     1      -3.014  -2.843   0.634
ATOM      4  H   RES     1      -3.656  -2.954  -1.021
ATOM      5  C   RES     1      -3.351  -0.938  -0.400
ATOM      6  O   RES     1      -4.027  -0.260  -1.167
ATOM      7  N   RES     1      -2.257  -0.435   0.247
ATOM      8  H   RES     1      -1.628  -1.091   0.688
ATOM      9  C   RES     1      -1.719   0.895  -0.082
ATOM     10  H   RES     1      -1.691   0.971  -1.178
ATOM     11  C   RES     1      -2.641   1.988   0.448
ATOM     12  H   RES     1      -3.618   1.911  -0.030
ATOM     13  H   RES     1      -2.222   2.976   0.233
ATOM     14  H   RES     1      -2.780   1.898   1.530
ATOM     15  C   RES     1      -0.307   0.994   0.452
ATOM     16  C   RES     1      -0.177   1.139   1.938
ATOM     17  H   RES     1      -0.551   2.113   2.275
ATOM     18  H   RES     1      -0.779   0.389   2.467
ATOM     19  H   RES     1       0.853   1.047   2.288
ATOM     20  C   RES     1       0.722   0.947  -0.409
ATOM     21  H   RES     1       0.494   0.827  -1.470
ATOM     22  C   RES     1       2.191   1.021  -0.105
ATOM     23  H   RES     1       2.339   1.283   0.951
ATOM     24  C   RES     1       2.882   2.060  -0.983
ATOM     25  H   RES     1       2.788   1.779  -2.035
ATOM     26  H   RES     1       2.433   3.046  -0.840
ATOM     27  H   RES     1       3.949   2.127  -0.753
ATOM     28  C   RES     1       2.793  -0.363  -0.364
ATOM     29  O   RES     1       3.063  -0.756  -1.492
ATOM     30  N   RES     1       2.960  -1.132   0.753
ATOM     31  H   RES     1       2.730  -0.734   1.650
ATOM     32  C   RES     1       3.466  -2.483   0.698
ATOM     33  H   RES     1       3.655  -2.717  -0.351
ATOM     34  H   RES     1       2.741  -3.200   1.095
ATOM     35  H   RES     1       4.403  -2.583   1.256
TER
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REMARK  Compound D structure 13
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.840061
REMARK   Sum of electronic and thermal Energies=    -690.821760
REMARK   Sum of electronic and thermal Enthalpies=  -690.820816
REMARK   Sum of electronic and thermal Free Energies=  -690.886837
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.596  -0.547   1.004
ATOM      2  C   RES     1      -4.750  -1.098   0.588
ATOM      3  H   RES     1      -4.289  -1.690   1.382
ATOM      4  H   RES     1      -5.154  -1.775  -0.169
ATOM      5  C   RES     1      -3.808  -0.125  -0.076
ATOM      6  O   RES     1      -4.178   0.660  -0.944
ATOM      7  N   RES     1      -2.513  -0.166   0.357
ATOM      8  H   RES     1      -2.225  -0.932   0.947
ATOM      9  C   RES     1      -1.471   0.630  -0.306
ATOM     10  H   RES     1      -1.653   0.552  -1.386
ATOM     11  C   RES     1      -1.585   2.098   0.094
ATOM     12  H   RES     1      -2.558   2.489  -0.206
ATOM     13  H   RES     1      -0.806   2.690  -0.399
ATOM     14  H   RES     1      -1.477   2.221   1.176
ATOM     15  C   RES     1      -0.115   0.043   0.010
ATOM     16  C   RES     1       0.381   0.224   1.414
ATOM     17  H   RES     1       0.711   1.257   1.586
ATOM     18  H   RES     1      -0.413   0.039   2.147
ATOM     19  H   RES     1       1.222  -0.428   1.658
ATOM     20  C   RES     1       0.588  -0.571  -0.957
ATOM     21  H   RES     1       0.122  -0.649  -1.940
ATOM     22  C   RES     1       1.947  -1.210  -0.803
ATOM     23  H   RES     1       2.349  -1.361  -1.815
ATOM     24  C   RES     1       1.867  -2.580  -0.134
ATOM     25  H   RES     1       1.470  -2.497   0.882
ATOM     26  H   RES     1       1.209  -3.244  -0.701
ATOM     27  H   RES     1       2.858  -3.032  -0.061
ATOM     28  C   RES     1       2.991  -0.329  -0.103
ATOM     29  O   RES     1       3.813  -0.785   0.684
ATOM     30  N   RES     1       2.974   0.984  -0.474
ATOM     31  H   RES     1       2.194   1.304  -1.029
ATOM     32  C   RES     1       3.860   1.961   0.110
ATOM     33  H   RES     1       4.659   1.422   0.620
ATOM     34  H   RES     1       3.346   2.593   0.845
ATOM     35  H   RES     1       4.295   2.603  -0.661
TER
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REMARK  Compound D structure 14
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.838395
REMARK   Sum of electronic and thermal Energies=    -690.819782
REMARK   Sum of electronic and thermal Enthalpies=  -690.818838
REMARK   Sum of electronic and thermal Free Energies=  -690.886699
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.298   0.812  -1.186
ATOM      2  C   RES     1      -4.810   0.887  -0.212
ATOM      3  H   RES     1      -4.780   1.948   0.048
ATOM      4  H   RES     1      -5.417   0.363   0.530
ATOM      5  C   RES     1      -3.395   0.373  -0.331
ATOM      6  O   RES     1      -2.603   0.834  -1.146
ATOM      7  N   RES     1      -3.059  -0.617   0.548
ATOM      8  H   RES     1      -3.778  -0.982   1.151
ATOM      9  C   RES     1      -1.747  -1.286   0.563
ATOM     10  H   RES     1      -1.777  -1.900   1.477
ATOM     11  C   RES     1      -1.600  -2.210  -0.635
ATOM     12  H   RES     1      -2.446  -2.901  -0.682
ATOM     13  H   RES     1      -0.684  -2.802  -0.570
ATOM     14  H   RES     1      -1.574  -1.630  -1.561
ATOM     15  C   RES     1      -0.629  -0.278   0.752
ATOM     16  C   RES     1      -0.889   0.747   1.813
ATOM     17  H   RES     1      -1.552   1.536   1.440
ATOM     18  H   RES     1      -1.388   0.305   2.684
ATOM     19  H   RES     1       0.026   1.232   2.162
ATOM     20  C   RES     1       0.486  -0.321   0.012
ATOM     21  H   RES     1       0.588  -1.063  -0.777
ATOM     22  C   RES     1       1.617   0.662   0.056
ATOM     23  H   RES     1       1.688   1.122   1.052
ATOM     24  C   RES     1       1.373   1.774  -0.976
ATOM     25  H   RES     1       1.322   1.344  -1.980
ATOM     26  H   RES     1       0.420   2.272  -0.777
ATOM     27  H   RES     1       2.175   2.520  -0.961
ATOM     28  C   RES     1       2.933  -0.033  -0.274
ATOM     29  O   RES     1       3.056  -0.769  -1.247
ATOM     30  N   RES     1       3.966   0.257   0.571
ATOM     31  H   RES     1       3.787   0.858   1.359
ATOM     32  C   RES     1       5.295  -0.275   0.387
ATOM     33  H   RES     1       5.277  -0.887  -0.516
ATOM     34  H   RES     1       5.598  -0.902   1.232
ATOM     35  H   RES     1       6.032   0.524   0.258
TER
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REMARK  Compound D structure 15
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.838489
REMARK   Sum of electronic and thermal Energies=    -690.819989
REMARK   Sum of electronic and thermal Enthalpies=  -690.819045
REMARK   Sum of electronic and thermal Free Energies=  -690.886307
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.463   0.175  -0.942
ATOM      2  C   RES     1      -4.564   0.795  -0.929
ATOM      3  H   RES     1      -4.390   1.121  -1.957
ATOM      4  H   RES     1      -4.751   1.674  -0.308
ATOM      5  C   RES     1      -3.395  -0.049  -0.480
ATOM      6  O   RES     1      -3.115  -1.107  -1.032
ATOM      7  N   RES     1      -2.694   0.461   0.578
ATOM      8  H   RES     1      -2.945   1.387   0.889
ATOM      9  C   RES     1      -1.489  -0.113   1.192
ATOM     10  H   RES     1      -1.447   0.339   2.191
ATOM     11  C   RES     1      -1.589  -1.625   1.385
ATOM     12  H   RES     1      -2.545  -1.896   1.842
ATOM     13  H   RES     1      -0.785  -1.948   2.053
ATOM     14  H   RES     1      -1.512  -2.165   0.441
ATOM     15  C   RES     1      -0.217   0.283   0.466
ATOM     16  C   RES     1      -0.174   0.021  -1.006
ATOM     17  H   RES     1      -0.397  -1.028  -1.233
ATOM     18  H   RES     1      -0.950   0.599  -1.520
ATOM     19  H   RES     1       0.784   0.279  -1.460
ATOM     20  C   RES     1       0.804   0.791   1.179
ATOM     21  H   RES     1       0.634   0.955   2.245
ATOM     22  C   RES     1       2.158   1.196   0.653
ATOM     23  H   RES     1       2.813   1.342   1.524
ATOM     24  C   RES     1       2.111   2.519  -0.109
ATOM     25  H   RES     1       1.464   2.441  -0.987
ATOM     26  H   RES     1       1.716   3.313   0.530
ATOM     27  H   RES     1       3.108   2.798  -0.455
ATOM     28  C   RES     1       2.884   0.127  -0.180
ATOM     29  O   RES     1       3.657   0.425  -1.085
ATOM     30  N   RES     1       2.669  -1.163   0.210
ATOM     31  H   RES     1       1.904  -1.334   0.846
ATOM     32  C   RES     1       3.219  -2.278  -0.524
ATOM     33  H   RES     1       4.084  -1.919  -1.083
ATOM     34  H   RES     1       2.498  -2.695  -1.238
ATOM     35  H   RES     1       3.535  -3.069   0.161
TER
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REMARK  Compound D structure 16
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.838605
REMARK   Sum of electronic and thermal Energies=    -690.820194
REMARK   Sum of electronic and thermal Enthalpies=  -690.819250
REMARK   Sum of electronic and thermal Free Energies=  -690.885956
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.618  -2.859   0.106
ATOM      2  C   RES     1      -3.780  -2.067  -0.628
ATOM      3  H   RES     1      -3.360  -2.381  -1.588
ATOM      4  H   RES     1      -4.861  -1.955  -0.740
ATOM      5  C   RES     1      -3.210  -0.775  -0.091
ATOM      6  O   RES     1      -3.560  -0.322   0.995
ATOM      7  N   RES     1      -2.304  -0.165  -0.911
ATOM      8  H   RES     1      -2.009  -0.677  -1.728
ATOM      9  C   RES     1      -1.576   1.088  -0.647
ATOM     10  H   RES     1      -1.223   1.408  -1.635
ATOM     11  C   RES     1      -2.483   2.189  -0.111
ATOM     12  H   RES     1      -3.354   2.315  -0.760
ATOM     13  H   RES     1      -1.928   3.131  -0.093
ATOM     14  H   RES     1      -2.850   1.971   0.892
ATOM     15  C   RES     1      -0.342   0.856   0.205
ATOM     16  C   RES     1      -0.567   0.324   1.585
ATOM     17  H   RES     1      -1.382   0.846   2.094
ATOM     18  H   RES     1      -0.876  -0.728   1.554
ATOM     19  H   RES     1       0.327   0.395   2.211
ATOM     20  C   RES     1       0.863   1.128  -0.322
ATOM     21  H   RES     1       0.903   1.481  -1.355
ATOM     22  C   RES     1       2.211   0.972   0.325
ATOM     23  H   RES     1       2.089   0.900   1.413
ATOM     24  C   RES     1       3.129   2.140  -0.008
ATOM     25  H   RES     1       3.306   2.182  -1.085
ATOM     26  H   RES     1       2.683   3.085   0.313
ATOM     27  H   RES     1       4.102   2.034   0.479
ATOM     28  C   RES     1       2.823  -0.341  -0.179
ATOM     29  O   RES     1       3.488  -0.406  -1.206
ATOM     30  N   RES     1       2.534  -1.430   0.592
ATOM     31  H   RES     1       1.938  -1.304   1.395
ATOM     32  C   RES     1       2.926  -2.769   0.222
ATOM     33  H   RES     1       3.603  -2.688  -0.629
ATOM     34  H   RES     1       2.064  -3.378  -0.074
ATOM     35  H   RES     1       3.445  -3.269   1.044
TER
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REMARK  Compound D structure 17
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.839466
REMARK   Sum of electronic and thermal Energies=    -690.821629
REMARK   Sum of electronic and thermal Enthalpies=  -690.820685
REMARK   Sum of electronic and thermal Free Energies=  -690.885733
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.997  -1.045  -1.686
ATOM      2  C   RES     1       4.116  -1.529  -1.256
ATOM      3  H   RES     1       3.415  -1.755  -2.064
ATOM      4  H   RES     1       4.456  -2.465  -0.807
ATOM      5  C   RES     1       3.546  -0.642  -0.178
ATOM      6  O   RES     1       4.188  -0.324   0.817
ATOM      7  N   RES     1       2.271  -0.202  -0.389
ATOM      8  H   RES     1       1.738  -0.589  -1.153
ATOM      9  C   RES     1       1.575   0.598   0.613
ATOM     10  H   RES     1       1.801   0.145   1.589
ATOM     11  C   RES     1       2.115   2.030   0.635
ATOM     12  H   RES     1       3.184   2.021   0.857
ATOM     13  H   RES     1       1.609   2.623   1.403
ATOM     14  H   RES     1       1.950   2.511  -0.333
ATOM     15  C   RES     1       0.075   0.592   0.413
ATOM     16  C   RES     1      -0.702   0.710   1.687
ATOM     17  H   RES     1      -0.619  -0.209   2.281
ATOM     18  H   RES     1      -0.292   1.513   2.311
ATOM     19  H   RES     1      -1.764   0.916   1.536
ATOM     20  C   RES     1      -0.488   0.544  -0.807
ATOM     21  H   RES     1       0.168   0.526  -1.679
ATOM     22  C   RES     1      -1.963   0.624  -1.118
ATOM     23  H   RES     1      -2.094   0.278  -2.154
ATOM     24  C   RES     1      -2.483   2.059  -1.050
ATOM     25  H   RES     1      -2.374   2.466  -0.041
ATOM     26  H   RES     1      -1.923   2.702  -1.734
ATOM     27  H   RES     1      -3.543   2.096  -1.308
ATOM     28  C   RES     1      -2.863  -0.310  -0.297
ATOM     29  O   RES     1      -3.999   0.009   0.036
ATOM     30  N   RES     1      -2.338  -1.542  -0.035
ATOM     31  H   RES     1      -1.353  -1.674  -0.208
ATOM     32  C   RES     1      -3.042  -2.516   0.764
ATOM     33  H   RES     1      -4.100  -2.252   0.756
ATOM     34  H   RES     1      -2.697  -2.522   1.805
ATOM     35  H   RES     1      -2.917  -3.518   0.347
TER
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REMARK  Compound D structure 18
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -690.836565
REMARK   Sum of electronic and thermal Energies=    -690.818162
REMARK   Sum of electronic and thermal Enthalpies=  -690.817217
REMARK   Sum of electronic and thermal Free Energies=  -690.883614
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.989   1.217   1.175
ATOM      2  C   RES     1      -3.945   1.206   1.496
ATOM      3  H   RES     1      -3.632   2.248   1.592
ATOM      4  H   RES     1      -3.884   0.727   2.476
ATOM      5  C   RES     1      -3.111   0.541   0.425
ATOM      6  O   RES     1      -3.075   0.963  -0.724
ATOM      7  N   RES     1      -2.407  -0.556   0.840
ATOM      8  H   RES     1      -2.445  -0.797   1.817
ATOM      9  C   RES     1      -1.525  -1.349  -0.012
ATOM     10  H   RES     1      -1.286  -2.241   0.589
ATOM     11  C   RES     1      -2.251  -1.846  -1.265
ATOM     12  H   RES     1      -3.220  -2.269  -0.991
ATOM     13  H   RES     1      -1.668  -2.628  -1.758
ATOM     14  H   RES     1      -2.419  -1.029  -1.968
ATOM     15  C   RES     1      -0.199  -0.678  -0.336
ATOM     16  C   RES     1       0.695  -1.499  -1.217
ATOM     17  H   RES     1       0.739  -2.542  -0.876
ATOM     18  H   RES     1       0.314  -1.526  -2.244
ATOM     19  H   RES     1       1.718  -1.121  -1.265
ATOM     20  C   RES     1       0.132   0.535   0.134
ATOM     21  H   RES     1      -0.604   1.061   0.739
ATOM     22  C   RES     1       1.396   1.298  -0.181
ATOM     23  H   RES     1       1.423   2.168   0.491
ATOM     24  C   RES     1       1.404   1.829  -1.613
ATOM     25  H   RES     1       1.390   1.007  -2.334
ATOM     26  H   RES     1       0.521   2.446  -1.793
ATOM     27  H   RES     1       2.304   2.417  -1.800
ATOM     28  C   RES     1       2.704   0.554   0.123
ATOM     29  O   RES     1       3.719   0.708  -0.548
ATOM     30  N   RES     1       2.676  -0.234   1.238
ATOM     31  H   RES     1       1.770  -0.439   1.633
ATOM     32  C   RES     1       3.803  -1.052   1.615
ATOM     33  H   RES     1       4.706  -0.588   1.217
ATOM     34  H   RES     1       3.734  -2.068   1.205
ATOM     35  H   RES     1       3.881  -1.116   2.703
TER
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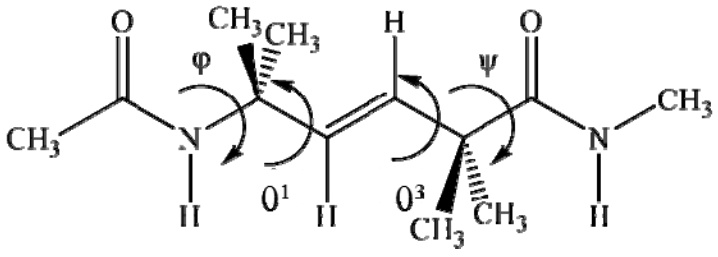
COMPOUND E



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REMARK  Compound E structure 01
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.130470
REMARK   Sum of electronic and thermal Energies=    -730.111038
REMARK   Sum of electronic and thermal Enthalpies=  -730.110094
REMARK   Sum of electronic and thermal Free Energies=  -730.177310
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -2.874   2.847   1.595
ATOM      2  C   RES     1      -3.383   2.255   0.832
ATOM      3  H   RES     1      -3.720   2.951   0.061
ATOM      4  H   RES     1      -4.257   1.776   1.281
ATOM      5  C   RES     1      -2.396   1.291   0.222
ATOM      6  O   RES     1      -1.364   1.691  -0.318
ATOM      7  N   RES     1      -2.730  -0.025   0.317
ATOM      8  H   RES     1      -3.610  -0.255   0.753
ATOM      9  C   RES     1      -1.943  -1.150  -0.245
ATOM     10  C   RES     1      -1.957  -1.070  -1.769
ATOM     11  H   RES     1      -1.493  -0.144  -2.117
ATOM     12  H   RES     1      -2.987  -1.101  -2.134
ATOM     13  H   RES     1      -1.417  -1.916  -2.204
ATOM     14  C   RES     1      -2.645  -2.427   0.218
ATOM     15  H   RES     1      -3.681  -2.461  -0.140
ATOM     16  H   RES     1      -2.650  -2.504   1.311
ATOM     17  H   RES     1      -2.125  -3.303  -0.176
ATOM     18  C   RES     1      -0.556  -1.103   0.349
ATOM     19  H   RES     1      -0.544  -1.072   1.440
ATOM     20  C   RES     1       0.592  -1.076  -0.331
ATOM     21  H   RES     1       0.556  -1.085  -1.423
ATOM     22  C   RES     1       1.973  -0.930   0.241
ATOM     23  C   RES     1       2.009  -1.079   1.764
ATOM     24  H   RES     1       1.637  -2.065   2.065
ATOM     25  H   RES     1       1.402  -0.317   2.265
ATOM     26  H   RES     1       3.037  -0.973   2.120
ATOM     27  C   RES     1       2.906  -1.961  -0.397
ATOM     28  H   RES     1       2.881  -1.899  -1.489
ATOM     29  H   RES     1       2.610  -2.974  -0.105
ATOM     30  H   RES     1       3.935  -1.780  -0.077
ATOM     31  C   RES     1       2.535   0.484  -0.070
ATOM     32  O   RES     1       3.745   0.704  -0.051
ATOM     33  N   RES     1       1.619   1.453  -0.303
ATOM     34  H   RES     1       0.626   1.248  -0.289
ATOM     35  C   RES     1       2.030   2.821  -0.511
ATOM     36  H   RES     1       2.703   2.901  -1.370
ATOM     37  H   RES     1       1.141   3.426  -0.691
ATOM     38  H   RES     1       2.565   3.212   0.360
TER
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REMARK  Compound E structure 02
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.129525
REMARK   Sum of electronic and thermal Energies=    -730.110094
REMARK   Sum of electronic and thermal Enthalpies=  -730.109150
REMARK   Sum of electronic and thermal Free Energies=  -730.176300
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       1.580   2.842   1.952
ATOM      2  C   RES     1       2.448   2.462   1.407
ATOM      3  H   RES     1       3.168   2.064   2.127
ATOM      4  H   RES     1       2.896   3.313   0.891
ATOM      5  C   RES     1       1.978   1.460   0.383
ATOM      6  O   RES     1       1.214   1.783  -0.527
ATOM      7  N   RES     1       2.440   0.191   0.551
ATOM      8  H   RES     1       3.059   0.017   1.328
ATOM      9  C   RES     1       2.145  -0.948  -0.337
ATOM     10  C   RES     1       2.897  -2.152   0.233
ATOM     11  H   RES     1       2.572  -2.370   1.255
ATOM     12  H   RES     1       3.980  -1.978   0.229
ATOM     13  H   RES     1       2.700  -3.039  -0.374
ATOM     14  C   RES     1       2.654  -0.645  -1.750
ATOM     15  H   RES     1       3.732  -0.454  -1.734
ATOM     16  H   RES     1       2.148   0.228  -2.166
ATOM     17  H   RES     1       2.469  -1.501  -2.406
ATOM     18  C   RES     1       0.666  -1.257  -0.386
ATOM     19  H   RES     1       0.385  -1.916  -1.209
ATOM     20  C   RES     1      -0.270  -0.803   0.448
ATOM     21  H   RES     1       0.038  -0.136   1.258
ATOM     22  C   RES     1      -1.750  -1.037   0.360
ATOM     23  C   RES     1      -2.129  -2.078  -0.696
ATOM     24  H   RES     1      -1.666  -3.045  -0.468
ATOM     25  H   RES     1      -1.814  -1.776  -1.700
ATOM     26  H   RES     1      -3.214  -2.207  -0.711
ATOM     27  C   RES     1      -2.276  -1.485   1.728
ATOM     28  H   RES     1      -2.004  -0.771   2.513
ATOM     29  H   RES     1      -1.858  -2.461   1.995
ATOM     30  H   RES     1      -3.366  -1.555   1.702
ATOM     31  C   RES     1      -2.502   0.266  -0.023
ATOM     32  O   RES     1      -3.723   0.343   0.104
ATOM     33  N   RES     1      -1.758   1.276  -0.530
ATOM     34  H   RES     1      -0.751   1.194  -0.621
ATOM     35  C   RES     1      -2.382   2.511  -0.946
ATOM     36  H   RES     1      -3.025   2.902  -0.152
ATOM     37  H   RES     1      -1.602   3.237  -1.174
ATOM     38  H   RES     1      -3.009   2.364  -1.832
TER
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REMARK  Compound E structure 03
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.122837
REMARK   Sum of electronic and thermal Energies=    -730.103095
REMARK   Sum of electronic and thermal Enthalpies=  -730.102150
REMARK   Sum of electronic and thermal Free Energies=  -730.171091
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.658  -0.984  -1.168
ATOM      2  C   RES     1      -4.953  -1.301  -0.397
ATOM      3  H   RES     1      -4.444  -2.207  -0.737
ATOM      4  H   RES     1      -5.540  -1.539   0.493
ATOM      5  C   RES     1      -4.026  -0.151  -0.080
ATOM      6  O   RES     1      -4.453   0.941   0.279
ATOM      7  N   RES     1      -2.696  -0.423  -0.234
ATOM      8  H   RES     1      -2.433  -1.377  -0.432
ATOM      9  C   RES     1      -1.594   0.512   0.093
ATOM     10  C   RES     1      -1.637   0.869   1.575
ATOM     11  H   RES     1      -1.514  -0.020   2.201
ATOM     12  H   RES     1      -2.598   1.331   1.809
ATOM     13  H   RES     1      -0.843   1.579   1.826
ATOM     14  C   RES     1      -1.726   1.780  -0.762
ATOM     15  H   RES     1      -2.657   2.302  -0.539
ATOM     16  H   RES     1      -1.710   1.532  -1.828
ATOM     17  H   RES     1      -0.887   2.453  -0.554
ATOM     18  C   RES     1      -0.324  -0.193  -0.318
ATOM     19  H   RES     1      -0.305  -0.497  -1.368
ATOM     20  C   RES     1       0.746  -0.417   0.451
ATOM     21  H   RES     1       0.715  -0.104   1.497
ATOM     22  C   RES     1       2.043  -1.061   0.036
ATOM     23  C   RES     1       2.372  -2.186   1.021
ATOM     24  H   RES     1       1.619  -2.977   0.955
ATOM     25  H   RES     1       2.393  -1.820   2.052
ATOM     26  H   RES     1       3.355  -2.605   0.798
ATOM     27  C   RES     1       2.003  -1.624  -1.388
ATOM     28  H   RES     1       1.808  -0.847  -2.135
ATOM     29  H   RES     1       1.223  -2.388  -1.478
ATOM     30  H   RES     1       2.964  -2.086  -1.629
ATOM     31  C   RES     1       3.212  -0.043   0.064
ATOM     32  O   RES     1       4.372  -0.407   0.224
ATOM     33  N   RES     1       2.866   1.254  -0.161
ATOM     34  H   RES     1       1.889   1.467  -0.305
ATOM     35  C   RES     1       3.843   2.311  -0.268
ATOM     36  H   RES     1       3.873   2.731  -1.279
ATOM     37  H   RES     1       3.633   3.116   0.441
ATOM     38  H   RES     1       4.819   1.881  -0.039
TER
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REMARK  Compound E structure 04
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.122548
REMARK   Sum of electronic and thermal Energies=    -730.102951
REMARK   Sum of electronic and thermal Enthalpies=  -730.102006
REMARK   Sum of electronic and thermal Free Energies=  -730.170583
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.515  -0.900  -0.936
ATOM      2  C   RES     1      -4.707  -1.265  -0.299
ATOM      3  H   RES     1      -4.516  -2.301  -0.588
ATOM      4  H   RES     1      -5.042  -1.246   0.742
ATOM      5  C   RES     1      -3.466  -0.446  -0.565
ATOM      6  O   RES     1      -3.004  -0.323  -1.696
ATOM      7  N   RES     1      -2.915   0.145   0.535
ATOM      8  H   RES     1      -3.297  -0.097   1.437
ATOM      9  C   RES     1      -1.658   0.930   0.542
ATOM     10  C   RES     1      -1.471   1.421   1.972
ATOM     11  H   RES     1      -1.359   0.590   2.677
ATOM     12  H   RES     1      -2.329   2.027   2.277
ATOM     13  H   RES     1      -0.579   2.048   2.051
ATOM     14  C   RES     1      -1.798   2.134  -0.397
ATOM     15  H   RES     1      -2.658   2.746  -0.107
ATOM     16  H   RES     1      -1.936   1.810  -1.430
ATOM     17  H   RES     1      -0.899   2.755  -0.336
ATOM     18  C   RES     1      -0.526   0.050   0.061
ATOM     19  H   RES     1      -0.707  -0.389  -0.920
ATOM     20  C   RES     1       0.618  -0.192   0.711
ATOM     21  H   RES     1       0.783   0.257   1.694
ATOM     22  C   RES     1       1.761  -1.048   0.231
ATOM     23  C   RES     1       2.108  -2.065   1.322
ATOM     24  H   RES     1       1.269  -2.749   1.479
ATOM     25  H   RES     1       2.329  -1.569   2.273
ATOM     26  H   RES     1       2.992  -2.638   1.036
ATOM     27  C   RES     1       1.444  -1.787  -1.074
ATOM     28  H   RES     1       1.227  -1.098  -1.897
ATOM     29  H   RES     1       0.574  -2.439  -0.943
ATOM     30  H   RES     1       2.297  -2.405  -1.367
ATOM     31  C   RES     1       3.022  -0.194  -0.048
ATOM     32  O   RES     1       4.154  -0.650   0.076
ATOM     33  N   RES     1       2.778   1.070  -0.494
ATOM     34  H   RES     1       1.815   1.354  -0.602
ATOM     35  C   RES     1       3.832   1.958  -0.922
ATOM     36  H   RES     1       4.781   1.510  -0.627
ATOM     37  H   RES     1       3.834   2.094  -2.010
ATOM     38  H   RES     1       3.736   2.938  -0.447
TER
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REMARK  Compound E structure 05
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.121925
REMARK   Sum of electronic and thermal Energies=    -730.102115
REMARK   Sum of electronic and thermal Enthalpies=  -730.101171
REMARK   Sum of electronic and thermal Free Energies=  -730.170374
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       2.468  -2.260  -2.385
ATOM      2  C   RES     1       3.187  -1.516  -2.033
ATOM      3  H   RES     1       3.321  -0.762  -2.814
ATOM      4  H   RES     1       4.133  -2.037  -1.879
ATOM      5  C   RES     1       2.708  -0.963  -0.712
ATOM      6  O   RES     1       2.594  -1.669   0.283
ATOM      7  N   RES     1       2.402   0.371  -0.721
ATOM      8  H   RES     1       2.503   0.872  -1.590
ATOM      9  C   RES     1       1.890   1.125   0.432
ATOM     10  C   RES     1       1.750   2.580  -0.026
ATOM     11  H   RES     1       1.072   2.661  -0.884
ATOM     12  H   RES     1       2.723   2.999  -0.304
ATOM     13  H   RES     1       1.340   3.193   0.781
ATOM     14  C   RES     1       2.883   1.054   1.596
ATOM     15  H   RES     1       3.857   1.446   1.287
ATOM     16  H   RES     1       3.008   0.026   1.938
ATOM     17  H   RES     1       2.521   1.661   2.432
ATOM     18  C   RES     1       0.536   0.622   0.884
ATOM     19  H   RES     1       0.233   1.001   1.862
ATOM     20  C   RES     1      -0.270  -0.201   0.212
ATOM     21  H   RES     1       0.069  -0.583  -0.754
ATOM     22  C   RES     1      -1.602  -0.739   0.660
ATOM     23  C   RES     1      -1.552  -2.268   0.577
ATOM     24  H   RES     1      -0.793  -2.657   1.262
ATOM     25  H   RES     1      -1.295  -2.602  -0.434
ATOM     26  H   RES     1      -2.527  -2.692   0.829
ATOM     27  C   RES     1      -1.963  -0.318   2.089
ATOM     28  H   RES     1      -2.036   0.770   2.192
ATOM     29  H   RES     1      -1.207  -0.678   2.794
ATOM     30  H   RES     1      -2.928  -0.748   2.369
ATOM     31  C   RES     1      -2.757  -0.243  -0.241
ATOM     32  O   RES     1      -3.799  -0.877  -0.365
ATOM     33  N   RES     1      -2.554   0.969  -0.831
ATOM     34  H   RES     1      -1.676   1.435  -0.656
ATOM     35  C   RES     1      -3.568   1.630  -1.616
ATOM     36  H   RES     1      -3.932   2.540  -1.126
ATOM     37  H   RES     1      -3.191   1.893  -2.609
ATOM     38  H   RES     1      -4.402   0.936  -1.726
TER
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REMARK  Compound E structure 06
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.122230
REMARK   Sum of electronic and thermal Energies=    -730.102595
REMARK   Sum of electronic and thermal Enthalpies=  -730.101651
REMARK   Sum of electronic and thermal Free Energies=  -730.170317
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.274   3.044   0.912
ATOM      2  C   RES     1      -3.753   2.247   0.340
ATOM      3  H   RES     1      -3.821   2.554  -0.707
ATOM      4  H   RES     1      -4.764   2.135   0.738
ATOM      5  C   RES     1      -2.995   0.959   0.562
ATOM      6  O   RES     1      -2.798   0.513   1.689
ATOM      7  N   RES     1      -2.560   0.340  -0.573
ATOM      8  H   RES     1      -2.743   0.791  -1.457
ATOM      9  C   RES     1      -1.812  -0.942  -0.623
ATOM     10  C   RES     1      -1.594  -1.246  -2.099
ATOM     11  H   RES     1      -1.001  -0.468  -2.593
ATOM     12  H   RES     1      -2.557  -1.329  -2.614
ATOM     13  H   RES     1      -1.071  -2.197  -2.223
ATOM     14  C   RES     1      -2.652  -2.053   0.014
ATOM     15  H   RES     1      -3.612  -2.150  -0.503
ATOM     16  H   RES     1      -2.843  -1.841   1.067
ATOM     17  H   RES     1      -2.121  -3.007  -0.061
ATOM     18  C   RES     1      -0.520  -0.787   0.149
ATOM     19  H   RES     1      -0.670  -0.554   1.202
ATOM     20  C   RES     1       0.715  -0.929  -0.342
ATOM     21  H   RES     1       0.851  -1.169  -1.400
ATOM     22  C   RES     1       2.007  -0.798   0.423
ATOM     23  C   RES     1       1.791  -0.602   1.927
ATOM     24  H   RES     1       1.254  -1.457   2.351
ATOM     25  H   RES     1       1.213   0.302   2.148
ATOM     26  H   RES     1       2.756  -0.518   2.432
ATOM     27  C   RES     1       2.851  -2.053   0.186
ATOM     28  H   RES     1       3.021  -2.224  -0.881
ATOM     29  H   RES     1       2.342  -2.930   0.597
ATOM     30  H   RES     1       3.828  -1.949   0.662
ATOM     31  C   RES     1       2.820   0.427  -0.063
ATOM     32  O   RES     1       4.044   0.454  -0.015
ATOM     33  N   RES     1       2.073   1.485  -0.490
ATOM     34  H   RES     1       1.067   1.394  -0.459
ATOM     35  C   RES     1       2.661   2.750  -0.856
ATOM     36  H   RES     1       3.740   2.605  -0.923
ATOM     37  H   RES     1       2.285   3.092  -1.825
ATOM     38  H   RES     1       2.460   3.525  -0.108
TER
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REMARK  Compound E structure 07
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.121583
REMARK   Sum of electronic and thermal Energies=    -730.101919
REMARK   Sum of electronic and thermal Enthalpies=  -730.100975
REMARK   Sum of electronic and thermal Free Energies=  -730.170183
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.348  -1.320   0.297
ATOM      2  C   RES     1      -4.650  -1.156  -0.526
ATOM      3  H   RES     1      -5.105  -0.462  -1.239
ATOM      4  H   RES     1      -4.504  -2.120  -1.017
ATOM      5  C   RES     1      -3.329  -0.688   0.037
ATOM      6  O   RES     1      -2.670  -1.378   0.806
ATOM      7  N   RES     1      -2.931   0.555  -0.370
ATOM      8  H   RES     1      -3.530   1.067  -1.001
ATOM      9  C   RES     1      -1.674   1.208   0.054
ATOM     10  C   RES     1      -1.696   1.449   1.560
ATOM     11  H   RES     1      -1.774   0.505   2.103
ATOM     12  H   RES     1      -2.552   2.075   1.824
ATOM     13  H   RES     1      -0.787   1.968   1.881
ATOM     14  C   RES     1      -1.621   2.546  -0.687
ATOM     15  H   RES     1      -2.488   3.168  -0.436
ATOM     16  H   RES     1      -1.598   2.401  -1.772
ATOM     17  H   RES     1      -0.722   3.098  -0.403
ATOM     18  C   RES     1      -0.515   0.354  -0.404
ATOM     19  H   RES     1      -0.543   0.116  -1.469
ATOM     20  C   RES     1       0.474  -0.121   0.357
ATOM     21  H   RES     1       0.464   0.096   1.427
ATOM     22  C   RES     1       1.600  -1.019  -0.082
ATOM     23  C   RES     1       1.590  -2.263   0.813
ATOM     24  H   RES     1       0.650  -2.807   0.685
ATOM     25  H   RES     1       1.685  -1.993   1.869
ATOM     26  H   RES     1       2.429  -2.915   0.559
ATOM     27  C   RES     1       1.481  -1.447  -1.549
ATOM     28  H   RES     1       1.497  -0.590  -2.231
ATOM     29  H   RES     1       0.547  -1.995  -1.709
ATOM     30  H   RES     1       2.315  -2.102  -1.811
ATOM     31  C   RES     1       2.979  -0.333   0.057
ATOM     32  O   RES     1       4.011  -0.981   0.188
ATOM     33  N   RES     1       2.965   1.026  -0.041
ATOM     34  H   RES     1       2.070   1.479  -0.161
ATOM     35  C   RES     1       4.169   1.820  -0.029
ATOM     36  H   RES     1       4.310   2.351  -0.977
ATOM     37  H   RES     1       4.155   2.553   0.784
ATOM     38  H   RES     1       5.009   1.142   0.121
TER
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REMARK  Compound E structure 08
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.120691
REMARK   Sum of electronic and thermal Energies=    -730.100973
REMARK   Sum of electronic and thermal Enthalpies=  -730.100029
REMARK   Sum of electronic and thermal Free Energies=  -730.169870
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       5.610  -1.133  -0.502
ATOM      2  C   RES     1       4.789  -1.254   0.208
ATOM      3  H   RES     1       5.098  -0.852   1.176
ATOM      4  H   RES     1       4.614  -2.327   0.312
ATOM      5  C   RES     1       3.549  -0.608  -0.365
ATOM      6  O   RES     1       3.106  -0.930  -1.464
ATOM      7  N   RES     1       2.980   0.349   0.422
ATOM      8  H   RES     1       3.364   0.486   1.344
ATOM      9  C   RES     1       1.738   1.097   0.106
ATOM     10  C   RES     1       1.932   1.885  -1.194
ATOM     11  H   RES     1       2.101   1.213  -2.037
ATOM     12  H   RES     1       2.793   2.556  -1.106
ATOM     13  H   RES     1       1.041   2.487  -1.395
ATOM     14  C   RES     1       1.520   2.065   1.261
ATOM     15  H   RES     1       2.377   2.739   1.355
ATOM     16  H   RES     1       1.382   1.540   2.212
ATOM     17  H   RES     1       0.633   2.678   1.087
ATOM     18  C   RES     1       0.600   0.116  -0.068
ATOM     19  H   RES     1       0.782  -0.617  -0.852
ATOM     20  C   RES     1      -0.544   0.115   0.619
ATOM     21  H   RES     1      -0.730   0.856   1.397
ATOM     22  C   RES     1      -1.694  -0.851   0.441
ATOM     23  C   RES     1      -1.442  -1.863  -0.671
ATOM     24  H   RES     1      -0.566  -2.472  -0.433
ATOM     25  H   RES     1      -1.240  -1.389  -1.639
ATOM     26  H   RES     1      -2.291  -2.546  -0.781
ATOM     27  C   RES     1      -1.912  -1.599   1.767
ATOM     28  H   RES     1      -2.110  -0.894   2.577
ATOM     29  H   RES     1      -1.024  -2.188   2.015
ATOM     30  H   RES     1      -2.767  -2.280   1.695
ATOM     31  C   RES     1      -2.941   0.036   0.226
ATOM     32  O   RES     1      -3.315   0.809   1.103
ATOM     33  N   RES     1      -3.582  -0.080  -0.971
ATOM     34  H   RES     1      -3.216  -0.713  -1.663
ATOM     35  C   RES     1      -4.736   0.719  -1.310
ATOM     36  H   RES     1      -5.000   1.306  -0.430
ATOM     37  H   RES     1      -4.522   1.402  -2.138
ATOM     38  H   RES     1      -5.586   0.088  -1.586
TER
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REMARK  Compound E structure 09
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.121757
REMARK   Sum of electronic and thermal Energies=    -730.102173
REMARK   Sum of electronic and thermal Enthalpies=  -730.101228
REMARK   Sum of electronic and thermal Free Energies=  -730.169713
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.134   0.361  -2.869
ATOM      2  C   RES     1       3.877  -0.465  -2.203
ATOM      3  H   RES     1       4.777  -1.073  -2.088
ATOM      4  H   RES     1       3.099  -1.069  -2.677
ATOM      5  C   RES     1       3.491   0.099  -0.856
ATOM      6  O   RES     1       4.251   0.822  -0.220
ATOM      7  N   RES     1       2.237  -0.240  -0.427
ATOM      8  H   RES     1       1.767  -0.978  -0.928
ATOM      9  C   RES     1       1.701   0.069   0.909
ATOM     10  C   RES     1       1.702   1.587   1.144
ATOM     11  H   RES     1       1.174   2.097   0.333
ATOM     12  H   RES     1       2.722   1.971   1.194
ATOM     13  H   RES     1       1.191   1.814   2.086
ATOM     14  C   RES     1       2.534  -0.629   1.987
ATOM     15  H   RES     1       3.570  -0.287   1.942
ATOM     16  H   RES     1       2.514  -1.715   1.855
ATOM     17  H   RES     1       2.138  -0.401   2.982
ATOM     18  C   RES     1       0.269  -0.408   0.980
ATOM     19  H   RES     1      -0.084  -0.578   1.998
ATOM     20  C   RES     1      -0.575  -0.569  -0.044
ATOM     21  H   RES     1      -0.221  -0.367  -1.060
ATOM     22  C   RES     1      -2.021  -0.988   0.029
ATOM     23  C   RES     1      -2.246  -2.171  -0.915
ATOM     24  H   RES     1      -1.673  -3.040  -0.575
ATOM     25  H   RES     1      -1.932  -1.931  -1.936
ATOM     26  H   RES     1      -3.306  -2.429  -0.949
ATOM     27  C   RES     1      -2.456  -1.375   1.446
ATOM     28  H   RES     1      -2.348  -0.544   2.152
ATOM     29  H   RES     1      -1.860  -2.216   1.816
ATOM     30  H   RES     1      -3.507  -1.675   1.442
ATOM     31  C   RES     1      -2.960   0.163  -0.414
ATOM     32  O   RES     1      -4.066  -0.061  -0.891
ATOM     33  N   RES     1      -2.493   1.420  -0.178
ATOM     34  H   RES     1      -1.577   1.518   0.235
ATOM     35  C   RES     1      -3.280   2.601  -0.443
ATOM     36  H   RES     1      -4.175   2.288  -0.981
ATOM     37  H   RES     1      -3.586   3.100   0.483
ATOM     38  H   RES     1      -2.723   3.314  -1.058
TER
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REMARK  Compound E structure 10
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.121500
REMARK   Sum of electronic and thermal Energies=    -730.101947
REMARK   Sum of electronic and thermal Enthalpies=  -730.101002
REMARK   Sum of electronic and thermal Free Energies=  -730.169451
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -5.028   1.651   1.593
ATOM      2  C   RES     1      -4.172   1.931   0.975
ATOM      3  H   RES     1      -3.408   2.381   1.615
ATOM      4  H   RES     1      -4.525   2.683   0.266
ATOM      5  C   RES     1      -3.705   0.716   0.208
ATOM      6  O   RES     1      -4.460   0.091  -0.530
ATOM      7  N   RES     1      -2.395   0.380   0.400
ATOM      8  H   RES     1      -1.842   0.971   1.001
ATOM      9  C   RES     1      -1.696  -0.752  -0.253
ATOM     10  C   RES     1      -1.702  -0.561  -1.767
ATOM     11  H   RES     1      -1.187   0.361  -2.054
ATOM     12  H   RES     1      -2.732  -0.510  -2.126
ATOM     13  H   RES     1      -1.207  -1.401  -2.263
ATOM     14  C   RES     1      -2.392  -2.069   0.117
ATOM     15  H   RES     1      -3.423  -2.066  -0.239
ATOM     16  H   RES     1      -2.396  -2.213   1.202
ATOM     17  H   RES     1      -1.859  -2.908  -0.339
ATOM     18  C   RES     1      -0.308  -0.763   0.340
ATOM     19  H   RES     1      -0.292  -0.837   1.431
ATOM     20  C   RES     1       0.848  -0.745  -0.331
ATOM     21  H   RES     1       0.820  -0.697  -1.423
ATOM     22  C   RES     1       2.234  -0.822   0.252
ATOM     23  C   RES     1       2.234  -0.976   1.776
ATOM     24  H   RES     1       1.712  -1.892   2.072
ATOM     25  H   RES     1       1.747  -0.131   2.274
ATOM     26  H   RES     1       3.262  -1.034   2.141
ATOM     27  C   RES     1       2.964  -2.013  -0.380
ATOM     28  H   RES     1       2.967  -1.945  -1.472
ATOM     29  H   RES     1       2.474  -2.950  -0.097
ATOM     30  H   RES     1       4.003  -2.033  -0.044
ATOM     31  C   RES     1       3.061   0.451  -0.050
ATOM     32  O   RES     1       4.286   0.438  -0.006
ATOM     33  N   RES     1       2.340   1.578  -0.305
ATOM     34  H   RES     1       1.334   1.507  -0.313
ATOM     35  C   RES     1       2.961   2.862  -0.529
ATOM     36  H   RES     1       4.041   2.709  -0.531
ATOM     37  H   RES     1       2.659   3.285  -1.492
ATOM     38  H   RES     1       2.709   3.575   0.264
TER
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REMARK  Compound E structure 11
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.120837
REMARK   Sum of electronic and thermal Energies=    -730.101167
REMARK   Sum of electronic and thermal Enthalpies=  -730.100223
REMARK   Sum of electronic and thermal Free Energies=  -730.169039
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.058   2.033  -2.141
ATOM      2  C   RES     1       3.442   2.181  -1.251
ATOM      3  H   RES     1       2.472   2.581  -1.558
ATOM      4  H   RES     1       3.952   2.923  -0.632
ATOM      5  C   RES     1       3.364   0.878  -0.491
ATOM      6  O   RES     1       4.372   0.293  -0.109
ATOM      7  N   RES     1       2.097   0.407  -0.283
ATOM      8  H   RES     1       1.335   1.030  -0.504
ATOM      9  C   RES     1       1.768  -0.777   0.525
ATOM     10  C   RES     1       2.215  -0.561   1.976
ATOM     11  H   RES     1       1.714   0.308   2.415
ATOM     12  H   RES     1       3.295  -0.402   2.016
ATOM     13  H   RES     1       1.970  -1.438   2.583
ATOM     14  C   RES     1       2.453  -2.022  -0.055
ATOM     15  H   RES     1       3.538  -1.923   0.008
ATOM     16  H   RES     1       2.167  -2.161  -1.101
ATOM     17  H   RES     1       2.143  -2.909   0.505
ATOM     18  C   RES     1       0.276  -1.006   0.492
ATOM     19  H   RES     1      -0.068  -1.679   1.279
ATOM     20  C   RES     1      -0.608  -0.535  -0.393
ATOM     21  H   RES     1      -0.262   0.104  -1.210
ATOM     22  C   RES     1      -2.088  -0.820  -0.437
ATOM     23  C   RES     1      -2.445  -1.341  -1.831
ATOM     24  H   RES     1      -1.944  -2.296  -2.016
ATOM     25  H   RES     1      -2.137  -0.637  -2.610
ATOM     26  H   RES     1      -3.525  -1.477  -1.919
ATOM     27  C   RES     1      -2.529  -1.839   0.618
ATOM     28  H   RES     1      -2.313  -1.499   1.637
ATOM     29  H   RES     1      -2.022  -2.796   0.464
ATOM     30  H   RES     1      -3.607  -2.008   0.543
ATOM     31  C   RES     1      -2.914   0.464  -0.176
ATOM     32  O   RES     1      -4.019   0.635  -0.678
ATOM     33  N   RES     1      -2.350   1.350   0.691
ATOM     34  H   RES     1      -1.458   1.108   1.098
ATOM     35  C   RES     1      -3.044   2.528   1.154
ATOM     36  H   RES     1      -3.926   2.659   0.526
ATOM     37  H   RES     1      -3.371   2.426   2.195
ATOM     38  H   RES     1      -2.409   3.415   1.071
TER
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REMARK  Compound E structure 12
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.119858
REMARK   Sum of electronic and thermal Energies=    -730.100133
REMARK   Sum of electronic and thermal Enthalpies=  -730.099189
REMARK   Sum of electronic and thermal Free Energies=  -730.168433
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.854   2.112   1.138
ATOM      2  C   RES     1       4.258   1.288   1.536
ATOM      3  H   RES     1       3.500   1.694   2.210
ATOM      4  H   RES     1       4.936   0.653   2.110
ATOM      5  C   RES     1       3.697   0.490   0.383
ATOM      6  O   RES     1       4.425   0.009  -0.482
ATOM      7  N   RES     1       2.340   0.352   0.381
ATOM      8  H   RES     1       1.825   0.722   1.166
ATOM      9  C   RES     1       1.563  -0.426  -0.613
ATOM     10  C   RES     1       1.979  -1.893  -0.566
ATOM     11  H   RES     1       1.804  -2.321   0.425
ATOM     12  H   RES     1       3.041  -1.980  -0.801
ATOM     13  H   RES     1       1.414  -2.475  -1.300
ATOM     14  C   RES     1       1.800   0.150  -2.015
ATOM     15  H   RES     1       2.854   0.075  -2.286
ATOM     16  H   RES     1       1.502   1.202  -2.055
ATOM     17  H   RES     1       1.202  -0.403  -2.746
ATOM     18  C   RES     1       0.116  -0.202  -0.246
ATOM     19  H   RES     1      -0.182   0.849  -0.240
ATOM     20  C   RES     1      -0.783  -1.139   0.058
ATOM     21  H   RES     1      -0.484  -2.190   0.065
ATOM     22  C   RES     1      -2.239  -0.925   0.411
ATOM     23  C   RES     1      -3.096  -1.745  -0.564
ATOM     24  H   RES     1      -2.889  -2.811  -0.431
ATOM     25  H   RES     1      -2.878  -1.518  -1.614
ATOM     26  H   RES     1      -4.165  -1.592  -0.383
ATOM     27  C   RES     1      -2.480  -1.442   1.836
ATOM     28  H   RES     1      -1.917  -0.849   2.559
ATOM     29  H   RES     1      -2.172  -2.489   1.914
ATOM     30  H   RES     1      -3.541  -1.380   2.098
ATOM     31  C   RES     1      -2.550   0.581   0.394
ATOM     32  O   RES     1      -2.245   1.307   1.336
ATOM     33  N   RES     1      -3.147   1.066  -0.731
ATOM     34  H   RES     1      -3.323   0.440  -1.500
ATOM     35  C   RES     1      -3.397   2.476  -0.920
ATOM     36  H   RES     1      -3.337   2.959   0.056
ATOM     37  H   RES     1      -2.654   2.938  -1.580
ATOM     38  H   RES     1      -4.392   2.637  -1.342
TER
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REMARK  Compound E structure 13
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.119684
REMARK   Sum of electronic and thermal Energies=    -730.100073
REMARK   Sum of electronic and thermal Enthalpies=  -730.099129
REMARK   Sum of electronic and thermal Free Energies=  -730.168218
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.817   2.063   1.438
ATOM      2  C   RES     1      -3.992   2.217   0.739
ATOM      3  H   RES     1      -3.162   2.685   1.275
ATOM      4  H   RES     1      -4.350   2.903  -0.031
ATOM      5  C   RES     1      -3.646   0.895   0.095
ATOM      6  O   RES     1      -4.468   0.265  -0.565
ATOM      7  N   RES     1      -2.371   0.461   0.319
ATOM      8  H   RES     1      -1.730   1.095   0.774
ATOM      9  C   RES     1      -1.775  -0.767  -0.260
ATOM     10  C   RES     1      -1.763  -0.669  -1.783
ATOM     11  H   RES     1      -1.195   0.204  -2.119
ATOM     12  H   RES     1      -2.787  -0.578  -2.150
ATOM     13  H   RES     1      -1.314  -1.566  -2.222
ATOM     14  C   RES     1      -2.581  -1.993   0.186
ATOM     15  H   RES     1      -3.604  -1.939  -0.187
ATOM     16  H   RES     1      -2.610  -2.059   1.278
ATOM     17  H   RES     1      -2.109  -2.903  -0.198
ATOM     18  C   RES     1      -0.398  -0.852   0.349
ATOM     19  H   RES     1      -0.401  -0.948   1.437
ATOM     20  C   RES     1       0.766  -0.809  -0.300
ATOM     21  H   RES     1       0.770  -0.702  -1.387
ATOM     22  C   RES     1       2.140  -0.852   0.331
ATOM     23  C   RES     1       2.104  -1.250   1.806
ATOM     24  H   RES     1       1.611  -2.219   1.927
ATOM     25  H   RES     1       1.579  -0.502   2.402
ATOM     26  H   RES     1       3.121  -1.333   2.202
ATOM     27  C   RES     1       3.000  -1.856  -0.443
ATOM     28  H   RES     1       2.985  -1.675  -1.524
ATOM     29  H   RES     1       2.611  -2.867  -0.293
ATOM     30  H   RES     1       4.040  -1.851  -0.097
ATOM     31  C   RES     1       2.664   0.605   0.262
ATOM     32  O   RES     1       2.227   1.467   1.018
ATOM     33  N   RES     1       3.588   0.878  -0.702
ATOM     34  H   RES     1       3.953   0.123  -1.260
ATOM     35  C   RES     1       4.143   2.199  -0.887
ATOM     36  H   RES     1       5.191   2.246  -0.570
ATOM     37  H   RES     1       4.078   2.505  -1.934
ATOM     38  H   RES     1       3.564   2.890  -0.275
TER
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REMARK  Compound E structure 14
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.120344
REMARK   Sum of electronic and thermal Energies=    -730.100941
REMARK   Sum of electronic and thermal Enthalpies=  -730.099997
REMARK   Sum of electronic and thermal Free Energies=  -730.168020
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       3.169   3.314   0.164
ATOM      2  C   RES     1       3.734   2.459  -0.212
ATOM      3  H   RES     1       4.737   2.529   0.215
ATOM      4  H   RES     1       3.809   2.536  -1.300
ATOM      5  C   RES     1       3.083   1.186   0.277
ATOM      6  O   RES     1       2.962   0.946   1.476
ATOM      7  N   RES     1       2.658   0.340  -0.703
ATOM      8  H   RES     1       2.709   0.666  -1.657
ATOM      9  C   RES     1       1.936  -0.939  -0.483
ATOM     10  C   RES     1       2.821  -1.890   0.327
ATOM     11  H   RES     1       3.025  -1.483   1.319
ATOM     12  H   RES     1       3.775  -2.053  -0.186
ATOM     13  H   RES     1       2.318  -2.856   0.439
ATOM     14  C   RES     1       1.684  -1.525  -1.865
ATOM     15  H   RES     1       2.635  -1.692  -2.382
ATOM     16  H   RES     1       1.061  -0.868  -2.481
ATOM     17  H   RES     1       1.176  -2.489  -1.786
ATOM     18  C   RES     1       0.663  -0.657   0.284
ATOM     19  H   RES     1       0.841  -0.203   1.257
ATOM     20  C   RES     1      -0.576  -0.924  -0.133
ATOM     21  H   RES     1      -0.751  -1.372  -1.112
ATOM     22  C   RES     1      -1.854  -0.670   0.635
ATOM     23  C   RES     1      -2.557  -2.019   0.868
ATOM     24  H   RES     1      -1.926  -2.669   1.480
ATOM     25  H   RES     1      -2.760  -2.513  -0.085
ATOM     26  H   RES     1      -3.512  -1.877   1.386
ATOM     27  C   RES     1      -1.604   0.006   1.978
ATOM     28  H   RES     1      -1.062   0.953   1.881
ATOM     29  H   RES     1      -0.993  -0.639   2.617
ATOM     30  H   RES     1      -2.544   0.186   2.511
ATOM     31  C   RES     1      -2.755   0.135  -0.326
ATOM     32  O   RES     1      -3.115  -0.349  -1.396
ATOM     33  N   RES     1      -3.112   1.390   0.065
ATOM     34  H   RES     1      -2.773   1.745   0.944
ATOM     35  C   RES     1      -3.927   2.253  -0.758
ATOM     36  H   RES     1      -3.379   3.152  -1.060
ATOM     37  H   RES     1      -4.202   1.692  -1.651
ATOM     38  H   RES     1      -4.838   2.557  -0.233
TER
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REMARK  Compound E structure 15
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.119667
REMARK   Sum of electronic and thermal Energies=    -730.100099
REMARK   Sum of electronic and thermal Enthalpies=  -730.099155
REMARK   Sum of electronic and thermal Free Energies=  -730.167849
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       3.975   2.694  -1.425
ATOM      2  C   RES     1       3.379   2.557  -0.520
ATOM      3  H   RES     1       2.385   2.979  -0.686
ATOM      4  H   RES     1       3.875   3.120   0.275
ATOM      5  C   RES     1       3.378   1.091  -0.156
ATOM      6  O   RES     1       4.423   0.475   0.033
ATOM      7  N   RES     1       2.141   0.519  -0.074
ATOM      8  H   RES     1       1.346   1.141  -0.087
ATOM      9  C   RES     1       1.885  -0.856   0.383
ATOM     10  C   RES     1       2.369  -1.027   1.827
ATOM     11  H   RES     1       1.847  -0.336   2.497
ATOM     12  H   RES     1       3.442  -0.836   1.887
ATOM     13  H   RES     1       2.178  -2.048   2.173
ATOM     14  C   RES     1       2.603  -1.857  -0.533
ATOM     15  H   RES     1       3.685  -1.729  -0.465
ATOM     16  H   RES     1       2.291  -1.714  -1.571
ATOM     17  H   RES     1       2.346  -2.879  -0.236
ATOM     18  C   RES     1       0.401  -1.127   0.317
ATOM     19  H   RES     1       0.094  -1.977   0.929
ATOM     20  C   RES     1      -0.502  -0.476  -0.419
ATOM     21  H   RES     1      -0.201   0.356  -1.056
ATOM     22  C   RES     1      -1.983  -0.766  -0.502
ATOM     23  C   RES     1      -2.330  -1.112  -1.960
ATOM     24  H   RES     1      -1.801  -2.019  -2.267
ATOM     25  H   RES     1      -2.044  -0.295  -2.626
ATOM     26  H   RES     1      -3.406  -1.284  -2.076
ATOM     27  C   RES     1      -2.406  -1.917   0.404
ATOM     28  H   RES     1      -2.173  -1.731   1.458
ATOM     29  H   RES     1      -1.883  -2.833   0.116
ATOM     30  H   RES     1      -3.477  -2.123   0.309
ATOM     31  C   RES     1      -2.682   0.579  -0.197
ATOM     32  O   RES     1      -2.417   1.579  -0.858
ATOM     33  N   RES     1      -3.592   0.590   0.816
ATOM     34  H   RES     1      -3.756  -0.254   1.339
ATOM     35  C   RES     1      -4.307   1.786   1.198
ATOM     36  H   RES     1      -4.027   2.575   0.500
ATOM     37  H   RES     1      -5.389   1.632   1.147
ATOM     38  H   RES     1      -4.044   2.103   2.212
TER
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REMARK  Compound E structure 16
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.119944
REMARK   Sum of electronic and thermal Energies=    -730.100389
REMARK   Sum of electronic and thermal Enthalpies=  -730.099445
REMARK   Sum of electronic and thermal Free Energies=  -730.167818
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.709   3.074  -0.394
ATOM      2  C   RES     1      -2.924   2.495  -0.883
ATOM      3  H   RES     1      -2.017   3.106  -0.876
ATOM      4  H   RES     1      -3.206   2.312  -1.924
ATOM      5  C   RES     1      -2.666   1.237  -0.087
ATOM      6  O   RES     1      -2.614   1.243   1.137
ATOM      7  N   RES     1      -2.478   0.110  -0.841
ATOM      8  H   RES     1      -2.430   0.227  -1.842
ATOM      9  C   RES     1      -2.039  -1.188  -0.310
ATOM     10  C   RES     1      -1.978  -2.148  -1.501
ATOM     11  H   RES     1      -1.278  -1.788  -2.262
ATOM     12  H   RES     1      -2.968  -2.270  -1.955
ATOM     13  H   RES     1      -1.633  -3.133  -1.175
ATOM     14  C   RES     1      -3.055  -1.711   0.710
ATOM     15  H   RES     1      -4.045  -1.789   0.250
ATOM     16  H   RES     1      -3.119  -1.048   1.572
ATOM     17  H   RES     1      -2.758  -2.709   1.050
ATOM     18  C   RES     1      -0.668  -1.105   0.329
ATOM     19  H   RES     1      -0.408  -1.981   0.926
ATOM     20  C   RES     1       0.188  -0.091   0.209
ATOM     21  H   RES     1      -0.088   0.779  -0.386
ATOM     22  C   RES     1       1.532   0.048   0.880
ATOM     23  C   RES     1       1.456   1.259   1.829
ATOM     24  H   RES     1       0.689   1.089   2.590
ATOM     25  H   RES     1       1.199   2.163   1.273
ATOM     26  H   RES     1       2.417   1.425   2.328
ATOM     27  C   RES     1       1.919  -1.192   1.678
ATOM     28  H   RES     1       1.955  -2.098   1.061
ATOM     29  H   RES     1       1.182  -1.372   2.467
ATOM     30  H   RES     1       2.887  -1.061   2.173
ATOM     31  C   RES     1       2.529   0.426  -0.237
ATOM     32  O   RES     1       2.351   1.431  -0.920
ATOM     33  N   RES     1       3.597  -0.402  -0.417
ATOM     34  H   RES     1       3.687  -1.218   0.164
ATOM     35  C   RES     1       4.599  -0.162  -1.429
ATOM     36  H   RES     1       4.643  -0.984  -2.150
ATOM     37  H   RES     1       4.326   0.754  -1.953
ATOM     38  H   RES     1       5.591  -0.033  -0.983
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REMARK  Compound E structure 17
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.119380
REMARK   Sum of electronic and thermal Energies=    -730.099719
REMARK   Sum of electronic and thermal Enthalpies=  -730.098774
REMARK   Sum of electronic and thermal Free Energies=  -730.167573
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.107  -2.997   0.084
ATOM      2  C   RES     1      -3.787  -2.226   0.787
ATOM      3  H   RES     1      -2.926  -2.597   1.349
ATOM      4  H   RES     1      -4.617  -2.061   1.479
ATOM      5  C   RES     1      -3.525  -0.949   0.024
ATOM      6  O   RES     1      -4.380  -0.443  -0.697
ATOM      7  N   RES     1      -2.276  -0.423   0.194
ATOM      8  H   RES     1      -1.697  -0.833   0.911
ATOM      9  C   RES     1      -1.832   0.868  -0.351
ATOM     10  C   RES     1      -2.688   2.002   0.226
ATOM     11  H   RES     1      -2.598   2.042   1.316
ATOM     12  H   RES     1      -3.737   1.847  -0.038
ATOM     13  H   RES     1      -2.365   2.966  -0.180
ATOM     14  C   RES     1      -1.939   0.860  -1.883
ATOM     15  H   RES     1      -2.982   0.775  -2.192
ATOM     16  H   RES     1      -1.372   0.023  -2.300
ATOM     17  H   RES     1      -1.525   1.790  -2.286
ATOM     18  C   RES     1      -0.386   1.099   0.014
ATOM     19  H   RES     1      -0.078   2.134  -0.143
ATOM     20  C   RES     1       0.508   0.203   0.438
ATOM     21  H   RES     1       0.235  -0.846   0.565
ATOM     22  C   RES     1       1.957   0.470   0.780
ATOM     23  C   RES     1       2.380   1.899   0.459
ATOM     24  H   RES     1       1.797   2.608   1.054
ATOM     25  H   RES     1       2.224   2.159  -0.594
ATOM     26  H   RES     1       3.432   2.064   0.713
ATOM     27  C   RES     1       2.161   0.209   2.283
ATOM     28  H   RES     1       1.882  -0.816   2.536
ATOM     29  H   RES     1       1.549   0.900   2.870
ATOM     30  H   RES     1       3.210   0.353   2.565
ATOM     31  C   RES     1       2.761  -0.619   0.036
ATOM     32  O   RES     1       2.559  -1.806   0.273
ATOM     33  N   RES     1       3.683  -0.198  -0.873
ATOM     34  H   RES     1       3.794   0.788  -1.042
ATOM     35  C   RES     1       4.482  -1.122  -1.646
ATOM     36  H   RES     1       4.218  -2.131  -1.328
ATOM     37  H   RES     1       4.279  -1.024  -2.717
ATOM     38  H   RES     1       5.550  -0.962  -1.473
TER
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REMARK  Compound E structure 18
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.119065
REMARK   Sum of electronic and thermal Energies=    -730.099540
REMARK   Sum of electronic and thermal Enthalpies=  -730.098596
REMARK   Sum of electronic and thermal Free Energies=  -730.167056
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.604  -2.127  -1.064
ATOM      2  C   RES     1      -4.734  -1.166  -0.560
ATOM      3  H   RES     1      -5.415  -1.336   0.277
ATOM      4  H   RES     1      -5.202  -0.464  -1.255
ATOM      5  C   RES     1      -3.398  -0.710  -0.022
ATOM      6  O   RES     1      -2.716  -1.422   0.706
ATOM      7  N   RES     1      -3.017   0.545  -0.406
ATOM      8  H   RES     1      -3.654   1.084  -0.973
ATOM      9  C   RES     1      -1.772   1.214   0.034
ATOM     10  C   RES     1      -1.810   1.441   1.542
ATOM     11  H   RES     1      -1.866   0.490   2.075
ATOM     12  H   RES     1      -2.685   2.043   1.805
ATOM     13  H   RES     1      -0.918   1.980   1.875
ATOM     14  C   RES     1      -1.734   2.557  -0.698
ATOM     15  H   RES     1      -2.611   3.166  -0.447
ATOM     16  H   RES     1      -1.706   2.417  -1.784
ATOM     17  H   RES     1      -0.842   3.116  -0.407
ATOM     18  C   RES     1      -0.594   0.382  -0.417
ATOM     19  H   RES     1      -0.642   0.097  -1.470
ATOM     20  C   RES     1       0.433  -0.001   0.341
ATOM     21  H   RES     1       0.466   0.272   1.395
ATOM     22  C   RES     1       1.592  -0.869  -0.087
ATOM     23  C   RES     1       1.550  -2.152   0.763
ATOM     24  H   RES     1       0.606  -2.679   0.595
ATOM     25  H   RES     1       1.631  -1.908   1.824
ATOM     26  H   RES     1       2.378  -2.820   0.501
ATOM     27  C   RES     1       1.527  -1.246  -1.563
ATOM     28  H   RES     1       1.504  -0.371  -2.224
ATOM     29  H   RES     1       0.617  -1.819  -1.761
ATOM     30  H   RES     1       2.373  -1.882  -1.846
ATOM     31  C   RES     1       2.868  -0.105   0.323
ATOM     32  O   RES     1       3.072   0.185   1.498
ATOM     33  N   RES     1       3.740   0.227  -0.672
ATOM     34  H   RES     1       3.518  -0.019  -1.623
ATOM     35  C   RES     1       4.959   0.957  -0.417
ATOM     36  H   RES     1       5.051   1.078   0.662
ATOM     37  H   RES     1       5.832   0.411  -0.789
ATOM     38  H   RES     1       4.940   1.948  -0.882
TER
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REMARK  Compound E structure 19
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.118615
REMARK   Sum of electronic and thermal Energies=    -730.098716
REMARK   Sum of electronic and thermal Enthalpies=  -730.097772
REMARK   Sum of electronic and thermal Free Energies=  -730.167027
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -3.568  -2.345  -1.357
ATOM      2  C   RES     1      -4.003  -1.403  -1.012
ATOM      3  H   RES     1      -4.905  -1.657  -0.452
ATOM      4  H   RES     1      -4.284  -0.807  -1.884
ATOM      5  C   RES     1      -3.025  -0.724  -0.083
ATOM      6  O   RES     1      -2.688  -1.227   0.982
ATOM      7  N   RES     1      -2.542   0.475  -0.531
ATOM      8  H   RES     1      -2.852   0.796  -1.435
ATOM      9  C   RES     1      -1.573   1.321   0.179
ATOM     10  C   RES     1      -2.096   1.675   1.576
ATOM     11  H   RES     1      -2.217   0.778   2.185
ATOM     12  H   RES     1      -3.061   2.184   1.499
ATOM     13  H   RES     1      -1.393   2.349   2.075
ATOM     14  C   RES     1      -1.427   2.603  -0.645
ATOM     15  H   RES     1      -2.379   3.143  -0.701
ATOM     16  H   RES     1      -1.085   2.382  -1.663
ATOM     17  H   RES     1      -0.693   3.268  -0.184
ATOM     18  C   RES     1      -0.217   0.662   0.300
ATOM     19  H   RES     1       0.480   1.216   0.934
ATOM     20  C   RES     1       0.178  -0.476  -0.271
ATOM     21  H   RES     1      -0.539  -1.037  -0.873
ATOM     22  C   RES     1       1.503  -1.171  -0.057
ATOM     23  C   RES     1       1.356  -2.125   1.133
ATOM     24  H   RES     1       0.525  -2.816   0.958
ATOM     25  H   RES     1       1.147  -1.573   2.052
ATOM     26  H   RES     1       2.276  -2.696   1.281
ATOM     27  C   RES     1       1.864  -1.983  -1.312
ATOM     28  H   RES     1       1.944  -1.349  -2.201
ATOM     29  H   RES     1       1.095  -2.740  -1.502
ATOM     30  H   RES     1       2.819  -2.500  -1.176
ATOM     31  C   RES     1       2.678  -0.211   0.213
ATOM     32  O   RES     1       3.536  -0.448   1.056
ATOM     33  N   RES     1       2.749   0.866  -0.623
ATOM     34  H   RES     1       1.948   1.062  -1.205
ATOM     35  C   RES     1       3.803   1.847  -0.534
ATOM     36  H   RES     1       4.571   1.444   0.128
ATOM     37  H   RES     1       4.243   2.040  -1.516
ATOM     38  H   RES     1       3.448   2.796  -0.116
TER
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REMARK  Compound E structure 20
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.118170
REMARK   Sum of electronic and thermal Energies=    -730.098450
REMARK   Sum of electronic and thermal Enthalpies=  -730.097506
REMARK   Sum of electronic and thermal Free Energies=  -730.166615
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1       4.868   1.606  -1.482
ATOM      2  C   RES     1       4.370   1.642  -0.510
ATOM      3  H   RES     1       3.695   2.501  -0.493
ATOM      4  H   RES     1       5.150   1.789   0.241
ATOM      5  C   RES     1       3.692   0.315  -0.261
ATOM      6  O   RES     1       4.318  -0.740  -0.274
ATOM      7  N   RES     1       2.343   0.389  -0.048
ATOM      8  H   RES     1       1.961   1.307   0.130
ATOM      9  C   RES     1       1.500  -0.745   0.361
ATOM     10  C   RES     1       1.944  -1.264   1.733
ATOM     11  H   RES     1       1.851  -0.484   2.495
ATOM     12  H   RES     1       2.984  -1.595   1.688
ATOM     13  H   RES     1       1.323  -2.113   2.038
ATOM     14  C   RES     1       1.582  -1.873  -0.679
ATOM     15  H   RES     1       2.584  -2.301  -0.706
ATOM     16  H   RES     1       1.332  -1.491  -1.674
ATOM     17  H   RES     1       0.865  -2.660  -0.422
ATOM     18  C   RES     1       0.065  -0.292   0.432
ATOM     19  H   RES     1      -0.576  -0.984   0.986
ATOM     20  C   RES     1      -0.493   0.779  -0.138
ATOM     21  H   RES     1       0.125   1.472  -0.715
ATOM     22  C   RES     1      -1.948   1.182  -0.028
ATOM     23  C   RES     1      -2.117   2.131   1.162
ATOM     24  H   RES     1      -1.460   2.999   1.045
ATOM     25  H   RES     1      -1.868   1.629   2.100
ATOM     26  H   RES     1      -3.150   2.479   1.234
ATOM     27  C   RES     1      -2.373   1.908  -1.315
ATOM     28  H   RES     1      -2.230   1.287  -2.205
ATOM     29  H   RES     1      -1.783   2.822  -1.444
ATOM     30  H   RES     1      -3.428   2.194  -1.268
ATOM     31  C   RES     1      -2.887  -0.028   0.166
ATOM     32  O   RES     1      -3.758  -0.050   1.028
ATOM     33  N   RES     1      -2.724  -1.033  -0.743
ATOM     34  H   RES     1      -1.909  -1.003  -1.338
ATOM     35  C   RES     1      -3.501  -2.248  -0.701
ATOM     36  H   RES     1      -4.319  -2.093   0.003
ATOM     37  H   RES     1      -3.916  -2.483  -1.686
ATOM     38  H   RES     1      -2.905  -3.102  -0.360
TER
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REMARK  Compound E structure 21
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.118350
REMARK   Sum of electronic and thermal Energies=    -730.098676
REMARK   Sum of electronic and thermal Enthalpies=  -730.097731
REMARK   Sum of electronic and thermal Free Energies=  -730.166561
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.668   2.544   0.081
ATOM      2  C   RES     1      -4.041   2.083  -0.685
ATOM      3  H   RES     1      -3.210   2.757  -0.912
ATOM      4  H   RES     1      -4.659   1.971  -1.578
ATOM      5  C   RES     1      -3.615   0.714  -0.208
ATOM      6  O   RES     1      -4.438  -0.146   0.093
ATOM      7  N   RES     1      -2.267   0.520  -0.137
ATOM      8  H   RES     1      -1.666   1.264  -0.458
ATOM      9  C   RES     1      -1.602  -0.741   0.273
ATOM     10  C   RES     1      -1.989  -1.864  -0.684
ATOM     11  H   RES     1      -1.690  -1.632  -1.711
ATOM     12  H   RES     1      -3.071  -2.008  -0.661
ATOM     13  H   RES     1      -1.509  -2.802  -0.387
ATOM     14  C   RES     1      -2.017  -1.097   1.706
ATOM     15  H   RES     1      -3.095  -1.260   1.760
ATOM     16  H   RES     1      -1.746  -0.295   2.398
ATOM     17  H   RES     1      -1.501  -2.008   2.023
ATOM     18  C   RES     1      -0.124  -0.434   0.270
ATOM     19  H   RES     1       0.167   0.379   0.941
ATOM     20  C   RES     1       0.818  -1.086  -0.412
ATOM     21  H   RES     1       0.532  -1.922  -1.056
ATOM     22  C   RES     1       2.311  -0.833  -0.387
ATOM     23  C   RES     1       2.993  -1.996   0.345
ATOM     24  H   RES     1       2.717  -2.948  -0.119
ATOM     25  H   RES     1       2.698  -2.012   1.395
ATOM     26  H   RES     1       4.083  -1.899   0.298
ATOM     27  C   RES     1       2.817  -0.793  -1.836
ATOM     28  H   RES     1       2.272  -0.074  -2.457
ATOM     29  H   RES     1       2.675  -1.772  -2.304
ATOM     30  H   RES     1       3.886  -0.560  -1.880
ATOM     31  C   RES     1       2.600   0.457   0.398
ATOM     32  O   RES     1       2.636   0.466   1.625
ATOM     33  N   RES     1       2.764   1.593  -0.341
ATOM     34  H   RES     1       2.730   1.532  -1.345
ATOM     35  C   RES     1       2.991   2.884   0.265
ATOM     36  H   RES     1       3.038   2.737   1.344
ATOM     37  H   RES     1       3.934   3.322  -0.075
ATOM     38  H   RES     1       2.178   3.582   0.038
TER
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REMARK  Compound E structure 22
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.118463
REMARK   Sum of electronic and thermal Energies=    -730.098877
REMARK   Sum of electronic and thermal Enthalpies=  -730.097933
REMARK   Sum of electronic and thermal Free Energies=  -730.166334
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.648  -1.727  -1.337
ATOM      2  C   RES     1      -3.805  -1.152  -1.723
ATOM      3  H   RES     1      -4.187  -0.303  -2.297
ATOM      4  H   RES     1      -3.252  -1.809  -2.398
ATOM      5  C   RES     1      -2.904  -0.766  -0.573
ATOM      6  O   RES     1      -2.471  -1.597   0.216
ATOM      7  N   RES     1      -2.619   0.570  -0.482
ATOM      8  H   RES     1      -2.948   1.171  -1.223
ATOM      9  C   RES     1      -1.652   1.154   0.476
ATOM     10  C   RES     1      -2.122   0.905   1.905
ATOM     11  H   RES     1      -2.211  -0.162   2.113
ATOM     12  H   RES     1      -3.102   1.367   2.057
ATOM     13  H   RES     1      -1.419   1.350   2.617
ATOM     14  C   RES     1      -1.630   2.655   0.195
ATOM     15  H   RES     1      -2.623   3.096   0.332
ATOM     16  H   RES     1      -1.293   2.865  -0.827
ATOM     17  H   RES     1      -0.941   3.156   0.881
ATOM     18  C   RES     1      -0.288   0.576   0.174
ATOM     19  H   RES     1       0.107   0.860  -0.806
ATOM     20  C   RES     1       0.406  -0.265   0.943
ATOM     21  H   RES     1      -0.021  -0.583   1.896
ATOM     22  C   RES     1       1.694  -0.965   0.580
ATOM     23  C   RES     1       2.599  -1.057   1.819
ATOM     24  H   RES     1       2.099  -1.633   2.605
ATOM     25  H   RES     1       2.844  -0.072   2.229
ATOM     26  H   RES     1       3.538  -1.564   1.576
ATOM     27  C   RES     1       1.338  -2.379   0.110
ATOM     28  H   RES     1       0.755  -2.347  -0.813
ATOM     29  H   RES     1       0.740  -2.887   0.872
ATOM     30  H   RES     1       2.244  -2.960  -0.081
ATOM     31  C   RES     1       2.468  -0.245  -0.541
ATOM     32  O   RES     1       2.835  -0.812  -1.564
ATOM     33  N   RES     1       2.773   1.061  -0.277
ATOM     34  H   RES     1       2.304   1.499   0.502
ATOM     35  C   RES     1       3.429   1.905  -1.245
ATOM     36  H   RES     1       3.910   1.257  -1.979
ATOM     37  H   RES     1       2.721   2.556  -1.774
ATOM     38  H   RES     1       4.188   2.529  -0.766
TER
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REMARK  Compound E structure 23
REMARK  ALL ENERGIES ARE EXPRESSED IN HARTREES
REMARK   Sum of electronic and zero-point Energies= -730.117827
REMARK   Sum of electronic and thermal Energies=    -730.098098
REMARK   Sum of electronic and thermal Enthalpies=  -730.097153
REMARK   Sum of electronic and thermal Free Energies=  -730.166196
REMARK   0 Virtual frequencies used

ATOM      1  H   RES     1      -4.936  -1.957  -0.831
ATOM      2  C   RES     1      -4.194  -1.346  -1.350
ATOM      3  H   RES     1      -4.718  -0.828  -2.157
ATOM      4  H   RES     1      -3.437  -2.004  -1.785
ATOM      5  C   RES     1      -3.645  -0.321  -0.385
ATOM      6  O   RES     1      -4.382   0.433   0.241
ATOM      7  N   RES     1      -2.283  -0.317  -0.264
ATOM      8  H   RES     1      -1.764  -0.852  -0.945
ATOM      9  C   RES     1      -1.517   0.685   0.493
ATOM     10  C   RES     1      -1.931   0.665   1.971
ATOM     11  H   RES     1      -1.807  -0.337   2.388
ATOM     12  H   RES     1      -2.972   0.971   2.080
ATOM     13  H   RES     1      -1.296   1.352   2.541
ATOM     14  C   RES     1      -1.748   2.081  -0.098
ATOM     15  H   RES     1      -2.808   2.340  -0.045
ATOM     16  H   RES     1      -1.427   2.120  -1.144
ATOM     17  H   RES     1      -1.179   2.830   0.462
ATOM     18  C   RES     1      -0.049   0.349   0.414
ATOM     19  H   RES     1       0.597   1.184   0.695
ATOM     20  C   RES     1       0.514  -0.821   0.096
ATOM     21  H   RES     1      -0.119  -1.683  -0.134
ATOM     22  C   RES     1       1.992  -1.145   0.116
ATOM     23  C   RES     1       2.304  -1.913   1.403
ATOM     24  H   RES     1       1.676  -2.807   1.469
ATOM     25  H   RES     1       2.123  -1.292   2.282
ATOM     26  H   RES     1       3.353  -2.219   1.423
ATOM     27  C   RES     1       2.333  -2.031  -1.093
ATOM     28  H   RES     1       2.080  -1.553  -2.045
ATOM     29  H   RES     1       1.780  -2.975  -1.036
ATOM     30  H   RES     1       3.401  -2.269  -1.111
ATOM     31  C   RES     1       2.869   0.122   0.072
ATOM     32  O   RES     1       3.713   0.369   0.925
ATOM     33  N   RES     1       2.673   0.918  -1.021
ATOM     34  H   RES     1       1.861   0.735  -1.593
ATOM     35  C   RES     1       3.343   2.187  -1.176
ATOM     36  H   RES     1       4.217   2.184  -0.524
ATOM     37  H   RES     1       3.667   2.329  -2.210
ATOM     38  H   RES     1       2.702   3.030  -0.889
TER
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