Supporting Information

# Do Anti-Bredt Natural Products Exist? Olefin Strain Energy as a Predictor of Isolability**

*Elizabeth H. Krenske* and Craig M. Williams**

# Supporting Information

**Contents** **Page**

General Description of Molecular Mechanics Calculations ..... 2
Determination of the Olefin Strain Energy Ranges Corresponding to Isolable, Observable and Unstable Alkenes with Contemporary Forcefields ..... 2
Figure S1. Bridgehead alkenes used to determine the olefin strain energy ranges corresponding to isolable, observable, and unstable alkenes ..... 3
Table S1. Forcefield energies of alkenes **S1**–**S25** and alkanes **S1**$H_2$–**S25**$H_2$ ..... 4
Table S2. Olefin strain energies of alkenes **S1**–**S25** ..... 7
Figure S2. Olefin strain energies of alkenes **S1**–**S25** computed with different force fields ..... 8
Figure S3. Olefin strain energies of alkenes **S1**–**S19** computed with different force fields, plotted against MM1 OS energy ..... 9
Olefin Strain Energy Calculations for Natural Products ..... 11
Table S3. Forcefield energies of bridgehead alkene natural products or putative bridgehead alkene natural products, and the corresponding alkanes ..... 11
Table S4. Olefin strain energies of bridgehead alkene natural products or putative bridgehead alkene natural products ..... 13
OPLS_2005 Optimized Geometries ..... 15
Density Functional Theory Calculations ..... 68
Table S5. DFT calculations on NPs giving a measure of the amount of strain energy not captured by the forcefield ..... 68
B3LYP-D3 Optimized Geometries and Associated Energies ..... 69
A Small Set of Alkenes for Rapid Estimation of OS Cutoffs for Other Forcefields ..... 73
References ..... 78

## General Description of Molecular Mechanics Calculations

Molecular mechanics (MM) calculations were performed in MacroModel 10.6[1] and Tinker 7.1.[2] The lowest-energy conformer of each bicyclic alkene and of the corresponding alkane resulting from hydrogenation of the bridgehead double bond was identified by means of a Monte Carlo Multiple Minimum (MCMM) conformational search in MacroModel 10.6 using the OPLS_2005 forcefield[3] (a modified version of OPLS-AA[4]) in the gas phase. For systems containing large rings that could potentially accommodate either inward- or outward-facing bridgehead hydrogens, all possible isomers were computed to identify the global minimum. For certain alkenes, hydrogenation of the bridgehead double bond may in principle give rise to multiple diastereomers, all of which were considered. For several of the natural products (or putative natural products) studied, the relative configuration at certain stereocentres was not completely determined in the original reports, and in these cases all possible diastereomers consistent with the published structures were considered. The lowest-energy conformer of each alkene and alkane identified by the OPLS_2005 conformational search was reoptimized using the MM2*,[5] MM3*,[6] OPLS (OPLS/AMBER),[7] and MMFF (MMFF94)[8] forcefields as implemented in MacroModel 10.6, and with the MM2,[5] MM3,[6] MMFF,[8] and OPLS-AA[4] forcefields as implemented in Tinker 7.1. Olefin strain (OS) energies were calculated by subtracting the total MM potential energy of the alkane from that of the corresponding alkene. (Note: The Tinker implementation of MMFF gave identical olefin strain energies to those listed in Table S2.)

## Determination of the Olefin Strain Energy Ranges Corresponding to Isolable, Observable and Unstable Alkenes with Contemporary Forcefields

The dataset for determination of the OS energy ranges corresponding to isolable, observable, and unstable bridgehead alkenes comprised 25 alkenes (**S1**–**S25**, Figure S1) taken from Schleyer's 1981 paper.[9]

For most of the alkenes **S21**–**S25**, and the corresponding alkanes, the lowest-energy conformer identified by the OPLS_2005 conformational search corresponded to that originally identified by Schleyer.[9] For six alkenes (**S1**, **S2**, **S5**, **S10**, **S15**, and **S17**), the conformer identified as most stable by the conformational search differed from that identified by Schleyer. These alkenes were reoptimized in Schleyer's lowest-energy conformation, resulting in a lower energy. For three other alkenes (**S3**, **S24**, and **S25**) and two alkanes (**S1**$H_2$ and **S4**$H_2$), the conformer identified by the OPLS_2005 search as most stable was lower in energy than Schleyer's most stable conformer. In these cases, the conformer identified as most stable by OPLS_2005 was used for analysis.

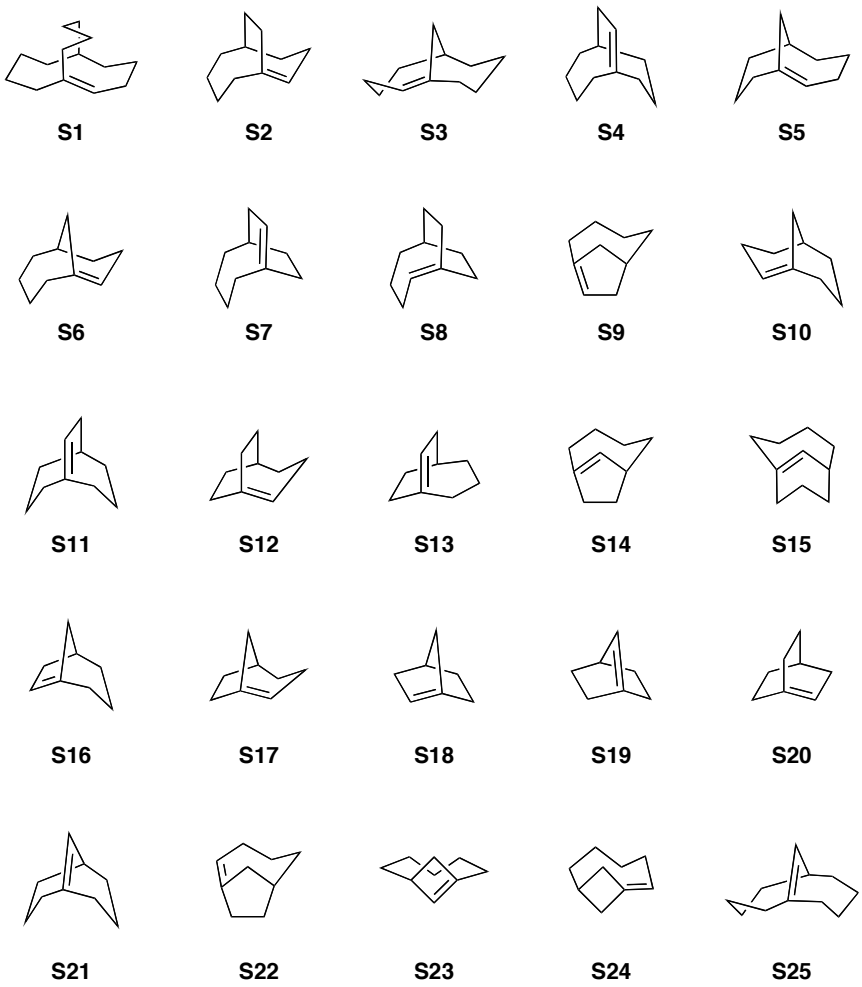



**Figure S1.** Bridgehead alkenes used to determine the olefin strain energy ranges corresponding to isolable, observable, and unstable alkenes.

The total potential energies of alkenes **S1**–**S25** and the corresponding alkenes **S1**$H_2$–**S25**$H_2$ calculated with OPLS_2005, MM2*, MM3*, OPLS, and MMFF in MacroModel 10.6 and with MM2, MM3, and OPLS-AA in Tinker 7.1 are listed in Table S1. The olefin strain energies of alkenes **S1**–**S25** are listed in Table S2 and are plotted in Figures S2 and S3.

**Table S1.** Forcefield energies of alkenes **S1**–**S25** and alkanes **S1**$H_2$–**S25**$H_2$.[a]

| | **S1** | **S1**$H_2$ | **S2** | **S2**$H_2$ |
|---|---|---|---|---|
| OPLS_2005 | 44.452 | 53.885 | 32.934 | 33.818 |
| MM2* | 48.695 | 56.447 | 32.588 | 37.262 |
| MM3* | 60.294 | 68.006 | 42.347 | 43.850 |
| OPLS | 44.452 | 49.459 | 32.107 | 27.485 |
| MMFF | 60.951 | 70.312 | 44.574 | 39.149 |
| MM2 | 48.540 | 56.448 | 32.355 | 37.263 |
| MM3 | 57.164 | 68.235 | 39.667 | 43.906 |
| OPLS-AA | 48.397 | 54.885 | 40.393 | 36.131 |
| | **S3** | **S3**$H_2$ | **S4** | **S4**$H_2$ |
| OPLS_2005 | 20.891 | 24.100 | 41.240 | 33.818 |
| MM2* | 21.870 | 27.187 | 37.542 | 37.262 |
| MM3* | 29.397 | 32.477 | 45.491 | 43.850 |
| OPLS | 19.407 | 16.695 | 36.446 | 27.485 |
| MMFF | 28.603 | 26.319 | 51.523 | 39.149 |
| MM2 | 21.697 | 27.186 | 37.116 | 37.263 |
| MM3 | 26.292 | 32.500 | 43.319 | 43.906 |
| OPLS-AA | 27.205 | 26.517 | 50.550 | 36.131 |
| | **S5** | **S5**$H_2$ | **S6** | **S6**$H_2$ |
| OPLS_2005 | 30.643 | 24.099 | 30.916 | 24.099 |
| MM2* | 25.014 | 24.196 | 24.982 | 24.196 |
| MM3* | 32.071 | 28.718 | 33.055 | 28.718 |
| OPLS | 24.699 | 14.022 | 25.288 | 14.022 |
| MMFF | 34.343 | 21.484 | 33.982 | 21.484 |
| MM2 | 24.788 | 24.197 | 24.740 | 24.197 |
| MM3 | 29.670 | 28.813 | 30.166 | 28.813 |
| OPLS-AA | 40.792 | 26.577 | 38.024 | 26.577 |
| | **S7** | **S7**$H_2$ | **S8** | **S8**$H_2$ |
| OPLS_2005 | 42.415 | 30.174 | 44.265 | 30.174 |
| MM2* | 34.350 | 29.599 | 36.453 | 29.599 |
| MM3* | 43.449 | 34.541 | 45.689 | 34.541 |
| OPLS | 38.082 | 21.665 | 40.987 | 21.665 |
| MMFF | 46.804 | 27.935 | 50.445 | 27.935 |
| MM2 | 33.913 | 29.599 | 36.089 | 29.599 |
| MM3 | 40.990 | 34.633 | 43.591 | 34.633 |
| OPLS-AA | 52.828 | 32.279 | 59.411 | 32.279 |
| | **S9** | **S9**$H_2$ | **S10** | **S10**$H_2$ |
| OPLS_2005 | 47.489 | 31.468 | 43.906 | 22.058 |
| MM2* | 30.526 | 24.362 | 29.494 | 18.263 |
| MM3* | 40.095 | 32.844 | 35.599 | 20.982 |
| OPLS | 37.791 | 17.533 | 34.914 | 10.026 |
| MMFF | 40.554 | 21.475 | 43.091 | 13.254 |
| MM2 | 30.204 | 24.362 | 28.614 | 18.263 |
| MM3 | 39.283 | 32.974 | 33.413 | 21.005 |
| OPLS-AA | 57.586 | 33.017 | 59.492 | 24.915 |

contd/

| | **S11** | **S11**$H_2$ | **S12** | **S12**$H_2$ |
|---|---|---|---|---|
| OPLS_2005 | 51.049 | 27.910 | 51.685 | 26.641 |
| MM2* | 42.512 | 29.949 | 39.288 | 24.354 |
| MM3* | 47.839 | 35.005 | 45.786 | 27.912 |
| OPLS | 41.153 | 20.217 | 44.436 | 15.207 |
| MMFF | 58.796 | 29.299 | 56.771 | 21.120 |
| MM2 | 41.288 | 29.949 | 37.955 | 24.354 |
| MM3 | 46.312 | 35.120 | 43.894 | 28.038 |
| OPLS-AA | 69.014 | 30.155 | 77.491 | 28.797 |
| | **S13** | **S13**$H_2$ | **S14** | **S14**$H_2$ |
| OPLS_2005 | 53.041 | 26.641 | 55.535 | 31.468 |
| MM2* | 39.199 | 24.354 | 38.914 | 24.362 |
| MM3* | 44.882 | 27.912 | 46.785 | 32.844 |
| OPLS | 42.840 | 15.207 | 47.795 | 17.533 |
| MMFF | 55.553 | 21.120 | 50.407 | 21.475 |
| MM2 | 37.744 | 24.354 | 37.517 | 24.362 |
| MM3 | 43.058 | 28.038 | 45.430 | 32.974 |
| OPLS-AA | 75.166 | 28.797 | 73.151 | 33.017 |
| | **S15** | **S15**$H_2$ | **S16** | **S16**$H_2$ |
| OPLS_2005 | 61.948 | 24.099 | 64.713 | 31.658 |
| MM2* | 50.141 | 24.196 | 39.098 | 19.265 |
| MM3* | 52.557 | 28.718 | 46.154 | 27.201 |
| OPLS | 46.413 | 14.022 | 53.443 | 12.848 |
| MMFF | 62.441 | 21.484 | 53.930 | 15.371 |
| MM2 | 45.433 | 24.197 | 36.062 | 19.266 |
| MM3 | 47.131 | 28.813 | 42.940 | 27.350 |
| OPLS-AA | 66.984 | 26.577 | 89.555 | 33.708 |
| | **S17** | **S17**$H_2$ | **S18** | **S18**$H_2$ |
| OPLS_2005 | 65.854 | 31.658 | 91.272 | 46.680 |
| MM2* | 41.656 | 19.265 | 51.692 | 23.093 |
| MM3* | 51.149 | 27.201 | 62.710 | 37.353 |
| OPLS | 50.904 | 12.848 | 72.782 | 19.122 |
| MMFF | 58.594 | 15.371 | 71.179 | 19.776 |
| MM2 | 40.010 | 19.266 | 44.753 | 23.094 |
| MM3 | 46.806 | 27.350 | 52.032 | 37.570 |
| OPLS-AA | 93.344 | 33.708 | 130.109 | 48.580 |
| | **S19** | **S19**$H_2$ | **S20** | **S20**$H_2$ |
| OPLS_2005 | 100.057 | 46.680 | 72.518 | 30.230 |
| MM2* | 59.359 | 23.093 | 47.561 | 19.638 |
| MM3* | 68.995 | 37.353 | 52.019 | 22.588 |
| OPLS | 87.065 | 19.122 | 58.660 | 12.005 |
| MMFF | 81.674 | 19.776 | 67.229 | 15.527 |
| MM2 | 47.893 | 23.094 | 42.953 | 19.639 |
| MM3 | 55.705 | 37.570 | 47.452 | 22.750 |
| OPLS-AA | 143.093 | 48.580 | 110.829 | 32.515 |

contd/

| | **S21** | **S21**$H_2$ | **S22** | **S22**$H_2$ |
|---|---|---|---|---|
| OPLS_2005 | 63.943 | 22.058 | 62.029 | 31.468 |
| MM2* | 45.999 | 18.263 | 44.760 | 24.362 |
| MM3* | 48.227 | 20.982 | 53.793 | 32.844 |
| OPLS | 53.327 | 10.026 | 46.980 | 17.533 |
| MMFF | 61.072 | 13.254 | 58.230 | 21.475 |
| MM2 | 41.721 | 18.263 | 43.718 | 24.362 |
| MM3 | 44.189 | 21.005 | 50.703 | 32.974 |
| OPLS-AA | 95.614 | 24.915 | 89.220 | 33.017 |
| | **S23**[b] | **S23**$H_2$ | **S24**[b] | **S24**$H_2$ |
| OPLS_2005 | 30.054 | 25.277 | 36.673 | 25.277 |
| MM2* | 55.823 | 47.609 | 56.860 | 47.609 |
| MM3* | 51.454 | 51.293 | 65.027 | 51.293 |
| OPLS | 76.512 | 34.216 | 66.683 | 34.216 |
| MMFF | 33.648 | 29.024 | 46.138 | 29.024 |
| MM2 | 65.341 | 45.958 | 62.924 | 45.958 |
| | **S25** | **S25**$H_2$ | | |
| OPLS_2005 | 46.200 | 24.100 | | |
| MM2* | 56.872 | 27.187 | | |
| MM3* | 60.188 | 32.477 | | |
| OPLS | 53.523 | 16.695 | | |
| MMFF | 77.823 | 26.319 | | |
| MM2 | 54.157 | 27.186 | | |
| MM3 | 57.506 | 32.500 | | |
| OPLS-AA | 87.969 | 26.517 | | |

[a] Energies given in kcal $mol^{-1}$. [b] MM3 and OPLS-AA energies of **S23** and **S24** were not determined.

**Table S2.** Olefin strain energies of alkenes **S1**–**S25**.[a]

| | **S1** | **S2** | **S3** | **S4** | **S5** |
|---|---|---|---|---|---|
| OPLS_2005 | –9.4 | –0.9 | –3.2 | 7.4 | 6.5 |
| MM2* | –7.8 | –4.7 | –5.3 | 0.3 | 0.8 |
| MM3* | –7.7 | –1.5 | –3.1 | 1.6 | 3.4 |
| OPLS | –5.0 | 4.6 | 2.7 | 9.0 | 10.7 |
| MMFF | –9.4 | 5.4 | 2.3 | 12.4 | 12.9 |
| MM2 | –7.9 | –4.9 | –5.5 | –0.1 | 0.6 |
| MM3 | –11.1 | –4.2 | –6.2 | –0.6 | 0.9 |
| OPLS-AA | –6.5 | 4.3 | 0.7 | 14.4 | 14.2 |
| | **S6** | **S7** | **S8** | **S9** | **S10** |
| OPLS_2005 | 6.8 | 12.2 | 14.1 | 16.0 | 21.8 |
| MM2* | 0.8 | 4.8 | 6.9 | 6.2 | 11.2 |
| MM3* | 4.3 | 8.9 | 11.1 | 7.3 | 14.6 |
| OPLS | 11.3 | 16.4 | 19.3 | 20.3 | 24.9 |
| MMFF | 12.5 | 18.9 | 22.5 | 19.1 | 29.8 |
| MM2 | 0.5 | 4.3 | 6.5 | 5.8 | 10.4 |
| MM3 | 1.4 | 6.4 | 9.0 | 6.3 | 12.4 |
| OPLS-AA | 11.4 | 20.5 | 27.1 | 24.6 | 34.6 |
| | **S11** | **S12** | **S13** | **S14** | **S15** |
| OPLS_2005 | 23.1 | 25.0 | 26.4 | 24.1 | 37.8 |
| MM2* | 12.6 | 14.9 | 14.8 | 14.6 | 25.9 |
| MM3* | 12.8 | 17.9 | 17.0 | 13.9 | 23.8 |
| OPLS | 20.9 | 29.2 | 27.6 | 30.3 | 32.4 |
| MMFF | 29.5 | 35.7 | 34.4 | 28.9 | 41.0 |
| MM2 | 11.3 | 13.6 | 13.4 | 13.2 | 21.2 |
| MM3 | 11.2 | 15.9 | 15.0 | 12.5 | 18.3 |
| OPLS-AA | 38.9 | 48.7 | 46.4 | 40.1 | 40.4 |
| | **S16** | **S17** | **S18** | **S19** | **S20** |
| OPLS_2005 | 33.1 | 34.2 | 44.6 | 53.4 | 42.3 |
| MM2* | 19.8 | 22.4 | 28.6 | 36.3 | 27.9 |
| MM3* | 19.0 | 23.9 | 25.4 | 31.6 | 29.4 |
| OPLS | 40.6 | 38.1 | 53.7 | 67.9 | 46.7 |
| MMFF | 38.6 | 43.2 | 51.4 | 61.9 | 51.7 |
| MM2 | 16.8 | 20.7 | 21.7 | 24.8 | 23.3 |
| MM3 | 15.6 | 19.5 | 14.5 | 18.1 | 24.7 |
| OPLS-AA | 55.8 | 59.6 | 81.5 | 94.5 | 78.3 |
| | **S21** | **S22** | **S23** | **S24** | **S25** |
| OPLS_2005 | 41.9 | 30.6 | 4.8 | 11.4 | 22.1 |
| MM2* | 27.7 | 20.4 | 8.2 | 9.3 | 29.7 |
| MM3* | 27.2 | 20.9 | 0.2 | 13.7 | 27.7 |
| OPLS | 43.3 | 29.4 | 42.3 | 32.5 | 36.8 |
| MMFF | 47.8 | 36.8 | 4.6 | 17.1 | 51.5 |
| MM2 | 23.5 | 19.4 | 19.4 | 17.0 | 27.0 |
| MM3 | 23.2 | 17.7 | | | 25.0 |
| OPLS-AA | 70.7 | 56.2 | | | 61.5 |

[a] Energies given in kcal mol$^{-1}$. [b] The MM3 and OPLS-AA olefin strain energies of **S23** and **S24** were not determined.

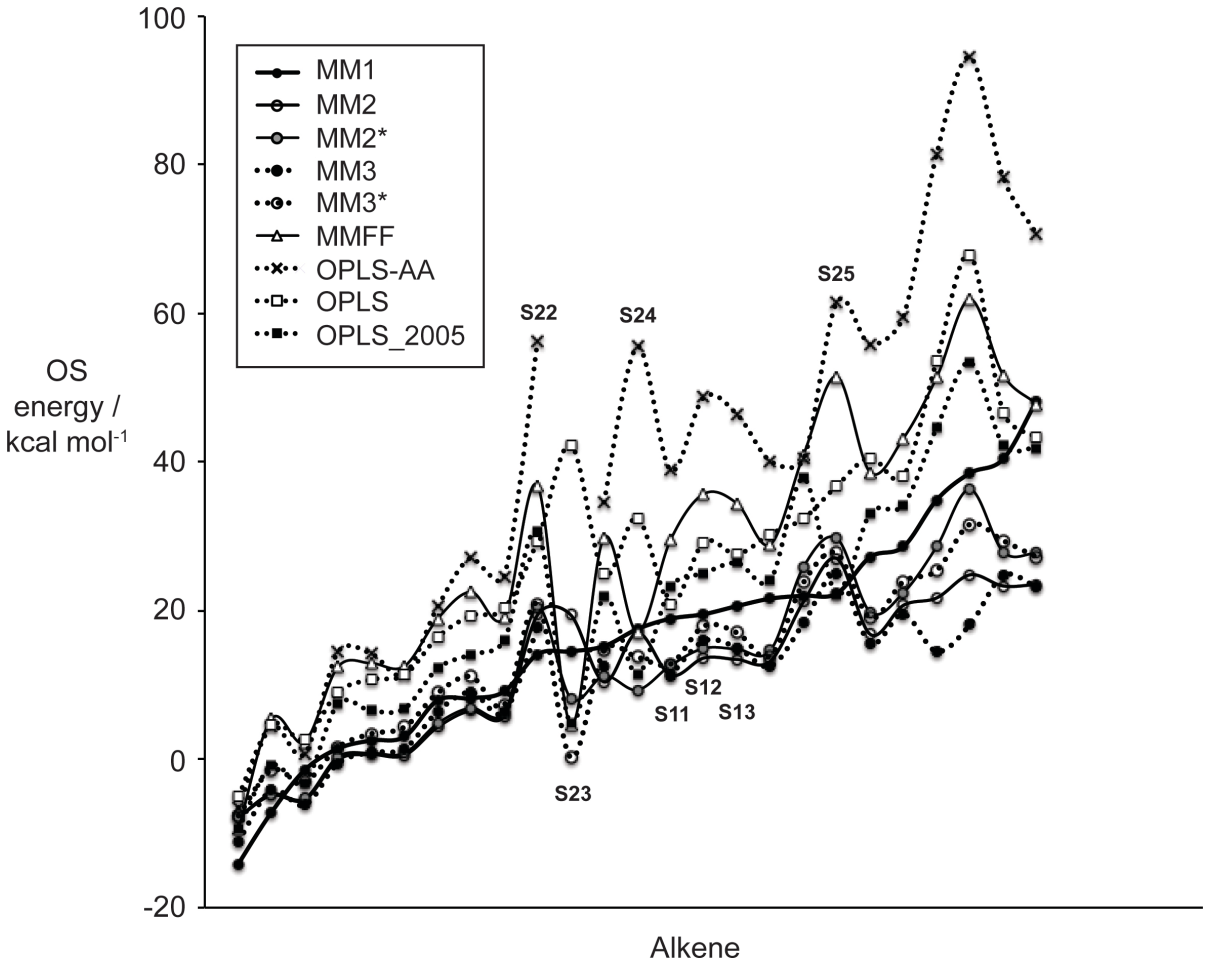



**Figure S2.** Olefin strain energies of alkenes **S1**–**S25** computed with different force fields. The alkenes are arranged in order of increasing MM1 OS energy [9] and not according to compound number.

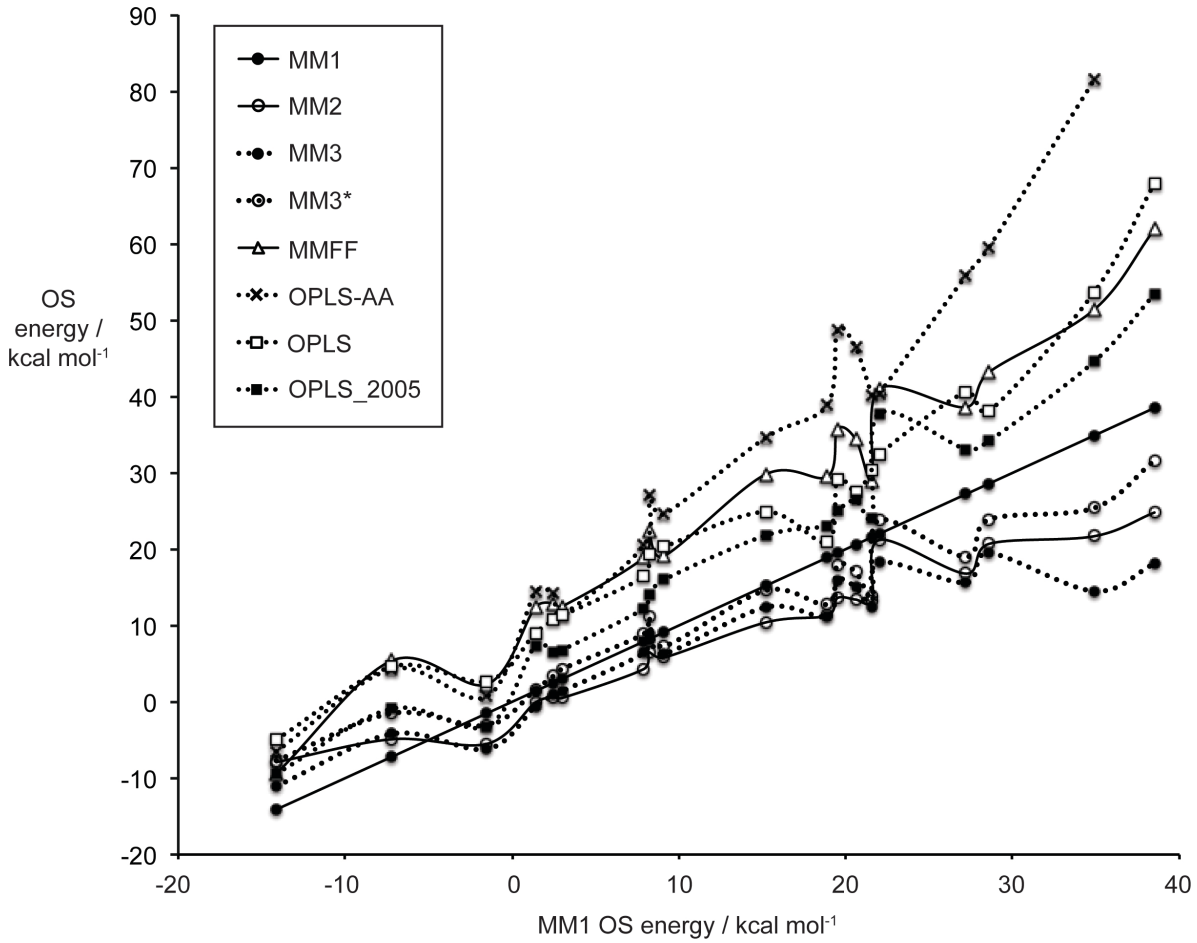



**Figure S3.** Olefin strain energies of alkenes **S1**–**S19** computed with different force fields, plotted against MM1 OS energy.[9]

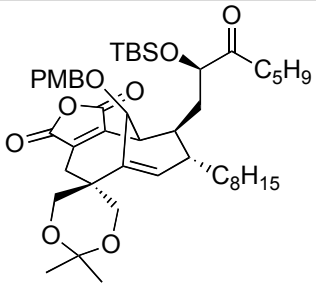
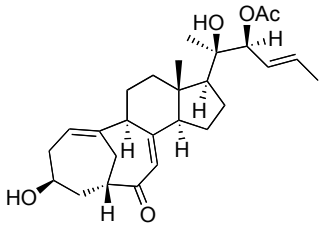
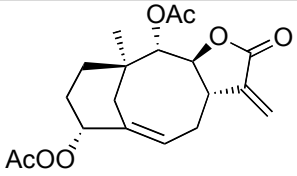
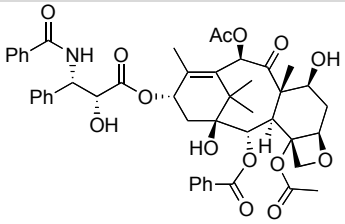
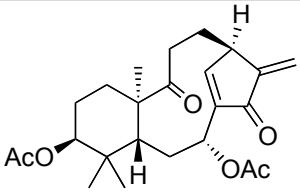
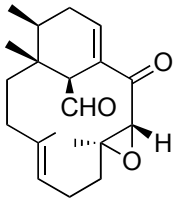
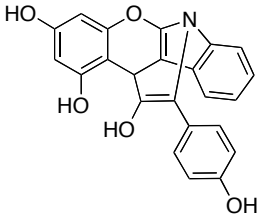
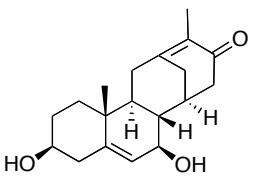
The OS energies of alkenes **S1**–**S25** computed with contemporary forcefields (OPLS_2005, MM2*, MM3*, OPLS, MMFF, MM2, MM3, and OPLS-AA) show similar general trends to the MM1 values, with several exceptions. The OS energies of alkene **S22** computed with the newer forcefields are larger than the MM1 trend would predict. Conversely, the contemporary forcefields (except OPLS) predict alkene **S23** to be much more stable than the MM1 trend predicts. Alkene **S23** contains a cyclobutene ring and would be expected to represent a difficult case for forcefield methods. The OS energies of alkene **S24** computed with OPLS_2005 and MMFF are smaller than the MM1 trend predicts, while those with OPLS and OPLS-AA are larger. The OPLS_2005 OS energy of **S25** is smaller than the MM1 trend predicts.

For the purpose of predicting the experimental behavior of bridgehead alkenes, the most critical region of Figure S2 is the region surrounding the "observable" alkenes, **S11**, **S12**, **S13**, and **S24**. Due to the erratic OS energy predictions for **S24**, and also for **S22**, **S23**, and **S25** which are found close to this region, alkenes **S22**–**S25** were excluded further from analysis and are not part of the data set of Figure 2 of the paper. Two further alkenes deserving comment are **S20** and **S21**. Most of the newer forcefields predict much smaller OS energies for these two alkenes than the MM1 trend predicts. Alkenes **S20** and **S21** are also not included in Figure 2 of the paper. Nonetheless, even taking into account their departure from the MM1 trend, **S20** and **S21** are unambiguously predicted to be highly unstable.

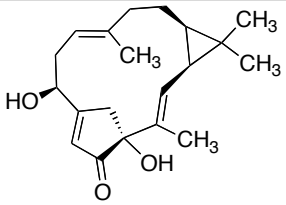
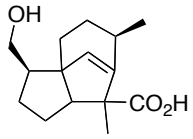
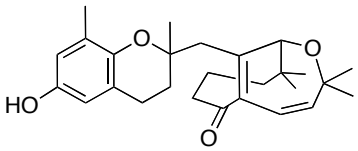
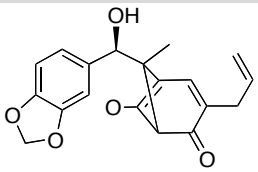
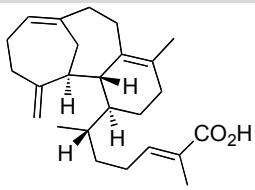
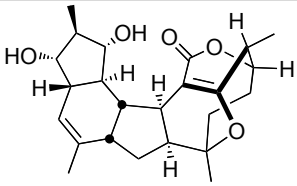
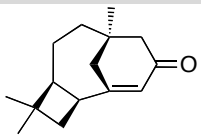
Alkenes **S11**, **S12**, and **S13** constitute the set of "observable" alkenes. For a given forcefield, the lowest OS energy out of the OS energies of alkenes **S11**–**S13** is taken as the isolable→observable "cutoff" (Figure 2 of the paper), while the highest OS energy is taken as the observable→unstable cutoff.

## Olefin Strain Energy Calculations for Natural Products

**Table S3.** Forcefield energies of bridgehead alkene natural products or putative bridgehead alkene natural products, and the corresponding alkanes.[a]

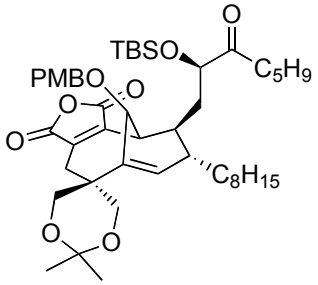
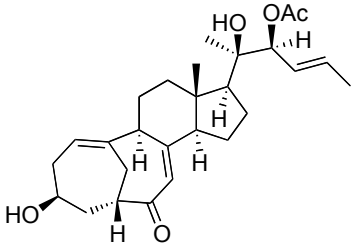
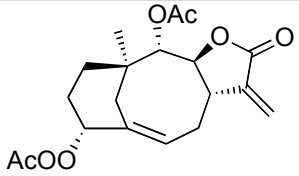
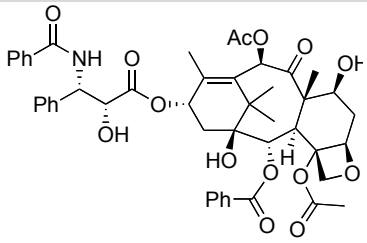
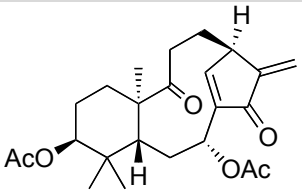
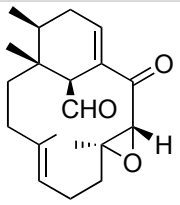
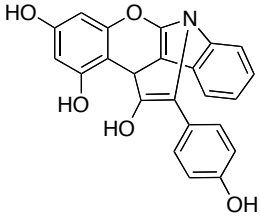
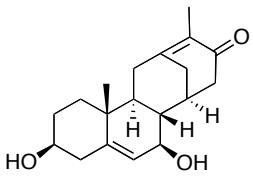
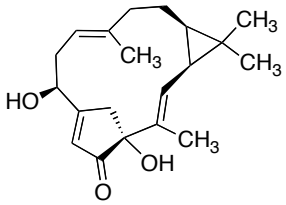
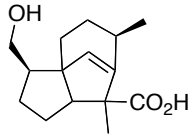
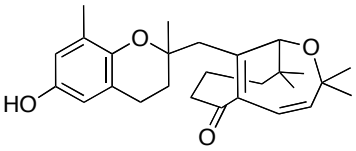
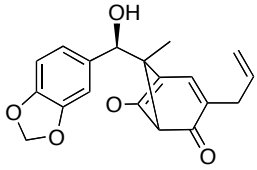
| | **5**[b] | **5**$H_2$ | **6** | **6**$H_2$ |
|---|---|---|---|---|
| |  | |  | |
| OPLS_2005 | –43.738 | –46.087 | 41.919 | 50.007 |
| MM3* | 45.050 | 25.562 | 118.399 | 110.793 |
| OPLS | 22.989 | 11.205 | 36.683 | 37.697 |
| MMFF | 56.115 | 35.027 | 129.245 | 125.023 |
| | **7** | **7**$H_2$ | **8** | **8**$H_2$ |
| |  | |  | |
| OPLS_2005 | 19.587 | 26.456 | 49.811 | 58.810 |
| MM3* | | | 191.913 | 193.050 |
| OPLS | | | 66.506 | 70.335 |
| MMFF | 88.935 | 92.889 | 236.390 | 250.925 |
| | **9** | **9**$H_2$ | **10** | **10**$H_2$ |
| |  | |  | |
| OPLS_2005 | 24.699 | 33.304 | 37.126 | 40.213 |
| MM3* | 65.570 | 72.018 | 70.572 | 56.484 |
| OPLS | 48.502 | 50.516 | 42.377 | 34.752 |
| MMFF | 64.849 | 80.660 | 86.559 | 69.948 |
| | **17** | **17**$H_2$ | **19** | **19**$H_2$ |
| |  | |  | |
| OPLS_2005 | 141.959 | 65.338 | 51.838 | 24.516 |
| MM3* | 176.322 | 24.540 | 61.253 | 47.278 |
| OPLS | 109.154 | 44.540 | 48.827 | 21.291 |
| MMFF | 189.427 | 72.953 | 88.936 | 61.971 |

contd/

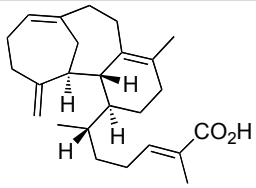
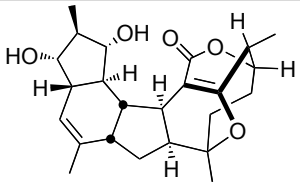
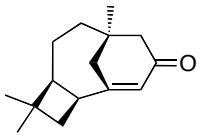
| | **21** | **21**$H_2$ | **22** | **22**$H_2$ |
|---|---|---|---|---|
| |  | |  | |
| OPLS_2005 | 19.955 | 22.528 | 111.411 | 73.458 |
| MM3* | 83.814 | 66.402 | 97.653 | 70.682 |
| OPLS | 25.281 | 32.420 | 79.954 | 31.435 |
| MMFF | 99.977 | 91.808 | 118.892 | 60.603 |
| | **23** | **23**$H_2$ | **24** | **24**$H_2$ |
| |  | |  | |
| OPLS_2005 | 43.785 | 6.642 | 103.194 | 37.498 |
| MM3* | 67.530 | 58.022 | 96.329 | 61.291 |
| OPLS | 51.718 | 31.602 | 138.048 | 51.096 |
| MMFF | 128.784 | 104.000 | 108.606 | 72.085 |
| | **25** | **25**$H_2$ | **26** | **26**$H_2$ |
| |  | |  | |
| OPLS_2005 | 15.016 | 18.546 | 83.219 | 73.089 |
| MM3* | 69.093 | 59.369 | 98.142 | 97.450 |
| OPLS | 23.146 | 20.384 | 70.563 | 59.473 |
| MMFF | 71.538 | 53.201 | 125.459 | 109.008 |
| | **27** | **27**$H_2$ | | |
| |  | | | |
| OPLS_2005 | 41.492 | 28.904 | | |
| MM3* | 61.634 | 62.750 | | |
| OPLS | 45.960 | 40.301 | | |
| MMFF | 64.997 | 53.897 | | |

[a] Energies given in kcal $mol^{-1}$. [b] The $C_5H_9$ group of **5** was modeled as Me, $C_8H_{15}$ as Me, PMB as Me, and TBS as TMS.

**Table S4.** Olefin strain energies of bridgehead alkene natural products or putative bridgehead alkene natural products.[a]

| | **5**[b] | **6** | **7** |
|---|---|---|---|
| |  |  |  |
| OPLS_2005 | 2.3 | –8.1 | –6.9 |
| MM3* | 19.5 | 7.6 | |
| OPLS | 11.8 | –1.0 | |
| MMFF | 21.1 | 4.2 | –4.0 |
| | **8** | **9** | **10** |
| |  |  |  |
| OPLS_2005 | –9.0 | –8.6 | –3.1 |
| MM3* | –1.1 | –6.4 | 14.1 |
| OPLS | –3.8 | –2.0 | 7.6 |
| MMFF | –14.5 | –15.8 | 16.6 |
| | **17** | **19** | **21** |
| |  |  |  |
| OPLS_2005 | 76.6 | 27.3 | –2.6 |
| MM3* | 151.8 | 14.0 | 17.4 |
| OPLS | 64.6 | 27.5 | –7.1 |
| MMFF | 116.5 | 27.0 | 8.2 |
| | **22** | **23** | **24** |
| |  |  |  |
| OPLS_2005 | 38.0 | 37.1 | 65.7 |
| MM3* | 27.0 | 9.5 | 35.0 |
| OPLS | 48.5 | 20.1 | 87.0 |
| MMFF | 58.3 | 24.8 | 36.5 |

contd/

| | **25** | **26** | **27** |
|---|---|---|---|
| |  |  |  |
| OPLS_2005 | –3.5 | 10.1 | 12.6 |
| MM3* | 9.7 | 0.7 | –1.1 |
| OPLS | 2.8 | 11.1 | 5.7 |
| MMFF | 18.3 | 16.5 | 11.1 |

[a] Energies given in kcal mol$^{-1}$. [b] The $C_5H_9$ group of **5** was modeled as Me, $C_8H_{15}$ as Me, PMB as Me, and TBS as TMS.

## OPLS_2005 Optimized Geometries

### S1

| | | | |
|---|---|---|---|
| C | 5.5943 | -0.7221 | -3.8038 |
| C | 6.2256 | 0.2520 | -2.7522 |
| C | 7.0015 | 1.5170 | -3.2175 |
| C | 6.4130 | 2.8694 | -2.7485 |
| C | 5.4033 | 3.5146 | -3.7241 |
| C | 4.2568 | 2.5972 | -4.1160 |
| C | 3.5876 | 1.9007 | -3.1800 |
| C | 2.5977 | 0.7767 | -3.3872 |
| C | 3.1115 | -0.5147 | -2.7229 |
| C | 4.1910 | -1.3313 | -3.4808 |
| C | 5.8922 | -0.5442 | -5.3221 |
| C | 4.8631 | 0.1704 | -6.2263 |
| C | 5.0118 | 1.6941 | -6.3868 |
| C | 3.9762 | 2.5185 | -5.6066 |
| H | 6.2279 | -1.5951 | -3.6304 |
| H | 6.9363 | -0.3356 | -2.1680 |
| H | 5.5002 | 0.5243 | -1.9920 |
| H | 7.1791 | 1.5484 | -4.2872 |
| H | 8.0018 | 1.4447 | -2.7882 |
| H | 5.9848 | 2.7735 | -1.7506 |
| H | 7.2367 | 3.5745 | -2.6302 |
| H | 5.9390 | 3.8270 | -4.6210 |
| H | 4.9892 | 4.4260 | -3.2917 |
| H | 3.8462 | 2.0657 | -2.1452 |
| H | 2.3595 | 0.6001 | -4.4328 |
| H | 1.6654 | 1.0800 | -2.9102 |
| H | 3.4420 | -0.3065 | -1.7051 |
| H | 2.2513 | -1.1736 | -2.5978 |
| H | 4.3621 | -2.2200 | -2.8709 |
| H | 3.7494 | -1.7299 | -4.3941 |
| H | 5.9456 | -1.5583 | -5.7227 |
| H | 6.8972 | -0.1658 | -5.5001 |
| H | 5.0030 | -0.2492 | -7.2237 |
| H | 3.8415 | -0.1021 | -5.9714 |
| H | 4.8624 | 1.9267 | -7.4420 |
| H | 6.0290 | 2.0191 | -6.1736 |
| H | 2.9715 | 2.1477 | -5.8028 |
| H | 3.9714 | 3.5399 | -5.9889 |

### S1$H_2$

| | | | |
|---|---|---|---|
| C | 9.5800 | 0.7589 | 0.2532 |
| C | 9.3387 | -0.7507 | 0.5941 |
| C | 8.0299 | -1.2168 | 1.2922 |
| C | 6.8648 | -1.6793 | 0.3816 |
| C | 5.7143 | -0.6592 | 0.2737 |
| C | 6.1713 | 0.6196 | -0.4366 |
| C | 6.1180 | 0.5566 | -1.9670 |
| C | 7.3482 | 1.2392 | -2.5968 |
| C | 8.6863 | 0.5160 | -2.3019 |
| C | 9.6349 | 1.1694 | -1.2574 |
| C | 9.0931 | 1.8305 | 1.2866 |
| C | 7.9362 | 2.8105 | 0.9421 |
| C | 6.5024 | 2.3889 | 1.3509 |
| C | 5.6298 | 1.9184 | 0.1705 |
| H | 10.1311 | -1.0244 | 1.2935 |
| H | 9.5462 | -1.3778 | -0.2724 |
| H | 7.6854 | -0.4909 | 2.0269 |
| H | 8.3029 | -2.0872 | 1.8906 |
| H | 6.4472 | -2.5960 | 0.8001 |
| H | 7.2314 | -1.9555 | -0.6072 |

| | | | |
|---|---|---|---|
| H | 5.3618 | -0.4279 | 1.2796 |
| H | 4.8610 | -1.0948 | -0.2474 |
| H | 5.1964 | 1.0125 | -2.3306 |
| H | 6.0888 | -0.4809 | -2.3022 |
| H | 7.1959 | 1.2491 | -3.6769 |
| H | 7.4013 | 2.2879 | -2.3041 |
| H | 8.5205 | -0.5389 | -2.0900 |
| H | 9.2357 | 0.5117 | -3.2444 |
| H | 10.6375 | 0.9033 | -1.5981 |
| H | 9.6182 | 2.2539 | -1.3613 |
| H | 9.9533 | 2.4788 | 1.4651 |
| H | 8.9212 | 1.3739 | 2.2608 |
| H | 7.9685 | 3.1200 | -0.1012 |
| H | 8.1453 | 3.7274 | 1.4950 |
| H | 6.0064 | 3.2521 | 1.7968 |
| H | 6.5293 | 1.6345 | 2.1374 |
| H | 4.5948 | 1.7833 | 0.4867 |
| H | 5.6103 | 2.7082 | -0.5814 |
| H | 7.2161 | 0.6623 | -0.2252 |
| H | 10.6503 | 0.8026 | 0.4697 |

**S2**

| | | | |
|---|---|---|---|
| C | -0.5211 | -4.6151 | -4.2112 |
| C | 0.8808 | -5.0039 | -3.6460 |
| C | 1.2560 | -6.4823 | -3.3605 |
| C | 1.4221 | -7.4086 | -4.5934 |
| C | 0.1788 | -8.2635 | -4.9110 |
| C | -1.0445 | -7.3820 | -4.9271 |
| C | -1.8219 | -7.2722 | -3.8387 |
| C | -1.7477 | -4.8513 | -3.2715 |
| C | -0.7261 | -4.9554 | -5.7108 |
| C | -1.1395 | -6.3976 | -6.0777 |
| H | -0.4425 | -3.5263 | -4.2260 |
| H | 1.0090 | -4.4603 | -2.7089 |
| H | 1.6427 | -4.5879 | -4.3065 |
| H | 0.5818 | -6.9185 | -2.6240 |
| H | 2.2225 | -6.4574 | -2.8554 |
| H | 2.2582 | -8.0870 | -4.4199 |
| H | 1.7047 | -6.8151 | -5.4636 |
| H | 0.0616 | -9.0407 | -4.1545 |
| H | 0.2880 | -8.7742 | -5.8684 |
| H | 0.1911 | -4.7127 | -6.2486 |
| H | -1.4759 | -4.2779 | -6.1216 |
| H | -2.1733 | -6.3945 | -6.4247 |
| H | -0.5579 | -6.7567 | -6.9274 |
| C | -2.6668 | -6.0498 | -3.6004 |
| H | -2.3699 | -3.9552 | -3.2739 |
| H | -1.6425 | -7.9059 | -2.9824 |
| H | -1.3916 | -4.9457 | -2.2450 |
| H | -3.3692 | -6.2405 | -2.7887 |
| H | -3.2691 | -5.8331 | -4.4828 |

**S2**$H_2$

| | | | |
|---|---|---|---|
| C | -5.3297 | -0.3446 | 1.9351 |
| C | -4.0390 | -0.5925 | 1.1185 |
| C | -3.0817 | 0.5809 | 0.8338 |
| C | -2.2258 | 1.0649 | 2.0156 |
| C | -2.8337 | 2.1483 | 2.9345 |
| C | -4.0603 | 1.7901 | 3.8159 |
| C | -4.1826 | 0.3065 | 4.2212 |
| C | -5.2173 | -0.5360 | 3.4604 |
| C | -6.2230 | 0.8434 | 1.5110 |
| C | -5.7845 | 2.2634 | 1.9104 |
| C | -5.3868 | 2.4543 | 3.3825 |

| | | | |
|---|---|---|---|
| H | -5.9447 | -1.2011 | 1.6516 |
| H | -4.3499 | -0.9747 | 0.1450 |
| H | -3.4796 | -1.4119 | 1.5716 |
| H | -3.5807 | 1.4028 | 0.3285 |
| H | -2.3795 | 0.2107 | 0.0855 |
| H | -1.3252 | 1.5074 | 1.5876 |
| H | -1.8542 | 0.2142 | 2.5848 |
| H | -3.0373 | 3.0490 | 2.3551 |
| H | -2.0319 | 2.4473 | 3.6115 |
| H | -3.8386 | 2.2888 | 4.7616 |
| H | -4.4668 | 0.2672 | 5.2738 |
| H | -3.2123 | -0.1850 | 4.2013 |
| H | -6.1997 | -0.3588 | 3.9001 |
| H | -5.0064 | -1.5859 | 3.6687 |
| H | -7.2161 | 0.6783 | 1.9313 |
| H | -6.3655 | 0.8134 | 0.4300 |
| H | -6.6250 | 2.9276 | 1.7059 |
| H | -4.9998 | 2.6341 | 1.2587 |
| H | -5.2944 | 3.5273 | 3.5564 |
| H | -6.1993 | 2.1296 | 4.0336 |

**S3**

| | | | |
|---|---|---|---|
| C | 4.1630 | 2.0104 | 12.1988 |
| C | 5.2689 | 1.0816 | 12.7614 |
| C | 4.8076 | -0.1302 | 13.6114 |
| C | 3.8748 | -1.1334 | 12.8969 |
| C | 2.4669 | -0.5880 | 12.7578 |
| C | 2.1685 | 0.5031 | 12.0347 |
| C | 0.8273 | 1.2027 | 12.1074 |
| C | 0.8640 | 2.4121 | 13.0663 |
| C | 2.0478 | 3.3947 | 12.8874 |
| C | 3.4193 | 2.8099 | 13.3015 |
| C | 3.2285 | 1.2437 | 11.2519 |
| H | 4.6726 | 2.7465 | 11.5751 |
| H | 5.9563 | 1.6816 | 13.3590 |
| H | 5.8666 | 0.7082 | 11.9288 |
| H | 4.3401 | 0.2109 | 14.5352 |
| H | 5.7016 | -0.6691 | 13.9273 |
| H | 3.8192 | -2.0599 | 13.4692 |
| H | 4.2720 | -1.4017 | 11.9174 |
| H | 0.0619 | 0.4990 | 12.4370 |
| H | 0.5360 | 1.5197 | 11.1054 |
| H | 0.8681 | 2.0454 | 14.0936 |
| H | -0.0712 | 2.9627 | 12.9588 |
| H | 1.8505 | 4.2572 | 13.5252 |
| H | 2.0809 | 3.7892 | 11.8714 |
| H | 4.0701 | 3.6244 | 13.6216 |
| H | 3.2772 | 2.1966 | 14.1909 |
| H | 3.7942 | 0.5445 | 10.6353 |
| H | 2.7538 | 1.9255 | 10.5457 |
| H | 1.7082 | -1.0452 | 13.3764 |

**S3**$H_2$

| | | | |
|---|---|---|---|
| C | 12.8820 | 6.2261 | -1.5415 |
| C | 14.2620 | 6.6426 | -2.0956 |
| C | 14.2557 | 7.6372 | -3.2728 |
| C | 13.4871 | 8.9497 | -3.0285 |
| C | 11.9589 | 8.7706 | -3.0614 |
| C | 11.3169 | 8.3312 | -1.7257 |
| C | 9.8736 | 7.8053 | -1.8840 |
| C | 9.7031 | 6.5054 | -2.6941 |
| C | 10.5368 | 5.3053 | -2.2062 |
| C | 12.0312 | 5.4259 | -2.5539 |
| C | 12.1699 | 7.4003 | -0.8417 |

| | | | |
|---|---|---|---|
| H | 14.8018 | 5.7464 | -2.4045 |
| H | 14.8554 | 7.0670 | -1.2846 |
| H | 13.8791 | 7.1523 | -4.1735 |
| H | 15.2927 | 7.8870 | -3.5002 |
| H | 13.7577 | 9.6410 | -3.8277 |
| H | 13.8084 | 9.4302 | -2.1038 |
| H | 11.7042 | 8.0821 | -3.8650 |
| H | 11.5021 | 9.7171 | -3.3535 |
| H | 9.2651 | 8.5828 | -2.3478 |
| H | 9.4404 | 7.6576 | -0.8938 |
| H | 9.9059 | 6.6898 | -3.7492 |
| H | 8.6494 | 6.2269 | -2.6546 |
| H | 10.1508 | 4.4149 | -2.7039 |
| H | 10.3925 | 5.1309 | -1.1395 |
| H | 12.4556 | 4.4236 | -2.6249 |
| H | 12.1252 | 5.8366 | -3.5575 |
| H | 12.9160 | 7.9981 | -0.3168 |
| H | 11.5415 | 7.0060 | -0.0422 |
| H | 13.1032 | 5.5257 | -0.7343 |
| H | 11.2198 | 9.2459 | -1.1383 |

### **S4**

| | | | |
|---|---|---|---|
| C | -3.2748 | 0.0977 | 10.1217 |
| C | -3.6937 | -0.9350 | 11.2281 |
| C | -3.9365 | -2.4487 | 10.9084 |
| C | -2.7222 | -3.4100 | 10.7225 |
| C | -2.0229 | -3.4167 | 9.3337 |
| C | -1.7010 | -2.0116 | 8.8802 |
| C | -1.1841 | -1.1598 | 9.7760 |
| C | -1.7440 | 0.2253 | 9.8864 |
| C | -4.0920 | 0.0453 | 8.8027 |
| C | -3.8593 | -1.1411 | 7.8359 |
| C | -2.3899 | -1.5258 | 7.6132 |
| H | -3.5422 | 1.0655 | 10.5499 |
| H | -4.6380 | -0.5679 | 11.6328 |
| H | -2.9972 | -0.8597 | 12.0640 |
| H | -4.6662 | -2.5782 | 10.1159 |
| H | -4.4628 | -2.8338 | 11.7828 |
| H | -3.0694 | -4.4275 | 10.9065 |
| H | -1.9961 | -3.2241 | 11.5140 |
| H | -2.6692 | -3.8982 | 8.5991 |
| H | -1.1045 | -4.0033 | 9.3724 |
| H | -0.7975 | -1.5479 | 10.7062 |
| H | -1.2610 | 0.7258 | 10.7264 |
| H | -1.5202 | 0.8142 | 8.9964 |
| H | -3.8791 | 0.9618 | 8.2506 |
| H | -5.1554 | 0.0992 | 9.0389 |
| H | -4.2910 | -0.8733 | 6.8710 |
| H | -4.4216 | -2.0192 | 8.1384 |
| H | -2.3160 | -2.3039 | 6.8528 |
| H | -1.8449 | -0.6710 | 7.2115 |

### **S4**$H_2$

Same as **S2**$H_2$.

### **S5**

| | | | |
|---|---|---|---|
| C | -2.5017 | -3.9447 | 2.8385 |
| C | -0.9730 | -3.6343 | 2.7952 |
| C | -1.8466 | -1.0066 | 3.7686 |
| C | -2.9701 | -1.6602 | 3.4295 |
| C | -3.7926 | -1.2906 | 2.2184 |
| C | -3.3551 | -2.2272 | 1.0627 |
| C | -3.2120 | -3.7246 | 1.4721 |

| | | | |
|---|---|---|---|
| C | -3.2199 | -3.0763 | 3.8733 |
| H | -2.6257 | -4.9874 | 3.1343 |
| H | -3.6500 | -0.2433 | 1.9493 |
| H | -4.8508 | -1.4245 | 2.4459 |
| H | -2.3916 | -1.8787 | 0.6895 |
| H | -4.0458 | -2.1333 | 0.2242 |
| H | -4.2112 | -4.1582 | 1.5317 |
| H | -2.6970 | -4.2786 | 0.6864 |
| H | -2.8677 | -3.2504 | 4.8898 |
| H | -4.2909 | -3.2827 | 3.8926 |
| C | -0.3631 | -3.1179 | 4.1317 |
| H | -0.4502 | -4.5417 | 2.4908 |
| C | -0.7030 | -1.6481 | 4.5443 |
| H | -0.7490 | -2.9082 | 2.0136 |
| H | -1.6276 | -0.0543 | 3.3076 |
| H | 0.7223 | -3.2036 | 4.0692 |
| H | -0.6440 | -3.7986 | 4.9362 |
| H | 0.1777 | -1.0266 | 4.3791 |
| H | -0.9148 | -1.5883 | 5.6124 |

**S5**$H_2$

| | | | |
|---|---|---|---|
| C | 2.5895 | -5.3032 | 2.8841 |
| C | 2.9701 | -4.9273 | 1.4360 |
| C | 3.7330 | -3.6093 | 1.2257 |
| C | 2.9752 | -2.3602 | 1.7018 |
| C | 3.1230 | -2.0598 | 3.2047 |
| C | 2.5409 | -3.0906 | 4.2077 |
| C | 3.6119 | -3.6584 | 5.1601 |
| C | 4.5473 | -4.6484 | 4.4500 |
| C | 3.7617 | -5.7838 | 3.7712 |
| C | 1.7212 | -4.2450 | 3.5944 |
| H | 2.0551 | -4.8845 | 0.8435 |
| H | 3.5518 | -5.7410 | 1.0011 |
| H | 3.9055 | -3.5062 | 0.1537 |
| H | 4.7279 | -3.6510 | 1.6637 |
| H | 1.9247 | -2.4149 | 1.4153 |
| H | 3.3733 | -1.5016 | 1.1596 |
| H | 2.6415 | -1.0993 | 3.3935 |
| H | 4.1769 | -1.8815 | 3.4208 |
| H | 1.8473 | -2.5293 | 4.8361 |
| H | 3.1201 | -4.1690 | 5.9893 |
| H | 4.1906 | -2.8503 | 5.6094 |
| H | 5.2455 | -5.0724 | 5.1724 |
| H | 5.1647 | -4.1224 | 3.7257 |
| H | 4.4383 | -6.4190 | 3.1985 |
| H | 3.3538 | -6.4220 | 4.5563 |
| H | 0.9437 | -3.8671 | 2.9302 |
| H | 1.1839 | -4.7403 | 4.4045 |
| H | 1.9479 | -6.1780 | 2.7648 |

**S6**

| | | | |
|---|---|---|---|
| C | 0.8274 | -2.7359 | -0.3798 |
| C | -0.4555 | -2.8663 | -1.1628 |
| C | -1.4216 | -1.7109 | -0.7990 |
| C | -0.7419 | -0.3609 | -0.4294 |
| C | -0.2383 | -0.2428 | 1.0381 |
| C | 0.9635 | -1.1344 | 1.4613 |
| C | 2.3397 | -0.6654 | 0.8820 |
| C | 3.0271 | -1.6802 | -0.0763 |
| C | 1.9806 | -2.3452 | -0.9439 |
| C | 0.6809 | -2.6035 | 1.1188 |
| H | -0.9193 | -3.8320 | -0.9591 |
| H | -0.2301 | -2.8441 | -2.2299 |
| H | -2.0643 | -2.0181 | 0.0268 |

| | | | |
|---|---|---|---|
| H | -2.0949 | -1.5547 | -1.6426 |
| H | -1.4811 | 0.4271 | -0.5771 |
| H | 0.0613 | -0.1313 | -1.1306 |
| H | -1.0774 | -0.4579 | 1.7010 |
| H | 0.0167 | 0.7988 | 1.2374 |
| H | 1.0339 | -1.0615 | 2.5477 |
| H | 3.0236 | -0.4298 | 1.6982 |
| H | 2.1996 | 0.2743 | 0.3464 |
| H | 3.5465 | -2.4524 | 0.4924 |
| H | 3.7728 | -1.1839 | -0.6980 |
| H | -0.3009 | -2.9299 | 1.4635 |
| H | 1.4115 | -3.2511 | 1.6055 |
| H | 2.0928 | -2.2785 | -2.0163 |

### **S6**$H_2$

Same as **S5**$H_2$.

### **S7**

| | | | |
|---|---|---|---|
| C | -7.9614 | -5.2591 | -1.5906 |
| C | -6.8086 | -4.2491 | -1.9325 |
| C | -6.2615 | -4.1237 | -3.3981 |
| C | -5.2790 | -5.2120 | -3.9308 |
| C | -5.9183 | -6.5193 | -4.4732 |
| C | -7.0104 | -6.9405 | -3.5274 |
| C | -6.6502 | -7.2232 | -2.2643 |
| C | -7.4610 | -6.6520 | -1.1332 |
| C | -8.9563 | -5.4588 | -2.7514 |
| C | -8.4053 | -6.4013 | -3.8479 |
| H | -5.9750 | -4.4014 | -1.2461 |
| H | -7.1923 | -3.2604 | -1.6772 |
| H | -5.7070 | -3.1849 | -3.4255 |
| H | -7.0739 | -3.9691 | -4.1075 |
| H | -4.5664 | -5.4520 | -3.1408 |
| H | -4.6792 | -4.7807 | -4.7331 |
| H | -5.1634 | -7.3035 | -4.5435 |
| H | -6.3174 | -6.3797 | -5.4783 |
| H | -5.6135 | -7.4243 | -2.0354 |
| H | -8.2910 | -7.3189 | -0.8964 |
| H | -6.8397 | -6.5714 | -0.2407 |
| H | -9.2406 | -4.4966 | -3.1787 |
| H | -9.8790 | -5.8870 | -2.3574 |
| H | -9.0714 | -7.2576 | -3.9577 |
| H | -8.4138 | -5.8952 | -4.8134 |
| H | -8.5136 | -4.8332 | -0.7513 |

### **S7**$H_2$

| | | | |
|---|---|---|---|
| C | 5.7830 | -1.2829 | 2.8873 |
| C | 6.0634 | -0.1187 | 3.8669 |
| C | 5.1178 | 1.0984 | 3.8437 |
| C | 4.9982 | 1.8122 | 2.4868 |
| C | 3.8168 | 1.3597 | 1.6063 |
| C | 3.7215 | -0.1354 | 1.2200 |
| C | 3.2549 | -1.0586 | 2.3698 |
| C | 4.3774 | -1.9000 | 3.0098 |
| C | 6.1619 | -0.9807 | 1.4186 |
| C | 4.9615 | -0.6910 | 0.4952 |
| H | 6.4763 | -2.0635 | 3.2060 |
| H | 7.0856 | 0.2296 | 3.7131 |
| H | 6.0542 | -0.5206 | 4.8809 |
| H | 5.5140 | 1.8168 | 4.5625 |
| H | 4.1350 | 0.8387 | 4.2334 |
| H | 5.9374 | 1.7627 | 1.9384 |
| H | 4.8538 | 2.8753 | 2.6830 |

| | | | |
|---|---|---|---|
| H | 3.8518 | 1.9449 | 0.6864 |
| H | 2.8857 | 1.6559 | 2.0911 |
| H | 2.9140 | -0.1634 | 0.4861 |
| H | 2.5012 | -1.7486 | 1.9881 |
| H | 2.7315 | -0.4808 | 3.1307 |
| H | 4.1392 | -2.1138 | 4.0524 |
| H | 4.3978 | -2.8697 | 2.5102 |
| H | 6.8822 | -0.1647 | 1.3735 |
| H | 6.6972 | -1.8370 | 1.0061 |
| H | 5.2630 | -0.0285 | -0.3169 |
| H | 4.6718 | -1.6273 | 0.0159 |

## S8

| | | | |
|---|---|---|---|
| C | -1.4465 | -0.5217 | 1.8069 |
| C | -1.3844 | 0.5557 | 0.6600 |
| C | -0.2626 | 1.6494 | 0.6773 |
| C | 1.1831 | 1.2402 | 0.2641 |
| C | 1.4330 | -0.2389 | 0.4393 |
| C | 1.1804 | -0.8870 | 1.5877 |
| C | 0.8553 | -0.1825 | 2.8973 |
| C | -0.6790 | -0.1237 | 3.0938 |
| C | -1.0076 | -1.9636 | 1.3716 |
| C | 0.5189 | -2.2344 | 1.4927 |
| H | -2.5017 | -0.6023 | 2.0737 |
| H | -2.3288 | 1.1001 | 0.7010 |
| H | -1.3993 | 0.0691 | -0.3156 |
| H | -0.2369 | 2.1252 | 1.6569 |
| H | -0.5697 | 2.4540 | 0.0082 |
| H | 1.9190 | 1.8118 | 0.8306 |
| H | 1.3521 | 1.4801 | -0.7862 |
| H | 1.4230 | -0.8051 | -0.4811 |
| H | 1.2960 | 0.8137 | 2.9228 |
| H | 1.3154 | -0.7313 | 3.7195 |
| H | -0.9879 | 0.8599 | 3.4484 |
| H | -0.9539 | -0.8193 | 3.8878 |
| H | -1.5325 | -2.7001 | 1.9812 |
| H | -1.3358 | -2.1521 | 0.3490 |
| H | 0.7449 | -2.8076 | 2.3928 |
| H | 0.8884 | -2.8099 | 0.6429 |

## S8$H_2$

Same as **S7**$H_2$.

## S9

| | | | |
|---|---|---|---|
| C | 1.2434 | 2.4199 | 2.9156 |
| C | 1.0442 | 3.7660 | 3.6829 |
| C | -0.3758 | 4.0969 | 4.2564 |
| C | -0.9807 | 3.1049 | 5.3013 |
| C | -1.5479 | 1.7753 | 4.7266 |
| C | -0.6820 | 1.3399 | 3.5754 |
| C | -0.9448 | 1.7383 | 2.3275 |
| C | 0.3151 | 2.2535 | 1.6834 |
| C | 0.7996 | 1.2727 | 3.8195 |
| H | 2.2914 | 2.3167 | 2.6304 |
| H | 1.3425 | 4.5808 | 3.0223 |
| H | 1.7570 | 3.7953 | 4.5080 |
| H | -1.0830 | 4.2473 | 3.4404 |
| H | -0.3022 | 5.0720 | 4.7392 |
| H | -1.7821 | 3.6059 | 5.8454 |
| H | -0.2217 | 2.8860 | 6.0531 |
| H | -2.5729 | 1.9116 | 4.3792 |
| H | -1.5690 | 1.0010 | 5.4942 |
| H | 0.6947 | 1.5195 | 0.9716 |

| | | | |
|---|---|---|---|
| H | 0.1485 | 3.1981 | 1.1646 |
| H | 1.1821 | 0.3173 | 3.4577 |
| H | 1.0933 | 1.3835 | 4.8636 |
| H | -1.9077 | 2.0979 | 1.9949 |

**S9**$H_2$

| | | | |
|---|---|---|---|
| C | 1.4303 | 3.0285 | 0.5652 |
| C | 0.0287 | 3.5476 | 0.1662 |
| C | -1.1128 | 2.5092 | 0.1155 |
| C | -0.7770 | 1.1884 | -0.5967 |
| C | -0.0130 | 0.1811 | 0.2880 |
| C | 1.3949 | 0.6133 | 0.7525 |
| C | 2.3383 | 0.9444 | -0.4094 |
| C | 2.2312 | 2.4609 | -0.6250 |
| C | 1.3921 | 1.8926 | 1.5940 |
| H | 1.9810 | 3.8736 | 0.9816 |
| H | 0.0939 | 4.0638 | -0.7923 |
| H | -0.2668 | 4.3192 | 0.8784 |
| H | -1.9610 | 2.9728 | -0.3897 |
| H | -1.4671 | 2.2947 | 1.1244 |
| H | -0.2454 | 1.3786 | -1.5288 |
| H | -1.7150 | 0.7172 | -0.8927 |
| H | 0.0776 | -0.7576 | -0.2600 |
| H | -0.6183 | -0.0540 | 1.1643 |
| H | 2.1094 | 0.3779 | -1.3129 |
| H | 3.3620 | 0.6938 | -0.1276 |
| H | 3.2281 | 2.9018 | -0.6635 |
| H | 1.7563 | 2.6862 | -1.5801 |
| H | 2.3027 | 1.9247 | 2.1943 |
| H | 0.5558 | 1.9561 | 2.2908 |
| H | 1.8110 | -0.2068 | 1.3397 |

**S10**

| | | | |
|---|---|---|---|
| C | 1.9494 | 1.7860 | -2.1328 |
| C | 3.0803 | 2.6338 | -2.7987 |
| C | 4.5042 | 2.4465 | -2.1834 |
| C | 4.5241 | 2.3466 | -0.6332 |
| C | 3.3916 | 1.4221 | -0.2724 |
| C | 3.5537 | 0.1013 | -0.4552 |
| C | 2.0113 | 0.2470 | -2.4327 |
| C | 2.0471 | 2.0153 | -0.6226 |
| H | 0.9909 | 2.1642 | -2.4911 |
| H | 2.8113 | 3.6862 | -2.6980 |
| H | 3.1110 | 2.4445 | -3.8723 |
| H | 5.1667 | 3.2455 | -2.5173 |
| H | 4.9256 | 1.5258 | -2.5894 |
| H | 4.3678 | 3.3223 | -0.1718 |
| H | 5.4795 | 1.9628 | -0.2728 |
| H | 1.2433 | 1.5086 | -0.0864 |
| H | 1.9947 | 3.0718 | -0.3563 |
| C | 2.4737 | -0.6339 | -1.2251 |
| H | 1.0326 | -0.1021 | -2.7642 |
| H | 4.5486 | -0.3171 | -0.5068 |
| H | 2.6803 | 0.0755 | -3.2768 |
| H | 1.6364 | -0.8223 | -0.5519 |
| H | 2.8374 | -1.6060 | -1.5590 |

**S10**$H_2$

| | | | |
|---|---|---|---|
| C | 0.8033 | 0.6302 | -0.5224 |
| C | 2.0424 | 0.5775 | 0.4014 |
| C | 2.2833 | 1.8674 | 1.2143 |
| C | 2.0565 | 3.1583 | 0.3989 |
| C | 0.8168 | 3.1173 | -0.5248 |
| C | -0.5457 | 3.1723 | 0.2048 |

| | | | |
|---|---|---|---|
| C | -0.9048 | 1.8845 | 0.9765 |
| C | -0.5597 | 0.5914 | 0.2073 |
| C | 0.8768 | 1.8725 | -1.4188 |
| H | 0.8464 | -0.2515 | -1.1638 |
| H | 2.9208 | 0.4003 | -0.2208 |
| H | 1.9790 | -0.2797 | 1.0727 |
| H | 3.3022 | 1.8622 | 1.6029 |
| H | 1.6597 | 1.8716 | 2.1039 |
| H | 2.9367 | 3.3247 | -0.2236 |
| H | 2.0024 | 4.0173 | 1.0685 |
| H | 0.8695 | 3.9972 | -1.1678 |
| H | -1.3220 | 3.3475 | -0.5413 |
| H | -0.5824 | 4.0312 | 0.8757 |
| H | -1.9700 | 1.8905 | 1.2097 |
| H | -0.4200 | 1.8828 | 1.9488 |
| H | -0.6058 | -0.2658 | 0.8798 |
| H | -1.3379 | 0.4232 | -0.5385 |
| H | 0.0542 | 1.8763 | -2.1354 |
| H | 1.7966 | 1.8669 | -2.0055 |

**S11**

| | | | |
|---|---|---|---|
| C | 11.4132 | 1.3482 | -0.6594 |
| C | 12.8735 | 1.2876 | -1.1747 |
| C | 13.5558 | -0.0995 | -1.2248 |
| C | 12.6612 | -1.2721 | -1.6700 |
| C | 11.3743 | -1.4382 | -0.8670 |
| C | 11.5278 | -1.7257 | 0.6077 |
| C | 11.8252 | -0.4070 | 1.3868 |
| C | 11.2251 | 0.9414 | 0.8496 |
| C | 10.4237 | 0.6477 | -1.6402 |
| C | 10.2565 | -0.7757 | -1.1907 |
| H | 11.1460 | 2.4051 | -0.7100 |
| H | 13.4930 | 1.9578 | -0.5775 |
| H | 12.8912 | 1.7082 | -2.1811 |
| H | 14.0163 | -0.3325 | -0.2688 |
| H | 14.4029 | -0.0360 | -1.9085 |
| H | 13.2250 | -2.2034 | -1.6096 |
| H | 12.4012 | -1.1510 | -2.7224 |
| H | 12.3082 | -2.4691 | 0.7738 |
| H | 10.6018 | -2.1666 | 0.9800 |
| H | 12.9000 | -0.2869 | 1.4975 |
| H | 11.4846 | -0.5435 | 2.4136 |
| H | 10.1586 | 0.9597 | 1.0773 |
| H | 11.6475 | 1.7402 | 1.4604 |
| H | 9.4468 | 1.1320 | -1.6191 |
| H | 10.7763 | 0.6905 | -2.6714 |
| H | 9.4321 | -0.8552 | -0.4959 |

**S11**$H_2$

| | | | |
|---|---|---|---|
| C | 1.9947 | 2.1200 | -2.7017 |
| C | 2.7992 | 2.5956 | -1.4736 |
| C | 3.1748 | 1.5075 | -0.4603 |
| C | 1.9778 | 0.7948 | 0.1809 |
| C | 1.0463 | 0.0407 | -0.7914 |
| C | 1.7732 | -0.9215 | -1.7629 |
| C | 1.8930 | -0.4459 | -3.2229 |
| C | 2.6052 | 0.9025 | -3.4387 |
| C | 0.4761 | 2.0249 | -2.4420 |
| C | -0.0161 | 0.9459 | -1.4507 |
| H | 2.0926 | 2.9484 | -3.4058 |
| H | 2.2572 | 3.3950 | -0.9668 |
| H | 3.7251 | 3.0527 | -1.8255 |
| H | 3.7619 | 1.9696 | 0.3341 |
| H | 3.8460 | 0.7817 | -0.9172 |

| | | | |
|---|---|---|---|
| H | 1.3974 | 1.5098 | 0.7652 |
| H | 2.3691 | 0.0797 | 0.9058 |
| H | 0.4685 | -0.6122 | -0.1346 |
| H | 1.2213 | -1.8623 | -1.7814 |
| H | 2.7556 | -1.1870 | -1.3724 |
| H | 0.9013 | -0.4084 | -3.6744 |
| H | 2.4270 | -1.2097 | -3.7891 |
| H | 3.6660 | 0.8088 | -3.2060 |
| H | 2.5758 | 1.1074 | -4.5098 |
| H | -0.0295 | 1.8750 | -3.3970 |
| H | 0.1221 | 2.9965 | -2.0947 |
| H | -0.5883 | 1.4389 | -0.6637 |
| H | -0.7425 | 0.3118 | -1.9607 |

**S12**

| | | | |
|---|---|---|---|
| C | 1.1543 | -2.4721 | -3.2288 |
| C | 0.1548 | -2.3442 | -4.4030 |
| C | -1.1550 | -1.6467 | -3.9612 |
| C | -1.0153 | -1.1153 | -2.5393 |
| C | -1.1443 | -1.9337 | -1.4820 |
| C | -0.8131 | -3.3945 | -1.6817 |
| C | 0.6622 | -3.5237 | -2.1724 |
| C | 1.4352 | -1.0450 | -2.6361 |
| C | 0.1563 | -0.1722 | -2.4465 |
| H | -0.0629 | -3.3239 | -4.8298 |
| H | 0.6167 | -1.7629 | -5.2020 |
| H | -2.0034 | -2.3287 | -4.0243 |
| H | -1.3861 | -0.8193 | -4.6329 |
| H | -0.7841 | -1.5669 | -0.5311 |
| H | -1.4950 | -3.8354 | -2.4089 |
| H | -0.9659 | -3.9408 | -0.7506 |
| H | 1.3255 | -3.4773 | -1.3080 |
| H | 0.7955 | -4.5262 | -2.5808 |
| H | 1.9550 | -1.1480 | -1.6829 |
| H | 2.1258 | -0.5094 | -3.2885 |
| H | 0.1740 | 0.3565 | -1.4924 |
| H | 0.0767 | 0.5827 | -3.2298 |
| H | 2.0999 | -2.8479 | -3.6226 |

**S12**$H_2$

| | | | |
|---|---|---|---|
| C | 1.3899 | -3.0564 | 1.0402 |
| C | 2.5462 | -2.0520 | 0.8692 |
| C | 2.4290 | -1.1911 | -0.4033 |
| C | 1.1793 | -1.5090 | -1.2472 |
| C | 1.3323 | -2.8252 | -2.0449 |
| C | 0.9015 | -4.0983 | -1.2964 |
| C | 1.5295 | -4.2740 | 0.0969 |
| C | 0.0288 | -2.3359 | 0.9139 |
| C | -0.0891 | -1.4706 | -0.3654 |
| H | 3.5053 | -2.5711 | 0.8831 |
| H | 2.5646 | -1.3890 | 1.7353 |
| H | 3.3311 | -1.2918 | -1.0080 |
| H | 2.3947 | -0.1412 | -0.1092 |
| H | 2.3609 | -2.9323 | -2.3910 |
| H | 0.7295 | -2.7551 | -2.9513 |
| H | 1.1421 | -4.9689 | -1.9075 |
| H | -0.1849 | -4.1105 | -1.2046 |
| H | 1.0536 | -5.1354 | 0.5674 |
| H | 2.5806 | -4.5462 | -0.0051 |
| H | -0.7848 | -3.0611 | 0.9561 |

| | | | |
|---|---|---|---|
| H | -0.1103 | -1.6920 | 1.7832 |
| H | -0.9601 | -1.7733 | -0.9479 |
| H | -0.2810 | -0.4382 | -0.0704 |
| H | 1.0928 | -0.7129 | -1.9886 |
| H | 1.4652 | -3.4487 | 2.0557 |

### S13

| | | | |
|---|---|---|---|
| C | 1.2658 | -2.8341 | -0.1425 |
| C | 1.8057 | -1.8166 | 0.8890 |
| C | 1.5975 | -0.3624 | 0.3946 |
| C | 0.7526 | -0.3311 | -0.8771 |
| C | 1.1056 | -1.1172 | -1.9087 |
| C | 1.7965 | -2.4127 | -1.5441 |
| C | -0.3037 | -2.9043 | -0.0994 |
| C | -1.0862 | -1.5834 | 0.2340 |
| C | -0.7305 | -0.3156 | -0.5964 |
| H | 1.6619 | -3.8233 | 0.0918 |
| H | 1.3266 | -1.9681 | 1.8568 |
| H | 2.8700 | -1.9886 | 1.0547 |
| H | 2.5676 | 0.0740 | 0.1536 |
| H | 1.1613 | 0.2683 | 1.1700 |
| H | 0.3868 | -1.2569 | -2.7036 |
| H | 2.8780 | -2.2707 | -1.5332 |
| H | 1.5742 | -3.1712 | -2.2954 |
| H | -0.5855 | -3.6416 | 0.6533 |
| H | -0.6696 | -3.3129 | -1.0422 |
| H | -0.9241 | -1.3528 | 1.2874 |
| H | -2.1576 | -1.7699 | 0.1545 |
| H | -1.2940 | -0.3003 | -1.5306 |
| H | -1.0022 | 0.5911 | -0.0548 |

### **S13**$H_2$

Same as **S12**$H_2$.

### S14

| | | | |
|---|---|---|---|
| C | 1.3542 | 3.6721 | -3.2600 |
| C | 0.4664 | 4.5228 | -2.3037 |
| C | -1.0027 | 4.0231 | -2.0622 |
| C | -1.2026 | 2.5994 | -1.4391 |
| C | -0.9310 | 1.3749 | -2.3718 |
| C | 0.2174 | 1.6866 | -3.3011 |
| C | -0.1441 | 2.3283 | -4.6243 |
| C | 0.7602 | 3.5696 | -4.6774 |
| C | 1.2767 | 2.2714 | -2.7448 |
| H | 2.3819 | 4.0377 | -3.2739 |
| H | 0.4294 | 5.5454 | -2.6811 |
| H | 0.9668 | 4.5936 | -1.3369 |
| H | -1.5799 | 4.1050 | -2.9825 |
| H | -1.4701 | 4.7389 | -1.3852 |
| H | -2.2237 | 2.5170 | -1.0650 |
| H | -0.5707 | 2.5234 | -0.5534 |
| H | -1.8160 | 1.1232 | -2.9573 |
| H | -0.6915 | 0.4953 | -1.7731 |
| H | -1.1977 | 2.6051 | -4.6620 |
| H | 0.0527 | 1.6438 | -5.4499 |
| H | 1.5604 | 3.4068 | -5.4008 |
| H | 0.2232 | 4.4695 | -4.9797 |
| H | 1.5221 | 2.1252 | -1.7023 |

### **S14**$H_2$

| | | | |
|---|---|---|---|
| C | 1.4303 | 3.0285 | 0.5652 |
| C | 0.0287 | 3.5476 | 0.1662 |
| C | -1.1128 | 2.5092 | 0.1155 |

| | | | |
|---|---|---|---|
| C | -0.7770 | 1.1884 | -0.5967 |
| C | -0.0130 | 0.1811 | 0.2880 |
| C | 1.3949 | 0.6133 | 0.7525 |
| C | 2.3383 | 0.9444 | -0.4094 |
| C | 2.2312 | 2.4609 | -0.6250 |
| C | 1.3921 | 1.8926 | 1.5940 |
| H | 1.9810 | 3.8736 | 0.9816 |
| H | 0.0939 | 4.0638 | -0.7923 |
| H | -0.2668 | 4.3192 | 0.8784 |
| H | -1.9610 | 2.9728 | -0.3897 |
| H | -1.4671 | 2.2947 | 1.1244 |
| H | -0.2454 | 1.3786 | -1.5288 |
| H | -1.7150 | 0.7172 | -0.8927 |
| H | 0.0776 | -0.7576 | -0.2600 |
| H | -0.6183 | -0.0540 | 1.1643 |
| H | 2.1094 | 0.3779 | -1.3129 |
| H | 3.3620 | 0.6938 | -0.1276 |
| H | 3.2281 | 2.9018 | -0.6635 |
| H | 1.7563 | 2.6862 | -1.5801 |
| H | 2.3027 | 1.9247 | 2.1943 |
| H | 0.5558 | 1.9561 | 2.2908 |
| H | 1.8110 | -0.2068 | 1.3397 |

## S15

| | | | |
|---|---|---|---|
| C | 0.9077 | -3.3987 | 0.7427 |
| C | -0.6187 | -3.3437 | 0.9680 |
| C | -1.4695 | -2.8020 | -0.1960 |
| C | -1.1561 | -1.3437 | -0.5801 |
| C | 0.0657 | -1.2012 | -1.5073 |
| C | 1.3872 | -1.6914 | -0.9203 |
| C | 2.1222 | -2.6193 | -1.8684 |
| C | 1.5077 | -4.0312 | -1.7328 |
| C | 1.3976 | -4.4906 | -0.2546 |
| C | 1.4879 | -2.0457 | 0.3709 |
| H | -0.8153 | -2.7289 | 1.8476 |
| H | -0.9738 | -4.3410 | 1.2301 |
| H | -2.5150 | -2.8541 | 0.1100 |
| H | -1.3918 | -3.4524 | -1.0664 |
| H | -1.0337 | -0.7321 | 0.3149 |
| H | -2.0203 | -0.9308 | -1.1018 |
| H | 0.1963 | -0.1528 | -1.7765 |
| H | -0.1477 | -1.7193 | -2.4429 |
| H | 3.1779 | -2.6492 | -1.5948 |
| H | 2.0771 | -2.2530 | -2.8948 |
| H | 2.0938 | -4.7512 | -2.3047 |
| H | 0.5161 | -4.0354 | -2.1840 |
| H | 0.7800 | -5.3864 | -0.1800 |
| H | 2.3951 | -4.8005 | 0.0604 |
| H | 2.5211 | -2.1920 | 0.6536 |
| H | 1.3273 | -3.6556 | 1.7172 |

## **S15**$H_2$

Same as **S5**$H_2$.

## S16

| | | | |
|---|---|---|---|
| C | 0.5448 | -1.5806 | 2.1343 |
| C | -0.3780 | -2.6630 | 2.7523 |
| C | -0.3824 | -3.7099 | 1.6624 |
| C | 0.5519 | -3.3901 | 0.7581 |
| C | 0.0359 | -2.8086 | -0.5369 |
| C | -0.7524 | -1.5139 | -0.1645 |
| C | -0.1581 | -0.7056 | 1.0431 |
| C | 1.5462 | -2.4563 | 1.3926 |

| | | | |
|---|---|---|---|
| H | 1.0150 | -0.9566 | 2.8954 |
| H | -1.3797 | -2.2827 | 2.9556 |
| H | 0.0345 | -3.0833 | 3.6704 |
| H | -0.6003 | -3.5231 | -1.0610 |
| H | 0.8759 | -2.5801 | -1.1941 |
| H | -1.7681 | -1.8073 | 0.1048 |
| H | -0.8615 | -0.8702 | -1.0378 |
| H | 0.5751 | 0.0021 | 0.6539 |
| H | -0.9394 | -0.0955 | 1.4977 |
| H | 2.1943 | -2.9998 | 2.0825 |
| H | 2.1709 | -1.9200 | 0.6765 |
| H | -1.3518 | -4.0801 | 1.3602 |

### **S16**$H_2$

| | | | |
|---|---|---|---|
| C | 1.1040 | -2.5669 | -0.2937 |
| C | -0.3966 | -2.6652 | 0.0676 |
| C | -0.9201 | -1.3726 | 0.7333 |
| C | -0.3825 | -0.0937 | 0.0525 |
| C | 1.1169 | -0.2127 | -0.3075 |
| C | 1.9755 | -0.6161 | 0.9053 |
| C | 1.9670 | -2.1588 | 0.9144 |
| C | 1.3027 | -1.3965 | -1.2566 |
| H | 1.4447 | -3.5070 | -0.7298 |
| H | -0.5720 | -3.5161 | 0.7270 |
| H | -0.9699 | -2.8636 | -0.8390 |
| H | -0.6165 | -1.3681 | 1.7807 |
| H | -2.0104 | -1.3666 | 0.7448 |
| H | -0.5485 | 0.7667 | 0.7019 |
| H | -0.9536 | 0.1003 | -0.8564 |
| H | 1.4679 | 0.7184 | -0.7546 |
| H | 1.5984 | -0.1927 | 1.8371 |
| H | 2.9972 | -0.2552 | 0.7791 |
| H | 2.9847 | -2.5323 | 0.7925 |
| H | 1.5853 | -2.5671 | 1.8510 |
| H | 0.5966 | -1.3975 | -2.0883 |
| H | 2.3105 | -1.4044 | -1.6753 |

### **S17**

| | | | |
|---|---|---|---|
| C | 1.5075 | -2.5483 | -0.5244 |
| C | -0.0555 | -2.6572 | -0.4211 |
| C | 0.0900 | -0.1363 | -0.1569 |
| C | 1.4054 | -0.2934 | -0.3852 |
| C | 2.2575 | -0.5884 | 0.8149 |
| C | 2.1975 | -2.1385 | 0.8159 |
| C | 1.8169 | -1.3358 | -1.3925 |
| H | 1.9319 | -3.4713 | -0.9216 |
| H | 1.8786 | -0.1428 | 1.7359 |
| H | 3.2739 | -0.2298 | 0.6461 |
| H | 3.2078 | -2.5460 | 0.8691 |
| H | 1.6526 | -2.5208 | 1.6796 |
| H | 2.8782 | -1.2548 | -1.6342 |
| H | 1.2475 | -1.2962 | -2.3226 |
| C | -0.8076 | -1.2886 | -0.5838 |
| H | -0.4228 | -3.3431 | -1.1854 |
| H | -0.3232 | -3.1155 | 0.5315 |
| H | -0.2139 | 0.3290 | 0.7700 |
| H | -1.7407 | -1.2776 | -0.0197 |
| H | -1.0728 | -1.1344 | -1.6305 |

### **S17**$H_2$

Same as **S16**$H_2$.

## S18

| | | | |
|---|---|---|---|
| C | 0.3955 | -2.1113 | -5.6945 |
| C | -0.1672 | -1.3097 | -4.5414 |
| C | -0.0392 | -2.3514 | -3.3940 |
| C | 0.4910 | -3.6157 | -4.1337 |
| C | -0.2322 | -3.4565 | -5.4597 |
| C | 1.9508 | -3.3821 | -4.6109 |
| C | 1.7237 | -2.2670 | -5.6126 |
| H | 0.3959 | -0.3939 | -4.3545 |
| H | -1.2087 | -1.0460 | -4.7314 |
| H | -1.0099 | -2.5401 | -2.9333 |
| H | 0.6454 | -2.0233 | -2.6109 |
| H | 0.3246 | -4.5576 | -3.6095 |
| H | 0.0577 | -4.1952 | -6.2101 |
| H | -1.3211 | -3.4275 | -5.3803 |
| H | 2.3762 | -4.2583 | -5.1022 |
| H | 2.6093 | -3.0737 | -3.7980 |
| H | 2.3577 | -1.4054 | -5.4584 |

## **S18**$H_2$

| | | | |
|---|---|---|---|
| C | 0.8212 | 2.5002 | -0.2404 |
| C | 1.9900 | 2.1640 | 0.7041 |
| C | 1.9792 | 0.6233 | 0.7229 |
| C | 0.8056 | 0.2806 | -0.2133 |
| C | -0.5202 | 0.6379 | 0.4837 |
| C | -0.5094 | 2.1787 | 0.4649 |
| C | 0.9129 | 1.3770 | -1.2670 |
| H | 0.8666 | 3.5091 | -0.6528 |
| H | 1.8572 | 2.5944 | 1.6976 |
| H | 2.9338 | 2.5363 | 0.3031 |
| H | 1.8405 | 0.2192 | 1.7266 |
| H | 2.9176 | 0.2281 | 0.3313 |
| H | 0.8367 | -0.7386 | -0.6010 |
| H | -0.5792 | 0.2334 | 1.4949 |
| H | -1.3718 | 0.2532 | -0.0793 |
| H | -1.3556 | 2.5614 | -0.1075 |
| H | -0.5625 | 2.6085 | 1.4659 |
| H | 1.8585 | 1.3637 | -1.8123 |
| H | 0.0878 | 1.3741 | -1.9818 |

## S19

| | | | |
|---|---|---|---|
| C | 0.7535 | 2.4863 | -0.2888 |
| C | 1.9592 | 2.1447 | 0.6238 |
| C | 1.9145 | 0.5928 | 0.6287 |
| C | 0.7227 | 0.3454 | -0.2789 |
| C | -0.5237 | 0.6506 | 0.5352 |
| C | -0.5498 | 2.1945 | 0.4831 |
| C | 0.7988 | 1.3020 | -1.2014 |
| H | 0.7957 | 3.4621 | -0.7745 |
| H | 1.8623 | 2.5722 | 1.6227 |
| H | 2.8948 | 2.5035 | 0.1922 |
| H | 1.7851 | 0.1707 | 1.6262 |
| H | 2.8198 | 0.1667 | 0.1932 |
| H | -0.4757 | 0.2573 | 1.5516 |
| H | -1.4032 | 0.2265 | 0.0485 |
| H | -1.4204 | 2.5487 | -0.0710 |
| H | -0.5662 | 2.6521 | 1.4730 |
| H | 1.6700 | 1.3434 | -1.8414 |

## **S19**$H_2$

Same as **S18**$H_2$.

## S20

| | | | |
|---|---|---|---|
| C | 1.0117 | -2.3703 | -0.1380 |
| C | 2.1055 | -1.8086 | 0.8026 |
| C | 1.9918 | -0.2591 | 0.8464 |
| C | 0.8135 | 0.1856 | -0.0190 |
| C | -0.4388 | -0.3941 | 0.6257 |
| C | -0.3686 | -1.9494 | 0.4639 |
| C | 1.1920 | -1.6598 | -1.5149 |
| C | 0.8883 | -0.1756 | -1.3135 |
| H | 1.0928 | -3.4538 | -0.2350 |
| H | 3.0959 | -2.1033 | 0.4533 |
| H | 1.9950 | -2.2255 | 1.8044 |
| H | 2.9050 | 0.1974 | 0.4623 |
| H | 1.8699 | 0.0983 | 1.8696 |
| H | -1.3338 | 0.0059 | 0.1470 |
| H | -0.4891 | -0.1083 | 1.6773 |
| H | -0.5297 | -2.4346 | 1.4273 |
| H | -1.1727 | -2.2916 | -0.1888 |
| H | 0.5099 | -2.0762 | -2.2572 |
| H | 2.2052 | -1.7849 | -1.8985 |
| H | 0.0147 | 0.0614 | -1.9045 |

## S20$H_2$

| | | | |
|---|---|---|---|
| C | 0.8338 | 2.6984 | 0.1333 |
| C | -0.5021 | 2.2195 | -0.4774 |
| C | -0.5506 | 0.6717 | -0.5124 |
| C | 0.7519 | 0.0830 | 0.0741 |
| C | 0.9091 | 0.5798 | 1.5286 |
| C | 0.9576 | 2.1275 | 1.5636 |
| C | 1.9958 | 2.1467 | -0.7226 |
| C | 1.9473 | 0.5990 | -0.7576 |
| H | 0.8680 | 3.7885 | 0.1580 |
| H | -0.6188 | 2.6201 | -1.4851 |
| H | -1.3402 | 2.6067 | 0.1035 |
| H | -0.6907 | 0.3251 | -1.5371 |
| H | -1.4121 | 0.3118 | 0.0516 |
| H | 0.7177 | -1.0071 | 0.0494 |
| H | 1.8174 | 0.1672 | 1.9696 |
| H | 0.0816 | 0.2177 | 2.1400 |
| H | 0.1536 | 2.5127 | 2.1920 |
| H | 1.8893 | 2.4621 | 2.0216 |
| H | 2.9516 | 2.4818 | -0.3178 |
| H | 1.9372 | 2.5457 | -1.7361 |
| H | 1.8653 | 0.2507 | -1.7880 |
| H | 2.8797 | 0.1868 | -0.3698 |

## S21

| | | | |
|---|---|---|---|
| C | 6.1402 | 4.2707 | 5.4051 |
| C | 7.2832 | 4.9170 | 4.5937 |
| C | 7.7408 | 4.0522 | 3.3957 |
| C | 6.6881 | 3.9278 | 2.2518 |
| C | 5.5257 | 2.9187 | 2.5304 |
| C | 5.9377 | 1.6663 | 3.3587 |
| C | 6.9618 | 2.0629 | 4.4077 |
| C | 6.3445 | 2.7537 | 5.6198 |
| C | 8.0356 | 2.6461 | 3.8606 |
| H | 5.1947 | 4.4459 | 4.8965 |
| H | 6.0380 | 4.7712 | 6.3684 |
| H | 8.1370 | 5.0611 | 5.2575 |
| H | 6.9926 | 5.9135 | 4.2592 |
| H | 8.6559 | 4.4858 | 2.9897 |
| H | 7.2111 | 3.5852 | 1.3578 |
| H | 6.2849 | 4.9075 | 1.9930 |
| H | 5.0751 | 2.6053 | 1.5882 |

| | | | |
|---|---|---|---|
| H | 4.7259 | 3.4365 | 3.0561 |
| H | 6.3908 | 0.9267 | 2.6969 |
| H | 5.0724 | 1.1839 | 3.8146 |
| H | 5.4167 | 2.2656 | 5.9199 |
| H | 7.0414 | 2.6153 | 6.4474 |
| H | 8.4431 | 2.1351 | 2.9991 |

### **S21**$H_2$

Same as **S10**$H_2$.

### **S22**

| | | | |
|---|---|---|---|
| C | -4.0343 | 2.7326 | -0.2253 |
| C | -2.6819 | 3.4704 | -0.5312 |
| C | -1.3592 | 2.9126 | 0.1060 |
| C | -0.8536 | 1.4968 | -0.3167 |
| C | -1.9488 | 0.6472 | -0.9210 |
| C | -3.1628 | 0.6128 | -0.3501 |
| C | -3.4185 | 0.8185 | 1.1341 |
| C | -4.0960 | 2.1987 | 1.2175 |
| C | -4.1963 | 1.4428 | -1.0471 |
| H | -4.8648 | 3.4109 | -0.4264 |
| H | -2.7909 | 4.4967 | -0.1785 |
| H | -2.5541 | 3.5576 | -1.6108 |
| H | -1.4560 | 2.9336 | 1.1911 |
| H | -0.5580 | 3.6238 | -0.0980 |
| H | -0.4202 | 0.9806 | 0.5406 |
| H | -0.0550 | 1.5870 | -1.0538 |
| H | -1.9362 | 0.7323 | -1.9985 |
| H | -2.5048 | 0.7590 | 1.7254 |
| H | -4.0926 | 0.0416 | 1.4961 |
| H | -5.1358 | 2.0775 | 1.5247 |
| H | -3.6253 | 2.8652 | 1.9405 |
| H | -5.1866 | 1.0025 | -0.9201 |
| H | -4.0166 | 1.5844 | -2.1140 |

### **S22**$H_2$

Same as **S14**$H_2$.

### **S23**

| | | | |
|---|---|---|---|
| C | -0.1589 | 1.2976 | 1.9351 |
| C | 0.5532 | -0.0623 | 2.0573 |
| C | -0.3050 | -1.3372 | 1.8029 |
| C | -1.5146 | -1.6202 | 2.7404 |
| C | -2.9027 | -1.1220 | 2.2472 |
| C | -3.2868 | 0.3199 | 2.6478 |
| C | -2.1493 | 1.2612 | 2.3650 |
| C | -1.4258 | 1.4272 | 1.0554 |
| C | -1.0854 | 1.4957 | 3.1316 |
| H | 0.5361 | 2.1186 | 1.7525 |
| H | 1.0233 | -0.1430 | 3.0383 |
| H | 1.3818 | -0.0826 | 1.3485 |
| H | 0.3776 | -2.1819 | 1.9044 |
| H | -0.6238 | -1.3777 | 0.7616 |
| H | -1.3121 | -1.2802 | 3.7566 |
| H | -1.5931 | -2.7052 | 2.8223 |
| H | -3.6717 | -1.7861 | 2.6436 |
| H | -2.9633 | -1.2314 | 1.1639 |
| H | -3.5289 | 0.3700 | 3.7100 |
| H | -4.1726 | 0.6443 | 2.1009 |
| H | -1.5164 | 0.6430 | 0.3053 |
| H | -1.5059 | 2.4044 | 0.5773 |
| H | -0.8954 | 1.3628 | 4.1928 |

## **S23**$H_2$

| | | | |
|---|---|---|---|
| C | -4.1975 | -0.0937 | -1.3374 |
| C | -3.8592 | 0.5362 | 0.0171 |
| C | -4.6067 | 1.8290 | 0.3961 |
| C | -4.4171 | 3.0317 | -0.5498 |
| C | -5.5007 | 3.1817 | -1.6362 |
| C | -5.1889 | 2.5481 | -3.0055 |
| C | -4.9444 | 1.0364 | -3.0353 |
| C | -3.5748 | 0.4995 | -2.6058 |
| C | -5.5733 | 0.0957 | -1.9954 |
| H | -2.7863 | 0.7257 | 0.0663 |
| H | -4.0501 | -0.1969 | 0.8018 |
| H | -4.2385 | 2.1237 | 1.3797 |
| H | -5.6663 | 1.6255 | 0.5504 |
| H | -3.4153 | 3.0488 | -0.9791 |
| H | -4.4717 | 3.9275 | 0.0705 |
| H | -5.6430 | 4.2487 | -1.8128 |
| H | -6.4655 | 2.8347 | -1.2663 |
| H | -4.3284 | 3.0590 | -3.4390 |
| H | -6.0188 | 2.7820 | -3.6735 |
| H | -5.1545 | 0.6530 | -4.0351 |
| H | -3.1916 | -0.2655 | -3.2835 |
| H | -2.8229 | 1.2679 | -2.4251 |
| H | -6.3405 | 0.5388 | -1.3630 |
| H | -5.9446 | -0.8264 | -2.4459 |
| H | -3.9576 | -1.1581 | -1.3143 |

## **S24**

| | | | |
|---|---|---|---|
| C | -1.6162 | 3.3529 | -0.5027 |
| C | -1.8303 | 2.3480 | 0.6654 |
| C | -2.7406 | 1.1077 | 0.4010 |
| C | -2.1335 | -0.1148 | -0.3503 |
| C | -1.8933 | 0.0301 | -1.8726 |
| C | -0.7798 | 1.0165 | -2.1150 |
| C | -1.0145 | 2.3331 | -2.0643 |
| C | -2.3023 | 3.0895 | -1.8660 |
| C | -0.2482 | 3.3400 | -1.2603 |
| H | -1.8308 | 4.3709 | -0.1734 |
| H | -2.2703 | 2.8954 | 1.5000 |
| H | -0.8675 | 2.0026 | 1.0433 |
| H | -3.6859 | 1.4044 | -0.0512 |
| H | -3.0294 | 0.7351 | 1.3845 |
| H | -2.8134 | -0.9560 | -0.2096 |
| H | -1.2051 | -0.4127 | 0.1388 |
| H | -2.8057 | 0.3421 | -2.3817 |
| H | -1.6061 | -0.9280 | -2.3069 |
| H | 0.2179 | 0.6603 | -1.9025 |
| H | -2.4241 | 4.0021 | -2.4524 |
| H | -3.2496 | 2.5565 | -1.8294 |
| H | 0.5919 | 3.0018 | -0.6528 |
| H | -0.0193 | 4.2928 | -1.7414 |

## **S24**$H_2$

Same as **S23**$H_2$.

## **S25**

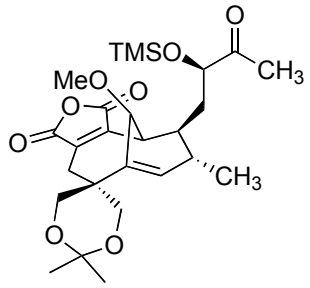
| | | | |
|---|---|---|---|
| C | 2.3466 | 6.5435 | -0.4324 |
| C | 1.5087 | 7.7640 | -0.8266 |
| C | 2.2269 | 8.5914 | -1.9610 |
| C | 3.1984 | 7.8433 | -2.9544 |
| C | 4.6215 | 7.4145 | -2.4356 |
| C | 4.5360 | 6.4680 | -1.2490 |
| C | 4.4836 | 4.9645 | -1.5362 |

| | | | |
|---|---|---|---|
| C | 4.0749 | 4.1134 | -0.2868 |
| C | 2.5783 | 4.1382 | 0.1706 |
| C | 1.9766 | 5.5066 | 0.6155 |
| C | 3.7868 | 6.9450 | -0.2640 |
| H | 1.3119 | 8.4058 | 0.0317 |
| H | 0.5333 | 7.4216 | -1.1808 |
| H | 2.7801 | 9.4129 | -1.5054 |
| H | 1.4487 | 9.0826 | -2.5482 |
| H | 3.3647 | 8.5050 | -3.8047 |
| H | 2.6902 | 6.9771 | -3.3792 |
| H | 5.1728 | 8.3024 | -2.1247 |
| H | 5.2078 | 6.9517 | -3.2285 |
| H | 5.4751 | 4.6629 | -1.8731 |
| H | 3.8100 | 4.7612 | -2.3712 |
| H | 4.7169 | 4.3810 | 0.5542 |
| H | 4.3218 | 3.0756 | -0.5116 |
| H | 2.4601 | 3.4358 | 0.9961 |
| H | 1.9654 | 3.7300 | -0.6371 |
| H | 0.8943 | 5.4211 | 0.7021 |
| H | 2.3491 | 5.7983 | 1.5986 |
| H | 3.8514 | 8.0053 | -0.0670 |
| H | 2.2108 | 5.9793 | -1.3564 |

### **S25**$H_2$

Same as **S3**$H_2$.

**5 (modelled with OTMS in place of OTBS, OMe in place of OPMB, Me in place of $C_8H_{15}$ and Me in place of $C_5H_9$)**




| | | | |
|---|---|---|---|
| C | -7.1771 | -5.0626 | -5.0631 |
| C | -7.5362 | -3.7577 | -4.3339 |
| C | -8.9023 | -3.9429 | -3.5950 |
| C | -9.2501 | -5.3651 | -3.1102 |
| C | -9.1613 | -6.5636 | -3.7084 |
| C | -8.6578 | -6.9679 | -5.1096 |
| C | -7.4502 | -7.9769 | -5.0790 |
| C | -6.0422 | -7.2855 | -5.1711 |
| C | -6.1035 | -5.8218 | -4.7648 |
| C | -8.2497 | -5.7317 | -5.9166 |
| C | -7.5964 | -2.5754 | -5.3227 |
| C | -6.4837 | -3.3357 | -3.2794 |
| H | -9.7250 | -3.6253 | -4.2349 |
| H | -8.9595 | -3.2520 | -2.7528 |
| H | -9.5135 | -7.4284 | -5.5919 |
| C | -7.5634 | -9.0773 | -6.1641 |
| H | -7.4804 | -8.4990 | -4.1229 |
| H | -5.7127 | -7.2774 | -6.2119 |
| C | -4.9799 | -8.0372 | -4.3525 |
| O | -9.3826 | -4.9227 | -6.2117 |
| H | -7.7784 | -6.0284 | -6.8564 |
| H | -5.3221 | -5.4743 | -4.1063 |
| C | -9.8631 | -5.5869 | -1.8037 |
| C | -9.7450 | -7.5401 | -2.7927 |
| O | -10.1369 | -6.9005 | -1.6734 |
| O | -9.8658 | -8.7479 | -2.9974 |
| O | -10.0935 | -4.7272 | -0.9547 |
| O | -5.2427 | -3.0252 | -3.9014 |
| C | -5.2947 | -2.0706 | -4.9185 |
| O | -6.3002 | -2.3241 | -5.8526 |
| C | -5.4502 | -0.6565 | -4.3246 |
| C | -3.9722 | -2.1889 | -5.6773 |
| C | -10.0664 | -5.2972 | -7.3992 |
| C | -8.7360 | -10.0666 | -5.9675 |
| C | -8.4199 | -11.4609 | -6.5361 |
| C | -7.3970 | -12.3044 | -5.7896 |
| O | -8.9692 | -11.8965 | -7.5462 |
| O | -9.8926 | -9.5301 | -6.5923 |
| H | -7.9866 | -1.6814 | -4.8365 |
| H | -8.2677 | -2.7717 | -6.1565 |
| H | -6.3287 | -4.1243 | -2.5423 |
| H | -6.8228 | -2.4701 | -2.7101 |
| H | -3.9979 | -7.5766 | -4.4682 |
| H | -5.2211 | -8.0361 | -3.2889 |
| H | -4.8883 | -9.0755 | -4.6710 |
| H | -6.3813 | -0.5440 | -3.7734 |
| H | -4.6231 | -0.4511 | -3.6449 |
| H | -5.4349 | 0.0818 | -5.1265 |
| H | -3.1348 | -2.0036 | -5.0046 |
| H | -3.8761 | -3.1929 | -6.0913 |
| H | -3.9425 | -1.4676 | -6.4942 |
| H | -10.4174 | -6.3287 | -7.3618 |
| H | -10.9358 | -4.6543 | -7.5359 |

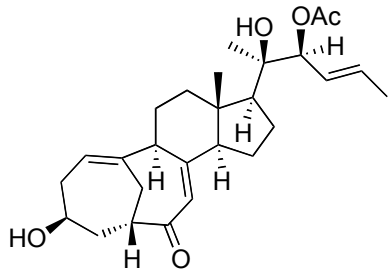
| | | | |
|---|---|---|---|
| H | -9.4259 | -5.1801 | -8.2742 |
| H | -8.9328 | -10.1964 | -4.9035 |
| H | -7.7218 | -13.3441 | -5.7608 |
| H | -6.4331 | -12.2552 | -6.2950 |
| H | -7.2769 | -11.9484 | -4.7668 |
| Si | -11.4779 | -10.0207 | -6.2727 |
| C | -11.5061 | -11.3615 | -4.9430 |
| C | -12.4247 | -8.4995 | -5.6861 |
| C | -12.2330 | -10.6483 | -7.8789 |
| H | -6.6266 | -9.6354 | -6.1739 |
| H | -7.6335 | -8.6241 | -7.1540 |
| H | -11.0298 | -11.0261 | -4.0222 |
| H | -12.5279 | -11.6433 | -4.6918 |
| H | -10.9979 | -12.2664 | -5.2738 |
| H | -13.4762 | -8.7271 | -5.5153 |
| H | -12.0185 | -8.1159 | -4.7522 |
| H | -12.3778 | -7.6964 | -6.4202 |
| H | -12.2225 | -9.8784 | -8.6492 |
| H | -11.6693 | -11.4970 | -8.2670 |
| H | -13.2643 | -10.9711 | -7.7443 |

**5**$H_2$

| | | | |
|---|---|---|---|
| C | -19.3349 | -9.1410 | -4.6658 |
| C | -20.6586 | -9.3737 | -5.4997 |
| C | -21.5016 | -10.5784 | -4.9838 |
| C | -20.8133 | -11.9268 | -5.1227 |
| C | -19.6142 | -12.3001 | -4.6970 |
| C | -18.5753 | -11.4859 | -3.9365 |
| C | -19.0372 | -11.1692 | -2.4726 |
| C | -18.8681 | -9.6609 | -2.1279 |
| C | -19.5972 | -8.7811 | -3.1710 |
| C | -18.2179 | -10.2181 | -4.7433 |
| C | -20.3654 | -9.5448 | -7.0136 |
| C | -21.5197 | -8.0853 | -5.4302 |
| H | -22.4454 | -10.6202 | -5.5298 |
| H | -21.7890 | -10.4503 | -3.9420 |
| H | -17.6641 | -12.0804 | -3.8760 |
| C | -18.3325 | -12.0877 | -1.4354 |
| H | -20.1083 | -11.3614 | -2.4003 |
| H | -17.8053 | -9.4146 | -2.1497 |
| C | -19.3694 | -9.2889 | -0.7191 |
| O | -17.8409 | -10.4976 | -6.0861 |
| H | -17.3320 | -9.7708 | -4.2888 |
| H | -20.6585 | -8.8308 | -2.9391 |
| C | -21.3938 | -13.0578 | -5.8408 |
| C | -19.3870 | -13.6591 | -5.1785 |
| O | -20.4890 | -14.0631 | -5.8465 |
| O | -18.3666 | -14.3293 | -5.0115 |
| O | -22.5093 | -13.1026 | -6.3575 |
| O | -22.6615 | -8.1773 | -6.2706 |
| C | -22.4089 | -8.4640 | -7.6097 |
| O | -21.5690 | -9.5617 | -7.7690 |
| C | -23.7524 | -8.8656 | -8.2199 |
| C | -21.8331 | -7.2297 | -8.3319 |
| C | -16.5779 | -11.1287 | -6.2535 |
| C | -18.5410 | -13.6063 | -1.6144 |
| C | -19.9864 | -14.0635 | -1.3723 |
| C | -20.3138 | -14.7620 | -0.0592 |
| O | -20.8564 | -13.8848 | -2.2225 |
| O | -17.6743 | -14.2789 | -0.7214 |
| H | -19.8799 | -10.4929 | -7.2326 |
| H | -19.6960 | -8.7659 | -7.3786 |
| H | -20.9331 | -7.2055 | -5.6951 |
| H | -21.8963 | -7.9003 | -4.4260 |
| H | -19.3572 | -8.2083 | -0.5721 |

| | | | |
|---|---|---|---|
| H | -20.3919 | -9.6308 | -0.5541 |
| H | -18.7413 | -9.7100 | 0.0652 |
| H | -24.1430 | -9.7418 | -7.7013 |
| H | -24.4689 | -8.0501 | -8.1225 |
| H | -23.6276 | -9.1101 | -9.2748 |
| H | -22.5273 | -6.3943 | -8.2407 |
| H | -20.8733 | -6.9253 | -7.9201 |
| H | -21.6956 | -7.4557 | -9.3895 |
| H | -16.5605 | -12.1315 | -5.8273 |
| H | -16.3644 | -11.2254 | -7.3180 |
| H | -15.7742 | -10.5422 | -5.8069 |
| H | -18.2661 | -13.8972 | -2.6239 |
| H | -21.3906 | -14.7714 | 0.1066 |
| H | -19.9539 | -15.7894 | -0.0806 |
| H | -19.8363 | -14.2428 | 0.7713 |
| Si | -16.6922 | -15.5544 | -1.2221 |
| C | -15.4662 | -14.8738 | -2.4805 |
| C | -15.8001 | -16.2292 | 0.2925 |
| C | -17.7791 | -16.8767 | -2.0106 |
| H | -18.6627 | -11.8436 | -0.4270 |
| H | -17.2624 | -11.8787 | -1.4517 |
| H | -14.8848 | -14.0517 | -2.0650 |
| H | -14.7641 | -15.6400 | -2.8076 |
| H | -15.9738 | -14.5006 | -3.3701 |
| H | -15.1390 | -17.0556 | 0.0340 |
| H | -15.1931 | -15.4602 | 0.7692 |
| H | -16.5054 | -16.5940 | 1.0384 |
| H | -17.1859 | -17.7234 | -2.3545 |
| H | -18.5182 | -17.2633 | -1.3103 |
| H | -18.3162 | -16.4903 | -2.8772 |
| H | -18.8760 | -8.2543 | -5.1066 |
| H | -19.3245 | -7.7375 | -3.0073 |

**6**




| | | | |
|---|---|---|---|
| C | 3.5002 | -3.8270 | 2.7872 |
| C | 1.9085 | -2.0217 | 2.1366 |
| C | 0.6967 | -2.4562 | 2.5219 |
| C | 0.4599 | -3.3252 | 3.7413 |
| C | 1.1491 | -4.7017 | 3.6099 |
| C | 2.6875 | -4.6816 | 3.7975 |
| C | 3.3976 | -4.3392 | 1.3311 |
| O | 3.1348 | -5.5264 | 1.1460 |
| C | 3.6795 | -3.4520 | 0.1801 |
| C | 3.1751 | -2.2125 | -0.0709 |
| C | 2.1650 | -1.4041 | 0.7764 |
| C | 3.5094 | -1.4612 | -1.3607 |
| C | 4.0703 | -0.0417 | -1.1383 |
| C | 2.9685 | 0.7565 | -0.4048 |
| C | 2.5582 | 0.0878 | 0.9226 |
| C | 4.3301 | 0.3721 | -2.6257 |
| C | 4.8156 | -0.9325 | -3.3161 |
| C | 4.4528 | -2.0981 | -2.3843 |
| H | -0.6182 | -3.4541 | 3.8470 |
| H | 0.7949 | -2.8082 | 4.6411 |
| H | 0.8857 | -5.1536 | 2.6518 |
| O | 0.6242 | -5.5240 | 4.6281 |

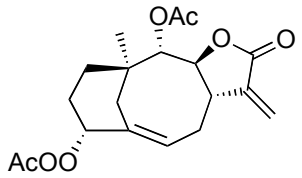
| | | | |
|---|---|---|---|
| H | 2.9175 | -4.3366 | 4.8065 |
| H | 3.0613 | -5.7060 | 3.7592 |
| H | 4.3317 | -3.9044 | -0.5485 |
| C | 5.3655 | -0.0715 | -0.2858 |
| H | 2.0863 | 0.8460 | -1.0406 |
| H | 3.2971 | 1.7706 | -0.1896 |
| H | 3.3710 | 0.2005 | 1.6388 |
| H | 1.7210 | 0.6374 | 1.3549 |
| C | 5.1389 | 1.6660 | -3.0151 |
| H | 3.3342 | 0.5285 | -3.0447 |
| H | 5.8856 | -0.9396 | -3.5130 |
| H | 4.3283 | -1.0397 | -4.2862 |
| H | 3.9890 | -2.9275 | -2.9199 |
| H | 5.3607 | -2.4707 | -1.9091 |
| H | -0.1608 | -2.2943 | 1.8847 |
| H | 1.2278 | -1.4298 | 0.2176 |
| O | 5.1208 | 1.6962 | -4.4312 |
| C | 6.6373 | 1.6432 | -2.6260 |
| C | 4.4598 | 2.9946 | -2.5602 |
| O | 5.2761 | 4.0682 | -3.0253 |
| C | 5.5427 | 5.1877 | -2.3125 |
| O | 6.2956 | 6.0663 | -2.7198 |
| C | 4.8631 | 5.3362 | -0.9524 |
| C | 3.0381 | 3.1722 | -3.0770 |
| C | 1.9697 | 3.4540 | -2.3130 |
| C | 0.5627 | 3.6202 | -2.8434 |
| H | 0.8993 | -6.4148 | 4.4668 |
| H | 5.6449 | 0.9275 | 0.0447 |
| H | 5.2554 | -0.6689 | 0.6181 |
| H | 6.2080 | -0.4954 | -0.8316 |
| H | 7.1208 | 0.6950 | -2.8502 |
| H | 6.7877 | 1.8514 | -1.5696 |
| H | 7.2038 | 2.4055 | -3.1621 |
| H | 5.0900 | 6.3178 | -0.5362 |
| H | 3.7813 | 5.2564 | -1.0478 |
| H | 5.2253 | 4.5840 | -0.2525 |
| H | 2.9098 | 3.0545 | -4.1437 |
| H | 2.0875 | 3.5758 | -1.2459 |
| H | -0.1026 | 2.8901 | -2.3819 |
| H | 0.1884 | 4.6183 | -2.6143 |
| H | 0.5246 | 3.4811 | -3.9246 |
| H | 5.4140 | 2.5594 | -4.6928 |
| C | 3.1531 | -2.3418 | 2.9345 |
| H | 2.5479 | -1.3686 | -1.8720 |
| H | 4.4390 | 2.9862 | -1.4737 |
| H | 3.9929 | -1.7289 | 2.6080 |
| H | 2.9955 | -2.0823 | 3.9819 |
| H | 4.5485 | -3.9401 | 3.0630 |

**6**$H_2$

| | | | |
|---|---|---|---|
| C | -13.1986 | 1.5216 | -9.9067 |
| C | -15.5777 | 2.5545 | -10.1399 |
| C | -16.2287 | 1.1535 | -10.0456 |
| C | -15.8982 | 0.3602 | -8.7685 |
| C | -14.5917 | -0.4481 | -8.8748 |
| C | -13.3015 | 0.3981 | -8.8436 |
| C | -13.2726 | 0.9973 | -11.3539 |
| O | -12.9439 | -0.1697 | -11.5627 |
| C | -13.6319 | 1.8615 | -12.4911 |
| C | -14.6319 | 2.7737 | -12.5968 |
| C | -15.6972 | 3.1756 | -11.5515 |
| C | -14.8808 | 3.5150 | -13.9139 |
| C | -14.8500 | 5.0510 | -13.7855 |
| C | -15.9853 | 5.4298 | -12.8104 |
| C | -15.8397 | 4.7195 | -11.4499 |

| | | | |
|---|---|---|---|
| C | -15.0848 | 5.4466 | -15.2821 |
| C | -14.3217 | 4.3675 | -16.0986 |
| C | -14.0091 | 3.2124 | -15.1366 |
| H | -16.7140 | -0.3449 | -8.6012 |
| H | -15.8891 | 1.0108 | -7.8931 |
| H | -14.6230 | -1.0653 | -9.7742 |
| O | -14.5452 | -1.3262 | -7.7720 |
| H | -13.1831 | 0.8386 | -7.8528 |
| H | -12.4444 | -0.2672 | -8.9597 |
| H | -13.0158 | 1.6733 | -13.3542 |
| C | -13.4878 | 5.5474 | -13.2351 |
| H | -16.9518 | 5.1649 | -13.2420 |
| H | -16.0096 | 6.5032 | -12.6367 |
| H | -14.9903 | 5.1440 | -10.9166 |
| H | -16.7116 | 4.9647 | -10.8421 |
| C | -14.9049 | 6.9208 | -15.8050 |
| H | -16.1349 | 5.2110 | -15.4661 |
| H | -13.3995 | 4.7372 | -16.5418 |
| H | -14.9418 | 4.0279 | -16.9294 |
| H | -14.2271 | 2.2375 | -15.5746 |
| H | -12.9481 | 3.2391 | -14.8871 |
| H | -15.9917 | 0.5478 | -10.9206 |
| H | -16.6444 | 2.8253 | -11.9659 |
| O | -15.2420 | 6.8649 | -17.1798 |
| C | -13.4534 | 7.4579 | -15.7617 |
| C | -15.9012 | 7.9399 | -15.1710 |
| O | -15.6496 | 9.2082 | -15.7738 |
| C | -15.6573 | 10.3853 | -15.1054 |
| O | -15.3786 | 11.4519 | -15.6432 |
| C | -16.0342 | 10.3531 | -13.6254 |
| C | -17.3671 | 7.5687 | -15.3533 |
| C | -18.2716 | 7.4909 | -14.3632 |
| C | -19.7230 | 7.1135 | -14.5621 |
| H | -13.8522 | -1.9538 | -7.9162 |
| H | -13.5339 | 6.5980 | -12.9534 |
| H | -13.1785 | 5.0083 | -12.3405 |
| H | -12.6824 | 5.4263 | -13.9592 |
| H | -13.3322 | 8.3409 | -16.3902 |
| H | -12.7211 | 6.7346 | -16.1135 |
| H | -13.1615 | 7.7655 | -14.7606 |
| H | -16.0933 | 11.3718 | -13.2418 |
| H | -17.0074 | 9.8860 | -13.4825 |
| H | -15.2830 | 9.8194 | -13.0442 |
| H | -17.6732 | 7.3548 | -16.3676 |
| H | -17.9765 | 7.7048 | -13.3461 |
| H | -19.9619 | 6.2192 | -13.9859 |
| H | -20.3727 | 7.9220 | -14.2259 |
| H | -19.9431 | 6.9124 | -15.6113 |
| H | -15.3443 | 7.7601 | -17.4758 |
| C | -14.1504 | 2.6797 | -9.5793 |
| H | -15.8919 | 3.2182 | -14.2034 |
| H | -15.6804 | 7.9820 | -14.1076 |
| H | -13.6940 | 3.6102 | -9.9161 |
| H | -14.2107 | 2.7924 | -8.4961 |
| H | -12.1900 | 1.9230 | -9.8091 |
| H | -17.3103 | 1.2880 | -10.0917 |
| H | -16.1904 | 3.1716 | -9.4800 |

**7**



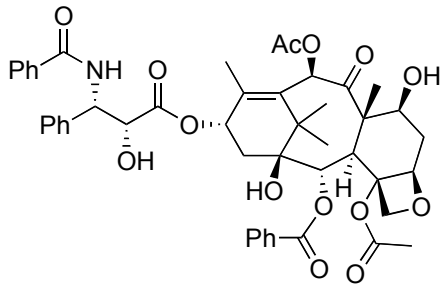

| | | | |
|---|---|---|---|
| C | 0.1709 | -3.8541 | -2.1530 |
| C | 0.0162 | -3.6768 | -0.8286 |
| C | 0.2352 | -4.7517 | 0.2233 |
| C | 1.7503 | -4.9915 | 0.4450 |
| C | 2.4772 | -5.8240 | -0.6431 |
| C | 2.9221 | -5.0089 | -1.8965 |
| C | 2.0073 | -5.2084 | -3.1591 |
| C | 0.5110 | -5.1884 | -2.7816 |
| C | 2.2203 | -4.0568 | -4.1864 |
| C | 1.7043 | -2.6707 | -3.7153 |
| C | 0.2719 | -2.7017 | -3.1375 |
| O | 3.5465 | -6.4191 | 0.0855 |
| C | 3.3120 | -6.5260 | 1.3955 |
| C | 2.1204 | -5.7366 | 1.6985 |
| H | -0.2767 | -5.6779 | -0.0382 |
| H | -0.2411 | -4.3955 | 1.1364 |
| H | 2.8628 | -3.9570 | -1.6285 |
| O | 4.2647 | -5.3111 | -2.2781 |
| H | -0.1041 | -5.3089 | -3.6750 |
| H | 0.2299 | -6.0264 | -2.1485 |
| H | 1.6992 | -4.3068 | -5.1120 |
| H | 3.2746 | -3.9825 | -4.4573 |
| H | 1.7508 | -1.9586 | -4.5403 |
| H | 2.3804 | -2.2775 | -2.9563 |
| H | 0.0713 | -1.7531 | -2.6361 |
| O | -0.6414 | -2.8513 | -4.2145 |
| O | 4.0058 | -7.1412 | 2.2004 |
| C | 1.5137 | -5.7375 | 2.8989 |
| H | -0.1247 | -2.6737 | -0.4502 |
| C | 2.3054 | -6.5612 | -3.8456 |
| C | 5.3531 | -4.6276 | -1.8500 |
| O | 6.4853 | -4.8551 | -2.2635 |
| C | 5.1291 | -3.5315 | -0.8092 |
| O | -2.0472 | -2.8205 | -3.6728 |
| H | 1.9023 | -6.3372 | 3.7109 |
| H | 0.6340 | -5.1457 | 3.0968 |
| H | 1.6289 | -6.7439 | -4.6811 |
| H | 3.3188 | -6.5979 | -4.2477 |
| H | 2.2014 | -7.3972 | -3.1537 |
| H | 6.0924 | -3.1447 | -0.4766 |
| H | 4.5637 | -2.7027 | -1.2333 |
| H | 4.6093 | -3.9228 | 0.0637 |
| H | 1.8568 | -6.6672 | -0.9450 |
| H | 2.2457 | -4.0241 | 0.5445 |
| C | -2.6147 | -1.6054 | -3.7084 |
| O | -2.0591 | -0.5643 | -4.0543 |
| C | -4.0614 | -1.6192 | -3.2419 |
| H | -4.6670 | -2.2232 | -3.9169 |
| H | -4.1312 | -2.0368 | -2.2381 |
| H | -4.4624 | -0.6059 | -3.2273 |

**7**$H_2$

| | | | |
|---|---|---|---|
| C | -0.0565 | -0.6793 | 1.6348 |
| C | -1.5981 | -0.6311 | 1.7892 |
| C | -2.3698 | -1.9638 | 1.6413 |
| C | -2.6991 | -2.6079 | 3.0072 |
| C | -1.5210 | -3.2599 | 3.7524 |

| | | | |
|---|---|---|---|
| C | -0.6008 | -2.2316 | 4.4610 |
| C | 0.7744 | -2.0142 | 3.7413 |
| C | 0.6617 | -1.9277 | 2.1928 |
| C | 1.4390 | -0.7010 | 4.2317 |
| C | 0.7480 | 0.5785 | 3.7145 |
| C | 0.6210 | 0.6003 | 2.1742 |
| O | -2.1790 | -4.1937 | 4.6025 |
| C | -3.3545 | -4.6080 | 4.1179 |
| C | -3.7068 | -3.7244 | 3.0072 |
| H | -1.8626 | -2.6603 | 0.9732 |
| H | -3.3114 | -1.7265 | 1.1455 |
| H | -1.1141 | -1.2751 | 4.4559 |
| O | -0.3445 | -2.5963 | 5.8186 |
| H | 1.6768 | -1.8976 | 1.7923 |
| H | 0.2573 | -2.8366 | 1.7536 |
| H | 2.4784 | -0.6775 | 3.8999 |
| H | 1.4811 | -0.6816 | 5.3217 |
| H | 1.3036 | 1.4511 | 4.0582 |
| H | -0.2376 | 0.6787 | 4.1661 |
| H | 0.0379 | 1.4683 | 1.8610 |
| O | 1.9090 | 0.6851 | 1.5789 |
| O | -4.0307 | -5.5314 | 4.5626 |
| C | -4.7402 | -3.9442 | 2.1753 |
| H | -1.9658 | 0.0529 | 1.0220 |
| C | 1.7252 | -3.1949 | 4.0590 |
| C | -1.0901 | -2.1945 | 6.8755 |
| O | -0.7838 | -2.4440 | 8.0368 |
| C | -2.3600 | -1.3990 | 6.5787 |
| O | 2.4922 | 2.0464 | 1.8519 |
| H | -5.3772 | -4.8085 | 2.3062 |
| H | -4.9724 | -3.2755 | 1.3613 |
| H | 2.6747 | -3.1028 | 3.5306 |
| H | 1.9679 | -3.2517 | 5.1210 |
| H | 1.2885 | -4.1528 | 3.7757 |
| H | -2.8889 | -1.2009 | 7.5111 |
| H | -2.1251 | -0.4403 | 6.1185 |
| H | -3.0292 | -1.9655 | 5.9337 |
| H | -0.9438 | -3.8836 | 3.0719 |
| H | -3.1468 | -1.8448 | 3.6454 |
| C | 2.2962 | 2.9251 | 0.8573 |
| O | 1.6416 | 2.7179 | -0.1631 |
| C | 2.9634 | 4.2660 | 1.1176 |
| H | 2.5283 | 4.7391 | 1.9972 |
| H | 4.0314 | 4.1285 | 1.2844 |
| H | 2.8272 | 4.9272 | 0.2621 |
| H | -1.8788 | -0.1455 | 2.7230 |
| H | 0.1176 | -0.6964 | 0.5569 |

**8**




| | | | |
|---|---|---|---|
| C | 1.7299 | -0.0182 | -1.8672 |
| C | 3.3186 | 0.0061 | -1.9681 |
| C | 4.0817 | 1.1649 | -1.1833 |
| C | 2.4450 | 2.3655 | -3.7689 |
| C | 1.0037 | 2.1519 | -3.2318 |
| C | 0.8626 | 0.6059 | -3.0574 |

| | | | |
|---|---|---|---|
| C | 2.8357 | 1.6970 | -4.8889 |
| C | 1.9355 | 0.6073 | -5.4877 |
| C | 1.0769 | -0.1267 | -4.4217 |
| H | 1.4769 | 0.4886 | -0.9391 |
| C | 4.0133 | -1.3896 | -1.7722 |
| C | 0.5800 | 2.9073 | -1.9290 |
| C | -0.0041 | 2.7640 | -4.2568 |
| O | -0.5015 | 0.4133 | -2.7143 |
| O | 2.6172 | -0.3778 | -6.2707 |
| H | 1.2546 | 1.1256 | -6.1579 |
| H | 0.1118 | -0.3062 | -4.8923 |
| H | 1.4765 | -1.1244 | -4.2458 |
| C | 4.1954 | 1.8725 | -5.5609 |
| C | 2.6003 | -0.2945 | -7.6209 |
| O | 2.1710 | 0.6614 | -8.2724 |
| C | 3.1616 | -1.5288 | -8.3500 |
| C | 2.2325 | -2.7733 | -8.2289 |
| C | 2.9419 | -4.0907 | -8.5472 |
| H | 0.8479 | 3.9638 | -1.9593 |
| H | -0.5015 | 2.8922 | -1.7873 |
| H | 0.9648 | 2.4920 | -1.0031 |
| H | -1.0398 | 2.6517 | -3.9332 |
| H | 0.1706 | 3.8351 | -4.3712 |
| H | 0.0156 | 2.3501 | -5.2561 |
| H | 4.1422 | -1.7501 | -7.9266 |
| O | 3.2984 | -1.1672 | -9.7177 |
| N | 1.0582 | -2.6108 | -9.0870 |
| H | 1.9328 | -2.8275 | -7.1832 |
| C | -0.2344 | -2.5332 | -8.7458 |
| O | -1.0735 | -2.1341 | -9.5449 |
| C | -0.6342 | -2.9028 | -7.3456 |
| H | 2.8305 | -0.3398 | -9.7966 |
| H | 1.2711 | -2.3734 | -10.0442 |
| C | 3.5349 | -4.3069 | -9.8121 |
| C | 4.1745 | -5.5267 | -10.1051 |
| C | 4.2188 | -6.5492 | -9.1395 |
| C | 3.6165 | -6.3522 | -7.8833 |
| C | 2.9782 | -5.1313 | -7.5914 |
| H | 3.5061 | -3.5370 | -10.5696 |
| H | 4.6289 | -5.6775 | -11.0739 |
| H | 4.7076 | -7.4859 | -9.3660 |
| H | 3.6395 | -7.1417 | -7.1460 |
| H | 2.5056 | -5.0098 | -6.6287 |
| C | -1.3679 | -1.9874 | -6.5619 |
| C | -1.7387 | -2.3170 | -5.2425 |
| C | -1.3927 | -3.5716 | -4.7061 |
| C | -0.6931 | -4.5048 | -5.4949 |
| C | -0.3245 | -4.1751 | -6.8143 |
| H | -1.6409 | -1.0254 | -6.9735 |
| H | -2.2865 | -1.6053 | -4.6402 |
| H | -1.6789 | -3.8231 | -3.6941 |
| H | -0.4525 | -5.4774 | -5.0905 |
| H | 0.1897 | -4.9025 | -7.4263 |
| O | 1.2983 | -1.3768 | -1.7611 |
| C | 0.4063 | -1.7724 | -0.8265 |
| O | -0.0758 | -1.0124 | 0.0149 |
| C | 0.0911 | -3.2267 | -0.9136 |
| C | 0.6969 | -4.0667 | -1.8807 |
| C | 0.3799 | -5.4382 | -1.9359 |
| C | -0.5468 | -5.9848 | -1.0289 |
| C | -1.1555 | -5.1596 | -0.0650 |
| C | -0.8372 | -3.7885 | -0.0076 |
| H | 3.5242 | 0.2131 | -3.0057 |
| H | -0.6614 | 0.7866 | -1.8576 |
| H | 1.4045 | -3.6715 | -2.5945 |

| | | | |
|---|---|---|---|
| H | 0.8458 | -6.0714 | -2.6770 |
| H | -0.7918 | -7.0364 | -1.0720 |
| H | -1.8680 | -5.5776 | 0.6319 |
| H | -1.3133 | -3.1660 | 0.7378 |
| C | 5.5112 | -1.4662 | -1.3992 |
| C | 6.3218 | -0.1925 | -1.1896 |
| C | 5.5861 | 1.0954 | -1.6138 |
| O | 3.7225 | -2.2877 | -2.8513 |
| C | 3.8208 | -2.1999 | -0.4804 |
| H | 6.0651 | -2.1875 | -2.0029 |
| O | 5.2143 | -2.0758 | -0.1208 |
| H | 7.2555 | -0.2592 | -1.7501 |
| H | 6.6289 | -0.1293 | -0.1447 |
| H | 5.6417 | 1.1521 | -2.7029 |
| O | 6.3534 | 2.1759 | -1.1132 |
| C | 4.3131 | -2.1887 | -4.0521 |
| O | 5.0917 | -1.3042 | -4.4000 |
| C | 3.9067 | -3.3102 | -4.9845 |
| H | 3.5343 | -3.2417 | -0.6378 |
| H | 3.1610 | -1.7380 | 0.2537 |
| H | 6.3818 | 2.1327 | -0.1659 |
| H | 4.2481 | -4.2676 | -4.5916 |
| H | 2.8217 | -3.3373 | -5.0783 |
| H | 4.3490 | -3.1633 | -5.9692 |
| C | 3.4514 | 3.1630 | -2.9336 |
| O | 3.1021 | 4.5476 | -2.9725 |
| H | 4.4459 | 3.0445 | -3.3494 |
| C | 3.9611 | 5.5685 | -2.7255 |
| O | 3.6128 | 6.7445 | -2.7514 |
| C | 5.4200 | 5.2136 | -2.4418 |
| H | 5.5110 | 4.6629 | -1.5067 |
| H | 5.8560 | 4.6315 | -3.2525 |
| H | 6.0028 | 6.1292 | -2.3414 |
| C | 3.9795 | 0.9678 | 0.3651 |
| H | 4.4657 | 1.7772 | 0.9124 |
| H | 2.9427 | 0.9430 | 0.7017 |
| H | 4.4546 | 0.0674 | 0.7379 |
| C | 3.5542 | 2.6116 | -1.4868 |
| O | 3.2533 | 3.3566 | -0.5495 |
| H | 4.0789 | 1.8770 | -6.6441 |
| H | 4.6767 | 2.8217 | -5.3335 |
| H | 4.8756 | 1.0637 | -5.3003 |

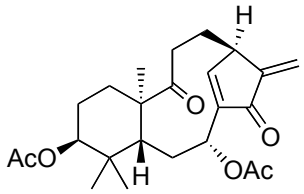
**8**$H_2$

| | | | |
|---|---|---|---|
| C | -0.5274 | 0.9604 | -3.2952 |
| C | 0.1057 | 2.3738 | -3.6063 |
| C | 1.6009 | 2.5509 | -3.1274 |
| C | -0.4542 | 2.2888 | -0.2237 |
| C | -0.9619 | 0.8469 | -0.6195 |
| C | -1.5564 | 0.8557 | -2.0803 |
| C | -1.4194 | 3.4647 | -0.5825 |
| C | -2.7798 | 3.0463 | -1.2012 |
| C | -2.7364 | 1.8673 | -2.2110 |
| H | 0.3026 | 0.2837 | -3.1107 |
| C | -0.1193 | 2.9270 | -5.0588 |
| C | 0.0908 | -0.2850 | -0.4195 |
| C | -2.0393 | 0.4265 | 0.4426 |
| O | -2.1320 | -0.4373 | -2.2003 |
| O | -3.3632 | 4.1794 | -1.8386 |
| H | -3.4394 | 2.7437 | -0.3916 |
| H | -3.6870 | 1.3431 | -2.0995 |
| H | -2.7795 | 2.2388 | -3.2298 |
| C | -1.6255 | 4.3594 | 0.6591 |
| C | -4.3403 | 4.9037 | -1.2351 |
| O | -4.8774 | 4.6267 | -0.1635 |

| | | | |
|---|---|---|---|
| C | -4.7036 | 6.1996 | -1.9818 |
| C | -3.7102 | 7.3667 | -1.7389 |
| C | -4.2593 | 8.6568 | -2.3476 |
| H | 0.6836 | -0.1234 | 0.4821 |
| H | -0.3767 | -1.2638 | -0.3025 |
| H | 0.7819 | -0.4226 | -1.2431 |
| H | -1.6028 | 0.3615 | 1.4406 |
| H | -2.8865 | 1.0933 | 0.5375 |
| H | -2.4663 | -0.5582 | 0.2488 |
| H | -5.6895 | 6.4984 | -1.6228 |
| O | -4.7996 | 5.9798 | -3.3793 |
| N | -2.3686 | 7.0263 | -2.2228 |
| H | -3.6587 | 7.5154 | -0.6578 |
| C | -1.1848 | 7.2378 | -1.6313 |
| O | -0.1925 | 6.5976 | -1.9676 |
| C | -1.0941 | 8.2194 | -0.4960 |
| H | -5.0045 | 6.8160 | -3.7741 |
| H | -2.3405 | 6.3603 | -2.9912 |
| C | -3.8528 | 9.0960 | -3.6297 |
| C | -4.3782 | 10.2837 | -4.1736 |
| C | -5.3142 | 11.0399 | -3.4433 |
| C | -5.7249 | 10.6080 | -2.1682 |
| C | -5.2001 | 9.4204 | -1.6230 |
| H | -3.1326 | 8.5302 | -4.2045 |
| H | -4.0604 | 10.6173 | -5.1513 |
| H | -5.7155 | 11.9526 | -3.8605 |
| H | -6.4418 | 11.1902 | -1.6068 |
| H | -5.5212 | 9.1030 | -0.6408 |
| C | -1.5978 | 9.5345 | -0.6179 |
| C | -1.4913 | 10.4427 | 0.4536 |
| C | -0.8602 | 10.0503 | 1.6492 |
| C | -0.3228 | 8.7545 | 1.7666 |
| C | -0.4313 | 7.8477 | 0.6940 |
| H | -2.0553 | 9.8615 | -1.5396 |
| H | -1.8840 | 11.4443 | 0.3527 |
| H | -0.7729 | 10.7482 | 2.4695 |
| H | 0.1806 | 8.4585 | 2.6759 |
| H | 0.0007 | 6.8620 | 0.7835 |
| O | -1.2012 | 0.5062 | -4.4723 |
| C | -0.9821 | -0.7246 | -4.9863 |
| O | -0.2239 | -1.5487 | -4.4723 |
| C | -1.7323 | -0.9630 | -6.2518 |
| C | -2.6476 | -0.0131 | -6.7681 |
| C | -3.3344 | -0.2637 | -7.9724 |
| C | -3.1162 | -1.4652 | -8.6721 |
| C | -2.2120 | -2.4177 | -8.1662 |
| C | -1.5246 | -2.1676 | -6.9621 |
| H | -0.4599 | 3.0632 | -3.0014 |
| H | -1.4377 | -1.0829 | -2.1890 |
| H | -2.8378 | 0.9139 | -6.2469 |
| H | -4.0319 | 0.4656 | -8.3584 |
| H | -3.6442 | -1.6579 | -9.5950 |
| H | -2.0451 | -3.3417 | -8.7009 |
| H | -0.8325 | -2.9079 | -6.5847 |
| C | 0.7617 | 4.0951 | -5.5556 |
| C | 1.8730 | 4.6631 | -4.6734 |
| C | 1.9533 | 4.0689 | -3.2468 |
| O | -1.5037 | 3.1280 | -5.3735 |
| C | 0.4391 | 2.1967 | -6.2914 |
| H | 0.1934 | 4.8951 | -6.0324 |
| O | 1.3499 | 3.2754 | -6.5951 |
| H | 1.7454 | 5.7428 | -4.5800 |
| H | 2.8262 | 4.5425 | -5.1901 |
| H | 1.2610 | 4.6366 | -2.6263 |
| O | 3.2573 | 4.3476 | -2.7721 |

| | | | |
|---|---|---|---|
| C | -2.1991 | 4.2172 | -5.0198 |
| O | -1.7904 | 5.1351 | -4.3116 |
| C | -3.6019 | 4.2060 | -5.6015 |
| H | -0.2826 | 2.0437 | -7.0967 |
| H | 0.9524 | 1.2600 | -6.0795 |
| H | 3.8925 | 3.9339 | -3.3411 |
| H | -3.6403 | 3.6042 | -6.5092 |
| H | -4.3016 | 3.7905 | -4.8766 |
| H | -3.9164 | 5.2202 | -5.8443 |
| C | 1.0430 | 2.7105 | -0.4602 |
| O | 1.7068 | 2.3869 | 0.7697 |
| H | 1.0779 | 3.7911 | -0.5821 |
| C | 2.7959 | 3.0228 | 1.2699 |
| O | 3.2821 | 2.7349 | 2.3590 |
| C | 3.4101 | 4.1449 | 0.4391 |
| H | 2.6736 | 4.8859 | 0.1324 |
| H | 4.1693 | 4.6591 | 1.0282 |
| H | 3.9029 | 3.7309 | -0.4386 |
| C | 2.6113 | 1.7376 | -4.0042 |
| H | 3.6148 | 1.7314 | -3.5748 |
| H | 2.3113 | 0.6943 | -4.1078 |
| H | 2.7583 | 2.1362 | -5.0023 |
| C | 1.7972 | 2.0689 | -1.6522 |
| O | 2.6029 | 1.1651 | -1.4146 |
| H | -2.2244 | 3.8537 | 1.4180 |
| H | -0.6739 | 4.6287 | 1.1180 |
| H | -2.1312 | 5.2917 | 0.4156 |
| H | -0.5184 | 2.2439 | 0.8648 |
| H | -0.9308 | 4.1126 | -1.3060 |

**9**




| | | | |
|---|---|---|---|
| C | 2.8363 | -2.3248 | -0.3092 |
| C | 2.2377 | -0.9508 | 0.1866 |
| C | 2.1555 | 0.2143 | -0.8895 |
| C | 1.6558 | -0.3184 | -2.2651 |
| C | 2.3415 | -1.6130 | -2.7260 |
| C | 2.1979 | -2.7206 | -1.6702 |
| C | 2.7800 | -0.4930 | 1.5902 |
| C | 1.1396 | 1.3066 | -0.4154 |
| C | -0.3751 | 1.0021 | -0.4237 |
| C | -1.2252 | 1.7455 | 0.6497 |
| C | -1.2068 | 1.1333 | 2.0744 |
| C | 0.2055 | 0.9269 | 2.5637 |
| C | 0.5398 | -0.3569 | 2.7311 |
| C | 1.9363 | -0.9357 | 2.8209 |
| C | -0.6360 | -1.1905 | 2.5053 |
| C | -1.7319 | -0.2949 | 2.1150 |
| C | 2.5154 | -3.4497 | 0.7048 |
| C | 4.3797 | -2.3369 | -0.4575 |
| C | 3.5333 | 0.9009 | -1.1247 |
| H | 1.7862 | 0.4486 | -3.0302 |
| H | 0.5854 | -0.5214 | -2.2505 |
| H | 3.3910 | -1.4350 | -2.9539 |
| H | 1.8951 | -1.9406 | -3.6653 |
| O | 0.8033 | -2.9764 | -1.4911 |
| H | 2.7152 | -3.6116 | -2.0234 |
| H | 3.8066 | -0.8223 | 1.7258 |
| H | 2.8544 | 0.5927 | 1.6327 |

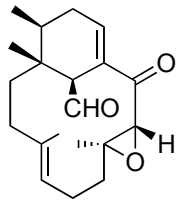
| | | | |
|---|---|---|---|
| O | 1.5337 | 2.4005 | -0.0094 |
| H | -0.5460 | -0.0715 | -0.3599 |
| H | -0.7349 | 1.3025 | -1.4075 |
| H | -2.2584 | 1.7806 | 0.3030 |
| H | -0.9139 | 2.7899 | 0.7055 |
| H | -1.7584 | 1.7568 | 2.7793 |
| O | 2.5597 | -0.4933 | 4.0211 |
| H | 1.8417 | -2.0208 | 2.8524 |
| O | -0.6910 | -2.4154 | 2.6010 |
| C | -2.9799 | -0.7178 | 1.8538 |
| H | 0.9112 | 1.7455 | 2.5907 |
| C | 0.1213 | -3.9731 | -2.1050 |
| O | -1.0871 | -4.1330 | -1.9667 |
| C | 0.9173 | -4.9116 | -3.0096 |
| H | 1.1927 | -1.2045 | 0.3480 |
| H | 2.7666 | -4.4310 | 0.3011 |
| H | 3.0823 | -3.3420 | 1.6296 |
| H | 1.4574 | -3.4779 | 0.9705 |
| H | 4.7202 | -3.3046 | -0.8277 |
| H | 4.7621 | -1.5995 | -1.1534 |
| H | 4.8966 | -2.1837 | 0.4885 |
| H | 4.1987 | 0.3248 | -1.7592 |
| H | 3.4191 | 1.8564 | -1.6397 |
| H | 4.0642 | 1.1107 | -0.1972 |
| H | 1.4375 | -4.3558 | -3.7886 |
| H | 1.6395 | -5.4828 | -2.4270 |
| H | 0.2410 | -5.6171 | -3.4923 |
| C | 3.5221 | -1.2336 | 4.5939 |
| O | 3.9820 | -2.2856 | 4.1533 |
| C | 4.0343 | -0.6227 | 5.8879 |
| H | -3.2359 | -1.7668 | 1.9161 |
| H | -3.7583 | -0.0255 | 1.5723 |
| H | 3.2221 | -0.5328 | 6.6087 |
| H | 4.8144 | -1.2498 | 6.3190 |
| H | 4.4475 | 0.3677 | 5.6995 |

**9**$H_2$

| | | | |
|---|---|---|---|
| C | -1.6176 | -3.3048 | 4.1864 |
| C | -0.3926 | -2.3957 | 4.6069 |
| C | -0.5792 | -0.8362 | 4.3664 |
| C | -1.9989 | -0.3460 | 4.7849 |
| C | -3.1441 | -1.2451 | 4.2994 |
| C | -2.9320 | -2.6978 | 4.7506 |
| C | 1.0021 | -2.9166 | 4.1182 |
| C | 0.4599 | -0.0593 | 5.2352 |
| C | 0.2858 | -0.0237 | 6.7608 |
| C | 1.5957 | -0.1058 | 7.5825 |
| C | 2.1661 | -1.5260 | 7.8220 |
| C | 2.8520 | -2.1750 | 6.5964 |
| C | 2.2503 | -3.5870 | 6.3989 |
| C | 1.7631 | -3.9762 | 4.9745 |
| C | 1.1970 | -3.7258 | 7.4871 |
| C | 1.1351 | -2.5237 | 8.3092 |
| C | -1.4900 | -4.7318 | 4.7680 |
| C | -1.7679 | -3.5167 | 2.6576 |
| C | -0.3723 | -0.4261 | 2.8772 |
| H | -2.1626 | 0.6695 | 4.4208 |
| H | -2.1020 | -0.2709 | 5.8664 |
| H | -3.2457 | -1.1904 | 3.2168 |
| H | -4.0882 | -0.8713 | 4.6968 |
| O | -2.8827 | -2.7093 | 6.1795 |
| H | -3.7574 | -3.3033 | 4.3787 |
| H | 0.8873 | -3.3148 | 3.1134 |
| H | 1.6865 | -2.0883 | 3.9548 |
| O | 1.4213 | 0.5139 | 4.7220 |

| | | | |
|---|---|---|---|
| H | -0.4131 | -0.7928 | 7.0842 |
| H | -0.1975 | 0.9275 | 6.9825 |
| H | 1.3929 | 0.3411 | 8.5562 |
| H | 2.3651 | 0.5303 | 7.1415 |
| H | 2.9158 | -1.4509 | 8.6117 |
| O | 2.9383 | -4.3414 | 4.2555 |
| H | 1.1466 | -4.8654 | 5.0895 |
| O | 0.5284 | -4.7462 | 7.6398 |
| C | 0.2572 | -2.3704 | 9.3158 |
| H | 2.7722 | -1.5506 | 5.7124 |
| C | -3.9230 | -3.0305 | 6.9833 |
| O | -3.8516 | -2.9865 | 8.2076 |
| C | -5.2269 | -3.4474 | 6.3065 |
| H | -0.3690 | -2.4920 | 5.6883 |
| H | -2.4153 | -5.2943 | 4.6396 |
| H | -0.7134 | -5.3123 | 4.2717 |
| H | -1.2762 | -4.7254 | 5.8356 |
| H | -2.6521 | -4.1168 | 2.4396 |
| H | -1.8819 | -2.6011 | 2.0904 |
| H | -0.9275 | -4.0592 | 2.2261 |
| H | -1.2377 | -0.6241 | 2.2529 |
| H | -0.2062 | 0.6482 | 2.7795 |
| H | 0.4858 | -0.9131 | 2.4164 |
| H | -5.5775 | -2.6731 | 5.6253 |
| H | -5.0918 | -4.3793 | 5.7583 |
| H | -5.9971 | -3.6086 | 7.0607 |
| C | 2.9103 | -5.3496 | 3.3653 |
| O | 1.9206 | -6.0071 | 3.0486 |
| C | 4.2703 | -5.6096 | 2.7387 |
| H | -0.4499 | -3.1512 | 9.5631 |
| H | 0.2256 | -1.4646 | 9.9013 |
| H | 4.6295 | -4.7137 | 2.2334 |
| H | 4.9901 | -5.8923 | 3.5062 |
| H | 4.2025 | -6.4173 | 2.0103 |
| H | 3.9237 | -2.2645 | 6.7770 |
| H | 3.0103 | -4.3144 | 6.6852 |

**10**




| | | | |
|---|---|---|---|
| C | 26.5053 | 16.5557 | 3.2559 |
| C | 26.7449 | 17.4968 | 4.4419 |
| C | 25.7809 | 17.8041 | 5.3350 |
| C | 24.3484 | 17.3107 | 5.2630 |
| C | 24.1416 | 16.1572 | 4.2543 |
| C | 24.9808 | 16.3487 | 2.9365 |
| C | 24.4271 | 17.6216 | 2.2120 |
| C | 25.0641 | 18.0365 | 0.8588 |
| C | 26.0263 | 19.2164 | 0.9296 |
| C | 29.2626 | 19.6345 | 2.8650 |
| C | 29.0006 | 18.2532 | 3.4292 |
| C | 28.0978 | 18.0864 | 4.6313 |
| C | 27.3092 | 19.0896 | 0.5301 |
| C | 28.3892 | 20.1617 | 0.5141 |
| C | 29.5993 | 19.7976 | 1.3907 |
| C | 27.3000 | 15.2625 | 3.4986 |
| H | 26.9566 | 17.0066 | 2.3751 |
| H | 23.7189 | 18.1611 | 4.9992 |
| H | 24.0284 | 17.0150 | 6.2630 |
| H | 23.0887 | 16.1840 | 3.9669 |

| | | | |
|---|---|---|---|
| C | 24.2940 | 14.8109 | 4.9975 |
| H | 24.4412 | 18.4781 | 2.8818 |
| H | 23.3652 | 17.4580 | 2.0217 |
| C | 28.8027 | 20.9363 | 3.5068 |
| O | 28.4857 | 18.4583 | 5.7405 |
| H | 28.0095 | 21.1375 | 0.8058 |
| H | 28.7206 | 20.2754 | -0.5185 |
| H | 30.0488 | 18.8720 | 1.0279 |
| H | 30.3719 | 20.5612 | 1.2923 |
| O | 28.2297 | 14.9674 | 2.7512 |
| C | 24.7308 | 15.1449 | 1.9820 |
| C | 25.4189 | 20.5107 | 1.4513 |
| H | 27.0102 | 14.6523 | 4.3504 |
| H | 24.1304 | 13.9440 | 4.3604 |
| H | 25.2604 | 14.7094 | 5.4861 |
| H | 23.5486 | 14.7367 | 5.7902 |
| H | 25.3038 | 15.2134 | 1.0593 |
| H | 25.0097 | 14.1854 | 2.4136 |
| H | 23.6784 | 15.0702 | 1.7058 |
| H | 27.6391 | 18.1263 | 0.1658 |
| H | 24.2640 | 18.3369 | 0.1809 |
| H | 25.5479 | 17.2008 | 0.3585 |
| H | 29.0754 | 17.4156 | 2.7409 |
| H | 29.4839 | 21.7472 | 3.2489 |
| H | 27.8009 | 21.1993 | 3.1700 |
| H | 28.7880 | 20.8544 | 4.5936 |
| H | 24.3838 | 20.6009 | 1.1208 |
| H | 25.4281 | 20.5270 | 2.5410 |
| H | 25.9342 | 21.3999 | 1.0951 |
| H | 25.9972 | 18.4796 | 6.1528 |
| O | 30.2476 | 18.9417 | 3.6380 |

**10**$H_2$

| | | | |
|---|---|---|---|
| C | 16.8259 | 18.1227 | 1.7719 |
| C | 16.6577 | 19.4249 | 0.9337 |
| C | 17.4841 | 19.3665 | -0.3706 |
| C | 18.9690 | 19.1112 | -0.0795 |
| C | 19.2035 | 17.8324 | 0.7586 |
| C | 18.3357 | 17.7998 | 2.0733 |
| C | 18.9169 | 18.8738 | 3.0509 |
| C | 18.2093 | 19.0672 | 4.4180 |
| C | 17.4577 | 20.3851 | 4.5558 |
| C | 14.3622 | 21.4491 | 2.5255 |
| C | 14.3202 | 20.0848 | 1.8710 |
| C | 15.1822 | 19.7885 | 0.6729 |
| C | 16.1291 | 20.4087 | 4.7873 |
| C | 15.2416 | 21.6367 | 4.9291 |
| C | 14.0159 | 21.5923 | 4.0000 |
| C | 16.0097 | 16.9481 | 1.1984 |
| H | 16.3457 | 18.3083 | 2.7311 |
| H | 19.3887 | 19.9800 | 0.4266 |
| H | 19.5177 | 19.0501 | -1.0204 |
| H | 20.2492 | 17.8658 | 1.0701 |
| C | 19.1289 | 16.5859 | -0.1524 |
| H | 18.9976 | 19.8377 | 2.5560 |
| H | 19.9538 | 18.6092 | 3.2641 |
| C | 15.1404 | 22.6395 | 1.9837 |
| O | 14.7251 | 19.7821 | -0.4697 |
| H | 15.7916 | 22.5580 | 4.7505 |
| H | 14.9033 | 21.6867 | 5.9645 |
| H | 13.3705 | 20.7616 | 4.2892 |
| H | 13.4165 | 22.4939 | 4.1327 |
| O | 15.2606 | 16.3056 | 1.9309 |
| C | 18.5127 | 16.4252 | 2.7803 |
| C | 18.3161 | 21.6341 | 4.4206 |

| | | | |
|---|---|---|---|
| H | 16.1177 | 16.7520 | 0.1330 |
| H | 19.4528 | 15.6796 | 0.3579 |
| H | 18.1359 | 16.4105 | -0.5582 |
| H | 19.7970 | 16.6985 | -1.0068 |
| H | 17.9411 | 16.3511 | 3.7038 |
| H | 18.1833 | 15.5841 | 2.1716 |
| H | 19.5577 | 16.2403 | 3.0316 |
| H | 15.6083 | 19.4667 | 4.8916 |
| H | 18.9614 | 19.0492 | 5.2080 |
| H | 17.5408 | 18.2408 | 4.6526 |
| H | 14.0016 | 19.2284 | 2.4614 |
| H | 14.6443 | 23.5709 | 2.2569 |
| H | 16.1536 | 22.6519 | 2.3841 |
| H | 15.2009 | 22.6046 | 0.8957 |
| H | 19.3165 | 21.4497 | 4.8131 |
| H | 18.4115 | 21.9267 | 3.3752 |
| H | 17.9172 | 22.4796 | 4.9782 |
| H | 17.3818 | 20.3052 | -0.9179 |
| O | 13.2749 | 21.0541 | 1.6818 |
| H | 17.0434 | 20.2525 | 1.5275 |
| H | 17.0988 | 18.5931 | -1.0365 |

### 11

Same as **S6**.

### 11$H_2$

Same as **S6**$H_2$.

### 12

Same as **S3**.

### 12$H_2$

Same as **S3**$H_2$.

### 13

| | | | |
|---|---|---|---|
| C | 4.7322 | -5.5673 | 8.4806 |
| C | 3.3533 | -6.1269 | 8.0452 |
| C | 3.3555 | -6.7245 | 6.6129 |
| C | 4.0439 | -5.8172 | 5.5674 |
| C | 5.3643 | -5.3243 | 6.1233 |
| C | 6.5603 | -5.7374 | 5.6700 |
| C | 7.8788 | -5.4982 | 6.3840 |
| C | 8.1078 | -6.4748 | 7.5611 |
| C | 7.2518 | -6.2590 | 8.8390 |
| C | 5.7688 | -6.6975 | 8.7394 |
| C | 5.1938 | -4.5633 | 7.4177 |
| H | 4.6009 | -5.0204 | 9.4154 |
| H | 2.6215 | -5.3187 | 8.0818 |
| H | 3.0061 | -6.8738 | 8.7603 |
| H | 3.8676 | -7.6868 | 6.6295 |
| H | 2.3339 | -6.9415 | 6.2998 |
| H | 3.4147 | -4.9547 | 5.3445 |
| H | 4.1916 | -6.3531 | 4.6291 |
| H | 7.9609 | -4.4646 | 6.7184 |
| H | 8.6723 | -5.6256 | 5.6470 |
| H | 9.1546 | -6.3847 | 7.8541 |
| H | 7.9968 | -7.5026 | 7.2128 |
| H | 7.3389 | -5.2352 | 9.2029 |
| H | 7.7084 | -6.8671 | 9.6210 |
| H | 5.6902 | -7.4786 | 7.9840 |
| H | 5.4888 | -7.1875 | 9.6727 |

| | | | |
|---|---|---|---|
| H | 4.4439 | -3.7840 | 7.2760 |
| H | 6.0944 | -4.0374 | 7.7245 |
| H | 6.6002 | -6.3894 | 4.8094 |

**13**$H_2$

| | | | |
|---|---|---|---|
| C | 6.1518 | -1.8968 | -2.0281 |
| C | 7.4469 | -2.0521 | -1.2032 |
| C | 7.1694 | -2.3359 | 0.2870 |
| C | 6.2185 | -3.5341 | 0.4829 |
| C | 4.9121 | -3.3926 | -0.3265 |
| C | 3.9311 | -2.3846 | 0.3206 |
| C | 2.7547 | -1.9256 | -0.5663 |
| C | 2.9383 | -0.5349 | -1.2124 |
| C | 4.0214 | -0.3972 | -2.3047 |
| C | 5.4718 | -0.5257 | -1.7940 |
| C | 5.2578 | -3.1329 | -1.8062 |
| H | 8.0714 | -1.1638 | -1.3065 |
| H | 8.0311 | -2.8773 | -1.6130 |
| H | 8.1108 | -2.5305 | 0.8017 |
| H | 6.7534 | -1.4489 | 0.7635 |
| H | 5.9959 | -3.6678 | 1.5423 |
| H | 6.7331 | -4.4433 | 0.1688 |
| H | 4.4070 | -4.3595 | -0.2983 |
| H | 4.4541 | -1.5141 | 0.7115 |
| H | 3.5191 | -2.8657 | 1.2087 |
| H | 1.8740 | -1.8580 | 0.0738 |
| H | 2.4946 | -2.6781 | -1.3103 |
| H | 3.1190 | 0.2043 | -0.4308 |
| H | 1.9840 | -0.2504 | -1.6576 |
| H | 3.9140 | 0.6033 | -2.7257 |
| H | 3.8290 | -1.0681 | -3.1417 |
| H | 6.0791 | 0.2230 | -2.3046 |
| H | 5.5169 | -0.2318 | -0.7472 |
| H | 4.3660 | -3.1010 | -2.4280 |
| H | 5.8001 | -4.0040 | -2.1769 |
| H | 6.4350 | -1.9125 | -3.0819 |

**14**

| | | | |
|---|---|---|---|
| C | 4.0175 | -7.6183 | -12.9269 |
| C | 5.0540 | -8.0712 | -12.1968 |
| C | 5.3532 | -7.5873 | -10.7820 |
| C | 4.4546 | -6.4103 | -10.3131 |
| C | 3.7978 | -5.6327 | -11.4780 |
| C | 4.8421 | -4.8242 | -12.3009 |
| C | 4.4663 | -4.4671 | -13.7621 |
| C | 4.8933 | -5.4928 | -14.8521 |
| C | 3.8569 | -6.5776 | -15.2456 |
| C | 3.8715 | -7.8809 | -14.4097 |
| C | 3.0253 | -6.6526 | -12.3184 |
| H | 5.2950 | -8.4236 | -10.0849 |
| H | 6.3918 | -7.2551 | -10.7785 |
| H | 5.0229 | -5.7348 | -9.6725 |
| H | 3.6622 | -6.8137 | -9.6808 |
| H | 3.0748 | -4.9276 | -11.0652 |
| H | 5.8050 | -5.3349 | -12.3110 |
| H | 5.0326 | -3.8982 | -11.7570 |
| H | 4.9967 | -3.5418 | -13.9915 |
| H | 3.4115 | -4.2057 | -13.8492 |
| H | 5.8523 | -5.9495 | -14.6048 |
| H | 5.0865 | -4.9151 | -15.7571 |
| H | 4.0354 | -6.8616 | -16.2835 |
| H | 2.8586 | -6.1398 | -15.2510 |
| H | 2.9554 | -8.4460 | -14.5845 |
| H | 4.6939 | -8.5163 | -14.7408 |

| | | | |
|---|---|---|---|
| H | 2.4102 | -6.1579 | -13.0669 |
| H | 2.3272 | -7.2165 | -11.6986 |
| H | 5.7859 | -8.7280 | -12.6440 |

### 14$H_2$

Same as **13**$H_2$.

### 15

| | | | |
|---|---|---|---|
| C | -2.6031 | 3.1697 | 6.7723 |
| C | -1.4376 | 2.1474 | 6.8220 |
| C | -1.7824 | 1.0219 | 5.8182 |
| C | -3.0896 | 1.4655 | 5.2137 |
| C | -3.6975 | 0.7574 | 4.0225 |
| C | -2.9620 | 1.0754 | 2.7012 |
| C | -2.9071 | 2.5777 | 2.3286 |
| C | -1.7729 | 3.3666 | 3.0265 |
| C | -2.2269 | 4.6313 | 3.7906 |
| C | -1.4346 | 4.8839 | 5.0961 |
| C | -2.1951 | 4.6244 | 6.4250 |
| C | -3.5522 | 2.5829 | 5.7671 |
| H | -1.3299 | 1.7400 | 7.8280 |
| H | -0.4820 | 2.6060 | 6.5690 |
| H | -1.9095 | 0.0600 | 6.3158 |
| H | -1.0105 | 0.9112 | 5.0571 |
| H | -4.7435 | 1.0537 | 3.9342 |
| H | -3.6958 | -0.3166 | 4.2111 |
| H | -3.4801 | 0.5442 | 1.9019 |
| H | -1.9545 | 0.6578 | 2.7192 |
| H | -3.8810 | 3.0329 | 2.5107 |
| H | -2.7550 | 2.6590 | 1.2515 |
| H | -1.2329 | 2.7071 | 3.7004 |
| H | -1.0231 | 3.6515 | 2.2873 |
| H | -3.2934 | 4.6076 | 4.0099 |
| H | -2.1050 | 5.4871 | 3.1253 |
| H | -1.1500 | 5.9369 | 5.1010 |
| H | -0.4849 | 4.3494 | 5.0838 |
| H | -1.5742 | 4.9962 | 7.2411 |
| H | -3.0882 | 5.2506 | 6.4418 |
| H | -4.4532 | 3.0957 | 5.4644 |
| H | -3.1180 | 3.1735 | 7.7342 |

### 15$H_2$

| | | | |
|---|---|---|---|
| C | -3.8444 | 5.4762 | 11.9499 |
| C | -2.7665 | 4.4863 | 11.4819 |
| C | -1.8855 | 5.2727 | 10.5110 |
| C | -1.9593 | 6.7458 | 10.9445 |
| C | -0.7131 | 7.2480 | 11.7180 |
| C | -0.5233 | 6.6994 | 13.1485 |
| C | -1.0319 | 7.6385 | 14.2629 |
| C | -1.7143 | 6.9314 | 15.4508 |
| C | -3.2013 | 6.5740 | 15.2312 |
| C | -3.4615 | 5.2046 | 14.5662 |
| C | -4.4320 | 5.2096 | 13.3589 |
| C | -3.2966 | 6.8920 | 11.6932 |
| H | -3.2030 | 3.6061 | 11.0085 |
| H | -2.1587 | 4.1174 | 12.3036 |
| H | -2.2984 | 5.1767 | 9.5058 |
| H | -0.8658 | 4.8875 | 10.4734 |
| H | -2.0091 | 7.3490 | 10.0363 |
| H | -0.7159 | 8.3385 | 11.7437 |
| H | 0.1688 | 6.9890 | 11.1305 |
| H | 0.5408 | 6.5307 | 13.3187 |
| H | -0.9648 | 5.7134 | 13.2300 |

| | | | |
|---|---|---|---|
| H | -1.6969 | 8.4067 | 13.8703 |
| H | -0.1729 | 8.1954 | 14.6399 |
| H | -1.1419 | 6.0586 | 15.7678 |
| H | -1.6739 | 7.6217 | 16.2946 |
| H | -3.7170 | 7.3809 | 14.7126 |
| H | -3.6780 | 6.5480 | 16.2123 |
| H | -3.9142 | 4.5710 | 15.3303 |
| H | -2.5325 | 4.6904 | 14.3380 |
| H | -4.9042 | 4.2269 | 13.3198 |
| H | -5.2497 | 5.9052 | 13.5513 |
| H | -3.1942 | 7.4710 | 12.6017 |
| H | -4.0059 | 7.4481 | 11.0786 |
| H | -4.6746 | 5.3566 | 11.2513 |

**16**

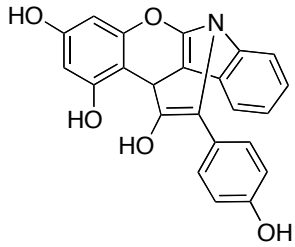
| | | | |
|---|---|---|---|
| C | 11.9116 | 4.9306 | 2.7847 |
| C | 12.7467 | 4.0945 | 3.4307 |
| C | 12.6461 | 3.7628 | 4.9110 |
| C | 11.6191 | 4.6375 | 5.6592 |
| C | 10.3611 | 4.9280 | 4.8177 |
| C | 9.5505 | 3.6384 | 4.5396 |
| C | 8.1402 | 3.8762 | 3.9596 |
| C | 7.4609 | 2.6083 | 3.3966 |
| C | 8.1681 | 1.9644 | 2.1838 |
| C | 8.1787 | 2.8326 | 0.9064 |
| C | 9.3863 | 2.5709 | -0.0175 |
| C | 10.7278 | 3.1087 | 0.5242 |
| C | 10.8600 | 4.6448 | 0.4650 |
| C | 12.0375 | 5.2028 | 1.2916 |
| C | 10.7940 | 5.6579 | 3.5243 |
| H | 13.6291 | 3.8627 | 5.3720 |
| H | 12.3671 | 2.7120 | 4.9945 |
| H | 12.0900 | 5.5871 | 5.9183 |
| H | 11.3506 | 4.1712 | 6.6079 |
| H | 9.7233 | 5.6010 | 5.3926 |
| H | 9.4475 | 3.0660 | 5.4622 |
| H | 10.1308 | 3.0074 | 3.8710 |
| H | 8.1619 | 4.6410 | 3.1882 |
| H | 7.5108 | 4.2922 | 4.7471 |
| H | 6.4341 | 2.8495 | 3.1186 |
| H | 7.3846 | 1.8682 | 4.1942 |
| H | 7.6729 | 1.0214 | 1.9489 |
| H | 9.1769 | 1.6712 | 2.4646 |
| H | 8.1364 | 3.8913 | 1.1480 |
| H | 7.2583 | 2.6385 | 0.3544 |
| H | 9.1966 | 3.0139 | -0.9960 |
| H | 9.4712 | 1.4972 | -0.1907 |
| H | 10.8743 | 2.7554 | 1.5432 |
| H | 11.5445 | 2.6713 | -0.0511 |
| H | 9.9372 | 5.1197 | 0.7904 |
| H | 10.9815 | 4.9463 | -0.5759 |
| H | 12.9720 | 4.7815 | 0.9187 |
| H | 12.1126 | 6.2811 | 1.1468 |
| H | 9.9418 | 5.8221 | 2.8709 |
| H | 11.1636 | 6.6539 | 3.7702 |
| H | 13.5245 | 3.5836 | 2.8818 |

**16**$H_2$

| | | | |
|---|---|---|---|
| C | -12.9689 | -10.6524 | -7.2485 |
| C | -12.3056 | -10.8152 | -5.8646 |
| C | -12.2322 | -9.4894 | -5.0854 |
| C | -13.6149 | -8.8264 | -4.9610 |
| C | -14.2615 | -8.6155 | -6.3426 |
| C | -15.6259 | -7.8955 | -6.2310 |

| | | | |
|---|---|---|---|
| C | -16.2320 | -7.4370 | -7.5752 |
| C | -15.4557 | -6.2953 | -8.2699 |
| C | -15.4120 | -6.3983 | -9.8090 |
| C | -14.5841 | -7.5783 | -10.3621 |
| C | -13.0688 | -7.4681 | -10.0992 |
| C | -12.2561 | -8.7050 | -10.5390 |
| C | -12.5295 | -9.9886 | -9.7270 |
| C | -12.0441 | -9.9313 | -8.2605 |
| C | -14.3489 | -9.9734 | -7.0761 |
| H | -13.1404 | -11.6562 | -7.6405 |
| H | -11.3084 | -11.2446 | -5.9685 |
| H | -12.8797 | -11.5346 | -5.2788 |
| H | -11.5420 | -8.8064 | -5.5815 |
| H | -11.8188 | -9.6684 | -4.0923 |
| H | -13.5123 | -7.8709 | -4.4451 |
| H | -14.2634 | -9.4443 | -4.3382 |
| H | -13.5945 | -7.9646 | -6.9019 |
| H | -15.5251 | -7.0233 | -5.5836 |
| H | -16.3344 | -8.5554 | -5.7287 |
| H | -16.3509 | -8.2927 | -8.2356 |
| H | -17.2520 | -7.0936 | -7.3985 |
| H | -14.4433 | -6.2088 | -7.8821 |
| H | -15.9270 | -5.3505 | -7.9962 |
| H | -15.0144 | -5.4680 | -10.2168 |
| H | -16.4331 | -6.4720 | -10.1856 |
| H | -14.7431 | -7.6408 | -11.4393 |
| H | -14.9732 | -8.5107 | -9.9612 |
| H | -12.8787 | -7.2669 | -9.0480 |
| H | -12.6896 | -6.5949 | -10.6314 |
| H | -12.4559 | -8.9009 | -11.5933 |
| H | -11.1922 | -8.4717 | -10.4793 |
| H | -12.0282 | -10.8249 | -10.2159 |
| H | -13.5856 | -10.2399 | -9.7890 |
| H | -11.0510 | -10.3807 | -8.2213 |
| H | -11.8837 | -8.9028 | -7.9464 |
| H | -15.0028 | -10.6390 | -6.5109 |
| H | -14.8287 | -9.8590 | -8.0435 |

**17**




| | | | |
|---|---|---|---|
| C | -4.4846 | -0.4357 | -1.3086 |
| C | -3.9579 | -1.3218 | -0.3480 |
| C | -3.9970 | -1.0074 | 1.0254 |
| C | -4.5311 | 0.2240 | 1.4494 |
| C | -5.0307 | 1.1325 | 0.4919 |
| C | -5.0116 | 0.8013 | -0.8804 |
| C | -3.3669 | -2.6806 | -0.6758 |
| C | -2.0828 | -2.8598 | 0.1760 |
| C | -2.6779 | -2.9221 | 1.4417 |
| O | -3.5393 | -1.9478 | 1.9257 |
| N | -3.0593 | -4.2231 | 1.5610 |
| C | -2.0348 | -5.0138 | 1.0338 |
| C | -1.4503 | -4.1018 | 0.1124 |
| C | -0.4442 | -4.5514 | -0.7688 |
| C | -0.0192 | -5.8974 | -0.6944 |
| C | -0.6166 | -6.7976 | 0.2191 |
| C | -1.6507 | -6.3640 | 1.0756 |
| O | -4.5091 | -0.7847 | -2.6298 |

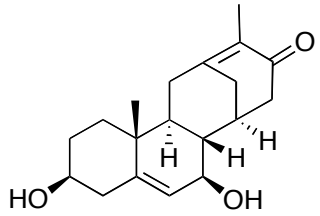
| | | | |
|---|---|---|---|
| H | -4.5567 | 0.4527 | 2.5043 |
| O | -5.5503 | 2.3329 | 0.8828 |
| H | -5.4180 | 1.5033 | -1.5935 |
| H | -0.0076 | -3.8734 | -1.4871 |
| H | 0.7594 | -6.2497 | -1.3571 |
| H | -0.2956 | -7.8300 | 0.2439 |
| H | -2.1513 | -7.0513 | 1.7416 |
| C | -4.4089 | -3.7603 | -0.2811 |
| C | -4.3200 | -4.4333 | 0.9106 |
| C | -5.2194 | -5.4965 | 1.4041 |
| C | -5.9166 | -6.3491 | 0.5195 |
| C | -6.7677 | -7.3526 | 1.0227 |
| C | -6.9276 | -7.5082 | 2.4137 |
| C | -6.2366 | -6.6609 | 3.2994 |
| C | -5.3856 | -5.6577 | 2.7967 |
| O | -7.7479 | -8.4758 | 2.9119 |
| O | -5.4131 | -3.8214 | -1.1669 |
| H | -4.8025 | -0.0846 | -3.1951 |
| H | -5.5329 | 2.4727 | 1.8176 |
| H | -5.7958 | -6.2475 | -0.5485 |
| H | -7.2898 | -7.9960 | 0.3304 |
| H | -6.3602 | -6.7794 | 4.3660 |
| H | -4.8620 | -5.0094 | 3.4843 |
| H | -8.1776 | -8.9885 | 2.2454 |
| H | -5.2991 | -3.0903 | -1.7607 |
| H | -3.1060 | -2.7600 | -1.7319 |

**17**$H_2$

| | | | |
|---|---|---|---|
| C | -4.6710 | -1.0867 | 1.3505 |
| C | -3.8557 | -2.2389 | 1.3942 |
| C | -3.6002 | -2.9839 | 0.2203 |
| C | -4.1862 | -2.5782 | -0.9948 |
| C | -5.0292 | -1.4504 | -1.0389 |
| C | -5.2718 | -0.7064 | 0.1345 |
| C | -3.1633 | -2.7143 | 2.6494 |
| C | -3.3248 | -4.2635 | 2.6626 |
| C | -2.4660 | -4.7191 | 1.4614 |
| O | -2.7794 | -4.0982 | 0.2295 |
| N | -1.1078 | -4.5347 | 2.0081 |
| C | -1.2192 | -5.1116 | 3.2770 |
| C | -2.5185 | -4.9394 | 3.7455 |
| C | -2.9119 | -5.3791 | 5.0202 |
| C | -1.9319 | -6.0038 | 5.8259 |
| C | -0.6049 | -6.1728 | 5.3543 |
| C | -0.2314 | -5.7211 | 4.0672 |
| O | -4.8623 | -0.3153 | 2.4603 |
| H | -3.9929 | -3.1412 | -1.8961 |
| O | -5.5986 | -1.0804 | -2.2237 |
| H | -5.9003 | 0.1713 | 0.1109 |
| H | -3.9249 | -5.2465 | 5.3718 |
| H | -2.1965 | -6.3546 | 6.8134 |
| H | 0.1318 | -6.6462 | 5.9869 |
| H | 0.7799 | -5.8287 | 3.7030 |
| C | -1.6825 | -2.3211 | 2.5148 |
| C | -0.7285 | -3.1959 | 2.1056 |
| C | 0.7058 | -2.8776 | 2.0052 |
| C | 1.4237 | -3.3022 | 0.8686 |
| C | 2.7953 | -3.0063 | 0.7464 |
| C | 3.4525 | -2.2881 | 1.7654 |
| C | 2.7396 | -1.8698 | 2.9049 |
| C | 1.3677 | -2.1636 | 3.0275 |
| O | 4.7792 | -1.9957 | 1.6601 |
| O | -1.4814 | -1.0233 | 2.7801 |
| H | -4.1523 | -0.4054 | 3.0799 |
| H | -6.1370 | -0.3067 | -2.1603 |

| | | | |
|---|---|---|---|
| H | 0.9170 | -3.8524 | 0.0883 |
| H | 3.3293 | -3.3360 | -0.1322 |
| H | 3.2488 | -1.3279 | 3.6887 |
| H | 0.8364 | -1.8580 | 3.9172 |
| H | 5.1759 | -2.3119 | 0.8634 |
| H | -0.5758 | -0.8431 | 2.5702 |
| H | -3.5992 | -2.2851 | 3.5510 |
| H | -4.3528 | -4.6198 | 2.5866 |
| H | -2.5880 | -5.7905 | 1.2870 |

**19**



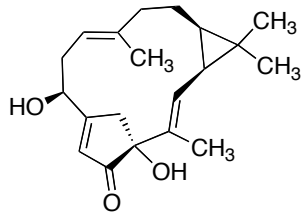

| | | | |
|---|---|---|---|
| C | -1.5320 | -3.1741 | 3.9687 |
| C | -2.9878 | -2.6176 | 3.7335 |
| C | -3.1112 | -1.0625 | 3.5431 |
| C | -2.1379 | -0.2450 | 4.4556 |
| C | -0.8072 | -0.9466 | 4.3527 |
| C | -0.8769 | -2.3001 | 5.0301 |
| C | -3.7477 | -3.3545 | 2.6110 |
| C | -5.0966 | -2.7307 | 2.3245 |
| C | -5.4957 | -1.5150 | 2.7469 |
| C | -4.5982 | -0.5649 | 3.5642 |
| C | -6.8903 | -0.9980 | 2.4126 |
| C | -6.8378 | 0.3882 | 1.7612 |
| C | -6.0695 | 1.3738 | 2.6470 |
| C | -4.6495 | 0.8560 | 2.9304 |
| H | -2.7581 | -0.8961 | 2.5238 |
| H | -2.4508 | -0.2395 | 5.4990 |
| H | -2.0658 | 0.7957 | 4.1435 |
| H | -1.4519 | -2.2641 | 5.9568 |
| H | 0.1209 | -2.6598 | 5.2894 |
| O | -3.9181 | -4.7111 | 2.9598 |
| H | -3.1900 | -3.3127 | 1.6758 |
| C | -5.1411 | -0.5012 | 5.0135 |
| H | -7.4820 | -0.9609 | 3.3273 |
| H | -7.4052 | -1.6958 | 1.7509 |
| O | -8.1552 | 0.8536 | 1.5696 |
| H | -6.3517 | 0.3114 | 0.7867 |
| H | -6.6040 | 1.5330 | 3.5842 |
| H | -6.0099 | 2.3487 | 2.1619 |
| H | -4.1021 | 0.8550 | 1.9867 |
| H | -4.1384 | 1.5769 | 3.5685 |
| H | -3.5161 | -2.8355 | 4.6619 |
| H | -5.7697 | -3.3340 | 1.7318 |
| C | -0.0504 | -0.7684 | 3.2452 |
| C | 0.3543 | -2.0103 | 2.5462 |
| C | -0.5433 | -3.2561 | 2.7522 |
| H | -1.6285 | -4.1857 | 4.3652 |
| O | 1.3122 | -2.0754 | 1.7784 |
| H | -4.3980 | -4.7588 | 3.7732 |
| H | -6.1934 | -0.2231 | 5.0479 |
| H | -5.0588 | -1.4601 | 5.5235 |
| H | -4.6171 | 0.2394 | 5.6162 |
| H | -8.1288 | 1.6675 | 1.0888 |
| C | -0.0547 | 0.4808 | 2.3772 |
| H | 0.1375 | -4.0910 | 2.9181 |
| H | -1.0625 | -3.4822 | 1.8232 |
| H | 0.8918 | 0.5794 | 1.8438 |

| | | | |
|---|---|---|---|
| H | -0.8570 | 0.4359 | 1.6406 |
| H | -0.1823 | 1.3785 | 2.9812 |

**19**$H_2$

| | | | |
|---|---|---|---|
| C | -1.6288 | -3.1590 | 4.1556 |
| C | -3.0504 | -2.7815 | 3.6274 |
| C | -3.1406 | -1.3501 | 3.0274 |
| C | -2.3912 | -0.3122 | 3.9130 |
| C | -0.9909 | -0.7619 | 4.3952 |
| C | -1.1417 | -2.0925 | 5.1495 |
| C | -3.6133 | -3.8251 | 2.6360 |
| C | -4.8828 | -3.3633 | 1.9583 |
| C | -5.3452 | -2.0993 | 1.9612 |
| C | -4.6110 | -0.9342 | 2.6524 |
| C | -6.6487 | -1.7509 | 1.2507 |
| C | -6.4697 | -0.5742 | 0.2858 |
| C | -5.8834 | 0.6380 | 1.0155 |
| C | -4.5423 | 0.2759 | 1.6746 |
| H | -2.6072 | -1.3950 | 2.0789 |
| H | -2.9715 | -0.1152 | 4.8130 |
| H | -2.3167 | 0.6467 | 3.4025 |
| H | -1.8473 | -1.9888 | 5.9756 |
| H | -0.1918 | -2.3899 | 5.5969 |
| O | -3.8516 | -5.0421 | 3.3104 |
| H | -2.9065 | -4.0156 | 1.8292 |
| C | -5.4247 | -0.5316 | 3.9085 |
| H | -7.4070 | -1.5131 | 1.9966 |
| H | -7.0266 | -2.6173 | 0.7062 |
| O | -7.7247 | -0.2345 | -0.2607 |
| H | -5.8054 | -0.8720 | -0.5278 |
| H | -6.5849 | 1.0006 | 1.7678 |
| H | -5.7331 | 1.4617 | 0.3170 |
| H | -3.8293 | 0.0616 | 0.8769 |
| H | -4.1576 | 1.1585 | 2.1850 |
| H | -3.7018 | -2.7842 | 4.5016 |
| H | -5.4345 | -4.1303 | 1.4334 |
| C | 0.1079 | -0.8702 | 3.2979 |
| C | -0.0792 | -2.1032 | 2.3944 |
| C | -0.5327 | -3.3921 | 3.0811 |
| H | -1.7281 | -4.0967 | 4.7042 |
| O | 0.1343 | -2.0701 | 1.1838 |
| H | -4.4768 | -4.8873 | 4.0024 |
| H | -6.4718 | -0.3403 | 3.6789 |
| H | -5.4120 | -1.3113 | 4.6691 |
| H | -5.0522 | 0.3848 | 4.3646 |
| H | -7.6017 | 0.4248 | -0.9273 |
| C | 0.2936 | 0.4298 | 2.4913 |
| H | 0.3468 | -3.8279 | 3.5541 |
| H | -0.8512 | -4.1125 | 2.3297 |
| H | 1.1731 | 0.3678 | 1.8491 |
| H | -0.5628 | 0.6290 | 1.8464 |
| H | 0.4286 | 1.2877 | 3.1495 |
| H | -0.6451 | -0.0177 | 5.1142 |
| H | 1.0497 | -1.0505 | 3.8165 |

**21**

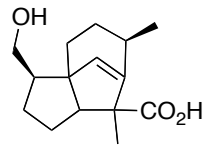



| | | | |
|---|---|---|---|
| C | 2.1460 | -7.5674 | -8.1928 |
| C | 1.5166 | -6.2220 | -7.7435 |
| C | 0.0301 | -6.4176 | -7.9736 |
| C | -0.2510 | -7.5172 | -8.6844 |
| C | 0.9920 | -8.2113 | -8.9699 |
| C | -0.9704 | -5.3898 | -7.4640 |
| C | -1.0025 | -5.2743 | -5.9246 |
| C | -1.3008 | -8.4610 | -3.5943 |
| C | 0.8360 | -9.8917 | -3.8823 |
| C | 2.0197 | -9.3809 | -4.6856 |
| C | 1.8048 | -8.5489 | -5.8958 |
| C | 2.5341 | -8.4982 | -7.0289 |
| C | 1.7182 | -10.8685 | -4.6400 |
| O | 3.2392 | -7.3320 | -9.0577 |
| H | 1.7447 | -5.9727 | -6.7076 |
| H | 1.8594 | -5.3892 | -8.3590 |
| H | -1.2226 | -7.8628 | -9.0019 |
| O | 1.1537 | -9.1597 | -9.7378 |
| O | -2.2726 | -5.6946 | -7.9236 |
| H | -0.6878 | -4.4257 | -7.8905 |
| H | -1.7303 | -4.5180 | -5.6293 |
| H | -0.0371 | -4.9101 | -5.5807 |
| H | -2.3752 | -8.5322 | -3.7701 |
| H | -1.1798 | -8.5118 | -2.5115 |
| C | 1.2110 | -11.5956 | -5.8787 |
| C | 2.6412 | -11.7780 | -3.8512 |
| H | 0.9392 | -7.9155 | -5.8334 |
| C | 3.7804 | -9.3535 | -7.2226 |
| C | -1.3773 | -6.5782 | -5.2299 |
| C | -0.8342 | -7.1093 | -4.1138 |
| C | 0.2704 | -6.4582 | -3.2953 |
| H | -2.8204 | -4.9299 | -7.8233 |
| H | 2.0489 | -11.9653 | -6.4704 |
| H | 0.5902 | -12.4444 | -5.5911 |
| H | 0.6199 | -10.9449 | -6.5216 |
| H | 3.4987 | -12.0692 | -4.4587 |
| H | 3.0133 | -11.2746 | -2.9584 |
| H | 2.1121 | -12.6790 | -3.5394 |
| H | -2.1702 | -7.1284 | -5.7183 |
| H | -0.0223 | -6.4186 | -2.2459 |
| H | 1.1905 | -7.0368 | -3.3610 |
| H | 0.4932 | -5.4376 | -3.5966 |
| C | -0.6209 | -9.6651 | -4.2783 |
| H | 0.9730 | -9.8893 | -2.8021 |
| H | -1.1690 | -10.5684 | -4.0088 |
| H | -0.7171 | -9.5734 | -5.3595 |
| H | 3.3311 | -8.1226 | -9.5744 |
| H | 3.9625 | -10.0166 | -6.3777 |
| H | 3.6763 | -9.9739 | -8.1129 |
| H | 4.6616 | -8.7222 | -7.3402 |
| H | 2.8678 | -9.0250 | -4.1031 |

**21**$H_2$

| | | | |
|---|---|---|---|
| C | 3.2669 | -5.0140 | -4.0208 |
| C | 2.5784 | -6.0335 | -4.9506 |
| C | 2.7007 | -5.4127 | -6.3577 |
| C | 2.3756 | -3.9328 | -6.1322 |
| C | 2.8917 | -3.7012 | -4.7198 |
| C | 1.9069 | -6.1464 | -7.4538 |
| C | 2.4723 | -7.5572 | -7.7555 |
| C | 6.4174 | -7.9151 | -7.9346 |
| C | 7.6525 | -6.6459 | -6.0271 |
| C | 6.9585 | -6.3084 | -4.7165 |
| C | 5.5074 | -6.0065 | -4.7081 |
| C | 4.8013 | -5.1728 | -3.9129 |
| C | 8.0118 | -5.3721 | -5.2784 |
| O | 2.6817 | -5.0464 | -2.7368 |
| H | 2.9867 | -7.0404 | -4.8730 |
| H | 1.5223 | -6.1222 | -4.6884 |
| H | 1.3024 | -3.7474 | -6.1608 |
| O | 2.9296 | -2.6023 | -4.1670 |
| O | 1.9898 | -5.3727 | -8.6321 |
| H | 0.8563 | -6.2204 | -7.1668 |
| H | 1.9389 | -7.9983 | -8.5979 |
| H | 2.2699 | -8.2111 | -6.9111 |
| H | 6.4156 | -7.8781 | -9.0251 |
| H | 7.0598 | -8.7574 | -7.6741 |
| C | 7.6179 | -3.9986 | -5.8062 |
| C | 9.3620 | -5.2910 | -4.5915 |
| H | 4.9855 | -6.5858 | -5.4404 |
| C | 5.4786 | -4.3704 | -2.8080 |
| C | 3.9597 | -7.5313 | -8.1009 |
| C | 4.9836 | -8.1714 | -7.4939 |
| C | 4.8448 | -9.1588 | -6.3454 |
| H | 1.4247 | -5.7511 | -9.2896 |
| H | 6.6058 | -3.9900 | -6.2082 |
| H | 7.6567 | -3.2600 | -5.0050 |
| H | 8.3015 | -3.6873 | -6.5964 |
| H | 9.3217 | -4.5941 | -3.7538 |
| H | 9.6617 | -6.2663 | -4.2068 |
| H | 10.1253 | -4.9513 | -5.2922 |
| H | 4.2033 | -6.8550 | -8.9090 |
| H | 5.1594 | -10.1492 | -6.6746 |
| H | 5.4896 | -8.8697 | -5.5156 |
| H | 3.8337 | -9.2484 | -5.9574 |
| C | 6.9989 | -6.5819 | -7.4088 |
| H | 8.3897 | -7.4445 | -5.9619 |
| H | 7.7750 | -6.2553 | -8.1017 |
| H | 6.2355 | -5.8056 | -7.4411 |
| H | 2.8314 | -4.1856 | -2.3661 |
| H | 6.5626 | -4.4771 | -2.8289 |
| H | 5.2530 | -3.3089 | -2.9084 |
| H | 5.1367 | -4.7044 | -1.8283 |
| H | 7.2404 | -6.9223 | -3.8628 |
| H | 3.7425 | -5.4045 | -6.6718 |
| H | 2.8682 | -3.2851 | -6.8569 |

## 22



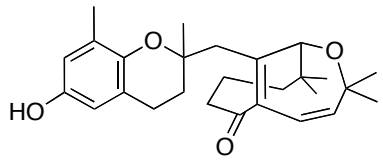

| | | | |
|---|---|---|---|
| C | 0.5654 | 3.1528 | 2.4444 |
| C | -0.1796 | 4.0564 | 3.4663 |
| C | 0.2859 | 3.8631 | 4.7190 |
| C | 0.4938 | 2.3828 | 4.7612 |
| C | 1.3004 | 2.2676 | 3.4782 |
| C | -0.9594 | 1.7526 | 4.7134 |
| C | -2.1245 | 2.7398 | 4.3063 |
| C | -1.6992 | 3.9723 | 3.4315 |
| C | -2.3597 | 5.2849 | 3.8851 |
| C | 1.5484 | 3.9511 | 1.5593 |
| C | -0.2996 | 2.2977 | 1.4781 |
| O | 2.7401 | 3.6873 | 1.4269 |
| O | 0.9260 | 4.9557 | 0.8885 |
| C | 1.6907 | 0.8022 | 3.3808 |
| C | 2.0159 | 0.4989 | 4.8695 |
| C | 1.4278 | 1.6532 | 5.7497 |
| C | 2.5055 | 2.5464 | 6.4013 |
| O | 3.2217 | 1.8014 | 7.3647 |
| H | -1.2162 | 1.3581 | 5.6969 |
| H | -0.9776 | 0.8761 | 4.0688 |
| H | -2.5624 | 3.1148 | 5.2325 |
| H | -2.9301 | 2.1902 | 3.8185 |
| H | -2.0393 | 3.8303 | 2.4079 |
| H | -3.4459 | 5.2171 | 3.8191 |
| H | -2.1074 | 5.5379 | 4.9150 |
| H | -2.0442 | 6.1166 | 3.2541 |
| H | 0.3301 | 1.6225 | 0.8975 |
| H | -1.0330 | 1.6767 | 1.9854 |
| H | -0.8360 | 2.9168 | 0.7581 |
| H | 1.5653 | 5.3944 | 0.3519 |
| H | 2.5459 | 0.6460 | 2.7221 |
| H | 0.8701 | 0.1826 | 3.0203 |
| H | 3.0937 | 0.4103 | 5.0073 |
| H | 1.5846 | -0.4609 | 5.1560 |
| H | 0.8387 | 1.2284 | 6.5640 |
| H | 3.2023 | 2.9534 | 5.6681 |
| H | 2.0405 | 3.3946 | 6.9054 |
| H | 3.6628 | 1.0880 | 6.9287 |
| H | 2.2572 | 2.7649 | 3.6604 |
| H | -0.2627 | 4.2352 | 5.5727 |

## 22$H_2$

| | | | |
|---|---|---|---|
| C | -4.6875 | 5.3928 | 1.2000 |
| C | -4.6027 | 3.8169 | 1.3699 |
| C | -3.9448 | 3.2913 | 0.0592 |
| C | -4.6885 | 4.1696 | -0.9563 |
| C | -4.3787 | 5.5126 | -0.3142 |
| C | -6.2139 | 3.7945 | -0.9614 |
| C | -6.6637 | 2.8517 | 0.1804 |
| C | -5.9724 | 3.1005 | 1.5442 |
| C | -5.8206 | 1.7809 | 2.3200 |
| C | -3.6063 | 6.0873 | 2.0691 |
| C | -6.0346 | 6.0662 | 1.5728 |
| O | -2.7353 | 6.8360 | 1.6365 |
| O | -3.7586 | 5.8129 | 3.3916 |
| C | -4.9051 | 6.5684 | -1.2774 |
| C | -4.5711 | 5.9222 | -2.6460 |
| C | -4.1903 | 4.4261 | -2.4010 |

| | | | |
|---|---|---|---|
| C | -2.6914 | 4.1359 | -2.6325 |
| O | -2.3782 | 4.2951 | -4.0011 |
| H | -6.4720 | 3.2887 | -1.8919 |
| H | -6.8386 | 4.6845 | -0.9684 |
| H | -6.4423 | 1.8334 | -0.1432 |
| H | -7.7480 | 2.8832 | 0.2930 |
| H | -6.6321 | 3.7041 | 2.1639 |
| H | -6.7845 | 1.2870 | 2.4463 |
| H | -5.1558 | 1.0852 | 1.8072 |
| H | -5.4119 | 1.9551 | 3.3159 |
| H | -5.9899 | 7.1430 | 1.4051 |
| H | -6.8732 | 5.6949 | 0.9892 |
| H | -6.2819 | 5.9201 | 2.6249 |
| H | -3.0923 | 6.2791 | 3.8695 |
| H | -4.4122 | 7.5313 | -1.1374 |
| H | -5.9779 | 6.7256 | -1.1703 |
| H | -3.7607 | 6.4653 | -3.1324 |
| H | -5.4350 | 5.9921 | -3.3079 |
| H | -4.7334 | 3.7907 | -3.1022 |
| H | -2.0498 | 4.7866 | -2.0378 |
| H | -2.4572 | 3.1084 | -2.3511 |
| H | -2.5475 | 5.1917 | -4.2481 |
| H | -3.2974 | 5.6457 | -0.3915 |
| H | -4.0779 | 2.2220 | -0.1089 |
| H | -3.9667 | 3.5522 | 2.2163 |
| H | -2.8698 | 3.4785 | 0.0699 |

**23**




| | | | |
|---|---|---|---|
| C | -0.0311 | -36.0907 | -12.9976 |
| C | 0.1998 | -35.7797 | -14.4867 |
| C | 1.5250 | -35.0979 | -14.8968 |
| C | 1.9398 | -33.7503 | -14.2256 |
| C | 2.7093 | -33.9412 | -12.8765 |
| C | 1.8381 | -35.5939 | -11.3113 |
| C | 1.2045 | -36.5634 | -12.2318 |
| H | -0.7996 | -36.8576 | -12.9032 |
| H | -0.4344 | -35.2149 | -12.4937 |
| H | -0.6368 | -35.1795 | -14.8446 |
| H | 0.1299 | -36.7196 | -15.0359 |
| H | 1.4402 | -34.9336 | -15.9718 |
| H | 2.3359 | -35.8227 | -14.8117 |
| C | 0.7329 | -32.8017 | -14.0637 |
| C | 2.9217 | -33.0573 | -15.1997 |
| O | 3.7489 | -34.9071 | -13.0866 |
| O | 1.5663 | -37.7339 | -12.3575 |
| H | 0.2512 | -32.6077 | -15.0225 |
| H | -0.0278 | -33.2077 | -13.4010 |
| H | 1.0386 | -31.8406 | -13.6493 |
| H | 3.2720 | -32.1003 | -14.8117 |
| H | 3.8027 | -33.6751 | -15.3799 |
| H | 2.4614 | -32.8590 | -16.1681 |
| C | 4.7490 | -35.1636 | -12.0854 |
| C | 5.5165 | -33.8804 | -11.7203 |
| C | 5.6984 | -36.1303 | -12.8047 |
| C | 4.2218 | -35.8626 | -10.8268 |
| C | 2.9332 | -36.0957 | -10.5066 |
| H | 6.3806 | -34.1057 | -11.0947 |
| H | 5.8805 | -33.3739 | -12.6145 |
| H | 4.9003 | -33.1748 | -11.1661 |

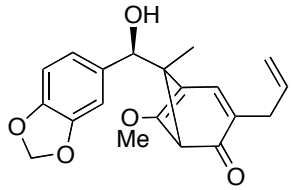
| | | | |
|---|---|---|---|
| H | 5.1766 | -37.0450 | -13.0900 |
| H | 6.0988 | -35.6862 | -13.7164 |
| H | 6.5416 | -36.4134 | -12.1743 |
| H | 4.9806 | -36.2462 | -10.1603 |
| H | 2.7076 | -36.6342 | -9.5995 |
| C | 1.8603 | -34.2856 | -11.6450 |
| C | 2.0408 | -33.2350 | -10.5376 |
| C | 0.7985 | -33.0348 | -9.6243 |
| C | -0.4232 | -32.6039 | -10.4538 |
| C | 1.0640 | -31.9727 | -8.5361 |
| C | 2.1503 | -32.4200 | -7.5530 |
| C | 1.9821 | -33.8756 | -7.1716 |
| C | 1.1062 | -34.7114 | -7.9068 |
| O | 0.4044 | -34.2611 | -9.0056 |
| C | 0.9138 | -36.0491 | -7.4950 |
| C | 1.6247 | -36.5589 | -6.3889 |
| C | 2.5164 | -35.7313 | -5.6801 |
| C | 2.6899 | -34.3911 | -6.0677 |
| C | -0.0541 | -36.9428 | -8.2482 |
| O | 3.2096 | -36.2166 | -4.6116 |
| H | 2.2504 | -32.2616 | -10.9804 |
| H | 2.9222 | -33.4859 | -9.9504 |
| H | -1.2861 | -32.4170 | -9.8141 |
| H | -0.2242 | -31.6925 | -11.0178 |
| H | -0.7197 | -33.3780 | -11.1592 |
| H | 0.1428 | -31.8160 | -7.9729 |
| H | 1.3227 | -31.0083 | -8.9740 |
| H | 2.1220 | -31.7989 | -6.6573 |
| H | 3.1398 | -32.2915 | -7.9918 |
| H | 1.4799 | -37.5860 | -6.0892 |
| H | 3.3638 | -33.7580 | -5.5094 |
| H | -0.2634 | -37.8602 | -7.6983 |
| H | -0.9999 | -36.4249 | -8.4102 |
| H | 0.3556 | -37.2137 | -9.2207 |
| H | 3.0220 | -37.1223 | -4.4211 |
| H | 3.2131 | -32.9941 | -12.6913 |

**23**$H_2$

| | | | |
|---|---|---|---|
| C | -32.3773 | -46.6428 | -19.5242 |
| C | -32.4452 | -45.0966 | -19.3549 |
| C | -33.8513 | -44.4837 | -19.0880 |
| C | -34.7150 | -44.0610 | -20.3204 |
| C | -34.6101 | -45.1018 | -21.4621 |
| C | -33.8314 | -47.4611 | -21.6092 |
| C | -32.4499 | -47.1553 | -20.9736 |
| H | -31.4136 | -46.9813 | -19.1427 |
| H | -33.1208 | -47.1458 | -18.9068 |
| H | -31.8284 | -44.8601 | -18.4874 |
| H | -31.9480 | -44.5924 | -20.1845 |
| H | -33.7149 | -43.6003 | -18.4624 |
| H | -34.4085 | -45.1656 | -18.4449 |
| C | -34.2046 | -42.7025 | -20.8462 |
| C | -36.1792 | -43.8790 | -19.8761 |
| O | -35.3749 | -44.7871 | -22.6094 |
| O | -31.4070 | -47.3346 | -21.6015 |
| H | -34.7919 | -42.3663 | -21.7015 |
| H | -34.2681 | -41.9249 | -20.0848 |
| H | -33.1655 | -42.7577 | -21.1711 |
| H | -36.8132 | -43.5927 | -20.7162 |
| H | -36.5915 | -44.7940 | -19.4546 |
| H | -36.2712 | -43.1028 | -19.1161 |
| C | -34.8224 | -45.1186 | -23.8870 |
| C | -33.8541 | -43.9953 | -24.2955 |
| C | -36.0477 | -45.0947 | -24.8105 |
| C | -34.1257 | -46.4850 | -24.0297 |

| | | | |
|---|---|---|---|
| C | -33.7333 | -47.4249 | -23.1358 |
| H | -33.5201 | -44.1161 | -25.3262 |
| H | -34.3306 | -43.0180 | -24.2157 |
| H | -32.9626 | -43.9774 | -23.6692 |
| H | -36.7667 | -45.8629 | -24.5249 |
| H | -36.5605 | -44.1338 | -24.7599 |
| H | -35.7724 | -45.2682 | -25.8510 |
| H | -33.9029 | -46.7227 | -25.0600 |
| H | -33.2317 | -48.2916 | -23.5413 |
| C | -34.9505 | -46.5583 | -21.0617 |
| C | -36.3884 | -47.0207 | -21.4511 |
| C | -37.0278 | -48.1319 | -20.5769 |
| C | -38.2476 | -48.7044 | -21.3301 |
| C | -37.4288 | -47.5933 | -19.1832 |
| C | -37.9649 | -48.7017 | -18.2741 |
| C | -37.1243 | -49.9564 | -18.3816 |
| C | -36.2251 | -50.1262 | -19.4632 |
| O | -36.0664 | -49.1788 | -20.4529 |
| C | -35.4296 | -51.2914 | -19.5283 |
| C | -35.5443 | -52.2850 | -18.5339 |
| C | -36.4502 | -52.1171 | -17.4692 |
| C | -37.2373 | -50.9546 | -17.3934 |
| C | -34.4489 | -51.4730 | -20.6711 |
| O | -36.5689 | -53.0726 | -16.5045 |
| H | -36.3807 | -47.3389 | -22.4928 |
| H | -37.0629 | -46.1645 | -21.4307 |
| H | -38.7010 | -49.5455 | -20.8067 |
| H | -39.0181 | -47.9461 | -21.4700 |
| H | -37.9615 | -49.0703 | -22.3165 |
| H | -38.1603 | -46.7891 | -19.2667 |
| H | -36.5583 | -47.1637 | -18.6906 |
| H | -38.9905 | -48.9524 | -18.5453 |
| H | -37.9891 | -48.3587 | -17.2393 |
| H | -34.9334 | -53.1731 | -18.5938 |
| H | -37.9255 | -50.8301 | -16.5703 |
| H | -34.0515 | -52.4874 | -20.7028 |
| H | -34.9367 | -51.2714 | -21.6253 |
| H | -33.6145 | -50.7804 | -20.5614 |
| H | -36.0057 | -53.8182 | -16.6408 |
| H | -34.0496 | -48.4924 | -21.3437 |
| H | -34.9200 | -46.6422 | -19.9839 |
| H | -33.5744 | -45.0087 | -21.7787 |

**24**




| | | | |
|---|---|---|---|
| C | -0.5035 | 4.0920 | 1.1895 |
| C | -1.4320 | 5.0519 | 0.9149 |
| C | -1.2301 | 6.3563 | 1.6341 |
| C | -0.0045 | 6.2975 | 2.5712 |
| C | 0.1436 | 4.9952 | 3.4271 |
| C | 0.5280 | 4.3681 | 2.0316 |
| C | 1.1174 | 5.5785 | 1.8331 |
| O | -1.9930 | 7.3135 | 1.5077 |
| H | 0.2207 | 7.2211 | 3.1033 |
| O | 1.5015 | 6.1288 | 0.6341 |
| C | -1.1476 | 4.3992 | 4.0520 |
| C | 1.3120 | 4.8884 | 4.4719 |
| C | 1.5791 | 6.2017 | 5.1921 |
| C | 0.8138 | 6.5579 | 6.3351 |

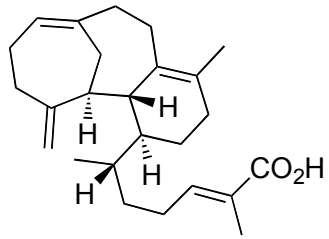
| | | | |
|---|---|---|---|
| C | 1.0454 | 7.7769 | 7.0126 |
| C | 2.0538 | 8.6180 | 6.5179 |
| C | 2.8009 | 8.2773 | 5.4098 |
| C | 2.5917 | 7.0732 | 4.7200 |
| O | 3.6987 | 9.2597 | 5.1467 |
| O | 1.1491 | 3.8157 | 5.3787 |
| C | -2.6370 | 4.9267 | -0.0109 |
| C | -2.8402 | 3.5206 | -0.5452 |
| C | -2.7712 | 3.1858 | -1.8426 |
| C | 2.0575 | 5.2222 | -0.3098 |
| H | -0.5619 | 3.1165 | 0.7318 |
| H | -1.3303 | 4.8107 | 5.0444 |
| H | -2.0553 | 4.5866 | 3.4827 |
| H | -1.0720 | 3.3168 | 4.1626 |
| H | 2.2446 | 4.6408 | 3.9601 |
| H | 0.0419 | 5.8914 | 6.6926 |
| H | 0.4665 | 8.0567 | 7.8803 |
| H | 1.8998 | 3.8101 | 5.9532 |
| H | -2.5180 | 5.6318 | -0.8348 |
| H | -3.5357 | 5.2248 | 0.5311 |
| H | -3.0562 | 2.7564 | 0.1885 |
| H | -2.9274 | 2.1661 | -2.1638 |
| H | -2.5590 | 3.9236 | -2.6032 |
| H | 2.7726 | 4.5408 | 0.1538 |
| H | 1.2832 | 4.6382 | -0.8076 |
| H | 2.5869 | 5.7846 | -1.0789 |
| C | 3.4875 | 10.2446 | 6.1259 |
| O | 2.4590 | 9.8253 | 6.9860 |
| H | 3.1850 | 6.8334 | 3.8497 |
| H | 3.2024 | 11.1816 | 5.6459 |
| H | 4.4040 | 10.3964 | 6.6973 |

**24**$H_2$

| | | | |
|---|---|---|---|
| C | -5.0437 | 2.1086 | 1.1524 |
| C | -4.1931 | 1.1165 | 0.7871 |
| C | -4.8309 | -0.2001 | 0.4835 |
| C | -6.3510 | -0.1471 | 0.6214 |
| C | -6.8822 | 0.4938 | 1.9633 |
| C | -6.5526 | 1.8309 | 1.1993 |
| C | -6.9342 | 1.0854 | -0.1035 |
| O | -4.1796 | -1.1924 | 0.1623 |
| H | -6.8272 | -1.0873 | 0.3448 |
| O | -8.3214 | 0.9930 | -0.4071 |
| C | -6.0784 | 0.1667 | 3.2491 |
| C | -8.3721 | 0.2185 | 2.3859 |
| C | -9.2397 | 1.4681 | 2.5760 |
| C | -10.4428 | 1.6556 | 1.8363 |
| C | -11.2436 | 2.8063 | 2.0180 |
| C | -10.8213 | 3.7544 | 2.9606 |
| C | -9.6688 | 3.5766 | 3.6947 |
| C | -8.8583 | 2.4428 | 3.5332 |
| O | -9.4949 | 4.6306 | 4.5313 |
| O | -8.9482 | -0.7175 | 1.5073 |
| C | -2.6745 | 1.2107 | 0.6816 |
| C | -2.1173 | 2.5300 | 1.1848 |
| C | -1.4585 | 3.4150 | 0.4213 |
| C | -8.8179 | 2.1612 | -1.0431 |
| H | -4.7032 | 3.1021 | 1.4029 |
| H | -6.1301 | -0.8991 | 3.4776 |
| H | -5.0206 | 0.4151 | 3.1977 |
| H | -6.4606 | 0.6975 | 4.1200 |
| H | -8.4202 | -0.2901 | 3.3508 |
| H | -10.7638 | 0.9159 | 1.1177 |
| H | -12.1535 | 2.9508 | 1.4549 |
| H | -8.9121 | -0.3004 | 0.6490 |

| | | | |
|---|---|---|---|
| H | -2.3843 | 1.0490 | -0.3577 |
| H | -2.2251 | 0.4034 | 1.2621 |
| H | -2.2717 | 2.7471 | 2.2327 |
| H | -1.0822 | 4.3384 | 0.8374 |
| H | -1.2832 | 3.2318 | -0.6293 |
| H | -8.3085 | 2.3448 | -1.9900 |
| H | -9.8806 | 2.0396 | -1.2534 |
| H | -8.7030 | 3.0400 | -0.4075 |
| C | -10.5889 | 5.4829 | 4.3064 |
| O | -11.4093 | 4.9256 | 3.3118 |
| H | -7.9643 | 2.3349 | 4.1260 |
| H | -10.2317 | 6.4607 | 3.9811 |
| H | -11.1598 | 5.5961 | 5.2288 |
| H | -7.1519 | 2.7107 | 1.4301 |
| H | -6.3591 | 1.3806 | -0.9854 |

**25**




| | | | |
|---|---|---|---|
| C | -2.7549 | 11.9015 | 2.8293 |
| C | -2.8306 | 10.7891 | 3.8848 |
| C | -2.0688 | 9.5444 | 3.4092 |
| C | -0.5881 | 9.6881 | 3.6647 |
| C | 0.1711 | 10.5316 | 2.9479 |
| C | -0.3910 | 11.4412 | 1.8740 |
| C | -1.3826 | 12.4716 | 2.4586 |
| C | -0.0971 | 8.9998 | 4.9174 |
| C | -0.5174 | 9.7795 | 6.1786 |
| C | -2.0074 | 10.1497 | 6.2731 |
| C | -2.4533 | 11.2799 | 5.3262 |
| C | -3.5781 | 12.1491 | 5.9613 |
| C | -4.7187 | 11.2101 | 6.4188 |
| C | -4.2543 | 10.1584 | 7.4375 |
| C | -2.8442 | 9.6271 | 7.2036 |
| C | -3.8689 | 12.3643 | 2.2359 |
| H | -3.8665 | 10.4597 | 3.8973 |
| H | -2.2496 | 9.3693 | 2.3479 |
| H | -2.4447 | 8.6546 | 3.9157 |
| H | 1.2067 | 10.6825 | 3.2164 |
| H | -0.8675 | 10.8495 | 1.0915 |
| H | 0.4448 | 11.9581 | 1.4019 |
| H | -0.9459 | 12.9670 | 3.3257 |
| H | -1.5251 | 13.2612 | 1.7198 |
| H | 0.9896 | 8.9128 | 4.8872 |
| H | -0.4849 | 7.9810 | 4.9496 |
| H | -0.1816 | 9.2362 | 7.0588 |
| H | 0.0484 | 10.7110 | 6.2174 |
| H | -1.5772 | 11.9062 | 5.1973 |
| H | -3.9687 | 12.7837 | 5.1697 |
| C | -3.0800 | 13.1086 | 7.0931 |
| H | -5.1393 | 10.6903 | 5.5609 |
| H | -5.5651 | 11.7647 | 6.8181 |
| H | -4.9618 | 9.3288 | 7.4503 |
| H | -4.2738 | 10.5970 | 8.4358 |
| C | -2.4491 | 8.5376 | 8.1882 |
| C | -1.9330 | 14.0387 | 6.6432 |
| C | -4.1909 | 13.9485 | 7.7834 |
| C | -4.8727 | 15.0421 | 6.9312 |
| C | -5.8955 | 14.4953 | 5.9477 |

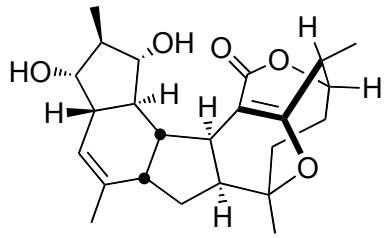
| | | | |
|---|---|---|---|
| C | -5.8959 | 14.6727 | 4.6050 |
| C | -6.9303 | 14.0453 | 3.7770 |
| C | -4.8288 | 15.4973 | 3.8964 |
| O | -6.9708 | 14.0749 | 2.5512 |
| O | -7.8913 | 13.3839 | 4.4764 |
| H | -3.8312 | 13.1470 | 1.4926 |
| H | -4.8449 | 11.9749 | 2.4853 |
| H | -2.6611 | 12.4806 | 7.8804 |
| H | -2.1152 | 8.9798 | 9.1269 |
| H | -3.3019 | 7.8932 | 8.4024 |
| H | -1.6641 | 7.8883 | 7.8041 |
| H | -1.7342 | 14.8123 | 7.3851 |
| H | -0.9959 | 13.4985 | 6.5140 |
| H | -2.1654 | 14.5351 | 5.7009 |
| H | -3.7322 | 14.4486 | 8.6375 |
| H | -4.9431 | 13.3037 | 8.2361 |
| H | -5.4143 | 15.7137 | 7.5980 |
| H | -4.6707 | 16.4479 | 4.4044 |
| H | -3.8859 | 14.9509 | 3.8771 |
| H | -5.0996 | 15.7309 | 2.8662 |
| H | -8.5021 | 13.0204 | 3.8561 |
| H | -4.1249 | 15.6616 | 6.4404 |
| H | -6.6694 | 13.9083 | 6.4208 |

**25**$H_2$

| | | | |
|---|---|---|---|
| C | 1.4191 | 14.1210 | 2.7080 |
| C | 0.0120 | 13.6215 | 3.0421 |
| C | -0.1688 | 12.1566 | 2.6012 |
| C | 0.2797 | 11.0573 | 3.5813 |
| C | 1.6562 | 11.2642 | 4.2547 |
| C | 2.7043 | 11.9975 | 3.4006 |
| C | 2.5927 | 13.5317 | 3.4796 |
| C | -0.8408 | 10.7001 | 4.5790 |
| C | -1.2141 | 11.7936 | 5.5958 |
| C | -1.6237 | 13.1373 | 4.9876 |
| C | -0.4484 | 13.9862 | 4.4900 |
| C | -0.7297 | 15.5098 | 4.6555 |
| C | -2.0877 | 15.8332 | 3.9895 |
| C | -3.2521 | 15.0327 | 4.5917 |
| C | -2.8955 | 13.6080 | 5.0013 |
| C | 1.6191 | 15.0581 | 1.7647 |
| H | -0.6449 | 14.1502 | 2.3560 |
| H | 0.3523 | 12.0179 | 1.6526 |
| H | -1.2184 | 11.9944 | 2.3520 |
| H | 1.5601 | 11.7836 | 5.2060 |
| H | 2.6793 | 11.6545 | 2.3656 |
| H | 3.6902 | 11.7224 | 3.7769 |
| H | 2.5447 | 13.8581 | 4.5184 |
| H | 3.5158 | 13.9612 | 3.0882 |
| H | -0.5498 | 9.8033 | 5.1273 |
| H | -1.7377 | 10.4194 | 4.0251 |
| H | -1.9961 | 11.4083 | 6.2464 |
| H | -0.3858 | 11.9677 | 6.2814 |
| H | 0.3850 | 13.7334 | 5.1336 |
| H | 0.0436 | 16.0342 | 4.1001 |
| C | -0.6332 | 16.0195 | 6.1324 |
| H | -2.0407 | 15.6183 | 2.9243 |
| H | -2.3127 | 16.8970 | 4.0222 |
| H | -4.0832 | 15.0150 | 3.8861 |
| H | -3.6140 | 15.5457 | 5.4834 |
| C | -4.0900 | 12.8215 | 5.5182 |
| C | 0.7152 | 15.6870 | 6.8068 |
| C | -0.9561 | 17.5269 | 6.3326 |
| C | 0.0486 | 18.5416 | 5.7427 |
| C | -0.0765 | 18.7147 | 4.2370 |

| | | | |
|---|---|---|---|
| C | 0.9031 | 18.5285 | 3.3203 |
| C | 0.6190 | 18.6928 | 1.8914 |
| C | 2.3174 | 18.1224 | 3.7155 |
| O | 1.4127 | 18.4740 | 0.9817 |
| O | -0.6427 | 19.1157 | 1.6100 |
| H | 2.6086 | 15.4210 | 1.5284 |
| H | 0.7970 | 15.4897 | 1.2132 |
| H | -1.3914 | 15.4823 | 6.7037 |
| H | -4.2908 | 13.0801 | 6.5579 |
| H | -4.9793 | 13.0566 | 4.9333 |
| H | -3.9501 | 11.7443 | 5.4431 |
| H | 0.8242 | 16.2102 | 7.7571 |
| H | 0.8067 | 14.6261 | 7.0363 |
| H | 1.5588 | 15.9670 | 6.1758 |
| H | -0.9980 | 17.7067 | 7.4078 |
| H | -1.9650 | 17.7588 | 5.9938 |
| H | -0.1479 | 19.5197 | 6.1828 |
| H | 2.6769 | 18.7224 | 4.5505 |
| H | 2.3371 | 17.0720 | 4.0059 |
| H | 3.0305 | 18.2565 | 2.9014 |
| H | -0.7209 | 19.1890 | 0.6727 |
| H | 1.0633 | 18.2876 | 6.0418 |
| H | -1.0684 | 19.0067 | 3.9236 |
| H | 0.3951 | 10.1699 | 2.9565 |
| H | 2.0471 | 10.2804 | 4.5176 |

**26**




| | | | |
|---|---|---|---|
| C | -1.0606 | -1.9583 | -3.2498 |
| C | -2.5855 | -1.7847 | -3.3077 |
| C | -2.8458 | -2.2407 | -4.7373 |
| C | -2.0433 | -3.5387 | -4.8825 |
| C | -0.8500 | -3.3445 | -3.9067 |
| C | -3.2039 | -0.3919 | -3.0901 |
| C | -4.7193 | -0.3769 | -3.4187 |
| C | -5.1767 | -1.3914 | -4.4770 |
| C | -4.3202 | -2.2460 | -5.0682 |
| C | -5.4440 | -0.5594 | -2.0797 |
| C | -4.4965 | -0.0897 | -0.9590 |
| C | -3.1096 | 0.0950 | -1.6326 |
| C | -2.6513 | 1.5479 | -1.5717 |
| C | -3.5491 | 2.5520 | -1.4501 |
| O | -4.8375 | 2.2548 | -1.1068 |
| C | -4.9107 | 1.1868 | -0.1555 |
| H | -0.5751 | -1.1807 | -3.8434 |
| O | -0.5312 | -1.9291 | -1.9408 |
| H | -3.0518 | -2.4880 | -2.6145 |
| O | -2.8179 | -4.6588 | -4.5001 |
| H | -1.7164 | -3.6761 | -5.9147 |
| C | 0.5180 | -3.4751 | -4.5882 |
| H | -0.9046 | -4.1060 | -3.1261 |
| H | -2.6892 | 0.3003 | -3.7594 |
| H | -6.4011 | -0.0427 | -2.0941 |
| H | -5.6648 | -1.6167 | -1.9254 |
| H | -2.3995 | -1.5161 | -5.4219 |
| H | -4.6529 | -2.9473 | -5.8205 |
| C | -6.6504 | -1.3627 | -4.8332 |
| H | -4.9612 | 0.6205 | -3.7904 |

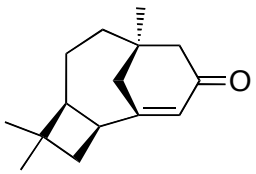
| | | | |
|---|---|---|---|
| H | -2.4028 | -0.5120 | -1.0686 |
| H | -4.4278 | -0.9146 | -0.2473 |
| C | -3.9334 | 1.3774 | 1.0827 |
| C | -6.3620 | 1.1633 | 0.3545 |
| C | -3.3346 | 2.7859 | 1.4135 |
| C | -2.4068 | 3.5025 | 0.3658 |
| C | -3.1467 | 3.8984 | -0.9174 |
| C | -4.3103 | 4.8892 | -0.7141 |
| H | -0.3523 | -1.0232 | -1.7077 |
| H | -3.1082 | -4.5298 | -3.6094 |
| H | 0.6414 | -4.4673 | -5.0228 |
| H | 1.3226 | -3.3252 | -3.8678 |
| H | 0.6397 | -2.7411 | -5.3847 |
| H | -6.8816 | -2.0726 | -5.6280 |
| H | -6.9371 | -0.3680 | -5.1747 |
| H | -7.2620 | -1.6185 | -3.9680 |
| H | -4.4418 | 1.0187 | 1.9783 |
| H | -3.0907 | 0.6912 | 1.0021 |
| H | -7.0885 | 1.1858 | -0.4560 |
| H | -6.5646 | 2.0378 | 0.9732 |
| H | -6.5582 | 0.2763 | 0.9571 |
| H | -4.1518 | 3.4518 | 1.6872 |
| H | -2.7524 | 2.6792 | 2.3292 |
| H | -2.4449 | 4.3537 | -1.6187 |
| H | -3.9528 | 5.8262 | -0.2872 |
| H | -5.0894 | 4.5028 | -0.0577 |
| H | -4.7834 | 5.1224 | -1.6682 |
| C | -1.2919 | 1.7713 | -1.0158 |
| O | -0.3119 | 1.1052 | -1.3514 |
| O | -1.2498 | 2.7276 | -0.0173 |
| H | -2.0261 | 4.4133 | 0.8288 |

**26**$H_2$

| | | | |
|---|---|---|---|
| C | 0.4936 | -4.8279 | 3.6469 |
| C | 1.8760 | -4.4524 | 4.2035 |
| C | 2.2452 | -5.7602 | 4.8932 |
| C | 1.9032 | -6.8517 | 3.8733 |
| C | 0.7279 | -6.2425 | 3.0620 |
| C | 2.0143 | -3.2861 | 5.2043 |
| C | 3.4470 | -3.2201 | 5.7934 |
| C | 4.1879 | -4.5608 | 5.8961 |
| C | 3.6380 | -5.7159 | 5.4771 |
| C | 4.2100 | -2.1811 | 4.9560 |
| C | 3.1859 | -1.4046 | 4.1036 |
| C | 1.8033 | -1.9004 | 4.5642 |
| C | 1.0335 | -0.9056 | 5.4834 |
| C | 1.9231 | 0.1915 | 6.1497 |
| O | 3.1562 | 0.5057 | 5.5000 |
| C | 3.3248 | 0.1386 | 4.1414 |
| H | -0.2352 | -4.8699 | 4.4590 |
| O | 0.0200 | -3.9483 | 2.6481 |
| H | 2.5597 | -4.2832 | 3.3689 |
| O | 3.0043 | -7.1166 | 3.0258 |
| H | 1.6220 | -7.7771 | 4.3788 |
| C | -0.5374 | -7.1095 | 3.0847 |
| H | 1.0368 | -6.1373 | 2.0199 |
| H | 1.2973 | -3.4642 | 6.0067 |
| H | 4.7705 | -1.5319 | 5.6285 |
| H | 4.9380 | -2.6553 | 4.2966 |
| H | 1.5781 | -5.9058 | 5.7456 |
| H | 4.1632 | -6.6563 | 5.5689 |
| C | 5.5666 | -4.5138 | 6.5264 |
| H | 3.3589 | -2.8230 | 6.8061 |
| H | 1.2277 | -2.0313 | 3.6509 |
| H | 3.3243 | -1.7308 | 3.0708 |

| | | | |
|---|---|---|---|
| C | 2.3150 | 0.8621 | 3.2039 |
| C | 4.7485 | 0.5992 | 3.7757 |
| C | 1.6306 | 2.1198 | 3.7863 |
| C | 0.6032 | 1.8840 | 4.9267 |
| C | 1.1800 | 1.5181 | 6.3031 |
| C | 2.0245 | 2.6331 | 6.9469 |
| H | -0.3995 | -3.2065 | 3.0681 |
| H | 3.2536 | -6.3099 | 2.5996 |
| H | -0.3436 | -8.0895 | 2.6482 |
| H | -1.3355 | -6.6409 | 2.5082 |
| H | -0.9013 | -7.2598 | 4.1011 |
| H | 6.0038 | -5.5100 | 6.6015 |
| H | 5.5082 | -4.0942 | 7.5308 |
| H | 6.2428 | -3.8959 | 5.9360 |
| H | 2.8308 | 1.1551 | 2.2887 |
| H | 1.5545 | 0.1765 | 2.8361 |
| H | 5.5003 | 0.2185 | 4.4654 |
| H | 4.8228 | 1.6866 | 3.8025 |
| H | 5.0270 | 0.2722 | 2.7737 |
| H | 2.3903 | 2.8326 | 4.1058 |
| H | 1.1019 | 2.6119 | 2.9696 |
| H | 0.3378 | 1.3549 | 6.9781 |
| H | 1.4446 | 3.5492 | 7.0586 |
| H | 2.9102 | 2.8715 | 6.3581 |
| H | 2.3666 | 2.3355 | 7.9382 |
| C | -0.2562 | -0.4102 | 4.7768 |
| O | -1.1044 | -1.2286 | 4.4217 |
| O | -0.3825 | 0.9264 | 4.5471 |
| H | 0.0615 | 2.8214 | 5.0558 |
| H | 0.6189 | -1.4726 | 6.3159 |
| H | 2.1996 | -0.1595 | 7.1444 |

**27**




| | | | |
|---|---|---|---|
| C | -0.1452 | -0.7590 | -0.4104 |
| C | -1.4046 | -0.7004 | -0.8889 |
| C | -2.4574 | -1.4966 | -0.2309 |
| C | -2.0148 | -2.6786 | 0.6644 |
| C | -0.4667 | -2.8714 | 0.7682 |
| C | 0.1331 | -1.4675 | 0.9040 |
| C | 1.0260 | -0.5650 | -1.3546 |
| C | 1.7598 | -1.8811 | -1.6950 |
| C | 1.5917 | -3.1844 | -0.8607 |
| C | 0.1287 | -3.5760 | -0.5005 |
| C | -0.1345 | -3.6990 | 2.0241 |
| O | -3.6554 | -1.2781 | -0.3934 |
| H | -1.6181 | -0.3141 | -1.8738 |
| H | -2.4898 | -3.5915 | 0.3053 |
| H | -2.4284 | -2.4865 | 1.6544 |
| H | 1.1867 | -1.4992 | 1.1688 |
| H | -0.3487 | -0.9175 | 1.7146 |
| C | 2.3479 | -0.0182 | -0.8156 |
| H | 0.7289 | -0.0307 | -2.2595 |
| C | 3.0927 | -1.0762 | -1.6634 |
| H | 1.5095 | -2.1173 | -2.7308 |
| H | 2.1886 | -3.1608 | 0.0492 |
| H | 2.0184 | -4.0049 | -1.4383 |
| H | -0.4943 | -3.3914 | -1.3766 |
| H | 0.0781 | -4.6564 | -0.3590 |
| H | 0.9410 | -3.8414 | 2.1355 |

| | | | |
|---|---|---|---|
| H | -0.4939 | -3.2107 | 2.9308 |
| H | -0.5939 | -4.6872 | 1.9824 |
| C | 4.3003 | -1.7351 | -0.9899 |
| C | 3.5773 | -0.5855 | -3.0331 |
| H | 2.5055 | -0.1385 | 0.2546 |
| H | 2.5485 | 1.0130 | -1.1085 |
| H | 5.1751 | -1.0840 | -1.0041 |
| H | 4.1078 | -1.9681 | 0.0572 |
| H | 4.5765 | -2.6660 | -1.4861 |
| H | 4.3790 | 0.1477 | -2.9378 |
| H | 3.9542 | -1.4075 | -3.6428 |
| H | 2.7779 | -0.1080 | -3.6005 |

**27**$H_2$

| | | | |
|---|---|---|---|
| C | -3.7894 | -1.8351 | 0.8043 |
| C | -3.2508 | -1.2144 | -0.5025 |
| C | -2.2347 | -0.1000 | -0.2649 |
| C | -1.1782 | -0.3354 | 0.8202 |
| C | -1.7164 | -1.0068 | 2.1155 |
| C | -2.6365 | -2.1961 | 1.7601 |
| C | -4.9326 | -1.0228 | 1.4325 |
| C | -4.7890 | 0.4030 | 2.0056 |
| C | -3.4546 | 0.9768 | 2.5097 |
| C | -2.4170 | -0.0099 | 3.0824 |
| C | -0.5019 | -1.5815 | 2.8764 |
| O | -2.2304 | 0.9202 | -0.9502 |
| H | -4.0702 | -0.8292 | -1.1093 |
| H | -0.6969 | 0.6137 | 1.0568 |
| H | -0.4108 | -0.9640 | 0.3691 |
| H | -3.0147 | -2.6756 | 2.6624 |
| H | -2.0382 | -2.9667 | 1.2709 |
| C | -5.5547 | -1.4158 | 2.7750 |
| H | -5.7464 | -0.9897 | 0.7048 |
| C | -5.9226 | 0.0575 | 3.0170 |
| H | -5.1926 | 1.1040 | 1.2722 |
| H | -3.6633 | 1.7179 | 3.2808 |
| H | -2.9922 | 1.5754 | 1.7263 |
| H | -1.6452 | 0.6093 | 3.5420 |
| H | -2.8594 | -0.5584 | 3.9135 |
| H | -0.8057 | -2.0701 | 3.8033 |
| H | 0.0360 | -2.3212 | 2.2820 |
| H | 0.2135 | -0.8009 | 3.1389 |
| C | -5.7743 | 0.5467 | 4.4613 |
| C | -7.3362 | 0.4612 | 2.5763 |
| H | -4.8399 | -1.7897 | 3.5068 |
| H | -6.4069 | -2.0918 | 2.6944 |
| H | -6.5567 | 0.1416 | 5.1039 |
| H | -4.8244 | 0.2449 | 4.9010 |
| H | -5.8296 | 1.6339 | 4.5246 |
| H | -8.0998 | 0.0005 | 3.2038 |
| H | -7.4775 | 1.5414 | 2.6273 |
| H | -7.5492 | 0.1630 | 1.5498 |
| H | -4.2284 | -2.7898 | 0.5120 |
| H | -2.7554 | -1.9817 | -1.0967 |

## Density Functional Theory Calculations

Density functional theory calculations were performed in Gaussian 09.[10] For validation of the forcefield-based OS energy predictions, the geometries of selected alkenes (**7**, **10**, **19**, **21**, **22**, and **26**) and the corresponding alkanes were reoptimized with M06-2X/6-31G(d).[11] Then, the difference in energy between the DFT-optimized (M06-2X) structure and the forcefield-optimized (OPLS_2005) structure was compared via single-point calculations with M06-2X/Def2-TZVPP. The difference in energy between the DFT-optimized and forcefield-optimized structures was taken as a measure of the amount of strain not captured by the forcefield calculation, and corrections to OS energy were calculated. The results of these calculations are listed in Table S5.

**Table S5.** DFT calculations on NPs giving a measure of the amount of strain energy not captured by the forcefield.

| Alkene | *E*(M06-2X/Def2-TZVPP) (Hartree) | | Alkane | *E*(M06-2X/Def2-TZVPP) (Hartree) | | Correction to OSE (kcal mol$^{-1}$) |
|---|---|---|---|---|---|---|
| | Forcefield-optimized geometry[a] | DFT-optimized geometry[b] | | Forcefield-optimized geometry[a] | DFT-optimized geometry[b] | |
| **7** | −1264.916884 | −1264.942901 | **7**$H_2$ | −1266.135200 | −1266.160843 | –0.2 |
| **10** | −1004.534663 | −1004.549322 | **10**$H_2$ | −1005.751180 | −1005.768574 | 1.7 |
| **19** | −965.263616 | −965.276861 | **19**$H_2$ | −966.519070 | −966.529357 | –1.9 |
| **21** | −1004.545903 | −1004.556458 | **21**$H_2$ | −1005.758196 | −1005.769217 | 0.3 |
| **22** | −810.376480 | −810.397738 | **22**$H_2$ | −811.688103 | −811.696477 | –8.1 |
| **26** | −1309.868195 | −1309.888150 | **26**$H_2$ | −1311.104175 | −1311.119835 | –2.7 |

[a] Geometry optimized with OPLS_2005. [b] Geometry optimized with M06-2X/6-31G(d).

For the study of the Michael addition of water to enone **27**, geometries were optimized at the B3LYP-D3/6-31G(d) level of theory[12] in implicit water, simulating the solvent with the SMD model.[13] Zero-point energy and thermochemical corrections were obtained from vibrational frequency calculations at this level of theory. Geometrical counterpoise corrections were computed with Grimme's gCP method.[14] Free energies in solution (25 °C) were calculated by adding the gCP correction to the B3LYP/6-31G(d) solution-phase free energy and correcting to a standard state of 1 mol L$^{-1}$. The Cartesian coordinates for the optimized geometries are listed, below, together with the following energies (all in Hartree):

B3LYP/6-31G(d) solution-phase electronic energy (E),

B3LYP/6-31G(d) solution-phase Gibbs free energy at 298.15 K and 1 mol L$^{-1}$ (G), and

gCP correction ($E_{gCP}$).

## B3LYP-D3 Optimized Geometries and Associated Energies

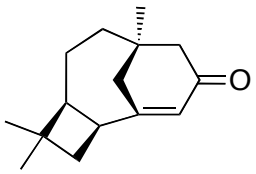
### $H_2O$

```
O     0.000000    0.000000    0.121396
H     0.000000    0.757511   -0.485585
H     0.000000   -0.757511   -0.485585
0 imaginary frequencies
E = -76.422652
G = -76.416350
E_gCP = 0.008557
```

### $OH^-$

```
O     0.000000    0.000000    0.108113
H     0.000000    0.000000   -0.864907
0 imaginary frequencies
E = -75.889591
G = -75.894524
E_gCP = 0.003870
```

### Alkene 27




```
C     0.889166    0.418280    1.231046
C     1.647968    1.129268    0.088098
C     2.954786    0.331263   -0.094160
C     2.776991   -1.187383   -0.129029
C     1.454417   -1.720960    0.175548
C     0.485285   -0.920780    0.688743
C     0.781567    1.108786   -1.210954
C    -0.743952    1.180755   -0.963601
C    -1.457557   -0.170680   -0.756356
C    -0.946234   -1.154518    0.385956
C     1.954707    2.574479    0.489366
H     1.085225    1.961326   -1.829200
H     1.005601    0.213053   -1.801237
H    -0.935083    1.860850   -0.127931
H    -1.220775    1.648349   -1.833389
C    -2.841421   -0.136498   -0.003956
H    -1.490757   -0.680958   -1.725797
C    -2.126416   -0.685174    1.266517
H    -1.096101   -2.183777    0.050973
H     1.224628   -2.708715   -0.218642
O     3.710364   -1.908372   -0.514126
H     3.632635    0.557522    0.741603
H     3.484643    0.617044   -1.011076
H     1.552746    0.310363    2.096364
H     0.028085    1.001725    1.557624
H     2.471041    2.615283    1.455765
H     2.593870    3.059503   -0.258165
H     1.030477    3.158374    0.573828
H    -2.647162   -1.464979    1.832226
H    -1.845889    0.120255    1.951898
C    -3.803134   -1.165705   -0.602923
C    -3.551498    1.203694    0.156398
H    -4.683749   -1.293129    0.038937
H    -4.151021   -0.842656   -1.592150
H    -3.329274   -2.147066   -0.720118
H    -4.441684    1.078883    0.785891
H    -2.915527    1.955999    0.632674
H    -3.882890    1.600757   -0.811243
```

0 imaginary frequencies
E = -660.119478
G = -659.814924
$E_{gCP}$ = 0.096203

## TS: $OH^-$ + Alkene 27

| | | | |
|---|---|---|---|
| C | 1.431334 | -1.451634 | -0.697804 |
| C | 0.479734 | -0.970230 | 0.167281 |
| C | 0.918805 | 0.052292 | 1.174426 |
| C | 1.663145 | 1.163670 | 0.408662 |
| C | 2.951709 | 0.505347 | -0.120563 |
| C | 2.723457 | -0.830661 | -0.830539 |
| C | -0.953317 | -1.009076 | -0.224741 |
| C | -2.143558 | -0.900036 | 0.747763 |
| C | -2.841435 | 0.082570 | -0.237978 |
| C | -3.775178 | -0.648582 | -1.205835 |
| C | 0.788808 | 1.698391 | -0.769453 |
| C | -0.734426 | 1.655113 | -0.514480 |
| C | -1.437856 | 0.341067 | -0.904287 |
| C | 1.999738 | 2.308494 | 1.368309 |
| O | 3.615984 | -1.278330 | -1.584405 |
| C | -3.578072 | 1.259159 | 0.394351 |
| O | 0.087429 | -2.656724 | 2.117184 |
| H | 1.091439 | 2.733603 | -0.967050 |
| H | 1.011256 | 1.139027 | -1.685326 |
| H | -0.925853 | 1.906273 | 0.533563 |
| H | -1.214786 | 2.450471 | -1.097547 |
| H | -1.440371 | 0.272759 | -1.998919 |
| H | -1.114516 | -1.827566 | -0.931596 |
| H | 1.171828 | -2.200155 | -1.444519 |
| H | 3.636405 | 0.325043 | 0.721237 |
| H | 3.483469 | 1.160199 | -0.822118 |
| H | 1.594556 | -0.404626 | 1.902715 |
| H | 0.073673 | 0.455636 | 1.734939 |
| H | 2.521830 | 1.936856 | 2.258218 |
| H | 2.642383 | 3.052800 | 0.882373 |
| H | 1.087357 | 2.818059 | 1.701382 |
| H | -2.663589 | -1.832919 | 0.987480 |
| H | -1.874508 | -0.399825 | 1.682705 |
| H | -4.661389 | -1.024762 | -0.679245 |
| H | -4.118558 | 0.026329 | -2.000148 |
| H | -3.283113 | -1.502752 | -1.685023 |
| H | -4.478679 | 0.901037 | 0.909688 |
| H | -2.964809 | 1.784965 | 1.132497 |
| H | -3.898512 | 1.986202 | -0.362551 |
| H | -0.260161 | -1.811516 | 2.434357 |

1 imaginary frequency
E = -736.022500
G = -735.709798
$E_{gCP}$ = 0.104302

## Michael adduct of $H_2O$ + 27

| | | | |
|---|---|---|---|
| C | -0.541955 | -1.255358 | -0.747048 |
| C | -1.193420 | -0.048590 | -1.427838 |
| C | -1.608579 | 1.104625 | -0.498554 |
| C | -2.509044 | 0.543275 | 0.630023 |
| C | -2.004353 | -0.723426 | 1.282680 |
| C | -1.468910 | -1.790985 | 0.356560 |
| C | -0.391971 | 1.871434 | 0.072780 |
| C | 0.413127 | 1.210157 | 1.199391 |
| C | 1.283863 | -0.016360 | 0.897888 |
| C | 2.624901 | 0.216517 | 0.100925 |
| C | 3.121922 | 1.645253 | -0.087845 |
| C | -2.434241 | 2.105090 | -1.323780 |

| | | | |
|---|---|---|---|
| O | -2.085145 | -0.910670 | 2.494136 |
| C | 0.878728 | -1.043239 | -0.213182 |
| C | 1.968623 | -0.450514 | -1.140323 |
| C | 3.748027 | -0.648655 | 0.679140 |
| H | 0.262092 | 2.134036 | -0.767118 |
| H | -0.769867 | 2.821725 | 0.472490 |
| H | -0.276836 | 0.955876 | 2.011096 |
| H | 1.073854 | 1.974724 | 1.628300 |
| H | 1.469279 | -0.508761 | 1.859578 |
| H | 1.201569 | -2.034502 | 0.121628 |
| H | -0.982256 | -2.573375 | 0.945427 |
| H | -3.478514 | 0.272388 | 0.184747 |
| H | -2.702138 | 1.292509 | 1.403911 |
| H | -2.090046 | -0.426346 | -1.934874 |
| H | -0.528181 | 0.335435 | -2.209819 |
| H | -3.281603 | 1.609783 | -1.811858 |
| H | -2.827669 | 2.907124 | -0.688275 |
| H | -1.815582 | 2.565161 | -2.103600 |
| H | 2.582618 | -1.159744 | -1.706651 |
| H | 1.569852 | 0.298543 | -1.831187 |
| H | 4.623868 | -0.648329 | 0.017897 |
| H | 4.066025 | -0.269190 | 1.658509 |
| H | 3.429759 | -1.689108 | 0.812249 |
| H | 3.986948 | 1.654861 | -0.763687 |
| H | 2.358805 | 2.297908 | -0.521468 |
| H | 3.444390 | 2.086922 | 0.863526 |
| O | -0.469175 | -2.332358 | -1.715935 |
| H | 0.142493 | -2.034948 | -2.411730 |
| H | -2.344599 | -2.233815 | -0.139597 |

0 imaginary frequencies
E = -736.574100
G = -736.243828
$E_{gCP}$ = 0.112619

## Cyclohexenone

| | | | |
|---|---|---|---|
| C | 0.383795 | 1.284937 | -0.063664 |
| C | -0.959727 | 1.320562 | 0.024071 |
| C | -1.812788 | 0.093084 | 0.141310 |
| C | -1.077183 | -1.159151 | -0.345700 |
| C | 0.326538 | -1.238821 | 0.262470 |
| C | 1.129593 | 0.022984 | 0.016251 |
| H | -1.467437 | 2.283315 | 0.016312 |
| H | -2.107670 | -0.022499 | 1.196550 |
| H | -2.746068 | 0.241404 | -0.413975 |
| H | -1.647895 | -2.059373 | -0.097158 |
| H | -0.992583 | -1.118817 | -1.438940 |
| H | 0.250928 | -1.355989 | 1.354540 |
| H | 0.894780 | -2.094451 | -0.114525 |
| O | 2.362741 | -0.001020 | -0.068468 |
| H | 0.972647 | 2.193002 | -0.163487 |

0 imaginary frequencies
E = -308.697577
G = -308.596783
$E_{gCP}$ = 0.033352

## TS: $OH^-$ + Cyclohexenone

| | | | |
|---|---|---|---|
| C | -1.357220 | -0.377987 | -0.006611 |
| C | -0.256408 | -1.077816 | 0.597537 |
| C | 0.940648 | -0.467603 | 0.874948 |
| C | 1.105472 | 1.019505 | 0.738404 |
| C | 0.273459 | 1.541518 | -0.434469 |
| C | -1.188752 | 1.108829 | -0.294783 |
| O | -2.452742 | -0.932008 | -0.252885 |
| H | 1.686700 | -1.004397 | 1.448571 |

```
H     0.768331    1.490627    1.676330
H     2.161550    1.271544    0.616153
H     0.342586    2.632279   -0.509095
H     0.700365    1.115979   -1.350761
H    -1.658050    1.648099    0.542413
H    -1.774012    1.352525   -1.188263
H    -0.402986   -2.135583    0.805403
O     2.396072   -1.012121   -0.950646
H     1.525678   -1.296723   -1.262652
1 imaginary frequency
E = -384.598247
G = -384.488593
E_gCP = 0.041040
```

## Michael adduct of $H_2O$ + Cyclohexenone

```
O    -2.268694   -0.690026   -0.397519
C    -1.278565   -0.178115    0.116137
C    -0.250863   -0.994178    0.870146
C     1.172469   -0.694087    0.370045
H    -0.314777   -0.720249    1.932041
H    -0.484787   -2.059545    0.776965
C     1.463044    0.805566    0.394547
O     1.322545   -1.134503   -0.989111
H     1.890718   -1.222662    1.010759
C     0.434604    1.597648   -0.420187
H     1.452986    1.138488    1.439628
H     2.472267    0.980683    0.005330
C    -1.004655    1.306738    0.050635
H     0.631051    2.671536   -0.338111
H     0.525303    1.335135   -1.479804
H    -1.131810    1.699244    1.070155
H    -1.749865    1.782290   -0.593115
H     1.061899   -2.070115   -1.018752
0 imaginary frequencies
E = -385.144251
G = -385.017012
E_gCP = 0.048160
```

## A Small Set of Alkenes for Rapid Estimation of OS Cutoffs for Other Forcefields

The geometries of alkenes **S1**–**S25** and alkanes **S1**$H_2$–**S25**$H_2$ may be re-minimized to compute olefin strain energies with other forcefields. However, if a full calibration of a new forcefield is not desired, a small set of alkenes may be utilized for a rapid estimation of the OS energy values corresponding to the isolable→observable and observable→unstable transition zones. Our definition of the isolable→observable "cutoff" for a given forcefield is simply the lowest OS energy out of those of **S11**–**S13**, while the observable→unstable cutoff is the highest OS energy out of those of **S11**–**S13** (these being the alkenes representing the "observable" range). Therefore, at its simplest, the task of calibration would involve minimizing **S11**–**S13** and the corresponding alkanes with the forcefield of choice, and computing their OS energies. We also suggest, however, that the OS energies of **S6** and **S17** be computed. These two alkenes are predicted to fall into the "isolable" and "unstable" categories, respectively, with relative confidence, without being extremely stable (for **S6**) or unstable (for **S17**). Therefore, computing **S6** and **S17** along with **S11**–**S13** would provide an rough indication of how similar the calibration curve is to the plots in Figure 2. The OPLS_2005 minimum energy geometries of **S6**, **S11**–**S13**, and **S17** and the corresponding alkanes are reproduced below.

### S6

| | | | |
|---|---|---|---|
| C | 0.8274 | -2.7359 | -0.3798 |
| C | -0.4555 | -2.8663 | -1.1628 |
| C | -1.4216 | -1.7109 | -0.7990 |
| C | -0.7419 | -0.3609 | -0.4294 |
| C | -0.2383 | -0.2428 | 1.0381 |
| C | 0.9635 | -1.1344 | 1.4613 |
| C | 2.3397 | -0.6654 | 0.8820 |
| C | 3.0271 | -1.6802 | -0.0763 |
| C | 1.9806 | -2.3452 | -0.9439 |
| C | 0.6809 | -2.6035 | 1.1188 |
| H | -0.9193 | -3.8320 | -0.9591 |
| H | -0.2301 | -2.8441 | -2.2299 |
| H | -2.0643 | -2.0181 | 0.0268 |
| H | -2.0949 | -1.5547 | -1.6426 |
| H | -1.4811 | 0.4271 | -0.5771 |
| H | 0.0613 | -0.1313 | -1.1306 |
| H | -1.0774 | -0.4579 | 1.7010 |
| H | 0.0167 | 0.7988 | 1.2374 |
| H | 1.0339 | -1.0615 | 2.5477 |
| H | 3.0236 | -0.4298 | 1.6982 |
| H | 2.1996 | 0.2743 | 0.3464 |
| H | 3.5465 | -2.4524 | 0.4924 |
| H | 3.7728 | -1.1839 | -0.6980 |
| H | -0.3009 | -2.9299 | 1.4635 |
| H | 1.4115 | -3.2511 | 1.6055 |
| H | 2.0928 | -2.2785 | -2.0163 |

### S6$H_2$

| | | | |
|---|---|---|---|
| C | 2.5895 | -5.3032 | 2.8841 |
| C | 2.9701 | -4.9273 | 1.4360 |

| | | | |
|---|---|---|---|
| C | 3.7330 | -3.6093 | 1.2257 |
| C | 2.9752 | -2.3602 | 1.7018 |
| C | 3.1230 | -2.0598 | 3.2047 |
| C | 2.5409 | -3.0906 | 4.2077 |
| C | 3.6119 | -3.6584 | 5.1601 |
| C | 4.5473 | -4.6484 | 4.4500 |
| C | 3.7617 | -5.7838 | 3.7712 |
| C | 1.7212 | -4.2450 | 3.5944 |
| H | 2.0551 | -4.8845 | 0.8435 |
| H | 3.5518 | -5.7410 | 1.0011 |
| H | 3.9055 | -3.5062 | 0.1537 |
| H | 4.7279 | -3.6510 | 1.6637 |
| H | 1.9247 | -2.4149 | 1.4153 |
| H | 3.3733 | -1.5016 | 1.1596 |
| H | 2.6415 | -1.0993 | 3.3935 |
| H | 4.1769 | -1.8815 | 3.4208 |
| H | 1.8473 | -2.5293 | 4.8361 |
| H | 3.1201 | -4.1690 | 5.9893 |
| H | 4.1906 | -2.8503 | 5.6094 |
| H | 5.2455 | -5.0724 | 5.1724 |
| H | 5.1647 | -4.1224 | 3.7257 |
| H | 4.4383 | -6.4190 | 3.1985 |
| H | 3.3538 | -6.4220 | 4.5563 |
| H | 0.9437 | -3.8671 | 2.9302 |
| H | 1.1839 | -4.7403 | 4.4045 |
| H | 1.9479 | -6.1780 | 2.7648 |

**S11**

| | | | |
|---|---|---|---|
| C | 11.4132 | 1.3482 | -0.6594 |
| C | 12.8735 | 1.2876 | -1.1747 |
| C | 13.5558 | -0.0995 | -1.2248 |
| C | 12.6612 | -1.2721 | -1.6700 |
| C | 11.3743 | -1.4382 | -0.8670 |
| C | 11.5278 | -1.7257 | 0.6077 |
| C | 11.8252 | -0.4070 | 1.3868 |
| C | 11.2251 | 0.9414 | 0.8496 |
| C | 10.4237 | 0.6477 | -1.6402 |
| C | 10.2565 | -0.7757 | -1.1907 |
| H | 11.1460 | 2.4051 | -0.7100 |
| H | 13.4930 | 1.9578 | -0.5775 |
| H | 12.8912 | 1.7082 | -2.1811 |
| H | 14.0163 | -0.3325 | -0.2688 |
| H | 14.4029 | -0.0360 | -1.9085 |
| H | 13.2250 | -2.2034 | -1.6096 |
| H | 12.4012 | -1.1510 | -2.7224 |
| H | 12.3082 | -2.4691 | 0.7738 |
| H | 10.6018 | -2.1666 | 0.9800 |
| H | 12.9000 | -0.2869 | 1.4975 |
| H | 11.4846 | -0.5435 | 2.4136 |
| H | 10.1586 | 0.9597 | 1.0773 |
| H | 11.6475 | 1.7402 | 1.4604 |
| H | 9.4468 | 1.1320 | -1.6191 |
| H | 10.7763 | 0.6905 | -2.6714 |
| H | 9.4321 | -0.8552 | -0.4959 |

**S11**$H_2$

| | | | |
|---|---|---|---|
| C | 1.9947 | 2.1200 | -2.7017 |
| C | 2.7992 | 2.5956 | -1.4736 |
| C | 3.1748 | 1.5075 | -0.4603 |
| C | 1.9778 | 0.7948 | 0.1809 |
| C | 1.0463 | 0.0407 | -0.7914 |
| C | 1.7732 | -0.9215 | -1.7629 |
| C | 1.8930 | -0.4459 | -3.2229 |
| C | 2.6052 | 0.9025 | -3.4387 |

| | | | |
|---|---|---|---|
| C | 0.4761 | 2.0249 | -2.4420 |
| C | -0.0161 | 0.9459 | -1.4507 |
| H | 2.0926 | 2.9484 | -3.4058 |
| H | 2.2572 | 3.3950 | -0.9668 |
| H | 3.7251 | 3.0527 | -1.8255 |
| H | 3.7619 | 1.9696 | 0.3341 |
| H | 3.8460 | 0.7817 | -0.9172 |
| H | 1.3974 | 1.5098 | 0.7652 |
| H | 2.3691 | 0.0797 | 0.9058 |
| H | 0.4685 | -0.6122 | -0.1346 |
| H | 1.2213 | -1.8623 | -1.7814 |
| H | 2.7556 | -1.1870 | -1.3724 |
| H | 0.9013 | -0.4084 | -3.6744 |
| H | 2.4270 | -1.2097 | -3.7891 |
| H | 3.6660 | 0.8088 | -3.2060 |
| H | 2.5758 | 1.1074 | -4.5098 |
| H | -0.0295 | 1.8750 | -3.3970 |
| H | 0.1221 | 2.9965 | -2.0947 |
| H | -0.5883 | 1.4389 | -0.6637 |
| H | -0.7425 | 0.3118 | -1.9607 |

**S12**

| | | | |
|---|---|---|---|
| C | 1.1543 | -2.4721 | -3.2288 |
| C | 0.1548 | -2.3442 | -4.4030 |
| C | -1.1550 | -1.6467 | -3.9612 |
| C | -1.0153 | -1.1153 | -2.5393 |
| C | -1.1443 | -1.9337 | -1.4820 |
| C | -0.8131 | -3.3945 | -1.6817 |
| C | 0.6622 | -3.5237 | -2.1724 |
| C | 1.4352 | -1.0450 | -2.6361 |
| C | 0.1563 | -0.1722 | -2.4465 |
| H | -0.0629 | -3.3239 | -4.8298 |
| H | 0.6167 | -1.7629 | -5.2020 |
| H | -2.0034 | -2.3287 | -4.0243 |
| H | -1.3861 | -0.8193 | -4.6329 |
| H | -0.7841 | -1.5669 | -0.5311 |
| H | -1.4950 | -3.8354 | -2.4089 |
| H | -0.9659 | -3.9408 | -0.7506 |
| H | 1.3255 | -3.4773 | -1.3080 |
| H | 0.7955 | -4.5262 | -2.5808 |
| H | 1.9550 | -1.1480 | -1.6829 |
| H | 2.1258 | -0.5094 | -3.2885 |
| H | 0.1740 | 0.3565 | -1.4924 |
| H | 0.0767 | 0.5827 | -3.2298 |
| H | 2.0999 | -2.8479 | -3.6226 |

**S12**$H_2$

| | | | |
|---|---|---|---|
| C | 1.3899 | -3.0564 | 1.0402 |
| C | 2.5462 | -2.0520 | 0.8692 |
| C | 2.4290 | -1.1911 | -0.4033 |
| C | 1.1793 | -1.5090 | -1.2472 |
| C | 1.3323 | -2.8252 | -2.0449 |
| C | 0.9015 | -4.0983 | -1.2964 |
| C | 1.5295 | -4.2740 | 0.0969 |
| C | 0.0288 | -2.3359 | 0.9139 |
| C | -0.0891 | -1.4706 | -0.3654 |
| H | 3.5053 | -2.5711 | 0.8831 |
| H | 2.5646 | -1.3890 | 1.7353 |
| H | 3.3311 | -1.2918 | -1.0080 |
| H | 2.3947 | -0.1412 | -0.1092 |
| H | 2.3609 | -2.9323 | -2.3910 |
| H | 0.7295 | -2.7551 | -2.9513 |
| H | 1.1421 | -4.9689 | -1.9075 |
| H | -0.1849 | -4.1105 | -1.2046 |

| | | | |
|---|---|---|---|
| H | 1.0536 | -5.1354 | 0.5674 |
| H | 2.5806 | -4.5462 | -0.0051 |
| H | -0.7848 | -3.0611 | 0.9561 |
| H | -0.1103 | -1.6920 | 1.7832 |
| H | -0.9601 | -1.7733 | -0.9479 |
| H | -0.2810 | -0.4382 | -0.0704 |
| H | 1.0928 | -0.7129 | -1.9886 |
| H | 1.4652 | -3.4487 | 2.0557 |

### S13

| | | | |
|---|---|---|---|
| C | 1.2658 | -2.8341 | -0.1425 |
| C | 1.8057 | -1.8166 | 0.8890 |
| C | 1.5975 | -0.3624 | 0.3946 |
| C | 0.7526 | -0.3311 | -0.8771 |
| C | 1.1056 | -1.1172 | -1.9087 |
| C | 1.7965 | -2.4127 | -1.5441 |
| C | -0.3037 | -2.9043 | -0.0994 |
| C | -1.0862 | -1.5834 | 0.2340 |
| C | -0.7305 | -0.3156 | -0.5964 |
| H | 1.6619 | -3.8233 | 0.0918 |
| H | 1.3266 | -1.9681 | 1.8568 |
| H | 2.8700 | -1.9886 | 1.0547 |
| H | 2.5676 | 0.0740 | 0.1536 |
| H | 1.1613 | 0.2683 | 1.1700 |
| H | 0.3868 | -1.2569 | -2.7036 |
| H | 2.8780 | -2.2707 | -1.5332 |
| H | 1.5742 | -3.1712 | -2.2954 |
| H | -0.5855 | -3.6416 | 0.6533 |
| H | -0.6696 | -3.3129 | -1.0422 |
| H | -0.9241 | -1.3528 | 1.2874 |
| H | -2.1576 | -1.7699 | 0.1545 |
| H | -1.2940 | -0.3003 | -1.5306 |
| H | -1.0022 | 0.5911 | -0.0548 |

### **S13**$H_2$

Same as **S12**$H_2$.

### S17

| | | | |
|---|---|---|---|
| C | 1.5075 | -2.5483 | -0.5244 |
| C | -0.0555 | -2.6572 | -0.4211 |
| C | 0.0900 | -0.1363 | -0.1569 |
| C | 1.4054 | -0.2934 | -0.3852 |
| C | 2.2575 | -0.5884 | 0.8149 |
| C | 2.1975 | -2.1385 | 0.8159 |
| C | 1.8169 | -1.3358 | -1.3925 |
| H | 1.9319 | -3.4713 | -0.9216 |
| H | 1.8786 | -0.1428 | 1.7359 |
| H | 3.2739 | -0.2298 | 0.6461 |
| H | 3.2078 | -2.5460 | 0.8691 |
| H | 1.6526 | -2.5208 | 1.6796 |
| H | 2.8782 | -1.2548 | -1.6342 |
| H | 1.2475 | -1.2962 | -2.3226 |
| C | -0.8076 | -1.2886 | -0.5838 |
| H | -0.4228 | -3.3431 | -1.1854 |
| H | -0.3232 | -3.1155 | 0.5315 |
| H | -0.2139 | 0.3290 | 0.7700 |
| H | -1.7407 | -1.2776 | -0.0197 |
| H | -1.0728 | -1.1344 | -1.6305 |

### **S17**$H_2$

| | | | |
|---|---|---|---|
| C | 1.1040 | -2.5669 | -0.2937 |
| C | -0.3966 | -2.6652 | 0.0676 |
| C | -0.9201 | -1.3726 | 0.7333 |

| | | | |
|---|---|---|---|
| C | -0.3825 | -0.0937 | 0.0525 |
| C | 1.1169 | -0.2127 | -0.3075 |
| C | 1.9755 | -0.6161 | 0.9053 |
| C | 1.9670 | -2.1588 | 0.9144 |
| C | 1.3027 | -1.3965 | -1.2566 |
| H | 1.4447 | -3.5070 | -0.7298 |
| H | -0.5720 | -3.5161 | 0.7270 |
| H | -0.9699 | -2.8636 | -0.8390 |
| H | -0.6165 | -1.3681 | 1.7807 |
| H | -2.0104 | -1.3666 | 0.7448 |
| H | -0.5485 | 0.7667 | 0.7019 |
| H | -0.9536 | 0.1003 | -0.8564 |
| H | 1.4679 | 0.7184 | -0.7546 |
| H | 1.5984 | -0.1927 | 1.8371 |
| H | 2.9972 | -0.2552 | 0.7791 |
| H | 2.9847 | -2.5323 | 0.7925 |
| H | 1.5853 | -2.5671 | 1.8510 |
| H | 0.5966 | -1.3975 | -2.0883 |
| H | 2.3105 | -1.4044 | -1.6753 |

## References


[1] a) MacroModel, version 10.6, Schrödinger, LLC, New York, NY, 2014. b) Maestro, version 9.9, Schrödinger, LLC, New York, NY, 2014.

[2] J. W. Ponder, *Tinker – Software Tools for Molecular Design*, Version 7.1; http://dasher.wustl.edu/tinker/

[3] J. L. Banks, H. S. Beard, Y. Cao, A. E. Cho, W. Damm, R. Farid, A. K. Felts, T. A. Halgren, D. T. Mainz, J. R. Maple, R. Murphy, D. M. Philipp, M. P. Repasky, L. Y. Zhang, B. J. Berne, R. A. Friesner, E. Gallicchio, R. M. Levy, *J. Comput. Chem.* **2005**, *26*, 1752–1780.

[4] W. L. Jorgensen, D. S. Maxwell, J. Tirado-Reves, *J. Am. Chem. Soc.* **1996**, *118*, 11225–11236.

[5] a) N. L. Allinger, *J. Am. Chem. Soc.* **1977**, *99*, 8127–8134. b) N. L. Allinger, Y. H. Yuh in *Molecular Mechanics,* ACS Monograph 177 (Eds.: U. Burkert, N. L. Allinger), American Chemical Society, Washington, DC, **1982**.

[6] N. L. Allinger, Y. H. Yuh, J.-H. Lii, *J. Am. Chem. Soc.* **1989**, *111*, 8551–8566.

[7] W. L. Jorgensen, J. Tirado-Rives, *J. Am. Chem. Soc.* **1988,** *110,* 1657–1666.

[8] a) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 490–519. b) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 520–552. c) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 553–586. c) T. A. Halgren, R. B. Nachbar, *J. Comput. Chem.* **1996**, *17*, 587–615. d) T. A. Halgren, *J. Comput. Chem.* **1996**, *17*, 616–641. e) T. A. Halgren, *J. Comput. Chem.* **1999**, *20*, 720–729. f) T. A. Halgren, *J. Comput. Chem.* **1999**, *20*, 730–748.

[9] W. F. Maier, P. v. R. Schleyer, *J. Am. Chem. Soc.* **1981**, *103*, 1891–1900.

[10] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2013.

[11] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215–241.

[12] B3LYP: a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785–789. b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 1372–1377. c) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652. d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623–11627. B3LYP-D3: e) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104. f) Becke–Johnson damping was used; see S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456–1465.

[13] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378–6396.

[14] H. Kruse, S. Grimme, *J. Chem. Phys.* **2012**, *136*, 154101.