

Supplementary Information

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Table S15. Calculated Energies (Hartrees) for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,12*R** of **5**. S408

Table S16. Coordinates (Angstroms) of calculated geometries for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,12*R** of **5**. S408

Table S1. ¹H (600 MHz), and ¹³C NMR (150 MHz) spectroscopic data of **4** in C₆D₆.

| No. | Marilzafurollene D (4) ^a | |
|-----|--|-------------------------------|
| | δ _C Mult. | δ _H (J in Hz) |
| 1 | 74.4, CH | 5.67, dd (2.0, 5.3) |
| 2 | 200.2, C | |
| 3 | 103.9, CH | 5.02, dd (5.3, 5.6) |
| 4 | 66.0, CH | 4.23, m |
| 5 | 38.6, CH ₂ | b 1.99, m |
| 6 | 79.3, CH | a 1.58, ddd (3.5, 8.3, 14.0) |
| 7 | 63.6, CH | 4.17, ddd (3.1, 3.5, 8.9) |
| 8 | 40.6, CH ₂ | 3.85, br dd (3.1, 5.0) |
| 9 | 79.7, CH | b 2.04, ddd (5.0, 9.8, 13.8) |
| 10 | 56.6, CH | a 1.85, dd (6.3, 13.8) |
| 11 | 42.9, CH ₂ | 4.14, ddd (2.8, 6.3, 9.8) |
| 12 | 69.9, CH | 4.27, m |
| 13 | 133.4, CH | b 2.00, ddd (2.6, 11.4, 14.3) |
| 14 | 125.3, C | a 1.66, m |
| 15 | 17.3, CH ₃ | 4.29, m |
| | | 5.30, br dd (6.4, 15.3) |
| | | 5.40, dq (6.3, 15.3) |
| | | 1.48, d, (6.3) |

^a Data recorded at 600/150 MHz (¹H/¹³C nuclei); Assignments were made based on COSY, HSQC and HMBC experiments.

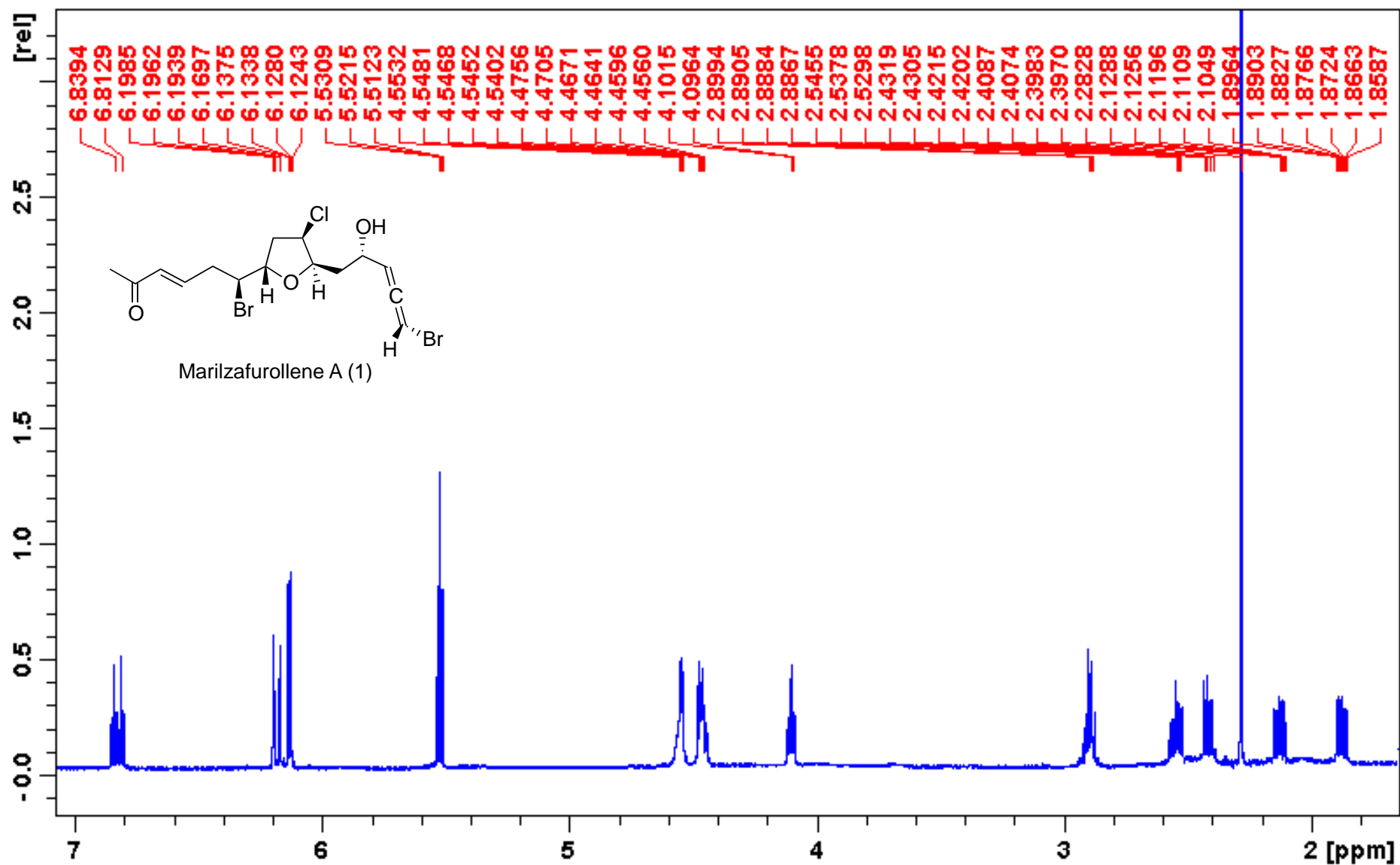
Figure S1. ^1H NMR spectrum (600 MHz, CDCl_3) of marilzafurollene A (1).

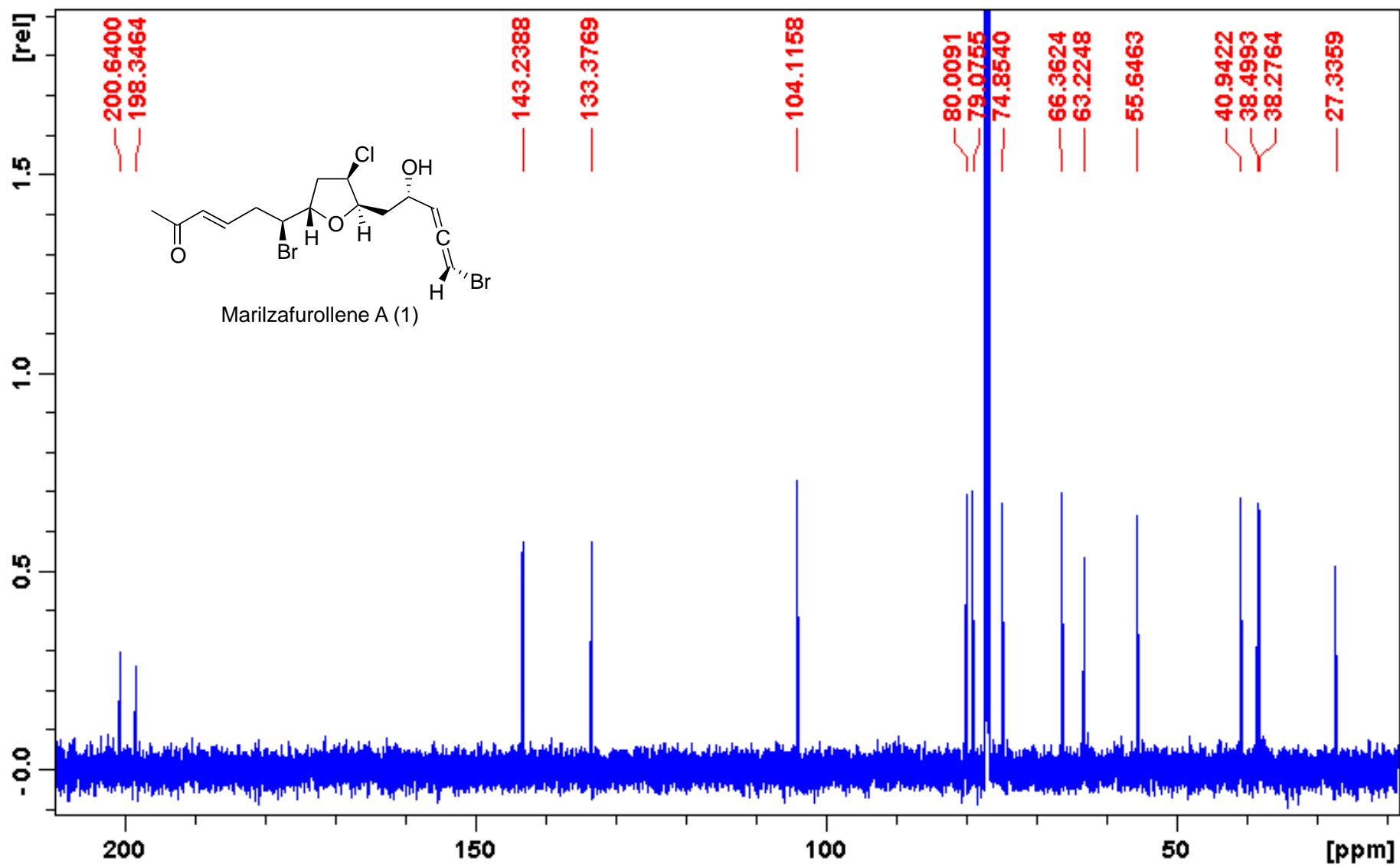
Figure S2. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 1.

Figure S4. HSQC NMR spectrum (600 MHz, CDCl₃) of compound 1.

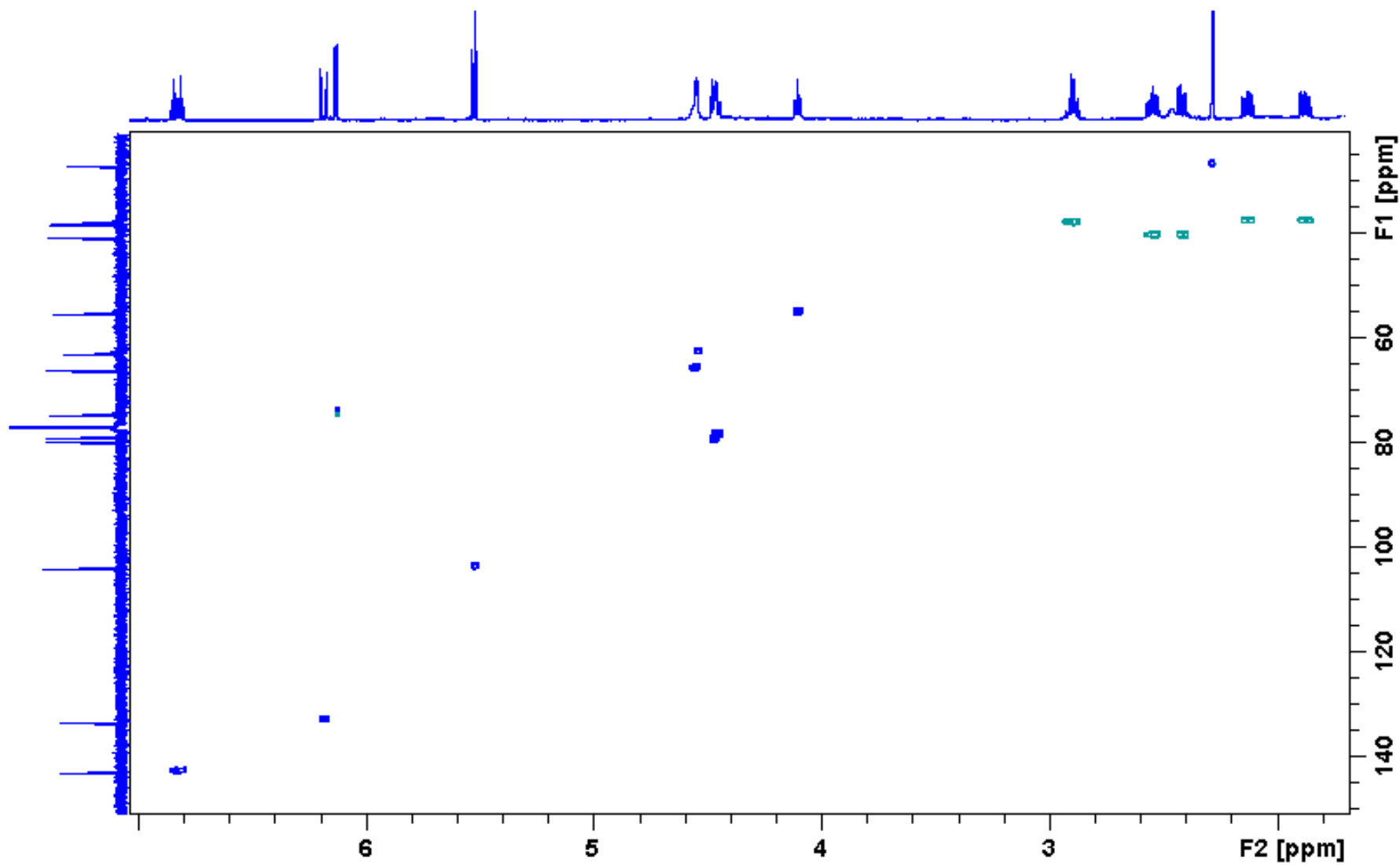


Figure S5. HMBC NMR spectrum (600 MHz, CDCl₃) of compound 1.

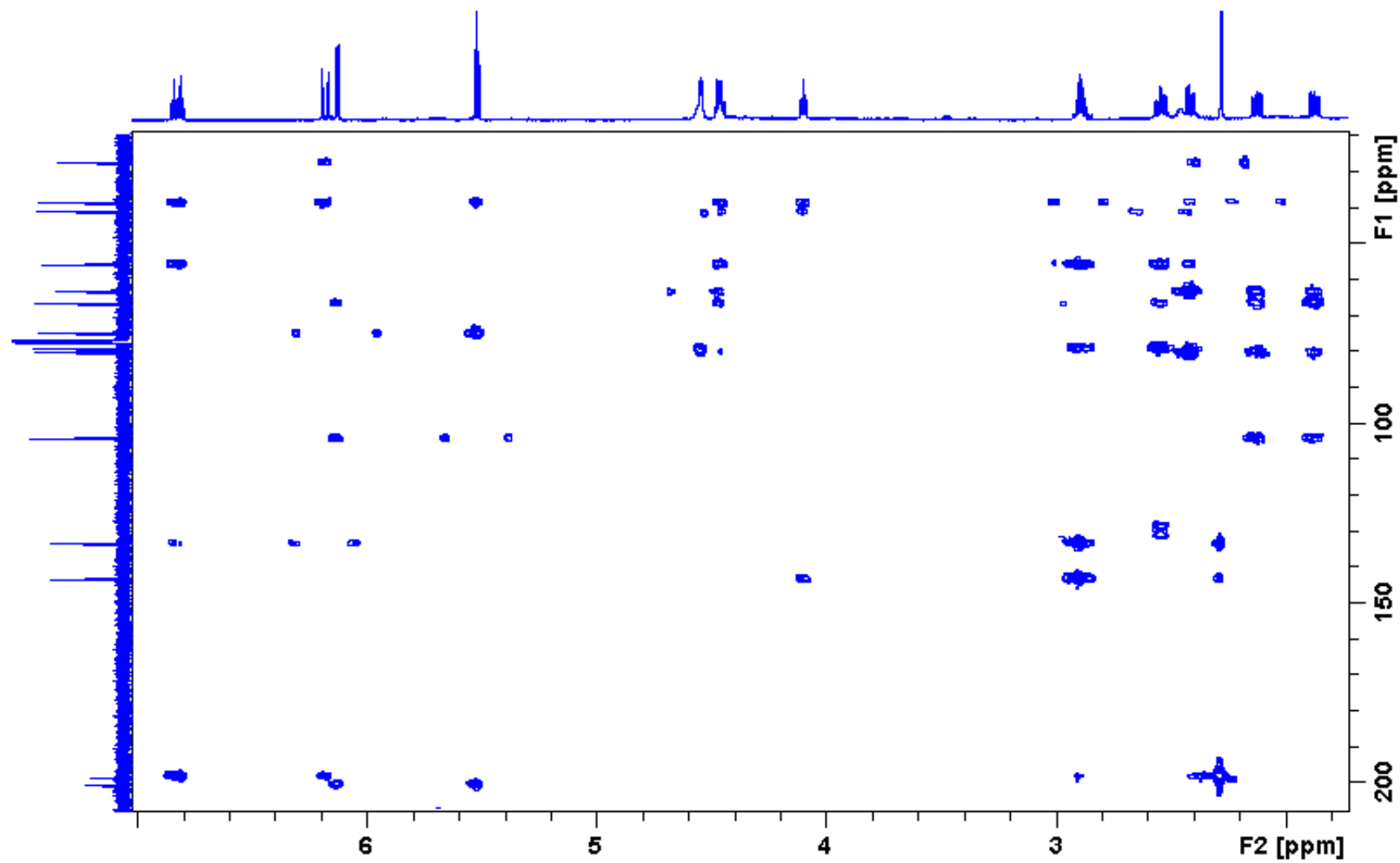


Figure S6. ROESY NMR spectrum (600 MHz, CDCl_3) of compound 1.

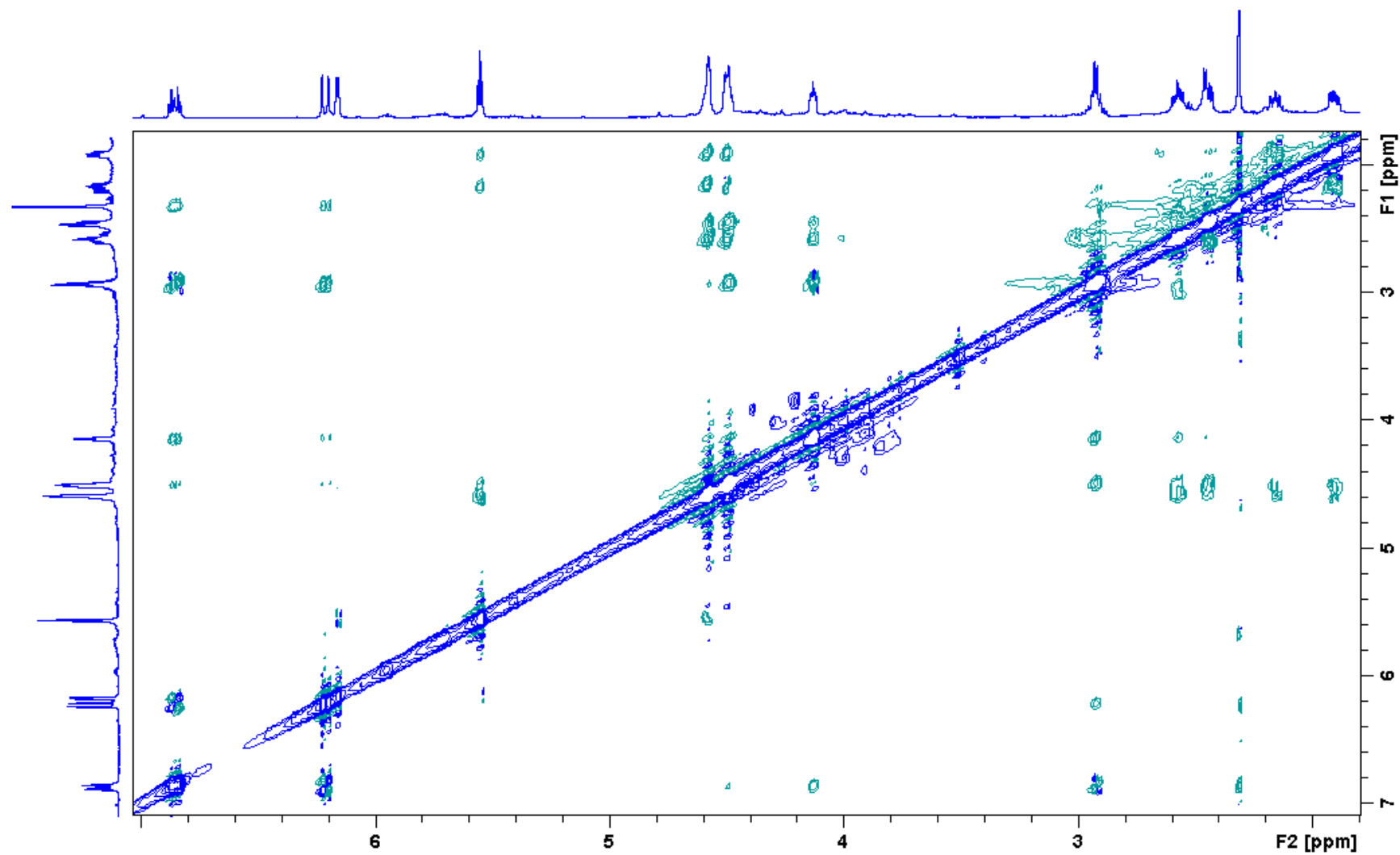


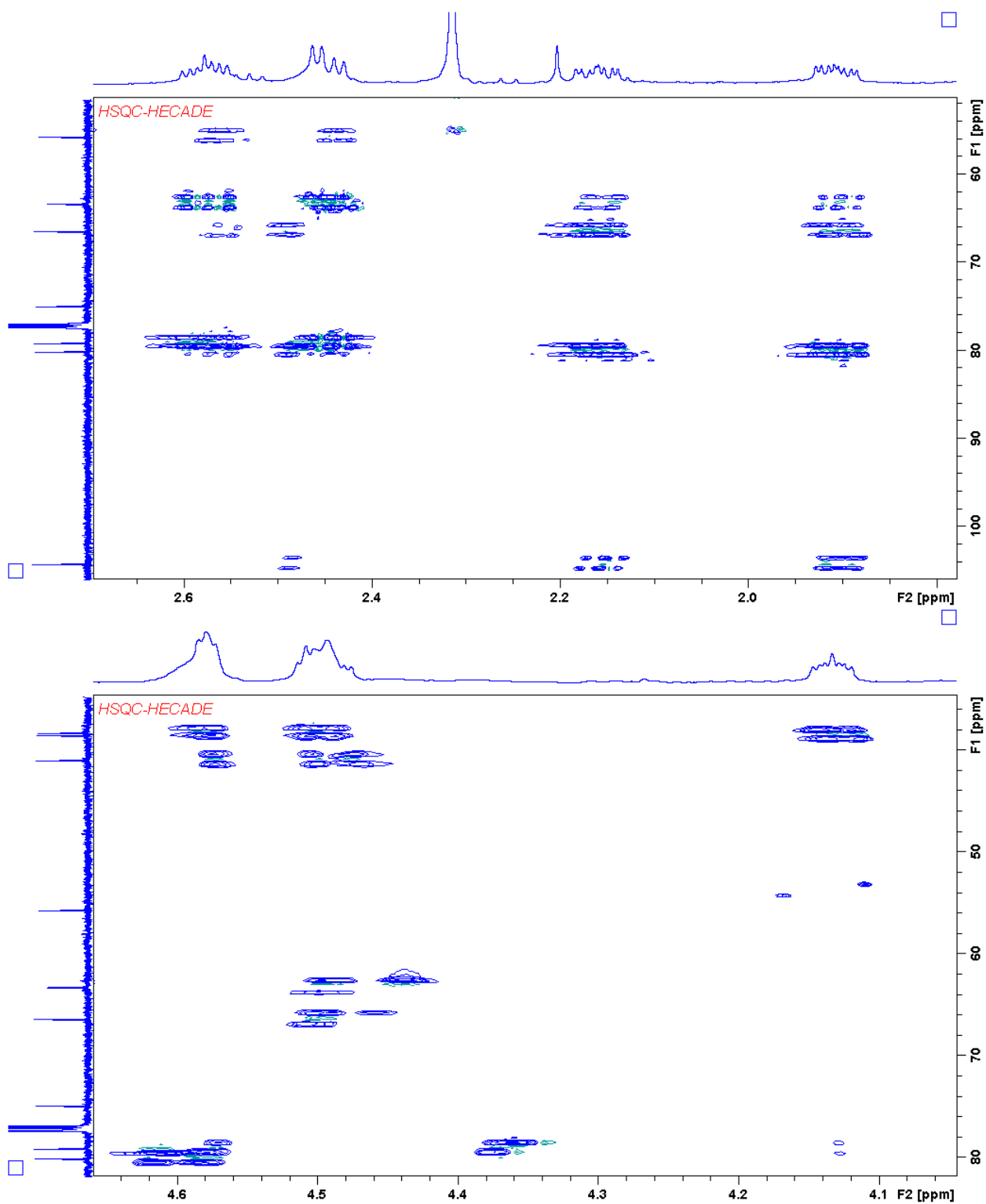
Figure S7. Selected sections of the HSQC-HECADE spectrum (600 MHz, CDCl₃) of compound **1**.

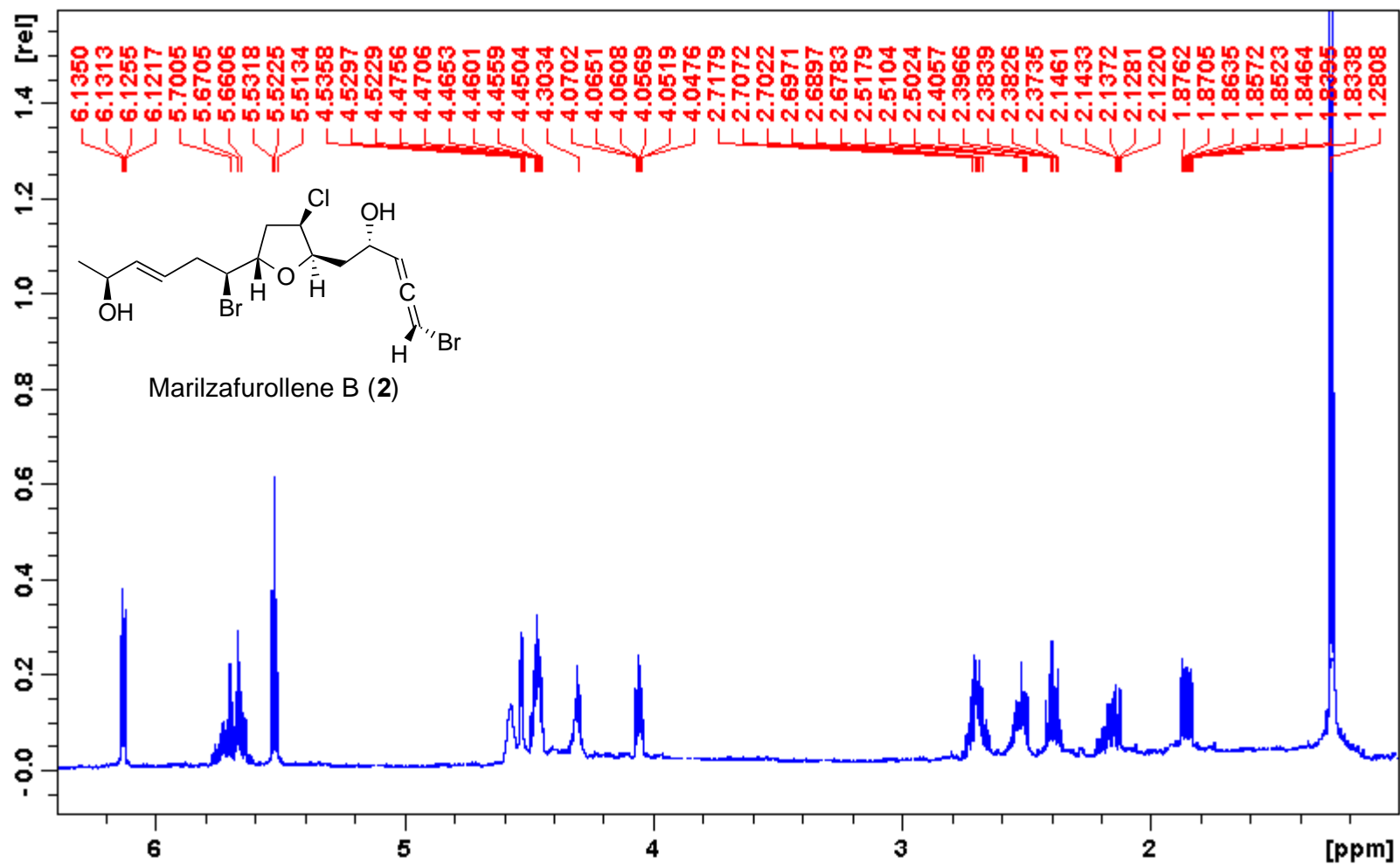
Figure S8. ^1H NMR spectrum (600 MHz, CDCl_3) of marilzafurollene B (2).

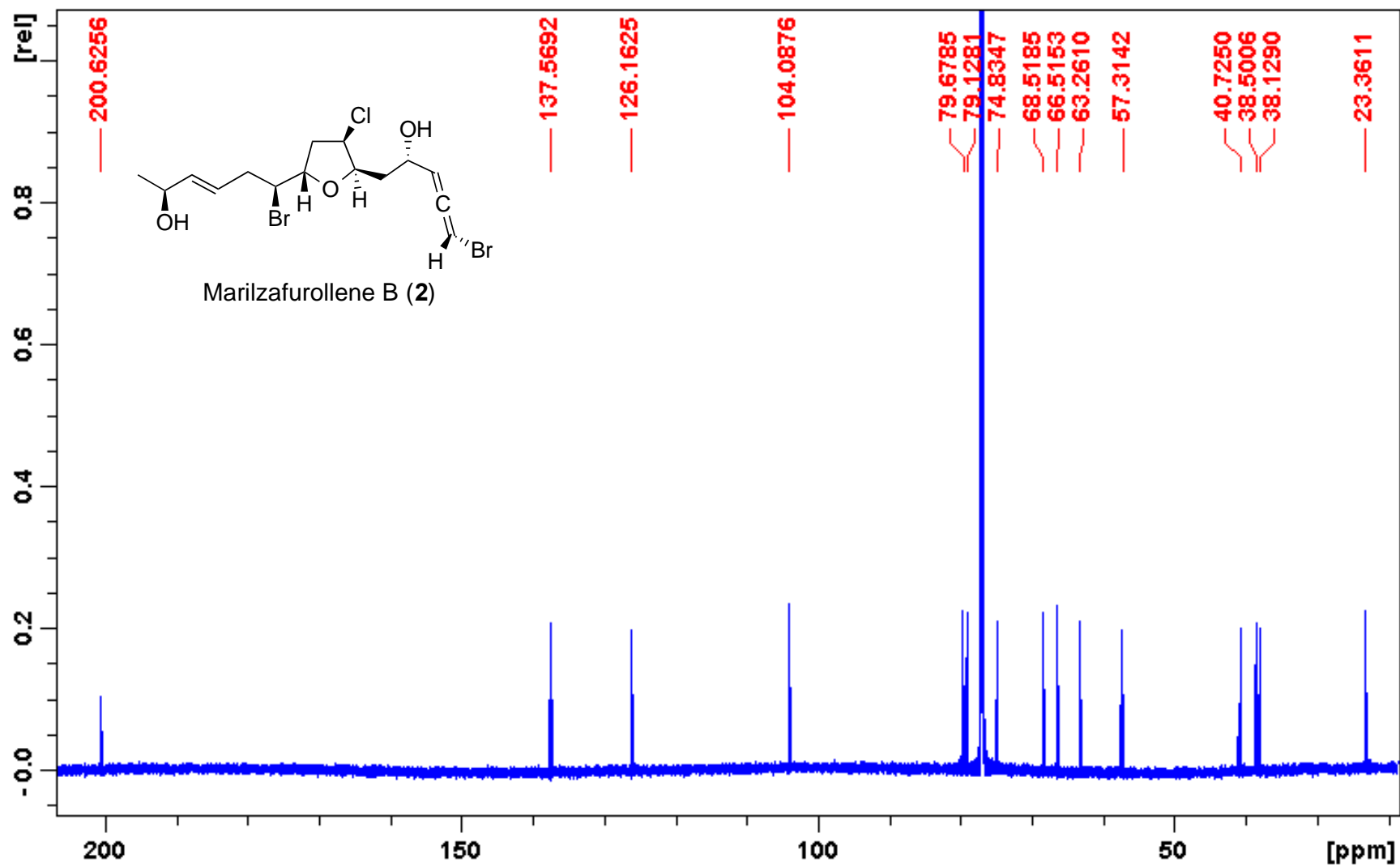
Figure S9. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 2.

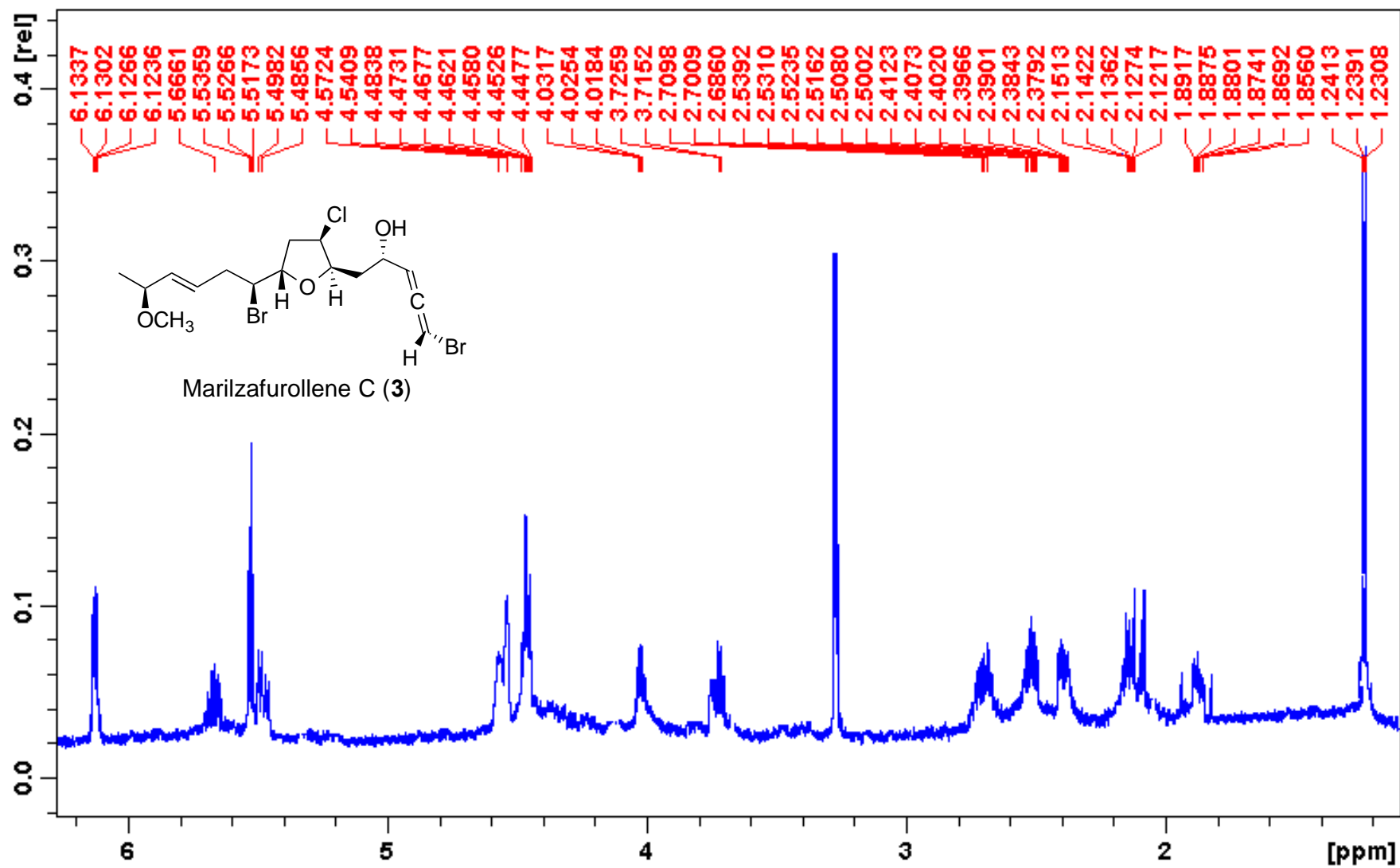
Figure S10. ^1H NMR spectrum (600 MHz, CDCl_3) of marilzafurollene C (3).

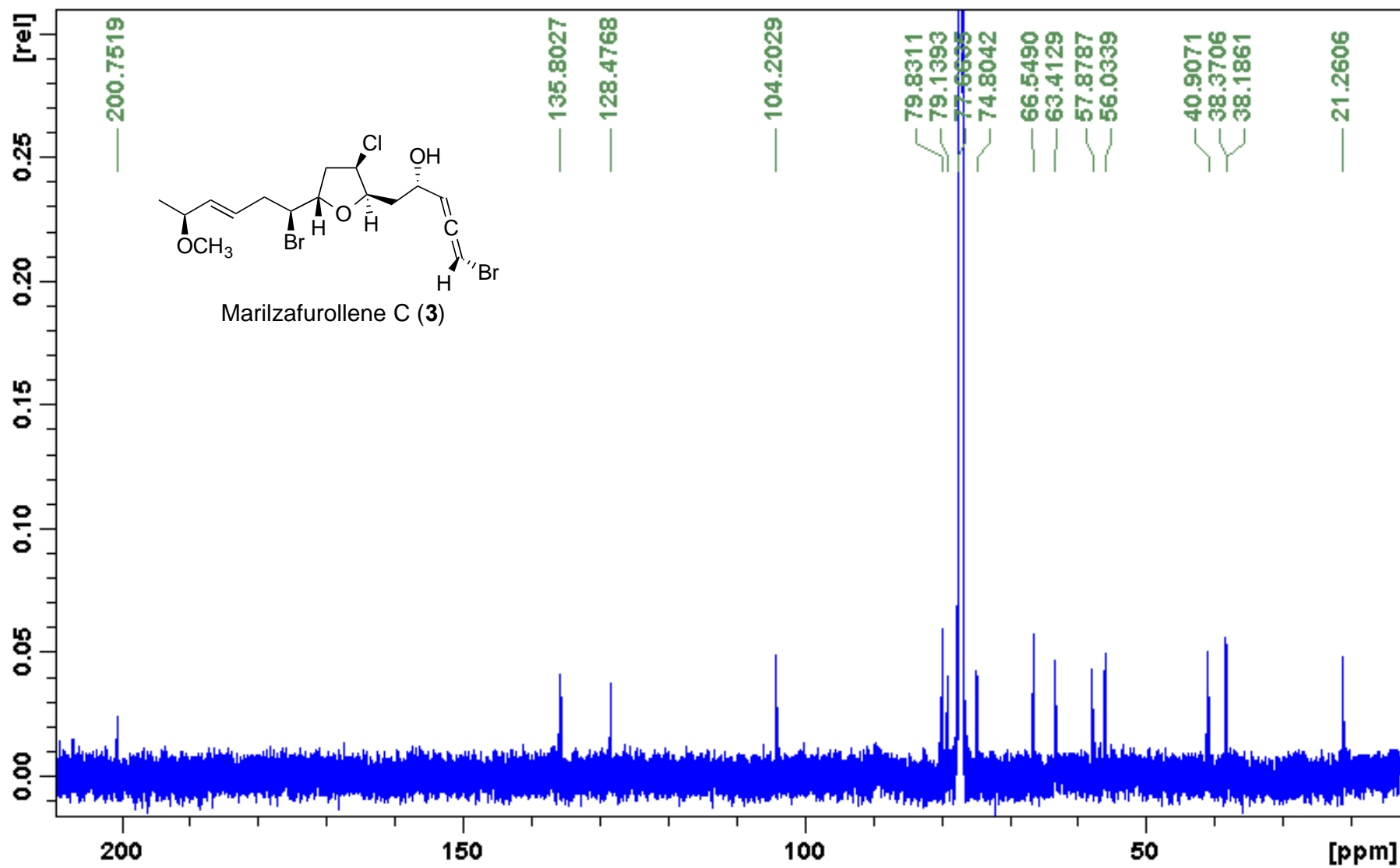
Figure S11. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **3**.

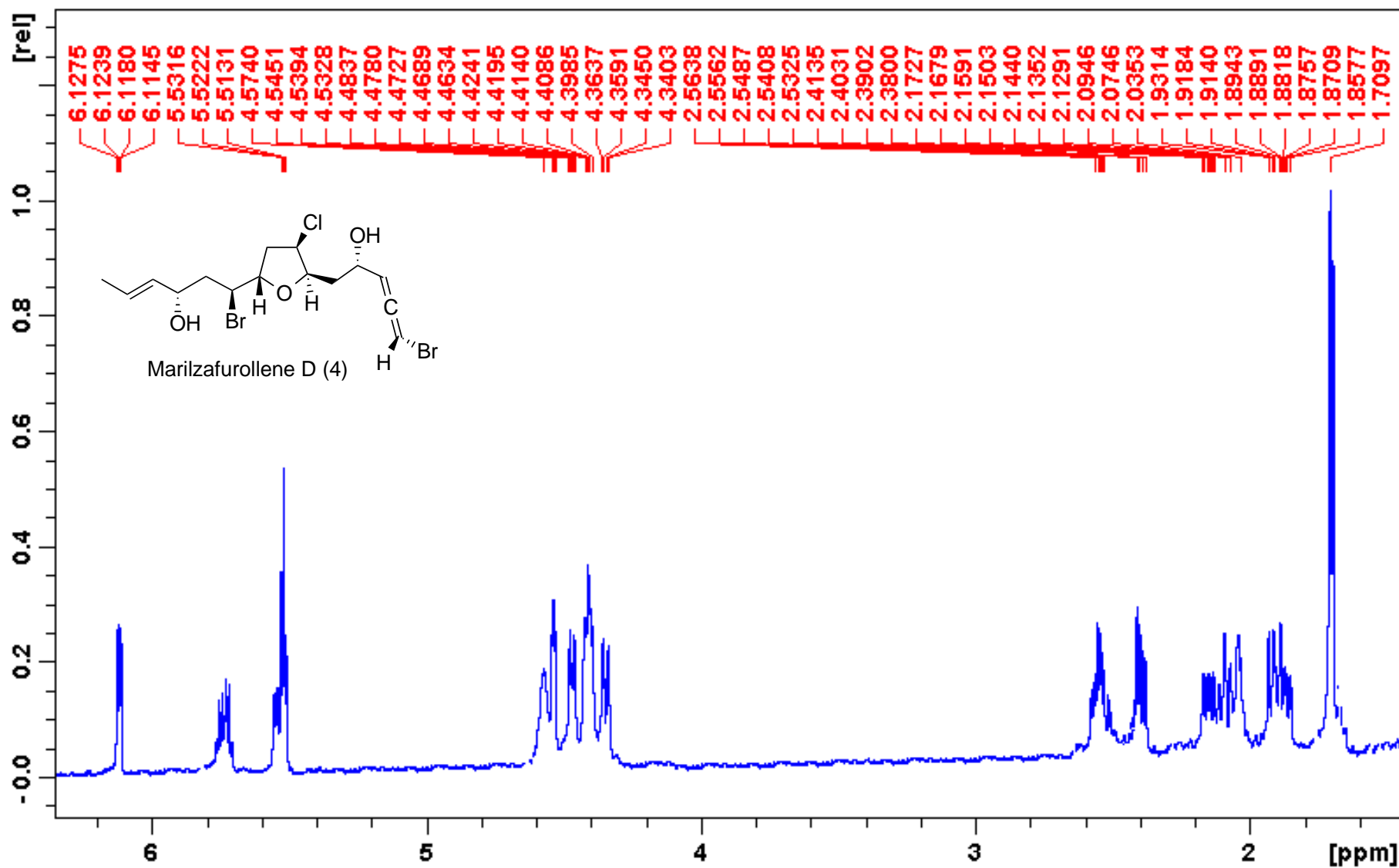
Figure S12. ^1H NMR spectrum (600 MHz, CDCl_3) of marilzafurollene D (4).

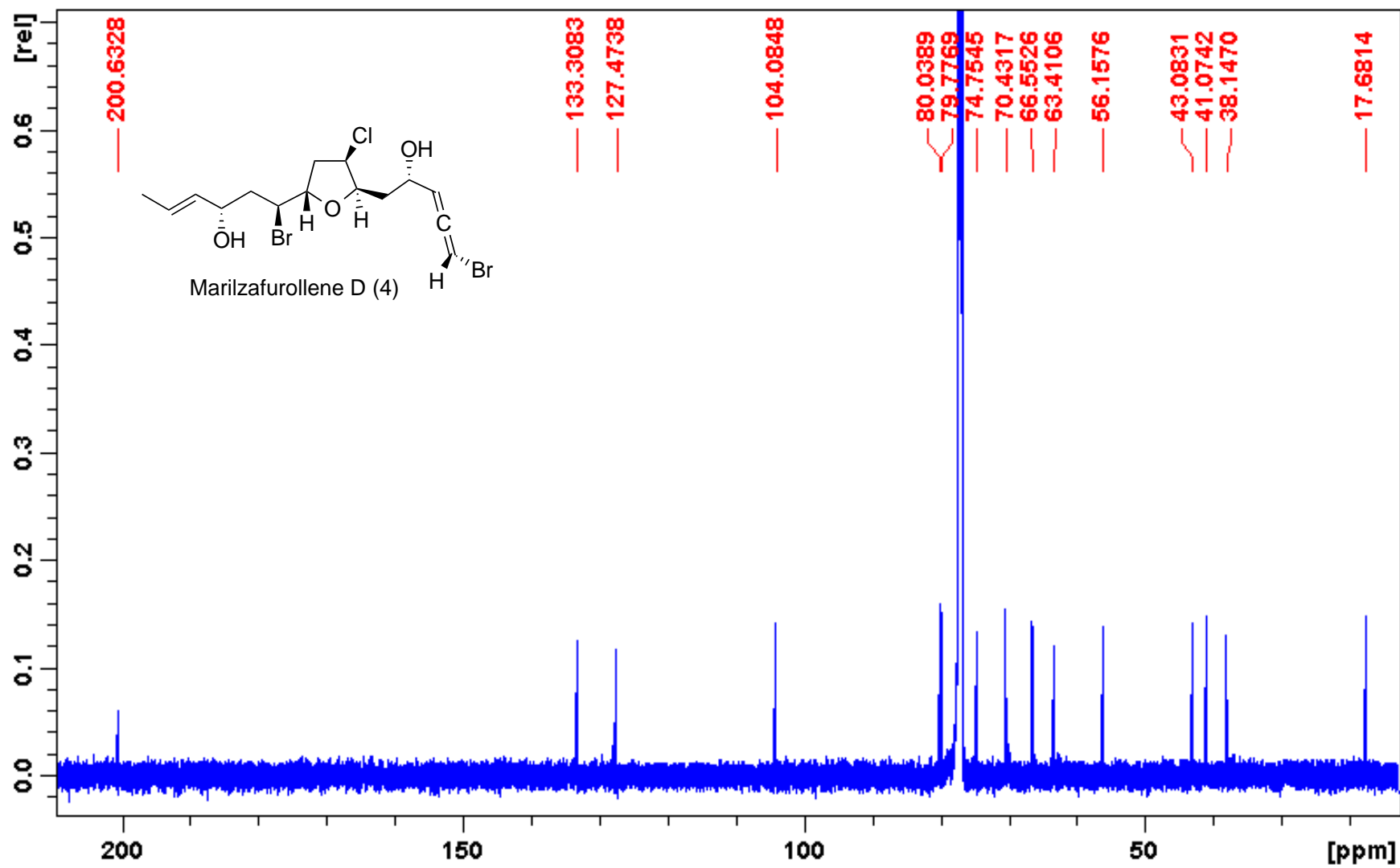
Figure S13. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound 4.

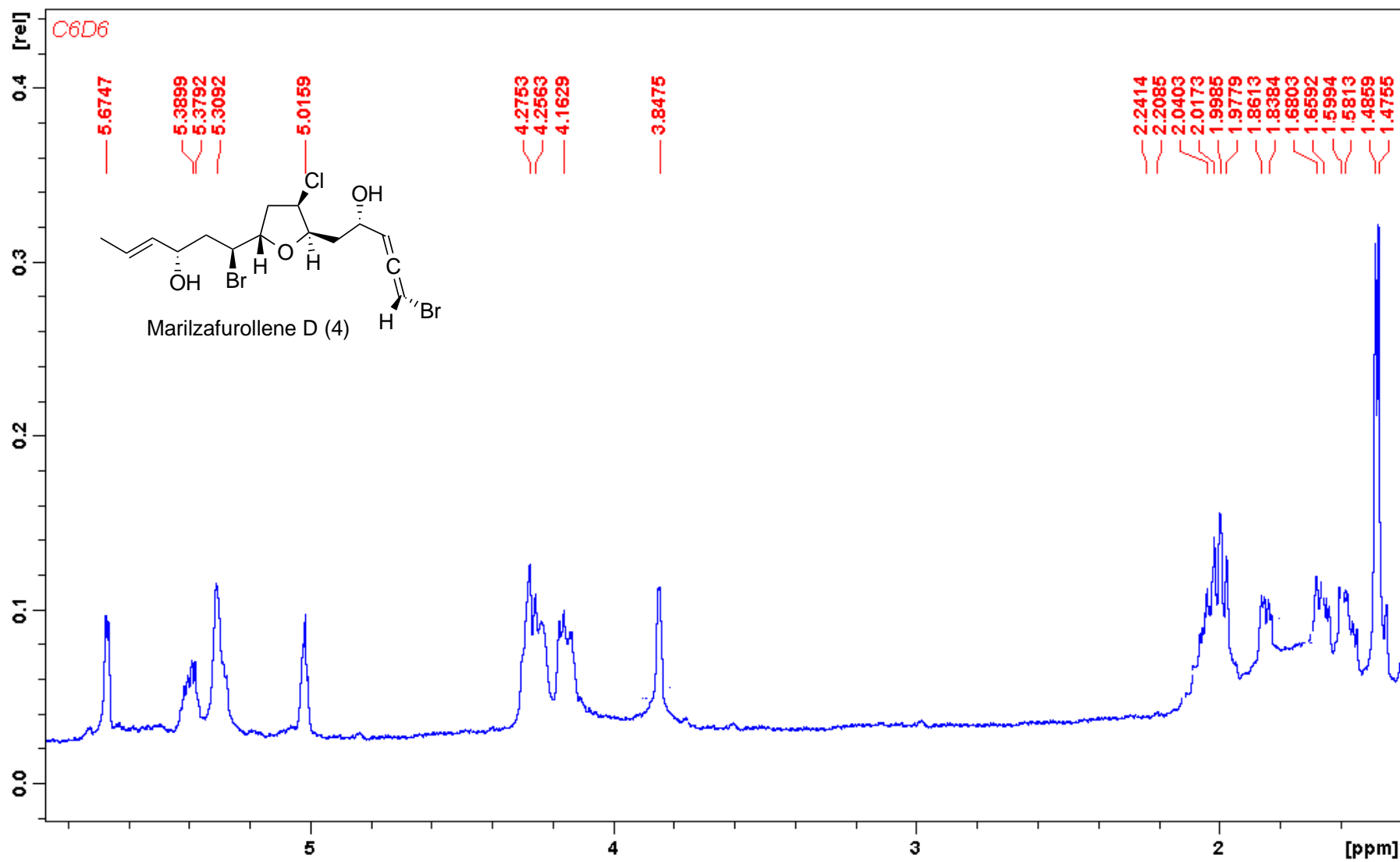
Figure S14. ^1H NMR spectrum (600 MHz, C_6D_6) of compound 4.

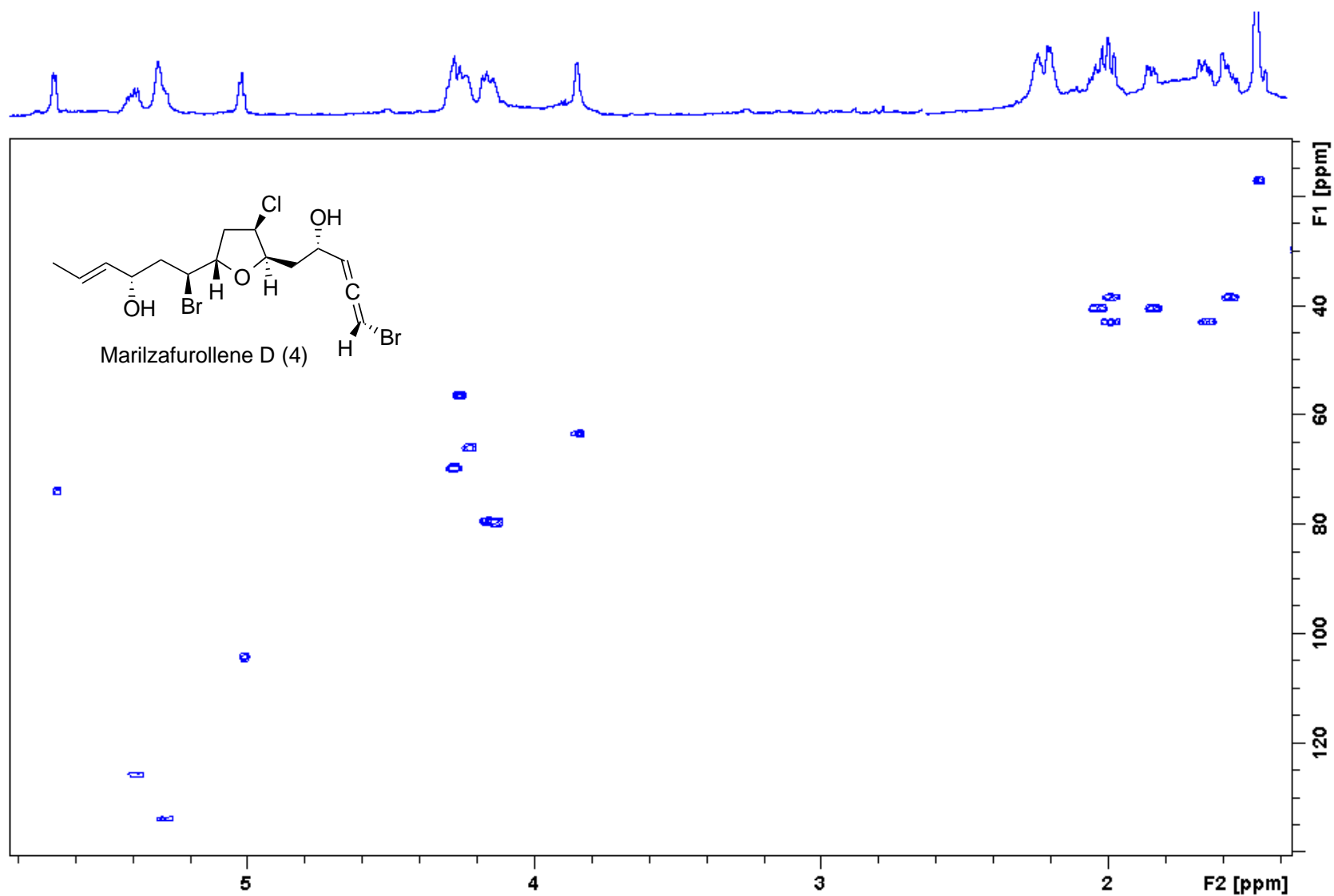
Figure S15. HSQC NMR spectrum (600 MHz, C₆D₆) of compound 4.

Figure S16. Selected sections of the HSQC-HECADE spectrum (600 MHz, C₆D₆) of compound 4.

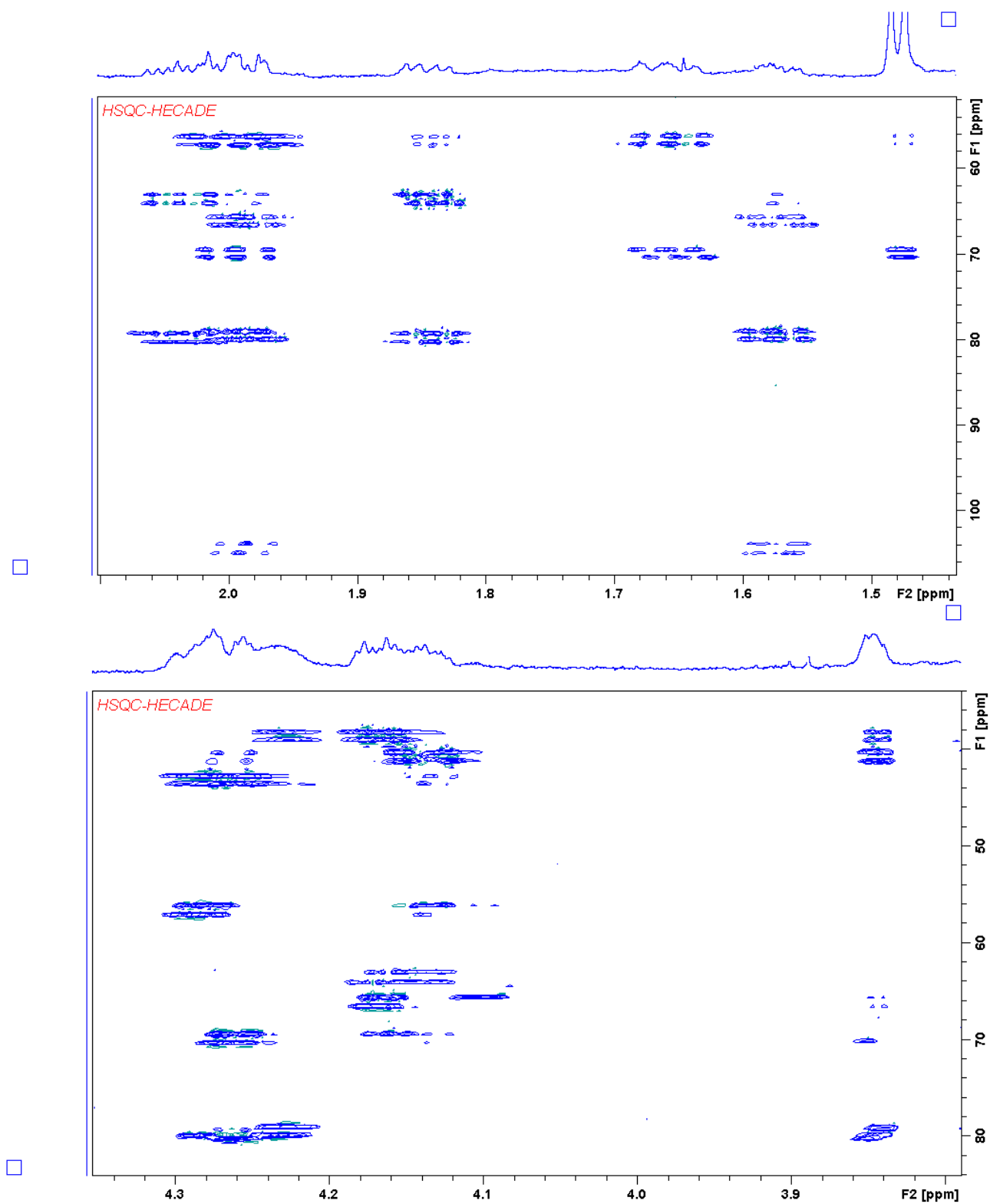


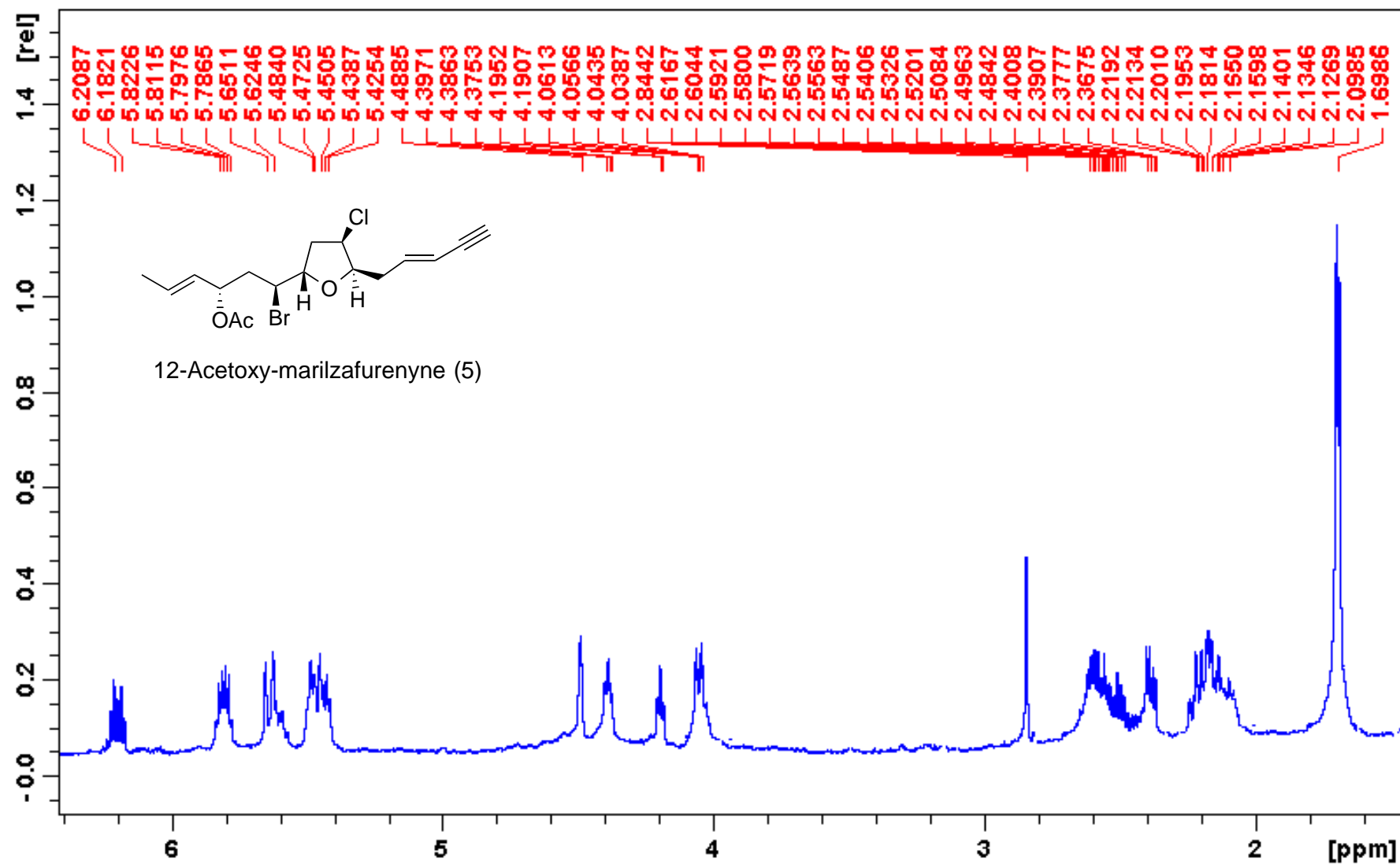
Figure S17. ^1H NMR spectrum (600 MHz, CDCl_3) of 12-acetoxy-marilzafurenyne (5).

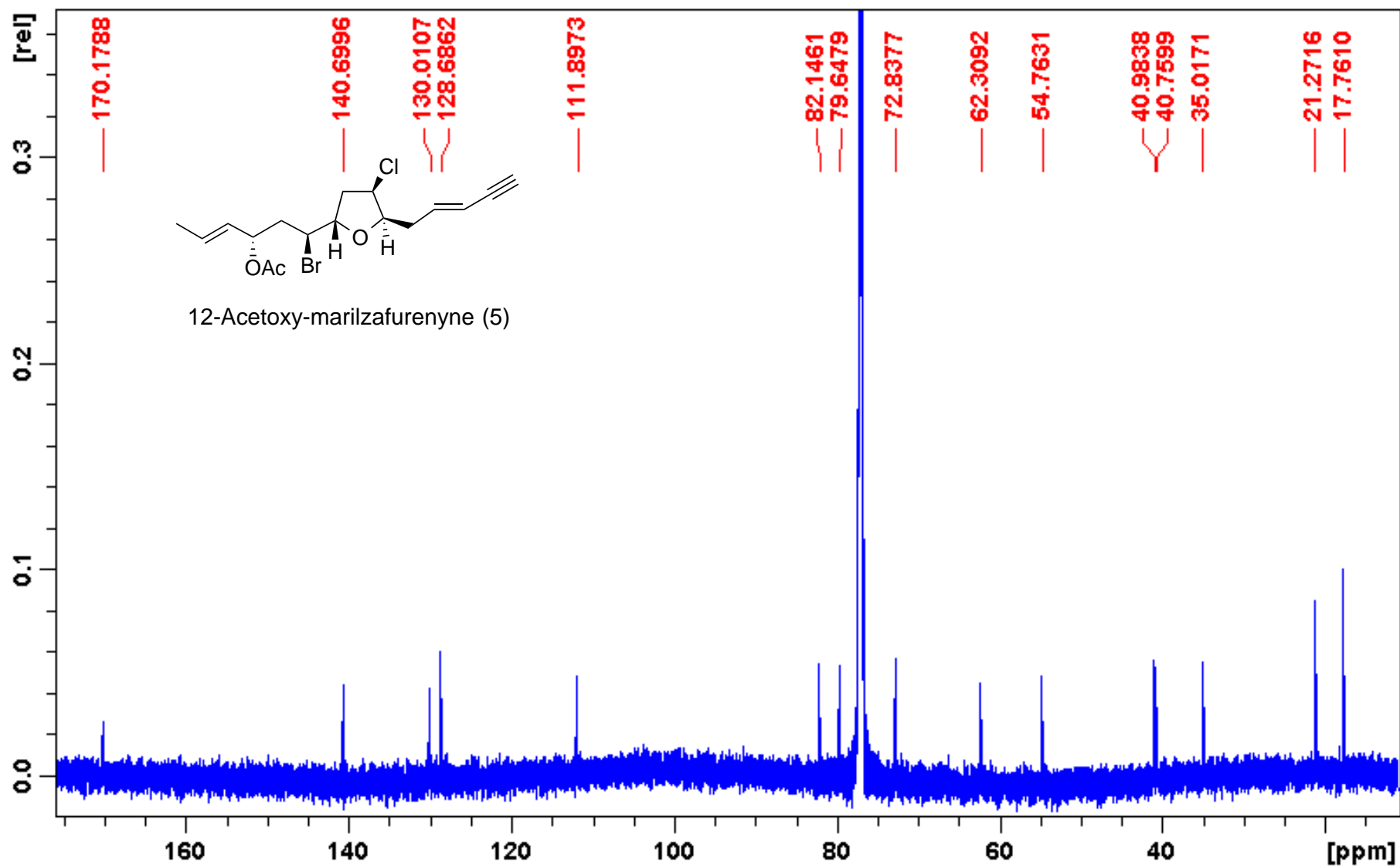
Figure S18. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **5**.

Table S2. Calculated ^{13}C and ^1H chemical shifts for marilzafurollene A (1).

| C | $S_{a,4S,6R,7R,9S,10S}$ | $S_{a,4R,6S,7S,9R,10R}$ | H | $S_{a,4S,6R,7R,9S,10S}$ | $S_{a,4R,6S,7S,9R,10R}$ |
|----|-------------------------|-------------------------|-----|-------------------------|-------------------------|
| 1 | 81.4 | 82.6 | 1 | 5.28 | 5.46 |
| 2 | 204.9 | 204.9 | 2 | - | - |
| 3 | 94.0 | 93.8 | 3 | 5.49 | 5.67 |
| 4 | 68.6 | 68.1 | 4 | 4.66 | 4.60 |
| 5 | 39.9 | 40.0 | 5b | 2.44 | 1.69 |
| | | | 5a | 1.84 | 2.26 |
| 6 | 81.4 | 81.9 | 6 | 4.42 | 4.38 |
| 7 | 66.3 | 66.4 | 7 | 4.20 | 4.21 |
| 8 | 39.5 | 39.6 | 8b | 2.68 | 1.82 |
| | | | 8a | 2.04 | 2.45 |
| 9 | 80.9 | 80.4 | 9 | 4.86 | 4.90 |
| 10 | 64.9 | 66.2 | 10 | 3.88 | 3.81 |
| 11 | 42.4 | 42.7 | 11b | 2.96 | 2.84 |
| | | | 11a | 2.93 | 2.81 |
| 12 | 142.9 | 142.3 | 12 | 6.91 | 7.08 |
| 13 | 132.4 | 132.9 | 13 | 6.17 | 6.29 |
| 14 | 197.1 | 197.4 | 14 | - | - |
| 15 | 23.2 | 23.1 | 15 | 2.28 | 2.10 |

Values were obtained after statistical analysis by linear regression of computed isotropic shieldings against experimental chemical shifts.

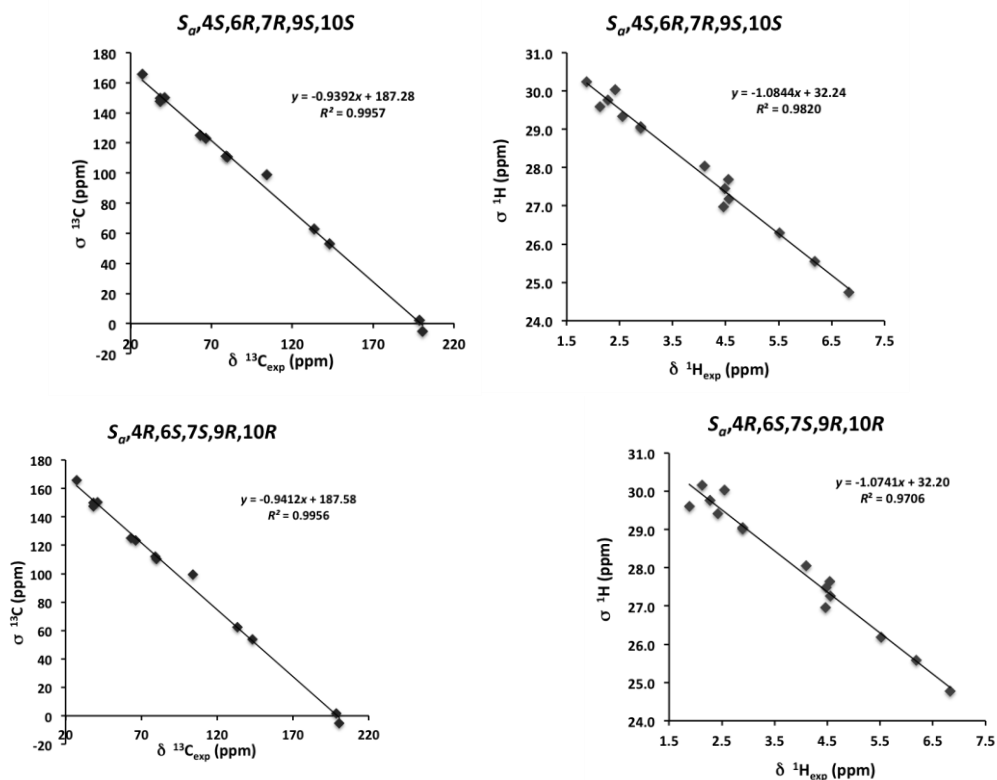
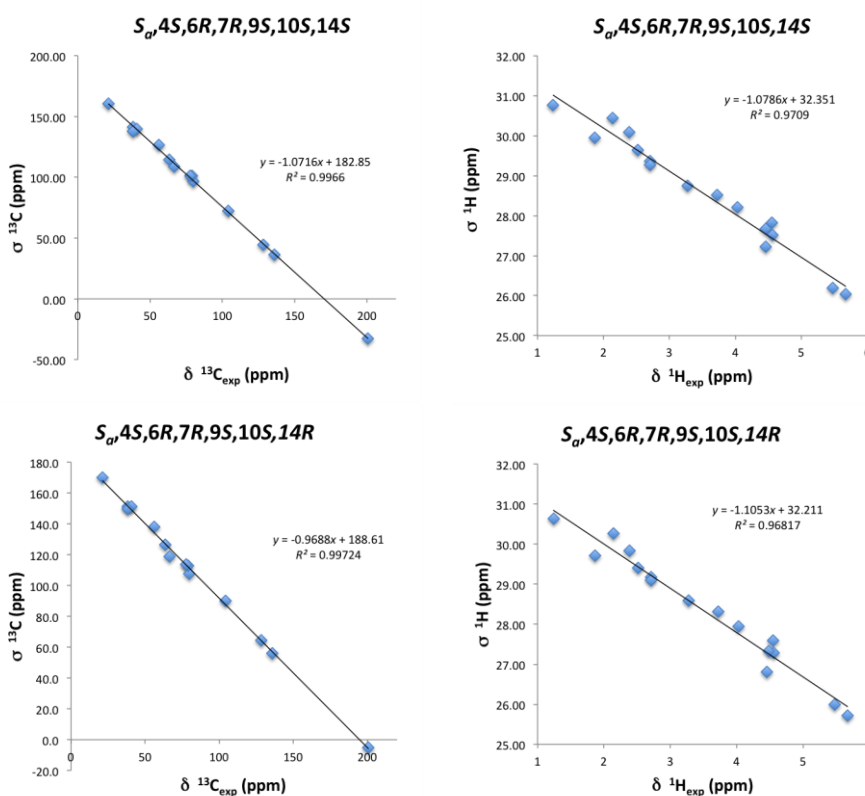
Figure S19. Correlation plots obtained for marilzafurollene A (1).

Table S3. Calculated ^{13}C and ^1H chemical shifts for marilzafurollene C (3).

| C | <i>S_a,4S,6R,7R,9S,10S,14S</i> | <i>S_a,4R,6S,7S,9R,10R,14R</i> | H | <i>S_a,4S,6R,7R,9S,10S,14S</i> | <i>S_a,4R,6S,7S,9R,10R,14R</i> |
|-----------|---|---|------------|---|---|
| 1 | 96.9 | 95.5 | 1 | 6.25 | 6.28 |
| 2 | 201.4 | 199.4 | 2 | - | - |
| 3 | 103.3 | 100.6 | 3 | 5.70 | 5.67 |
| 4 | 69.3 | 71.0 | 4 | 4.49 | 4.46 |
| 5 | 38.8 | 37.5 | 5b | 1.78 | 1.77 |
| | | | 5a | 2.24 | 2.26 |
| 6 | 80.6 | 82.5 | 6 | 4.35 | 4.41 |
| 7 | 64.1 | 62.9 | 7 | 4.21 | 4.18 |
| 8 | 40.2 | 37.2 | 8b | 2.53 | 2.54 |
| | | | 8a | 2.11 | 2.15 |
| 9 | 76.5 | 77.3 | 9 | 4.76 | 4.89 |
| 10 | 71.2 | 71.7 | 10 | 3.85 | 3.86 |
| 11 | 42.4 | 39.1 | 11b | 2.78 | 2.75 |
| | | | 11a | 2.87 | 2.82 |
| 12 | 129.2 | 127.2 | 12 | 5.85 | 5.88 |
| 13 | 137.0 | 136.1 | 13 | 5.72 | 5.62 |
| 14 | 76.1 | 76.1 | 14 | 3.56 | 3.52 |
| 15 | 20.8 | 17.7 | 15 | 1.45 | 1.43 |
| 16 | 52.4 | 51.0 | 16 | 3.27 | 3.28 |

Values were obtained after statistical analysis by linear regression of computed isotropic shieldings against experimental chemical shifts.

Figure S20. Correlation plots obtained for marilzafurollene C (3).**Table S4.** Calculated ^{13}C and ^1H chemical shifts for 12-acetoxy-marilzafurenyne (5).

| C | 4S,6R,7R,9S,10S,12S | 4R,6S,7S,9R,10R,12R | H | 4S,6R,7R,9S,10S,12S | 4R,6S,7S,9R,10R,12R |
|----|---------------------|---------------------|-----|---------------------|---------------------|
| 1 | 73.9 | 73.4 | 1 | 3.08 | 3.03 |
| 2 | 74.9 | 75.3 | 2 | - | - |
| 3 | 107.5 | 107.6 | 3 | 5.46 | 5.45 |
| 4 | 144.5 | 145.5 | 4 | 6.39 | 6.42 |
| 5 | 38.0 | 38.2 | 5b | 2.67 | 2.62 |
| 6 | 83.5 | 83.8 | 5a | 2.31 | 2.28 |
| 7 | 64.7 | 65.3 | 6 | 4.22 | 4.18 |
| 8 | 40.1 | 40.5 | 7 | 4.08 | 4.01 |
| 9 | 80.9 | 77.1 | 8b | 2.56 | 2.42 |
| 10 | 70.0 | 71.7 | 8a | 2.16 | 2.21 |
| 11 | 44.1 | 45.1 | 9 | 4.58 | 5.25 |
| 12 | 70.6 | 71.4 | 10 | 3.93 | 3.83 |
| 13 | 128.7 | 129.9 | 11b | 2.24 | 2.14 |
| 14 | 132.8 | 129.8 | 11a | 2.12 | 2.46 |
| 15 | 17.8 | 17.9 | 12 | 5.43 | 5.18 |
| 16 | 170.2 | 171.5 | 13 | 5.40 | 5.61 |
| 17 | 20.8 | 20.9 | 14 | 6.04 | 5.92 |
| | | | 15 | 1.90 | 1.86 |
| | | | 16 | - | - |
| | | | 17 | 2.12 | 2.11 |

Values were obtained after statistical analysis by linear regression of computed isotropic shieldings against experimental chemical shifts.

Figure S21. Correlation plots obtained for 12-acetoxy-marilzafurenyne (5).

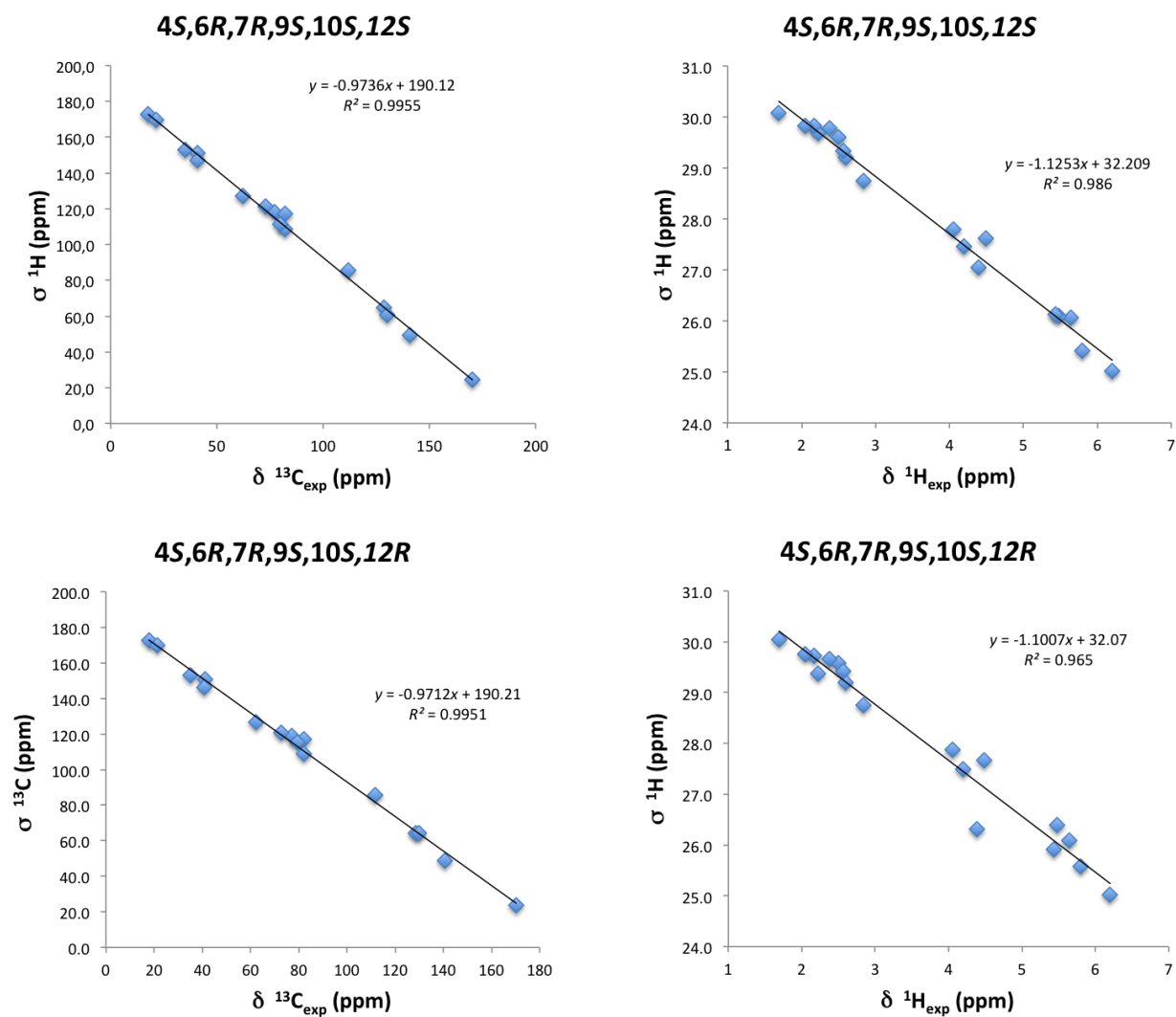


Table S5. Calculated Energies (Hartrees) for diastereoisomer $S_a,4S,6R,7R,9S,10S$ of **1**.

| Entry ID | Gas Phase Energy |
|----------|------------------|
| 1 | -849,889,732 |
| 2 | -849,888,667 |
| 3 | -849,888,966 |
| 4 | -84,988,891 |
| 5 | -849,888,974 |
| 6 | -849,888,926 |
| 7 | -849,888,972 |
| 8 | -849,889,026 |
| 9 | -849,888,969 |
| 10 | -849,888,891 |
| 11 | -849,887,938 |
| 12 | -849,886,933 |
| 13 | -849,889,308 |
| 14 | -849,888,746 |
| 15 | -849,889,561 |
| 16 | -849,885,682 |
| 17 | -849,888,414 |
| 18 | -84,988,757 |
| 19 | -849,886,403 |
| 20 | -849,889,367 |
| 21 | -849,889,111 |
| 22 | -849,887,528 |
| 23 | -849,887,684 |
| 24 | -849,888,722 |
| 25 | -849,886,912 |
| 26 | -849,888,443 |
| 27 | -84,988,468 |
| 28 | -849,886,486 |
| 29 | -849,889,128 |
| 30 | -849,888,472 |
| 31 | -849,888,025 |
| 32 | -849,886,947 |
| 33 | -849,888,084 |
| 34 | -849,887,247 |
| 35 | -849,885,538 |
| 36 | -849,884,153 |
| 37 | -849,891,294 |
| 38 | -849,887,349 |
| 39 | -849,887,769 |
| 40 | -849,887,456 |
| 41 | -849,884,487 |
| 42 | -849,884,354 |
| 43 | -849,884,733 |
| 44 | -849,884,722 |
| 45 | -849,883,607 |

Table S5. *Cont.*

| | |
|----|--------------|
| 46 | −849,887,933 |
| 47 | −849,886,773 |
| 48 | −849,884,928 |
| 49 | −849,887,161 |
| 50 | −849,888,234 |
| 51 | −849,885,235 |
| 52 | −849,886,184 |
| 53 | −849,887,786 |
| 54 | −849,886,996 |
| 55 | −849,887,917 |
| 56 | −849,889,128 |
| 57 | −849,884,162 |
| 58 | −849,884,633 |
| 59 | −849,886,797 |
| 60 | −84,988,321 |
| 61 | −849,885,029 |
| 62 | −849,884,135 |
| 63 | −849,884,101 |
| 64 | −849,883,757 |
| 65 | −849,887,386 |
| 66 | −849,888,699 |
| 67 | −849,883,317 |
| 68 | −849,883,094 |
| 69 | −849,887,465 |

Table S6. Coordinates (Angstroms) of calculated geometries for diastereoisomer $S_a,4S,6R,7R,9S,10S$ of **1**.

| Marilzafurollene_A_1 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83250 | -3.28330 | -0.59460 |
| O | -2.12440 | -2.71510 | -0.89840 |
| C | -0.66080 | -4.68810 | -1.19310 |
| C | -0.63790 | -3.16120 | 0.91540 |
| C | -2.61620 | -2.05240 | 0.28790 |
| C | -1.42240 | -1.90560 | 1.23820 |
| C | -3.35450 | -0.77040 | -0.09270 |
| Cl | -0.41540 | -0.45810 | 0.92620 |
| C | -4.62620 | -1.03170 | -0.90860 |
| C | -0.83370 | -4.72950 | -2.72030 |
| Br | -1.98070 | -5.94670 | -0.43350 |
| C | 0.24120 | -3.97420 | -3.45540 |
| C | 0.00500 | -2.88900 | -4.20890 |
| C | 1.11880 | -2.18700 | -4.90980 |
| C | 0.75570 | -0.98210 | -5.73730 |
| O | 2.28530 | -2.56060 | -4.79750 |
| C | -5.71960 | -1.66540 | -0.10150 |
| O | -5.12420 | 0.22950 | -1.36010 |
| C | -6.17620 | -2.87270 | -0.27490 |
| C | -6.62750 | -4.07550 | -0.43690 |
| H | -7.39630 | -4.35450 | -1.14500 |
| Br | -6.02170 | -5.38290 | 0.71160 |
| H | -0.10020 | -2.62190 | -1.07460 |
| H | 0.31240 | -5.10280 | -0.90650 |
| H | -1.08880 | -4.00080 | 1.45380 |
| H | 0.41840 | -3.12350 | 1.19990 |
| H | -3.31850 | -2.75540 | 0.75300 |
| H | -1.73270 | -1.85470 | 2.28550 |
| H | -3.60160 | -0.19280 | 0.80750 |
| H | -2.70500 | -0.13030 | -0.70360 |
| H | -4.39090 | -1.62620 | -1.79910 |
| H | -0.79420 | -5.76930 | -3.07110 |
| H | -1.82730 | -4.35650 | -3.00160 |
| H | 1.25700 | -4.35760 | -3.36280 |
| H | -0.99300 | -2.48160 | -4.32540 |
| H | 1.02360 | -0.07470 | -5.19030 |
| H | 1.29960 | -1.02160 | -6.68520 |
| H | -0.31380 | -0.96370 | -5.96400 |
| H | -6.14890 | -1.06280 | 0.69470 |
| H | -5.89080 | 0.03660 | -1.92840 |

Table S6. Cont.

| Marilzafurollene_A_2 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28290 | -0.59440 |
| O | -2.12420 | -2.71530 | -0.89870 |
| C | -0.65790 | -4.68700 | -1.19150 |
| C | -0.63600 | -3.15840 | 0.91460 |
| C | -2.61580 | -2.05250 | 0.28790 |
| C | -1.42060 | -1.90270 | 1.23610 |
| C | -3.35700 | -0.77180 | -0.09080 |
| Cl | -0.41370 | -0.45650 | 0.91720 |
| C | -4.63090 | -1.03380 | -0.90270 |
| C | -0.80340 | -4.67080 | -2.72290 |
| Br | -1.99790 | -5.93380 | -0.44890 |
| C | -0.33080 | -5.94290 | -3.38030 |
| C | -1.12320 | -6.74980 | -4.10290 |
| C | -0.58600 | -7.99490 | -4.72420 |
| C | -1.56490 | -8.86190 | -5.47170 |
| O | 0.60620 | -8.28840 | -4.65130 |
| C | -5.71750 | -1.67900 | -0.09560 |
| O | -5.13780 | 0.22870 | -1.34050 |
| C | -6.18590 | -2.87840 | -0.29110 |
| C | -6.65010 | -4.07330 | -0.47450 |
| H | -7.42790 | -4.32940 | -1.18130 |
| Br | -6.06460 | -5.40510 | 0.65640 |
| H | -0.10080 | -2.62700 | -1.08420 |
| H | 0.31290 | -5.09910 | -0.89390 |
| H | -1.08580 | -3.99810 | 1.45420 |
| H | 0.42070 | -3.11980 | 1.19750 |
| H | -3.31610 | -2.75660 | 0.75470 |
| H | -1.72880 | -1.84900 | 2.28390 |
| H | -3.60190 | -0.19440 | 0.81010 |
| H | -2.71020 | -0.13070 | -0.70350 |
| H | -4.39610 | -1.61990 | -1.79880 |
| H | -1.84020 | -4.45280 | -3.01010 |
| H | -0.19210 | -3.85730 | -3.13410 |
| H | 0.72190 | -6.19420 | -3.25390 |
| H | -2.17500 | -6.53370 | -4.25130 |
| H | -1.48080 | -8.66230 | -6.54280 |
| H | -1.34000 | -9.91300 | -5.26950 |
| H | -2.59080 | -8.67050 | -5.14550 |
| H | -6.13430 | -1.09090 | 0.71800 |
| H | -5.89500 | 0.03570 | -1.92140 |

Table S6. Cont.

| Marilzafurollene_A_3 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65510 | -4.68240 | -1.20130 |
| C | -0.63920 | -3.16520 | 0.91520 |
| C | -2.61590 | -2.05250 | 0.28780 |
| C | -1.42260 | -1.90940 | 1.23990 |
| C | -3.35110 | -0.76830 | -0.09100 |
| Cl | -0.41140 | -0.46390 | 0.93060 |
| C | -4.61550 | -1.02210 | -0.92040 |
| C | -0.81760 | -4.65660 | -2.73080 |
| Br | -1.97740 | -5.94390 | -0.45360 |
| C | -0.34060 | -5.91890 | -3.40350 |
| C | -1.13180 | -6.72220 | -4.13150 |
| C | -0.58840 | -7.95440 | -4.77290 |
| C | -1.56130 | -8.81350 | -5.53710 |
| O | 0.60490 | -8.24430 | -4.70230 |
| C | -5.71140 | -1.67700 | -0.13410 |
| O | -5.11800 | 0.24470 | -1.35060 |
| C | -6.19010 | -2.86640 | -0.36270 |
| C | -6.66510 | -4.05080 | -0.58250 |
| H | -7.43960 | -4.27970 | -1.30210 |
| Br | -6.06230 | -5.43050 | 0.47930 |
| H | -0.10100 | -2.62340 | -1.07980 |
| H | 0.32140 | -5.08980 | -0.91620 |
| H | -1.09210 | -4.00570 | 1.45080 |
| H | 0.41690 | -3.12960 | 1.20080 |
| H | -3.32080 | -2.75450 | 0.75100 |
| H | -1.73360 | -1.85950 | 2.28700 |
| H | -3.60530 | -0.19660 | 0.81090 |
| H | -2.69670 | -0.12380 | -0.69190 |
| H | -4.36960 | -1.59820 | -1.82000 |
| H | -1.85930 | -4.44580 | -3.00520 |
| H | -0.21800 | -3.83460 | -3.14240 |
| H | 0.71440 | -6.16440 | -3.28600 |
| H | -2.18550 | -6.51060 | -4.27240 |
| H | -1.44710 | -8.62420 | -6.60730 |
| H | -1.35720 | -9.86580 | -5.32010 |
| H | -2.59260 | -8.60390 | -5.24060 |
| H | -6.13030 | -1.10330 | 0.68870 |
| H | -5.87170 | 0.05760 | -1.93780 |

Table S6. Cont.

| Marilzafurollene_A_4 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65310 | -4.68090 | -1.20400 |
| C | -0.64110 | -3.16840 | 0.91570 |
| C | -2.61590 | -2.05250 | 0.28790 |
| C | -1.42350 | -1.91220 | 1.24150 |
| C | -3.34830 | -0.76660 | -0.09070 |
| Cl | -0.41040 | -0.46730 | 0.93590 |
| C | -4.61390 | -1.01760 | -0.91900 |
| C | -0.81270 | -4.65220 | -2.73370 |
| Br | -1.97560 | -5.94550 | -0.46160 |
| C | -0.33510 | -5.91390 | -3.40700 |
| C | -1.12760 | -6.72010 | -4.13040 |
| C | -0.58500 | -7.95380 | -4.76950 |
| C | -1.56230 | -8.82350 | -5.51580 |
| O | 0.61040 | -8.23740 | -4.71000 |
| C | -5.71120 | -1.66780 | -0.13060 |
| O | -5.11280 | 0.25000 | -1.35110 |
| C | -6.18480 | -2.86140 | -0.34810 |
| C | -6.65480 | -4.04980 | -0.55620 |
| H | -7.42770 | -4.28910 | -1.27430 |
| Br | -6.05170 | -5.41540 | 0.52360 |
| H | -0.10080 | -2.62190 | -1.07750 |
| H | 0.32320 | -5.08820 | -0.91800 |
| H | -1.09570 | -4.00940 | 1.44890 |
| H | 0.41470 | -3.13450 | 1.20280 |
| H | -3.32240 | -2.75360 | 0.74980 |
| H | -1.73560 | -1.86370 | 2.28830 |
| H | -3.60080 | -0.19410 | 0.81130 |
| H | -2.69270 | -0.12370 | -0.69210 |
| H | -4.37050 | -1.59610 | -1.81780 |
| H | -1.85380 | -4.44060 | -3.00970 |
| H | -0.21200 | -3.82980 | -3.14300 |
| H | 0.72070 | -6.15750 | -3.29250 |
| H | -2.18230 | -6.51100 | -4.26700 |
| H | -1.35660 | -9.87260 | -5.28520 |
| H | -2.59200 | -8.61000 | -5.21670 |
| H | -1.45430 | -8.64920 | -6.58920 |
| H | -6.13310 | -1.08810 | 0.68630 |
| H | -5.86710 | 0.06410 | -1.93810 |

Table S6. Cont.

| Marilzafurollene_A_5 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65540 | -4.68270 | -1.20060 |
| C | -0.63850 | -3.16460 | 0.91510 |
| C | -2.61590 | -2.05260 | 0.28780 |
| C | -1.42240 | -1.90910 | 1.23980 |
| C | -3.35100 | -0.76820 | -0.09060 |
| Cl | -0.41160 | -0.46340 | 0.93040 |
| C | -4.61450 | -1.02080 | -0.92160 |
| C | -0.81890 | -4.65760 | -2.73010 |
| Br | -1.97690 | -5.94420 | -0.45150 |
| C | -0.34110 | -5.91960 | -3.40270 |
| C | -1.13170 | -6.72340 | -4.13080 |
| C | -0.58750 | -7.95530 | -4.77200 |
| C | -1.56010 | -8.81590 | -5.53500 |
| O | 0.60600 | -8.24430 | -4.70170 |
| C | -5.70960 | -1.68150 | -0.13900 |
| O | -5.11920 | 0.24700 | -1.34650 |
| C | -6.19810 | -2.86360 | -0.38440 |
| C | -6.68470 | -4.03980 | -0.62220 |
| H | -7.46200 | -4.24950 | -1.34470 |
| Br | -6.09630 | -5.44230 | 0.41740 |
| H | -0.10110 | -2.62370 | -1.08030 |
| H | 0.32140 | -5.08980 | -0.91590 |
| H | -1.09060 | -4.00510 | 1.45120 |
| H | 0.41780 | -3.12840 | 1.20010 |
| H | -3.32080 | -2.75460 | 0.75090 |
| H | -1.73330 | -1.85920 | 2.28690 |
| H | -3.60610 | -0.19740 | 0.81160 |
| H | -2.69620 | -0.12290 | -0.69020 |
| H | -4.36670 | -1.59240 | -1.82360 |
| H | -1.86100 | -4.44800 | -3.00390 |
| H | -0.22030 | -3.83510 | -3.14230 |
| H | 0.71410 | -6.16460 | -3.28490 |
| H | -2.18540 | -6.51220 | -4.27180 |
| H | -1.43990 | -8.63440 | -6.60590 |
| H | -1.36110 | -9.86740 | -5.30960 |
| H | -2.59210 | -8.60020 | -5.24540 |
| H | -6.12280 | -1.11670 | 0.69270 |
| H | -5.87340 | 0.06120 | -1.93350 |

Table S6. Cont.

| Marilzafurollene_A_6 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65640 | -4.68370 | -1.19860 |
| C | -0.63750 | -3.16280 | 0.91490 |
| C | -2.61590 | -2.05260 | 0.28780 |
| C | -1.42190 | -1.90750 | 1.23890 |
| C | -3.35270 | -0.76920 | -0.09070 |
| Cl | -0.41230 | -0.46150 | 0.92760 |
| C | -4.61610 | -1.02370 | -0.92130 |
| C | -0.81960 | -4.66070 | -2.72810 |
| Br | -1.97990 | -5.94280 | -0.44810 |
| C | -0.34290 | -5.92430 | -3.39860 |
| C | -1.13730 | -6.73440 | -4.11540 |
| C | -0.59560 | -7.96830 | -4.75490 |
| C | -1.57720 | -8.84720 | -5.48450 |
| O | 0.60210 | -8.24470 | -4.70930 |
| C | -5.71020 | -1.68520 | -0.13790 |
| O | -5.12240 | 0.24330 | -1.34670 |
| C | -6.19700 | -2.86830 | -0.38220 |
| C | -6.68190 | -4.04540 | -0.61900 |
| H | -7.45830 | -4.25700 | -1.34180 |
| Br | -6.09620 | -5.44490 | 0.42630 |
| H | -0.10110 | -2.62460 | -1.08160 |
| H | 0.31990 | -5.09150 | -0.91310 |
| H | -1.08850 | -4.00310 | 1.45210 |
| H | 0.41900 | -3.12560 | 1.19900 |
| H | -3.31980 | -2.75510 | 0.75170 |
| H | -1.73220 | -1.85690 | 2.28620 |
| H | -3.60840 | -0.19860 | 0.81160 |
| H | -2.69890 | -0.12320 | -0.69050 |
| H | -4.36800 | -1.59550 | -1.82300 |
| H | -1.86150 | -4.45060 | -3.00240 |
| H | -0.22040 | -3.83940 | -3.14180 |
| H | 0.71410 | -6.16490 | -3.28920 |
| H | -2.19330 | -6.52830 | -4.24650 |
| H | -1.35830 | -9.89430 | -5.25700 |
| H | -2.60360 | -8.64280 | -5.16780 |
| H | -1.48890 | -8.67240 | -6.55960 |
| H | -6.12450 | -1.12010 | 0.69300 |
| H | -5.87680 | 0.05630 | -1.93300 |

Table S6. Cont.

| Marilzafurollene_A_7 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65340 | -4.68110 | -1.20370 |
| C | -0.64060 | -3.16770 | 0.91560 |
| C | -2.61590 | -2.05250 | 0.28780 |
| C | -1.42320 | -1.91160 | 1.24120 |
| C | -3.34900 | -0.76690 | -0.09070 |
| Cl | -0.41060 | -0.46660 | 0.93480 |
| C | -4.61350 | -1.01820 | -0.92060 |
| C | -0.81540 | -4.65280 | -2.73330 |
| Br | -1.97400 | -5.94580 | -0.45870 |
| C | -0.33630 | -5.91310 | -3.40810 |
| C | -1.12600 | -6.71670 | -4.13740 |
| C | -0.58060 | -7.94700 | -4.78070 |
| C | -1.55310 | -8.80820 | -5.54300 |
| O | 0.61370 | -8.23350 | -4.71320 |
| C | -5.71030 | -1.67250 | -0.13510 |
| O | -5.11430 | 0.24970 | -1.34990 |
| C | -6.18690 | -2.86320 | -0.36130 |
| C | -6.65990 | -4.04890 | -0.57860 |
| H | -7.43360 | -4.28060 | -1.29820 |
| Br | -6.05780 | -5.42490 | 0.48840 |
| H | -0.10090 | -2.62220 | -1.07800 |
| H | 0.32360 | -5.08780 | -0.91910 |
| H | -1.09490 | -4.00860 | 1.44940 |
| H | 0.41520 | -3.13340 | 1.20240 |
| H | -3.32210 | -2.75380 | 0.75000 |
| H | -1.73510 | -1.86290 | 2.28810 |
| H | -3.60270 | -0.19530 | 0.81140 |
| H | -2.69330 | -0.12320 | -0.69100 |
| H | -4.36810 | -1.59380 | -1.82070 |
| H | -1.85740 | -4.44310 | -3.00770 |
| H | -0.21690 | -3.82910 | -3.14320 |
| H | 0.71920 | -6.15700 | -3.29100 |
| H | -2.18010 | -6.50680 | -4.27780 |
| H | -1.44800 | -8.61200 | -6.61290 |
| H | -1.34040 | -9.86030 | -5.33360 |
| H | -2.58360 | -8.60740 | -5.23740 |
| H | -6.13080 | -1.09780 | 0.68620 |
| H | -5.86820 | 0.06410 | -1.93730 |

Table S6. Cont.

| Marilzafurollene_A_8 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65200 | -4.68000 | -1.20590 |
| C | -0.64190 | -3.17010 | 0.91590 |
| C | -2.61590 | -2.05250 | 0.28790 |
| C | -1.42390 | -1.91390 | 1.24240 |
| C | -3.34670 | -0.76550 | -0.09040 |
| Cl | -0.40990 | -0.46910 | 0.93920 |
| C | -4.61210 | -1.01430 | -0.91970 |
| C | -0.81310 | -4.64940 | -2.73550 |
| Br | -1.97180 | -5.94710 | -0.46360 |
| C | -0.33170 | -5.90800 | -3.41190 |
| C | -1.11950 | -6.71110 | -4.14370 |
| C | -0.57180 | -7.93970 | -4.78840 |
| C | -1.54200 | -8.79960 | -5.55520 |
| O | 0.62250 | -8.22570 | -4.71860 |
| C | -5.71040 | -1.66460 | -0.13280 |
| O | -5.10970 | 0.25440 | -1.35010 |
| C | -6.18940 | -2.85480 | -0.35690 |
| C | -6.66400 | -4.04020 | -0.57180 |
| H | -7.43960 | -4.27220 | -1.28930 |
| Br | -6.05320 | -5.41700 | 0.48910 |
| H | -0.10080 | -2.62100 | -1.07630 |
| H | 0.32520 | -5.08620 | -0.92130 |
| H | -1.09740 | -4.01130 | 1.44800 |
| H | 0.41370 | -3.13690 | 1.20370 |
| H | -3.32350 | -2.75310 | 0.74890 |
| H | -1.73680 | -1.86630 | 2.28910 |
| H | -3.59890 | -0.19320 | 0.81170 |
| H | -2.69000 | -0.12310 | -0.69110 |
| H | -4.36870 | -1.59160 | -1.81920 |
| H | -1.85520 | -4.44090 | -3.01020 |
| H | -0.21550 | -3.82420 | -3.14370 |
| H | 0.72390 | -6.15110 | -3.29360 |
| H | -2.17360 | -6.50210 | -4.28550 |
| H | -1.32620 | -9.85220 | -5.35160 |
| H | -2.57290 | -8.60340 | -5.24830 |
| H | -1.43750 | -8.59740 | -6.62400 |
| H | -6.12850 | -1.08810 | 0.68840 |
| H | -5.86480 | 0.07010 | -1.93650 |

Table S6. Cont.

| Marilzafurollene_A_9 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65520 | -4.68260 | -1.20090 |
| C | -0.63890 | -3.16490 | 0.91520 |
| C | -2.61590 | -2.05250 | 0.28780 |
| C | -1.42240 | -1.90910 | 1.23970 |
| C | -3.35140 | -0.76840 | -0.09080 |
| Cl | -0.41150 | -0.46360 | 0.93010 |
| C | -4.61550 | -1.02220 | -0.92060 |
| C | -0.81850 | -4.65750 | -2.73030 |
| Br | -1.97680 | -5.94400 | -0.45190 |
| C | -0.34240 | -5.92030 | -3.40250 |
| C | -1.13470 | -6.72440 | -4.12860 |
| C | -0.59230 | -7.95730 | -4.76940 |
| C | -1.56630 | -8.81670 | -5.53200 |
| O | 0.60090 | -8.24760 | -4.69960 |
| C | -5.71110 | -1.67870 | -0.13510 |
| O | -5.11890 | 0.24470 | -1.34960 |
| C | -6.18980 | -2.86770 | -0.36580 |
| C | -6.66480 | -4.05160 | -0.58780 |
| H | -7.43900 | -4.27930 | -1.30830 |
| Br | -6.06300 | -5.43310 | 0.47210 |
| H | -0.10100 | -2.62360 | -1.08010 |
| H | 0.32160 | -5.08970 | -0.91610 |
| H | -1.09160 | -4.00530 | 1.45100 |
| H | 0.41720 | -3.12920 | 1.20060 |
| H | -3.32060 | -2.75460 | 0.75110 |
| H | -1.73330 | -1.85910 | 2.28690 |
| H | -3.60610 | -0.19710 | 0.81130 |
| H | -2.69710 | -0.12340 | -0.69130 |
| H | -4.36910 | -1.59720 | -1.82070 |
| H | -1.86030 | -4.44650 | -3.00420 |
| H | -0.21880 | -3.83590 | -3.14260 |
| H | 0.71270 | -6.16590 | -3.28610 |
| H | -2.18860 | -6.51270 | -4.26830 |
| H | -2.59720 | -8.60670 | -5.23440 |
| H | -1.45320 | -8.62810 | -6.60250 |
| H | -1.36210 | -9.86890 | -5.31460 |
| H | -6.13030 | -1.10630 | 0.68850 |
| H | -5.87360 | 0.05780 | -1.93550 |

Table S6. Cont.

| Marilzafurollene_A_10 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65620 | -4.68380 | -1.19820 |
| C | -0.63730 | -3.16240 | 0.91480 |
| C | -2.61590 | -2.05260 | 0.28780 |
| C | -1.42190 | -1.90720 | 1.23870 |
| C | -3.35330 | -0.76940 | -0.09040 |
| Cl | -0.41230 | -0.46110 | 0.92700 |
| C | -4.61600 | -1.02390 | -0.92190 |
| C | -0.81960 | -4.66170 | -2.72770 |
| Br | -1.97880 | -5.94330 | -0.44700 |
| C | -0.34550 | -5.92710 | -3.39660 |
| C | -1.14110 | -6.73590 | -4.11350 |
| C | -0.60210 | -7.97320 | -4.74840 |
| C | -1.58320 | -8.84710 | -5.48470 |
| O | 0.59360 | -8.25670 | -4.69330 |
| C | -5.70950 | -1.68870 | -0.14060 |
| O | -5.12380 | 0.24330 | -1.34500 |
| C | -6.19580 | -2.87110 | -0.38880 |
| C | -6.68020 | -4.04770 | -0.62950 |
| H | -7.45620 | -4.25720 | -1.35330 |
| Br | -6.09690 | -5.44970 | 0.41380 |
| H | -0.10120 | -2.62470 | -1.08190 |
| H | 0.32020 | -5.09120 | -0.91280 |
| H | -1.08830 | -4.00270 | 1.45230 |
| H | 0.41910 | -3.12520 | 1.19900 |
| H | -3.31950 | -2.75520 | 0.75190 |
| H | -1.73200 | -1.85650 | 2.28610 |
| H | -3.60970 | -0.19950 | 0.81210 |
| H | -2.69950 | -0.12250 | -0.68940 |
| H | -4.36650 | -1.59340 | -1.82480 |
| H | -1.86120 | -4.45000 | -3.00200 |
| H | -0.21900 | -3.84190 | -3.14210 |
| H | 0.71050 | -6.17110 | -3.28430 |
| H | -2.19610 | -6.52640 | -4.24740 |
| H | -1.47770 | -8.68210 | -6.55980 |
| H | -1.37930 | -9.89460 | -5.24560 |
| H | -2.61170 | -8.62850 | -5.18490 |
| H | -6.12440 | -1.12640 | 0.69190 |
| H | -5.87770 | 0.05640 | -1.93200 |

Table S6. Cont.

| Marilzafurollene_A_11 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83220 | -3.28330 | -0.59430 |
| O | -2.12490 | -2.71510 | -0.89900 |
| C | -0.67780 | -4.70800 | -1.14950 |
| C | -0.61620 | -3.12110 | 0.90960 |
| C | -2.61600 | -2.05240 | 0.28810 |
| C | -1.41080 | -1.86810 | 1.21600 |
| C | -3.38430 | -0.79070 | -0.09970 |
| Cl | -0.42980 | -0.41520 | 0.84930 |
| C | -4.67890 | -1.09190 | -0.86620 |
| C | -0.83930 | -4.79410 | -2.67600 |
| Br | -2.02390 | -5.92120 | -0.36120 |
| C | 0.26100 | -4.09010 | -3.42430 |
| C | 0.05620 | -3.04570 | -4.24180 |
| C | 1.19520 | -2.39670 | -4.95330 |
| C | 0.86380 | -1.24940 | -5.87080 |
| O | 2.35570 | -2.76480 | -4.77830 |
| C | -5.75280 | -1.66760 | 0.00620 |
| O | -5.20190 | 0.13750 | -1.37450 |
| C | -6.13690 | -2.91230 | 0.00670 |
| C | -6.52040 | -4.14900 | 0.01400 |
| H | -7.24560 | -4.57160 | -0.66830 |
| Br | -5.87370 | -5.24260 | 1.34840 |
| H | -0.10170 | -2.64120 | -1.10230 |
| H | 0.28670 | -5.12900 | -0.84320 |
| H | -1.04650 | -3.95420 | 1.47460 |
| H | 0.44400 | -3.06370 | 1.17610 |
| H | -3.29540 | -2.76460 | 0.77180 |
| H | -1.70480 | -1.79540 | 2.26660 |
| H | -3.61220 | -0.19430 | 0.79320 |
| H | -2.76110 | -0.15860 | -0.74510 |
| H | -4.48550 | -1.74440 | -1.72560 |
| H | -0.82200 | -5.84530 | -2.99270 |
| H | -1.82090 | -4.40570 | -2.97770 |
| H | 1.26980 | -4.47890 | -3.28720 |
| H | -0.93370 | -2.63610 | -4.40800 |
| H | 1.08780 | -0.30660 | -5.36580 |
| H | 1.46140 | -1.33580 | -6.78270 |
| H | -0.19100 | -1.26440 | -6.15840 |
| H | -6.24510 | -0.97860 | 0.68720 |
| H | -4.57510 | 0.44880 | -2.05060 |

Table S6. Cont.

| Marilzafurollene_A_12 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83300 | -3.28300 | -0.59430 |
| O | -2.12440 | -2.71530 | -0.89880 |
| C | -0.66530 | -4.69380 | -1.17750 |
| C | -0.62570 | -3.14050 | 0.91180 |
| C | -2.61580 | -2.05260 | 0.28790 |
| C | -1.41500 | -1.88570 | 1.22590 |
| C | -3.36830 | -0.78130 | -0.09940 |
| Cl | -0.42030 | -0.43660 | 0.88100 |
| C | -4.64540 | -1.06210 | -0.90210 |
| C | -0.82990 | -4.69290 | -2.70700 |
| Br | -1.99620 | -5.93300 | -0.40710 |
| C | -0.36300 | -5.97030 | -3.35770 |
| C | -1.16310 | -6.78470 | -4.06330 |
| C | -0.63050 | -8.03370 | -4.68080 |
| C | -1.61660 | -8.91250 | -5.40450 |
| O | 0.56370 | -8.32230 | -4.62230 |
| C | -5.73610 | -1.66820 | -0.07250 |
| O | -5.16060 | 0.18120 | -1.38380 |
| C | -6.13420 | -2.90650 | -0.14180 |
| C | -6.53280 | -4.13670 | -0.20750 |
| H | -7.24970 | -4.51240 | -0.92510 |
| Br | -5.93690 | -5.30570 | 1.08590 |
| H | -0.10210 | -2.63460 | -1.09620 |
| H | 0.30880 | -5.10310 | -0.88690 |
| H | -1.06630 | -3.97690 | 1.46400 |
| H | 0.43280 | -3.09300 | 1.18650 |
| H | -3.30670 | -2.75960 | 0.76320 |
| H | -1.71550 | -1.82170 | 2.27530 |
| H | -3.61330 | -0.19650 | 0.79660 |
| H | -2.72750 | -0.14290 | -0.72090 |
| H | -4.43080 | -1.68720 | -1.77680 |
| H | -1.87050 | -4.47940 | -2.98360 |
| H | -0.22500 | -3.88260 | -3.13370 |
| H | 0.69150 | -6.21880 | -3.24190 |
| H | -2.21690 | -6.57150 | -4.20060 |
| H | -1.41050 | -9.95850 | -5.16050 |
| H | -2.64280 | -8.69260 | -5.09790 |
| H | -1.51910 | -8.75420 | -6.48140 |
| H | -6.23280 | -1.00770 | 0.63300 |
| H | -4.52450 | 0.50910 | -2.04330 |

Table S6. Cont.

| Marilzafurollene_A_13 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83280 | -3.28320 | -0.59480 |
| O | -2.12440 | -2.71480 | -0.89750 |
| C | -0.66170 | -4.68740 | -1.19590 |
| C | -0.63250 | -3.15690 | 0.91460 |
| C | -2.61600 | -2.05280 | 0.28710 |
| C | -1.42350 | -1.90650 | 1.24060 |
| C | -3.35720 | -0.77050 | -0.08590 |
| Cl | -0.41740 | -0.45600 | 0.94120 |
| C | -4.57120 | -1.00800 | -0.99150 |
| C | -0.91470 | -4.74650 | -2.71150 |
| Br | -1.91030 | -5.97450 | -0.36450 |
| C | 0.06000 | -3.92520 | -3.51150 |
| C | -0.29980 | -2.86700 | -4.25460 |
| C | 0.71230 | -2.09560 | -5.03160 |
| C | 0.20050 | -0.96630 | -5.88660 |
| O | 1.91240 | -2.35450 | -4.95850 |
| C | -5.66760 | -1.78930 | -0.33180 |
| O | -5.11650 | 0.26900 | -1.33050 |
| C | -6.23590 | -2.84630 | -0.83850 |
| C | -6.80450 | -3.89080 | -1.35100 |
| H | -7.69810 | -3.86630 | -1.96030 |
| Br | -5.97110 | -5.52000 | -1.14440 |
| H | -0.10250 | -2.62250 | -1.07940 |
| H | 0.33380 | -5.07860 | -0.95700 |
| H | -1.07600 | -3.99550 | 1.45990 |
| H | 0.42500 | -3.11380 | 1.19440 |
| H | -3.32120 | -2.75580 | 0.74900 |
| H | -1.73660 | -1.86180 | 2.28740 |
| H | -3.66420 | -0.23480 | 0.82170 |
| H | -2.68800 | -0.09210 | -0.63040 |
| H | -4.25180 | -1.48430 | -1.92590 |
| H | -0.82670 | -5.78400 | -3.06030 |
| H | -1.94580 | -4.44330 | -2.93680 |
| H | 1.10400 | -4.23490 | -3.47930 |
| H | -1.33030 | -2.53450 | -4.31190 |
| H | 0.34070 | -0.02010 | -5.35830 |
| H | 0.75270 | -0.95230 | -6.83040 |
| H | -0.85960 | -1.09800 | -6.12090 |
| H | -6.04020 | -1.40750 | 0.61480 |
| H | -5.86080 | 0.10000 | -1.93500 |

Table S6. Cont.

| Marilzafurollene_A_14 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83270 | -3.28290 | -0.59370 |
| O | -2.12550 | -2.71470 | -0.89870 |
| C | -0.68640 | -4.71060 | -1.14370 |
| C | -0.61390 | -3.11560 | 0.90970 |
| C | -2.61490 | -2.05320 | 0.28730 |
| C | -1.41050 | -1.86310 | 1.21520 |
| C | -3.41000 | -0.80410 | -0.08330 |
| Cl | -0.42950 | -0.41150 | 0.84880 |
| C | -4.61740 | -1.08860 | -0.98650 |
| C | -0.85420 | -4.80070 | -2.66950 |
| Br | -2.04160 | -5.91160 | -0.34720 |
| C | 0.24160 | -4.09670 | -3.42420 |
| C | 0.03380 | -3.04030 | -4.22550 |
| C | 1.16800 | -2.38960 | -4.94310 |
| C | 0.83460 | -1.22040 | -5.83180 |
| O | 2.32690 | -2.77440 | -4.79540 |
| C | -5.63190 | -2.01510 | -0.37310 |
| O | -5.23040 | 0.16470 | -1.29870 |
| C | -6.63430 | -1.66990 | 0.38500 |
| C | -7.63080 | -1.32310 | 1.13580 |
| H | -7.55500 | -1.08680 | 2.18860 |
| Br | -9.29190 | -1.17810 | 0.35200 |
| H | -0.10170 | -2.64440 | -1.10530 |
| H | 0.27600 | -5.13680 | -0.83820 |
| H | -1.04050 | -3.94830 | 1.47810 |
| H | 0.44690 | -3.05580 | 1.17350 |
| H | -3.28630 | -2.77280 | 0.77360 |
| H | -1.70490 | -1.79080 | 2.26580 |
| H | -3.73700 | -0.28410 | 0.82640 |
| H | -2.77220 | -0.09550 | -0.62670 |
| H | -4.27880 | -1.51790 | -1.93630 |
| H | -0.83760 | -5.85270 | -2.98370 |
| H | -1.83740 | -4.41410 | -2.96830 |
| H | 1.24920 | -4.49450 | -3.30500 |
| H | -0.95490 | -2.61990 | -4.37150 |
| H | 1.40950 | -1.29970 | -6.75880 |
| H | -0.22660 | -1.21260 | -6.09490 |
| H | 1.08580 | -0.29090 | -5.31510 |
| H | -5.44970 | -3.07730 | -0.51990 |
| H | -6.08660 | -0.03430 | -1.71680 |

Table S6. Cont.

| Marilzafurollene_A_15 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59450 |
| O | -2.12400 | -2.71540 | -0.89850 |
| C | -0.65630 | -4.68220 | -1.20310 |
| C | -0.63930 | -3.16510 | 0.91520 |
| C | -2.61590 | -2.05250 | 0.28790 |
| C | -1.42220 | -1.90870 | 1.23930 |
| C | -3.35180 | -0.76890 | -0.09160 |
| Cl | -0.41120 | -0.46360 | 0.92810 |
| C | -4.62080 | -1.02550 | -0.91320 |
| C | -0.81480 | -4.65250 | -2.73400 |
| Br | -1.97820 | -5.94210 | -0.45290 |
| C | -0.34280 | -5.91610 | -3.41550 |
| C | 0.72660 | -5.96170 | -4.22500 |
| C | 1.21360 | -7.18440 | -4.92410 |
| C | 0.47760 | -8.48740 | -4.75450 |
| O | 2.21880 | -7.09680 | -5.63020 |
| C | -5.71560 | -1.66780 | -0.11490 |
| O | -5.12030 | 0.23900 | -1.35360 |
| C | -6.18560 | -2.86590 | -0.31460 |
| C | -6.65140 | -4.05920 | -0.50380 |
| H | -7.42420 | -4.31270 | -1.21700 |
| Br | -6.04330 | -5.40420 | 0.59880 |
| H | -0.10080 | -2.62320 | -1.07910 |
| H | 0.32050 | -5.08980 | -0.91920 |
| H | -1.09250 | -4.00530 | 1.45100 |
| H | 0.41680 | -3.12980 | 1.20080 |
| H | -3.32000 | -2.75470 | 0.75160 |
| H | -1.73270 | -1.85790 | 2.28660 |
| H | -3.60130 | -0.19380 | 0.80950 |
| H | -2.69970 | -0.12730 | -0.69800 |
| H | -4.38160 | -1.61150 | -1.80830 |
| H | -1.86180 | -4.48210 | -3.01530 |
| H | -0.24870 | -3.80090 | -3.13370 |
| H | -0.93890 | -6.80640 | -3.23010 |
| H | 1.32150 | -5.07500 | -4.42480 |
| H | 0.49300 | -8.79480 | -3.70570 |
| H | -0.54970 | -8.38970 | -5.11500 |
| H | 0.97520 | -9.26210 | -5.34600 |
| H | -6.13830 | -1.07800 | 0.69440 |
| H | -5.87540 | 0.04900 | -1.93810 |

Table S6. Cont.

| Marilzafurollene_A_16 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83250 | -3.28330 | -0.59440 |
| O | -2.12480 | -2.71480 | -0.89820 |
| C | -0.67920 | -4.70420 | -1.15970 |
| C | -0.61990 | -3.12970 | 0.91080 |
| C | -2.61580 | -2.05270 | 0.28740 |
| C | -1.41470 | -1.87810 | 1.22300 |
| C | -3.38340 | -0.78730 | -0.09010 |
| Cl | -0.42860 | -0.42460 | 0.87730 |
| C | -4.64570 | -1.07220 | -0.91840 |
| C | -0.85750 | -4.78150 | -2.68500 |
| Br | -2.01650 | -5.92600 | -0.36550 |
| C | 0.22060 | -4.05300 | -3.44210 |
| C | -0.01150 | -2.99010 | -4.22800 |
| C | 1.10460 | -2.31390 | -4.95020 |
| C | 0.74610 | -1.13860 | -5.82120 |
| O | 2.27010 | -2.68640 | -4.82380 |
| C | -5.73940 | -1.83710 | -0.22710 |
| O | -5.20430 | 0.17460 | -1.34050 |
| C | -6.06060 | -1.75630 | 1.03370 |
| C | -6.38350 | -1.66880 | 2.28500 |
| H | -6.20890 | -2.44420 | 3.01920 |
| Br | -6.93110 | -0.02510 | 2.91450 |
| H | -0.10130 | -2.63780 | -1.09700 |
| H | 0.28910 | -5.12490 | -0.86560 |
| H | -1.05150 | -3.96540 | 1.47080 |
| H | 0.43990 | -3.07460 | 1.17980 |
| H | -3.29980 | -2.76650 | 0.76330 |
| H | -1.71490 | -1.81480 | 2.27260 |
| H | -3.64180 | -0.21470 | 0.80960 |
| H | -2.74820 | -0.12970 | -0.69760 |
| H | -4.36620 | -1.61280 | -1.82960 |
| H | -0.82740 | -5.82990 | -3.00980 |
| H | -1.84910 | -4.40750 | -2.97210 |
| H | 1.23490 | -4.43750 | -3.33830 |
| H | -1.00820 | -2.58330 | -4.35750 |
| H | 1.06660 | -0.21590 | -5.33090 |
| H | 1.24760 | -1.24300 | -6.78730 |
| H | -0.33080 | -1.09110 | -6.00350 |
| H | -6.43230 | -2.34860 | -0.89120 |
| H | -5.55990 | 0.61030 | -0.54550 |

Table S6. Cont.

| Marilzafurollene_A_17 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59460 |
| O | -2.12400 | -2.71540 | -0.89840 |
| C | -0.65580 | -4.68260 | -1.20130 |
| C | -0.63870 | -3.16440 | 0.91500 |
| C | -2.61590 | -2.05250 | 0.28780 |
| C | -1.42220 | -1.90840 | 1.23920 |
| C | -3.35220 | -0.76900 | -0.09130 |
| Cl | -0.41120 | -0.46320 | 0.92810 |
| C | -4.61610 | -1.02410 | -0.92100 |
| C | -0.81750 | -4.65660 | -2.73140 |
| Br | -1.97470 | -5.94530 | -0.45270 |
| C | -0.36130 | -5.92820 | -3.40750 |
| C | -1.17000 | -6.68920 | -4.16140 |
| C | -0.76070 | -7.94490 | -4.85080 |
| C | 0.64780 | -8.45640 | -4.69870 |
| O | -1.59270 | -8.53890 | -5.53750 |
| C | -5.71190 | -1.67910 | -0.13470 |
| O | -5.11910 | 0.24210 | -1.35270 |
| C | -6.17930 | -2.87500 | -0.35290 |
| C | -6.64360 | -4.06560 | -0.56220 |
| H | -7.40920 | -4.30890 | -1.28660 |
| Br | -6.06460 | -5.42170 | 0.54270 |
| H | -0.10120 | -2.62380 | -1.08050 |
| H | 0.32140 | -5.08930 | -0.91750 |
| H | -1.09120 | -4.00470 | 1.45110 |
| H | 0.41750 | -3.12840 | 1.20010 |
| H | -3.32000 | -2.75480 | 0.75160 |
| H | -1.73260 | -1.85770 | 2.28650 |
| H | -3.60720 | -0.19730 | 0.81050 |
| H | -2.69820 | -0.12400 | -0.69210 |
| H | -4.36950 | -1.60080 | -1.82010 |
| H | -1.85560 | -4.42740 | -3.00470 |
| H | -0.20380 | -3.84450 | -3.14220 |
| H | 0.68230 | -6.19460 | -3.26060 |
| H | -2.21170 | -6.42130 | -4.31470 |
| H | 1.35680 | -7.73480 | -5.11260 |
| H | 0.86560 | -8.65400 | -3.64590 |
| H | 0.75180 | -9.39550 | -5.25070 |
| H | -6.14150 | -1.09950 | 0.67830 |
| H | -5.87060 | 0.05380 | -1.94240 |

Table S6. Cont.

| Marilzafurollene_A_18 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83300 | -3.28290 | -0.59430 |
| O | -2.12430 | -2.71530 | -0.89880 |
| C | -0.66610 | -4.69310 | -1.18050 |
| C | -0.62600 | -3.14110 | 0.91190 |
| C | -2.61570 | -2.05260 | 0.28790 |
| C | -1.41500 | -1.88600 | 1.22600 |
| C | -3.36850 | -0.78130 | -0.09930 |
| Cl | -0.41990 | -0.43730 | 0.88090 |
| C | -4.64610 | -1.06230 | -0.90110 |
| C | -0.83050 | -4.68760 | -2.71100 |
| Br | -1.99260 | -5.93290 | -0.40490 |
| C | -0.36620 | -5.96390 | -3.37370 |
| C | 0.69930 | -6.02650 | -4.18720 |
| C | 1.17930 | -7.26200 | -4.86840 |
| C | 0.44010 | -8.55980 | -4.67420 |
| O | 2.18160 | -7.18900 | -5.58030 |
| C | -5.73670 | -1.66720 | -0.07040 |
| O | -5.16100 | 0.18090 | -1.38340 |
| C | -6.12900 | -2.90790 | -0.13200 |
| C | -6.52110 | -4.14050 | -0.18980 |
| H | -7.23410 | -4.52510 | -0.90660 |
| Br | -5.92340 | -5.29660 | 1.11440 |
| H | -0.10200 | -2.63390 | -1.09510 |
| H | 0.30950 | -5.10150 | -0.89370 |
| H | -1.06690 | -3.97730 | 1.46400 |
| H | 0.43250 | -3.09390 | 1.18670 |
| H | -3.30650 | -2.75970 | 0.76320 |
| H | -1.71550 | -1.82190 | 2.27540 |
| H | -3.61280 | -0.19620 | 0.79660 |
| H | -2.72790 | -0.14320 | -0.72140 |
| H | -4.43250 | -1.68820 | -1.77540 |
| H | -1.87790 | -4.51730 | -2.99110 |
| H | -0.26240 | -3.84500 | -3.12660 |
| H | -0.96430 | -6.84910 | -3.17080 |
| H | 1.29630 | -5.14520 | -4.40430 |
| H | 0.46050 | -8.85060 | -3.62080 |
| H | -0.58880 | -8.46440 | -5.03040 |
| H | 0.93190 | -9.34520 | -5.25620 |
| H | -6.23790 | -1.00410 | 0.62940 |
| H | -4.52670 | 0.50630 | -2.04600 |

Table S6. Cont.

| Marilzafurollene_A_19 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83300 | -3.28290 | -0.59430 |
| O | -2.12430 | -2.71530 | -0.89870 |
| C | -0.66710 | -4.69510 | -1.17540 |
| C | -0.62410 | -3.13720 | 0.91130 |
| C | -2.61580 | -2.05260 | 0.28790 |
| C | -1.41400 | -1.88230 | 1.22380 |
| C | -3.37220 | -0.78360 | -0.09960 |
| Cl | -0.42100 | -0.43330 | 0.87370 |
| C | -4.64930 | -1.06850 | -0.90090 |
| C | -0.83240 | -4.69650 | -2.70530 |
| Br | -1.99460 | -5.93310 | -0.40030 |
| C | -0.38830 | -5.98420 | -3.35850 |
| C | -1.20430 | -6.75130 | -4.09820 |
| C | -0.80710 | -8.02310 | -4.76490 |
| C | 0.59590 | -8.54620 | -4.60170 |
| O | -1.64410 | -8.62030 | -5.44250 |
| C | -5.73830 | -1.67620 | -0.07010 |
| O | -5.16760 | 0.17320 | -1.38360 |
| C | -6.12010 | -2.92040 | -0.12380 |
| C | -6.50160 | -4.15680 | -0.17300 |
| H | -7.20770 | -4.55360 | -0.89000 |
| Br | -5.91080 | -5.29330 | 1.15150 |
| H | -0.10240 | -2.63620 | -1.09860 |
| H | 0.30770 | -5.10390 | -0.88630 |
| H | -1.06330 | -3.97280 | 1.46560 |
| H | 0.43480 | -3.08830 | 1.18450 |
| H | -3.30410 | -2.76080 | 0.76510 |
| H | -1.71290 | -1.81610 | 2.27350 |
| H | -3.61780 | -0.19880 | 0.79620 |
| H | -2.73370 | -0.14390 | -0.72220 |
| H | -4.43430 | -1.69410 | -1.77500 |
| H | -1.86930 | -4.46390 | -2.98050 |
| H | -0.21300 | -3.89740 | -3.13270 |
| H | 0.65300 | -6.25760 | -3.20720 |
| H | -2.24360 | -6.47650 | -4.25630 |
| H | 0.68920 | -9.49890 | -5.13200 |
| H | 1.31230 | -7.84190 | -5.03220 |
| H | 0.81240 | -8.72230 | -3.54480 |
| H | -6.24780 | -1.01200 | 0.62280 |
| H | -4.53520 | 0.49920 | -2.04760 |

Table S6. Cont.

| Marilzafurollene_A_20 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83390 | -3.28370 | -0.59780 |
| O | -2.12020 | -2.71610 | -0.89470 |
| C | -0.51190 | -4.51160 | -1.46060 |
| C | -0.82940 | -3.47540 | 0.91230 |
| C | -2.61910 | -2.05110 | 0.28730 |
| C | -1.55000 | -2.22050 | 1.37820 |
| C | -3.02480 | -0.63070 | -0.10620 |
| Cl | -0.39070 | -0.85930 | 1.49450 |
| C | -4.23680 | -0.62220 | -1.04960 |
| C | -0.30640 | -4.18440 | -2.95700 |
| Br | -1.87990 | -5.91050 | -1.27570 |
| C | -1.45480 | -3.49000 | -3.64870 |
| C | -1.49570 | -2.16250 | -3.84640 |
| C | -2.68420 | -1.44530 | -4.37870 |
| C | -3.66830 | -2.17840 | -5.25100 |
| O | -2.85330 | -0.26670 | -4.05650 |
| C | -5.53440 | -0.73730 | -0.30700 |
| O | -4.27350 | 0.62620 | -1.74160 |
| C | -6.27700 | -1.80610 | -0.25190 |
| C | -7.01560 | -2.86830 | -0.19800 |
| H | -7.86680 | -3.05730 | -0.83840 |
| Br | -6.54760 | -4.18620 | 1.00140 |
| H | -0.09100 | -2.51420 | -0.84880 |
| H | 0.40390 | -4.98340 | -1.08590 |
| H | -1.42230 | -4.34910 | 1.20430 |
| H | 0.17740 | -3.59890 | 1.32260 |
| H | -3.50280 | -2.61940 | 0.59930 |
| H | -1.99510 | -2.33270 | 2.37080 |
| H | -3.23800 | -0.02760 | 0.78520 |
| H | -2.19160 | -0.14050 | -0.62680 |
| H | -4.16480 | -1.41320 | -1.80440 |
| H | 0.59510 | -3.56350 | -3.04770 |
| H | -0.08520 | -5.10470 | -3.51300 |
| H | -2.29750 | -4.12130 | -3.92050 |
| H | -0.69160 | -1.51440 | -3.51220 |
| H | -3.14920 | -2.85800 | -5.93230 |
| H | -4.37390 | -2.73160 | -4.62620 |
| H | -4.21620 | -1.45350 | -5.86030 |
| H | -5.85850 | 0.14490 | 0.23820 |
| H | -3.70750 | 0.50780 | -2.53690 |

Table S6. Cont.

| Marilzafurollene_A_21 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83280 | -3.28330 | -0.59490 |
| O | -2.12400 | -2.71520 | -0.89800 |
| C | -0.66220 | -4.68850 | -1.19210 |
| C | -0.63850 | -3.16270 | 0.91540 |
| C | -2.61640 | -2.05230 | 0.28780 |
| C | -1.42420 | -1.90860 | 1.24070 |
| C | -3.35200 | -0.76860 | -0.09200 |
| Cl | -0.41560 | -0.46080 | 0.93710 |
| C | -4.62020 | -1.02510 | -0.91470 |
| C | -0.83080 | -4.73280 | -2.72010 |
| Br | -1.98670 | -5.94380 | -0.43410 |
| C | 0.26340 | -4.00700 | -3.46270 |
| C | 0.03510 | -2.93830 | -4.24180 |
| C | 1.07840 | -2.20510 | -5.01260 |
| C | 2.51360 | -2.65710 | -4.94470 |
| O | 0.73740 | -1.23870 | -5.69520 |
| C | -5.71600 | -1.66700 | -0.11740 |
| O | -5.11940 | 0.23950 | -1.35510 |
| C | -6.18560 | -2.86520 | -0.31670 |
| C | -6.65150 | -4.05860 | -0.50520 |
| H | -7.42210 | -4.31290 | -1.22050 |
| Br | -6.05580 | -5.39980 | 0.60890 |
| H | -0.10010 | -2.62290 | -1.07590 |
| H | 0.30910 | -5.10530 | -0.90230 |
| H | -1.08850 | -4.00340 | 1.45280 |
| H | 0.41790 | -3.12480 | 1.19990 |
| H | -3.32100 | -2.75450 | 0.75090 |
| H | -1.73670 | -1.86150 | 2.28750 |
| H | -3.60230 | -0.19370 | 0.80900 |
| H | -2.69930 | -0.12700 | -0.69780 |
| H | -4.38020 | -1.61100 | -1.80960 |
| H | -0.81160 | -5.77520 | -3.06510 |
| H | -1.81650 | -4.34250 | -3.00560 |
| H | 1.26400 | -4.41780 | -3.35190 |
| H | -0.96640 | -2.53220 | -4.35820 |
| H | 2.60600 | -3.67630 | -5.32850 |
| H | 3.12840 | -1.99960 | -5.56690 |
| H | 2.87960 | -2.59510 | -3.91660 |
| H | -6.14060 | -1.07610 | 0.69000 |
| H | -5.86840 | 0.04930 | -1.94740 |

Table S6. Cont.

| Marilzafurollene_A_22 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83270 | -3.28320 | -0.59460 |
| O | -2.12430 | -2.71520 | -0.89840 |
| C | -0.66560 | -4.69290 | -1.18240 |
| C | -0.63140 | -3.14950 | 0.91370 |
| C | -2.61610 | -2.05240 | 0.28780 |
| C | -1.41890 | -1.89460 | 1.23190 |
| C | -3.36050 | -0.77630 | -0.09930 |
| Cl | -0.41860 | -0.44590 | 0.90290 |
| C | -4.63360 | -1.04780 | -0.91140 |
| C | -0.84260 | -4.74810 | -2.70920 |
| Br | -1.98550 | -5.94280 | -0.40830 |
| C | 0.23100 | -4.00110 | -3.46080 |
| C | -0.02590 | -2.93650 | -4.23650 |
| C | 0.99640 | -2.17430 | -5.00680 |
| C | 2.44280 | -2.58880 | -4.94220 |
| O | 0.62880 | -1.21350 | -5.68350 |
| C | -5.73230 | -1.65370 | -0.09220 |
| O | -5.14050 | 0.20010 | -1.39000 |
| C | -6.12740 | -2.89300 | -0.16290 |
| C | -6.52200 | -4.12440 | -0.22990 |
| H | -7.23030 | -4.50370 | -0.95410 |
| Br | -5.93610 | -5.28860 | 1.07240 |
| H | -0.10110 | -2.62730 | -1.08310 |
| H | 0.30770 | -5.10700 | -0.89550 |
| H | -1.07640 | -3.98710 | 1.46020 |
| H | 0.42610 | -3.10610 | 1.19280 |
| H | -3.31270 | -2.75690 | 0.75850 |
| H | -1.72420 | -1.83690 | 2.28020 |
| H | -3.60840 | -0.19360 | 0.79740 |
| H | -2.71280 | -0.13860 | -0.71430 |
| H | -4.41600 | -1.66920 | -1.78800 |
| H | -0.80440 | -5.79160 | -3.04910 |
| H | -1.83790 | -4.37910 | -2.99000 |
| H | 1.24120 | -4.38900 | -3.35510 |
| H | -1.03710 | -2.55380 | -4.34700 |
| H | 2.56140 | -3.60380 | -5.32980 |
| H | 3.03950 | -1.91320 | -5.56280 |
| H | 2.80850 | -2.52100 | -3.91440 |
| H | -6.23690 | -0.99270 | 0.60710 |
| H | -4.49920 | 0.52820 | -2.04450 |

Table S6. Cont.

| Marilzafurolene_A_23 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83320 | -3.28260 | -0.59360 |
| O | -2.12520 | -2.71490 | -0.89890 |
| C | -0.67870 | -4.70450 | -1.15400 |
| C | -0.61700 | -3.12210 | 0.91020 |
| C | -2.61470 | -2.05330 | 0.28730 |
| C | -1.41110 | -1.86840 | 1.21780 |
| C | -3.40530 | -0.80090 | -0.08200 |
| Cl | -0.42450 | -0.41940 | 0.85540 |
| C | -4.61050 | -1.07820 | -0.99040 |
| C | -0.82480 | -4.72440 | -2.68530 |
| Br | -2.04210 | -5.90900 | -0.38000 |
| C | -0.37430 | -6.01980 | -3.31140 |
| C | -1.17500 | -6.81990 | -4.03260 |
| C | -0.65650 | -8.08600 | -4.62720 |
| C | -1.63720 | -8.93330 | -5.39470 |
| O | 0.52420 | -8.41280 | -4.51650 |
| C | -5.62770 | -2.00770 | -0.38610 |
| O | -5.22160 | 0.17800 | -1.29460 |
| C | -6.63590 | -1.66650 | 0.36620 |
| C | -7.63820 | -1.32420 | 1.11120 |
| H | -7.57030 | -1.09170 | 2.16540 |
| Br | -9.29490 | -1.18330 | 0.31720 |
| H | -0.10190 | -2.64490 | -1.10820 |
| H | 0.28510 | -5.12490 | -0.84540 |
| H | -1.04780 | -3.95620 | 1.47360 |
| H | 0.44330 | -3.06610 | 1.17680 |
| H | -3.28900 | -2.77170 | 0.77130 |
| H | -1.70660 | -1.79760 | 2.26820 |
| H | -3.73380 | -0.28330 | 0.82850 |
| H | -2.76380 | -0.09210 | -0.62050 |
| H | -4.26970 | -1.50110 | -1.94220 |
| H | -1.85770 | -4.49540 | -2.97770 |
| H | -0.19930 | -3.93210 | -3.11620 |
| H | 0.67020 | -6.29370 | -3.16540 |
| H | -2.21830 | -6.58060 | -4.20290 |
| H | -1.48130 | -8.78500 | -6.46620 |
| H | -1.48130 | -9.98450 | -5.13640 |
| H | -2.66860 | -8.67470 | -5.14040 |
| H | -5.44340 | -3.06910 | -0.53540 |
| H | -6.07120 | -0.01740 | -1.72760 |

Table S6. Cont.

| Marilzafurollene_A_24 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28320 | -0.59490 |
| O | -2.12390 | -2.71520 | -0.89790 |
| C | -0.66000 | -4.68440 | -1.20070 |
| C | -0.64230 | -3.16930 | 0.91640 |
| C | -2.61640 | -2.05230 | 0.28770 |
| C | -1.42590 | -1.91410 | 1.24360 |
| C | -3.34670 | -0.76590 | -0.09290 |
| Cl | -0.41400 | -0.46710 | 0.94650 |
| C | -4.61420 | -1.01790 | -0.91820 |
| C | -0.82830 | -4.73210 | -2.72950 |
| Br | -1.98250 | -5.94510 | -0.44350 |
| C | 0.24330 | -3.98040 | -3.47440 |
| C | 1.18020 | -4.57010 | -4.23340 |
| C | 2.20270 | -3.75750 | -4.95520 |
| C | 3.16360 | -4.50070 | -5.84560 |
| O | 2.27390 | -2.53820 | -4.81090 |
| C | -5.71430 | -1.65400 | -0.12220 |
| O | -5.10740 | 0.24840 | -1.36090 |
| C | -6.18780 | -2.85110 | -0.31970 |
| C | -6.65710 | -4.04340 | -0.50650 |
| H | -7.42820 | -4.29670 | -1.22160 |
| Br | -6.05690 | -5.38700 | 0.60220 |
| H | -0.09950 | -2.61870 | -1.06840 |
| H | 0.31170 | -5.10110 | -0.91210 |
| H | -1.09620 | -4.01050 | 1.44980 |
| H | 0.41330 | -3.13470 | 1.20420 |
| H | -3.32450 | -2.75260 | 0.74830 |
| H | -1.74060 | -1.86930 | 2.28990 |
| H | -3.59670 | -0.19040 | 0.80770 |
| H | -2.69060 | -0.12640 | -0.69730 |
| H | -4.37500 | -1.60590 | -1.81190 |
| H | -0.83170 | -5.77790 | -3.06580 |
| H | -1.80380 | -4.32340 | -3.02260 |
| H | 0.21970 | -2.89340 | -3.39910 |
| H | 1.22770 | -5.64640 | -4.35250 |
| H | 2.78520 | -5.49600 | -6.09390 |
| H | 3.28810 | -3.94600 | -6.77980 |
| H | 4.12610 | -4.59700 | -5.33720 |
| H | -6.13770 | -1.06030 | 0.68380 |
| H | -5.85530 | 0.06030 | -1.95510 |

Table S6. Cont.

| Marilzafurollene_A_25 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83280 | -3.28320 | -0.59480 |
| O | -2.12410 | -2.71520 | -0.89810 |
| C | -0.66850 | -4.69350 | -1.18200 |
| C | -0.63040 | -3.14800 | 0.91360 |
| C | -2.61620 | -2.05240 | 0.28770 |
| C | -1.41940 | -1.89410 | 1.23210 |
| C | -3.36070 | -0.77680 | -0.10110 |
| Cl | -0.42160 | -0.44350 | 0.90550 |
| C | -4.63300 | -1.05000 | -0.91400 |
| C | -0.84840 | -4.76260 | -2.70860 |
| Br | -1.98980 | -5.93930 | -0.39790 |
| C | 0.21270 | -4.01530 | -3.47260 |
| C | 1.14770 | -4.60960 | -4.23040 |
| C | 2.15850 | -3.79980 | -4.97160 |
| C | 3.12140 | -4.54910 | -5.85470 |
| O | 2.21910 | -2.57770 | -4.84780 |
| C | -5.73330 | -1.65180 | -0.09370 |
| O | -5.13820 | 0.19670 | -1.39780 |
| C | -6.12280 | -2.89350 | -0.15270 |
| C | -6.51160 | -4.12730 | -0.20820 |
| H | -7.21520 | -4.51720 | -0.93140 |
| Br | -5.93470 | -5.27280 | 1.11460 |
| H | -0.10070 | -2.62770 | -1.08240 |
| H | 0.30410 | -5.10900 | -0.89460 |
| H | -1.07320 | -3.98570 | 1.46150 |
| H | 0.42740 | -3.10290 | 1.19150 |
| H | -3.31290 | -2.75670 | 0.75850 |
| H | -1.72540 | -1.83780 | 2.28040 |
| H | -3.60960 | -0.19340 | 0.79470 |
| H | -2.71270 | -0.13960 | -0.71630 |
| H | -4.41540 | -1.67490 | -1.78810 |
| H | -0.84920 | -5.81290 | -3.03060 |
| H | -1.82830 | -4.36280 | -2.99940 |
| H | 0.18260 | -2.92750 | -3.41310 |
| H | 1.20200 | -5.68710 | -4.33440 |
| H | 3.24120 | -4.00540 | -6.79600 |
| H | 4.08550 | -4.63420 | -5.34730 |
| H | 2.74730 | -5.54910 | -6.09010 |
| H | -6.24330 | -0.98570 | 0.59680 |
| H | -4.49530 | 0.52130 | -2.05250 |

Table S6. Cont.

| Marilzafurollene_A_26 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59440 |
| O | -2.12410 | -2.71530 | -0.89850 |
| C | -0.65750 | -4.68460 | -1.19790 |
| C | -0.63530 | -3.15860 | 0.91440 |
| C | -2.61580 | -2.05260 | 0.28780 |
| C | -1.42020 | -1.90290 | 1.23600 |
| C | -3.35690 | -0.77210 | -0.09170 |
| Cl | -0.41300 | -0.45670 | 0.91720 |
| C | -4.62370 | -1.03330 | -0.91510 |
| C | -0.82290 | -4.66160 | -2.72810 |
| Br | -1.97660 | -5.94110 | -0.43660 |
| C | -0.31150 | -5.90820 | -3.40730 |
| C | 0.72180 | -5.92180 | -4.26410 |
| C | 1.16630 | -7.19120 | -4.91130 |
| C | 2.30950 | -7.09610 | -5.88740 |
| O | 0.64120 | -8.27030 | -4.64290 |
| C | -5.71540 | -1.68580 | -0.12080 |
| O | -5.13050 | 0.23010 | -1.35080 |
| C | -6.19230 | -2.87760 | -0.34030 |
| C | -6.66660 | -4.06390 | -0.55140 |
| H | -7.43750 | -4.29880 | -1.27310 |
| Br | -6.09560 | -5.42760 | 0.54810 |
| H | -0.10140 | -2.62540 | -1.08310 |
| H | 0.32060 | -5.09000 | -0.91510 |
| H | -1.08470 | -3.99780 | 1.45490 |
| H | 0.42160 | -3.11980 | 1.19670 |
| H | -3.31670 | -2.75650 | 0.75410 |
| H | -1.72830 | -1.84910 | 2.28380 |
| H | -3.60960 | -0.19860 | 0.80950 |
| H | -2.70720 | -0.12710 | -0.69710 |
| H | -4.38000 | -1.61410 | -1.81230 |
| H | -1.87580 | -4.52510 | -3.00560 |
| H | -0.28460 | -3.79400 | -3.13160 |
| H | -0.83890 | -6.83680 | -3.19000 |
| H | 1.26600 | -5.02000 | -4.51960 |
| H | 2.43520 | -6.07290 | -6.25190 |
| H | 3.23070 | -7.42160 | -5.39780 |
| H | 2.09890 | -7.73550 | -6.74930 |
| H | -6.13640 | -1.10590 | 0.69650 |
| H | -5.88540 | 0.03770 | -1.93490 |

Table S6. Cont.

| Marilzafurollene_A_27 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28290 | -0.59420 |
| O | -2.12460 | -2.71500 | -0.89840 |
| C | -0.67380 | -4.69950 | -1.16610 |
| C | -0.62100 | -3.13230 | 0.91070 |
| C | -2.61550 | -2.05290 | 0.28750 |
| C | -1.41380 | -1.87940 | 1.22290 |
| C | -3.38270 | -0.78680 | -0.08870 |
| Cl | -0.42470 | -0.42830 | 0.87450 |
| C | -4.64430 | -1.06940 | -0.91890 |
| C | -0.83050 | -4.70910 | -2.69640 |
| Br | -2.02210 | -5.92020 | -0.39200 |
| C | -0.37480 | -5.99690 | -3.33440 |
| C | -1.17770 | -6.80280 | -4.04640 |
| C | -0.65580 | -8.06270 | -4.65090 |
| C | -1.64320 | -8.92560 | -5.39170 |
| O | 0.53160 | -8.37260 | -4.56830 |
| C | -5.73590 | -1.84220 | -0.23300 |
| O | -5.20700 | 0.17890 | -1.33140 |
| C | -6.05830 | -1.76990 | 1.02810 |
| C | -6.38240 | -1.69130 | 2.27970 |
| H | -6.20600 | -2.47090 | 3.00910 |
| Br | -6.93900 | -0.05430 | 2.91860 |
| H | -0.10180 | -2.64010 | -1.10260 |
| H | 0.29490 | -5.11570 | -0.86720 |
| H | -1.05540 | -3.96840 | 1.46810 |
| H | 0.43850 | -3.07970 | 1.18100 |
| H | -3.29940 | -2.76680 | 0.76320 |
| H | -1.71320 | -1.81460 | 2.27260 |
| H | -3.64200 | -0.21600 | 0.81190 |
| H | -2.74710 | -0.12790 | -0.69410 |
| H | -4.36340 | -1.60270 | -1.83400 |
| H | -1.86710 | -4.48590 | -2.98020 |
| H | -0.21400 | -3.90910 | -3.12610 |
| H | 0.67440 | -6.26040 | -3.20400 |
| H | -2.22610 | -6.57410 | -4.19960 |
| H | -1.52080 | -8.77310 | -6.46680 |
| H | -1.46170 | -9.97430 | -5.14010 |
| H | -2.67120 | -8.68550 | -5.10700 |
| H | -6.42680 | -2.35160 | -0.90070 |
| H | -5.56340 | 0.60780 | -0.53310 |

Table S6. Cont.

| Marilzafurollene_A_28 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28290 | -0.59420 |
| O | -2.12440 | -2.71530 | -0.89880 |
| C | -0.66680 | -4.69510 | -1.17590 |
| C | -0.62290 | -3.13550 | 0.91110 |
| C | -2.61570 | -2.05260 | 0.28790 |
| C | -1.41330 | -1.88060 | 1.22280 |
| C | -3.37340 | -0.78460 | -0.10000 |
| Cl | -0.42180 | -0.43120 | 0.87010 |
| C | -4.65370 | -1.07230 | -0.89520 |
| C | -0.83530 | -4.69530 | -2.70590 |
| Br | -1.99240 | -5.93100 | -0.39240 |
| C | -0.33430 | -5.95610 | -3.36620 |
| C | 0.69850 | -5.99150 | -4.22310 |
| C | 1.13200 | -7.27450 | -4.85080 |
| C | 2.27680 | -7.20490 | -5.82720 |
| O | 0.59620 | -8.34450 | -4.56720 |
| C | -5.74140 | -1.67090 | -0.05620 |
| O | -5.17050 | 0.16710 | -1.38550 |
| C | -6.12140 | -2.91630 | -0.09380 |
| C | -6.50030 | -4.15410 | -0.12690 |
| H | -7.20790 | -4.56110 | -0.83660 |
| Br | -5.89830 | -5.27440 | 1.20630 |
| H | -0.10250 | -2.63580 | -1.09830 |
| H | 0.30950 | -5.10190 | -0.88890 |
| H | -1.06090 | -3.97050 | 1.46720 |
| H | 0.43620 | -3.08540 | 1.18320 |
| H | -3.30280 | -2.76120 | 0.76600 |
| H | -1.71150 | -1.81340 | 2.27260 |
| H | -3.61580 | -0.19740 | 0.79510 |
| H | -2.73720 | -0.14680 | -0.72670 |
| H | -4.44320 | -1.70490 | -1.76540 |
| H | -1.88770 | -4.55550 | -2.98350 |
| H | -0.29160 | -3.83810 | -3.12430 |
| H | -0.86920 | -6.87700 | -3.13460 |
| H | 1.25030 | -5.09840 | -4.49240 |
| H | 2.05440 | -7.84440 | -6.68610 |
| H | 2.42200 | -6.18600 | -6.19620 |
| H | 3.19180 | -7.54500 | -5.33570 |
| H | -6.24980 | -0.99940 | 0.63030 |
| H | -4.53950 | 0.48620 | -2.05430 |

Table S6. Cont.

| Marilzafurollene_A_29 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59470 |
| O | -2.12390 | -2.71530 | -0.89820 |
| C | -0.66070 | -4.68420 | -1.19990 |
| C | -0.63670 | -3.16050 | 0.91520 |
| C | -2.61610 | -2.05240 | 0.28780 |
| C | -1.42240 | -1.90550 | 1.23860 |
| C | -3.35430 | -0.77060 | -0.09310 |
| Cl | -0.41490 | -0.45810 | 0.92730 |
| C | -4.61930 | -1.02970 | -0.91990 |
| C | -0.86740 | -4.74090 | -2.72390 |
| Br | -1.94890 | -5.95810 | -0.40750 |
| C | 0.13230 | -3.92550 | -3.50570 |
| C | 1.11070 | -4.47180 | -4.24390 |
| C | 2.10120 | -3.70390 | -5.05020 |
| C | 2.02030 | -2.20090 | -5.10160 |
| O | 2.97160 | -4.32570 | -5.66030 |
| C | -5.71410 | -1.68020 | -0.12830 |
| O | -5.12250 | 0.23430 | -1.35760 |
| C | -6.18210 | -2.87710 | -0.33910 |
| C | -6.64680 | -4.06880 | -0.54080 |
| H | -7.41520 | -4.31600 | -1.26100 |
| Br | -6.05690 | -5.42100 | 0.56310 |
| H | -0.10110 | -2.62050 | -1.07350 |
| H | 0.32300 | -5.08810 | -0.93450 |
| H | -1.08640 | -3.99920 | 1.45580 |
| H | 0.41990 | -3.12180 | 1.19840 |
| H | -3.31900 | -2.75540 | 0.75240 |
| H | -1.73290 | -1.85500 | 2.28590 |
| H | -3.60850 | -0.19710 | 0.80770 |
| H | -2.70200 | -0.12640 | -0.69660 |
| H | -4.37440 | -1.61120 | -1.81630 |
| H | -0.82090 | -5.78610 | -3.05930 |
| H | -1.87390 | -4.39190 | -2.98910 |
| H | -0.00280 | -2.84710 | -3.46480 |
| H | 1.24070 | -5.54920 | -4.29840 |
| H | 1.05760 | -1.88920 | -5.51490 |
| H | 2.16730 | -1.78180 | -4.10290 |
| H | 2.81170 | -1.81930 | -5.75400 |
| H | -6.14110 | -1.09660 | 0.68330 |
| H | -5.87750 | 0.04340 | -1.94200 |

Table S6. Cont.

| Marilzafurolene_A_30 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.83330 | -3.28280 | -0.59440 |
| O | -2.12440 | -2.71490 | -0.89780 |
| C | -0.67780 | -4.70370 | -1.15770 |
| C | -0.61050 | -3.11760 | 0.90780 |
| C | -2.61540 | -2.05310 | 0.28700 |
| C | -1.41040 | -1.86850 | 1.21720 |
| C | -3.39440 | -0.79280 | -0.08290 |
| Cl | -0.42590 | -0.41600 | 0.85870 |
| C | -4.61400 | -1.06470 | -0.97110 |
| C | -0.89810 | -4.73460 | -2.68030 |
| Br | -1.96510 | -5.94030 | -0.31420 |
| C | -0.47180 | -6.03340 | -3.32380 |
| C | -1.31340 | -6.82500 | -4.00690 |
| C | -0.93490 | -8.11020 | -4.65850 |
| C | 0.47370 | -8.62740 | -4.52850 |
| O | -1.79090 | -8.72350 | -5.29680 |
| C | -5.67760 | -1.88060 | -0.29940 |
| O | -5.20270 | 0.19690 | -1.29550 |
| C | -6.24810 | -2.93020 | -0.81900 |
| C | -6.82190 | -3.96520 | -1.34480 |
| H | -7.72320 | -3.93060 | -1.94200 |
| Br | -6.01780 | -5.60730 | -1.12660 |
| H | -0.10530 | -2.64570 | -1.11450 |
| H | 0.30950 | -5.10050 | -0.89570 |
| H | -1.03330 | -3.95020 | 1.47850 |
| H | 0.45090 | -3.05520 | 1.16840 |
| H | -3.29570 | -2.76810 | 0.76780 |
| H | -1.70540 | -1.80000 | 2.26790 |
| H | -3.70340 | -0.26140 | 0.82660 |
| H | -2.75070 | -0.09890 | -0.63820 |
| H | -4.29390 | -1.52790 | -1.91190 |
| H | -1.94580 | -4.51320 | -2.92180 |
| H | -0.29960 | -3.94060 | -3.14510 |
| H | 0.57770 | -6.29420 | -3.21340 |
| H | -2.36140 | -6.56270 | -4.12390 |
| H | 0.73030 | -8.76370 | -3.47470 |
| H | 0.54780 | -9.59990 | -5.02480 |
| H | 1.17230 | -7.93980 | -5.01200 |
| H | -6.03660 | -1.52230 | 0.66150 |
| H | -5.94270 | 0.00840 | -1.89950 |

Table S6. Cont.

| Marilzafurollene_A_31 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83260 | -3.28350 | -0.59520 |
| O | -2.12410 | -2.71480 | -0.89690 |
| C | -0.64960 | -4.67820 | -1.21540 |
| C | -0.63890 | -3.17210 | 0.91630 |
| C | -2.61650 | -2.05250 | 0.28700 |
| C | -1.42960 | -1.92410 | 1.25160 |
| C | -3.33350 | -0.75700 | -0.09000 |
| Cl | -0.41490 | -0.47330 | 0.97930 |
| C | -4.52360 | -0.96420 | -1.03460 |
| C | -0.94900 | -4.73620 | -2.72270 |
| Br | -1.83870 | -6.00570 | -0.35990 |
| C | -0.05830 | -3.85140 | -3.55200 |
| C | -0.52070 | -2.83140 | -4.29150 |
| C | 0.39960 | -1.98790 | -5.10570 |
| C | -0.23250 | -0.89770 | -5.93050 |
| O | 1.61740 | -2.15620 | -5.08200 |
| C | -5.65240 | -1.72810 | -0.41500 |
| O | -5.05500 | 0.31790 | -1.37790 |
| C | -6.14030 | -2.84360 | -0.87830 |
| C | -6.63410 | -3.94140 | -1.35500 |
| H | -7.42040 | -3.98800 | -2.09640 |
| Br | -5.94610 | -5.53770 | -0.74800 |
| H | -0.10360 | -2.61420 | -1.07030 |
| H | 0.36190 | -5.04680 | -1.01040 |
| H | -1.08720 | -4.01330 | 1.45320 |
| H | 0.41730 | -3.13370 | 1.20120 |
| H | -3.33640 | -2.74700 | 0.73880 |
| H | -1.75040 | -1.89120 | 2.29650 |
| H | -3.65920 | -0.22870 | 0.81540 |
| H | -2.64010 | -0.08070 | -0.60560 |
| H | -4.19730 | -1.44240 | -1.96590 |
| H | -0.81230 | -5.76420 | -3.08400 |
| H | -2.00430 | -4.49450 | -2.90790 |
| H | 1.00670 | -4.07980 | -3.54710 |
| H | -1.57590 | -2.58270 | -4.32050 |
| H | 0.33360 | -0.77260 | -6.85770 |
| H | -1.26040 | -1.15740 | -6.19920 |
| H | -0.22720 | 0.03610 | -5.36280 |
| H | -6.13750 | -1.27080 | 0.44250 |
| H | -4.37200 | 0.77410 | -1.89950 |

Table S6. Cont.

| Marilzafurollene_A_32 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28310 | -0.59450 |
| O | -2.12420 | -2.71530 | -0.89850 |
| C | -0.67150 | -4.69700 | -1.17300 |
| C | -0.62180 | -3.13300 | 0.91130 |
| C | -2.61600 | -2.05250 | 0.28790 |
| C | -1.41410 | -1.87920 | 1.22300 |
| C | -3.37440 | -0.78500 | -0.10030 |
| Cl | -0.42470 | -0.42800 | 0.87250 |
| C | -4.65150 | -1.07220 | -0.90080 |
| C | -0.88200 | -4.78140 | -2.69530 |
| Br | -1.96740 | -5.94580 | -0.35340 |
| C | 0.12740 | -3.99510 | -3.49430 |
| C | 1.09570 | -4.56970 | -4.22450 |
| C | 2.09580 | -3.83220 | -5.04710 |
| C | 2.03900 | -2.32920 | -5.12460 |
| O | 2.95400 | -4.47860 | -5.64870 |
| C | -5.73850 | -1.68230 | -0.06940 |
| O | -5.17270 | 0.16850 | -1.38280 |
| C | -6.12560 | -2.92450 | -0.13140 |
| C | -6.51290 | -4.15870 | -0.18950 |
| H | -7.22380 | -4.54600 | -0.90690 |
| Br | -5.91640 | -5.31100 | 1.11850 |
| H | -0.10240 | -2.63280 | -1.09200 |
| H | 0.30980 | -5.10280 | -0.90210 |
| H | -1.05760 | -3.96680 | 1.47060 |
| H | 0.43750 | -3.08080 | 1.18210 |
| H | -3.30310 | -2.76130 | 0.76590 |
| H | -1.71300 | -1.81310 | 2.27280 |
| H | -3.62050 | -0.19980 | 0.79510 |
| H | -2.73720 | -0.14480 | -0.72370 |
| H | -4.43550 | -1.69710 | -1.77530 |
| H | -0.84970 | -5.83350 | -3.01000 |
| H | -1.88420 | -4.42450 | -2.96570 |
| H | 0.00890 | -2.91430 | -3.47340 |
| H | 1.20910 | -5.64980 | -4.25940 |
| H | 2.19670 | -1.89520 | -4.13390 |
| H | 2.83400 | -1.97200 | -5.78640 |
| H | 1.07990 | -2.00910 | -5.53980 |
| H | -6.24260 | -1.02150 | 0.63060 |
| H | -4.54080 | 0.49700 | -2.04610 |

Table S6. Cont.

| Marilzafurollene_A_33 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83340 | -3.28250 | -0.59360 |
| O | -2.12510 | -2.71490 | -0.89890 |
| C | -0.67910 | -4.70280 | -1.15920 |
| C | -0.61800 | -3.12450 | 0.91050 |
| C | -2.61460 | -2.05340 | 0.28730 |
| C | -1.41150 | -1.87050 | 1.21900 |
| C | -3.40380 | -0.80000 | -0.08210 |
| Cl | -0.42350 | -0.42190 | 0.85900 |
| C | -4.60560 | -1.07490 | -0.99560 |
| C | -0.83060 | -4.71650 | -2.69090 |
| Br | -2.03380 | -5.91140 | -0.37740 |
| C | -0.37970 | -6.00880 | -3.33150 |
| C | 0.69190 | -6.09840 | -4.13450 |
| C | 1.15940 | -7.35000 | -4.79480 |
| C | 0.39780 | -8.63340 | -4.59180 |
| O | 2.16980 | -7.30190 | -5.49710 |
| C | -5.62230 | -2.01070 | -0.40040 |
| O | -5.21910 | 0.18150 | -1.29410 |
| C | -6.62910 | -1.67730 | 0.35720 |
| C | -7.62990 | -1.34260 | 1.10770 |
| H | -7.55970 | -1.12010 | 2.16390 |
| Br | -9.28850 | -1.19590 | 0.31910 |
| H | -0.10180 | -2.64340 | -1.10600 |
| H | 0.28790 | -5.12130 | -0.85790 |
| H | -1.04970 | -3.95860 | 1.47300 |
| H | 0.44210 | -3.06940 | 1.17790 |
| H | -3.29030 | -2.77120 | 0.77040 |
| H | -1.70770 | -1.80060 | 2.26920 |
| H | -3.73530 | -0.28440 | 0.82840 |
| H | -2.76050 | -0.08990 | -0.61680 |
| H | -4.26080 | -1.49110 | -1.94900 |
| H | -1.87290 | -4.53470 | -2.98230 |
| H | -0.24650 | -3.88840 | -3.11340 |
| H | -0.99260 | -6.88230 | -3.12210 |
| H | 1.30390 | -5.22910 | -4.35810 |
| H | -0.62570 | -8.52640 | -4.96010 |
| H | 0.88310 | -9.43390 | -5.15840 |
| H | 0.40250 | -8.91080 | -3.53450 |
| H | -5.43770 | -3.07060 | -0.56050 |
| H | -6.06670 | -0.01360 | -1.73110 |

Table S6. Cont.

| Marilzafurollene_A_34 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83340 | -3.28250 | -0.59370 |
| O | -2.12510 | -2.71490 | -0.89880 |
| C | -0.67940 | -4.70400 | -1.15560 |
| C | -0.61690 | -3.12230 | 0.91010 |
| C | -2.61470 | -2.05330 | 0.28730 |
| C | -1.41110 | -1.86860 | 1.21790 |
| C | -3.40520 | -0.80100 | -0.08240 |
| Cl | -0.42420 | -0.41980 | 0.85540 |
| C | -4.60790 | -1.07800 | -0.99420 |
| C | -0.83180 | -4.72310 | -2.68670 |
| Br | -2.03420 | -5.91240 | -0.37560 |
| C | -0.40050 | -6.02550 | -3.31900 |
| C | -1.22030 | -6.79020 | -4.05680 |
| C | -0.83530 | -8.07580 | -4.70370 |
| C | 0.56160 | -8.61150 | -4.52980 |
| O | -1.67780 | -8.67430 | -5.37360 |
| C | -5.62430 | -2.01180 | -0.39530 |
| O | -5.22140 | 0.17780 | -1.29540 |
| C | -6.62970 | -1.67560 | 0.36300 |
| C | -7.62900 | -1.33780 | 1.11410 |
| H | -7.55720 | -1.11410 | 2.17000 |
| Br | -9.28650 | -1.18000 | 0.32530 |
| H | -0.10220 | -2.64490 | -1.10850 |
| H | 0.28700 | -5.12250 | -0.85260 |
| H | -1.04750 | -3.95620 | 1.47370 |
| H | 0.44350 | -3.06620 | 1.17640 |
| H | -3.28930 | -2.77160 | 0.77110 |
| H | -1.70660 | -1.79780 | 2.26820 |
| H | -3.73620 | -0.28460 | 0.82790 |
| H | -2.76310 | -0.09090 | -0.61860 |
| H | -4.26420 | -1.49680 | -1.94680 |
| H | -1.86290 | -4.47940 | -2.97380 |
| H | -0.19750 | -3.93850 | -3.11910 |
| H | 0.63530 | -6.31180 | -3.15440 |
| H | -2.25410 | -6.50290 | -4.22830 |
| H | 0.76990 | -8.78450 | -3.47080 |
| H | 0.64900 | -9.56740 | -5.05540 |
| H | 1.28730 | -7.91630 | -4.95950 |
| H | -5.44140 | -3.07210 | -0.55400 |
| H | -6.07020 | -0.01820 | -1.72970 |

Table S6. Cont.

| Marilzafurollene_A_35 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59430 |
| O | -2.12440 | -2.71510 | -0.89840 |
| C | -0.67290 | -4.69730 | -1.17250 |
| C | -0.62300 | -3.13640 | 0.91130 |
| C | -2.61550 | -2.05280 | 0.28750 |
| C | -1.41480 | -1.88310 | 1.22510 |
| C | -3.37960 | -0.78480 | -0.08850 |
| Cl | -0.42320 | -0.43260 | 0.88140 |
| C | -4.63950 | -1.06400 | -0.92230 |
| C | -0.83010 | -4.69920 | -2.70380 |
| Br | -2.01490 | -5.92240 | -0.39550 |
| C | -0.37270 | -5.98310 | -3.35670 |
| C | 0.69660 | -6.05880 | -4.16410 |
| C | 1.17010 | -7.30190 | -4.83610 |
| C | 0.41800 | -8.59200 | -4.64040 |
| O | 2.17750 | -7.24150 | -5.54180 |
| C | -5.73240 | -1.83760 | -0.23940 |
| O | -5.19970 | 0.18550 | -1.33390 |
| C | -6.07080 | -1.75110 | 1.01670 |
| C | -6.41230 | -1.65880 | 2.26270 |
| H | -6.23570 | -2.42480 | 3.00610 |
| Br | -7.02710 | -0.02870 | 2.86430 |
| H | -0.10150 | -2.63780 | -1.09920 |
| H | 0.29800 | -5.11180 | -0.87860 |
| H | -1.05950 | -3.97290 | 1.46640 |
| H | 0.43610 | -3.08570 | 1.18320 |
| H | -3.30190 | -2.76560 | 0.76160 |
| H | -1.71560 | -1.82010 | 2.27450 |
| H | -3.64030 | -0.21510 | 0.81240 |
| H | -2.74140 | -0.12590 | -0.69120 |
| H | -4.35700 | -1.59590 | -1.83770 |
| H | -1.87480 | -4.52240 | -2.98970 |
| H | -0.25350 | -3.86350 | -3.12150 |
| H | -0.97920 | -6.86220 | -3.15260 |
| H | 1.30200 | -5.18360 | -4.38270 |
| H | -0.60780 | -8.48910 | -5.00350 |
| H | 0.90620 | -9.38460 | -5.21570 |
| H | 0.42910 | -8.87800 | -3.58550 |
| H | -6.40980 | -2.36350 | -0.90820 |
| H | -5.56320 | 0.61090 | -0.53690 |

Table S6. Cont.

| Marilzafurollene_A_36 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59440 |
| O | -2.12440 | -2.71510 | -0.89830 |
| C | -0.67200 | -4.69730 | -1.17160 |
| C | -0.62340 | -3.13670 | 0.91120 |
| C | -2.61560 | -2.05280 | 0.28750 |
| C | -1.41500 | -1.88340 | 1.22520 |
| C | -3.37860 | -0.78430 | -0.08910 |
| Cl | -0.42290 | -0.43310 | 0.88200 |
| C | -4.64100 | -1.06290 | -0.91940 |
| C | -0.83100 | -4.70180 | -2.70220 |
| Br | -2.01240 | -5.92510 | -0.39830 |
| C | -0.38970 | -5.99330 | -3.34990 |
| C | -1.20610 | -6.75970 | -4.09000 |
| C | -0.81120 | -8.03470 | -4.75190 |
| C | 0.59290 | -8.55590 | -4.59300 |
| O | -1.65150 | -8.63650 | -5.42140 |
| C | -5.73590 | -1.83020 | -0.23250 |
| O | -5.19820 | 0.18730 | -1.33360 |
| C | -6.05830 | -1.75420 | 1.02840 |
| C | -6.38220 | -1.67140 | 2.27980 |
| H | -6.21030 | -2.45070 | 3.01050 |
| Br | -6.92370 | -0.02850 | 2.91670 |
| H | -0.10180 | -2.63800 | -1.09980 |
| H | 0.29890 | -5.11140 | -0.87710 |
| H | -1.06020 | -3.97330 | 1.46590 |
| H | 0.43570 | -3.08630 | 1.18350 |
| H | -3.30220 | -2.76540 | 0.76130 |
| H | -1.71600 | -1.82070 | 2.27460 |
| H | -3.63630 | -0.21250 | 0.81130 |
| H | -2.74060 | -0.12770 | -0.69450 |
| H | -4.36210 | -1.59850 | -1.83370 |
| H | -1.86570 | -4.46530 | -2.98240 |
| H | -0.20630 | -3.90660 | -3.12910 |
| H | 0.65010 | -6.26980 | -3.19480 |
| H | -2.24400 | -6.48190 | -4.25180 |
| H | 0.81050 | -8.73740 | -3.53730 |
| H | 0.68790 | -9.50510 | -5.12920 |
| H | 1.30760 | -7.84790 | -5.02010 |
| H | -6.42910 | -2.33740 | -0.89960 |
| H | -5.55550 | 0.61750 | -0.53640 |

Table S6. Cont.

| Marilzafurollene_A_37 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83790 | -3.27920 | -0.59100 |
| O | -2.12350 | -2.71750 | -0.90390 |
| C | -0.37370 | -4.31550 | -1.62540 |
| C | -0.95920 | -3.69150 | 0.86660 |
| C | -2.61160 | -2.05410 | 0.28970 |
| C | -1.69090 | -2.49260 | 1.45190 |
| C | -2.70430 | -0.55210 | -0.00110 |
| Cl | -0.50010 | -1.26250 | 1.98230 |
| C | -3.72310 | -0.21250 | -1.09750 |
| C | -0.51440 | -3.85000 | -3.09140 |
| Br | -1.36780 | -6.00930 | -1.46350 |
| C | -0.00660 | -2.44980 | -3.34340 |
| C | -0.85750 | -1.42710 | -3.52390 |
| C | -0.48020 | 0.00600 | -3.60900 |
| C | 0.93080 | 0.38670 | -3.96570 |
| O | -1.34160 | 0.84700 | -3.34120 |
| C | -5.13730 | -0.28000 | -0.60510 |
| O | -3.50700 | 1.13450 | -1.52080 |
| C | -5.99740 | -1.20760 | -0.91560 |
| C | -6.85360 | -2.12770 | -1.22710 |
| H | -7.48230 | -2.10860 | -2.10720 |
| Br | -7.02820 | -3.56630 | -0.08960 |
| H | -0.12060 | -2.44830 | -0.64480 |
| H | 0.66560 | -4.59410 | -1.41700 |
| H | -1.60330 | -4.56850 | 0.98740 |
| H | 0.00620 | -3.90980 | 1.33260 |
| H | -3.61070 | -2.46480 | 0.47260 |
| H | -2.26960 | -2.75490 | 2.34230 |
| H | -2.95000 | 0.00120 | 0.91420 |
| H | -1.72730 | -0.18250 | -0.33950 |
| H | -3.59770 | -0.85530 | -1.97510 |
| H | 0.03280 | -4.53780 | -3.74900 |
| H | -1.56500 | -3.91840 | -3.40630 |
| H | 1.06840 | -2.29770 | -3.30130 |
| H | -1.93100 | -1.59630 | -3.51690 |
| H | 1.30680 | -0.24600 | -4.77410 |
| H | 0.94440 | 1.42170 | -4.32030 |
| H | 1.57090 | 0.29950 | -3.08450 |
| H | -5.45570 | 0.51630 | 0.06200 |
| H | -2.73850 | 1.11530 | -2.13410 |

Table S6. Cont.

| Marilzafurollene_A_38 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83340 | -3.28250 | -0.59350 |
| O | -2.12520 | -2.71490 | -0.89890 |
| C | -0.67950 | -4.70460 | -1.15500 |
| C | -0.61490 | -3.11930 | 0.90970 |
| C | -2.61460 | -2.05340 | 0.28730 |
| C | -1.41010 | -1.86590 | 1.21610 |
| C | -3.40770 | -0.80270 | -0.08220 |
| Cl | -0.42520 | -0.41660 | 0.84980 |
| C | -4.61090 | -1.08230 | -0.99260 |
| C | -0.83800 | -4.72410 | -2.68590 |
| Br | -2.03040 | -5.91070 | -0.36290 |
| C | -0.35020 | -6.00130 | -3.32430 |
| C | 0.68460 | -6.06260 | -4.17730 |
| C | 1.10500 | -7.36070 | -4.78220 |
| C | 2.24860 | -7.31910 | -5.76160 |
| O | 0.56050 | -8.42040 | -4.47740 |
| C | -5.62490 | -2.01790 | -0.39240 |
| O | -5.22700 | 0.17220 | -1.29360 |
| C | -6.63000 | -1.68360 | 0.36700 |
| C | -7.62920 | -1.34780 | 1.11920 |
| H | -7.55670 | -1.12400 | 2.17500 |
| Br | -9.28810 | -1.19430 | 0.33250 |
| H | -0.10250 | -2.64510 | -1.10910 |
| H | 0.28910 | -5.12040 | -0.85530 |
| H | -1.04370 | -3.95230 | 1.47600 |
| H | 0.44570 | -3.06150 | 1.17440 |
| H | -3.28730 | -2.77250 | 0.77250 |
| H | -1.70440 | -1.79340 | 2.26670 |
| H | -3.73870 | -0.28650 | 0.82820 |
| H | -2.76750 | -0.09170 | -0.61940 |
| H | -4.26730 | -1.50080 | -1.94540 |
| H | -1.88660 | -4.57380 | -2.97250 |
| H | -0.27960 | -3.88070 | -3.11270 |
| H | -0.89630 | -6.91210 | -3.07960 |
| H | 1.24730 | -5.18050 | -4.46010 |
| H | 2.02630 | -7.98480 | -6.60040 |
| H | 2.39080 | -6.31160 | -6.16190 |
| H | 3.16480 | -7.64260 | -5.26130 |
| H | -5.43990 | -3.07790 | -0.55110 |
| H | -6.07610 | -0.02570 | -1.72650 |

Table S6. Cont.

| Marilzafurollene_A_39 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28280 | -0.59380 |
| O | -2.12510 | -2.71480 | -0.89850 |
| C | -0.68270 | -4.70630 | -1.15270 |
| C | -0.61930 | -3.12550 | 0.91130 |
| C | -2.61490 | -2.05330 | 0.28720 |
| C | -1.41350 | -1.87240 | 1.22110 |
| C | -3.40280 | -0.79910 | -0.08190 |
| Cl | -0.42490 | -0.42270 | 0.86850 |
| C | -4.60170 | -1.07130 | -1.00010 |
| C | -0.84540 | -4.78760 | -2.67980 |
| Br | -2.03710 | -5.91530 | -0.36770 |
| C | 0.25690 | -4.08590 | -3.43330 |
| C | 0.03890 | -3.03490 | -4.23900 |
| C | 1.09240 | -2.32120 | -5.01430 |
| C | 2.52900 | -2.75890 | -4.90080 |
| O | 0.75850 | -1.38170 | -5.73670 |
| C | -5.61690 | -2.01470 | -0.41440 |
| O | -5.21860 | 0.18520 | -1.29090 |
| C | -6.62830 | -1.69000 | 0.34070 |
| C | -7.63380 | -1.36410 | 1.08900 |
| H | -7.56880 | -1.14640 | 2.14650 |
| Br | -9.29130 | -1.22860 | 0.29600 |
| H | -0.10130 | -2.64030 | -1.09960 |
| H | 0.27960 | -5.13260 | -0.84730 |
| H | -1.05100 | -3.96010 | 1.47300 |
| H | 0.44060 | -3.07060 | 1.17940 |
| H | -3.29190 | -2.77060 | 0.76900 |
| H | -1.71190 | -1.80570 | 2.27090 |
| H | -3.73720 | -0.28550 | 0.82880 |
| H | -2.75780 | -0.08770 | -0.61290 |
| H | -4.25290 | -1.47960 | -1.95560 |
| H | -0.83180 | -5.83840 | -2.99850 |
| H | -1.82700 | -4.39720 | -2.97900 |
| H | 1.25510 | -4.49720 | -3.30450 |
| H | -0.96010 | -2.62900 | -4.37540 |
| H | 2.63970 | -3.78390 | -5.26380 |
| H | 3.15440 | -2.10660 | -5.51810 |
| H | 2.86800 | -2.67550 | -3.86500 |
| H | -5.42660 | -3.07280 | -0.57930 |
| H | -6.06250 | -0.00950 | -1.73510 |

Table S6. Cont.

| Marilzafurollene_A_40 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83300 | -3.28280 | -0.59400 |
| O | -2.12500 | -2.71470 | -0.89820 |
| C | -0.68480 | -4.70680 | -1.15230 |
| C | -0.61840 | -3.12410 | 0.91120 |
| C | -2.61510 | -2.05320 | 0.28710 |
| C | -1.41400 | -1.87190 | 1.22120 |
| C | -3.40340 | -0.79960 | -0.08310 |
| Cl | -0.42750 | -0.42040 | 0.87030 |
| C | -4.59890 | -1.07260 | -1.00540 |
| C | -0.85060 | -4.80250 | -2.67910 |
| Br | -2.03960 | -5.91240 | -0.35690 |
| C | 0.24020 | -4.10160 | -3.44510 |
| C | 1.16460 | -4.73820 | -4.18120 |
| C | 2.20810 | -3.97410 | -4.92570 |
| C | 3.15230 | -4.76870 | -5.78910 |
| O | 2.30900 | -2.75300 | -4.81930 |
| C | -5.61580 | -2.01590 | -0.42250 |
| O | -5.21530 | 0.18370 | -1.29890 |
| C | -6.63150 | -1.69060 | 0.32660 |
| C | -7.64100 | -1.36400 | 1.06910 |
| H | -7.58130 | -1.14300 | 2.12630 |
| Br | -9.29510 | -1.23420 | 0.26810 |
| H | -0.10100 | -2.64050 | -1.09870 |
| H | 0.27710 | -5.13390 | -0.84650 |
| H | -1.04830 | -3.95870 | 1.47430 |
| H | 0.44170 | -3.06770 | 1.17850 |
| H | -3.29210 | -2.77060 | 0.76880 |
| H | -1.71280 | -1.80610 | 2.27100 |
| H | -3.74110 | -0.28720 | 0.82710 |
| H | -2.75770 | -0.08690 | -0.61140 |
| H | -4.24690 | -1.48110 | -1.95950 |
| H | -0.87780 | -5.85860 | -2.97990 |
| H | -1.81550 | -4.38100 | -2.98880 |
| H | 0.24280 | -3.01240 | -3.40640 |
| H | 1.18700 | -5.81870 | -4.26490 |
| H | 4.10700 | -4.88320 | -5.26990 |
| H | 2.74380 | -5.75700 | -6.01720 |
| H | 3.30240 | -4.24110 | -6.73520 |
| H | -5.42310 | -3.07410 | -0.58360 |
| H | -6.05670 | -0.01190 | -1.74750 |

Table S6. Cont.

| Marilzafurollene_A_41 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83230 | -3.28320 | -0.59400 |
| O | -2.12520 | -2.71490 | -0.89910 |
| C | -0.68590 | -4.71370 | -1.13710 |
| C | -0.60850 | -3.10660 | 0.90750 |
| C | -2.61560 | -2.05260 | 0.28790 |
| C | -1.40690 | -1.85450 | 1.20820 |
| C | -3.39920 | -0.79940 | -0.09540 |
| Cl | -0.43300 | -0.40150 | 0.82360 |
| C | -4.67940 | -1.10970 | -0.88720 |
| C | -0.86820 | -4.81400 | -2.66050 |
| Br | -2.02440 | -5.91850 | -0.32030 |
| C | 0.21650 | -4.10900 | -3.43010 |
| C | -0.00630 | -3.06690 | -4.24610 |
| C | 1.11830 | -2.41670 | -4.97930 |
| C | 0.76750 | -1.27620 | -5.89810 |
| O | 2.28300 | -2.77920 | -4.82120 |
| C | -5.78810 | -1.79460 | -0.14050 |
| O | -5.23150 | 0.11860 | -1.36890 |
| C | -5.94130 | -1.87170 | 1.15180 |
| C | -6.10320 | -1.95560 | 2.43420 |
| H | -5.93420 | -2.85190 | 3.01580 |
| Br | -6.47980 | -0.40910 | 3.36200 |
| H | -0.10270 | -2.64790 | -1.11170 |
| H | 0.28180 | -5.13300 | -0.83890 |
| H | -1.03090 | -3.93660 | 1.48280 |
| H | 0.45310 | -3.04220 | 1.16700 |
| H | -3.28440 | -2.77340 | 0.77370 |
| H | -1.69590 | -1.77450 | 2.25970 |
| H | -3.64160 | -0.20840 | 0.79670 |
| H | -2.77710 | -0.15390 | -0.72870 |
| H | -4.43470 | -1.71530 | -1.76770 |
| H | -0.84860 | -5.86780 | -2.96830 |
| H | -1.85630 | -4.43470 | -2.95200 |
| H | 1.22870 | -4.49440 | -3.31010 |
| H | -1.00010 | -2.66040 | -4.39560 |
| H | 1.00960 | -0.33000 | -5.40790 |
| H | 1.33970 | -1.37400 | -6.82500 |
| H | -0.29480 | -1.28780 | -6.15670 |
| H | -6.61890 | -2.12210 | -0.76070 |
| H | -4.55830 | 0.52830 | -1.93900 |

Table S6. Cont.

| Marilzafurollene_A_42 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59430 |
| O | -2.12450 | -2.71510 | -0.89830 |
| C | -0.67230 | -4.69810 | -1.17060 |
| C | -0.62100 | -3.13330 | 0.91080 |
| C | -2.61550 | -2.05290 | 0.28750 |
| C | -1.41390 | -1.88040 | 1.22340 |
| C | -3.38110 | -0.78600 | -0.08890 |
| Cl | -0.42400 | -0.42950 | 0.87610 |
| C | -4.64330 | -1.06690 | -0.91880 |
| C | -0.83660 | -4.70350 | -2.70110 |
| Br | -2.00980 | -5.92290 | -0.38540 |
| C | -0.34470 | -5.97200 | -3.35350 |
| C | 0.68490 | -6.02000 | -4.21360 |
| C | 1.10880 | -7.31120 | -4.83070 |
| C | 2.24050 | -7.25450 | -5.82300 |
| O | 0.57660 | -8.37700 | -4.52540 |
| C | -5.73650 | -1.83630 | -0.23160 |
| O | -5.20300 | 0.18230 | -1.33280 |
| C | -6.06040 | -1.75910 | 1.02880 |
| C | -6.38620 | -1.67560 | 2.27970 |
| H | -6.21240 | -2.45310 | 3.01180 |
| Br | -6.93880 | -0.03490 | 2.91240 |
| H | -0.10200 | -2.63850 | -1.10090 |
| H | 0.30040 | -5.11000 | -0.87890 |
| H | -1.05540 | -3.96920 | 1.46850 |
| H | 0.43850 | -3.08060 | 1.18090 |
| H | -3.30030 | -2.76630 | 0.76270 |
| H | -1.71360 | -1.81610 | 2.27300 |
| H | -3.63960 | -0.21460 | 0.81150 |
| H | -2.74460 | -0.12810 | -0.69460 |
| H | -4.36360 | -1.60190 | -1.83330 |
| H | -1.88700 | -4.55610 | -2.98210 |
| H | -0.28420 | -3.85300 | -3.12170 |
| H | -0.88350 | -6.88820 | -3.11290 |
| H | 1.24020 | -5.13230 | -4.49340 |
| H | 2.01720 | -7.92240 | -6.65980 |
| H | 2.36480 | -6.24500 | -6.22420 |
| H | 3.16640 | -7.56660 | -5.33360 |
| H | -6.42730 | -2.34690 | -0.89850 |
| H | -5.56140 | 0.61140 | -0.53550 |

Table S6. Cont.

| Marilzafurollene_A_43 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83280 | -3.28310 | -0.59460 |
| O | -2.12450 | -2.71500 | -0.89800 |
| C | -0.67680 | -4.70170 | -1.16420 |
| C | -0.62400 | -3.13650 | 0.91180 |
| C | -2.61590 | -2.05270 | 0.28740 |
| C | -1.41640 | -1.88400 | 1.22640 |
| C | -3.37880 | -0.78400 | -0.08840 |
| Cl | -0.42460 | -0.43260 | 0.88800 |
| C | -4.63990 | -1.06160 | -0.92100 |
| C | -0.84060 | -4.77270 | -2.69170 |
| Br | -2.02200 | -5.92460 | -0.38590 |
| C | 0.26050 | -4.06470 | -3.44130 |
| C | 0.04020 | -3.01170 | -4.24370 |
| C | 1.09230 | -2.29230 | -5.01550 |
| C | 2.53010 | -2.72630 | -4.90190 |
| O | 0.75690 | -1.35120 | -5.73510 |
| C | -5.73510 | -1.83180 | -0.23790 |
| O | -5.19830 | 0.18880 | -1.33280 |
| C | -6.05920 | -1.76020 | 1.02290 |
| C | -6.38490 | -1.68220 | 2.27410 |
| H | -6.21350 | -2.46390 | 3.00220 |
| Br | -6.93240 | -0.04310 | 2.91540 |
| H | -0.10080 | -2.63560 | -1.09360 |
| H | 0.28820 | -5.12520 | -0.86310 |
| H | -1.06010 | -3.97320 | 1.46680 |
| H | 0.43500 | -3.08550 | 1.18430 |
| H | -3.30290 | -2.76530 | 0.76050 |
| H | -1.71890 | -1.82330 | 2.27540 |
| H | -3.63800 | -0.21360 | 0.81250 |
| H | -2.74010 | -0.12620 | -0.69190 |
| H | -4.35910 | -1.59450 | -1.83640 |
| H | -0.82560 | -5.82130 | -3.01770 |
| H | -1.82290 | -4.38180 | -2.98750 |
| H | 1.25980 | -4.47350 | -3.31290 |
| H | -0.96000 | -2.60830 | -4.37940 |
| H | 2.64370 | -3.75080 | -5.26560 |
| H | 3.15390 | -2.07200 | -5.51860 |
| H | 2.86830 | -2.64270 | -3.86590 |
| H | -6.42710 | -2.33690 | -0.90760 |
| H | -5.55160 | 0.61930 | -0.53400 |

Table S6. Cont.

| Marilzafurollene_A_44 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83280 | -3.28320 | -0.59470 |
| O | -2.12440 | -2.71490 | -0.89770 |
| C | -0.67720 | -4.69990 | -1.16900 |
| C | -0.62530 | -3.13910 | 0.91240 |
| C | -2.61600 | -2.05270 | 0.28730 |
| C | -1.41790 | -1.88700 | 1.22860 |
| C | -3.37620 | -0.78270 | -0.08970 |
| Cl | -0.42610 | -0.43440 | 0.89690 |
| C | -4.63440 | -1.05840 | -0.92720 |
| C | -0.84580 | -4.77940 | -2.69640 |
| Br | -2.02010 | -5.92470 | -0.38400 |
| C | 0.23960 | -4.06390 | -3.45670 |
| C | 1.16420 | -4.68700 | -4.20420 |
| C | 2.20200 | -3.90920 | -4.94210 |
| C | 3.14270 | -4.68820 | -5.82340 |
| O | 2.30160 | -2.68980 | -4.81670 |
| C | -5.73080 | -1.83060 | -0.24820 |
| O | -5.19190 | 0.19280 | -1.33800 |
| C | -6.06930 | -1.74840 | 1.00810 |
| C | -6.40990 | -1.66020 | 2.25460 |
| H | -6.23680 | -2.43080 | 2.99410 |
| Br | -7.00830 | -0.02760 | 2.86610 |
| H | -0.10040 | -2.63350 | -1.08960 |
| H | 0.28840 | -5.12360 | -0.87020 |
| H | -1.06190 | -3.97650 | 1.46590 |
| H | 0.43340 | -3.08860 | 1.18590 |
| H | -3.30530 | -2.76420 | 0.75890 |
| H | -1.72240 | -1.82920 | 2.27730 |
| H | -3.63810 | -0.21320 | 0.81100 |
| H | -2.73480 | -0.12470 | -0.69010 |
| H | -4.35070 | -1.58930 | -1.84280 |
| H | -0.86770 | -5.83220 | -3.00900 |
| H | -1.81360 | -4.35990 | -2.99930 |
| H | 0.23770 | -2.97540 | -3.40370 |
| H | 1.19030 | -5.76620 | -4.30240 |
| H | 3.28590 | -4.14560 | -6.76210 |
| H | 4.10080 | -4.80840 | -5.31170 |
| H | 2.73520 | -5.67370 | -6.06430 |
| H | -6.41010 | -2.35030 | -0.91980 |
| H | -5.55050 | 0.62000 | -0.53980 |

Table S6. Cont.

| Marilzafurollene_A_45 | | | |
|------------------------------|-----------|----------|----------|
| C | -0.83280 | -3.28300 | -0.59400 |
| O | -2.12480 | -2.71520 | -0.89920 |
| C | -0.67460 | -4.70340 | -1.15690 |
| C | -0.61600 | -3.12170 | 0.90930 |
| C | -2.61550 | -2.05270 | 0.28800 |
| C | -1.40950 | -1.86760 | 1.21540 |
| C | -3.38660 | -0.79150 | -0.09520 |
| Cl | -0.42500 | -0.41810 | 0.84470 |
| C | -4.66580 | -1.08830 | -0.89390 |
| C | -0.83810 | -4.72380 | -2.68640 |
| Br | -2.01710 | -5.92090 | -0.36870 |
| C | -0.38200 | -6.01460 | -3.31780 |
| C | -1.18640 | -6.82860 | -4.01900 |
| C | -0.66340 | -8.09090 | -4.61750 |
| C | -1.65210 | -8.96400 | -5.34460 |
| O | 0.52590 | -8.39520 | -4.54070 |
| C | -5.78550 | -1.76190 | -0.15310 |
| O | -5.20210 | 0.14600 | -1.37770 |
| C | -5.94450 | -1.84080 | 1.13830 |
| C | -6.11240 | -1.92610 | 2.41980 |
| H | -5.95600 | -2.82590 | 2.99970 |
| Br | -6.47540 | -0.37790 | 3.35020 |
| H | -0.10250 | -2.64430 | -1.10890 |
| H | 0.29610 | -5.11610 | -0.85950 |
| H | -1.04720 | -3.95450 | 1.47410 |
| H | 0.44430 | -3.06540 | 1.17560 |
| H | -3.29260 | -2.76970 | 0.76770 |
| H | -1.70270 | -1.79300 | 2.26610 |
| H | -3.62790 | -0.20090 | 0.79750 |
| H | -2.75610 | -0.14970 | -0.72380 |
| H | -4.42300 | -1.69630 | -1.77320 |
| H | -1.87660 | -4.50520 | -2.96690 |
| H | -0.22580 | -3.92510 | -3.12430 |
| H | 0.66890 | -6.27350 | -3.19210 |
| H | -2.23660 | -6.60500 | -4.16720 |
| H | -1.53140 | -8.82640 | -6.42190 |
| H | -10.00910 | -5.07870 | |
| H | -2.67970 | -8.71990 | -5.06200 |
| H | -6.61760 | -2.07780 | -0.77750 |
| H | -4.52580 | 0.54190 | -1.95420 |

Table S6. Cont.

| Marilzafurollene_A_46 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83330 | -3.28270 | -0.59380 |
| O | -2.12490 | -2.71490 | -0.89850 |
| C | -0.68410 | -4.70540 | -1.15430 |
| C | -0.61500 | -3.11880 | 0.91020 |
| C | -2.61490 | -2.05330 | 0.28720 |
| C | -1.41160 | -1.86640 | 1.21770 |
| C | -3.40690 | -0.80220 | -0.08380 |
| Cl | -0.42780 | -0.41530 | 0.85630 |
| C | -4.60750 | -1.08110 | -0.99770 |
| C | -0.88350 | -4.80560 | -2.67700 |
| Br | -2.00870 | -5.92440 | -0.33000 |
| C | 0.14260 | -4.04270 | -3.47740 |
| C | 1.11120 | -4.63870 | -4.18960 |
| C | 2.12700 | -3.92430 | -5.01360 |
| C | 2.08520 | -2.42240 | -5.11680 |
| O | 2.98550 | -4.58870 | -5.59480 |
| C | -5.62350 | -2.01650 | -0.40070 |
| O | -5.22190 | 0.17380 | -1.30070 |
| C | -6.63360 | -1.68170 | 0.35190 |
| C | -7.63790 | -1.34540 | 1.09700 |
| H | -7.57250 | -1.11960 | 2.15280 |
| Br | -9.29150 | -1.19400 | 0.29880 |
| H | -0.10230 | -2.64110 | -1.10150 |
| H | 0.28880 | -5.12190 | -0.86980 |
| H | -1.04220 | -3.95130 | 1.47810 |
| H | 0.44570 | -3.05970 | 1.17440 |
| H | -3.28870 | -2.77190 | 0.77160 |
| H | -1.70740 | -1.79630 | 2.26800 |
| H | -3.74020 | -0.28630 | 0.82600 |
| H | -2.76520 | -0.09110 | -0.61900 |
| H | -4.26130 | -1.49970 | -1.94960 |
| H | -0.86300 | -5.86180 | -2.97870 |
| H | -1.87850 | -4.43840 | -2.96000 |
| H | 0.03610 | -2.96040 | -3.47380 |
| H | 1.21330 | -5.72040 | -4.20750 |
| H | 2.23870 | -1.97320 | -4.13220 |
| H | 2.88890 | -2.08390 | -5.77790 |
| H | 1.13260 | -2.10030 | -5.54550 |
| H | -5.43690 | -3.07660 | -0.55640 |
| H | -6.07010 | -0.02340 | -1.73560 |

Table S6. Cont.

| Marilzafurollene_A_47 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83270 | -3.28390 | -0.59650 |
| O | -2.12250 | -2.71520 | -0.89580 |
| C | -0.62320 | -4.67330 | -1.21680 |
| C | -0.66870 | -3.20680 | 0.92000 |
| C | -2.61790 | -2.05170 | 0.28710 |
| C | -1.43960 | -1.94780 | 1.26180 |
| C | -3.31000 | -0.74760 | -0.10450 |
| Cl | -0.40350 | -0.50970 | 1.00540 |
| C | -4.55780 | -0.96850 | -0.96920 |
| C | -0.55500 | -4.68110 | -2.75680 |
| Br | -1.99000 | -5.95520 | -0.61540 |
| C | -1.76440 | -4.15110 | -3.48570 |
| C | -1.75810 | -3.01660 | -4.20220 |
| C | -2.94710 | -2.44790 | -4.89480 |
| C | -4.24710 | -3.20850 | -4.89800 |
| O | -2.83820 | -1.35350 | -5.44910 |
| C | -5.70350 | -1.55730 | -0.20420 |
| O | -5.01020 | 0.30100 | -1.44440 |
| C | -6.12930 | -2.78360 | -0.31200 |
| C | -6.55350 | -4.00270 | -0.41310 |
| H | -7.25930 | -4.34860 | -1.15620 |
| Br | -5.95580 | -5.22870 | 0.82530 |
| H | -0.09570 | -2.60920 | -1.05260 |
| H | 0.31500 | -5.09370 | -0.83540 |
| H | -1.14740 | -4.05610 | 1.41930 |
| H | 0.38120 | -3.19530 | 1.22910 |
| H | -3.34920 | -2.73810 | 0.73100 |
| H | -1.76790 | -1.91830 | 2.30440 |
| H | -3.57410 | -0.17250 | 0.79220 |
| H | -2.62210 | -0.11940 | -0.68480 |
| H | -4.32460 | -1.58120 | -1.84760 |
| H | 0.33300 | -4.11000 | -3.05900 |
| H | -0.38020 | -5.70620 | -3.10900 |
| H | -2.67190 | -4.74120 | -3.38610 |
| H | -0.86080 | -2.41190 | -4.29410 |
| H | -4.98150 | -2.66410 | -5.49940 |
| H | -4.10620 | -4.19560 | -5.34580 |
| H | -4.63390 | -3.29670 | -3.87950 |
| H | -6.20770 | -0.89800 | 0.49720 |
| H | -4.35810 | 0.59870 | -2.10360 |

Table S6. Cont.

| Marilzafurollene_A_48 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28300 | -0.59450 |
| O | -2.12430 | -2.71510 | -0.89800 |
| C | -0.67650 | -4.69880 | -1.17000 |
| C | -0.62120 | -3.13290 | 0.91130 |
| C | -2.61580 | -2.05270 | 0.28740 |
| C | -1.41520 | -1.88080 | 1.22480 |
| C | -3.38060 | -0.78560 | -0.09010 |
| Cl | -0.42650 | -0.42830 | 0.88200 |
| C | -4.64080 | -1.06620 | -0.92310 |
| C | -0.88130 | -4.78540 | -2.69290 |
| Br | -1.98580 | -5.93780 | -0.35250 |
| C | 0.13150 | -4.00120 | -3.48940 |
| C | 1.10650 | -4.57700 | -4.20940 |
| C | 2.10970 | -3.84070 | -5.02950 |
| C | 2.04590 | -2.33870 | -5.11940 |
| O | 2.97630 | -4.48750 | -5.61870 |
| C | -5.73580 | -1.83570 | -0.23900 |
| O | -5.19900 | 0.18310 | -1.33850 |
| C | -6.06100 | -1.76110 | 1.02130 |
| C | -6.38770 | -1.68000 | 2.27210 |
| H | -6.21530 | -2.45920 | 3.00270 |
| Br | -6.93930 | -0.04000 | 2.90780 |
| H | -0.10190 | -2.63440 | -1.09300 |
| H | 0.30110 | -5.11030 | -0.89390 |
| H | -1.05460 | -3.96800 | 1.47060 |
| H | 0.43830 | -3.07940 | 1.18120 |
| H | -3.30130 | -2.76590 | 0.76190 |
| H | -1.71640 | -1.81850 | 2.27410 |
| H | -3.64100 | -0.21460 | 0.81000 |
| H | -2.74280 | -0.12750 | -0.69410 |
| H | -4.35890 | -1.60110 | -1.83700 |
| H | -0.84910 | -5.83800 | -3.00570 |
| H | -1.88210 | -4.42760 | -2.96760 |
| H | 0.00910 | -2.92060 | -3.47590 |
| H | 1.22400 | -5.65690 | -4.23700 |
| H | 1.08850 | -2.02680 | -5.54470 |
| H | 2.19350 | -1.89610 | -4.13090 |
| H | 2.84420 | -1.98260 | -5.77770 |
| H | -6.42660 | -2.34380 | -0.90780 |
| H | -5.55990 | 0.61210 | -0.54220 |

Table S6. Cont.

| Marilzafurollene_A_49 | | | |
|------------------------------|----------|-----------|----------|
| C | -0.83320 | -3.28290 | -0.59460 |
| O | -2.12390 | -2.71530 | -0.89830 |
| C | -0.65540 | -4.68580 | -1.19880 |
| C | -0.63720 | -3.16160 | 0.91480 |
| C | -2.61600 | -2.05250 | 0.28770 |
| C | -1.42160 | -1.90580 | 1.23780 |
| C | -3.35480 | -0.77070 | -0.09190 |
| Cl | -0.41250 | -0.46000 | 0.92380 |
| C | -4.61940 | -1.02940 | -0.91950 |
| C | -0.81710 | -4.65950 | -2.73060 |
| Br | -1.98790 | -5.93640 | -0.44930 |
| C | -0.37530 | -5.86180 | -3.53400 |
| C | 0.24470 | -6.96900 | -3.09610 |
| C | 0.60640 | -8.06530 | -4.04460 |
| C | 1.23240 | -9.30060 | -3.45180 |
| O | 0.42750 | -7.95590 | -5.25650 |
| C | -5.71310 | -1.68490 | -0.13050 |
| O | -5.12530 | 0.23530 | -1.35220 |
| C | -6.18940 | -2.87600 | -0.35570 |
| C | -6.66370 | -4.06120 | -0.57290 |
| H | -7.43180 | -4.29280 | -1.29860 |
| Br | -6.10260 | -5.42810 | 0.52780 |
| H | -0.10100 | -2.62470 | -1.08150 |
| H | 0.32130 | -5.08530 | -0.90660 |
| H | -1.08810 | -4.00160 | 1.45270 |
| H | 0.41930 | -3.12410 | 1.19870 |
| H | -3.31860 | -2.75550 | 0.75270 |
| H | -1.73110 | -1.85400 | 2.28530 |
| H | -3.60960 | -0.19850 | 0.80950 |
| H | -2.70280 | -0.12530 | -0.69440 |
| H | -4.37290 | -1.60710 | -1.81800 |
| H | -1.86680 | -4.46350 | -2.98690 |
| H | -0.24420 | -3.80960 | -3.12490 |
| H | -0.60050 | -5.78320 | -4.59920 |
| H | 0.50480 | -7.12650 | -2.05740 |
| H | 0.98470 | -9.39820 | -2.39130 |
| H | 0.84380 | -10.18270 | -3.96850 |
| H | 2.31760 | -9.24830 | -3.56900 |
| H | -6.13670 | -1.10780 | 0.68730 |
| H | -5.87590 | 0.04460 | -1.94230 |

Table S6. Cont.

| Marilzafurollene_A_50 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83250 | -3.28350 | -0.59500 |
| O | -2.12420 | -2.71500 | -0.89780 |
| C | -0.66170 | -4.68760 | -1.19520 |
| C | -0.63770 | -3.16250 | 0.91490 |
| C | -2.61650 | -2.05230 | 0.28760 |
| C | -1.42330 | -1.90800 | 1.23910 |
| C | -3.34920 | -0.76740 | -0.09740 |
| Cl | -0.41910 | -0.45770 | 0.93080 |
| C | -4.63560 | -1.02580 | -0.89480 |
| C | -0.83660 | -4.72820 | -2.72240 |
| Br | -1.98220 | -5.94610 | -0.43550 |
| C | 0.22880 | -3.96150 | -3.45920 |
| C | -0.02220 | -2.88020 | -4.21370 |
| C | 1.08080 | -2.16450 | -4.91730 |
| C | 0.69840 | -0.97090 | -5.75230 |
| O | 2.25330 | -2.51730 | -4.80010 |
| C | -5.74110 | -1.60510 | -0.06140 |
| O | -5.11360 | 0.21490 | -1.42210 |
| C | -6.15480 | -2.83900 | -0.12210 |
| C | -6.56420 | -4.06620 | -0.17610 |
| H | -7.29920 | -4.43940 | -0.87650 |
| Br | -5.91320 | -5.24600 | 1.08060 |
| H | -0.10010 | -2.62160 | -1.07430 |
| H | 0.31160 | -5.10300 | -0.91020 |
| H | -1.08790 | -4.00290 | 1.45270 |
| H | 0.41860 | -3.12400 | 1.19940 |
| H | -3.32110 | -2.75280 | 0.75200 |
| H | -1.73470 | -1.85920 | 2.28620 |
| H | -3.58080 | -0.18010 | 0.80050 |
| H | -2.70140 | -0.13970 | -0.72270 |
| H | -4.42570 | -1.66860 | -1.75710 |
| H | -0.78810 | -5.76730 | -3.07420 |
| H | -1.83430 | -4.36450 | -3.00110 |
| H | 1.24940 | -4.33210 | -3.36750 |
| H | -1.02570 | -2.48590 | -4.32950 |
| H | 1.26650 | -0.99040 | -6.68650 |
| H | -0.36500 | -0.98930 | -6.00590 |
| H | 0.92230 | -0.05590 | -5.19830 |
| H | -6.22100 | -0.94570 | 0.65580 |
| H | -5.16310 | 0.85130 | -0.68870 |

Table S6. Cont.

| Marilzafurollene_A_51 | | | |
|------------------------------|----------|-----------|----------|
| C | -0.83310 | -3.28300 | -0.59440 |
| O | -2.12420 | -2.71530 | -0.89860 |
| C | -0.66450 | -4.69620 | -1.17720 |
| C | -0.62490 | -3.13870 | 0.91160 |
| C | -2.61590 | -2.05250 | 0.28780 |
| C | -1.41470 | -1.88380 | 1.22490 |
| C | -3.37080 | -0.78290 | -0.10010 |
| Cl | -0.42120 | -0.43460 | 0.87780 |
| C | -4.64810 | -1.06710 | -0.90130 |
| C | -0.83070 | -4.69300 | -2.70870 |
| Br | -2.00240 | -5.92700 | -0.40460 |
| C | -0.39850 | -5.91020 | -3.49440 |
| C | 0.21680 | -7.01400 | -3.04130 |
| C | 0.56920 | -8.12690 | -3.97410 |
| C | 1.19200 | -9.35580 | -3.36500 |
| O | 0.38510 | -8.03560 | -5.18660 |
| C | -5.73850 | -1.67070 | -0.06930 |
| O | -5.16380 | 0.17450 | -1.38700 |
| C | -6.12300 | -2.91420 | -0.12060 |
| C | -6.50710 | -4.14990 | -0.16810 |
| H | -7.21320 | -4.54610 | -0.88540 |
| Br | -5.91990 | -5.28570 | 1.15850 |
| H | -0.10210 | -2.63490 | -1.09670 |
| H | 0.31080 | -5.09660 | -0.88170 |
| H | -1.06430 | -3.97470 | 1.46500 |
| H | 0.43390 | -3.09000 | 1.18530 |
| H | -3.30520 | -2.76020 | 0.76430 |
| H | -1.71460 | -1.81900 | 2.27440 |
| H | -3.61600 | -0.19750 | 0.79540 |
| H | -2.73150 | -0.14410 | -0.72290 |
| H | -4.43400 | -1.69520 | -1.77400 |
| H | -1.88000 | -4.49450 | -2.96510 |
| H | -0.25390 | -3.85290 | -3.11790 |
| H | -0.62690 | -5.84730 | -4.56010 |
| H | 0.47970 | -7.15660 | -2.00120 |
| H | 0.95900 | -9.42980 | -2.29930 |
| H | 0.78790 | -10.24440 | -3.85830 |
| H | 2.27580 | -9.31610 | -3.49840 |
| H | -6.24690 | -1.00390 | 0.62180 |
| H | -4.53090 | 0.49700 | -2.05240 |

Table S6. Cont.

| Marilzafurollene_A_52 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28360 | -0.59610 |
| O | -2.12290 | -2.71510 | -0.89610 |
| C | -0.62060 | -4.67750 | -1.20500 |
| C | -0.66430 | -3.20230 | 0.92040 |
| C | -2.61730 | -2.05210 | 0.28700 |
| C | -1.43940 | -1.94780 | 1.26360 |
| C | -3.31430 | -0.74420 | -0.08270 |
| Cl | -0.40230 | -0.50880 | 1.01600 |
| C | -4.53940 | -0.93510 | -0.98360 |
| C | -0.57470 | -4.70960 | -2.74460 |
| Br | -1.95920 | -5.96970 | -0.56230 |
| C | -1.80070 | -4.21370 | -3.46930 |
| C | -1.79670 | -3.15440 | -4.29290 |
| C | -2.99570 | -2.63610 | -5.00800 |
| C | -4.32900 | -3.31050 | -4.82070 |
| O | -2.86580 | -1.65870 | -5.74620 |
| C | -5.66190 | -1.67020 | -0.31520 |
| O | -5.03760 | 0.36230 | -1.31660 |
| C | -6.27120 | -2.71120 | -0.80670 |
| C | -6.88130 | -3.74270 | -1.29750 |
| H | -7.79140 | -3.69610 | -1.88070 |
| Br | -6.03310 | -5.37480 | -1.19370 |
| H | -0.09720 | -2.61120 | -1.05740 |
| H | 0.32800 | -5.08280 | -0.83250 |
| H | -1.13680 | -4.05140 | 1.42520 |
| H | 0.38680 | -3.18630 | 1.22540 |
| H | -3.34910 | -2.74110 | 0.72800 |
| H | -1.76950 | -1.92220 | 2.30580 |
| H | -3.60080 | -0.19990 | 0.82670 |
| H | -2.62220 | -0.08920 | -0.62730 |
| H | -4.24320 | -1.42370 | -1.91900 |
| H | 0.30120 | -4.13180 | -3.06850 |
| H | -0.39050 | -5.73910 | -3.07900 |
| H | -2.71630 | -4.77040 | -3.28610 |
| H | -0.88940 | -2.58850 | -4.48170 |
| H | -4.28210 | -4.34370 | -5.17430 |
| H | -4.62480 | -3.27350 | -3.76970 |
| H | -5.08660 | -2.78110 | -5.40660 |
| H | -6.00680 | -1.27430 | 0.63620 |
| H | -5.76150 | 0.22570 | -1.95300 |

Table S6. Cont.

| Marilzafurollene_A_53 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83260 | -3.28360 | -0.59570 |
| O | -2.12330 | -2.71520 | -0.89700 |
| C | -0.63960 | -4.69790 | -1.16280 |
| C | -0.64150 | -3.15760 | 0.91580 |
| C | -2.61720 | -2.05190 | 0.28750 |
| C | -1.42390 | -1.90130 | 1.23690 |
| C | -3.35910 | -0.77140 | -0.09020 |
| Cl | -0.41400 | -0.45730 | 0.91670 |
| C | -4.62080 | -1.02950 | -0.92160 |
| C | -0.57210 | -4.78190 | -2.69980 |
| Br | -2.01510 | -5.94190 | -0.50640 |
| C | -1.78440 | -4.31620 | -3.46700 |
| C | -2.52750 | -5.12750 | -4.23570 |
| C | -3.72660 | -4.70160 | -5.01000 |
| C | -4.19780 | -3.27360 | -4.93350 |
| O | -4.31020 | -5.53690 | -5.70150 |
| C | -5.71030 | -1.70750 | -0.14670 |
| O | -5.13580 | 0.23610 | -1.33960 |
| C | -6.19210 | -2.88910 | -0.40730 |
| C | -6.67210 | -4.06550 | -0.65730 |
| H | -7.44410 | -4.27420 | -1.38570 |
| Br | -6.09070 | -5.47060 | 0.38260 |
| H | -0.09800 | -2.63110 | -1.08620 |
| H | 0.29640 | -5.10860 | -0.76520 |
| H | -1.09640 | -3.99860 | 1.44990 |
| H | 0.41430 | -3.12240 | 1.20320 |
| H | -3.31860 | -2.75600 | 0.75330 |
| H | -1.73300 | -1.84630 | 2.28440 |
| H | -3.61710 | -0.20200 | 0.81190 |
| H | -2.70760 | -0.12270 | -0.68960 |
| H | -4.36680 | -1.59180 | -1.82730 |
| H | 0.27900 | -4.17770 | -3.04060 |
| H | -0.33160 | -5.81500 | -2.98560 |
| H | -2.02590 | -3.26030 | -3.37560 |
| H | -2.28940 | -6.18240 | -4.33550 |
| H | -4.47360 | -3.02500 | -3.90580 |
| H | -3.42110 | -2.59870 | -5.30180 |
| H | -5.08400 | -3.15110 | -5.56400 |
| H | -6.13000 | -1.15440 | 0.68970 |
| H | -5.91680 | 0.05090 | -1.89060 |

Table S6. Cont.

| Marilzafurollene_A_54 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83320 | -3.28290 | -0.59450 |
| O | -2.12400 | -2.71540 | -0.89860 |
| C | -0.65340 | -4.68460 | -1.20070 |
| C | -0.63900 | -3.16420 | 0.91520 |
| C | -2.61600 | -2.05250 | 0.28800 |
| C | -1.42190 | -1.90770 | 1.23870 |
| C | -3.35170 | -0.76910 | -0.09250 |
| Cl | -0.41160 | -0.46250 | 0.92530 |
| C | -4.62920 | -1.02830 | -0.90010 |
| C | -0.81210 | -4.65530 | -2.73320 |
| Br | -1.98970 | -5.93570 | -0.45980 |
| C | -0.38490 | -5.86280 | -3.54140 |
| C | 0.28010 | -6.94370 | -3.10430 |
| C | 0.67060 | -8.10270 | -3.95840 |
| C | 0.26170 | -8.13890 | -5.40760 |
| O | 1.32900 | -9.01130 | -3.45070 |
| C | -5.72100 | -1.65140 | -0.08250 |
| O | -5.12420 | 0.23340 | -1.35360 |
| C | -6.20290 | -2.84810 | -0.26100 |
| C | -6.68110 | -4.03980 | -0.42820 |
| H | -7.46510 | -4.29660 | -1.12780 |
| Br | -6.05160 | -5.38080 | 0.66740 |
| H | -0.10070 | -2.62350 | -1.07960 |
| H | 0.32220 | -5.08370 | -0.90550 |
| H | -1.09190 | -4.00450 | 1.45110 |
| H | 0.41710 | -3.12850 | 1.20060 |
| H | -3.31960 | -2.75480 | 0.75220 |
| H | -1.73180 | -1.85600 | 2.28600 |
| H | -3.59190 | -0.18790 | 0.80730 |
| H | -2.70320 | -0.13310 | -0.70870 |
| H | -4.40200 | -1.62850 | -1.78880 |
| H | -1.86060 | -4.44990 | -2.98780 |
| H | -0.23290 | -3.80980 | -3.12780 |
| H | -0.66690 | -5.79260 | -4.59090 |
| H | 0.59220 | -7.05390 | -2.07120 |
| H | 0.59210 | -9.08300 | -5.85150 |
| H | -0.82660 | -8.08580 | -5.49470 |
| H | 0.73540 | -7.31840 | -5.95240 |
| H | -6.12980 | -1.04800 | 0.72390 |
| H | -5.88630 | 0.04040 | -1.92800 |

Table S6. Cont.

| Marilzafurollene_A_55 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28360 | -0.59610 |
| O | -2.12270 | -2.71530 | -0.89640 |
| C | -0.61640 | -4.67150 | -1.21660 |
| C | -0.67270 | -3.21460 | 0.92150 |
| C | -2.61750 | -2.05190 | 0.28730 |
| C | -1.44270 | -1.95760 | 1.26830 |
| C | -3.30450 | -0.74000 | -0.08740 |
| Cl | -0.39930 | -0.52160 | 1.03060 |
| C | -4.54050 | -0.93420 | -0.97280 |
| C | -0.54440 | -4.68420 | -2.75570 |
| Br | -1.97390 | -5.96280 | -0.61330 |
| C | -1.75590 | -4.17260 | -3.49370 |
| C | -1.73740 | -3.09380 | -4.29150 |
| C | -2.92320 | -2.55990 | -5.01710 |
| C | -4.26020 | -3.23750 | -4.86790 |
| O | -2.77970 | -1.56840 | -5.73340 |
| C | -5.67620 | -1.60490 | -0.26080 |
| O | -5.00620 | 0.35990 | -1.36050 |
| C | -6.17250 | -2.76910 | -0.56810 |
| C | -6.66760 | -3.92870 | -0.86240 |
| H | -7.42970 | -4.10160 | -1.61040 |
| Br | -6.09420 | -5.38230 | 0.11330 |
| H | -0.09580 | -2.60610 | -1.04760 |
| H | 0.32380 | -5.08610 | -0.83330 |
| H | -1.15370 | -4.06530 | 1.41610 |
| H | 0.37650 | -3.20640 | 1.23330 |
| H | -3.35390 | -2.73750 | 0.72510 |
| H | -1.77630 | -1.93540 | 2.30940 |
| H | -3.57790 | -0.18360 | 0.81850 |
| H | -2.61090 | -0.09860 | -0.64620 |
| H | -4.26860 | -1.47190 | -1.88840 |
| H | 0.33940 | -4.10650 | -3.05750 |
| H | -0.35940 | -5.71010 | -3.10060 |
| H | -2.67360 | -4.73520 | -3.34270 |
| H | -0.82760 | -2.52230 | -4.44860 |
| H | -4.21050 | -4.25720 | -5.25830 |
| H | -4.56910 | -3.23870 | -3.81950 |
| H | -5.01020 | -2.68520 | -5.44240 |
| H | -6.10750 | -1.06820 | 0.58030 |
| H | -5.72500 | 0.21560 | -2.00100 |

Table S6. Cont.

| Marilzafurollene_A_56 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83350 | -3.28390 | -0.59770 |
| O | -2.12130 | -2.71480 | -0.89270 |
| C | -0.66060 | -4.70170 | -1.16290 |
| C | -0.62790 | -3.13910 | 0.91030 |
| C | -2.61830 | -2.05220 | 0.28530 |
| C | -1.42280 | -1.88840 | 1.22950 |
| C | -3.37750 | -0.78530 | -0.10240 |
| Cl | -0.42430 | -0.43820 | 0.90350 |
| C | -4.56380 | -1.05140 | -1.03770 |
| C | -0.70810 | -4.80390 | -2.70080 |
| Br | -1.97260 | -5.95880 | -0.39960 |
| C | -1.97200 | -4.33670 | -3.37480 |
| C | -2.85980 | -5.15580 | -3.95890 |
| C | -4.10810 | -4.61990 | -4.57480 |
| C | -5.11100 | -5.63090 | -5.06480 |
| O | -4.30390 | -3.41220 | -4.70090 |
| C | -5.66050 | -1.84980 | -0.39930 |
| O | -5.13010 | 0.21290 | -1.39120 |
| C | -6.19530 | -2.92090 | -0.91230 |
| C | -6.73180 | -3.97520 | -1.43880 |
| H | -7.48650 | -3.95550 | -2.21340 |
| Br | -6.10120 | -5.62420 | -0.91510 |
| H | -0.10190 | -2.64030 | -1.10420 |
| H | 0.30470 | -5.09830 | -0.82600 |
| H | -1.06520 | -3.97810 | 1.46120 |
| H | 0.43050 | -3.08870 | 1.18540 |
| H | -3.31490 | -2.75910 | 0.75460 |
| H | -1.72840 | -1.83310 | 2.27790 |
| H | -3.71600 | -0.25710 | 0.79830 |
| H | -2.71230 | -0.09150 | -0.63160 |
| H | -4.21240 | -1.52390 | -1.96280 |
| H | 0.11960 | -4.21250 | -3.11340 |
| H | -0.50070 | -5.84200 | -2.99420 |
| H | -2.15850 | -3.26310 | -3.37040 |
| H | -2.72060 | -6.23040 | -3.97440 |
| H | -4.97630 | -6.59420 | -4.56520 |
| H | -6.11970 | -5.27460 | -4.83700 |
| H | -4.99670 | -5.76090 | -6.14370 |
| H | -6.07880 | -1.45600 | 0.52290 |
| H | -5.77180 | 0.02990 | -2.10080 |

Table S6. Cont.

| Marilzafurollene_A_57 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28290 | -0.59410 |
| O | -2.12460 | -2.71530 | -0.89920 |
| C | -0.67280 | -4.70060 | -1.16480 |
| C | -0.61910 | -3.12740 | 0.91020 |
| C | -2.61560 | -2.05260 | 0.28810 |
| C | -1.41080 | -1.87270 | 1.21830 |
| C | -3.38160 | -0.78840 | -0.09530 |
| Cl | -0.42260 | -0.42400 | 0.85370 |
| C | -4.66220 | -1.08060 | -0.89340 |
| C | -0.83360 | -4.71110 | -2.69560 |
| Br | -2.01080 | -5.92300 | -0.37790 |
| C | -0.37570 | -5.99770 | -3.34260 |
| C | 0.69200 | -6.07640 | -4.15170 |
| C | 1.16620 | -7.32260 | -4.81760 |
| C | 0.41700 | -8.61290 | -4.61250 |
| O | 2.17170 | -7.26440 | -5.52610 |
| C | -5.78330 | -1.75020 | -0.15120 |
| O | -5.19440 | 0.15530 | -1.37740 |
| C | -5.94820 | -1.81530 | 1.14020 |
| C | -6.12240 | -1.88640 | 2.42180 |
| H | -5.96820 | -2.77930 | 3.01280 |
| Br | -6.49990 | -0.32950 | 3.33190 |
| H | -0.10210 | -2.64110 | -1.10440 |
| H | 0.29940 | -5.11220 | -0.87100 |
| H | -1.05340 | -3.96090 | 1.47150 |
| H | 0.44070 | -3.07400 | 1.17900 |
| H | -3.29610 | -2.76800 | 0.76540 |
| H | -1.70590 | -1.80040 | 2.26860 |
| H | -3.62040 | -0.19660 | 0.79710 |
| H | -2.74870 | -0.14930 | -0.72440 |
| H | -4.42200 | -1.69000 | -1.77250 |
| H | -1.87920 | -4.53740 | -2.98000 |
| H | -0.25920 | -3.87680 | -3.11920 |
| H | -0.98030 | -6.87670 | -3.13220 |
| H | 1.29570 | -5.20160 | -4.37660 |
| H | 0.90650 | -9.40850 | -5.18260 |
| H | 0.42960 | -8.89170 | -3.55560 |
| H | -0.60940 | -8.51460 | -4.97540 |
| H | -6.61250 | -2.07310 | -0.77600 |
| H | -4.51790 | 0.54750 | -1.95600 |

Table S6. Cont.

| Marilzafurollene_A_58 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83300 | -3.28290 | -0.59430 |
| O | -2.12430 | -2.71530 | -0.89880 |
| C | -0.66360 | -4.69570 | -1.17770 |
| C | -0.62490 | -3.13890 | 0.91170 |
| C | -2.61580 | -2.05260 | 0.28790 |
| C | -1.41460 | -1.88400 | 1.22500 |
| C | -3.37060 | -0.78260 | -0.09960 |
| Cl | -0.42080 | -0.43490 | 0.87730 |
| C | -4.64740 | -1.06610 | -0.90180 |
| C | -0.83530 | -4.69250 | -2.70910 |
| Br | -1.99850 | -5.92900 | -0.40470 |
| C | -0.41600 | -5.91400 | -3.50010 |
| C | 0.24960 | -6.98910 | -3.04960 |
| C | 0.63340 | -8.16230 | -3.88740 |
| C | 0.21820 | -8.21980 | -5.33410 |
| O | 1.29180 | -9.06450 | -3.36850 |
| C | -5.73760 | -1.67180 | -0.07120 |
| O | -5.16380 | 0.17590 | -1.38570 |
| C | -6.12310 | -2.91490 | -0.12620 |
| C | -6.50840 | -4.15010 | -0.17680 |
| H | -7.21590 | -4.54360 | -0.89420 |
| Br | -5.92120 | -5.29010 | 1.14620 |
| H | -0.10230 | -2.63460 | -1.09650 |
| H | 0.31300 | -5.09340 | -0.88370 |
| H | -1.06470 | -3.97490 | 1.46500 |
| H | 0.43380 | -3.09050 | 1.18560 |
| H | -3.30530 | -2.76020 | 0.76420 |
| H | -1.71430 | -1.81890 | 2.27450 |
| H | -3.61620 | -0.19790 | 0.79620 |
| H | -2.73100 | -0.14340 | -0.72150 |
| H | -4.43250 | -1.69250 | -1.77540 |
| H | -1.88550 | -4.48990 | -2.95870 |
| H | -0.25820 | -3.85470 | -3.12290 |
| H | -0.70420 | -5.86030 | -4.54880 |
| H | 0.56740 | -7.08350 | -2.01670 |
| H | -0.87050 | -8.16750 | -5.41720 |
| H | 0.68980 | -7.40760 | -5.89310 |
| H | 0.54660 | -9.17040 | -5.76540 |
| H | -6.24500 | -1.00710 | 0.62260 |
| H | -4.52860 | 0.50250 | -2.04680 |

Table S6. Cont.

| Marilzafurollene_A_59 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83310 | -3.28310 | -0.59480 |
| O | -2.12390 | -2.71520 | -0.89780 |
| C | -0.65820 | -4.68450 | -1.19800 |
| C | -0.63640 | -3.16200 | 0.91420 |
| C | -2.61610 | -2.05250 | 0.28750 |
| C | -1.42220 | -1.90780 | 1.23860 |
| C | -3.35010 | -0.76750 | -0.09510 |
| Cl | -0.41660 | -0.45880 | 0.92800 |
| C | -4.62870 | -1.02230 | -0.90600 |
| C | -0.81720 | -4.66180 | -2.72790 |
| Br | -1.98670 | -5.94000 | -0.45030 |
| C | -0.34680 | -5.92920 | -3.39550 |
| C | -1.14340 | -6.73230 | -4.11770 |
| C | -0.60850 | -7.97220 | -4.75090 |
| C | -1.59010 | -8.83860 | -5.49550 |
| O | 0.58460 | -8.26470 | -4.68680 |
| C | -5.73190 | -1.63630 | -0.09470 |
| O | -5.11980 | 0.22470 | -1.40540 |
| C | -6.14920 | -2.86500 | -0.21120 |
| C | -6.56420 | -4.08630 | -0.32410 |
| H | -7.29500 | -4.42230 | -1.04740 |
| Br | -5.96950 | -5.31530 | 0.91300 |
| H | -0.10100 | -2.62550 | -1.08280 |
| H | 0.31650 | -5.09440 | -0.90990 |
| H | -1.08570 | -4.00310 | 1.45180 |
| H | 0.42030 | -3.12330 | 1.19750 |
| H | -3.32050 | -2.75340 | 0.75210 |
| H | -1.73260 | -1.85820 | 2.28590 |
| H | -3.59050 | -0.18740 | 0.80520 |
| H | -2.69980 | -0.13270 | -0.71040 |
| H | -4.40470 | -1.64100 | -1.78220 |
| H | -1.85710 | -4.44550 | -3.00500 |
| H | -0.21190 | -3.84460 | -3.14060 |
| H | 0.70700 | -6.17980 | -3.27770 |
| H | -2.19630 | -6.51570 | -4.25740 |
| H | -1.40830 | -9.88630 | -5.24020 |
| H | -2.62060 | -8.59940 | -5.21900 |
| H | -1.46150 | -8.68800 | -6.57030 |
| H | -6.21320 | -1.00660 | 0.64780 |
| H | -5.18200 | 0.84240 | -0.65720 |

Table S6. Cont.

| Marilzafurollene_A_60 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28290 | -0.59410 |
| O | -2.12470 | -2.71520 | -0.89910 |
| C | -0.67460 | -4.70330 | -1.15770 |
| C | -0.61620 | -3.12190 | 0.90930 |
| C | -2.61560 | -2.05260 | 0.28800 |
| C | -1.40940 | -1.86750 | 1.21520 |
| C | -3.38650 | -0.79140 | -0.09520 |
| Cl | -0.42430 | -0.41850 | 0.84360 |
| C | -4.66750 | -1.08820 | -0.89090 |
| C | -0.83690 | -4.72280 | -2.68780 |
| Br | -2.01330 | -5.92250 | -0.36910 |
| C | -0.40140 | -6.02200 | -3.32380 |
| C | -1.22110 | -6.79130 | -4.05690 |
| C | -0.83240 | -8.07430 | -4.70690 |
| C | 0.56730 | -8.60430 | -4.53750 |
| O | -1.67380 | -8.67520 | -5.37570 |
| C | -5.78640 | -1.75900 | -0.14650 |
| O | -5.20320 | 0.14590 | -1.37580 |
| C | -5.94430 | -1.83310 | 1.14530 |
| C | -6.11170 | -1.91370 | 2.42720 |
| H | -5.95640 | -2.81160 | 3.01020 |
| Br | -6.47400 | -0.36200 | 3.35220 |
| H | -0.10270 | -2.64420 | -1.10890 |
| H | 0.29690 | -5.11510 | -0.86170 |
| H | -1.04770 | -3.95450 | 1.47400 |
| H | 0.44410 | -3.06590 | 1.17560 |
| H | -3.29270 | -2.76960 | 0.76780 |
| H | -1.70230 | -1.79240 | 2.26590 |
| H | -3.62580 | -0.19970 | 0.79730 |
| H | -2.75670 | -0.15070 | -0.72570 |
| H | -4.42720 | -1.69820 | -1.76950 |
| H | -1.87150 | -4.48580 | -2.96790 |
| H | -0.21070 | -3.93380 | -3.12390 |
| H | 0.63720 | -6.30200 | -3.16590 |
| H | -2.25770 | -6.51020 | -4.22180 |
| H | 1.28850 | -7.90760 | -4.97230 |
| H | 0.78100 | -8.77320 | -3.47890 |
| H | 0.65600 | -9.56150 | -5.06030 |
| H | -6.61960 | -2.07630 | -0.76880 |
| H | -4.52930 | 0.53770 | -1.95780 |

Table S6. Cont.

| Marilzafurollene_A_61 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83270 | -3.28360 | -0.59570 |
| O | -2.12320 | -2.71520 | -0.89700 |
| C | -0.64060 | -4.70210 | -1.15340 |
| C | -0.63400 | -3.14570 | 0.91380 |
| C | -2.61720 | -2.05190 | 0.28750 |
| C | -1.42100 | -1.89190 | 1.23180 |
| C | -3.36300 | -0.77500 | -0.09600 |
| Cl | -0.41900 | -0.44490 | 0.89980 |
| C | -4.60870 | -1.03490 | -0.95220 |
| C | -0.60310 | -4.79950 | -2.69060 |
| Br | -1.99230 | -5.95160 | -0.45880 |
| C | -1.84800 | -4.38370 | -3.43440 |
| C | -2.57630 | -5.22790 | -4.18150 |
| C | -3.81120 | -4.85570 | -4.92610 |
| C | -4.34370 | -3.45020 | -4.83700 |
| O | -4.37360 | -5.71670 | -5.60370 |
| C | -5.71240 | -1.71230 | -0.20010 |
| O | -5.13640 | 0.22280 | -1.38030 |
| C | -6.08600 | -2.94930 | -0.36510 |
| C | -6.46260 | -4.17800 | -0.52420 |
| H | -7.14190 | -4.51690 | -1.29480 |
| Br | -5.95530 | -5.40530 | 0.75290 |
| H | -0.10010 | -2.63510 | -1.09450 |
| H | 0.30640 | -5.10110 | -0.77000 |
| H | -1.08040 | -3.98530 | 1.45720 |
| H | 0.42310 | -3.10320 | 1.19500 |
| H | -3.31450 | -2.75650 | 0.75750 |
| H | -1.72600 | -1.83280 | 2.28020 |
| H | -3.64000 | -0.21260 | 0.80500 |
| H | -2.70490 | -0.11880 | -0.67950 |
| H | -4.35000 | -1.60170 | -1.85370 |
| H | 0.22060 | -4.17290 | -3.05660 |
| H | -0.33610 | -5.82800 | -2.96980 |
| H | -2.12900 | -3.33800 | -3.34290 |
| H | -2.29870 | -6.27330 | -4.28230 |
| H | -3.60920 | -2.74220 | -5.22900 |
| H | -5.25280 | -3.36990 | -5.44070 |
| H | -4.59960 | -3.21130 | -3.80180 |
| H | -6.24790 | -1.10680 | 0.52610 |
| H | -4.47180 | 0.62140 | -1.96880 |

Table S6. Cont.

| Marilzafurollene_A_62 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83250 | -3.28320 | -0.59430 |
| O | -2.12460 | -2.71510 | -0.89880 |
| C | -0.67400 | -4.70230 | -1.16230 |
| C | -0.62250 | -3.13210 | 0.91160 |
| C | -2.61590 | -2.05250 | 0.28790 |
| C | -1.41370 | -1.87780 | 1.22220 |
| C | -3.37710 | -0.78520 | -0.09480 |
| Cl | -0.42240 | -0.42870 | 0.86920 |
| C | -4.65500 | -1.07100 | -0.89940 |
| C | -0.84670 | -4.77760 | -2.68870 |
| Br | -2.00770 | -5.93070 | -0.37430 |
| C | 0.23820 | -4.05450 | -3.44720 |
| C | -0.00390 | -3.00220 | -4.24420 |
| C | 1.03020 | -2.26490 | -5.02310 |
| C | 2.47210 | -2.69200 | -4.94230 |
| O | 0.67580 | -1.31360 | -5.72000 |
| C | -5.78260 | -1.73810 | -0.16480 |
| O | -5.18030 | 0.16820 | -1.38250 |
| C | -5.94690 | -1.82040 | 1.12570 |
| C | -6.12070 | -1.90920 | 2.40630 |
| H | -5.97390 | -2.81230 | 2.98340 |
| Br | -6.47720 | -0.36200 | 3.34090 |
| H | -0.10140 | -2.63610 | -1.09520 |
| H | 0.29500 | -5.12030 | -0.86640 |
| H | -1.05880 | -3.96650 | 1.46970 |
| H | 0.43680 | -3.08070 | 1.18290 |
| H | -3.29980 | -2.76660 | 0.76230 |
| H | -1.71230 | -1.81020 | 2.27190 |
| H | -3.61820 | -0.19550 | 0.79850 |
| H | -2.73970 | -0.14590 | -0.71900 |
| H | -4.41290 | -1.67880 | -1.77910 |
| H | -0.81940 | -5.82640 | -3.01330 |
| H | -1.83660 | -4.40110 | -2.97810 |
| H | 1.24410 | -4.45000 | -3.32870 |
| H | -1.01060 | -2.61200 | -4.36830 |
| H | 3.07840 | -2.03590 | -5.57420 |
| H | 2.83330 | -2.60570 | -3.91420 |
| H | 2.58260 | -3.71630 | -5.30750 |
| H | -6.61490 | -2.04520 | -0.79330 |
| H | -4.50010 | 0.55870 | -1.95810 |

Table S6. Cont.

| Marilzafurollene_A_63 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83240 | -3.28300 | -0.59350 |
| O | -2.12580 | -2.71460 | -0.89900 |
| C | -0.69660 | -4.72300 | -1.11390 |
| C | -0.59890 | -3.08810 | 0.90470 |
| C | -2.61490 | -2.05320 | 0.28740 |
| C | -1.40340 | -1.83850 | 1.19970 |
| C | -3.42490 | -0.81530 | -0.08960 |
| Cl | -0.44210 | -0.38280 | 0.79730 |
| C | -4.65920 | -1.13240 | -0.94630 |
| C | -0.86490 | -4.84480 | -2.63730 |
| Br | -2.05880 | -5.89810 | -0.29120 |
| C | 0.24290 | -4.17500 | -3.40570 |
| C | 0.05020 | -3.15160 | -4.25230 |
| C | 1.19690 | -2.53750 | -4.98230 |
| C | 0.87890 | -1.41740 | -5.93740 |
| O | 2.35330 | -2.91160 | -4.79310 |
| C | -5.65980 | -2.01840 | -0.25950 |
| O | -5.30330 | 0.09390 | -1.29530 |
| C | -6.53690 | -1.64750 | 0.63090 |
| C | -7.40670 | -1.28090 | 1.51760 |
| H | -7.17570 | -1.07320 | 2.55340 |
| Br | -9.18340 | -1.25780 | 1.02970 |
| H | -0.10330 | -2.65800 | -1.12420 |
| H | 0.26310 | -5.14920 | -0.79990 |
| H | -1.01010 | -3.91590 | 1.49120 |
| H | 0.46430 | -3.01410 | 1.15520 |
| H | -3.27290 | -2.77720 | 0.78500 |
| H | -1.68690 | -1.75200 | 2.25220 |
| H | -3.72650 | -0.27190 | 0.81500 |
| H | -2.80500 | -0.12120 | -0.67090 |
| H | -4.35740 | -1.61220 | -1.88460 |
| H | -0.86310 | -5.90380 | -2.92770 |
| H | -1.84180 | -4.45020 | -2.94570 |
| H | 1.24710 | -4.57200 | -3.25860 |
| H | -0.93460 | -2.73490 | -4.43040 |
| H | 1.11590 | -0.46120 | -5.46450 |
| H | 1.47370 | -1.54210 | -6.84660 |
| H | -0.17650 | -1.42810 | -6.22290 |
| H | -5.55900 | -3.08260 | -0.45630 |
| H | -4.67550 | 0.59950 | -1.83910 |

Table S6. Cont.

| Marilzafurollene_A_64 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83260 | -3.28320 | -0.59450 |
| O | -2.12450 | -2.71510 | -0.89850 |
| C | -0.67670 | -4.70240 | -1.16290 |
| C | -0.62170 | -3.13100 | 0.91150 |
| C | -2.61600 | -2.05250 | 0.28780 |
| C | -1.41420 | -1.87740 | 1.22240 |
| C | -3.37730 | -0.78590 | -0.09670 |
| Cl | -0.42500 | -0.42660 | 0.87150 |
| C | -4.65230 | -1.07300 | -0.90550 |
| C | -0.85350 | -4.79010 | -2.68890 |
| Br | -2.01070 | -5.92770 | -0.36490 |
| C | 0.21930 | -4.06660 | -3.45940 |
| C | 1.14910 | -4.68310 | -4.20570 |
| C | 2.17310 | -3.89700 | -4.95410 |
| C | 3.12980 | -4.67160 | -5.82180 |
| O | 2.24950 | -2.67420 | -4.84660 |
| C | -5.78140 | -1.74150 | -0.17450 |
| O | -5.17750 | 0.16580 | -1.39000 |
| C | -5.95020 | -1.82300 | 1.11550 |
| C | -6.12780 | -1.91140 | 2.39550 |
| H | -5.97940 | -2.81340 | 2.97390 |
| Br | -6.49780 | -0.36560 | 3.32710 |
| H | -0.10110 | -2.63620 | -1.09400 |
| H | 0.29190 | -5.12160 | -0.86760 |
| H | -1.05650 | -3.96550 | 1.47080 |
| H | 0.43770 | -3.07830 | 1.18210 |
| H | -3.30010 | -2.76640 | 0.76220 |
| H | -1.71330 | -1.81100 | 2.27210 |
| H | -3.62160 | -0.19650 | 0.79590 |
| H | -2.73870 | -0.14580 | -0.71910 |
| H | -4.40690 | -1.68030 | -1.78460 |
| H | -0.86660 | -5.84450 | -2.99680 |
| H | -1.82740 | -4.38180 | -2.98780 |
| H | 0.20320 | -2.97780 | -3.41490 |
| H | 1.19010 | -5.76260 | -4.29490 |
| H | 3.28010 | -4.13110 | -6.76060 |
| H | 4.08290 | -4.78310 | -5.29890 |
| H | 2.73160 | -5.66060 | -6.06440 |
| H | -6.61040 | -2.05170 | -0.80580 |
| H | -4.49560 | 0.55680 | -1.96310 |

Table S6. Cont.

| Marilzafurollene_A_65 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83270 | -3.28400 | -0.59680 |
| O | -2.12230 | -2.71510 | -0.89520 |
| C | -0.65480 | -4.70180 | -1.15870 |
| C | -0.63900 | -3.14980 | 0.91300 |
| C | -2.61810 | -2.05170 | 0.28680 |
| C | -1.42160 | -1.89080 | 1.22830 |
| C | -3.36370 | -0.78120 | -0.11390 |
| Cl | -0.42010 | -0.44580 | 0.88830 |
| C | -4.66160 | -1.07450 | -0.87860 |
| C | -0.55710 | -4.78630 | -2.69420 |
| Br | -2.07750 | -5.91300 | -0.53700 |
| C | -1.70300 | -4.21090 | -3.48350 |
| C | -2.53010 | -4.93760 | -4.25040 |
| C | -3.64220 | -4.28730 | -5.00330 |
| C | -4.56510 | -5.19440 | -5.77400 |
| O | -3.78610 | -3.06580 | -5.01820 |
| C | -5.75260 | -1.59180 | 0.01020 |
| O | -5.14790 | 0.15280 | -1.42650 |
| C | -6.17470 | -2.82350 | 0.04650 |
| C | -6.59450 | -4.04770 | 0.08560 |
| H | -7.34070 | -4.46280 | -0.57830 |
| Br | -5.88360 | -5.16310 | 1.36790 |
| H | -0.09620 | -2.63760 | -1.09250 |
| H | 0.26160 | -5.13580 | -0.74090 |
| H | -1.09220 | -3.99010 | 1.45020 |
| H | 0.41690 | -3.11180 | 1.19880 |
| H | -3.31370 | -2.75580 | 0.75910 |
| H | -1.72490 | -1.82780 | 2.27690 |
| H | -3.58430 | -0.17220 | 0.77220 |
| H | -2.72970 | -0.16590 | -0.76520 |
| H | -4.48420 | -1.76140 | -1.71470 |
| H | 0.34970 | -4.25310 | -3.00890 |
| H | -0.39750 | -5.83330 | -2.98550 |
| H | -1.84370 | -3.13210 | -3.42090 |
| H | -2.42940 | -6.01280 | -4.34060 |
| H | -4.51350 | -6.22100 | -5.40100 |
| H | -5.59440 | -4.84520 | -5.65250 |
| H | -4.28800 | -5.17860 | -6.83090 |
| H | -6.21770 | -0.86960 | 0.67560 |
| H | -4.58290 | 0.34940 | -2.19490 |

Table S6. Cont.

| Marilzafurollene_A_66 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83330 | -3.28380 | -0.59720 |
| O | -2.12160 | -2.71530 | -0.89470 |
| C | -0.64160 | -4.68720 | -1.18910 |
| C | -0.65420 | -3.17900 | 0.91650 |
| C | -2.61830 | -2.05170 | 0.28670 |
| C | -1.43160 | -1.92030 | 1.24620 |
| C | -3.34120 | -0.76500 | -0.10570 |
| Cl | -0.41080 | -0.47870 | 0.95300 |
| C | -4.60110 | -1.02370 | -0.94180 |
| C | -0.56060 | -4.73890 | -2.72730 |
| Br | -2.03350 | -5.93570 | -0.57350 |
| C | -1.75130 | -4.22760 | -3.49570 |
| C | -2.51570 | -4.99210 | -4.29080 |
| C | -3.67820 | -4.41400 | -5.02640 |
| C | -4.49000 | -5.36180 | -5.87020 |
| O | -3.94930 | -3.21560 | -4.97140 |
| C | -5.72020 | -1.61590 | -0.13820 |
| O | -5.07220 | 0.23650 | -1.42520 |
| C | -6.17590 | -2.82960 | -0.26210 |
| C | -6.62910 | -4.03730 | -0.37490 |
| H | -7.37670 | -4.34900 | -1.09180 |
| Br | -6.04940 | -5.29150 | 0.84400 |
| H | -0.09620 | -2.62350 | -1.07320 |
| H | 0.28760 | -5.11240 | -0.79080 |
| H | -1.11970 | -4.02440 | 1.43460 |
| H | 0.39890 | -3.15400 | 1.21410 |
| H | -3.33200 | -2.74840 | 0.74360 |
| H | -1.74840 | -1.87630 | 2.29180 |
| H | -3.59820 | -0.18390 | 0.78930 |
| H | -2.67830 | -0.13080 | -0.70820 |
| H | -4.36050 | -1.64180 | -1.81470 |
| H | 0.30790 | -4.14730 | -3.04510 |
| H | -0.34160 | -5.77040 | -3.03500 |
| H | -1.97980 | -3.16690 | -3.39460 |
| H | -2.32290 | -6.05060 | -4.42080 |
| H | -4.33770 | -6.39880 | -5.55890 |
| H | -5.55170 | -5.12850 | -5.75010 |
| H | -4.20000 | -5.25170 | -6.91800 |
| H | -6.17160 | -0.97230 | 0.61240 |
| H | -5.73220 | 0.03220 | -2.11160 |

Table S6. Cont.

| Marilzafurollene_A_67 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83290 | -3.28290 | -0.59400 |
| O | -2.12480 | -2.71520 | -0.89920 |
| C | -0.67530 | -4.70430 | -1.15630 |
| C | -0.61380 | -3.11810 | 0.90880 |
| C | -2.61550 | -2.05270 | 0.28800 |
| C | -1.40840 | -1.86420 | 1.21320 |
| C | -3.38920 | -0.79330 | -0.09520 |
| Cl | -0.42580 | -0.41450 | 0.83720 |
| C | -4.67220 | -1.09350 | -0.88650 |
| C | -0.84360 | -4.72530 | -2.68620 |
| Br | -2.01110 | -5.91970 | -0.35470 |
| C | -0.35470 | -6.00060 | -3.32770 |
| C | 0.67430 | -6.05830 | -4.18790 |
| C | 1.09520 | -7.35510 | -4.79550 |
| C | 2.23210 | -7.30980 | -5.78240 |
| O | 0.55620 | -8.41660 | -4.48710 |
| C | -5.78880 | -1.76250 | -0.13700 |
| O | -5.21000 | 0.13890 | -1.37360 |
| C | -5.94020 | -1.83770 | 1.15550 |
| C | -6.10070 | -1.91980 | 2.43820 |
| H | -5.94200 | -2.81840 | 3.01920 |
| Br | -6.45540 | -0.36890 | 3.36730 |
| H | -0.10290 | -2.64480 | -1.11010 |
| H | 0.29800 | -5.11390 | -0.86330 |
| H | -1.04280 | -3.94980 | 1.47670 |
| H | 0.44690 | -3.05990 | 1.17310 |
| H | -3.29050 | -2.77060 | 0.76940 |
| H | -1.70000 | -1.78740 | 2.26420 |
| H | -3.62680 | -0.20020 | 0.79680 |
| H | -2.76210 | -0.15280 | -0.72870 |
| H | -4.43390 | -1.70600 | -1.76390 |
| H | -1.89470 | -4.57970 | -2.96580 |
| H | -0.29180 | -3.87960 | -3.11690 |
| H | -0.89550 | -6.91360 | -3.07910 |
| H | 1.23160 | -5.17420 | -4.47500 |
| H | 2.00560 | -7.97500 | -6.62050 |
| H | 2.36940 | -6.30150 | -6.18240 |
| H | 3.15220 | -7.63190 | -5.28870 |
| H | -6.62480 | -2.07930 | -0.75560 |
| H | -4.53810 | 0.52900 | -1.95900 |

Table S6. Cont.

| Marilzafurollene_A_68 | | | |
|------------------------------|----------|-----------|----------|
| C | -0.83300 | -3.28270 | -0.59360 |
| O | -2.12530 | -2.71490 | -0.89900 |
| C | -0.68300 | -4.70950 | -1.14280 |
| C | -0.60960 | -3.10960 | 0.90780 |
| C | -2.61480 | -2.05320 | 0.28740 |
| C | -1.40760 | -1.85750 | 1.21060 |
| C | -3.40640 | -0.80390 | -0.09100 |
| Cl | -0.43140 | -0.40540 | 0.83030 |
| C | -4.63740 | -1.10230 | -0.95910 |
| C | -0.84170 | -4.74310 | -2.67260 |
| Br | -2.03960 | -5.90780 | -0.34780 |
| C | -0.39270 | -6.04330 | -3.28960 |
| C | -1.19990 | -6.85810 | -3.98670 |
| C | -0.68330 | -8.12990 | -4.57050 |
| C | -1.67440 | -9.00160 | -5.29590 |
| O | 0.50320 | -8.44270 | -4.48370 |
| C | -5.65520 | -1.97730 | -0.28360 |
| O | -5.26300 | 0.13330 | -1.30880 |
| C | -6.52200 | -1.60120 | 0.61440 |
| C | -7.38120 | -1.22900 | 1.50910 |
| H | -7.14320 | -1.04190 | 2.54730 |
| Br | -9.15750 | -1.15210 | 1.02490 |
| H | -0.10300 | -2.65060 | -1.11680 |
| H | 0.28320 | -5.12700 | -0.83810 |
| H | -1.03310 | -3.94130 | 1.48000 |
| H | 0.45190 | -3.04670 | 1.16810 |
| H | -3.28520 | -2.77200 | 0.77600 |
| H | -1.69790 | -1.77970 | 2.26190 |
| H | -3.70850 | -0.26020 | 0.81330 |
| H | -2.77340 | -0.11520 | -0.66460 |
| H | -4.33430 | -1.58280 | -1.89670 |
| H | -1.87750 | -4.51960 | -2.95880 |
| H | -0.22190 | -3.95330 | -3.11600 |
| H | 0.65570 | -6.30900 | -3.15660 |
| H | -2.24760 | -6.62820 | -4.14220 |
| H | -1.49970 | -10.04610 | -5.02290 |
| H | -2.70150 | -8.74960 | -5.01860 |
| H | -1.54880 | -8.87140 | -6.37370 |
| H | -5.57730 | -3.04030 | -0.49650 |
| H | -4.62810 | 0.62740 | -1.85500 |

Table S6. Cont.

| Marilzafurollene_A_69 | | | |
|------------------------------|----------|----------|----------|
| C | -0.83300 | -3.28390 | -0.59710 |
| O | -2.12200 | -2.71500 | -0.89430 |
| C | -0.65890 | -4.70300 | -1.15850 |
| C | -0.63140 | -3.14030 | 0.91100 |
| C | -2.61810 | -2.05190 | 0.28630 |
| C | -1.42050 | -1.88500 | 1.22590 |
| C | -3.37610 | -0.78620 | -0.10790 |
| Cl | -0.42320 | -0.43710 | 0.88610 |
| C | -4.62390 | -1.08010 | -0.95030 |
| C | -0.63270 | -4.78700 | -2.69760 |
| Br | -2.02550 | -5.93680 | -0.46180 |
| C | -1.83160 | -4.23730 | -3.42580 |
| C | -1.78270 | -3.19080 | -4.26470 |
| C | -3.01720 | -2.67910 | -4.92800 |
| C | -2.86870 | -1.45100 | -5.78740 |
| O | -4.10310 | -3.24260 | -4.80190 |
| C | -5.72200 | -1.72950 | -0.16250 |
| O | -5.13920 | 0.16740 | -1.42180 |
| C | -6.15780 | -2.94290 | -0.34620 |
| C | -6.59050 | -4.14990 | -0.52720 |
| H | -7.31270 | -4.43660 | -1.27980 |
| Br | -6.08260 | -5.43720 | 0.68940 |
| H | -0.09910 | -2.64020 | -1.10010 |
| H | 0.28290 | -5.12000 | -0.78200 |
| H | -1.07530 | -3.97910 | 1.45770 |
| H | 0.42610 | -3.09470 | 1.19000 |
| H | -3.31050 | -2.75930 | 0.76010 |
| H | -1.72280 | -1.82280 | 2.27490 |
| H | -3.65240 | -0.21340 | 0.78660 |
| H | -2.73030 | -0.13220 | -0.70770 |
| H | -4.35710 | -1.67520 | -1.83140 |
| H | 0.27160 | -4.27040 | -3.04620 |
| H | -0.51150 | -5.83450 | -3.00340 |
| H | -2.78660 | -4.72660 | -3.23710 |
| H | -0.85650 | -2.66850 | -4.47280 |
| H | -2.83840 | -1.74700 | -6.83890 |
| H | -3.71880 | -0.78590 | -5.61100 |
| H | -1.95660 | -0.90140 | -5.53920 |
| H | -6.19320 | -1.12440 | 0.60750 |
| H | -5.85850 | -0.05310 | -2.04020 |

Table S7. Calculated Energies (Hartrees) for diastereoisomer $S_a,4R,6S,7S,9R,10R$ of **1**.

| Entry ID | Gas Phase Energy |
|----------|------------------|
| 1 | -849,892312 |
| 2 | -849,891362 |
| 3 | -849,889723 |
| 4 | -849,888014 |
| 5 | -849,890752 |
| 6 | -849,888881 |
| 7 | -849,891284 |
| 8 | -849,887862 |
| 9 | -849,890823 |
| 10 | -849,8903 |
| 11 | -849,89047 |
| 12 | -849,887116 |
| 13 | -849,887459 |
| 14 | -849,885981 |
| 15 | -849,886131 |
| 16 | -849,886643 |
| 17 | -849,89112 |
| 18 | -849,889149 |
| 19 | -849,888072 |
| 20 | -849,889069 |
| 21 | -849,888506 |
| 22 | -849,887669 |
| 23 | -849,887238 |
| 24 | -849,886538 |
| 25 | -849,88672 |
| 26 | -849,888164 |
| 27 | -849,887177 |
| 28 | -849,886464 |
| 29 | -849,88626 |
| 30 | -849,887009 |
| 31 | -849,8872 |
| 32 | -849,88652 |
| 33 | -849,887065 |
| 34 | -849,886281 |
| 35 | -849,88669 |
| 36 | -849,886453 |
| 37 | -849,886943 |
| 38 | -849,889594 |
| 39 | -849,888768 |
| 40 | -849,88626 |
| 41 | -849,888689 |
| 42 | -849,887404 |
| 43 | -849,887051 |
| 44 | -849,889586 |

| | |
|----|-------------|
| 45 | -849,888582 |
| 46 | -849,888918 |
| 47 | -849,886761 |
| 48 | -849,888629 |
| 49 | -849,887692 |
| 50 | -849,890553 |
| 51 | -849,890372 |
| 52 | -849,887395 |
| 53 | -849,88919 |
| 54 | -849,886823 |

Table S8. Coordinates (Angstroms) of calculated geometries for diastereoisomer $S_a,4R,6S,7S,9R,10R$ of **1**.

| Marilzafurollene-A_1 | | | |
|-----------------------------|----------|----------|----------|
| C | -0.60640 | 1.28380 | 1.68150 |
| O | 0.17000 | 0.12240 | 1.31470 |
| C | -1.72510 | 0.93540 | 2.67640 |
| C | 0.38090 | 2.36100 | 2.13110 |
| C | 1.56710 | 0.47880 | 1.38080 |
| C | 1.62790 | 2.00840 | 1.34520 |
| C | 2.36450 | -0.27280 | 0.31760 |
| Cl | 1.52880 | 2.70040 | -0.30250 |
| C | 2.29850 | -1.79620 | 0.48100 |
| C | -2.72540 | -0.10030 | 2.13690 |
| Br | -0.97130 | 0.18590 | 4.34580 |
| C | -3.53510 | 0.41310 | 0.97640 |
| C | -3.48450 | -0.11370 | -0.25700 |
| C | -4.31440 | 0.44640 | -1.36260 |
| C | -4.20020 | -0.21980 | -2.70840 |
| O | -5.03940 | 1.42470 | -1.18950 |
| C | 2.93750 | -2.28660 | 1.74600 |
| O | 3.01600 | -2.38530 | -0.60520 |
| C | 2.30180 | -2.87100 | 2.72130 |
| C | 1.65840 | -3.44090 | 3.68990 |
| H | 1.18210 | -2.91230 | 4.50510 |
| Br | 1.44310 | -5.26950 | 3.62550 |
| H | -1.07230 | 1.63320 | 0.75160 |
| H | -2.24820 | 1.84530 | 2.99180 |
| H | 0.00310 | 3.37320 | 1.95440 |
| H | 0.60660 | 2.28500 | 3.19970 |
| H | 1.91020 | 0.16460 | 2.37500 |
| H | 2.54270 | 2.39800 | 1.80010 |
| H | 1.97530 | -0.04340 | -0.68240 |
| H | 3.41020 | 0.06090 | 0.32400 |
| H | 1.25880 | -2.13620 | 0.40530 |
| H | -2.20400 | -1.02690 | 1.86290 |
| H | -3.43520 | -0.37840 | 2.92720 |

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| H | -4.20010 | 1.25220 | 1.17880 |
| H | -2.83780 | -0.95090 | -0.49430 |
| H | -3.55110 | 0.37780 | -3.35330 |
| H | -3.78970 | -1.22910 | -2.61720 |
| H | -5.19580 | -0.30150 | -3.15340 |
| H | 4.00960 | -2.13820 | 1.84280 |
| H | 2.91420 | -3.34930 | -0.51110 |
| Marilzafurollene-A_2 | | | |
| C | 0.13020 | 1.71480 | 1.05350 |
| O | 0.88890 | 0.49740 | 0.89270 |
| C | -1.37580 | 1.44060 | 1.18540 |
| C | 0.77630 | 2.50160 | 2.19330 |
| C | 2.03480 | 0.56570 | 1.76770 |
| C | 2.21950 | 2.04290 | 2.12680 |
| C | 3.23040 | -0.15260 | 1.14680 |
| Cl | 3.10270 | 2.98570 | 0.88780 |
| C | 2.97040 | -1.64180 | 0.88820 |
| C | -1.92890 | 0.72920 | -0.06170 |
| Br | -1.74120 | 0.30780 | 2.76490 |
| C | -3.43540 | 0.71020 | -0.11970 |
| C | -4.16800 | -0.41380 | -0.15270 |
| C | -5.65740 | -0.35480 | -0.21270 |
| C | -6.39370 | -1.66870 | -0.21180 |
| O | -6.25690 | 0.71670 | -0.28470 |
| C | 2.75020 | -2.43310 | 2.14310 |
| O | 4.12840 | -2.18470 | 0.25110 |
| C | 1.63970 | -3.03800 | 2.45550 |
| C | 0.52880 | -3.62810 | 2.76330 |
| H | -0.27180 | -3.17220 | 3.33070 |
| Br | 0.24810 | -5.33110 | 2.11880 |
| H | 0.28260 | 2.28230 | 0.12570 |
| H | -1.91160 | 2.37790 | 1.37320 |
| H | 0.63730 | 3.58220 | 2.08650 |
| H | 0.36290 | 2.21930 | 3.16700 |
| H | 1.74140 | 0.04350 | 2.68750 |
| H | 2.75400 | 2.17700 | 3.07120 |
| H | 3.48490 | 0.29810 | 0.17920 |
| H | 4.11590 | -0.03090 | 1.78400 |
| H | 2.13110 | -1.76020 | 0.19280 |
| H | -1.58540 | 1.25930 | -0.95930 |
| H | -1.52920 | -0.29060 | -0.13330 |
| H | -3.93390 | 1.67870 | -0.14660 |
| H | -3.70940 | -1.39570 | -0.13100 |
| H | -7.27960 | -1.58280 | 0.42380 |
| H | -6.69060 | -1.91700 | -1.23380 |
| H | -5.76980 | -2.47170 | 0.19000 |
| H | 3.58810 | -2.50250 | 2.83150 |

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| H | 3.91550 | -3.11090 | 0.03830 |
| Marilzafurollene-A_3 | | | |
| C | -0.57480 | 1.20940 | 1.67730 |
| O | 0.18940 | 0.03560 | 1.32240 |
| C | -1.71290 | 0.88120 | 2.65730 |
| C | 0.42170 | 2.27230 | 2.14090 |
| C | 1.59080 | 0.36760 | 1.42060 |
| C | 1.67780 | 1.89600 | 1.38150 |
| C | 2.39430 | -0.39780 | 0.37200 |
| Cl | 1.62280 | 2.58160 | -0.27130 |
| C | 2.31530 | -1.92080 | 0.54150 |
| C | -2.72520 | -0.13600 | 2.10550 |
| Br | -0.99550 | 0.12100 | 4.33750 |
| C | -3.51600 | 0.39540 | 0.94010 |
| C | -3.48380 | -0.14220 | -0.28920 |
| C | -4.29650 | 0.43650 | -1.39810 |
| C | -4.22160 | -0.25460 | -2.73410 |
| O | -4.97740 | 1.44780 | -1.23540 |
| C | 2.96740 | -2.41370 | 1.79760 |
| O | 3.02100 | -2.53120 | -0.54130 |
| C | 2.33110 | -2.85710 | 2.84480 |
| C | 1.68930 | -3.28640 | 3.88430 |
| H | 1.26780 | -2.65030 | 4.65120 |
| Br | 1.38400 | -5.09750 | 4.02680 |
| H | -1.02180 | 1.56430 | 0.74040 |
| H | -2.22350 | 1.80080 | 2.96520 |
| H | 0.06420 | 3.28970 | 1.95230 |
| H | 0.62520 | 2.19820 | 3.21400 |
| H | 1.90770 | 0.05000 | 2.42190 |
| H | 2.59000 | 2.27200 | 1.85270 |
| H | 2.01780 | -0.16840 | -0.63290 |
| H | 3.44280 | -0.07350 | 0.38870 |
| H | 1.27540 | -2.26450 | 0.48820 |
| H | -2.21680 | -1.07010 | 1.83310 |
| H | -3.44680 | -0.40400 | 2.88850 |
| H | -4.15310 | 1.25760 | 1.13580 |
| H | -2.86780 | -1.00400 | -0.51980 |
| H | -3.56140 | 0.31070 | -3.39650 |
| H | -3.84320 | -1.27530 | -2.63160 |
| H | -5.22500 | -0.31030 | -3.16530 |
| H | 4.05350 | -2.40540 | 1.81870 |
| H | 2.50530 | -2.35200 | -1.34670 |
| Marilzafurollene-A_4 | | | |
| C | -0.87590 | 0.94090 | 1.83400 |
| O | -0.33320 | -0.33260 | 1.42260 |
| C | -2.17350 | 0.78200 | 2.64210 |
| C | 0.25470 | 1.70870 | 2.51740 |

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| C | 1.09500 | -0.30300 | 1.63700 |
| C | 1.48290 | 1.16840 | 1.81350 |
| C | 1.81100 | -1.07440 | 0.52970 |
| Cl | 1.73910 | 2.04050 | 0.27100 |
| C | 1.50170 | -2.57960 | 0.55350 |
| C | -3.28720 | 0.04840 | 1.87660 |
| Br | -1.84900 | -0.24370 | 4.30140 |
| C | -3.78810 | 0.81880 | 0.68440 |
| C | -3.67410 | 0.38730 | -0.58130 |
| C | -4.19210 | 1.20290 | -1.71750 |
| C | -4.03350 | 0.62820 | -3.10050 |
| O | -4.70240 | 2.30720 | -1.53540 |
| C | 1.99470 | -3.33030 | 1.75810 |
| O | 2.08980 | -3.18910 | -0.59780 |
| C | 3.10700 | -3.11170 | 2.40160 |
| C | 4.20620 | -2.88500 | 3.04780 |
| H | 5.12210 | -3.44700 | 2.92160 |
| Br | 4.17850 | -1.59480 | 4.36330 |
| H | -1.11820 | 1.47180 | 0.90480 |
| H | -2.52610 | 1.76090 | 2.98620 |
| H | 0.12810 | 2.79350 | 2.44310 |
| H | 0.32730 | 1.46450 | 3.58200 |
| H | 1.25880 | -0.80190 | 2.59990 |
| H | 2.39770 | 1.28730 | 2.40060 |
| H | 1.49850 | -0.69880 | -0.45320 |
| H | 2.89450 | -0.91150 | 0.58890 |
| H | 0.41950 | -2.72840 | 0.46740 |
| H | -2.94720 | -0.95080 | 1.57410 |
| H | -4.14740 | -0.11580 | 2.53900 |
| H | -4.27690 | 1.77100 | 0.88890 |
| H | -3.19730 | -0.55640 | -0.82200 |
| H | -3.18720 | 1.10950 | -3.59670 |
| H | -3.86520 | -0.45150 | -3.06400 |
| H | -4.95050 | 0.80580 | -3.66940 |
| H | 1.37540 | -4.16440 | 2.07780 |
| H | 3.05510 | -3.13420 | -0.48760 |
| Marilzafurollene-A_5 | | | |
| C | 0.15780 | 1.71440 | 0.99100 |
| O | 0.89500 | 0.48010 | 0.86660 |
| C | -1.35200 | 1.47050 | 1.13990 |
| C | 0.82380 | 2.52680 | 2.10060 |
| C | 2.05310 | 0.56140 | 1.72460 |
| C | 2.26010 | 2.04660 | 2.03680 |
| C | 3.23180 | -0.18980 | 1.11020 |
| Cl | 3.14530 | 2.94010 | 0.76320 |
| C | 2.94820 | -1.68090 | 0.89090 |
| C | -1.92500 | 0.72710 | -0.07980 |

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| Br | -1.72870 | 0.40130 | 2.75930 |
| C | -3.43530 | 0.70980 | -0.12220 |
| C | -4.15520 | -0.42280 | -0.14140 |
| C | -5.64290 | -0.48920 | -0.18930 |
| C | -6.44810 | 0.78340 | -0.20590 |
| O | -6.18310 | -1.59550 | -0.21690 |
| C | 2.72820 | -2.43790 | 2.16660 |
| O | 4.09220 | -2.25560 | 0.25650 |
| C | 1.60610 | -3.00230 | 2.51190 |
| C | 0.48280 | -3.54990 | 2.85150 |
| H | -0.32160 | -3.03560 | 3.36070 |
| Br | 0.19190 | -5.30150 | 2.35980 |
| H | 0.31410 | 2.24780 | 0.04390 |
| H | -1.87070 | 2.42290 | 1.29710 |
| H | 0.69820 | 3.60540 | 1.96160 |
| H | 0.41510 | 2.28000 | 3.08580 |
| H | 1.76560 | 0.07070 | 2.66340 |
| H | 2.80400 | 2.20220 | 2.97250 |
| H | 3.48250 | 0.23280 | 0.12910 |
| H | 4.12570 | -0.06480 | 1.73500 |
| H | 2.10080 | -1.80420 | 0.20620 |
| H | -1.58990 | 1.23110 | -0.99540 |
| H | -1.52820 | -0.29530 | -0.12730 |
| H | -3.92020 | 1.68230 | -0.15050 |
| H | -3.67200 | -1.39580 | -0.11940 |
| H | -6.24550 | 1.36980 | 0.69400 |
| H | -6.21980 | 1.36130 | -1.10510 |
| H | -7.51390 | 0.53530 | -0.21860 |
| H | 3.57430 | -2.51190 | 2.84450 |
| H | 3.86080 | -3.18110 | 0.06010 |
| Marilzafurollene-A_6 | | | |
| C | 0.15800 | 1.62640 | 1.04560 |
| O | 0.89270 | 0.39420 | 0.88390 |
| C | -1.35320 | 1.38240 | 1.17700 |
| C | 0.81920 | 2.39980 | 2.18560 |
| C | 2.03820 | 0.43770 | 1.76110 |
| C | 2.25240 | 1.91100 | 2.12110 |
| C | 3.21700 | -0.30010 | 1.13120 |
| Cl | 3.15740 | 2.83390 | 0.88230 |
| C | 2.93710 | -1.78910 | 0.88620 |
| C | -1.91890 | 0.68010 | -0.06940 |
| Br | -1.74140 | 0.25930 | 2.75780 |
| C | -3.42510 | 0.69420 | -0.13200 |
| C | -4.18200 | -0.41370 | -0.16040 |
| C | -5.66940 | -0.32260 | -0.22910 |
| C | -6.43530 | -1.61950 | -0.22620 |
| O | -6.24470 | 0.76170 | -0.30850 |

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| C | 2.77110 | -2.57750 | 2.15000 |
| O | 4.06240 | -2.35240 | 0.20850 |
| C | 1.64010 | -3.04690 | 2.59540 |
| C | 0.51060 | -3.50060 | 3.03750 |
| H | -0.20950 | -2.91600 | 3.59440 |
| Br | 0.05060 | -5.23540 | 2.62150 |
| H | 0.32190 | 2.19090 | 0.11790 |
| H | -1.87040 | 2.33030 | 1.36340 |
| H | 0.70300 | 3.48300 | 2.07790 |
| H | 0.39880 | 2.12700 | 3.15900 |
| H | 1.73570 | -0.08030 | 2.67990 |
| H | 2.78850 | 2.03410 | 3.06610 |
| H | 3.46280 | 0.14310 | 0.15800 |
| H | 4.11210 | -0.18560 | 1.75610 |
| H | 2.06480 | -1.91930 | 0.23480 |
| H | -1.56130 | 1.19980 | -0.96760 |
| H | -1.54180 | -0.34850 | -0.13730 |
| H | -3.90210 | 1.67330 | -0.16790 |
| H | -3.74480 | -1.40510 | -0.12960 |
| H | -5.82170 | -2.44150 | 0.15230 |
| H | -7.30500 | -1.52040 | 0.42950 |
| H | -6.75940 | -1.84980 | -1.24410 |
| H | 3.67210 | -2.77000 | 2.72580 |
| H | 4.06980 | -1.96800 | -0.68550 |
| Marilzafurollene-A_7 | | | |
| C | -0.02800 | 1.39930 | 1.01470 |
| O | 0.81200 | 0.23070 | 0.90800 |
| C | -1.49060 | 1.03040 | 1.30760 |
| C | 0.64330 | 2.34750 | 2.00710 |
| C | 2.02380 | 0.48100 | 1.65180 |
| C | 2.10950 | 1.99780 | 1.84730 |
| C | 3.21510 | -0.20140 | 0.98350 |
| Cl | 2.79600 | 2.87310 | 0.44490 |
| C | 3.06600 | -1.72540 | 0.89800 |
| C | -2.08300 | 0.15370 | 0.18960 |
| Br | -1.62920 | 0.05180 | 3.02040 |
| C | -3.58690 | 0.02200 | 0.25790 |
| C | -4.41460 | 0.54350 | -0.66070 |
| C | -5.89990 | 0.42380 | -0.63480 |
| C | -6.57000 | -0.34530 | 0.47330 |
| O | -6.54910 | 0.96510 | -1.53040 |
| C | 3.04250 | -2.39610 | 2.23910 |
| O | 4.19980 | -2.23770 | 0.19540 |
| C | 2.01980 | -3.03330 | 2.73400 |
| C | 0.99370 | -3.65450 | 3.22220 |
| H | 0.16500 | -3.17130 | 3.72280 |
| Br | 0.88580 | -5.47620 | 2.97030 |

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| H | 0.00080 | 1.87490 | 0.02520 |
| H | -2.08460 | 1.94070 | 1.44710 |
| H | 0.40200 | 3.39710 | 1.81080 |
| H | 0.34250 | 2.13570 | 3.03820 |
| H | 1.86460 | 0.03600 | 2.64240 |
| H | 2.71060 | 2.27060 | 2.71900 |
| H | 3.33510 | 0.16400 | -0.04420 |
| H | 4.14240 | 0.05650 | 1.51120 |
| H | 2.17640 | -1.98260 | 0.31090 |
| H | -1.80820 | 0.58340 | -0.78270 |
| H | -1.64900 | -0.85400 | 0.21160 |
| H | -3.97630 | -0.54770 | 1.09820 |
| H | -4.03420 | 1.10510 | -1.50930 |
| H | -6.35730 | 0.12220 | 1.43810 |
| H | -7.65310 | -0.33220 | 0.31730 |
| H | -6.23650 | -1.38620 | 0.46480 |
| H | 3.95180 | -2.33880 | 2.83140 |
| H | 4.05080 | -3.19490 | 0.09480 |
| Marilzafurollene-A_8 | | | |
| C | -0.87700 | 1.14340 | 1.78110 |
| O | -0.28820 | -0.13650 | 1.46080 |
| C | -2.17200 | 0.99570 | 2.59540 |
| C | 0.22260 | 1.99530 | 2.41430 |
| C | 1.13530 | -0.04270 | 1.68520 |
| C | 1.47340 | 1.45000 | 1.75470 |
| C | 1.89590 | -0.87840 | 0.65930 |
| Cl | 1.70460 | 2.22040 | 0.15520 |
| C | 1.53590 | -2.36940 | 0.69910 |
| C | -3.26120 | 0.18520 | 1.87370 |
| Br | -1.82110 | 0.08090 | 4.31330 |
| C | -3.78800 | 0.87420 | 0.64340 |
| C | -3.66370 | 0.37980 | -0.59820 |
| C | -4.21000 | 1.11810 | -1.77350 |
| C | -4.03380 | 0.47840 | -3.12550 |
| O | -4.75670 | 2.21270 | -1.64710 |
| C | 1.81550 | -3.03430 | 2.01870 |
| O | 2.27850 | -3.02870 | -0.32920 |
| C | 2.99170 | -3.35820 | 2.47760 |
| C | 4.16280 | -3.67070 | 2.93350 |
| H | 4.64480 | -4.62800 | 2.78740 |
| Br | 5.10770 | -2.37550 | 3.84170 |
| H | -1.13230 | 1.60010 | 0.81660 |
| H | -2.55420 | 1.98270 | 2.87990 |
| H | 0.05960 | 3.06730 | 2.26390 |
| H | 0.29550 | 1.82850 | 3.49380 |
| H | 1.30670 | -0.45970 | 2.68600 |
| H | 2.38010 | 1.64270 | 2.33460 |

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| H | 1.67370 | -0.52820 | -0.35660 |
| H | 2.97730 | -0.74930 | 0.79640 |
| H | 0.47560 | -2.50130 | 0.45510 |
| H | -2.88850 | -0.81690 | 1.62450 |
| H | -4.11530 | 0.02890 | 2.54590 |
| H | -4.30600 | 1.82030 | 0.79860 |
| H | -3.15850 | -0.55990 | -0.79100 |
| H | -3.20300 | 0.95960 | -3.64730 |
| H | -3.83200 | -0.59230 | -3.03390 |
| H | -4.95590 | 0.59800 | -3.70120 |
| H | 0.96650 | -3.11980 | 2.69300 |
| H | 2.15440 | -3.98480 | -0.19950 |
| Marilzafurollene-A_9 | | | |
| C | -0.59890 | 1.28820 | 1.68060 |
| O | 0.17480 | 0.12200 | 1.32720 |
| C | -1.73310 | 0.94940 | 2.66060 |
| C | 0.38950 | 2.35930 | 2.14130 |
| C | 1.57300 | 0.47440 | 1.39170 |
| C | 1.63980 | 2.00420 | 1.36170 |
| C | 2.36640 | -0.27610 | 0.32470 |
| Cl | 1.55320 | 2.70470 | -0.28300 |
| C | 2.29380 | -1.80010 | 0.48000 |
| C | -2.73330 | -0.08130 | 2.11050 |
| Br | -1.00720 | 0.20060 | 4.34220 |
| C | -3.53830 | 0.43420 | 0.94370 |
| C | -3.48290 | -0.11080 | -0.28150 |
| C | -4.27170 | 0.35180 | -1.45800 |
| C | -5.20600 | 1.52460 | -1.31660 |
| O | -4.13920 | -0.24300 | -2.52790 |
| C | 2.92700 | -2.29960 | 1.74440 |
| O | 3.01380 | -2.38600 | -0.60620 |
| C | 2.28560 | -2.88030 | 2.71810 |
| C | 1.63680 | -3.44570 | 3.68570 |
| H | 1.08150 | -2.91250 | 4.44610 |
| Br | 1.57000 | -5.28640 | 3.72210 |
| H | -1.05080 | 1.63800 | 0.74390 |
| H | -2.25470 | 1.86350 | 2.96630 |
| H | 0.01720 | 3.37390 | 1.96650 |
| H | 0.60860 | 2.27740 | 3.21080 |
| H | 1.91630 | 0.15570 | 2.38430 |
| H | 2.55340 | 2.38830 | 1.82360 |
| H | 1.97790 | -0.04020 | -0.67400 |
| H | 3.41360 | 0.05290 | 0.33220 |
| H | 1.25310 | -2.13570 | 0.39890 |
| H | -2.21270 | -1.00960 | 1.84070 |
| H | -3.44970 | -0.35790 | 2.89540 |
| H | -4.19620 | 1.27350 | 1.15580 |

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| H | -2.83140 | -0.95500 | -0.49180 |
| H | -5.68390 | 1.72310 | -2.28090 |
| H | -5.98780 | 1.29730 | -0.58740 |
| H | -4.64840 | 2.41730 | -1.02180 |
| H | 4.00010 | -2.15970 | 1.84300 |
| H | 2.89360 | -3.34920 | -0.52720 |
| Marilzafurollene-A_10 | | | |
| C | -0.01540 | 1.39680 | 0.94960 |
| O | 0.81550 | 0.21880 | 0.88250 |
| C | -1.47740 | 1.05140 | 1.27350 |
| C | 0.67340 | 2.38180 | 1.89330 |
| C | 2.03360 | 0.48850 | 1.60860 |
| C | 2.13490 | 2.01140 | 1.73730 |
| C | 3.21440 | -0.23390 | 0.96440 |
| Cl | 2.81750 | 2.81810 | 0.29240 |
| C | 3.04990 | -1.75870 | 0.94510 |
| C | -2.08610 | 0.12720 | 0.20360 |
| Br | -1.60200 | 0.15320 | 3.03090 |
| C | -3.59090 | 0.03950 | 0.27010 |
| C | -4.40850 | 0.46750 | -0.70490 |
| C | -5.88980 | 0.33650 | -0.57710 |
| C | -6.72000 | 0.80440 | -1.74360 |
| O | -6.41200 | -0.10970 | 0.44300 |
| C | 3.02440 | -2.37080 | 2.31390 |
| O | 4.17610 | -2.31220 | 0.26160 |
| C | 2.00010 | -2.98430 | 2.83490 |
| C | 0.97240 | -3.58240 | 3.34800 |
| H | 0.13200 | -3.07580 | 3.80400 |
| Br | 0.87760 | -5.41640 | 3.20060 |
| H | 0.00560 | 1.83020 | -0.05930 |
| H | -2.06390 | 1.97120 | 1.37740 |
| H | 0.44010 | 3.42390 | 1.65230 |
| H | 0.37980 | 2.21960 | 2.93540 |
| H | 1.87590 | 0.08840 | 2.61840 |
| H | 2.74580 | 2.31620 | 2.59150 |
| H | 3.33270 | 0.08570 | -0.07860 |
| H | 4.14710 | 0.03690 | 1.47590 |
| H | 2.15570 | -2.03180 | 0.37240 |
| H | -1.79750 | 0.49420 | -0.79010 |
| H | -1.67760 | -0.88800 | 0.28590 |
| H | -4.01700 | -0.41950 | 1.16190 |
| H | -4.02880 | 0.91690 | -1.61520 |
| H | -7.12940 | 1.79310 | -1.52220 |
| H | -6.12380 | 0.85590 | -2.65870 |
| H | -7.53320 | 0.09300 | -1.91290 |
| H | 3.93310 | -2.28910 | 2.90420 |
| H | 4.01880 | -3.27180 | 0.20620 |

| Marilzafurollene-A_11 | | | |
|------------------------------|----------|----------|----------|
| C | -0.48990 | 1.13260 | 1.40400 |
| O | 0.38880 | 0.01020 | 1.17750 |
| C | -1.74550 | 0.72740 | 2.19190 |
| C | 0.35690 | 2.24850 | 2.01660 |
| C | 1.73880 | 0.43060 | 1.46650 |
| C | 1.73270 | 1.96200 | 1.44880 |
| C | 2.72950 | -0.27070 | 0.54010 |
| Cl | 1.87890 | 2.67130 | -0.18770 |
| C | 2.70960 | -1.79770 | 0.68170 |
| C | -2.60020 | -0.34860 | 1.49960 |
| Br | -1.25040 | 0.00340 | 3.96830 |
| C | -3.23420 | 0.12370 | 0.21780 |
| C | -4.55330 | 0.31760 | 0.06320 |
| C | -5.11120 | 0.77430 | -1.24340 |
| C | -6.60950 | 0.88970 | -1.34420 |
| O | -4.37970 | 1.06850 | -2.18720 |
| C | 3.16030 | -2.27510 | 2.03000 |
| O | 3.62080 | -2.33840 | -0.27710 |
| C | 2.40590 | -2.90100 | 2.88790 |
| C | 1.64480 | -3.51220 | 3.73880 |
| H | 0.94780 | -3.01890 | 4.40340 |
| Br | 1.67530 | -5.35410 | 3.75850 |
| H | -0.80350 | 1.46900 | 0.40830 |
| H | -2.35370 | 1.61160 | 2.41430 |
| H | -0.03310 | 3.24440 | 1.78300 |
| H | 0.40530 | 2.17070 | 3.10750 |
| H | 1.93390 | 0.12030 | 2.50110 |
| H | 2.53950 | 2.38640 | 2.05260 |
| H | 2.49410 | -0.04620 | -0.50790 |
| H | 3.74410 | 0.10980 | 0.71510 |
| H | 1.71300 | -2.18390 | 0.43720 |
| H | -1.99560 | -1.23760 | 1.27880 |
| H | -3.38850 | -0.68840 | 2.18500 |
| H | -2.56580 | 0.28520 | -0.62780 |
| H | -5.25650 | 0.14950 | 0.87080 |
| H | -7.10500 | 0.30130 | -0.56720 |
| H | -6.89860 | 1.93870 | -1.24360 |
| H | -6.93400 | 0.50430 | -2.31500 |
| H | 4.19490 | -2.07860 | 2.29820 |
| H | 3.53830 | -3.30700 | -0.21760 |
| Marilzafurollene-A_12 | | | |
| C | -0.14240 | 1.32930 | 1.38480 |
| O | 0.50100 | 0.14050 | 0.87920 |
| C | -1.67320 | 1.24350 | 1.29360 |
| C | 0.43950 | 1.59860 | 2.77090 |
| C | 1.57400 | -0.20770 | 1.78170 |

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|------------------------------|----------|----------|----------|
| C | 1.83780 | 1.02820 | 2.64820 |
| C | 2.76250 | -0.76580 | 1.00080 |
| Cl | 2.92320 | 2.23060 | 1.88460 |
| C | 2.45110 | -2.10250 | 0.30950 |
| C | -2.14020 | 1.05380 | -0.15990 |
| Br | -2.35320 | -0.26750 | 2.37070 |
| C | -3.61910 | 1.28160 | -0.34520 |
| C | -4.46960 | 0.34310 | -0.78910 |
| C | -5.92230 | 0.64140 | -0.94920 |
| C | -6.80590 | -0.48910 | -1.40720 |
| O | -6.37570 | 1.76540 | -0.73920 |
| C | 2.16430 | -3.26160 | 1.22160 |
| O | 3.56560 | -2.47020 | -0.50630 |
| C | 2.73370 | -3.50080 | 2.36950 |
| C | 3.29150 | -3.73380 | 3.51490 |
| H | 4.11430 | -4.41880 | 3.67110 |
| Br | 2.55720 | -2.93860 | 5.00620 |
| H | 0.18000 | 2.14320 | 0.72150 |
| H | -2.12390 | 2.13820 | 1.73780 |
| H | 0.40260 | 2.65860 | 3.04180 |
| H | -0.09560 | 1.04690 | 3.55060 |
| H | 1.16600 | -0.98590 | 2.43820 |
| H | 2.27990 | 0.76960 | 3.61430 |
| H | 3.06030 | -0.06100 | 0.21380 |
| H | 3.63410 | -0.87560 | 1.65840 |
| H | 1.59890 | -1.97080 | -0.36660 |
| H | -1.62650 | 1.78180 | -0.80090 |
| H | -1.85510 | 0.06090 | -0.53100 |
| H | -3.99190 | 2.27750 | -0.10780 |
| H | -4.13660 | -0.65820 | -1.03680 |
| H | -6.32820 | -1.45820 | -1.23960 |
| H | -7.73720 | -0.47060 | -0.83420 |
| H | -7.02060 | -0.37100 | -2.47220 |
| H | 1.45680 | -3.99400 | 0.84110 |
| H | 4.30690 | -2.66360 | 0.09370 |
| Marilzafurollene-A_13 | | | |
| C | -0.84590 | 0.89100 | 1.83940 |
| O | -0.26450 | -0.36200 | 1.41530 |
| C | -2.15280 | 0.68630 | 2.62190 |
| C | 0.25230 | 1.67580 | 2.55630 |
| C | 1.15470 | -0.31010 | 1.68330 |
| C | 1.50870 | 1.16670 | 1.87970 |
| C | 1.91940 | -1.06080 | 0.59530 |
| Cl | 1.78240 | 2.05370 | 0.34820 |
| C | 1.64960 | -2.57380 | 0.61560 |
| C | -3.23600 | -0.05820 | 1.82410 |
| Br | -1.83230 | -0.36270 | 4.26720 |

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|------------------------------|----------|----------|----------|
| C | -3.73680 | 0.72460 | 0.63990 |
| C | -3.60610 | 0.31610 | -0.63190 |
| C | -4.12800 | 1.14370 | -1.75790 |
| C | -3.95930 | 0.59160 | -3.14890 |
| O | -4.65060 | 2.23960 | -1.56120 |
| C | 2.16110 | -3.31510 | 1.81720 |
| O | 2.27460 | -3.17400 | -0.52060 |
| C | 3.20270 | -3.00320 | 2.53620 |
| C | 4.23970 | -2.68970 | 3.24540 |
| H | 5.24060 | -3.05860 | 3.06490 |
| Br | 3.99490 | -1.55890 | 4.67910 |
| H | -1.08510 | 1.43150 | 0.91490 |
| H | -2.53420 | 1.65010 | 2.97820 |
| H | 0.10530 | 2.75830 | 2.48690 |
| H | 0.30290 | 1.42550 | 3.62080 |
| H | 1.29160 | -0.81220 | 2.64840 |
| H | 2.40640 | 1.30020 | 2.48960 |
| H | 1.61980 | -0.69060 | -0.39370 |
| H | 2.99660 | -0.86990 | 0.67930 |
| H | 0.57280 | -2.76000 | 0.52670 |
| H | -2.86710 | -1.04240 | 1.50710 |
| H | -4.10230 | -0.25600 | 2.46910 |
| H | -4.24130 | 1.66620 | 0.85580 |
| H | -3.11590 | -0.61720 | -0.88440 |
| H | -3.13070 | 1.10510 | -3.64290 |
| H | -3.75650 | -0.48260 | -3.12770 |
| H | -4.88440 | 0.74790 | -3.71080 |
| H | 1.66010 | -4.25450 | 2.03440 |
| H | 1.87910 | -2.76560 | -1.30980 |
| Marilzafurollene-A_14 | | | |
| C | -0.84040 | 1.20960 | 1.80490 |
| O | -0.33870 | -0.11530 | 1.52710 |
| C | -2.13370 | 1.17420 | 2.63430 |
| C | 0.32060 | 2.01080 | 2.39210 |
| C | 1.09480 | -0.09970 | 1.69620 |
| C | 1.52280 | 1.37200 | 1.72600 |
| C | 1.76100 | -0.99460 | 0.65290 |
| Cl | 1.77840 | 2.09170 | 0.10700 |
| C | 1.31310 | -2.46140 | 0.73430 |
| C | -3.26760 | 0.37020 | 1.97590 |
| Br | -1.81190 | 0.35370 | 4.40560 |
| C | -3.74480 | 0.96600 | 0.67860 |
| C | -3.65490 | 0.33660 | -0.50360 |
| C | -4.14940 | 0.98010 | -1.75480 |
| C | -4.04900 | 0.17410 | -3.02330 |
| O | -4.59520 | 2.12640 | -1.75480 |
| C | 1.64060 | -3.13510 | 2.03740 |

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|------------------------------|----------|----------|----------|
| O | 1.92310 | -3.18990 | -0.33350 |
| C | 2.83030 | -3.46870 | 2.45270 |
| C | 4.01180 | -3.79680 | 2.86880 |
| H | 4.38350 | -4.81130 | 2.92770 |
| Br | 5.11430 | -2.45120 | 3.47570 |
| H | -1.07890 | 1.64550 | 0.82640 |
| H | -2.46660 | 2.19420 | 2.85780 |
| H | 0.21930 | 3.08610 | 2.21400 |
| H | 0.40800 | 1.86970 | 3.47400 |
| H | 1.28000 | -0.51240 | 2.69630 |
| H | 2.44950 | 1.52050 | 2.28730 |
| H | 1.51370 | -0.64760 | -0.35830 |
| H | 2.85290 | -0.92720 | 0.74060 |
| H | 0.23180 | -2.52620 | 0.57000 |
| H | -2.95720 | -0.67250 | 1.82720 |
| H | -4.13270 | 0.33120 | 2.65110 |
| H | -4.19510 | 1.95680 | 0.73110 |
| H | -3.21770 | -0.65170 | -0.59220 |
| H | -3.97100 | -0.89480 | -2.80680 |
| H | -4.95190 | 0.33020 | -3.62020 |
| H | -3.16930 | 0.49490 | -3.58680 |
| H | 0.81470 | -3.22350 | 2.73930 |
| H | 2.88130 | -3.19800 | -0.16560 |
| Marilzafurollene-A_15 | | | |
| C | -0.14160 | 1.47860 | 1.34410 |
| O | 0.50480 | 0.24560 | 0.96220 |
| C | -1.67090 | 1.39000 | 1.23300 |
| C | 0.41600 | 1.87210 | 2.71070 |
| C | 1.55990 | -0.01910 | 1.91250 |
| C | 1.81490 | 1.29060 | 2.66610 |
| C | 2.75720 | -0.66210 | 1.21790 |
| Cl | 2.91560 | 2.41830 | 1.81650 |
| C | 2.42660 | -2.00170 | 0.54650 |
| C | -2.11290 | 1.07540 | -0.20650 |
| Br | -2.37600 | -0.02030 | 2.42500 |
| C | -3.58700 | 1.29130 | -0.43800 |
| C | -4.43430 | 0.32140 | -0.81570 |
| C | -5.88220 | 0.61070 | -1.02800 |
| C | -6.76360 | -0.55130 | -1.40360 |
| O | -6.33290 | 1.75040 | -0.92370 |
| C | 1.91430 | -3.05390 | 1.49080 |
| O | 3.61420 | -2.48010 | -0.08920 |
| C | 2.61800 | -3.67040 | 2.39840 |
| C | 3.32020 | -4.26810 | 3.30750 |
| H | 3.78050 | -5.23990 | 3.19060 |
| Br | 3.61500 | -3.37380 | 4.89160 |
| H | 0.19720 | 2.22690 | 0.61490 |

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|------------------------------|----------|----------|----------|
| H | -2.12550 | 2.32130 | 1.58940 |
| H | 0.37760 | 2.95240 | 2.88320 |
| H | -0.13540 | 1.39450 | 3.52700 |
| H | 1.13750 | -0.73000 | 2.63450 |
| H | 2.23850 | 1.12090 | 3.65980 |
| H | 3.13990 | -0.00120 | 0.42990 |
| H | 3.58050 | -0.79290 | 1.93200 |
| H | 1.68540 | -1.84610 | -0.24580 |
| H | -1.58420 | 1.74270 | -0.89920 |
| H | -1.82620 | 0.05280 | -0.48410 |
| H | -3.95900 | 2.30530 | -0.29390 |
| H | -4.10240 | -0.69870 | -0.97070 |
| H | -7.70390 | -0.48140 | -0.84950 |
| H | -6.96060 | -0.52270 | -2.47820 |
| H | -6.29340 | -1.50460 | -1.14730 |
| H | 0.83600 | -3.19380 | 1.50220 |
| H | 3.43130 | -3.38880 | -0.38420 |
| Marilzafurollene-A_16 | | | |
| C | -0.09720 | 1.29120 | 1.38540 |
| O | 0.55200 | 0.09420 | 0.90550 |
| C | -1.62750 | 1.20070 | 1.28770 |
| C | 0.47640 | 1.58980 | 2.76930 |
| C | 1.60830 | -0.24410 | 1.83250 |
| C | 1.87280 | 1.01010 | 2.67100 |
| C | 2.79970 | -0.82820 | 1.07640 |
| Cl | 2.96910 | 2.18760 | 1.88380 |
| C | 2.48900 | -2.19240 | 0.44030 |
| C | -2.08620 | 0.98090 | -0.16410 |
| Br | -2.31100 | -0.28940 | 2.39110 |
| C | -3.56350 | 1.20690 | -0.36400 |
| C | -4.41190 | 0.26320 | -0.80100 |
| C | -5.86240 | 0.56240 | -0.98000 |
| C | -6.74230 | -0.56870 | -1.44360 |
| O | -6.31670 | 1.68800 | -0.78090 |
| C | 2.24590 | -3.32310 | 1.39820 |
| O | 3.59430 | -2.58870 | -0.37400 |
| C | 2.74970 | -3.45030 | 2.59360 |
| C | 3.25510 | -3.57270 | 3.77960 |
| H | 4.18200 | -4.08450 | 4.00150 |
| Br | 2.32200 | -2.84970 | 5.19400 |
| H | 0.22720 | 2.09260 | 0.70800 |
| H | -2.08190 | 2.10340 | 1.71150 |
| H | 0.44280 | 2.65600 | 3.01500 |
| H | -0.06750 | 1.05960 | 3.55780 |
| H | 1.18280 | -1.00250 | 2.50050 |
| H | 2.30710 | 0.77320 | 3.64610 |
| H | 3.09420 | -0.15070 | 0.26460 |

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|------------------------------|----------|----------|----------|
| H | 3.67240 | -0.91110 | 1.73640 |
| H | 1.61790 | -2.10480 | -0.21940 |
| H | -1.56760 | 1.69460 | -0.81700 |
| H | -1.80030 | -0.01990 | -0.51260 |
| H | -3.93690 | 2.20690 | -0.14510 |
| H | -4.07850 | -0.74200 | -1.03170 |
| H | -6.26320 | -1.53740 | -1.27790 |
| H | -7.67520 | -0.55360 | -0.87310 |
| H | -6.95410 | -0.44810 | -2.50890 |
| H | 1.67100 | -4.15530 | 1.00110 |
| H | 3.69100 | -1.91270 | -1.06690 |
| Marilzafurollene-A_17 | | | |
| C | -0.46590 | 1.17020 | 1.41000 |
| O | 0.37590 | 0.02300 | 1.17000 |
| C | -1.70420 | 0.80710 | 2.24400 |
| C | 0.42880 | 2.27570 | 1.97100 |
| C | 1.74490 | 0.41320 | 1.40950 |
| C | 1.77630 | 1.94370 | 1.36140 |
| C | 2.68780 | -0.33040 | 0.46660 |
| Cl | 1.88000 | 2.61640 | -0.29410 |
| C | 2.63560 | -1.85340 | 0.64000 |
| C | -2.59080 | -0.28090 | 1.61250 |
| Br | -1.17170 | 0.13480 | 4.02940 |
| C | -3.20680 | 0.12360 | 0.29640 |
| C | -4.51150 | 0.40090 | 0.14930 |
| C | -5.16390 | 0.77900 | -1.13610 |
| C | -4.34850 | 0.83540 | -2.40120 |
| O | -6.36720 | 1.04020 | -1.13030 |
| C | 3.11960 | -2.31530 | 1.98210 |
| O | 3.49910 | -2.43560 | -0.33810 |
| C | 2.37830 | -2.90190 | 2.87830 |
| C | 1.63050 | -3.47430 | 3.76720 |
| H | 0.98920 | -2.94720 | 4.46130 |
| Br | 1.57840 | -5.31560 | 3.79660 |
| H | -0.80710 | 1.49790 | 0.42020 |
| H | -2.29530 | 1.70610 | 2.45220 |
| H | 0.05540 | 3.27660 | 1.73130 |
| H | 0.51440 | 2.21790 | 3.06070 |
| H | 1.96440 | 0.11750 | 2.44350 |
| H | 2.61440 | 2.35940 | 1.92730 |
| H | 2.42440 | -0.12070 | -0.57770 |
| H | 3.71650 | 0.02800 | 0.60160 |
| H | 1.62190 | -2.21900 | 0.43730 |
| H | -2.01460 | -1.20130 | 1.45100 |
| H | -3.38980 | -0.55360 | 2.31540 |
| H | -2.52990 | 0.14900 | -0.55450 |
| H | -5.19420 | 0.36310 | 0.99380 |

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|------------------------------|----------|----------|----------|
| H | -4.99920 | 1.10810 | -3.23760 |
| H | -3.56790 | 1.59530 | -2.31200 |
| H | -3.91320 | -0.14460 | -2.61310 |
| H | 4.16790 | -2.14290 | 2.21070 |
| H | 3.40190 | -3.40070 | -0.25060 |
| Marilzafurollene-A_18 | | | |
| C | 0.00240 | 1.31610 | 1.00780 |
| O | 0.82330 | 0.13270 | 0.91150 |
| C | -1.46670 | 0.97490 | 1.30290 |
| C | 0.68900 | 2.26240 | 1.99160 |
| C | 2.03540 | 0.36650 | 1.66010 |
| C | 2.14870 | 1.88350 | 1.84020 |
| C | 3.21400 | -0.34210 | 0.99680 |
| Cl | 2.85590 | 2.72900 | 0.42940 |
| C | 3.04810 | -1.86650 | 0.93770 |
| C | -2.07170 | 0.09380 | 0.19520 |
| Br | -1.62470 | 0.02190 | 3.02790 |
| C | -3.57780 | -0.01060 | 0.26150 |
| C | -4.39410 | 0.51250 | -0.66640 |
| C | -5.88130 | 0.41900 | -0.64280 |
| C | -6.56740 | -0.32320 | 0.47380 |
| O | -6.51860 | 0.95920 | -1.54750 |
| C | 3.06550 | -2.51850 | 2.28710 |
| O | 4.15500 | -2.41130 | 0.21590 |
| C | 2.02280 | -3.01640 | 2.88930 |
| C | 0.97830 | -3.49890 | 3.48380 |
| H | 0.26280 | -2.90950 | 4.04140 |
| Br | 0.62340 | -5.29600 | 3.28850 |
| H | 0.03950 | 1.78200 | 0.01400 |
| H | -2.04550 | 1.89680 | 1.42940 |
| H | 0.46830 | 3.31410 | 1.78280 |
| H | 0.38150 | 2.06840 | 3.02420 |
| H | 1.86500 | -0.06630 | 2.65390 |
| H | 2.75270 | 2.15440 | 2.71050 |
| H | 3.33040 | 0.00680 | -0.03700 |
| H | 4.14780 | -0.08730 | 1.51430 |
| H | 2.13680 | -2.13820 | 0.39170 |
| H | -1.78710 | 0.50550 | -0.78200 |
| H | -1.65550 | -0.92100 | 0.23180 |
| H | -3.97900 | -0.56190 | 1.10850 |
| H | -4.00200 | 1.05560 | -1.52170 |
| H | -6.34760 | 0.15250 | 1.43300 |
| H | -7.64980 | -0.29190 | 0.31570 |
| H | -6.25320 | -1.37020 | 0.47910 |
| H | 4.02870 | -2.58170 | 2.78550 |
| H | 4.04720 | -2.13300 | -0.71040 |

| Marilzafurollene-A_19 | | | |
|------------------------------|----------|----------|----------|
| C | 0.18500 | 1.63460 | 0.97120 |
| O | 0.89980 | 0.38640 | 0.84900 |
| C | -1.32850 | 1.41820 | 1.12340 |
| C | 0.86800 | 2.43930 | 2.07620 |
| C | 2.05320 | 0.44460 | 1.71490 |
| C | 2.29320 | 1.92680 | 2.01750 |
| C | 3.21510 | -0.33490 | 1.10420 |
| Cl | 3.19960 | 2.78900 | 0.73660 |
| C | 2.90950 | -1.82700 | 0.91650 |
| C | -1.91540 | 0.67990 | -0.09270 |
| Br | -1.72190 | 0.36280 | 2.74760 |
| C | -3.42540 | 0.69350 | -0.13540 |
| C | -4.16910 | -0.42380 | -0.14440 |
| C | -5.65790 | -0.45760 | -0.19020 |
| C | -6.43510 | 0.83240 | -0.20020 |
| O | -6.22230 | -1.55170 | -0.22000 |
| C | 2.73170 | -2.56360 | 2.20950 |
| O | 4.02400 | -2.43450 | 0.25980 |
| C | 1.59610 | -3.01440 | 2.66270 |
| C | 0.46200 | -3.45080 | 3.11030 |
| H | -0.27070 | -2.84180 | 3.62310 |
| Br | 0.01280 | -5.20440 | 2.76770 |
| H | 0.34900 | 2.16200 | 0.02200 |
| H | -1.83010 | 2.38020 | 1.27740 |
| H | 0.76690 | 3.51950 | 1.92960 |
| H | 0.45240 | 2.20890 | 3.06250 |
| H | 1.75050 | -0.03390 | 2.65490 |
| H | 2.84010 | 2.07700 | 2.95230 |
| H | 3.46070 | 0.06790 | 0.11350 |
| H | 4.11670 | -0.21180 | 1.71790 |
| H | 2.03390 | -1.96640 | 0.27130 |
| H | -1.56990 | 1.17240 | -1.01070 |
| H | -1.53940 | -0.35060 | -0.13470 |
| H | -3.88970 | 1.67570 | -0.17300 |
| H | -3.70690 | -1.40670 | -0.11430 |
| H | -6.19780 | 1.40760 | -1.09880 |
| H | -7.50610 | 0.60780 | -0.20880 |
| H | -6.21560 | 1.41170 | 0.70040 |
| H | 3.62660 | -2.73080 | 2.80220 |
| H | 4.03230 | -2.08990 | -0.65020 |
| Marilzafurollene-A_20 | | | |
| C | -0.56780 | 1.22930 | 1.68910 |
| O | 0.18890 | 0.04840 | 1.34700 |
| C | -1.71630 | 0.91550 | 2.66100 |
| C | 0.43460 | 2.28650 | 2.15190 |
| C | 1.59250 | 0.37540 | 1.42760 |

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|------------------------------|----------|----------|----------|
| C | 1.68640 | 1.90370 | 1.38820 |
| C | 2.37910 | -0.39420 | 0.36940 |
| Cl | 1.62900 | 2.59180 | -0.26350 |
| C | 2.29020 | -1.91680 | 0.53780 |
| C | -2.72590 | -0.10650 | 2.11170 |
| Br | -1.01800 | 0.17380 | 4.35720 |
| C | -3.50660 | 0.40470 | 0.92660 |
| C | -3.44320 | -0.15980 | -0.28940 |
| C | -4.20570 | 0.29790 | -1.48470 |
| C | -5.13530 | 1.47760 | -1.37140 |
| O | -4.05460 | -0.30600 | -2.54710 |
| C | 2.95080 | -2.41560 | 1.78720 |
| O | 2.98090 | -2.53120 | -0.55220 |
| C | 2.32100 | -2.86100 | 2.83730 |
| C | 1.68450 | -3.29370 | 3.87870 |
| H | 1.25460 | -2.65950 | 4.64250 |
| Br | 1.39100 | -5.10680 | 4.02170 |
| H | -1.00620 | 1.58180 | 0.74700 |
| H | -2.22790 | 1.83980 | 2.95240 |
| H | 0.08200 | 3.30600 | 1.96540 |
| H | 0.64150 | 2.20940 | 3.22410 |
| H | 1.91960 | 0.05630 | 2.42520 |
| H | 2.60210 | 2.27520 | 1.85630 |
| H | 1.99350 | -0.16090 | -0.63100 |
| H | 3.43010 | -0.07760 | 0.37510 |
| H | 1.24730 | -2.25270 | 0.49440 |
| H | -2.21690 | -1.04680 | 1.86210 |
| H | -3.45700 | -0.36030 | 2.89080 |
| H | -4.15280 | 1.25820 | 1.11670 |
| H | -2.80270 | -1.01770 | -0.47710 |
| H | -5.60270 | 1.66290 | -2.34340 |
| H | -5.92570 | 1.26600 | -0.64670 |
| H | -4.57560 | 2.37170 | -1.08500 |
| H | 4.03710 | -2.41090 | 1.79970 |
| H | 2.45120 | -2.35800 | -1.35010 |
| Marilzafurollene-A_21 | | | |
| C | -0.46940 | 1.06470 | 1.41890 |
| O | 0.39000 | -0.07550 | 1.20500 |
| C | -1.73950 | 0.68860 | 2.19780 |
| C | 0.39380 | 2.16820 | 2.03070 |
| C | 1.74580 | 0.32220 | 1.49990 |
| C | 1.76670 | 1.85350 | 1.47140 |
| C | 2.72250 | -0.40090 | 0.57580 |
| Cl | 1.93220 | 2.54570 | -0.17120 |
| C | 2.69790 | -1.92580 | 0.74580 |
| C | -2.60680 | -0.37730 | 1.50560 |
| Br | -1.27510 | -0.02860 | 3.98470 |

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|------------------------------|----------|----------|----------|
| C | -3.21150 | 0.09190 | 0.20870 |
| C | -4.52430 | 0.30690 | 0.03010 |
| C | -5.05210 | 0.75780 | -1.29090 |
| C | -6.54650 | 0.89330 | -1.42000 |
| O | -4.29950 | 1.03180 | -2.22420 |
| C | 3.20820 | -2.38060 | 2.07950 |
| O | 3.56720 | -2.50150 | -0.23180 |
| C | 2.47020 | -2.87440 | 3.03310 |
| C | 1.72720 | -3.35590 | 3.97810 |
| H | 1.13470 | -2.75780 | 4.65760 |
| Br | 1.56630 | -5.18700 | 4.10350 |
| H | -0.76860 | 1.40100 | 0.41870 |
| H | -2.33360 | 1.58550 | 2.40670 |
| H | 0.02340 | 3.16980 | 1.78980 |
| H | 0.43510 | 2.09480 | 3.12210 |
| H | 1.93180 | 0.01470 | 2.53670 |
| H | 2.57860 | 2.26840 | 2.07510 |
| H | 2.47460 | -0.19160 | -0.47250 |
| H | 3.74130 | -0.02370 | 0.73240 |
| H | 1.69210 | -2.32210 | 0.56290 |
| H | -2.01790 | -1.28140 | 1.30440 |
| H | -3.41180 | -0.69200 | 2.18350 |
| H | -2.52700 | 0.23190 | -0.62780 |
| H | -5.24360 | 0.15990 | 0.82750 |
| H | -7.06420 | 0.31860 | -0.64710 |
| H | -6.82270 | 1.94710 | -1.33360 |
| H | -6.85880 | 0.50400 | -2.39310 |
| H | 4.27770 | -2.29180 | 2.24810 |
| H | 3.14330 | -2.36220 | -1.09670 |
| Marilzafurollene-A_22 | | | |
| C | -0.31070 | 1.00560 | 1.25960 |
| O | 0.40990 | -0.17890 | 0.85960 |
| C | -1.82920 | 0.77420 | 1.29560 |
| C | 0.33090 | 1.50600 | 2.55210 |
| C | 1.56530 | -0.31230 | 1.71640 |
| C | 1.76630 | 1.04580 | 2.39690 |
| C | 2.74970 | -0.86730 | 0.92720 |
| Cl | 2.68170 | 2.22430 | 1.40690 |
| C | 2.51920 | -2.30300 | 0.42950 |
| C | -2.36610 | 0.35310 | -0.08420 |
| Br | -2.28790 | -0.62840 | 2.60980 |
| C | -3.87200 | 0.41940 | -0.19240 |
| C | -4.51670 | 1.29420 | -0.97980 |
| C | -5.99760 | 1.38070 | -1.12230 |
| C | -6.88030 | 0.42820 | -0.35940 |
| O | -6.46720 | 2.24070 | -1.86830 |
| C | 2.38940 | -3.35420 | 1.49520 |

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|------------------------------|----------|----------|----------|
| O | 3.61340 | -2.68090 | -0.40890 |
| C | 3.04440 | -3.39790 | 2.62130 |
| C | 3.68710 | -3.43740 | 3.74500 |
| H | 4.57390 | -4.03010 | 3.92660 |
| Br | 2.97550 | -2.51860 | 5.17500 |
| H | -0.11130 | 1.74980 | 0.47670 |
| H | -2.33520 | 1.67830 | 1.65260 |
| H | 0.21150 | 2.58560 | 2.68820 |
| H | -0.09810 | 1.01980 | 3.43410 |
| H | 1.27370 | -1.02780 | 2.49490 |
| H | 2.29180 | 0.95670 | 3.35170 |
| H | 2.93440 | -0.24800 | 0.04000 |
| H | 3.66590 | -0.81940 | 1.52920 |
| H | 1.62130 | -2.32880 | -0.19800 |
| H | -1.92610 | 1.00420 | -0.85090 |
| H | -2.04900 | -0.66780 | -0.33220 |
| H | -4.42300 | -0.30840 | 0.39840 |
| H | -3.97440 | 2.01770 | -1.58210 |
| H | -6.73910 | 0.56330 | 0.71610 |
| H | -7.92770 | 0.63890 | -0.59650 |
| H | -6.66440 | -0.60240 | -0.65240 |
| H | 1.72740 | -4.18310 | 1.25800 |
| H | 4.40150 | -2.73830 | 0.15900 |
| Marilzafurollene-A_23 | | | |
| C | -0.31490 | 1.17600 | 1.23340 |
| O | 0.40810 | -0.04290 | 0.95910 |
| C | -1.83420 | 0.95120 | 1.27050 |
| C | 0.31070 | 1.79680 | 2.48110 |
| C | 1.55370 | -0.09060 | 1.83750 |
| C | 1.74870 | 1.32700 | 2.38620 |
| C | 2.74570 | -0.73020 | 1.13050 |
| Cl | 2.67090 | 2.40980 | 1.29850 |
| C | 2.47860 | -2.16580 | 0.65930 |
| C | -2.35370 | 0.40560 | -0.07190 |
| Br | -2.31280 | -0.32510 | 2.70140 |
| C | -3.85770 | 0.46380 | -0.20660 |
| C | -4.48880 | 1.26220 | -1.08140 |
| C | -5.96730 | 1.33810 | -1.25240 |
| C | -6.86380 | 0.46330 | -0.41610 |
| O | -6.42350 | 2.12510 | -2.08240 |
| C | 2.12390 | -3.12070 | 1.76550 |
| O | 3.65200 | -2.63430 | -0.00950 |
| C | 2.94970 | -3.60860 | 2.64800 |
| C | 3.77220 | -4.08400 | 3.52810 |
| H | 4.31810 | -5.01190 | 3.42230 |
| Br | 4.09100 | -3.08020 | 5.04010 |
| H | -0.10280 | 1.84150 | 0.38570 |

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|------------------------------|----------|----------|----------|
| H | -2.34280 | 1.88480 | 1.53620 |
| H | 0.18840 | 2.88410 | 2.51390 |
| H | -0.12860 | 1.39420 | 3.39950 |
| H | 1.25420 | -0.72520 | 2.68160 |
| H | 2.26380 | 1.33090 | 3.35070 |
| H | 3.01400 | -0.15150 | 0.23770 |
| H | 3.62700 | -0.70710 | 1.78450 |
| H | 1.67130 | -2.16830 | -0.08210 |
| H | -1.90160 | 0.98280 | -0.88910 |
| H | -2.03590 | -0.63420 | -0.22050 |
| H | -4.41920 | -0.20430 | 0.44210 |
| H | -3.93600 | 1.92520 | -1.74110 |
| H | -6.73810 | 0.69930 | 0.64380 |
| H | -7.90690 | 0.65200 | -0.68790 |
| H | -6.64650 | -0.59080 | -0.60710 |
| H | 1.06120 | -3.30110 | 1.91030 |
| H | 3.51810 | -3.58180 | -0.18490 |
| Marilzafurollene-A_24 | | | |
| C | -0.10040 | 1.52670 | 1.26920 |
| O | 0.51480 | 0.26360 | 0.93810 |
| C | -1.63330 | 1.46240 | 1.19210 |
| C | 0.49290 | 1.97760 | 2.60260 |
| C | 1.58340 | 0.02580 | 1.88030 |
| C | 1.87960 | 1.36730 | 2.55940 |
| C | 2.75300 | -0.67900 | 1.19850 |
| Cl | 2.98130 | 2.42860 | 1.62880 |
| C | 2.37810 | -2.03630 | 0.58870 |
| C | -2.10960 | 1.08160 | -0.22080 |
| Br | -2.34180 | 0.13500 | 2.47190 |
| C | -3.59050 | 1.28980 | -0.43430 |
| C | -4.42790 | 0.30090 | -0.78390 |
| C | -5.89140 | 0.46270 | -1.01120 |
| C | -6.53210 | 1.81310 | -0.82620 |
| O | -6.54780 | -0.52250 | -1.35040 |
| C | 1.85200 | -3.03310 | 1.58440 |
| O | 3.54370 | -2.57030 | -0.04340 |
| C | 2.56410 | -3.69460 | 2.45290 |
| C | 3.27520 | -4.34330 | 3.31920 |
| H | 3.70690 | -5.32100 | 3.15260 |
| Br | 3.63490 | -3.52030 | 4.92810 |
| H | 0.23690 | 2.23010 | 0.49620 |
| H | -2.06290 | 2.42060 | 1.50530 |
| H | 0.47800 | 3.06580 | 2.72080 |
| H | -0.04970 | 1.55250 | 3.45320 |
| H | 1.16160 | -0.63780 | 2.64630 |
| H | 2.32180 | 1.24100 | 3.55140 |
| H | 3.14240 | -0.06320 | 0.37800 |

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|------------------------------|----------|----------|----------|
| H | 3.58220 | -0.80170 | 1.90720 |
| H | 1.62920 | -1.89470 | -0.19890 |
| H | -1.59420 | 1.71460 | -0.95460 |
| H | -1.82930 | 0.04650 | -0.45530 |
| H | -3.94980 | 2.30720 | -0.30110 |
| H | -4.07000 | -0.71540 | -0.92400 |
| H | -6.11350 | 2.52900 | -1.53820 |
| H | -7.60710 | 1.73090 | -1.01380 |
| H | -6.39090 | 2.15990 | 0.20080 |
| H | 0.76920 | -3.09110 | 1.66640 |
| H | 3.32840 | -3.48090 | -0.31000 |
| Marilzafurollene-A_25 | | | |
| C | -0.10840 | 1.34990 | 1.34020 |
| O | 0.50410 | 0.13400 | 0.86240 |
| C | -1.64200 | 1.28890 | 1.27790 |
| C | 0.50440 | 1.65350 | 2.70570 |
| C | 1.58810 | -0.20420 | 1.75540 |
| C | 1.89010 | 1.05420 | 2.57570 |
| C | 2.75080 | -0.80910 | 0.97070 |
| Cl | 2.98100 | 2.21180 | 1.75280 |
| C | 2.40010 | -2.15840 | 0.32390 |
| C | -2.13720 | 1.05470 | -0.16020 |
| Br | -2.33150 | -0.16520 | 2.42290 |
| C | -3.62060 | 1.28380 | -0.33160 |
| C | -4.46410 | 0.33570 | -0.76850 |
| C | -5.93010 | 0.52050 | -0.95920 |
| C | -6.56540 | 1.84610 | -0.63130 |
| O | -6.59300 | -0.42510 | -1.38690 |
| C | 2.10390 | -3.28380 | 1.27430 |
| O | 3.49350 | -2.57290 | -0.49820 |
| C | 2.69140 | -3.50500 | 2.41670 |
| C | 3.26730 | -3.72000 | 3.55660 |
| H | 4.07480 | -4.42240 | 3.71570 |
| Br | 2.58610 | -2.86320 | 5.03890 |
| H | 0.21580 | 2.13560 | 0.64450 |
| H | -2.06870 | 2.20820 | 1.69460 |
| H | 0.49120 | 2.72220 | 2.94240 |
| H | -0.02490 | 1.13690 | 3.51290 |
| H | 1.17940 | -0.95330 | 2.44450 |
| H | 2.34630 | 0.81930 | 3.54130 |
| H | 3.04860 | -0.13370 | 0.15820 |
| H | 3.63180 | -0.91770 | 1.61590 |
| H | 1.54000 | -2.02800 | -0.34240 |
| H | -1.63070 | 1.75950 | -0.83210 |
| H | -1.86160 | 0.04900 | -0.50310 |
| H | -3.97640 | 2.28260 | -0.09140 |
| H | -4.10960 | -0.66130 | -1.01540 |

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|------------------------------|----------|----------|----------|
| H | -6.41080 | 2.08770 | 0.42350 |
| H | -6.15400 | 2.62950 | -1.27300 |
| H | -7.64280 | 1.78420 | -0.81290 |
| H | 1.36960 | -4.00770 | 0.92990 |
| H | 4.23810 | -2.77120 | 0.09610 |
| Marilzafurollene-A_26 | | | |
| C | 0.01370 | 1.31300 | 0.94210 |
| O | 0.82530 | 0.12030 | 0.89120 |
| C | -1.45470 | 0.99740 | 1.26820 |
| C | 0.71790 | 2.29920 | 1.87310 |
| C | 2.04410 | 0.37710 | 1.62090 |
| C | 2.17270 | 1.89970 | 1.72790 |
| C | 3.21190 | -0.37320 | 0.98520 |
| Cl | 2.87510 | 2.67040 | 0.27240 |
| C | 3.03130 | -1.89700 | 0.99970 |
| C | -2.07710 | 0.06640 | 0.21210 |
| Br | -1.59910 | 0.13110 | 3.03980 |
| C | -3.58350 | 0.00860 | 0.27510 |
| C | -4.38980 | 0.43600 | -0.70940 |
| C | -5.87380 | 0.33600 | -0.58430 |
| C | -6.69130 | 0.79860 | -1.76180 |
| O | -6.40770 | -0.08170 | 0.44180 |
| C | 3.04720 | -2.48340 | 2.37870 |
| O | 4.13040 | -2.48670 | 0.30190 |
| C | 2.00530 | -2.96140 | 2.99820 |
| C | 0.96150 | -3.42670 | 3.60740 |
| H | 0.23020 | -2.81870 | 4.12320 |
| Br | 0.62650 | -5.23450 | 3.49060 |
| H | 0.04310 | 1.73220 | -0.07260 |
| H | -2.02530 | 1.92890 | 1.35560 |
| H | 0.50480 | 3.34160 | 1.61540 |
| H | 0.41810 | 2.15870 | 2.91650 |
| H | 1.87590 | -0.00660 | 2.63510 |
| H | 2.78670 | 2.20600 | 2.57920 |
| H | 3.32540 | -0.07500 | -0.06460 |
| H | 4.15130 | -0.10310 | 1.48470 |
| H | 2.11550 | -2.18520 | 0.47000 |
| H | -1.77860 | 0.41090 | -0.78670 |
| H | -1.68820 | -0.95470 | 0.31320 |
| H | -4.02090 | -0.42720 | 1.17320 |
| H | -3.99880 | 0.86260 | -1.62580 |
| H | -6.08930 | 0.83140 | -2.67400 |
| H | -7.51200 | 0.09470 | -1.92680 |
| H | -7.09010 | 1.79490 | -1.55570 |
| H | 4.00840 | -2.51630 | 2.88370 |
| H | 4.02080 | -2.25450 | -0.63670 |

| Marilzafurollene-A_27 | | | |
|------------------------------|----------|----------|----------|
| C | -0.27590 | 0.96480 | 1.28130 |
| O | 0.44680 | -0.22930 | 0.91300 |
| C | -1.79550 | 0.73900 | 1.30330 |
| C | 0.35240 | 1.49000 | 2.57060 |
| C | 1.59210 | -0.34740 | 1.78720 |
| C | 1.78850 | 1.02450 | 2.44030 |
| C | 2.78040 | -0.91730 | 1.01540 |
| Cl | 2.71560 | 2.17910 | 1.43250 |
| C | 2.56100 | -2.37410 | 0.57730 |
| C | -2.31570 | 0.28750 | -0.07340 |
| Br | -2.27710 | -0.63050 | 2.64320 |
| C | -3.81940 | 0.36000 | -0.20460 |
| C | -4.44690 | 1.21730 | -1.02460 |
| C | -5.92510 | 1.30980 | -1.19090 |
| C | -6.82550 | 0.38460 | -0.41520 |
| O | -6.37760 | 2.15200 | -1.96700 |
| C | 2.49440 | -3.38760 | 1.68340 |
| O | 3.64140 | -2.77390 | -0.26790 |
| C | 3.10550 | -3.32300 | 2.83290 |
| C | 3.71690 | -3.25480 | 3.97230 |
| H | 4.70090 | -3.66070 | 4.16590 |
| Br | 2.84710 | -2.42730 | 5.36960 |
| H | -0.06540 | 1.69240 | 0.48590 |
| H | -2.30270 | 1.65300 | 1.63230 |
| H | 0.23360 | 2.57230 | 2.68350 |
| H | -0.08700 | 1.02230 | 3.45750 |
| H | 1.29010 | -1.04670 | 2.57600 |
| H | 2.30470 | 0.95580 | 3.40180 |
| H | 2.95150 | -0.32710 | 0.10590 |
| H | 3.69990 | -0.83730 | 1.60870 |
| H | 1.64250 | -2.44920 | -0.01650 |
| H | -1.86100 | 0.91720 | -0.84930 |
| H | -2.00150 | -0.74100 | -0.29200 |
| H | -4.38360 | -0.34790 | 0.39780 |
| H | -3.89130 | 1.92080 | -1.63830 |
| H | -6.69960 | 0.54920 | 0.65810 |
| H | -7.86770 | 0.59500 | -0.67430 |
| H | -6.61200 | -0.65520 | -0.67580 |
| H | 1.96150 | -4.30410 | 1.44520 |
| H | 3.62320 | -2.18880 | -1.04490 |
| Marilzafurollene-A_28 | | | |
| C | -0.82220 | 1.15020 | 1.80540 |
| O | -0.28440 | -0.15760 | 1.51000 |
| C | -2.12930 | 1.06920 | 2.61000 |
| C | 0.30690 | 1.96720 | 2.43320 |
| C | 1.14020 | -0.12100 | 1.74470 |

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|------------------------------|----------|----------|----------|
| C | 1.54040 | 1.35720 | 1.79870 |
| C | 1.86450 | -0.99590 | 0.72430 |
| Cl | 1.82700 | 2.09290 | 0.19140 |
| C | 1.44880 | -2.47280 | 0.78910 |
| C | -3.23690 | 0.26340 | 1.91070 |
| Br | -1.82350 | 0.20750 | 4.36460 |
| C | -3.71080 | 0.89170 | 0.62770 |
| C | -3.61820 | 0.29250 | -0.56970 |
| C | -4.11370 | 0.96550 | -1.80500 |
| C | -4.01890 | 0.18620 | -3.09040 |
| O | -4.55390 | 2.11350 | -1.77900 |
| C | 1.75740 | -3.13850 | 2.09870 |
| O | 2.12830 | -3.19390 | -0.24060 |
| C | 2.94800 | -3.39700 | 2.56140 |
| C | 4.13580 | -3.65380 | 3.00760 |
| H | 4.70320 | -4.54090 | 2.76030 |
| Br | 4.96910 | -2.36660 | 4.02890 |
| H | -1.05170 | 1.60040 | 0.83140 |
| H | -2.48480 | 2.07670 | 2.85440 |
| H | 0.19060 | 3.04200 | 2.26070 |
| H | 0.36390 | 1.81970 | 3.51630 |
| H | 1.28830 | -0.53690 | 2.74970 |
| H | 2.44750 | 1.51900 | 2.38750 |
| H | 1.64380 | -0.64950 | -0.29320 |
| H | 2.95090 | -0.90370 | 0.84950 |
| H | 0.37520 | -2.57230 | 0.59120 |
| H | -2.90190 | -0.76690 | 1.73240 |
| H | -4.10960 | 0.18450 | 2.57250 |
| H | -4.16350 | 1.88000 | 0.70420 |
| H | -3.18180 | -0.69350 | -0.68240 |
| H | -3.12160 | 0.49240 | -3.63380 |
| H | -3.97770 | -0.88920 | -2.89640 |
| H | -4.90750 | 0.38310 | -3.69660 |
| H | 0.90510 | -3.34420 | 2.74040 |
| H | 1.85200 | -2.80510 | -1.08800 |
| Marilzafurollene-A_29 | | | |
| C | -0.06510 | 1.31070 | 1.34290 |
| O | 0.55300 | 0.08830 | 0.88700 |
| C | -1.59830 | 1.24760 | 1.27000 |
| C | 0.53610 | 1.63590 | 2.70900 |
| C | 1.61760 | -0.24490 | 1.80630 |
| C | 1.91960 | 1.02670 | 2.60490 |
| C | 2.78500 | -0.87290 | 1.04790 |
| Cl | 3.02450 | 2.16060 | 1.76740 |
| C | 2.43850 | -2.24920 | 0.45770 |
| C | -2.08270 | 0.99640 | -0.16880 |
| Br | -2.29530 | -0.19340 | 2.42680 |

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|------------------------------|----------|----------|----------|
| C | -3.56550 | 1.21900 | -0.35340 |
| C | -4.40280 | 0.26370 | -0.78670 |
| C | -5.86800 | 0.44150 | -0.98930 |
| C | -6.51120 | 1.76630 | -0.67340 |
| O | -6.52390 | -0.50910 | -1.41690 |
| C | 2.19150 | -3.34630 | 1.45280 |
| O | 3.52230 | -2.68960 | -0.36280 |
| C | 2.71650 | -3.44930 | 2.64140 |
| C | 3.24300 | -3.54780 | 3.82040 |
| H | 4.16170 | -4.07520 | 4.03990 |
| Br | 2.35560 | -2.76090 | 5.23010 |
| H | 0.26410 | 2.08630 | 0.63840 |
| H | -2.02870 | 2.17150 | 1.67250 |
| H | 0.52670 | 2.70890 | 2.92560 |
| H | -0.00490 | 1.13800 | 3.52020 |
| H | 1.18870 | -0.97600 | 2.50190 |
| H | 2.36540 | 0.80860 | 3.57920 |
| H | 3.07770 | -0.22500 | 0.21160 |
| H | 3.66720 | -0.95300 | 1.69530 |
| H | 1.55770 | -2.16470 | -0.18960 |
| H | -1.57350 | 1.69540 | -0.84470 |
| H | -1.80160 | -0.01200 | -0.49890 |
| H | -3.92630 | 2.21900 | -0.12600 |
| H | -4.04340 | -0.73460 | -1.02110 |
| H | -7.58770 | 1.69740 | -0.85750 |
| H | -6.36110 | 2.01680 | 0.38000 |
| H | -6.10170 | 2.54680 | -1.31980 |
| H | 1.59040 | -4.17660 | 1.09220 |
| H | 3.61620 | -2.03840 | -1.07950 |
| Marilzafurollene-A_30 | | | |
| C | -0.85670 | 1.14870 | 1.77190 |
| O | -0.26920 | -0.13340 | 1.46220 |
| C | -2.15670 | 1.00930 | 2.57920 |
| C | 0.24110 | 2.00090 | 2.40770 |
| C | 1.15440 | -0.03960 | 1.68540 |
| C | 1.49370 | 1.45310 | 1.75370 |
| C | 1.91580 | -0.87680 | 0.66130 |
| Cl | 1.73090 | 2.22270 | 0.15480 |
| C | 1.54850 | -2.36620 | 0.69450 |
| C | -3.24590 | 0.19950 | 1.85610 |
| Br | -1.81890 | 0.10290 | 4.30400 |
| C | -3.77900 | 0.88700 | 0.62380 |
| C | -3.66860 | 0.36920 | -0.60950 |
| C | -4.19490 | 1.00220 | -1.85150 |
| C | -4.89690 | 2.33240 | -1.77250 |
| O | -4.04190 | 0.41510 | -2.92300 |
| C | 1.80660 | -3.03440 | 2.01680 |

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|------------------------------|----------|----------|----------|
| O | 2.30360 | -3.02790 | -0.32310 |
| C | 2.97500 | -3.36180 | 2.49280 |
| C | 4.13860 | -3.67780 | 2.96520 |
| H | 4.62310 | -4.63380 | 2.81900 |
| Br | 5.07150 | -2.38760 | 3.89280 |
| H | -1.10610 | 1.60080 | 0.80360 |
| H | -2.53700 | 1.99910 | 2.85650 |
| H | 0.07950 | 3.07280 | 2.25510 |
| H | 0.31010 | 1.83560 | 3.48770 |
| H | 1.32570 | -0.45550 | 2.68680 |
| H | 2.39850 | 1.64580 | 2.33660 |
| H | 1.70060 | -0.52320 | -0.35500 |
| H | 2.99700 | -0.75300 | 0.80410 |
| H | 0.49120 | -2.49280 | 0.43510 |
| H | -2.87320 | -0.80310 | 1.60880 |
| H | -4.09980 | 0.04360 | 2.52880 |
| H | -4.28830 | 1.83290 | 0.79190 |
| H | -3.16750 | -0.58060 | -0.77720 |
| H | -5.79760 | 2.24670 | -1.15930 |
| H | -4.22250 | 3.09100 | -1.36720 |
| H | -5.19510 | 2.64290 | -2.77860 |
| H | 0.94700 | -3.12050 | 2.67740 |
| H | 2.15560 | -3.98260 | -0.20890 |
| Marilzafurollene-A_31 | | | |
| C | -0.83590 | 0.90560 | 1.84960 |
| O | -0.26670 | -0.35810 | 1.44490 |
| C | -2.15160 | 0.72730 | 2.62320 |
| C | 0.26710 | 1.68420 | 2.56530 |
| C | 1.15590 | -0.31090 | 1.69640 |
| C | 1.51920 | 1.16470 | 1.88870 |
| C | 1.90510 | -1.06500 | 0.59990 |
| Cl | 1.79680 | 2.04830 | 0.35590 |
| C | 1.63010 | -2.57700 | 0.62380 |
| C | -3.23740 | -0.01700 | 1.82810 |
| Br | -1.85700 | -0.29870 | 4.28730 |
| C | -3.72750 | 0.75020 | 0.62530 |
| C | -3.58640 | 0.30500 | -0.63290 |
| C | -4.06630 | 1.01700 | -1.85040 |
| C | -4.77280 | 2.34000 | -1.71270 |
| O | -3.87040 | 0.50030 | -2.95080 |
| C | 2.15770 | -3.32070 | 1.81700 |
| O | 2.23560 | -3.17830 | -0.52230 |
| C | 3.20860 | -3.01030 | 2.52300 |
| C | 4.25530 | -2.69860 | 3.21870 |
| H | 5.25420 | -3.06390 | 3.02120 |
| Br | 4.02960 | -1.57430 | 4.66060 |
| H | -1.06230 | 1.43820 | 0.91720 |

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|------------------------------|----------|----------|----------|
| H | -2.52500 | 1.70070 | 2.96110 |
| H | 0.12770 | 2.76760 | 2.49420 |
| H | 0.31700 | 1.43440 | 3.63000 |
| H | 1.30120 | -0.81320 | 2.66020 |
| H | 2.41860 | 1.29370 | 2.49710 |
| H | 1.59500 | -0.69400 | -0.38560 |
| H | 2.98390 | -0.87800 | 0.67080 |
| H | 0.55150 | -2.75960 | 0.55160 |
| H | -2.87690 | -1.01070 | 1.53110 |
| H | -4.10980 | -0.19570 | 2.47060 |
| H | -4.22990 | 1.69130 | 0.83530 |
| H | -3.09050 | -0.63940 | -0.84160 |
| H | -5.68790 | 2.21920 | -1.12730 |
| H | -4.10960 | 3.07440 | -1.24850 |
| H | -5.04790 | 2.70690 | -2.70630 |
| H | 1.66060 | -4.26140 | 2.03740 |
| H | 1.81760 | -2.77830 | -1.30450 |
| Marilzafurollene-A_32 | | | |
| C | -0.28890 | 1.18240 | 1.15430 |
| O | 0.40930 | -0.06220 | 0.93670 |
| C | -1.81030 | 0.98550 | 1.23990 |
| C | 0.37590 | 1.86710 | 2.34720 |
| C | 1.57180 | -0.07830 | 1.79360 |
| C | 1.80320 | 1.36630 | 2.24990 |
| C | 2.73720 | -0.78220 | 1.10380 |
| Cl | 2.71820 | 2.36370 | 1.07760 |
| C | 2.43420 | -2.23800 | 0.72500 |
| C | -2.36950 | 0.36500 | -0.05300 |
| Br | -2.27190 | -0.19160 | 2.75870 |
| C | -3.86950 | 0.47580 | -0.17310 |
| C | -4.49250 | 1.18690 | -1.12620 |
| C | -5.98270 | 1.24160 | -1.19260 |
| C | -6.58740 | 2.03650 | -2.32020 |
| O | -6.68640 | 0.68460 | -0.35200 |
| C | 2.08500 | -3.11760 | 1.89370 |
| O | 3.58460 | -2.76820 | 0.06250 |
| C | 2.92120 | -3.57600 | 2.78230 |
| C | 3.75400 | -4.02240 | 3.66770 |
| H | 4.26970 | -4.97110 | 3.60440 |
| Br | 4.14050 | -2.94170 | 5.10930 |
| H | -0.08740 | 1.79240 | 0.26340 |
| H | -2.29770 | 1.94230 | 1.45860 |
| H | 0.27270 | 2.95640 | 2.31540 |
| H | -0.04860 | 1.52990 | 3.29830 |
| H | 1.27900 | -0.65450 | 2.68090 |
| H | 2.34040 | 1.41960 | 3.20080 |
| H | 2.99800 | -0.26350 | 0.17270 |

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|------------------------------|----------|----------|----------|
| H | 3.63180 | -0.73730 | 1.73820 |
| H | 1.61170 | -2.26910 | 0.00130 |
| H | -1.90880 | 0.86370 | -0.91580 |
| H | -2.09480 | -0.69460 | -0.12890 |
| H | -4.46240 | -0.07720 | 0.55510 |
| H | -3.94360 | 1.74090 | -1.87880 |
| H | -6.91050 | 3.01000 | -1.94320 |
| H | -5.86930 | 2.18270 | -3.13160 |
| H | -7.44380 | 1.48980 | -2.72480 |
| H | 1.02220 | -3.25980 | 2.07580 |
| H | 3.43070 | -3.72210 | -0.05110 |
| Marilzafurollene-A_33 | | | |
| C | -0.86310 | 0.93300 | 1.81400 |
| O | -0.31720 | -0.34210 | 1.41450 |
| C | -2.16500 | 0.77890 | 2.61560 |
| C | 0.26230 | 1.70490 | 2.50120 |
| C | 1.11000 | -0.30980 | 1.63490 |
| C | 1.49540 | 1.16280 | 1.80760 |
| C | 1.83340 | -1.08490 | 0.53500 |
| Cl | 1.76000 | 2.02990 | 0.26370 |
| C | 1.52670 | -2.59060 | 0.56260 |
| C | -3.27890 | 0.05060 | 1.84510 |
| Br | -1.85160 | -0.24680 | 4.27670 |
| C | -3.79390 | 0.83430 | 0.66340 |
| C | -3.69910 | 0.39820 | -0.60230 |
| C | -4.20780 | 1.12930 | -1.79680 |
| C | -4.86740 | 2.47250 | -1.62540 |
| O | -4.07550 | 0.61180 | -2.90620 |
| C | 2.00840 | -3.33440 | 1.77620 |
| O | 2.12910 | -3.20510 | -0.57850 |
| C | 3.11670 | -3.11510 | 2.42630 |
| C | 4.21220 | -2.88830 | 3.07870 |
| H | 5.12740 | -3.45330 | 2.96100 |
| Br | 4.17890 | -1.59310 | 4.38920 |
| H | -1.10060 | 1.45800 | 0.88020 |
| H | -2.51530 | 1.75920 | 2.95830 |
| H | 0.13510 | 2.78920 | 2.42150 |
| H | 0.32820 | 1.46520 | 3.56730 |
| H | 1.26980 | -0.80420 | 2.60070 |
| H | 2.40640 | 1.28500 | 2.39990 |
| H | 1.52640 | -0.71370 | -0.45140 |
| H | 2.91640 | -0.92010 | 0.60010 |
| H | 0.44580 | -2.74200 | 0.46550 |
| H | -2.93620 | -0.94370 | 1.53010 |
| H | -4.13560 | -0.12480 | 2.50930 |
| H | -4.27610 | 1.78050 | 0.89670 |
| H | -3.22510 | -0.55180 | -0.83520 |

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|------------------------------|----------|----------|----------|
| H | -4.16940 | 3.17990 | -1.17020 |
| H | -5.15520 | 2.86060 | -2.60730 |
| H | -5.77060 | 2.37340 | -1.01790 |
| H | 1.38530 | -4.16590 | 2.09540 |
| H | 3.09300 | -3.14090 | -0.46170 |
| Marilzafurollene-A_34 | | | |
| C | -0.78430 | 0.90940 | 1.53400 |
| O | -0.07180 | -0.32120 | 1.28490 |
| C | -2.18210 | 0.65740 | 2.12050 |
| C | 0.14250 | 1.80230 | 2.35880 |
| C | 1.29220 | -0.14740 | 1.72550 |
| C | 1.51520 | 1.35920 | 1.89360 |
| C | 2.25230 | -0.89110 | 0.80110 |
| Cl | 1.94860 | 2.20730 | 0.37810 |
| C | 1.99120 | -2.40180 | 0.73660 |
| C | -3.09260 | -0.20090 | 1.22500 |
| Br | -2.05170 | -0.27820 | 3.86040 |
| C | -3.46280 | 0.46970 | -0.07150 |
| C | -4.70170 | 0.89330 | -0.36730 |
| C | -4.99640 | 1.53730 | -1.68080 |
| C | -6.42990 | 1.91080 | -1.95260 |
| O | -4.10520 | 1.77650 | -2.49380 |
| C | 2.10070 | -3.10290 | 2.06240 |
| O | 2.93320 | -2.97260 | -0.17480 |
| C | 3.20510 | -3.32540 | 2.71810 |
| C | 4.30470 | -3.53090 | 3.37020 |
| H | 4.89210 | -4.43760 | 3.31680 |
| Br | 4.95620 | -2.15710 | 4.41150 |
| H | -0.90780 | 1.38360 | 0.55260 |
| H | -2.66930 | 1.61030 | 2.35650 |
| H | -0.06520 | 2.86730 | 2.21400 |
| H | 0.05570 | 1.59960 | 3.43100 |
| H | 1.33930 | -0.59390 | 2.72720 |
| H | 2.30330 | 1.58210 | 2.61820 |
| H | 2.16220 | -0.51300 | -0.22510 |
| H | 3.28980 | -0.70150 | 1.10540 |
| H | 0.99520 | -2.58820 | 0.31890 |
| H | -2.61120 | -1.15940 | 0.99250 |
| H | -4.01090 | -0.45500 | 1.77170 |
| H | -2.66750 | 0.58260 | -0.80820 |
| H | -5.52680 | 0.78300 | 0.32690 |
| H | -7.11360 | 1.34970 | -1.30970 |
| H | -6.56400 | 2.98110 | -1.77750 |
| H | -6.67230 | 1.66920 | -2.99140 |
| H | 1.15970 | -3.30300 | 2.56950 |
| H | 2.84310 | -3.93880 | -0.10600 |

| Marilzafurollene-A_35 | | | |
|------------------------------|----------|----------|----------|
| C | -0.75120 | 0.68380 | 1.57930 |
| O | -0.03630 | -0.52540 | 1.24580 |
| C | -2.15370 | 0.39120 | 2.13450 |
| C | 0.16920 | 1.51550 | 2.47210 |
| C | 1.32280 | -0.38840 | 1.71780 |
| C | 1.54500 | 1.10250 | 1.98970 |
| C | 2.28440 | -1.05930 | 0.73940 |
| Cl | 1.99180 | 2.04500 | 0.53400 |
| C | 2.11510 | -2.58620 | 0.69290 |
| C | -3.05490 | -0.40370 | 1.17350 |
| Br | -2.03980 | -0.66000 | 3.80750 |
| C | -3.40630 | 0.35130 | -0.08130 |
| C | -4.63970 | 0.79880 | -0.36410 |
| C | -4.91530 | 1.52770 | -1.63670 |
| C | -6.34370 | 1.92560 | -1.90100 |
| O | -4.01300 | 1.81400 | -2.42190 |
| C | 2.50210 | -3.32740 | 1.94040 |
| O | 2.93150 | -3.11310 | -0.35490 |
| C | 3.40490 | -2.96760 | 2.80910 |
| C | 4.30490 | -2.60670 | 3.66730 |
| H | 5.34580 | -2.89820 | 3.62390 |
| Br | 3.77680 | -1.54300 | 5.07580 |
| H | -0.86750 | 1.22780 | 0.63390 |
| H | -2.64400 | 1.32570 | 2.43000 |
| H | -0.03510 | 2.58850 | 2.39890 |
| H | 0.07240 | 1.23980 | 3.52700 |
| H | 1.35260 | -0.90640 | 2.68380 |
| H | 2.32810 | 1.27560 | 2.73300 |
| H | 2.10630 | -0.68170 | -0.27580 |
| H | 3.32330 | -0.80330 | 0.98250 |
| H | 1.07620 | -2.83770 | 0.44940 |
| H | -2.57290 | -1.34660 | 0.88490 |
| H | -3.98060 | -0.68990 | 1.69090 |
| H | -2.60150 | 0.50800 | -0.79930 |
| H | -5.47390 | 0.64760 | 0.31140 |
| H | -7.03770 | 1.32760 | -1.30420 |
| H | -6.47520 | 2.98300 | -1.65820 |
| H | -6.57430 | 1.75340 | -2.95610 |
| H | 2.04500 | -4.30560 | 2.06220 |
| H | 2.61200 | -2.71980 | -1.18550 |
| Marilzafurollene-A_36 | | | |
| C | -0.29370 | 1.00080 | 1.18950 |
| O | 0.39200 | -0.22320 | 0.85210 |
| C | -1.81560 | 0.80780 | 1.27420 |
| C | 0.39000 | 1.57050 | 2.43080 |
| C | 1.56700 | -0.32440 | 1.68640 |

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|------------------------------|----------|----------|----------|
| C | 1.81150 | 1.07020 | 2.27200 |
| C | 2.71870 | -0.95260 | 0.90360 |
| Cl | 2.72580 | 2.16210 | 1.18640 |
| C | 2.45270 | -2.41630 | 0.51800 |
| C | -2.39280 | 0.30330 | -0.06060 |
| Br | -2.27260 | -0.48950 | 2.69290 |
| C | -3.89270 | 0.43750 | -0.15590 |
| C | -4.51730 | 1.23000 | -1.04130 |
| C | -6.00730 | 1.30370 | -1.08850 |
| C | -6.61450 | 2.19040 | -2.14390 |
| O | -6.70900 | 0.68820 | -0.28780 |
| C | 2.34450 | -3.38430 | 1.66210 |
| O | 3.51350 | -2.87070 | -0.32530 |
| C | 3.04410 | -3.36010 | 2.76180 |
| C | 3.73070 | -3.32760 | 3.85940 |
| H | 4.60090 | -3.93860 | 4.05980 |
| Br | 3.11300 | -2.25850 | 5.22740 |
| H | -0.09720 | 1.68730 | 0.35490 |
| H | -2.29290 | 1.74620 | 1.57840 |
| H | 0.29560 | 2.65900 | 2.49830 |
| H | -0.02600 | 1.15230 | 3.35290 |
| H | 1.28310 | -0.98210 | 2.51690 |
| H | 2.35880 | 1.03180 | 3.21790 |
| H | 2.88410 | -0.40070 | -0.03080 |
| H | 3.65380 | -0.87700 | 1.47280 |
| H | 1.53420 | -2.47320 | -0.07670 |
| H | -1.93500 | 0.86850 | -0.88300 |
| H | -2.12930 | -0.74870 | -0.22790 |
| H | -4.48420 | -0.16800 | 0.53050 |
| H | -3.96950 | 1.83850 | -1.75160 |
| H | -6.93730 | 3.12840 | -1.68550 |
| H | -5.89820 | 2.40560 | -2.94150 |
| H | -7.47150 | 1.67910 | -2.59150 |
| H | 1.64490 | -4.20390 | 1.51980 |
| H | 4.31830 | -2.90260 | 0.22080 |
| Marilzafurollene-A_37 | | | |
| C | -0.78030 | 0.72200 | 1.54360 |
| O | -0.08800 | -0.49900 | 1.20770 |
| C | -2.17630 | 0.45190 | 2.12590 |
| C | 0.16640 | 1.54640 | 2.41520 |
| C | 1.28180 | -0.37650 | 1.64830 |
| C | 1.52820 | 1.11250 | 1.91200 |
| C | 2.21990 | -1.06390 | 0.65780 |
| Cl | 1.96660 | 2.04660 | 0.44880 |
| C | 2.01000 | -2.58480 | 0.58940 |
| C | -3.10650 | -0.33410 | 1.18540 |
| Br | -2.04510 | -0.59420 | 3.80130 |

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|------------------------------|----------|----------|----------|
| C | -3.48200 | 0.42730 | -0.05870 |
| C | -4.71870 | 0.88360 | -0.31140 |
| C | -5.01930 | 1.61920 | -1.57440 |
| C | -6.45230 | 2.01960 | -1.80800 |
| O | -4.13290 | 1.90870 | -2.37640 |
| C | 2.33350 | -3.34860 | 1.84210 |
| O | 2.82850 | -3.11660 | -0.45490 |
| C | 3.30750 | -3.09660 | 2.67100 |
| C | 4.26890 | -2.84160 | 3.50050 |
| H | 5.22850 | -3.34140 | 3.50330 |
| Br | 3.94240 | -1.62790 | 4.84800 |
| H | -0.90560 | 1.26080 | 0.59640 |
| H | -2.64780 | 1.39440 | 2.42690 |
| H | -0.02520 | 2.62160 | 2.33960 |
| H | 0.08420 | 1.27780 | 3.47320 |
| H | 1.32700 | -0.89100 | 2.61600 |
| H | 2.32480 | 1.27640 | 2.64290 |
| H | 2.05140 | -0.67290 | -0.35390 |
| H | 3.26560 | -0.83820 | 0.90230 |
| H | 0.97140 | -2.79500 | 0.31020 |
| H | -2.63930 | -1.28020 | 0.88350 |
| H | -4.02220 | -0.61380 | 1.72390 |
| H | -2.69280 | 0.58120 | -0.79450 |
| H | -5.53800 | 0.73480 | 0.38260 |
| H | -6.70640 | 1.84560 | -2.85740 |
| H | -7.13440 | 1.42470 | -1.19460 |
| H | -6.57610 | 3.07780 | -1.56460 |
| H | 1.72550 | -4.23130 | 2.02330 |
| H | 3.75440 | -2.99900 | -0.17940 |
| Marilzafurollene-A_38 | | | |
| C | -0.09270 | 2.13750 | 1.71690 |
| O | 0.38050 | 0.89040 | 1.16750 |
| C | -1.48090 | 2.02480 | 2.36510 |
| C | 1.00870 | 2.66080 | 2.64080 |
| C | 1.74710 | 0.70010 | 1.59020 |
| C | 2.26180 | 2.07440 | 2.02460 |
| C | 2.54920 | -0.03290 | 0.51770 |
| Cl | 2.81360 | 3.10510 | 0.66940 |
| C | 1.98350 | -1.41720 | 0.17990 |
| C | -2.64050 | 1.78570 | 1.37970 |
| Br | -1.51990 | 0.63590 | 3.76200 |
| C | -2.60090 | 0.51420 | 0.56910 |
| C | -3.54470 | -0.43670 | 0.64680 |
| C | -3.54590 | -1.70140 | -0.13960 |
| C | -2.39120 | -2.01560 | -1.05340 |
| O | -4.50680 | -2.46340 | -0.02680 |
| C | 2.01760 | -2.37480 | 1.33300 |

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|------------------------------|----------|----------|----------|
| O | 2.78960 | -1.97910 | -0.85710 |
| C | 0.96410 | -2.86060 | 1.92540 |
| C | -0.08960 | -3.32960 | 2.51410 |
| H | -0.57600 | -2.86760 | 3.36320 |
| Br | -0.88760 | -4.82380 | 1.79040 |
| H | -0.17710 | 2.82630 | 0.86600 |
| H | -1.69100 | 2.95370 | 2.90900 |
| H | 1.00700 | 3.75300 | 2.71590 |
| H | 0.89890 | 2.26800 | 3.65750 |
| H | 1.69820 | 0.07360 | 2.49020 |
| H | 3.09270 | 2.00300 | 2.73170 |
| H | 2.55260 | 0.54310 | -0.41620 |
| H | 3.59880 | -0.12040 | 0.82680 |
| H | 0.96760 | -1.31640 | -0.21910 |
| H | -3.58760 | 1.83850 | 1.93380 |
| H | -2.66780 | 2.62320 | 0.67040 |
| H | -1.75920 | 0.40870 | -0.11060 |
| H | -4.39490 | -0.33310 | 1.31490 |
| H | -1.45460 | -2.01930 | -0.49070 |
| H | -2.53190 | -3.01210 | -1.48290 |
| H | -2.34960 | -1.28960 | -1.86920 |
| H | 2.99810 | -2.67370 | 1.69370 |
| H | 2.39170 | -2.83910 | -1.08180 |
| Marilzafurollene-A_39 | | | |
| C | -0.43480 | 1.09770 | 1.40750 |
| O | 0.39560 | -0.06080 | 1.17970 |
| C | -1.68440 | 0.75430 | 2.23340 |
| C | 0.46790 | 2.19620 | 1.97010 |
| C | 1.76540 | 0.31080 | 1.44300 |
| C | 1.81900 | 1.84020 | 1.38240 |
| C | 2.71000 | -0.45230 | 0.51760 |
| Cl | 1.95490 | 2.49430 | -0.27860 |
| C | 2.64730 | -1.97340 | 0.71040 |
| C | -2.57880 | -0.32630 | 1.60030 |
| Br | -1.17570 | 0.08700 | 4.02730 |
| C | -3.18580 | 0.08310 | 0.28140 |
| C | -4.48740 | 0.37260 | 0.12980 |
| C | -5.13220 | 0.75650 | -1.15780 |
| C | -4.31210 | 0.80590 | -2.42000 |
| O | -6.33320 | 1.02820 | -1.15600 |
| C | 3.15290 | -2.42360 | 2.04740 |
| O | 3.49470 | -2.58580 | -0.26410 |
| C | 2.40500 | -2.87080 | 3.01620 |
| C | 1.65180 | -3.30620 | 3.97540 |
| H | 1.11090 | -2.67360 | 4.66650 |
| Br | 1.39660 | -5.12510 | 4.11710 |
| H | -0.76390 | 1.42400 | 0.41320 |

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|----------------------------|----------|----------|----------|
| H | -2.26620 | 1.66170 | 2.43120 |
| H | 0.11170 | 3.19960 | 1.71580 |
| H | 0.53770 | 2.14810 | 3.06140 |
| H | 1.96330 | 0.02000 | 2.48240 |
| H | 2.65510 | 2.24950 | 1.95590 |
| H | 2.45440 | -0.25240 | -0.53060 |
| H | 3.74030 | -0.10000 | 0.65540 |
| H | 1.63030 | -2.34580 | 0.53890 |
| H | -2.01090 | -1.25230 | 1.44240 |
| H | -3.38340 | -0.59030 | 2.30030 |
| H | -2.50590 | 0.10200 | -0.56700 |
| H | -5.17330 | 0.34130 | 0.97200 |
| H | -4.95710 | 1.08640 | -3.25830 |
| H | -3.52390 | 1.55750 | -2.32740 |
| H | -3.88630 | -0.17830 | -2.63160 |
| H | 4.22730 | -2.38120 | 2.20190 |
| H | 3.07000 | -2.44750 | -1.12870 |
| Marilzafurollene-A_ | | | |
| C | -0.24920 | 0.97080 | 1.20680 |
| O | 0.45100 | -0.25060 | 0.88690 |
| C | -1.77060 | 0.76640 | 1.27580 |
| C | 0.41470 | 1.55740 | 2.45130 |
| C | 1.60640 | -0.34320 | 1.75070 |
| C | 1.83970 | 1.05930 | 2.32050 |
| C | 2.77150 | -0.98060 | 0.99690 |
| Cl | 2.76560 | 2.13710 | 1.22980 |
| C | 2.52070 | -2.45810 | 0.65570 |
| C | -2.32890 | 0.24930 | -0.06220 |
| Br | -2.23310 | -0.52560 | 2.69740 |
| C | -3.82890 | 0.36780 | -0.17420 |
| C | -4.45250 | 1.15010 | -1.06930 |
| C | -5.94270 | 1.20730 | -1.13220 |
| C | -6.54860 | 2.08170 | -2.19850 |
| O | -6.64580 | 0.58830 | -0.33540 |
| C | 2.45970 | -3.39930 | 1.82420 |
| O | 3.57830 | -2.92820 | -0.18220 |
| C | 3.08260 | -3.26640 | 2.96150 |
| C | 3.70580 | -3.13030 | 4.08840 |
| H | 4.68540 | -3.53730 | 4.30070 |
| Br | 2.85830 | -2.20430 | 5.43670 |
| H | -0.04850 | 1.65190 | 0.36890 |
| H | -2.25860 | 1.70290 | 1.56870 |
| H | 0.31650 | 2.64640 | 2.50390 |
| H | -0.01460 | 1.14990 | 3.37220 |
| H | 1.30210 | -0.98970 | 2.58250 |
| H | 2.37400 | 1.03610 | 3.27420 |
| H | 2.93640 | -0.45140 | 0.04940 |

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|------------------------------|----------|----------|----------|
| H | 3.70250 | -0.87980 | 1.56880 |
| H | 1.58980 | -2.55470 | 0.08470 |
| H | -1.86810 | 0.81480 | -0.88270 |
| H | -2.05310 | -0.80090 | -0.22120 |
| H | -4.42140 | -0.24120 | 0.50840 |
| H | -3.90400 | 1.76150 | -1.77640 |
| H | -5.82660 | 2.30020 | -2.98990 |
| H | -7.39550 | 1.55880 | -2.65180 |
| H | -6.88600 | 3.01870 | -1.74850 |
| H | 1.91580 | -4.32390 | 1.65080 |
| H | 3.55270 | -2.39410 | -0.99490 |
| Marilzafurollene-A_41 | | | |
| C | -0.51940 | 1.95130 | 1.94480 |
| O | -0.13220 | 0.60100 | 1.64070 |
| C | -1.90450 | 2.04170 | 2.60000 |
| C | 0.65520 | 2.52520 | 2.72400 |
| C | 1.31140 | 0.52420 | 1.62850 |
| C | 1.83490 | 1.92820 | 1.97360 |
| C | 1.73930 | -0.09290 | 0.29700 |
| Cl | 2.22710 | 2.94300 | 0.55000 |
| C | 1.31040 | -1.56270 | 0.17920 |
| C | -3.06680 | 1.65900 | 1.65620 |
| Br | -2.00630 | 0.96290 | 4.23950 |
| C | -2.98950 | 0.28710 | 1.03090 |
| C | -2.53200 | 0.07490 | -0.21370 |
| C | -2.29760 | -1.27630 | -0.78830 |
| C | -3.06470 | -2.45690 | -0.25530 |
| O | -1.44360 | -1.40020 | -1.66970 |
| C | 2.25220 | -2.48950 | 0.88810 |
| O | 1.32980 | -1.93510 | -1.19910 |
| C | 1.98060 | -3.14680 | 1.97970 |
| C | 1.71200 | -3.80140 | 3.06440 |
| H | 2.01300 | -3.49610 | 4.05740 |
| Br | 0.76940 | -5.37710 | 2.91370 |
| H | -0.58610 | 2.47890 | 0.98340 |
| H | -2.07140 | 3.06830 | 2.94650 |
| H | 0.64790 | 3.61880 | 2.76140 |
| H | 0.66970 | 2.15210 | 3.75390 |
| H | 1.58030 | -0.14510 | 2.45460 |
| H | 2.74340 | 1.88540 | 2.58080 |
| H | 1.27090 | 0.45680 | -0.53020 |
| H | 2.82430 | -0.00660 | 0.15830 |
| H | 0.28870 | -1.71240 | 0.54560 |
| H | -4.02230 | 1.73250 | 2.19140 |
| H | -3.11850 | 2.41350 | 0.85950 |
| H | -3.25950 | -0.54540 | 1.67620 |
| H | -2.19170 | 0.89400 | -0.83950 |

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|------------------------------|----------|----------|----------|
| H | -4.10140 | -2.18090 | -0.04460 |
| H | -3.07960 | -3.24590 | -1.01300 |
| H | -2.57980 | -2.83390 | 0.64860 |
| H | 3.22080 | -2.64380 | 0.42050 |
| H | 0.44090 | -1.70480 | -1.55030 |
| Marilzafurollene-A_42 | | | |
| C | -0.75340 | 0.78330 | 1.56940 |
| O | -0.11360 | -0.46590 | 1.23470 |
| C | -2.13430 | 0.57070 | 2.20810 |
| C | 0.25340 | 1.59910 | 2.37940 |
| C | 1.27620 | -0.37680 | 1.61820 |
| C | 1.57890 | 1.11000 | 1.83140 |
| C | 2.15180 | -1.11880 | 0.61000 |
| Cl | 1.98080 | 1.99200 | 0.32560 |
| C | 1.89150 | -2.63330 | 0.58960 |
| C | -3.11210 | -0.23860 | 1.33760 |
| Br | -1.97200 | -0.39890 | 3.92570 |
| C | -3.46270 | 0.43030 | 0.03190 |
| C | -4.66320 | 0.97620 | -0.21610 |
| C | -5.05770 | 1.62280 | -1.49950 |
| C | -4.08490 | 1.66060 | -2.64860 |
| O | -6.18220 | 2.11660 | -1.58790 |
| C | 2.24290 | -3.37640 | 1.84720 |
| O | 2.64790 | -3.21600 | -0.47410 |
| C | 3.25600 | -3.13370 | 2.63060 |
| C | 4.25650 | -2.88730 | 3.41520 |
| H | 5.19910 | -3.41830 | 3.39640 |
| Br | 4.01950 | -1.62990 | 4.74120 |
| H | -0.90100 | 1.30310 | 0.61450 |
| H | -2.57590 | 1.53670 | 2.47800 |
| H | 0.09150 | 2.67750 | 2.28340 |
| H | 0.20920 | 1.36020 | 3.44650 |
| H | 1.34390 | -0.86770 | 2.59670 |
| H | 2.41100 | 1.26770 | 2.52310 |
| H | 1.95540 | -0.74780 | -0.40420 |
| H | 3.21300 | -0.92110 | 0.80730 |
| H | 0.83600 | -2.81620 | 0.35890 |
| H | -2.69730 | -1.22970 | 1.11240 |
| H | -4.03400 | -0.42760 | 1.90450 |
| H | -2.68490 | 0.41940 | -0.72820 |
| H | -5.44790 | 0.97690 | 0.53560 |
| H | -3.19790 | 2.23620 | -2.37170 |
| H | -3.81090 | 0.64470 | -2.94440 |
| H | -4.55800 | 2.14980 | -3.50560 |
| H | 1.61670 | -4.23540 | 2.07500 |
| H | 3.58750 | -3.13120 | -0.23570 |

| Marilzafurollene-A_43 | | | |
|------------------------------|----------|----------|----------|
| C | -0.75410 | 0.97750 | 1.53250 |
| O | -0.08360 | -0.27800 | 1.29170 |
| C | -2.13590 | 0.77900 | 2.17400 |
| C | 0.22640 | 1.87000 | 2.29300 |
| C | 1.29850 | -0.13020 | 1.68360 |
| C | 1.56830 | 1.37440 | 1.79160 |
| C | 2.20740 | -0.93220 | 0.75600 |
| Cl | 1.96220 | 2.15910 | 0.23120 |
| C | 1.89930 | -2.43540 | 0.74810 |
| C | -3.09140 | -0.10080 | 1.34860 |
| Br | -1.96760 | -0.08050 | 3.94890 |
| C | -3.45290 | 0.48600 | 0.00680 |
| C | -4.66570 | 0.98710 | -0.27370 |
| C | -5.07170 | 1.55270 | -1.59140 |
| C | -4.09440 | 1.55660 | -2.73730 |
| O | -6.20930 | 2.00890 | -1.71020 |
| C | 2.03550 | -3.09810 | 2.09100 |
| O | 2.78880 | -3.06130 | -0.17950 |
| C | 3.15610 | -3.38010 | 2.69420 |
| C | 4.27160 | -3.65080 | 3.29350 |
| H | 4.80560 | -4.58750 | 3.20620 |
| Br | 5.04360 | -2.32690 | 4.31670 |
| H | -0.90330 | 1.42620 | 0.54250 |
| H | -2.59750 | 1.75120 | 2.38110 |
| H | 0.04160 | 2.93520 | 2.12110 |
| H | 0.17570 | 1.70420 | 3.37380 |
| H | 1.36550 | -0.54430 | 2.69810 |
| H | 2.38980 | 1.59970 | 2.47720 |
| H | 2.09800 | -0.58380 | -0.27870 |
| H | 3.25870 | -0.76560 | 1.02390 |
| H | 0.88340 | -2.60350 | 0.37260 |
| H | -2.65270 | -1.09290 | 1.18030 |
| H | -4.01080 | -0.27920 | 1.92290 |
| H | -2.67230 | 0.45340 | -0.74980 |
| H | -5.45310 | 1.00910 | 0.47490 |
| H | -3.22340 | 2.16760 | -2.48680 |
| H | -3.79380 | 0.53400 | -2.97980 |
| H | -4.57530 | 1.98960 | -3.61980 |
| H | 1.11210 | -3.22100 | 2.65220 |
| H | 2.67580 | -4.02200 | -0.07540 |
| Marilzafurollene-A_44 | | | |
| C | -0.37230 | 1.92640 | 1.98460 |
| O | 0.12040 | 0.71620 | 1.37410 |
| C | -1.56480 | 1.68420 | 2.92230 |
| C | 0.82990 | 2.61310 | 2.63450 |
| C | 1.55960 | 0.71190 | 1.47150 |

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|------------------------------|----------|----------|----------|
| C | 1.98120 | 2.15420 | 1.76350 |
| C | 2.18290 | 0.03940 | 0.25070 |
| Cl | 2.09430 | 3.19000 | 0.30850 |
| C | 1.71750 | -1.40820 | 0.05390 |
| C | -2.86790 | 1.26860 | 2.21340 |
| Br | -1.13130 | 0.36260 | 4.31970 |
| C | -2.81020 | 0.02460 | 1.36300 |
| C | -3.04520 | 0.02120 | 0.04180 |
| C | -2.98940 | -1.18800 | -0.82590 |
| C | -2.64270 | -2.52480 | -0.22590 |
| O | -3.23630 | -1.06390 | -2.02610 |
| C | 2.11480 | -2.32260 | 1.17370 |
| O | 2.33500 | -1.90900 | -1.13320 |
| C | 1.28600 | -2.87100 | 2.01600 |
| C | 0.45800 | -3.40140 | 2.85860 |
| H | 0.19900 | -2.97260 | 3.81770 |
| Br | -0.37670 | -4.97180 | 2.37900 |
| H | -0.72030 | 2.56030 | 1.15830 |
| H | -1.76760 | 2.60300 | 3.48550 |
| H | 0.70910 | 3.69960 | 2.69360 |
| H | 0.99460 | 2.25100 | 3.65520 |
| H | 1.79690 | 0.11930 | 2.36450 |
| H | 2.94830 | 2.20940 | 2.27050 |
| H | 1.91300 | 0.58310 | -0.66330 |
| H | 3.27780 | 0.07840 | 0.31720 |
| H | 0.63400 | -1.43190 | -0.10990 |
| H | -3.65640 | 1.11870 | 2.96270 |
| H | -3.20070 | 2.11560 | 1.59880 |
| H | -2.56430 | -0.89650 | 1.88510 |
| H | -3.29110 | 0.93520 | -0.49060 |
| H | -1.64940 | -2.48710 | 0.22700 |
| H | -3.39480 | -2.81280 | 0.51290 |
| H | -2.62850 | -3.28220 | -1.01550 |
| H | 3.17590 | -2.53090 | 1.28240 |
| H | 1.96390 | -2.79670 | -1.28380 |
| Marilzafurollene-A_45 | | | |
| C | -0.57800 | 1.65920 | 2.16130 |
| O | -0.42730 | 0.30670 | 1.69900 |
| C | -2.00610 | 1.97440 | 2.62700 |
| C | 0.54230 | 1.85140 | 3.17350 |
| C | 0.95040 | -0.09450 | 1.88100 |
| C | 1.68420 | 1.10350 | 2.50380 |
| C | 1.46170 | -0.63360 | 0.54490 |
| Cl | 2.49620 | 2.17190 | 1.31550 |
| C | 0.79550 | -1.97110 | 0.17830 |
| C | -3.04510 | 1.98540 | 1.48280 |
| Br | -2.59900 | 0.74600 | 4.04160 |

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|------------------------------|----------|----------|----------|
| C | -3.14810 | 0.71860 | 0.66790 |
| C | -2.53000 | 0.55580 | -0.51320 |
| C | -2.48590 | -0.73580 | -1.24770 |
| C | -3.58170 | -1.74760 | -1.04180 |
| O | -1.52290 | -0.96100 | -1.98470 |
| C | 1.34300 | -3.19400 | 0.85850 |
| O | 0.94330 | -2.19010 | -1.22540 |
| C | 2.39560 | -3.27110 | 1.62250 |
| C | 3.44620 | -3.35430 | 2.37520 |
| H | 4.42520 | -3.65900 | 2.02980 |
| Br | 3.25690 | -2.97740 | 4.16830 |
| H | -0.37550 | 2.30630 | 1.29680 |
| H | -2.01790 | 2.95980 | 3.10730 |
| H | 0.75130 | 2.90500 | 3.38220 |
| H | 0.30890 | 1.35840 | 4.12360 |
| H | 0.92490 | -0.89680 | 2.62760 |
| H | 2.45510 | 0.78620 | 3.21150 |
| H | 1.22820 | 0.08390 | -0.25300 |
| H | 2.55270 | -0.74220 | 0.55430 |
| H | -0.27980 | -1.93240 | 0.38700 |
| H | -4.04150 | 2.20930 | 1.88530 |
| H | -2.80440 | 2.82290 | 0.81410 |
| H | -3.69890 | -0.09870 | 1.12740 |
| H | -1.91660 | 1.34030 | -0.94510 |
| H | -3.62430 | -2.41110 | -1.91060 |
| H | -3.37450 | -2.33820 | -0.14600 |
| H | -4.55300 | -1.25310 | -0.95530 |
| H | 0.80310 | -4.11440 | 0.65150 |
| H | 0.21560 | -1.68720 | -1.65420 |
| Marilzafurollene-A_46 | | | |
| C | 0.03250 | 1.43510 | 0.78790 |
| O | 0.87100 | 0.26100 | 0.77000 |
| C | -1.45780 | 1.07900 | 0.92500 |
| C | 0.60200 | 2.37890 | 1.84620 |
| C | 1.99860 | 0.50210 | 1.63840 |
| C | 2.07420 | 2.01810 | 1.84310 |
| C | 3.24910 | -0.18920 | 1.10010 |
| Cl | 2.91240 | 2.88870 | 0.52270 |
| C | 3.09770 | -1.71180 | 0.99420 |
| C | -1.93300 | 0.20020 | -0.24770 |
| Br | -1.77760 | 0.09670 | 2.61210 |
| C | -3.41680 | -0.00110 | -0.45650 |
| C | -4.43270 | 0.57460 | 0.20580 |
| C | -5.84940 | 0.25030 | -0.14140 |
| C | -6.92170 | 0.89270 | 0.69930 |
| O | -6.13040 | -0.48540 | -1.08600 |
| C | 2.92020 | -2.38510 | 2.32240 |

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|------------------------------|----------|----------|----------|
| O | 4.29800 | -2.23240 | 0.41990 |
| C | 1.84640 | -3.02110 | 2.69570 |
| C | 0.77000 | -3.64150 | 3.06110 |
| H | -0.11960 | -3.15570 | 3.43980 |
| Br | 0.70110 | -5.46670 | 2.82060 |
| H | 0.16910 | 1.91030 | -0.19280 |
| H | -2.04700 | 1.99860 | 1.00040 |
| H | 0.39080 | 3.43010 | 1.62560 |
| H | 0.19170 | 2.17010 | 2.83950 |
| H | 1.73190 | 0.05810 | 2.60610 |
| H | 2.58110 | 2.28640 | 2.77410 |
| H | 3.48220 | 0.17720 | 0.09240 |
| H | 4.11630 | 0.05970 | 1.72520 |
| H | 2.27640 | -1.95990 | 0.31150 |
| H | -1.55550 | 0.63560 | -1.18250 |
| H | -1.47630 | -0.79560 | -0.17010 |
| H | -3.65490 | -0.70460 | -1.25650 |
| H | -4.28480 | 1.28380 | 1.01000 |
| H | -7.31490 | 1.76830 | 0.17700 |
| H | -7.72410 | 0.16950 | 0.87080 |
| H | -6.53040 | 1.19560 | 1.67440 |
| H | 3.75600 | -2.33080 | 3.01470 |
| H | 4.15290 | -3.18810 | 0.30090 |
| Marilzafurollene-A_47 | | | |
| C | -0.72060 | 0.73100 | 1.57790 |
| O | -0.04690 | -0.49990 | 1.23810 |
| C | -2.10950 | 0.48010 | 2.18520 |
| C | 0.25050 | 1.55710 | 2.42110 |
| C | 1.32650 | -0.39470 | 1.67610 |
| C | 1.59890 | 1.09470 | 1.90690 |
| C | 2.24490 | -1.11620 | 0.69210 |
| Cl | 2.02510 | 1.99070 | 0.41590 |
| C | 2.03300 | -2.63850 | 0.68840 |
| C | -3.05450 | -0.32970 | 1.27980 |
| Br | -1.96190 | -0.52020 | 3.88640 |
| C | -3.40110 | 0.36460 | -0.01380 |
| C | -4.61150 | 0.88580 | -0.26700 |
| C | -5.00280 | 1.55670 | -1.53890 |
| C | -4.01180 | 1.65550 | -2.66860 |
| O | -6.13990 | 2.01970 | -1.63400 |
| C | 2.42730 | -3.35880 | 1.94560 |
| O | 2.81070 | -3.21400 | -0.36310 |
| C | 3.35880 | -3.00260 | 2.78500 |
| C | 4.28690 | -2.64520 | 3.61420 |
| H | 5.31710 | -2.97130 | 3.55970 |
| Br | 3.81980 | -1.52850 | 5.00300 |
| H | -0.85930 | 1.26150 | 0.62770 |

| | | | |
|------------------------------|----------|----------|----------|
| H | -2.57460 | 1.43220 | 2.46520 |
| H | 0.07320 | 2.63330 | 2.32820 |
| H | 0.18010 | 1.31000 | 3.48510 |
| H | 1.36350 | -0.89100 | 2.65310 |
| H | 2.40930 | 1.26220 | 2.62170 |
| H | 2.05250 | -0.75880 | -0.32780 |
| H | 3.29600 | -0.88360 | 0.90390 |
| H | 0.98230 | -2.86670 | 0.47420 |
| H | -2.61280 | -1.30460 | 1.03630 |
| H | -3.98020 | -0.55450 | 1.82690 |
| H | -2.61150 | 0.39500 | -0.76090 |
| H | -5.40790 | 0.84550 | 0.47120 |
| H | -3.14450 | 2.24370 | -2.35790 |
| H | -3.70730 | 0.65650 | -2.99120 |
| H | -4.48230 | 2.16020 | -3.51790 |
| H | 1.94530 | -4.31970 | 2.10350 |
| H | 2.48470 | -2.83270 | -1.19660 |
| Marilzafurollene-A_48 | | | |
| C | 0.03040 | 1.43590 | 0.78920 |
| O | 0.87060 | 0.26280 | 0.76940 |
| C | -1.45900 | 1.07740 | 0.92780 |
| C | 0.59980 | 2.38000 | 1.84730 |
| C | 1.99750 | 0.50440 | 1.63880 |
| C | 2.07240 | 2.02050 | 1.84310 |
| C | 3.24850 | -0.18670 | 1.10170 |
| Cl | 2.90880 | 2.89080 | 0.52140 |
| C | 3.09750 | -1.70930 | 0.99670 |
| C | -1.93300 | 0.19590 | -0.24400 |
| Br | -1.77570 | 0.09280 | 2.61390 |
| C | -3.41770 | -0.02140 | -0.44820 |
| C | -4.42750 | 0.59290 | 0.18800 |
| C | -5.87430 | 0.33060 | -0.06390 |
| C | -6.28430 | -0.72490 | -1.05690 |
| O | -6.70770 | 0.99510 | 0.55300 |
| C | 2.92030 | -2.38200 | 2.32530 |
| O | 4.29760 | -2.23010 | 0.42210 |
| C | 1.84360 | -3.01110 | 2.70210 |
| C | 0.76440 | -3.62410 | 3.07170 |
| H | -0.11640 | -3.13320 | 3.46430 |
| Br | 0.68050 | -5.44830 | 2.82880 |
| H | 0.16500 | 1.91170 | -0.19140 |
| H | -2.04860 | 1.99660 | 1.00390 |
| H | 0.38760 | 3.43120 | 1.62710 |
| H | 0.19030 | 2.17070 | 2.84080 |
| H | 1.73010 | 0.06070 | 2.60640 |
| H | 2.57980 | 2.28950 | 2.77360 |
| H | 3.48200 | 0.17920 | 0.09390 |

| | | | |
|------------------------------|----------|----------|----------|
| H | 4.11530 | 0.06280 | 1.72710 |
| H | 2.27610 | -1.95820 | 0.31440 |
| H | -1.56180 | 0.63220 | -1.18090 |
| H | -1.46810 | -0.79620 | -0.16620 |
| H | -3.63680 | -0.76400 | -1.21400 |
| H | -4.25970 | 1.34670 | 0.94980 |
| H | -5.94530 | -0.45030 | -2.05900 |
| H | -5.88040 | -1.69720 | -0.76310 |
| H | -7.37590 | -0.80070 | -1.07190 |
| H | 3.75860 | -2.33280 | 3.01510 |
| H | 4.15420 | -3.18640 | 0.30660 |
| Marilzafurollene-A_49 | | | |
| C | -0.34190 | 1.86710 | 1.98060 |
| O | 0.11520 | 0.64010 | 1.37640 |
| C | -1.55580 | 1.66660 | 2.90090 |
| C | 0.87680 | 2.51210 | 2.64180 |
| C | 1.55230 | 0.58710 | 1.48260 |
| C | 2.01930 | 2.01440 | 1.77980 |
| C | 2.14930 | -0.10050 | 0.25710 |
| Cl | 2.17970 | 3.04480 | 0.32500 |
| C | 1.64560 | -1.53700 | 0.06440 |
| C | -2.85540 | 1.27440 | 2.17160 |
| Br | -1.18060 | 0.35120 | 4.32010 |
| C | -2.81240 | 0.01140 | 1.34860 |
| C | -2.95440 | -0.00700 | 0.01440 |
| C | -2.89040 | -1.23430 | -0.82670 |
| C | -2.70730 | -2.57970 | -0.17590 |
| O | -2.98750 | -1.11590 | -2.04890 |
| C | 2.07450 | -2.47210 | 1.15400 |
| O | 2.20230 | -2.05100 | -1.14730 |
| C | 1.30240 | -2.91240 | 2.10700 |
| C | 0.53230 | -3.33460 | 3.05860 |
| H | 0.43750 | -2.86160 | 4.02690 |
| Br | -0.53160 | -4.80100 | 2.72620 |
| H | -0.65780 | 2.51130 | 1.14940 |
| H | -1.74460 | 2.59720 | 3.44940 |
| H | 0.79280 | 3.60200 | 2.70050 |
| H | 1.02080 | 2.14390 | 3.66330 |
| H | 1.76660 | -0.01560 | 2.37420 |
| H | 2.98380 | 2.03700 | 2.29450 |
| H | 1.88470 | 0.45210 | -0.65300 |
| H | 3.24530 | -0.09010 | 0.31440 |
| H | 0.55530 | -1.55400 | -0.04660 |
| H | -3.66480 | 1.16280 | 2.90510 |
| H | -3.15030 | 2.11710 | 1.53210 |
| H | -2.64820 | -0.90970 | 1.90220 |
| H | -3.10950 | 0.90770 | -0.54980 |

| | | | |
|------------------------------|----------|----------|----------|
| H | -3.52630 | -2.77780 | 0.52030 |
| H | -2.71800 | -3.35750 | -0.94550 |
| H | -1.74400 | -2.61890 | 0.33770 |
| H | 3.10840 | -2.80480 | 1.13170 |
| H | 1.77420 | -1.56870 | -1.87650 |
| Marilzafurollene-A_50 | | | |
| C | -0.19380 | 2.12080 | 1.85070 |
| O | 0.29590 | 0.91130 | 1.24220 |
| C | -1.57110 | 1.93570 | 2.50540 |
| C | 0.91430 | 2.62410 | 2.77700 |
| C | 1.67210 | 0.72670 | 1.62370 |
| C | 2.16830 | 2.08900 | 2.11220 |
| C | 2.44740 | 0.05490 | 0.49330 |
| Cl | 2.67860 | 3.19080 | 0.79770 |
| C | 1.86460 | -1.30890 | 0.09740 |
| C | -2.73010 | 1.67190 | 1.52350 |
| Br | -1.54260 | 0.49820 | 3.85630 |
| C | -2.58130 | 0.49530 | 0.59490 |
| C | -3.32340 | -0.62030 | 0.66210 |
| C | -3.10270 | -1.74280 | -0.29620 |
| C | -3.89510 | -3.00050 | -0.05640 |
| O | -2.33750 | -1.63740 | -1.25300 |
| C | 1.96820 | -2.33620 | 1.18500 |
| O | 2.62020 | -1.80400 | -1.01010 |
| C | 0.95740 | -2.83170 | 1.84040 |
| C | -0.05220 | -3.30600 | 2.49800 |
| H | -0.52690 | -2.80930 | 3.33360 |
| Br | -0.77530 | -4.90540 | 1.94060 |
| H | -0.30860 | 2.84460 | 1.03310 |
| H | -1.81490 | 2.83520 | 3.08320 |
| H | 0.89400 | 3.71160 | 2.90030 |
| H | 0.83130 | 2.18500 | 3.77700 |
| H | 1.65690 | 0.05690 | 2.49320 |
| H | 3.01240 | 2.00130 | 2.80160 |
| H | 2.42640 | 0.68060 | -0.40780 |
| H | 3.50450 | -0.04940 | 0.76910 |
| H | 0.82830 | -1.19120 | -0.24120 |
| H | -3.66620 | 1.57710 | 2.09030 |
| H | -2.85710 | 2.56350 | 0.89560 |
| H | -1.81820 | 0.58160 | -0.17880 |
| H | -4.08900 | -0.75560 | 1.41710 |
| H | -3.32120 | -3.86120 | -0.41160 |
| H | -4.08470 | -3.14230 | 1.01120 |
| H | -4.84320 | -2.94170 | -0.59650 |
| H | 2.96790 | -2.67360 | 1.44450 |
| H | 2.12480 | -2.57060 | -1.35070 |

| Marilzafurollene-A_51 | | | |
|------------------------------|----------|----------|----------|
| C | -0.62970 | 1.64320 | 2.02530 |
| O | -0.05570 | 0.32530 | 2.00190 |
| C | -1.97430 | 1.69370 | 2.76610 |
| C | 0.50880 | 2.53270 | 2.49630 |
| C | 1.33390 | 0.46310 | 1.61150 |
| C | 1.67300 | 1.96970 | 1.69410 |
| C | 1.52130 | -0.22380 | 0.25430 |
| Cl | 1.77840 | 2.81160 | 0.11550 |
| C | 1.25480 | -1.73470 | 0.30020 |
| C | -2.96780 | 0.58930 | 2.34330 |
| Br | -1.74210 | 1.54150 | 4.71710 |
| C | -3.09300 | 0.41600 | 0.84780 |
| C | -2.53020 | -0.63030 | 0.22270 |
| C | -2.44190 | -0.81300 | -1.24780 |
| C | -3.39220 | -0.07380 | -2.15000 |
| O | -1.55260 | -1.54610 | -1.68650 |
| C | 2.37950 | -2.49520 | 0.93640 |
| O | 1.14460 | -2.21740 | -1.03970 |
| C | 2.33340 | -3.06580 | 2.10680 |
| C | 2.28930 | -3.63170 | 3.27080 |
| H | 2.66520 | -3.19000 | 4.18370 |
| Br | 1.53190 | -5.30670 | 3.39180 |
| H | -0.84480 | 1.90170 | 0.97900 |
| H | -2.42770 | 2.68170 | 2.62640 |
| H | 0.31610 | 3.59750 | 2.33610 |
| H | 0.72880 | 2.38090 | 3.55800 |
| H | 1.91330 | -0.05990 | 2.38070 |
| H | 2.63460 | 2.13550 | 2.18840 |
| H | 0.82260 | 0.20680 | -0.47510 |
| H | 2.53180 | -0.03960 | -0.13200 |
| H | 0.31150 | -1.96080 | 0.80830 |
| H | -2.67860 | -0.36830 | 2.79820 |
| H | -3.96290 | 0.81600 | 2.74750 |
| H | -3.59380 | 1.20790 | 0.29750 |
| H | -1.99500 | -1.38750 | 0.78950 |
| H | -3.42510 | -0.57310 | -3.12290 |
| H | -4.40380 | -0.08700 | -1.73560 |
| H | -3.04920 | 0.95490 | -2.28460 |
| H | 3.28870 | -2.59380 | 0.34980 |
| H | 0.23700 | -1.99250 | -1.34410 |
| Marilzafurollene-A_52 | | | |
| C | -0.03190 | 2.07510 | 1.68460 |
| O | 0.40530 | 0.80710 | 1.15320 |
| C | -1.43570 | 2.02120 | 2.30670 |
| C | 1.07150 | 2.56650 | 2.62370 |
| C | 1.75630 | 0.57020 | 1.60160 |

| | | | |
|------------------------------|----------|----------|----------|
| C | 2.31290 | 1.92840 | 2.03620 |
| C | 2.54740 | -0.19290 | 0.54180 |
| Cl | 2.92810 | 2.92650 | 0.68320 |
| C | 1.94200 | -1.55940 | 0.19690 |
| C | -2.58330 | 1.79570 | 1.30410 |
| Br | -1.54730 | 0.66930 | 3.73540 |
| C | -2.57900 | 0.49650 | 0.53750 |
| C | -3.56180 | -0.41290 | 0.62660 |
| C | -3.59640 | -1.70500 | -0.11330 |
| C | -2.42270 | -2.11160 | -0.96420 |
| O | -4.60000 | -2.41200 | -0.01550 |
| C | 1.95540 | -2.52550 | 1.34160 |
| O | 2.72820 | -2.15330 | -0.83820 |
| C | 0.90430 | -2.89890 | 2.01510 |
| C | -0.14410 | -3.25970 | 2.68390 |
| H | -0.55820 | -2.71240 | 3.52020 |
| Br | -1.04840 | -4.76450 | 2.12630 |
| H | -0.07530 | 2.75850 | 0.82620 |
| H | -1.62560 | 2.96920 | 2.82460 |
| H | 1.10880 | 3.65870 | 2.68870 |
| H | 0.93010 | 2.18830 | 3.64190 |
| H | 1.67080 | -0.04990 | 2.50310 |
| H | 3.12750 | 1.83220 | 2.75910 |
| H | 2.58160 | 0.38240 | -0.39190 |
| H | 3.58950 | -0.31440 | 0.86440 |
| H | 0.92490 | -1.44240 | -0.19460 |
| H | -3.53840 | 1.90400 | 1.83610 |
| H | -2.56300 | 2.60950 | 0.56750 |
| H | -1.72840 | 0.33300 | -0.11900 |
| H | -4.42230 | -0.25120 | 1.26970 |
| H | -1.50830 | -2.12220 | -0.36620 |
| H | -2.58780 | -3.12340 | -1.34650 |
| H | -2.32160 | -1.43160 | -1.81370 |
| H | 2.91880 | -2.94870 | 1.61180 |
| H | 2.60590 | -1.60590 | -1.63320 |
| Marilzafurollene-A_53 | | | |
| C | -0.59390 | 1.25210 | 1.67480 |
| O | 0.12940 | 0.05460 | 1.31730 |
| C | -1.71780 | 0.96370 | 2.68290 |
| C | 0.44230 | 2.29190 | 2.10090 |
| C | 1.54030 | 0.35330 | 1.35310 |
| C | 1.66380 | 1.87930 | 1.30440 |
| C | 2.28210 | -0.43700 | 0.27630 |
| Cl | 1.57760 | 2.56120 | -0.34820 |
| C | 2.16770 | -1.95800 | 0.45460 |
| C | -2.75810 | -0.04620 | 2.17080 |
| Br | -0.98030 | 0.22070 | 4.36250 |

| | | | |
|------------------------------|----------|----------|----------|
| C | -3.54900 | 0.46660 | 0.99720 |
| C | -3.51720 | -0.09370 | -0.22200 |
| C | -4.32570 | 0.46640 | -1.34300 |
| C | -4.23870 | -0.24090 | -2.66980 |
| O | -5.01320 | 1.47590 | -1.19740 |
| C | 2.84010 | -2.46810 | 1.69600 |
| O | 2.78540 | -2.60090 | -0.66330 |
| C | 2.21420 | -2.94620 | 2.73440 |
| C | 1.58100 | -3.40980 | 3.76450 |
| H | 1.10110 | -2.79730 | 4.51630 |
| Br | 1.36980 | -5.23500 | 3.90050 |
| H | -1.05290 | 1.60850 | 0.74420 |
| H | -2.20570 | 1.89790 | 2.98320 |
| H | 0.10480 | 3.31700 | 1.91740 |
| H | 0.67860 | 2.21790 | 3.16720 |
| H | 1.89100 | 0.03130 | 2.34180 |
| H | 2.59960 | 2.23320 | 1.74580 |
| H | 1.87420 | -0.20280 | -0.71500 |
| H | 3.33860 | -0.14030 | 0.25300 |
| H | 1.11350 | -2.25740 | 0.44010 |
| H | -2.27310 | -0.99900 | 1.92110 |
| H | -3.47660 | -0.27610 | 2.96870 |
| H | -4.18310 | 1.33430 | 1.17720 |
| H | -2.90090 | -0.95980 | -0.43610 |
| H | -3.58410 | 0.32430 | -3.33800 |
| H | -3.84730 | -1.25510 | -2.55380 |
| H | -5.24040 | -0.31500 | -3.10250 |
| H | 3.92410 | -2.42040 | 1.73390 |
| H | 3.70680 | -2.29500 | -0.71250 |
| Marilzafurollene-A_54 | | | |
| C | 0.06250 | 1.34820 | 0.77320 |
| O | 0.88120 | 0.15960 | 0.76930 |
| C | -1.43380 | 1.02050 | 0.91670 |
| C | 0.64990 | 2.29660 | 1.81770 |
| C | 2.00980 | 0.38980 | 1.63930 |
| C | 2.11470 | 1.90700 | 1.82200 |
| C | 3.24610 | -0.33080 | 1.10710 |
| Cl | 2.97160 | 2.73930 | 0.48850 |
| C | 3.07520 | -1.85430 | 1.03810 |
| C | -1.92540 | 0.13170 | -0.24150 |
| Br | -1.76990 | 0.07190 | 2.61950 |
| C | -3.41270 | -0.04450 | -0.44790 |
| C | -4.41790 | 0.55870 | 0.20620 |
| C | -5.84030 | 0.25630 | -0.13770 |
| C | -6.90130 | 0.92710 | 0.69510 |
| O | -6.13440 | -0.48520 | -1.07380 |
| C | 2.94130 | -2.49800 | 2.38490 |

| | | | |
|----|----------|----------|----------|
| O | 4.24900 | -2.41190 | 0.44340 |
| C | 1.83940 | -3.00140 | 2.86480 |
| C | 0.73660 | -3.49120 | 3.33470 |
| H | -0.05000 | -2.90470 | 3.79060 |
| Br | 0.42340 | -5.29220 | 3.10600 |
| H | 0.20590 | 1.80770 | -0.21400 |
| H | -2.00650 | 1.95160 | 0.97770 |
| H | 0.45980 | 3.34830 | 1.58080 |
| H | 0.23480 | 2.11140 | 2.81370 |
| H | 1.73320 | -0.03590 | 2.61210 |
| H | 2.62620 | 2.17930 | 2.74920 |
| H | 3.47360 | 0.01130 | 0.08970 |
| H | 4.12230 | -0.08000 | 1.71890 |
| H | 2.22600 | -2.12190 | 0.39820 |
| H | -1.53960 | 0.54470 | -1.18310 |
| H | -1.48770 | -0.87110 | -0.14770 |
| H | -3.66390 | -0.75430 | -1.23850 |
| H | -4.25690 | 1.27540 | 1.00110 |
| H | -7.29220 | 1.79240 | 0.15410 |
| H | -7.70730 | 0.21420 | 0.89070 |
| H | -6.50060 | 1.25210 | 1.65920 |
| H | 3.84110 | -2.55250 | 2.99110 |
| H | 4.24180 | -2.14230 | -0.49170 |

Table S9. Calculated Energies (Hartrees) for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,14*S** of **3**.

| Entry ID | Gas Phase Energy |
|----------|------------------|
| 1 | -1335,914446 |
| 2 | -1335,916256 |
| 3 | -1335,911134 |
| 4 | -1335,91517 |
| 5 | -1335,91346 |
| 6 | -1335,913569 |
| 7 | -1335,913417 |
| 8 | -1335,915523 |
| 9 | -1335,911506 |
| 10 | -1335,915896 |
| 11 | -1335,916525 |
| 12 | -1335,91004 |
| 13 | -1335,914391 |
| 14 | -1335,910539 |
| 15 | -1335,912527 |
| 16 | -1335,914866 |
| 17 | -1335,912661 |
| 18 | -1335,910434 |
| 19 | -1335,914381 |

| | |
|----|--------------|
| 20 | -1335,909918 |
| 21 | -1335,912263 |
| 22 | -1335,914974 |
| 23 | -1335,911609 |
| 24 | -1335,912037 |
| 25 | -1335,913897 |
| 26 | -1335,912701 |
| 27 | -1335,910775 |
| 28 | -1335,911195 |
| 29 | -1335,914683 |
| 30 | -1335,911719 |
| 31 | -1335,91515 |
| 32 | -1335,911583 |
| 33 | -1335,915222 |
| 34 | -1335,915761 |
| 35 | -1335,914861 |
| 36 | -1335,910835 |
| 37 | -1335,908888 |
| 38 | -1335,912922 |
| 39 | -1335,912555 |
| 40 | -1335,914515 |
| 41 | -1335,910589 |
| 42 | -1335,91306 |
| 43 | -1335,910704 |
| 44 | -1335,914248 |
| 45 | -1335,91281 |
| 46 | -1335,909631 |
| 47 | -1335,912855 |
| 48 | -1335,906209 |
| 49 | -1335,91171 |
| 50 | -1335,913508 |
| 51 | -1335,914507 |
| 52 | -1335,911226 |
| 53 | -1335,910697 |
| 54 | -1335,908852 |
| 55 | -1335,911472 |
| 56 | -1335,912174 |
| 57 | -1335,909609 |
| 58 | -1335,911884 |
| 59 | -1335,906562 |
| 60 | -1335,911257 |
| 61 | -1335,91464 |
| 62 | -1335,914206 |
| 63 | -1335,912782 |
| 64 | -1335,910404 |
| 65 | -1335,913251 |
| 66 | -1335,906259 |

| | |
|-----|--------------|
| 67 | -1335,91363 |
| 68 | -1335,91121 |
| 69 | -1335,910968 |
| 70 | -1335,913105 |
| 71 | -1335,911797 |
| 72 | -1335,912348 |
| 73 | -1335,914211 |
| 74 | -1335,912671 |
| 75 | -1335,910164 |
| 76 | -1335,908801 |
| 77 | -1335,912049 |
| 78 | -1335,913949 |
| 79 | -1335,909965 |
| 80 | -1335,913957 |
| 81 | -1335,908301 |
| 82 | -1335,910315 |
| 83 | -1335,911187 |
| 84 | -1335,913139 |
| 85 | -1335,912342 |
| 86 | -1335,909157 |
| 87 | -1335,911956 |
| 88 | -1335,913616 |
| 89 | -1335,906279 |
| 90 | -1335,914129 |
| 91 | -1335,908341 |
| 92 | -1335,914187 |
| 93 | -1335,909781 |
| 94 | -1335,913575 |
| 95 | -1335,911571 |
| 96 | -1335,913443 |
| 97 | -1335,908821 |
| 98 | -1335,907442 |
| 99 | -1335,906272 |
| 100 | -1335,909431 |
| 101 | -1335,910797 |
| 102 | -1335,910265 |
| 103 | -1335,911906 |
| 104 | -1335,914471 |
| 105 | -1335,912234 |
| 106 | -1335,914976 |
| 107 | -1335,913506 |
| 108 | -1335,909822 |
| 109 | -1335,908804 |
| 110 | -1335,915056 |
| 111 | -1335,91099 |
| 112 | -1335,909737 |
| 113 | -1335,913668 |

| | |
|-----|--------------|
| 114 | -1335,911323 |
| 115 | -1335,906175 |
| 116 | -1335,906472 |
| 117 | -1335,907731 |
| 118 | -1335,911137 |
| 119 | -1335,909504 |
| 120 | -1335,910704 |
| 121 | -1335,909266 |
| 122 | -1335,910932 |
| 123 | -1335,912148 |
| 124 | -1335,911438 |
| 125 | -1335,913825 |
| 126 | -1335,90975 |
| 127 | -1335,910236 |
| 128 | -1335,91279 |
| 129 | -1335,911724 |
| 130 | -1335,910216 |
| 131 | -1335,909309 |
| 132 | -1335,912317 |
| 133 | -1335,909104 |
| 134 | -1335,907802 |
| 135 | -1335,911302 |
| 136 | -1335,909562 |
| 137 | -1335,910724 |
| 138 | -1335,910953 |
| 139 | -1335,912951 |
| 140 | -1335,910395 |
| 141 | -1335,913709 |
| 142 | -1335,915466 |
| 143 | -1335,913115 |
| 144 | -1335,907243 |
| 145 | -1335,91047 |
| 146 | -1335,913401 |
| 147 | -1335,913185 |
| 148 | -1335,913168 |
| 149 | -1335,913169 |
| 150 | -1335,907502 |
| 151 | -1335,910645 |
| 152 | -1335,912831 |
| 153 | -1335,911961 |
| 154 | -1335,911163 |
| 155 | -1335,912695 |
| 156 | -1335,913543 |
| 157 | -1335,912967 |
| 158 | -1335,912393 |
| 159 | -1335,911443 |
| 160 | -1335,911457 |

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|-----|--------------|
| 161 | -1335,910828 |
| 162 | -1335,910443 |
| 163 | -1335,911635 |
| 164 | -1335,911104 |
| 165 | -1335,90902 |
| 166 | -1335,913207 |
| 167 | -1335,912907 |
| 168 | -1335,913864 |
| 169 | -1335,910721 |
| 170 | -1335,908344 |
| 171 | -1335,909066 |
| 172 | -1335,911942 |
| 173 | -1335,908846 |
| 174 | -1335,909078 |
| 175 | -1335,912925 |
| 176 | -1335,910267 |
| 177 | -1335,912499 |
| 178 | -1335,911099 |
| 179 | -1335,911123 |
| 180 | -1335,911018 |
| 181 | -1335,905061 |
| 182 | -1335,908958 |

Table S10. Coordinates (Angstroms) of calculated geometries for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,14*S** of **3**.

| Marilzafurollene C_2 | | | |
|-----------------------------|----------|----------|----------|
| C | 2.91730 | -1.56500 | -1.12860 |
| O | 2.26350 | -1.81540 | 0.11490 |
| C | 3.00560 | -0.05030 | -1.39630 |
| C | 2.14800 | -2.36860 | -2.18670 |
| C | 1.12820 | -2.64820 | -0.09490 |
| C | 3.89730 | 0.66540 | -0.36770 |
| Br | 1.17760 | 0.75610 | -1.34790 |
| C | 1.47080 | -3.44290 | -1.35900 |
| C | 0.78130 | -3.46670 | 1.16460 |
| C | 4.09850 | 2.13280 | -0.69310 |
| Cl | 2.62950 | -4.76710 | -1.03540 |
| C | 0.43640 | -2.59320 | 2.38490 |
| C | -0.77520 | -1.71070 | 2.14860 |
| O | 0.18190 | -3.44330 | 3.48440 |
| C | -0.71270 | -0.39870 | 2.11950 |
| C | 5.28820 | 2.70000 | -0.95340 |
| C | 5.48680 | 4.16910 | -1.27690 |
| C | 6.10410 | 4.34260 | -2.66690 |
| O | 6.36670 | 4.78560 | -0.34810 |
| C | -0.62090 | 0.90910 | 2.07310 |
| Br | -0.83080 | 2.04700 | 3.67910 |

| | | | |
|-----------------------------|----------|----------|----------|
| C | 5.81260 | 4.96760 | 0.94800 |
| H | 3.92370 | -1.97930 | -1.05040 |
| H | 3.40640 | 0.11520 | -2.39760 |
| H | 1.38840 | -1.75200 | -2.66780 |
| H | 2.79150 | -2.77000 | -2.97000 |
| H | 0.28910 | -1.99530 | -0.34000 |
| H | 3.45740 | 0.58280 | 0.62710 |
| H | 4.86970 | 0.17360 | -0.31750 |
| H | 0.59310 | -3.87020 | -1.84500 |
| H | -0.05140 | -4.13490 | 0.94260 |
| H | 1.62400 | -4.10680 | 1.42650 |
| H | 3.20600 | 2.74250 | -0.70810 |
| H | 1.30420 | -1.97480 | 2.62740 |
| H | -1.71640 | -2.21890 | 1.99670 |
| H | 0.18840 | -2.92180 | 4.27490 |
| H | 6.18540 | 2.09800 | -0.93730 |
| H | 4.52310 | 4.68220 | -1.26230 |
| H | 6.23300 | 5.39870 | -2.90420 |
| H | 7.08340 | 3.86730 | -2.72700 |
| H | 5.46910 | 3.90440 | -3.43730 |
| H | -0.42590 | 1.48130 | 1.17750 |
| H | 5.56420 | 4.01630 | 1.41990 |
| H | 6.53740 | 5.47380 | 1.58550 |
| H | 4.91350 | 5.58380 | 0.91040 |
| Marilzafurollene C_1 | | | |
| C | 2.94210 | -1.27340 | -1.05170 |
| O | 2.15660 | -1.23740 | 0.14050 |
| C | 3.30180 | 0.15300 | -1.50700 |
| C | 2.13830 | -2.09410 | -2.06880 |
| C | 0.94870 | -1.97200 | -0.04990 |
| C | 4.22300 | 0.86680 | -0.50330 |
| Br | 1.63250 | 1.22570 | -1.74000 |
| C | 1.26790 | -2.95780 | -1.17930 |
| C | 0.45180 | -2.58410 | 1.27410 |
| C | 4.68890 | 2.22040 | -1.00350 |
| Cl | 2.21170 | -4.36380 | -0.60220 |
| C | 0.04190 | -1.52400 | 2.31140 |
| C | -0.61140 | -2.15540 | 3.52480 |
| O | 1.19910 | -0.82770 | 2.71950 |
| C | -1.84140 | -1.89250 | 3.90340 |
| C | 5.97180 | 2.55120 | -1.22580 |
| C | 6.43490 | 3.90740 | -1.72460 |
| C | 7.16790 | 3.77510 | -3.06190 |
| O | 7.33830 | 4.51050 | -0.80970 |
| C | -3.07530 | -1.62950 | 4.26320 |
| Br | -4.62070 | -2.66940 | 3.59260 |
| C | 6.73340 | 4.96580 | 0.39300 |

| | | | |
|-----------------------------|----------|----------|----------|
| H | 3.85630 | -1.82170 | -0.81820 |
| H | 3.79580 | 0.10720 | -2.47900 |
| H | 1.50370 | -1.44870 | -2.67650 |
| H | 2.76830 | -2.67060 | -2.74670 |
| H | 0.19950 | -1.26930 | -0.41970 |
| H | 3.70510 | 1.00290 | 0.44700 |
| H | 5.09390 | 0.24400 | -0.29480 |
| H | 0.37650 | -3.33170 | -1.68430 |
| H | -0.41030 | -3.21630 | 1.05650 |
| H | 1.20940 | -3.24170 | 1.70210 |
| H | 3.91360 | 2.95200 | -1.18370 |
| H | -0.640 | -0.81110 | 1.85020 |
| H | -0.00380 | -2.85170 | 4.08420 |
| H | 1.74110 | -0.71120 | 1.94240 |
| H | 6.75280 | 1.82650 | -1.04500 |
| H | 5.57170 | 4.56020 | -1.86890 |
| H | 7.48740 | 4.75150 | -3.42650 |
| H | 8.05600 | 3.15010 | -2.96620 |
| H | 6.52400 | 3.33160 | -3.82170 |
| H | -3.36530 | -0.84130 | 4.94260 |
| H | 7.48610 | 5.44230 | 1.02090 |
| H | 5.95420 | 5.70150 | 0.18950 |
| H | 6.29770 | 4.14500 | 0.96370 |
| Marilzafurollene C_3 | | | |
| C | 2.89580 | -1.53350 | -1.08610 |
| O | 2.24770 | -1.77410 | 0.16270 |
| C | 2.98370 | -0.02130 | -1.36750 |
| C | 2.12140 | -2.34490 | -2.13420 |
| C | 1.11120 | -2.60800 | -0.03530 |
| C | 3.88410 | 0.70270 | -0.35250 |
| Br | 1.15660 | 0.78690 | -1.31290 |
| C | 1.44740 | -3.41210 | -1.29520 |
| C | 0.77940 | -3.41940 | 1.23250 |
| C | 4.08310 | 2.16720 | -0.69200 |
| Cl | 2.60640 | -4.73470 | -0.96550 |
| C | 0.40880 | -2.53900 | 2.44060 |
| C | -0.84320 | -1.71440 | 2.20450 |
| O | 0.20550 | -3.37380 | 3.56260 |
| C | -0.83710 | -0.40300 | 2.12440 |
| C | 5.27060 | 2.73150 | -0.96810 |
| C | 5.46690 | 4.19780 | -1.30560 |
| C | 6.07190 | 4.35930 | -2.70240 |
| O | 6.35520 | 4.82150 | -0.38980 |
| C | -0.80520 | 0.90450 | 2.02090 |
| Br | -1.02950 | 2.10360 | 3.58030 |
| C | 5.81240 | 5.01500 | 0.90940 |
| H | 3.90240 | -1.94750 | -1.00950 |

| | | | |
|-----------------------------|----------|----------|----------|
| H | 3.37710 | 0.13520 | -2.37320 |
| H | 1.35990 | -1.73160 | -2.61660 |
| H | 2.76100 | -2.75270 | -2.91730 |
| H | 0.26910 | -1.95830 | -0.27860 |
| H | 3.45220 | 0.62910 | 0.64650 |
| H | 4.85660 | 0.21100 | -0.30590 |
| H | 0.56730 | -3.84240 | -1.77420 |
| H | -0.03840 | -4.10790 | 1.01590 |
| H | 1.63690 | -4.03750 | 1.49840 |
| H | 3.19070 | 2.77720 | -0.70370 |
| H | 1.24420 | -1.87090 | 2.66420 |
| H | -1.76600 | -2.26610 | 2.10180 |
| H | 1.05030 | -3.62840 | 3.90640 |
| H | 6.16770 | 2.12920 | -0.95530 |
| H | 4.50350 | 4.71140 | -1.28690 |
| H | 6.19910 | 5.41340 | -2.94970 |
| H | 7.05060 | 3.88320 | -2.76720 |
| H | 5.43000 | 3.91500 | -3.46350 |
| H | -0.65700 | 1.44480 | 1.09710 |
| H | 5.56720 | 4.06800 | 1.39150 |
| H | 6.54300 | 5.52600 | 1.53640 |
| H | 4.91340 | 5.63170 | 0.87430 |
| Marilzafurollene C_4 | | | |
| C | 2.97030 | -1.57910 | -1.36500 |
| O | 2.31690 | -1.47270 | -0.09960 |
| C | 3.63930 | -0.24470 | -1.74360 |
| C | 1.90750 | -2.07430 | -2.35480 |
| C | 0.95050 | -1.86300 | -0.22270 |
| C | 4.78320 | 0.12240 | -0.78270 |
| Br | 2.27990 | 1.21900 | -1.72550 |
| C | 0.91910 | -2.78080 | -1.44970 |
| C | 0.41900 | -2.46060 | 1.09440 |
| C | 5.51970 | 1.37820 | -1.20680 |
| Cl | 1.51780 | -4.42540 | -1.07870 |
| C | 0.37680 | -1.43980 | 2.24510 |
| C | -0.32000 | -2.00580 | 3.46660 |
| O | 1.70190 | -1.09670 | 2.58660 |
| C | -1.40870 | -1.48490 | 3.98490 |
| C | 5.63380 | 2.48260 | -0.45050 |
| C | 6.35840 | 3.74580 | -0.87620 |
| C | 7.52340 | 4.05190 | 0.06830 |
| O | 5.49210 | 4.87100 | -0.85100 |
| C | -2.50280 | -0.96130 | 4.48480 |
| Br | -4.30970 | -1.51560 | 3.89540 |
| C | 4.48250 | 4.85470 | -1.85170 |
| H | 3.73340 | -2.35330 | -1.26840 |
| H | 4.02600 | -0.31290 | -2.76150 |

| | | | |
|-----------------------------|----------|----------|----------|
| H | 1.41110 | -1.23680 | -2.84560 |
| H | 2.31560 | -2.71870 | -3.13380 |
| H | 0.37880 | -0.96400 | -0.46110 |
| H | 4.39260 | 0.24420 | 0.22880 |
| H | 5.50710 | -0.69210 | -0.73960 |
| H | -0.07490 | -2.87250 | -1.88900 |
| H | -0.59050 | -2.83470 | 0.91760 |
| H | 1.01430 | -3.32450 | 1.39270 |
| H | 5.97220 | 1.35850 | -2.18780 |
| H | -0.13850 | -0.53650 | 1.91070 |
| H | 0.13110 | -2.88230 | 3.90840 |
| H | 2.19230 | -1.03720 | 1.76970 |
| H | 5.18200 | 2.50780 | 0.53100 |
| H | 6.75650 | 3.61760 | -1.88470 |
| H | 8.05230 | 4.95120 | -0.24770 |
| H | 7.17300 | 4.21430 | 1.08790 |
| H | 8.24220 | 3.23240 | 0.08590 |
| H | -2.52840 | -0.19640 | 5.24710 |
| H | 3.89610 | 5.77140 | -1.79130 |
| H | 4.91640 | 4.80100 | -2.85090 |
| H | 3.79730 | 4.01610 | -1.72340 |
| Marilzafurollene C_5 | | | |
| C | 2.90470 | -1.84780 | -1.41580 |
| O | 2.27630 | -1.98780 | -0.14240 |
| C | 3.37130 | -0.39510 | -1.63130 |
| C | 1.89690 | -2.36780 | -2.45140 |
| C | 0.94580 | -2.46430 | -0.31060 |
| C | 4.45380 | 0.01870 | -0.61990 |
| Br | 1.81960 | 0.85280 | -1.46160 |
| C | 0.99420 | -3.25790 | -1.62010 |
| C | 0.44660 | -3.21780 | 0.93850 |
| C | 5.01190 | 1.40110 | -0.89740 |
| Cl | 1.76260 | -4.86050 | -1.41540 |
| C | 0.45340 | -2.35760 | 2.21560 |
| C | -0.42250 | -1.12420 | 2.09770 |
| O | -0.00590 | -3.15130 | 3.29060 |
| C | 0.05450 | 0.09930 | 2.13670 |
| C | 4.93450 | 2.43620 | -0.04470 |
| C | 5.48360 | 3.82290 | -0.32270 |
| C | 6.52570 | 4.21800 | 0.72660 |
| O | 4.45540 | 4.80180 | -0.28170 |
| C | 0.56070 | 1.30920 | 2.16490 |
| Br | 0.78170 | 2.32760 | 3.84790 |
| C | 3.54050 | 4.73330 | -1.36740 |
| H | 3.77140 | -2.51070 | -1.41800 |
| H | 3.75940 | -0.29060 | -2.64540 |
| H | 1.30980 | -1.54990 | -2.86930 |

| | | | |
|-----------------------------|----------|----------|----------|
| H | 2.37010 | -2.89120 | -3.28260 |
| H | 0.30940 | -1.59450 | -0.48030 |
| H | 4.04840 | -0.02340 | 0.39230 |
| H | 5.28220 | -0.68970 | -0.65120 |
| H | 0.00990 | -3.40690 | -2.06520 |
| H | -0.55970 | -3.59450 | 0.75250 |
| H | 1.07210 | -4.09340 | 1.11260 |
| H | 5.49710 | 1.53680 | -1.85330 |
| H | 1.48320 | -2.06040 | 2.42910 |
| H | -1.48150 | -1.29740 | 1.97230 |
| H | 0.19760 | -2.70550 | 4.10100 |
| H | 4.44710 | 2.30640 | 0.91110 |
| H | 5.96060 | 3.83830 | -1.30470 |
| H | 6.93040 | 5.20820 | 0.51690 |
| H | 6.09030 | 4.24250 | 1.72590 |
| H | 7.35850 | 3.51450 | 0.73930 |
| H | 0.89960 | 1.85620 | 1.29660 |
| H | 2.98950 | 3.79230 | -1.37470 |
| H | 2.81310 | 5.54040 | -1.28120 |
| H | 4.05210 | 4.84560 | -2.32410 |
| Marilzafurollene C_6 | | | |
| C | 2.90800 | -1.81890 | -1.42170 |
| O | 2.29720 | -1.96840 | -0.14060 |
| C | 3.36470 | -0.36340 | -1.63780 |
| C | 1.88870 | -2.33770 | -2.44610 |
| C | 0.97290 | -2.46810 | -0.29270 |
| C | 4.47610 | 0.04480 | -0.65610 |
| Br | 1.81460 | 0.87750 | -1.41070 |
| C | 1.01290 | -3.24920 | -1.60990 |
| C | 0.50780 | -3.24310 | 0.95620 |
| C | 5.03020 | 1.42620 | -0.94670 |
| Cl | 1.80780 | -4.84200 | -1.43100 |
| C | 0.48100 | -2.38510 | 2.23440 |
| C | -0.46240 | -1.20170 | 2.12430 |
| O | 0.07300 | -3.20330 | 3.31160 |
| C | -0.05640 | 0.04680 | 2.17410 |
| C | 4.98150 | 2.45980 | -0.09010 |
| C | 5.52720 | 3.84510 | -0.38180 |
| C | 6.60100 | 4.23470 | 0.63710 |
| O | 4.50430 | 4.82760 | -0.30940 |
| C | 0.37570 | 1.28470 | 2.21430 |
| Br | 0.52140 | 2.30200 | 3.90640 |
| C | 3.55710 | 4.76330 | -1.36740 |
| H | 3.77710 | -2.47830 | -1.44050 |
| H | 3.72230 | -0.24910 | -2.66200 |
| H | 1.28430 | -1.52120 | -2.84180 |
| H | 2.35310 | -2.84430 | -3.29250 |

| | | | |
|-----------------------------|----------|----------|----------|
| H | 0.31850 | -1.60860 | -0.44510 |
| H | 4.09940 | 0.00040 | 0.36690 |
| H | 5.30170 | -0.66520 | -0.71320 |
| H | 0.02410 | -3.40890 | -2.04110 |
| H | -0.48280 | -3.66040 | 0.77240 |
| H | 1.16940 | -4.09280 | 1.12580 |
| H | 5.48770 | 1.56240 | -1.91600 |
| H | 1.49500 | -2.03320 | 2.43970 |
| H | -1.50960 | -1.43370 | 1.99430 |
| H | 0.25870 | -2.74830 | 4.12120 |
| H | 4.52170 | 2.32970 | 0.87920 |
| H | 5.97530 | 3.86040 | -1.37730 |
| H | 7.00310 | 5.22370 | 0.41710 |
| H | 6.19520 | 4.25920 | 1.64870 |
| H | 7.43120 | 3.52810 | 0.62440 |
| H | 0.68700 | 1.85740 | 1.35220 |
| H | 3.00260 | 3.82430 | -1.35870 |
| H | 2.83580 | 5.57310 | -1.25910 |
| H | 4.04040 | 4.87420 | -2.33880 |
| Marilzafurollene C_7 | | | |
| C | 2.90460 | -1.85380 | -1.41490 |
| O | 2.27270 | -1.99170 | -0.14300 |
| C | 3.37330 | -0.40170 | -1.63040 |
| C | 1.89900 | -2.37400 | -2.45270 |
| C | 0.94090 | -2.46320 | -0.31440 |
| C | 4.45030 | 0.01300 | -0.61350 |
| Br | 1.82160 | 0.84770 | -1.47180 |
| C | 0.99060 | -3.25940 | -1.62230 |
| C | 0.43460 | -3.21190 | 0.93470 |
| C | 5.00860 | 1.39590 | -0.88800 |
| Cl | 1.75320 | -4.86410 | -1.41220 |
| C | 0.44780 | -2.35130 | 2.21150 |
| C | -0.41390 | -1.10810 | 2.09140 |
| O | -0.02230 | -3.13940 | 3.28580 |
| C | 0.07730 | 0.10990 | 2.12940 |
| C | 4.92530 | 2.43090 | -0.03570 |
| C | 5.47440 | 3.81820 | -0.31050 |
| C | 6.50990 | 4.21450 | 0.74480 |
| O | 4.44490 | 4.79590 | -0.27540 |
| C | 0.59810 | 1.31360 | 2.15630 |
| Br | 0.83140 | 2.33090 | 3.83820 |
| C | 3.53650 | 4.72670 | -1.36650 |
| H | 3.77070 | -2.51750 | -1.41390 |
| H | 3.76720 | -0.29930 | -2.64260 |
| H | 1.31550 | -1.55580 | -2.87510 |
| H | 2.37370 | -2.90100 | -3.28070 |
| H | 0.30840 | -1.59120 | -0.48770 |

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| H | 4.03950 | -0.02910 | 0.39650 |
| H | 5.27930 | -0.69490 | -0.64030 |
| H | 0.00720 | -3.40600 | -2.07010 |
| H | -0.57460 | -3.58030 | 0.74790 |
| H | 1.05260 | -4.09260 | 1.11000 |
| H | 5.49890 | 1.53210 | -1.84120 |
| H | 1.48030 | -2.06540 | 2.42710 |
| H | -1.47470 | -1.26920 | 1.96540 |
| H | 0.18420 | -2.69540 | 4.09650 |
| H | 4.43280 | 2.30050 | 0.91740 |
| H | 5.95710 | 3.83420 | -1.28970 |
| H | 6.91470 | 5.20520 | 0.53750 |
| H | 6.06880 | 4.23850 | 1.74160 |
| H | 7.34350 | 3.51200 | 0.76240 |
| H | 0.94360 | 1.85560 | 1.28760 |
| H | 2.98670 | 3.78500 | -1.37720 |
| H | 2.80780 | 5.53290 | -1.28440 |
| H | 4.05360 | 4.83970 | -2.32010 |
| Marilzafurollene C_8 | | | |
| C | 3.04750 | -1.35300 | -1.07540 |
| O | 2.18950 | -1.34460 | 0.06620 |
| C | 3.36430 | 0.08510 | -1.52580 |
| C | 2.34850 | -2.22180 | -2.12930 |
| C | 1.03300 | -2.14010 | -0.18740 |
| C | 4.18490 | 0.85360 | -0.47620 |
| Br | 1.66210 | 1.07100 | -1.87530 |
| C | 1.46800 | -3.11890 | -1.28380 |
| C | 0.48730 | -2.76440 | 1.11180 |
| C | 4.61420 | 2.22380 | -0.96410 |
| Cl | 2.44100 | -4.47230 | -0.63410 |
| C | -0.03670 | -1.71750 | 2.11050 |
| C | -0.72940 | -2.37080 | 3.29040 |
| O | 1.05940 | -0.96200 | 2.57750 |
| C | -2.00280 | -2.20520 | 3.56780 |
| C | 5.89070 | 2.61540 | -1.11210 |
| C | 6.31680 | 3.98800 | -1.59870 |
| C | 7.13590 | 3.87950 | -2.88740 |
| O | 7.13210 | 4.64360 | -0.63840 |
| C | -3.27790 | -2.05490 | 3.83920 |
| Br | -3.95630 | -0.61040 | 5.01070 |
| C | 6.43320 | 5.07990 | 0.51960 |
| H | 3.97130 | -1.85320 | -0.77990 |
| H | 3.91960 | 0.05460 | -2.46480 |
| H | 1.72190 | -1.61430 | -2.78260 |
| H | 3.04620 | -2.77310 | -2.76020 |
| H | 0.27400 | -1.47870 | -0.60980 |
| H | 3.60280 | 0.97310 | 0.43840 |

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| H | 5.07070 | 0.27710 | -0.20640 |
| H | 0.62820 | -3.54010 | -1.83770 |
| H | -0.32710 | -3.44140 | 0.84990 |
| H | 1.24940 | -3.37920 | 1.59230 |
| H | 3.81670 | 2.91440 | -1.20030 |
| H | -0.72970 | -1.04330 | 1.60180 |
| H | -0.11070 | -2.99630 | 3.91720 |
| H | 1.63790 | -0.82060 | 1.83160 |
| H | 6.69340 | 1.93200 | -0.87510 |
| H | 5.43330 | 4.59600 | -1.80330 |
| H | 7.42930 | 4.86690 | -3.24400 |
| H | 8.04590 | 3.29990 | -2.73020 |
| H | 6.56210 | 3.39760 | -3.67930 |
| H | -4.06750 | -2.68740 | 3.46090 |
| H | 6.00400 | 4.24400 | 1.07300 |
| H | 7.12210 | 5.59900 | 1.18610 |
| H | 5.63310 | 5.77430 | 0.26010 |
| Marilzafurollene C_9 | | | |
| C | 3.13900 | -1.27500 | -1.94060 |
| O | 2.50940 | -0.84220 | -0.73250 |
| C | 2.91060 | -0.25420 | -3.07570 |
| C | 2.57750 | -2.67550 | -2.21880 |
| C | 1.60200 | -1.83680 | -0.26640 |
| C | 3.77660 | 1.01770 | -2.97490 |
| Br | 0.98430 | 0.26440 | -3.14340 |
| C | 2.15030 | -3.14390 | -0.84170 |
| C | 1.44840 | -1.75680 | 1.26310 |
| C | 3.68530 | 1.71860 | -1.63210 |
| Cl | 3.57470 | -3.72960 | 0.06810 |
| C | 0.71530 | -0.48250 | 1.71930 |
| C | 0.49530 | -0.47280 | 3.21880 |
| O | 1.49140 | 0.63840 | 1.35790 |
| C | -0.69380 | -0.43400 | 3.77510 |
| C | 4.74790 | 2.03160 | -0.87210 |
| C | 4.67610 | 2.69860 | 0.48780 |
| C | 5.26110 | 4.11180 | 0.43130 |
| O | 5.43750 | 1.97330 | 1.44250 |
| C | -1.88830 | -0.40690 | 4.31690 |
| Br | -2.89530 | -2.05580 | 4.74820 |
| C | 4.82420 | 0.76830 | 1.87940 |
| H | 4.20800 | -1.36830 | -1.74190 |
| H | 3.13440 | -0.73120 | -4.03120 |
| H | 1.70260 | -2.61400 | -2.86740 |
| H | 3.29920 | -3.33940 | -2.69550 |
| H | 0.63350 | -1.64460 | -0.73240 |
| H | 4.81900 | 0.75860 | -3.16490 |
| H | 3.48790 | 1.72100 | -3.75650 |

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|------------------------------|----------|----------|----------|
| H | 1.40990 | -3.94410 | -0.86970 |
| H | 0.88480 | -2.62710 | 1.60230 |
| H | 2.42440 | -1.81850 | 1.74640 |
| H | 2.69000 | 1.96330 | -1.28790 |
| H | -0.24510 | -0.41360 | 1.20330 |
| H | 1.38480 | -0.49800 | 3.83100 |
| H | 1.91360 | 0.42690 | 0.52720 |
| H | 5.74280 | 1.79490 | -1.22030 |
| H | 3.63580 | 2.76570 | 0.81360 |
| H | 6.30880 | 4.09440 | 0.13040 |
| H | 4.71660 | 4.73460 | -0.27870 |
| H | 5.20370 | 4.59320 | 1.40760 |
| H | -2.42840 | 0.49220 | 4.57550 |
| H | 4.59530 | 0.09710 | 1.05040 |
| H | 5.49620 | 0.24240 | 2.55710 |
| H | 3.90420 | 0.97800 | 2.42500 |
| Marilzafurollene C_10 | | | |
| C | 2.82030 | -0.50310 | -1.02720 |
| O | 1.95170 | -0.57190 | 0.10430 |
| C | 2.63260 | 0.83110 | -1.77820 |
| C | 2.53640 | -1.75960 | -1.86060 |
| C | 1.18060 | -1.77120 | 0.05410 |
| C | 3.02070 | 2.07100 | -0.95310 |
| Br | 0.71890 | 1.03190 | -2.30690 |
| C | 1.99920 | -2.72440 | -0.82380 |
| C | 0.83220 | -2.27260 | 1.46900 |
| C | 4.49790 | 2.12630 | -0.61180 |
| Cl | 3.36260 | -3.46270 | 0.06910 |
| C | -0.09230 | -1.31270 | 2.23810 |
| C | -0.56220 | -1.91980 | 3.54510 |
| O | 0.62190 | -0.12680 | 2.50990 |
| C | -1.82590 | -2.14090 | 3.82740 |
| C | 5.35780 | 3.03540 | -1.10020 |
| C | 6.83520 | 3.09230 | -0.75900 |
| C | 7.19530 | 4.43380 | -0.11560 |
| O | 7.63620 | 2.95800 | -1.92390 |
| C | -3.09080 | -2.36780 | 4.09120 |
| Br | -3.98120 | -4.07490 | 3.63030 |
| C | 7.64630 | 1.64960 | -2.47820 |
| H | 3.84160 | -0.57960 | -0.65300 |
| H | 3.21540 | 0.81930 | -2.70060 |
| H | 1.76620 | -1.56870 | -2.60800 |
| H | 3.41710 | -2.13440 | -2.38280 |
| H | 0.25630 | -1.53660 | -0.47740 |
| H | 2.75360 | 2.96910 | -1.51140 |
| H | 2.44420 | 2.10250 | -0.02770 |
| H | 1.40080 | -3.52790 | -1.25480 |

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|------------------------------|----------|----------|----------|
| H | 0.33690 | -3.24030 | 1.37650 |
| H | 1.73910 | -2.45060 | 2.04810 |
| H | 4.85780 | 1.37410 | 0.07590 |
| H | -0.95440 | -1.06180 | 1.61570 |
| H | 0.20950 | -2.16980 | 4.25850 |
| H | 1.14970 | 0.06260 | 1.73730 |
| H | 5.00620 | 3.79130 | -1.78800 |
| H | 7.08060 | 2.29600 | -0.05340 |
| H | 8.25390 | 4.46800 | 0.14240 |
| H | 6.99180 | 5.26430 | -0.79200 |
| H | 6.62520 | 4.59740 | 0.79930 |
| H | -3.75620 | -1.66630 | 4.57300 |
| H | 8.30530 | 1.62740 | -3.34610 |
| H | 8.01730 | 0.91860 | -1.75870 |
| H | 6.65350 | 1.34170 | -2.80820 |
| Marilzafurollene C_11 | | | |
| C | 2.68170 | -0.59440 | -1.59160 |
| O | 1.96690 | -0.55290 | -0.35580 |
| C | 2.36230 | 0.64930 | -2.44630 |
| C | 2.32380 | -1.93510 | -2.24590 |
| C | 1.22320 | -1.75730 | -0.18060 |
| C | 2.84290 | 1.96490 | -1.81010 |
| Br | 0.38950 | 0.78550 | -2.71310 |
| C | 1.94170 | -2.79060 | -1.05560 |
| C | 1.07350 | -2.10800 | 1.31240 |
| C | 4.35390 | 2.06300 | -1.72150 |
| Cl | 3.42070 | -3.42720 | -0.27590 |
| C | 0.24160 | -1.07540 | 2.09300 |
| C | -0.03970 | -1.54160 | 3.50770 |
| O | 0.96370 | 0.13570 | 2.14060 |
| C | -1.25060 | -1.73530 | 3.97840 |
| C | 5.04070 | 2.15950 | -0.57100 |
| C | 6.55180 | 2.25740 | -0.47490 |
| C | 7.12380 | 1.08260 | 0.32240 |
| O | 6.95000 | 3.44760 | 0.18970 |
| C | -2.46540 | -1.93580 | 4.43150 |
| Br | -3.38090 | -3.68410 | 4.27590 |
| C | 6.74230 | 4.63520 | -0.56270 |
| H | 3.74480 | -0.61310 | -1.34680 |
| H | 2.80760 | 0.54060 | -3.43630 |
| H | 1.46190 | -1.82990 | -2.90500 |
| H | 3.14020 | -2.35490 | -2.83420 |
| H | 0.23270 | -1.58760 | -0.60710 |
| H | 2.49060 | 2.80800 | -2.40490 |
| H | 2.40080 | 2.08060 | -0.81940 |
| H | 1.30820 | -3.63730 | -1.32230 |
| H | 0.58830 | -3.08220 | 1.38820 |

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|------------------------------|----------|----------|----------|
| H | 2.05200 | -2.21930 | 1.78110 |
| H | 4.88910 | 2.05240 | -2.66030 |
| H | -0.69970 | -0.89580 | 1.56840 |
| H | 0.82430 | -1.71200 | 4.13330 |
| H | 1.38580 | 0.24030 | 1.29060 |
| H | 4.50850 | 2.17050 | 0.36990 |
| H | 6.98550 | 2.23690 | -1.47660 |
| H | 8.21080 | 1.14370 | 0.37770 |
| H | 6.73960 | 1.07340 | 1.34280 |
| H | 6.86720 | 0.12970 | -0.14130 |
| H | -3.07220 | -1.18850 | 4.92160 |
| H | 5.68540 | 4.80140 | -0.77380 |
| H | 7.10510 | 5.49270 | 0.00400 |
| H | 7.28660 | 4.60490 | -1.50730 |
| Marilzafurollene C_12 | | | |
| C | 2.64260 | -1.22510 | -1.96920 |
| O | 2.52770 | -1.04030 | -0.55700 |
| C | 1.80030 | -0.18290 | -2.73690 |
| C | 2.24260 | -2.68400 | -2.22900 |
| C | 2.03600 | -2.22650 | 0.05410 |
| C | 2.40750 | 1.23440 | -2.76010 |
| Br | -0.04380 | -0.09730 | -1.97500 |
| C | 2.49100 | -3.34370 | -0.88660 |
| C | 2.48700 | -2.32480 | 1.52340 |
| C | 2.72110 | 1.78400 | -1.38170 |
| Cl | 4.23290 | -3.70960 | -0.70710 |
| C | 1.90180 | -1.20820 | 2.40730 |
| C | 0.39130 | -1.28890 | 2.52340 |
| O | 2.47160 | -1.31360 | 3.69560 |
| C | -0.41380 | -0.35010 | 2.08030 |
| C | 3.92360 | 2.25100 | -1.00740 |
| C | 4.25430 | 2.76290 | 0.38100 |
| C | 4.60530 | 4.25220 | 0.34430 |
| O | 5.37820 | 2.08200 | 0.92030 |
| C | -1.19760 | 0.59460 | 1.61730 |
| Br | -1.77320 | 2.13220 | 2.72290 |
| C | 5.12440 | 0.73060 | 1.28190 |
| H | 3.69540 | -1.10710 | -2.23070 |
| H | 1.69070 | -0.51220 | -3.77120 |
| H | 1.18180 | -2.75150 | -2.47370 |
| H | 2.80200 | -3.14260 | -3.04480 |
| H | 0.94650 | -2.18970 | 0.01250 |
| H | 3.32270 | 1.22600 | -3.35330 |
| H | 1.72200 | 1.91900 | -3.26040 |
| H | 1.93180 | -4.27010 | -0.75220 |
| H | 2.20770 | -3.29850 | 1.92720 |
| H | 3.57520 | -2.27580 | 1.56960 |

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| H | 1.90670 | 1.77550 | -0.67110 |
| H | 2.18580 | -0.24100 | 1.98680 |
| H | -0.00690 | -2.17610 | 2.99440 |
| H | 2.23240 | -0.54560 | 4.19550 |
| H | 4.73830 | 2.26470 | -1.71670 |
| H | 3.39300 | 2.62560 | 1.03810 |
| H | 4.83190 | 4.62130 | 1.34460 |
| H | 5.47730 | 4.43720 | -0.28330 |
| H | 3.77660 | 4.84220 | -0.04790 |
| H | -1.59640 | 0.62810 | 0.61350 |
| H | 4.80320 | 0.12970 | 0.43030 |
| H | 6.03550 | 0.28190 | 1.67710 |
| H | 4.36280 | 0.67100 | 2.05910 |
| Marilzafurollene C_13 | | | |
| C | 2.72890 | -0.68090 | -1.00020 |
| O | 2.19340 | -1.13390 | 0.24260 |
| C | 2.19500 | 0.72700 | -1.33860 |
| C | 2.39450 | -1.76780 | -2.03170 |
| C | 1.51860 | -2.37340 | 0.05500 |
| C | 2.62950 | 1.81240 | -0.33770 |
| Br | 0.19900 | 0.69720 | -1.36450 |
| C | 2.20320 | -2.99650 | -1.16530 |
| C | 1.50520 | -3.21610 | 1.34570 |
| C | 4.12570 | 2.06380 | -0.33320 |
| Cl | 3.79870 | -3.69910 | -0.76300 |
| C | 0.76480 | -2.53540 | 2.51160 |
| C | -0.69960 | -2.28310 | 2.20410 |
| O | 0.86140 | -3.36910 | 3.64820 |
| C | -1.21900 | -1.07930 | 2.11850 |
| C | 4.70560 | 3.20700 | -0.73530 |
| C | 6.20150 | 3.46210 | -0.72910 |
| C | 6.54820 | 4.65070 | 0.17090 |
| O | 6.67480 | 3.77200 | -2.03170 |
| C | -1.71240 | 0.13200 | 2.01750 |
| Br | -2.48090 | 1.09790 | 3.56530 |
| C | 6.70290 | 2.66480 | -2.92180 |
| H | 3.81330 | -0.65220 | -0.88990 |
| H | 2.52010 | 1.01300 | -2.34010 |
| H | 1.46150 | -1.54230 | -2.54860 |
| H | 3.16920 | -1.89120 | -2.78880 |
| H | 0.49200 | -2.14220 | -0.23320 |
| H | 2.11600 | 2.74450 | -0.57620 |
| H | 2.31600 | 1.53860 | 0.67060 |
| H | 1.60140 | -3.77010 | -1.64350 |
| H | 1.05180 | -4.18600 | 1.13870 |
| H | 2.52980 | -3.41910 | 1.65780 |
| H | 4.74510 | 1.25460 | 0.02690 |

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| H | 1.26500 | -1.59070 | 2.73920 |
| H | -1.31430 | -3.15800 | 2.04890 |
| H | 0.60390 | -2.86890 | 4.41010 |
| H | 4.09330 | 4.02130 | -1.09560 |
| H | 6.72340 | 2.58080 | -0.35080 |
| H | 7.62430 | 4.82440 | 0.18580 |
| H | 6.06960 | 5.56540 | -0.17980 |
| H | 6.22620 | 4.47460 | 1.19750 |
| H | -1.74770 | 0.70850 | 1.10420 |
| H | 5.70560 | 2.25950 | -3.09580 |
| H | 7.10410 | 2.98200 | -3.88440 |
| H | 7.34200 | 1.86750 | -2.54030 |
| Marilzafurollene C_14 | | | |
| C | 2.66480 | -1.90140 | -1.44580 |
| O | 2.31290 | -2.02020 | -0.06790 |
| C | 3.52610 | -0.64370 | -1.66800 |
| C | 1.34610 | -1.97300 | -2.22810 |
| C | 0.90410 | -2.19220 | 0.06280 |
| C | 2.87830 | 0.66890 | -1.19050 |
| Br | 3.98700 | -0.50340 | -3.60310 |
| C | 0.45360 | -2.75750 | -1.28840 |
| C | 0.56230 | -3.03580 | 1.30590 |
| C | 3.83870 | 1.84010 | -1.24700 |
| Cl | 0.80220 | -4.50600 | -1.44000 |
| C | 0.88000 | -2.31950 | 2.63140 |
| C | -0.03980 | -1.13960 | 2.88600 |
| O | 0.73540 | -3.24300 | 3.69070 |
| C | 0.37130 | 0.10680 | 2.94310 |
| C | 4.26570 | 2.52310 | -0.17210 |
| C | 5.21640 | 3.70370 | -0.22430 |
| C | 6.51380 | 3.39200 | 0.52560 |
| O | 4.64620 | 4.85230 | 0.38640 |
| C | 0.76310 | 1.35830 | 2.97780 |
| Br | 0.79370 | 2.50290 | 1.36300 |
| C | 3.55490 | 5.41530 | -0.32960 |
| H | 3.25920 | -2.78170 | -1.69550 |
| H | 4.46620 | -0.78430 | -1.13200 |
| H | 0.92450 | -0.98070 | -2.38280 |
| H | 1.45850 | -2.43940 | -3.20730 |
| H | 0.46520 | -1.19810 | 0.16320 |
| H | 2.00230 | 0.91510 | -1.78930 |
| H | 2.53040 | 0.55030 | -0.16380 |
| H | -0.60910 | -2.60640 | -1.48090 |
| H | -0.49310 | -3.31040 | 1.28340 |
| H | 1.12090 | -3.97100 | 1.25930 |
| H | 4.18480 | 2.12390 | -2.23100 |
| H | 1.91890 | -1.98100 | 2.61880 |

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| H | -1.08440 | -1.37560 | 3.02730 |
| H | 1.46630 | -3.84490 | 3.66910 |
| H | 3.92160 | 2.24130 | 0.81290 |
| H | 5.46360 | 3.92970 | -1.26350 |
| H | 7.20240 | 4.23550 | 0.47550 |
| H | 6.32120 | 3.18290 | 1.57820 |
| H | 7.01790 | 2.52560 | 0.09690 |
| H | 1.09680 | 1.87730 | 3.86460 |
| H | 2.71040 | 4.72760 | -0.38860 |
| H | 3.21160 | 6.31520 | 0.18050 |
| H | 3.84840 | 5.69620 | -1.34180 |
| Marilzafurollene C_15 | | | |
| C | 2.83300 | -1.08730 | -0.45360 |
| O | 1.53620 | -0.56530 | -0.15120 |
| C | 3.62900 | -0.05880 | -1.27860 |
| C | 2.59830 | -2.43020 | -1.16110 |
| C | 0.55690 | -1.59880 | -0.23210 |
| C | 3.89330 | 1.23860 | -0.49590 |
| Br | 2.63280 | 0.37450 | -2.95440 |
| C | 1.09910 | -2.44480 | -1.38630 |
| C | 0.44890 | -2.31700 | 1.13470 |
| C | 4.79480 | 2.19720 | -1.24950 |
| Cl | 0.43050 | -4.09870 | -1.46210 |
| C | -0.04370 | -1.40140 | 2.26980 |
| C | -0.32590 | -2.18600 | 3.53590 |
| O | 0.95160 | -0.43800 | 2.53730 |
| C | -1.50900 | -2.24270 | 4.10360 |
| C | 5.99660 | 2.61360 | -0.81690 |
| C | 6.89570 | 3.57430 | -1.57260 |
| C | 8.23690 | 2.91680 | -1.90730 |
| O | 7.17800 | 4.73090 | -0.79840 |
| C | -2.69870 | -2.29980 | 4.65380 |
| Br | -4.02500 | -3.68860 | 4.17290 |
| C | 6.07450 | 5.61310 | -0.64390 |
| H | 3.35460 | -1.27810 | 0.48590 |
| H | 4.58300 | -0.49750 | -1.57630 |
| H | 3.15610 | -2.53980 | -2.09160 |
| H | 2.89090 | -3.24860 | -0.50230 |
| H | -0.41230 | -1.17270 | -0.49430 |
| H | 2.95060 | 1.74210 | -0.27780 |
| H | 4.34840 | 1.00220 | 0.46680 |
| H | 0.86600 | -1.95330 | -2.33210 |
| H | -0.26110 | -3.13920 | 1.03600 |
| H | 1.39830 | -2.77680 | 1.41100 |
| H | 4.41840 | 2.55630 | -2.19730 |
| H | -0.94950 | -0.88220 | 1.94820 |
| H | 0.51300 | -2.71240 | 3.96700 |

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|------------------------------|----------|----------|----------|
| H | 1.25930 | -0.11830 | 1.69320 |
| H | 6.37820 | 2.26170 | 0.13080 |
| H | 6.41490 | 3.86940 | -2.50750 |
| H | 8.09670 | 2.02520 | -2.51890 |
| H | 8.87660 | 3.60290 | -2.46270 |
| H | 8.77090 | 2.62450 | -1.00280 |
| H | -3.06510 | -1.61440 | 5.40410 |
| H | 5.24920 | 5.14040 | -0.11050 |
| H | 6.38410 | 6.48530 | -0.06810 |
| H | 5.71030 | 5.96350 | -1.61040 |
| Marilzafurollene C_16 | | | |
| C | 2.44500 | -0.64620 | -1.48460 |
| O | 2.15020 | -0.97320 | -0.12690 |
| C | 1.68690 | 0.62810 | -1.91230 |
| C | 2.11640 | -1.90000 | -2.30700 |
| C | 1.62740 | -2.29490 | -0.04920 |
| C | 2.13370 | 1.88510 | -1.14670 |
| Br | -0.26890 | 0.38510 | -1.59440 |
| C | 2.20760 | -3.00660 | -1.27530 |
| C | 1.91070 | -2.93870 | 1.32250 |
| C | 3.56410 | 2.28770 | -1.45040 |
| Cl | 3.91960 | -3.47200 | -1.04510 |
| C | 1.26290 | -2.18280 | 2.49710 |
| C | -0.25080 | -2.14010 | 2.39890 |
| O | 1.62970 | -2.82850 | 3.69920 |
| C | -0.93020 | -1.02560 | 2.24970 |
| C | 4.55110 | 2.31790 | -0.53970 |
| C | 5.98480 | 2.71720 | -0.83470 |
| C | 6.94480 | 1.56620 | -0.52390 |
| O | 6.38580 | 3.82340 | -0.03940 |
| C | -1.58750 | 0.09710 | 2.08060 |
| Br | -2.24610 | 1.18130 | 3.60040 |
| C | 5.78020 | 5.05600 | -0.40440 |
| H | 3.52080 | -0.47620 | -1.54610 |
| H | 1.81480 | 0.79060 | -2.98340 |
| H | 1.09940 | -1.85400 | -2.69700 |
| H | 2.78830 | -2.04400 | -3.15350 |
| H | 0.54880 | -2.22430 | -0.19690 |
| H | 1.48960 | 2.72370 | -1.41250 |
| H | 2.00860 | 1.72750 | -0.07420 |
| H | 1.64750 | -3.89980 | -1.55370 |
| H | 1.56420 | -3.97260 | 1.31450 |
| H | 2.98730 | -2.97930 | 1.48940 |
| H | 3.77630 | 2.56280 | -2.47370 |
| H | 1.66280 | -1.16600 | 2.52120 |
| H | -0.76130 | -3.09080 | 2.45290 |
| H | 1.42580 | -2.25300 | 4.42310 |

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|------------------------------|----------|----------|----------|
| H | 4.34120 | 2.04240 | 0.48420 |
| H | 6.08470 | 2.97270 | -1.89140 |
| H | 7.97330 | 1.84650 | -0.75160 |
| H | 6.90160 | 1.28930 | 0.52970 |
| H | 6.70280 | 0.68140 | -1.11340 |
| H | -1.82860 | 0.53090 | 1.12070 |
| H | 4.69740 | 5.02860 | -0.27800 |
| H | 6.16720 | 5.85320 | 0.23020 |
| H | 6.00440 | 5.31510 | -1.43990 |
| Marilzafurollene C_17 | | | |
| C | 2.67070 | -1.90740 | -1.48390 |
| O | 2.30820 | -2.02690 | -0.10910 |
| C | 3.54270 | -0.65600 | -1.69840 |
| C | 1.35680 | -1.96830 | -2.27440 |
| C | 0.90160 | -2.22660 | 0.01070 |
| C | 2.90120 | 0.66070 | -1.22380 |
| Br | 4.01820 | -0.51650 | -3.63020 |
| C | 0.46380 | -2.77320 | -1.35280 |
| C | 0.56070 | -3.09540 | 1.23720 |
| C | 3.86970 | 1.82540 | -1.27500 |
| Cl | 0.82330 | -4.51690 | -1.53250 |
| C | 0.86420 | -2.40460 | 2.57910 |
| C | -0.05140 | -1.22210 | 2.83730 |
| O | 0.68780 | -3.35150 | 3.61290 |
| C | 0.36980 | 0.01810 | 2.93860 |
| C | 4.29740 | 2.50450 | -0.19780 |
| C | 5.25660 | 3.67850 | -0.24550 |
| C | 6.54890 | 3.35720 | 0.50940 |
| O | 4.69220 | 4.83080 | 0.36360 |
| C | 0.76950 | 1.26550 | 3.01260 |
| Br | 0.85750 | 2.44330 | 1.42440 |
| C | 3.60730 | 5.40150 | -0.35600 |
| H | 3.26020 | -2.79150 | -1.73180 |
| H | 4.47780 | -0.80440 | -1.15590 |
| H | 0.93230 | -0.97480 | -2.41230 |
| H | 1.47540 | -2.41660 | -3.26130 |
| H | 0.44760 | -1.24090 | 0.12490 |
| H | 2.03020 | 0.91280 | -1.82750 |
| H | 2.54680 | 0.54340 | -0.19920 |
| H | -0.59860 | -2.62570 | -1.54920 |
| H | -0.49130 | -3.38110 | 1.20320 |
| H | 1.12910 | -4.02450 | 1.18180 |
| H | 4.22170 | 2.10780 | -2.25730 |
| H | 1.90880 | -2.08390 | 2.58420 |
| H | -1.10300 | -1.44990 | 2.93740 |
| H | 1.12650 | -3.03680 | 4.39080 |
| H | 3.94770 | 2.22410 | 0.78560 |

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|------------------------------|----------|----------|----------|
| H | 5.50950 | 3.90330 | -1.28360 |
| H | 7.24370 | 4.19580 | 0.46230 |
| H | 6.35070 | 3.14900 | 1.56110 |
| H | 7.04850 | 2.48740 | 0.08210 |
| H | 1.07980 | 1.76360 | 3.91970 |
| H | 3.90580 | 5.67980 | -1.36740 |
| H | 2.75800 | 4.71990 | -0.41720 |
| H | 3.26890 | 6.30410 | 0.15270 |
| Marilzafurollene C_18 | | | |
| C | 2.89090 | -1.78890 | -1.36950 |
| O | 2.28330 | -1.93000 | -0.08580 |
| C | 3.34470 | -0.33470 | -1.59990 |
| C | 1.87090 | -2.31840 | -2.38760 |
| C | 0.95970 | -2.43310 | -0.23050 |
| C | 4.45250 | 0.08780 | -0.62020 |
| Br | 1.79160 | 0.90550 | -1.39160 |
| C | 0.99760 | -3.22350 | -1.54230 |
| C | 0.50730 | -3.20420 | 1.02520 |
| C | 5.01120 | 1.46260 | -0.93210 |
| Cl | 1.79370 | -4.81460 | -1.35250 |
| C | 0.46620 | -2.33440 | 2.29540 |
| C | -0.51860 | -1.18470 | 2.18960 |
| O | 0.10520 | -3.15140 | 3.39050 |
| C | -0.15260 | 0.07720 | 2.18290 |
| C | 4.96250 | 2.51100 | -0.09360 |
| C | 5.51360 | 3.88930 | -0.40740 |
| C | 6.58760 | 4.29170 | 0.60640 |
| O | 4.49450 | 4.87690 | -0.35280 |
| C | 0.23900 | 1.32910 | 2.15830 |
| Br | 0.42890 | 2.41730 | 3.80120 |
| C | 3.54700 | 4.79720 | -1.40950 |
| H | 3.76150 | -2.44660 | -1.38460 |
| H | 3.70470 | -0.23120 | -2.62440 |
| H | 1.26450 | -1.50660 | -2.78990 |
| H | 2.33480 | -2.83180 | -3.23020 |
| H | 0.30130 | -1.57670 | -0.38440 |
| H | 4.07150 | 0.06120 | 0.40190 |
| H | 5.27710 | -0.62460 | -0.66210 |
| H | 0.00800 | -3.38720 | -1.97050 |
| H | -0.47740 | -3.63750 | 0.84540 |
| H | 1.18310 | -4.04200 | 1.19670 |
| H | 5.47260 | 1.58100 | -1.90190 |
| H | 1.46580 | -1.93630 | 2.48650 |
| H | -1.56190 | -1.45410 | 2.11720 |
| H | 0.86640 | -3.64410 | 3.66330 |
| H | 4.49870 | 2.39900 | 0.87610 |
| H | 5.96310 | 3.88660 | -1.40230 |

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|------------------------------|----------|----------|----------|
| H | 6.99360 | 5.27550 | 0.37060 |
| H | 6.18070 | 4.33440 | 1.61700 |
| H | 7.41520 | 3.58200 | 0.60640 |
| H | 0.49100 | 1.87770 | 1.26210 |
| H | 2.98860 | 3.86090 | -1.38370 |
| H | 2.82900 | 5.61180 | -1.31600 |
| H | 4.03080 | 4.88840 | -2.38280 |
| Marilzafurollene C_19 | | | |
| C | 3.09660 | -1.65480 | -1.36420 |
| O | 2.34150 | -1.55580 | -0.15620 |
| C | 3.73900 | -0.29970 | -1.71470 |
| C | 2.13620 | -2.20940 | -2.42450 |
| C | 1.00640 | -2.00620 | -0.37740 |
| C | 4.78650 | 0.13090 | -0.67360 |
| Br | 2.32400 | 1.10560 | -1.83320 |
| C | 1.10900 | -2.94270 | -1.58650 |
| C | 0.39890 | -2.60680 | 0.90530 |
| C | 5.50370 | 1.40890 | -1.06330 |
| Cl | 1.74200 | -4.55540 | -1.14020 |
| C | 0.22370 | -1.57260 | 2.03140 |
| C | -0.54060 | -2.15190 | 3.20580 |
| O | 1.50360 | -1.16850 | 2.46600 |
| C | -1.70930 | -1.70310 | 3.60420 |
| C | 5.51240 | 2.52980 | -0.32300 |
| C | 6.21760 | 3.81450 | -0.71550 |
| C | 7.29010 | 4.18480 | 0.31200 |
| O | 5.30780 | 4.90320 | -0.78190 |
| C | -2.88390 | -1.26860 | 3.99600 |
| Br | -3.09560 | 0.16820 | 5.34150 |
| C | 4.38230 | 4.82740 | -1.85830 |
| H | 3.88030 | -2.39470 | -1.19350 |
| H | 4.20830 | -0.36820 | -2.69720 |
| H | 1.64650 | -1.40130 | -2.96830 |
| H | 2.63040 | -2.84810 | -3.15710 |
| H | 0.41830 | -1.13610 | -0.67550 |
| H | 4.31160 | 0.25350 | 0.30100 |
| H | 5.53670 | -0.65190 | -0.55680 |
| H | 0.15730 | -3.08210 | -2.10050 |
| H | -0.57650 | -3.02750 | 0.65710 |
| H | 1.00520 | -3.43930 | 1.26440 |
| H | 6.03370 | 1.39130 | -2.00480 |
| H | -0.30220 | -0.69710 | 1.64350 |
| H | -0.06650 | -2.97430 | 3.72130 |
| H | 2.05120 | -1.09440 | 1.68780 |
| H | 4.98280 | 2.55290 | 0.61880 |
| H | 6.69990 | 3.68580 | -1.68650 |
| H | 7.80620 | 5.09980 | 0.02070 |

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|------------------------------|----------|----------|----------|
| H | 6.85300 | 4.34980 | 1.29710 |
| H | 8.03750 | 3.39630 | 0.40310 |
| H | -3.83110 | -1.64040 | 3.63380 |
| H | 3.75700 | 5.72010 | -1.86340 |
| H | 4.89590 | 4.77390 | -2.81900 |
| H | 3.72280 | 3.96380 | -1.76670 |
| Marilzafurollene C_20 | | | |
| C | 2.61480 | -1.14200 | -1.76660 |
| O | 1.48130 | -1.09150 | -0.90570 |
| C | 2.46620 | -0.14190 | -2.92880 |
| C | 2.75600 | -2.62270 | -2.14990 |
| C | 1.43110 | -2.29790 | -0.15470 |
| C | 2.30020 | 1.31700 | -2.45810 |
| Br | 0.87430 | -0.62070 | -4.03080 |
| C | 1.72930 | -3.31400 | -1.26160 |
| C | 2.45650 | -2.24640 | 1.00690 |
| C | 3.38250 | 1.75850 | -1.48800 |
| Cl | 2.28870 | -4.89930 | -0.65950 |
| C | 2.30810 | -0.98950 | 1.88300 |
| C | 1.05770 | -1.02170 | 2.73930 |
| O | 3.44340 | -0.86290 | 2.71180 |
| C | 0.07770 | -0.15640 | 2.61320 |
| C | 3.13530 | 2.19140 | -0.23740 |
| C | 4.16270 | 2.59510 | 0.81390 |
| C | 5.61500 | 2.31160 | 0.40670 |
| O | 3.94090 | 1.88680 | 2.02920 |
| C | -0.88420 | 0.72440 | 2.47280 |
| Br | -0.90590 | 2.43590 | 3.46660 |
| C | 2.92190 | 2.45110 | 2.84730 |
| H | 3.49410 | -0.86980 | -1.18150 |
| H | 3.33710 | -0.21680 | -3.58140 |
| H | 2.55860 | -2.81820 | -3.20390 |
| H | 3.76740 | -2.96790 | -1.93350 |
| H | 0.42770 | -2.44260 | 0.24710 |
| H | 2.30090 | 1.98700 | -3.31820 |
| H | 1.32600 | 1.42900 | -1.97990 |
| H | 0.81820 | -3.48460 | -1.83720 |
| H | 2.36120 | -3.13960 | 1.62520 |
| H | 3.47010 | -2.28160 | 0.60790 |
| H | 4.39570 | 1.69270 | -1.85540 |
| H | 2.28840 | -0.10850 | 1.23960 |
| H | 1.00630 | -1.80750 | 3.47860 |
| H | 3.78940 | 0.01830 | 2.58790 |
| H | 2.10480 | 2.25490 | 0.08000 |
| H | 4.06610 | 3.66880 | 0.98660 |
| H | 6.30020 | 2.60430 | 1.20250 |
| H | 5.77330 | 1.25050 | 0.21170 |

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|------------------------------|----------|----------|----------|
| H | 5.89750 | 2.87140 | -0.48510 |
| H | -1.73650 | 0.60940 | 1.81910 |
| H | 1.95850 | 2.47520 | 2.33880 |
| H | 2.80210 | 1.85220 | 3.75020 |
| H | 3.17820 | 3.46590 | 3.15430 |
| Marilzafurollene C_21 | | | |
| C | 3.04110 | -1.16440 | -1.41450 |
| O | 1.72560 | -0.68380 | -1.12770 |
| C | 3.60360 | -0.43900 | -2.65360 |
| C | 2.91220 | -2.68790 | -1.56300 |
| C | 0.91530 | -1.74690 | -0.63430 |
| C | 3.72430 | 1.08370 | -2.46720 |
| Br | 2.41380 | -0.77550 | -4.21870 |
| C | 1.41500 | -2.91840 | -1.48230 |
| C | 1.11640 | -1.88920 | 0.89410 |
| C | 4.67690 | 1.46900 | -1.35170 |
| Cl | 0.99970 | -4.52630 | -0.82650 |
| C | 0.69330 | -0.63920 | 1.68640 |
| C | 0.71490 | -0.89260 | 3.18070 |
| O | 1.58750 | 0.40950 | 1.38560 |
| C | -0.34730 | -0.79400 | 3.94690 |
| C | 4.30940 | 2.12180 | -0.23650 |
| C | 5.24940 | 2.50040 | 0.89220 |
| C | 4.79640 | 1.86510 | 2.20890 |
| O | 5.27810 | 3.90660 | 1.09090 |
| C | -1.41890 | -0.70050 | 4.69800 |
| Br | -2.62130 | -2.23800 | 5.02840 |
| C | 5.93560 | 4.62990 | 0.05970 |
| H | 3.67390 | -0.96030 | -0.54920 |
| H | 4.58110 | -0.85170 | -2.90770 |
| H | 3.33780 | -3.07640 | -2.48860 |
| H | 3.41960 | -3.18220 | -0.73370 |
| H | -0.13510 | -1.54160 | -0.84430 |
| H | 4.08180 | 1.54030 | -3.39060 |
| H | 2.73870 | 1.51020 | -2.27480 |
| H | 0.98120 | -2.84810 | -2.48120 |
| H | 0.51400 | -2.72940 | 1.24190 |
| H | 2.14890 | -2.14790 | 1.13110 |
| H | 5.71100 | 1.18480 | -1.48540 |
| H | -0.31010 | -0.33730 | 1.37730 |
| H | 1.67080 | -1.16450 | 3.60380 |
| H | 1.72230 | 0.39310 | 0.44150 |
| H | 3.27650 | 2.40940 | -0.09830 |
| H | 6.25640 | 2.14430 | 0.66640 |
| H | 3.79860 | 2.20540 | 2.48850 |
| H | 4.76410 | 0.77800 | 2.13140 |
| H | 5.47610 | 2.12260 | 3.02100 |

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|------------------------------|----------|----------|----------|
| H | -1.74460 | 0.19960 | 5.19870 |
| H | 5.94320 | 5.69110 | 0.30810 |
| H | 6.97110 | 4.30590 | -0.05190 |
| H | 5.42930 | 4.51830 | -0.89970 |
| Marilzafurollene C_22 | | | |
| C | 2.97130 | -1.70130 | -1.33220 |
| O | 2.35570 | -1.54120 | -0.05440 |
| C | 4.05030 | -0.62400 | -1.55260 |
| C | 1.82350 | -1.73760 | -2.34900 |
| C | 0.93580 | -1.64150 | -0.17750 |
| C | 3.54150 | 0.82740 | -1.46860 |
| Br | 4.91250 | -0.92810 | -3.32470 |
| C | 0.69140 | -2.32250 | -1.53060 |
| C | 0.31260 | -2.32590 | 1.05520 |
| C | 4.67480 | 1.83430 | -1.48650 |
| Cl | 0.86970 | -4.10060 | -1.43870 |
| C | 0.47740 | -1.51100 | 2.34990 |
| C | -0.30500 | -2.12230 | 3.49540 |
| O | 1.84660 | -1.48200 | 2.68940 |
| C | -1.26710 | -1.49380 | 4.13140 |
| C | 4.94410 | 2.69610 | -0.49180 |
| C | 6.07870 | 3.70350 | -0.51120 |
| C | 7.04770 | 3.45500 | 0.64740 |
| O | 5.59080 | 5.02990 | -0.37210 |
| C | -2.23430 | -0.85870 | 4.74980 |
| Br | -4.11910 | -0.95570 | 4.15210 |
| C | 4.90670 | 5.52290 | -1.51610 |
| H | 3.45370 | -2.68020 | -1.32630 |
| H | 4.82710 | -0.76900 | -0.79970 |
| H | 1.55130 | -0.73500 | -2.67590 |
| H | 2.06140 | -2.32280 | -3.23790 |
| H | 0.55350 | -0.62140 | -0.24710 |
| H | 2.87310 | 1.05300 | -2.29880 |
| H | 2.96260 | 0.96210 | -0.55390 |
| H | -0.29350 | -2.10460 | -1.94550 |
| H | -0.75190 | -2.47040 | 0.86400 |
| H | 0.73260 | -3.32290 | 1.19430 |
| H | 5.29260 | 1.83760 | -2.37380 |
| H | 0.14180 | -0.48550 | 2.17910 |
| H | -0.02930 | -3.12810 | 3.77720 |
| H | 2.33760 | -1.43950 | 1.87260 |
| H | 4.32920 | 2.69960 | 0.39690 |
| H | 6.63290 | 3.61470 | -1.44770 |
| H | 7.87040 | 4.16990 | 0.62450 |
| H | 6.54700 | 3.55640 | 1.61060 |
| H | 7.47630 | 2.45390 | 0.59460 |
| H | -2.10440 | -0.23610 | 5.62300 |

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|------------------------------|----------|----------|----------|
| H | 5.55200 | 5.51670 | -2.39550 |
| H | 4.01190 | 4.93960 | -1.73580 |
| H | 4.59540 | 6.55220 | -1.33820 |
| Marilzafurollene C_23 | | | |
| C | 2.96160 | -1.35970 | -0.61240 |
| O | 1.66540 | -1.11960 | -0.06000 |
| C | 3.45870 | -0.09740 | -1.34170 |
| C | 2.82090 | -2.60030 | -1.50720 |
| C | 0.85000 | -2.27980 | -0.18950 |
| C | 3.64500 | 1.09270 | -0.38560 |
| Br | 2.16260 | 0.40660 | -2.77560 |
| C | 1.32380 | -2.83700 | -1.53350 |
| C | 1.06410 | -3.20360 | 1.03360 |
| C | 4.26430 | 2.29590 | -1.06990 |
| Cl | 0.90050 | -4.54940 | -1.81090 |
| C | 0.69340 | -2.54690 | 2.37580 |
| C | -0.78290 | -2.20930 | 2.46780 |
| O | 1.02720 | -3.44540 | 3.41360 |
| C | -1.23500 | -0.98660 | 2.63030 |
| C | 5.44300 | 2.84380 | -0.73040 |
| C | 6.05930 | 4.04880 | -1.41630 |
| C | 7.41500 | 3.69190 | -2.03090 |
| O | 6.28250 | 5.10620 | -0.49500 |
| C | -1.66740 | 0.24100 | 2.79560 |
| Br | -1.95790 | 1.03160 | 4.58690 |
| C | 5.09710 | 5.75080 | -0.04850 |
| H | 3.64440 | -1.59770 | 0.20490 |
| H | 4.40950 | -0.31600 | -1.83050 |
| H | 3.23550 | -2.47000 | -2.50720 |
| H | 3.33090 | -3.44650 | -1.04550 |
| H | -0.19920 | -1.99010 | -0.25280 |
| H | 2.68300 | 1.38540 | 0.03710 |
| H | 4.27450 | 0.79530 | 0.45410 |
| H | 0.87600 | -2.25440 | -2.34000 |
| H | 0.47560 | -4.11340 | 0.91110 |
| H | 2.10440 | -3.52670 | 1.07370 |
| H | 3.69510 | 2.72350 | -1.88360 |
| H | 1.29260 | -1.64270 | 2.50710 |
| H | -1.46860 | -3.04060 | 2.38850 |
| H | 0.95190 | -2.99100 | 4.24120 |
| H | 6.01610 | 2.42380 | 0.08370 |
| H | 5.39990 | 4.39400 | -2.21540 |
| H | 7.85030 | 4.55440 | -2.53590 |
| H | 8.12110 | 3.36320 | -1.26790 |
| H | 7.31630 | 2.89220 | -2.76540 |
| H | -1.90220 | 0.92610 | 1.99390 |
| H | 4.44430 | 5.06720 | 0.49550 |

| | | | |
|------------------------------|----------|----------|----------|
| H | 5.35850 | 6.56590 | 0.62630 |
| H | 4.53930 | 6.17530 | -0.88420 |
| Marilzafurollene C_24 | | | |
| C | 2.92710 | -1.51350 | -1.17750 |
| O | 2.25760 | -1.82500 | 0.04360 |
| C | 3.17510 | 0.00330 | -1.28530 |
| C | 2.07040 | -2.11390 | -2.30150 |
| C | 1.03400 | -2.49710 | -0.23440 |
| C | 4.14200 | 0.50790 | -0.20100 |
| Br | 1.44360 | 0.98890 | -1.12770 |
| C | 1.28060 | -3.18750 | -1.57940 |
| C | 0.59980 | -3.39940 | 0.93780 |
| C | 4.49450 | 1.97250 | -0.37290 |
| Cl | 2.28550 | -4.65840 | -1.41350 |
| C | 0.36600 | -2.62720 | 2.24930 |
| C | -0.72820 | -1.58300 | 2.12650 |
| O | 0.01070 | -3.55370 | 3.25520 |
| C | -0.50620 | -0.29370 | 2.24580 |
| C | 5.73200 | 2.43820 | -0.61700 |
| C | 6.10350 | 3.90180 | -0.79530 |
| C | 6.91060 | 4.40620 | 0.40340 |
| O | 4.96250 | 4.74220 | -0.92070 |
| C | -0.25520 | 0.98970 | 2.35010 |
| Br | -0.33600 | 1.95050 | 4.07890 |
| C | 4.39350 | 4.75890 | -2.22360 |
| H | 3.88410 | -2.03750 | -1.16020 |
| H | 3.58800 | 0.23110 | -2.26920 |
| H | 1.38240 | -1.37110 | -2.70590 |
| H | 2.66330 | -2.50000 | -3.13100 |
| H | 0.27380 | -1.73160 | -0.39720 |
| H | 3.70120 | 0.36640 | 0.78670 |
| H | 5.05730 | -0.08490 | -0.21890 |
| H | 0.35880 | -3.46150 | -2.09350 |
| H | -0.30700 | -3.93830 | 0.66090 |
| H | 1.36230 | -4.15770 | 1.11630 |
| H | 3.67390 | 2.67090 | -0.28440 |
| H | 1.30340 | -2.14880 | 2.54390 |
| H | -1.72360 | -1.95260 | 1.92670 |
| H | 0.07980 | -3.12430 | 4.09640 |
| H | 6.55310 | 1.74010 | -0.69640 |
| H | 6.72570 | 3.99070 | -1.68790 |
| H | 7.20040 | 5.44790 | 0.26500 |
| H | 6.32810 | 4.34310 | 1.32300 |
| H | 7.82160 | 3.82350 | 0.54170 |
| H | 0.01430 | 1.63390 | 1.52540 |
| H | 4.08330 | 3.76460 | -2.54650 |
| H | 3.51250 | 5.40060 | -2.22800 |

| | | | |
|------------------------------|----------|----------|----------|
| H | 5.09890 | 5.15620 | -2.95440 |
| Marilzafurollene C_25 | | | |
| C | 2.93960 | -1.20690 | -1.08800 |
| O | 2.19730 | -1.24290 | 0.13160 |
| C | 3.43800 | 0.22090 | -1.37790 |
| C | 2.02300 | -1.80320 | -2.16430 |
| C | 0.91190 | -1.81750 | -0.09750 |
| C | 4.45960 | 0.70200 | -0.33360 |
| Br | 1.88830 | 1.48150 | -1.40860 |
| C | 1.09000 | -2.67840 | -1.35300 |
| C | 0.38940 | -2.53910 | 1.15980 |
| C | 5.05510 | 2.05170 | -0.68360 |
| Cl | 1.89210 | -4.23710 | -0.99520 |
| C | 0.12720 | -1.58400 | 2.33740 |
| C | -0.55840 | -2.29370 | 3.48810 |
| O | 1.36470 | -1.07260 | 2.78170 |
| C | -1.74190 | -1.95420 | 3.94570 |
| C | 6.35620 | 2.26970 | -0.94330 |
| C | 6.97090 | 3.61420 | -1.29880 |
| C | 7.83810 | 4.13450 | -0.14990 |
| O | 5.98960 | 4.60750 | -1.57100 |
| C | -2.92990 | -1.61200 | 4.38460 |
| Br | -4.59640 | -2.39060 | 3.65240 |
| C | 5.44580 | 4.54290 | -2.88320 |
| H | 3.79560 | -1.87210 | -0.96310 |
| H | 3.89650 | 0.24850 | -2.36770 |
| H | 1.44470 | -1.02330 | -2.66020 |
| H | 2.56720 | -2.35080 | -2.93420 |
| H | 0.23320 | -0.99910 | -0.34530 |
| H | 3.98770 | 0.77040 | 0.64740 |
| H | 5.26320 | -0.02950 | -0.24030 |
| H | 0.14910 | -2.89000 | -1.86240 |
| H | -0.54230 | -3.04460 | 0.90160 |
| H | 1.08270 | -3.32170 | 1.47020 |
| H | 4.36200 | 2.88090 | -0.71610 |
| H | -0.48970 | -0.74890 | 1.99760 |
| H | -0.01560 | -3.11570 | 3.93150 |
| H | 1.89300 | -0.90920 | 2.00360 |
| H | 7.04930 | 1.44160 | -0.90180 |
| H | 7.60910 | 3.47810 | -2.17400 |
| H | 8.30090 | 5.08570 | -0.41340 |
| H | 7.24320 | 4.29290 | 0.75000 |
| H | 8.63630 | 3.43300 | 0.09380 |
| H | -3.11440 | -0.89130 | 5.16790 |
| H | 4.68570 | 5.31530 | -3.00070 |
| H | 6.21600 | 4.71600 | -3.63570 |
| H | 4.97580 | 3.57960 | -3.08350 |

| Marilzafurollene C_26 | | | |
|------------------------------|----------|----------|----------|
| C | 3.26570 | -1.77560 | -1.82380 |
| O | 2.67620 | -1.32910 | -0.60160 |
| C | 3.58540 | -0.58710 | -2.75530 |
| C | 2.28120 | -2.79730 | -2.40990 |
| C | 1.41100 | -1.95360 | -0.40480 |
| C | 4.76920 | 0.29270 | -2.30110 |
| Br | 1.96530 | 0.55710 | -2.98600 |
| C | 1.51390 | -3.26460 | -1.18890 |
| C | 1.08240 | -2.06530 | 1.09610 |
| C | 4.57890 | 0.92430 | -0.93440 |
| Cl | 2.47010 | -4.49820 | -0.31490 |
| C | 0.87650 | -0.69540 | 1.76790 |
| C | 0.41600 | -0.84270 | 3.20440 |
| O | 2.10090 | 0.00510 | 1.74360 |
| C | -0.72780 | -0.37450 | 3.64910 |
| C | 4.39910 | 2.23680 | -0.71480 |
| C | 4.19380 | 2.85430 | 0.65560 |
| C | 2.83430 | 3.55200 | 0.73810 |
| O | 5.18800 | 3.83040 | 0.93260 |
| C | -1.87820 | 0.08930 | 4.07630 |
| Br | -3.54000 | -0.98540 | 4.02700 |
| C | 6.47760 | 3.28940 | 1.18430 |
| H | 4.18990 | -2.29670 | -1.56910 |
| H | 3.82680 | -0.97860 | -3.74480 |
| H | 1.59280 | -2.31390 | -3.10400 |
| H | 2.77490 | -3.60880 | -2.94520 |
| H | 0.65830 | -1.32830 | -0.88880 |
| H | 5.68260 | -0.30220 | -2.27160 |
| H | 4.93810 | 1.07720 | -3.03980 |
| H | 0.54190 | -3.69570 | -1.43120 |
| H | 0.17020 | -2.65330 | 1.20660 |
| H | 1.86460 | -2.61720 | 1.61880 |
| H | 4.58650 | 0.24640 | -0.09290 |
| H | 0.14110 | -0.12040 | 1.20040 |
| H | 1.08940 | -1.36390 | 3.86900 |
| H | 2.50340 | -0.17920 | 0.89760 |
| H | 4.38840 | 2.92350 | -1.54870 |
| H | 4.22400 | 2.07420 | 1.41920 |
| H | 2.68010 | 3.98330 | 1.72710 |
| H | 2.75500 | 4.35570 | 0.00600 |
| H | 2.02310 | 2.84620 | 0.55520 |
| H | -2.03120 | 1.07680 | 4.48680 |
| H | 7.17130 | 4.09680 | 1.41840 |
| H | 6.46040 | 2.60690 | 2.03500 |
| H | 6.86980 | 2.75660 | 0.31730 |

| Marilzafurollene C_27 | | | |
|------------------------------|----------|----------|----------|
| C | 3.24430 | -1.29710 | -1.96050 |
| O | 2.57740 | -0.93720 | -0.74850 |
| C | 2.93830 | -0.27940 | -3.07990 |
| C | 2.79890 | -2.73340 | -2.26480 |
| C | 1.75160 | -2.00930 | -0.30320 |
| C | 3.69710 | 1.05710 | -2.95390 |
| Br | 0.97630 | 0.08110 | -3.15030 |
| C | 2.40510 | -3.25810 | -0.89820 |
| C | 1.58760 | -1.96880 | 1.22710 |
| C | 3.54280 | 1.72680 | -1.60100 |
| Cl | 3.86800 | -3.74430 | 0.00920 |
| C | 0.75230 | -0.76640 | 1.70290 |
| C | 0.52950 | -0.80090 | 3.20190 |
| O | 1.43780 | 0.41840 | 1.36310 |
| C | -0.65560 | -0.91390 | 3.75740 |
| C | 4.57310 | 2.11510 | -0.83120 |
| C | 4.44130 | 2.75320 | 0.53810 |
| C | 4.90800 | 4.21060 | 0.50540 |
| O | 5.25670 | 2.07880 | 1.48550 |
| C | -1.83580 | -1.04200 | 4.31640 |
| Br | -2.96640 | 0.51270 | 4.78990 |
| C | 4.74120 | 0.82250 | 1.90380 |
| H | 4.31660 | -1.30710 | -1.75800 |
| H | 3.20440 | -0.72060 | -4.04180 |
| H | 1.92460 | -2.73170 | -2.91710 |
| H | 3.57380 | -3.32870 | -2.74850 |
| H | 0.77230 | -1.88760 | -0.77010 |
| H | 4.75790 | 0.88690 | -3.14190 |
| H | 3.35540 | 1.74700 | -3.72600 |
| H | 1.73120 | -4.11430 | -0.94400 |
| H | 1.09620 | -2.88820 | 1.54850 |
| H | 2.56410 | -1.95920 | 1.71310 |
| H | 2.52950 | 1.88280 | -1.25790 |
| H | -0.20970 | -0.76550 | 1.18520 |
| H | 1.41490 | -0.72200 | 3.81580 |
| H | 1.87370 | 0.25790 | 0.52820 |
| H | 5.58540 | 1.96720 | -1.17800 |
| H | 3.39780 | 2.72950 | 0.85970 |
| H | 4.80730 | 4.67070 | 1.48840 |
| H | 5.95460 | 4.28430 | 0.20940 |
| H | 4.31640 | 4.79710 | -0.19800 |
| H | -2.29960 | -1.98430 | 4.56890 |
| H | 5.45200 | 0.34270 | 2.57620 |
| H | 3.80640 | 0.95010 | 2.44950 |
| H | 4.56860 | 0.14690 | 1.06480 |

| Marilzafurollene C_28 | | | |
|------------------------------|----------|----------|----------|
| C | 2.69120 | -0.67110 | -0.97150 |
| O | 2.15760 | -1.10910 | 0.27770 |
| C | 2.15660 | 0.73220 | -1.32780 |
| C | 2.35670 | -1.77110 | -1.98910 |
| C | 1.47810 | -2.34800 | 0.10510 |
| C | 2.58620 | 1.82980 | -0.33810 |
| Br | 0.16080 | 0.69990 | -1.36100 |
| C | 2.16150 | -2.98790 | -1.10720 |
| C | 1.47000 | -3.17270 | 1.40700 |
| C | 4.08260 | 2.07950 | -0.32730 |
| Cl | 3.75460 | -3.68980 | -0.69400 |
| C | 0.71380 | -2.48530 | 2.55920 |
| C | -0.75960 | -2.28460 | 2.25620 |
| O | 0.84090 | -3.28040 | 3.72060 |
| C | -1.31040 | -1.10070 | 2.10980 |
| C | 4.66670 | 3.21630 | -0.74110 |
| C | 6.16280 | 3.46940 | -0.72840 |
| C | 6.50490 | 4.67010 | 0.15730 |
| O | 6.64520 | 3.76050 | -2.03190 |
| C | -1.83660 | 0.08920 | 1.94120 |
| Br | -2.61720 | 1.13050 | 3.43320 |
| C | 6.67780 | 2.64100 | -2.90640 |
| H | 3.77560 | -0.64020 | -0.86260 |
| H | 2.48500 | 1.00710 | -2.33130 |
| H | 1.42530 | -1.55100 | -2.51100 |
| H | 3.13270 | -1.90580 | -2.74310 |
| H | 0.45130 | -2.11880 | -0.18370 |
| H | 2.07510 | 2.75930 | -0.59160 |
| H | 2.26600 | 1.56920 | 0.67160 |
| H | 1.55790 | -3.76580 | -1.57620 |
| H | 1.02870 | -4.15070 | 1.21130 |
| H | 2.49720 | -3.35830 | 1.72100 |
| H | 4.69850 | 1.27450 | 0.04780 |
| H | 1.17640 | -1.51610 | 2.76130 |
| H | -1.35410 | -3.18140 | 2.16260 |
| H | 1.69870 | -3.13430 | 4.09400 |
| H | 4.05780 | 4.02640 | -1.11650 |
| H | 6.68090 | 2.59290 | -0.33420 |
| H | 7.58110 | 4.84260 | 0.17730 |
| H | 6.03000 | 5.58040 | -0.20950 |
| H | 6.17540 | 4.50880 | 1.18400 |
| H | -1.89510 | 0.60730 | 0.99480 |
| H | 7.08610 | 2.94430 | -3.87050 |
| H | 7.31290 | 1.84810 | -2.50950 |
| H | 5.68090 | 2.23490 | -3.08170 |

| Marilzafurollene C_29 | | | |
|------------------------------|----------|----------|----------|
| C | 2.80400 | -1.17180 | -0.87310 |
| O | 1.91680 | -0.92970 | 0.21970 |
| C | 3.32010 | 0.15640 | -1.45690 |
| C | 2.03340 | -2.05740 | -1.86120 |
| C | 0.67310 | -1.59060 | -0.00740 |
| C | 4.19770 | 0.92700 | -0.45630 |
| Br | 1.77340 | 1.30390 | -1.98900 |
| C | 1.01390 | -2.73480 | -0.96860 |
| C | -0.00340 | -1.98760 | 1.31940 |
| C | 4.81790 | 2.17000 | -1.06460 |
| Cl | 1.77990 | -4.11680 | -0.12950 |
| C | -0.41730 | -0.76880 | 2.17620 |
| C | -1.25040 | -1.09050 | 3.40980 |
| O | 0.75460 | -0.09720 | 2.58340 |
| C | -1.63390 | -2.28950 | 3.78950 |
| C | 6.13890 | 2.37960 | -1.19110 |
| C | 6.75640 | 3.62540 | -1.79860 |
| C | 7.59850 | 3.27270 | -3.02730 |
| O | 7.61610 | 4.27600 | -0.87430 |
| C | -2.02650 | -3.48760 | 4.15220 |
| Br | -3.73270 | -4.27680 | 3.53210 |
| C | 6.94010 | 4.92250 | 0.19570 |
| H | 3.64460 | -1.74810 | -0.48310 |
| H | 3.89790 | -0.04730 | -2.35990 |
| H | 1.51520 | -1.45240 | -2.60550 |
| H | 2.67390 | -2.76010 | -2.39480 |
| H | 0.02740 | -0.88800 | -0.53770 |
| H | 3.60550 | 1.21910 | 0.41190 |
| H | 4.99130 | 0.27710 | -0.08520 |
| H | 0.14610 | -3.10720 | -1.51420 |
| H | -0.88950 | -2.57620 | 1.07710 |
| H | 0.64980 | -2.64010 | 1.90020 |
| H | 4.12550 | 2.92470 | -1.41080 |
| H | -1.00340 | -0.08470 | 1.56020 |
| H | -1.53130 | -0.23170 | 4.00200 |
| H | 1.37240 | -0.15120 | 1.85710 |
| H | 6.83730 | 1.63140 | -0.84460 |
| H | 5.96690 | 4.31300 | -2.10890 |
| H | 8.02990 | 4.16990 | -3.47140 |
| H | 8.41940 | 2.60470 | -2.76570 |
| H | 6.99470 | 2.78180 | -3.79090 |
| H | -1.47430 | -4.14650 | 4.80620 |
| H | 6.38650 | 4.21380 | 0.81270 |
| H | 7.66700 | 5.42150 | 0.83650 |
| H | 6.24680 | 5.67880 | -0.17440 |

| Marilzafurollene C_30 | | | |
|------------------------------|----------|----------|----------|
| C | 2.41080 | -0.64230 | -1.45380 |
| O | 2.11780 | -0.95370 | -0.09180 |
| C | 1.65540 | 0.62910 | -1.89520 |
| C | 2.07800 | -1.90440 | -2.26190 |
| C | 1.58390 | -2.26970 | 0.00040 |
| C | 2.10210 | 1.89280 | -1.14060 |
| Br | -0.30150 | 0.39210 | -1.58030 |
| C | 2.16000 | -2.99920 | -1.21710 |
| C | 1.86920 | -2.89690 | 1.37890 |
| C | 3.53430 | 2.28960 | -1.44370 |
| Cl | 3.86850 | -3.47360 | -0.97820 |
| C | 1.20870 | -2.13570 | 2.54340 |
| C | -0.30660 | -2.13700 | 2.46030 |
| O | 1.60360 | -2.73890 | 3.75880 |
| C | -1.01830 | -1.05050 | 2.26160 |
| C | 4.51880 | 2.32550 | -0.53050 |
| C | 5.95410 | 2.71940 | -0.82480 |
| C | 6.91040 | 1.56750 | -0.50600 |
| O | 6.35650 | 3.82870 | -0.03450 |
| C | -1.70980 | 0.04150 | 2.03680 |
| Br | -2.39020 | 1.19210 | 3.49740 |
| C | 5.75490 | 5.06110 | -0.40720 |
| H | 3.48690 | -0.47540 | -1.51880 |
| H | 1.78610 | 0.78120 | -2.96750 |
| H | 1.06240 | -1.85790 | -2.65560 |
| H | 2.75140 | -2.06200 | -3.10470 |
| H | 0.50540 | -2.19410 | -0.14610 |
| H | 1.46040 | 2.72990 | -1.41670 |
| H | 1.97320 | 1.74620 | -0.06710 |
| H | 1.59420 | -3.89180 | -1.48610 |
| H | 1.53120 | -3.93390 | 1.38020 |
| H | 2.94630 | -2.92630 | 1.54380 |
| H | 3.74990 | 2.55550 | -2.46880 |
| H | 1.56970 | -1.10420 | 2.54550 |
| H | -0.79000 | -3.09610 | 2.57380 |
| H | 2.48260 | -2.45400 | 3.96530 |
| H | 4.30530 | 2.05930 | 0.49520 |
| H | 6.05680 | 2.96910 | -1.88270 |
| H | 7.94010 | 1.84400 | -0.73320 |
| H | 6.86460 | 1.29640 | 0.54900 |
| H | 6.66730 | 0.68030 | -1.09130 |
| H | -1.97090 | 0.41310 | 1.05640 |
| H | 5.98200 | 5.31420 | -1.44350 |
| H | 4.67170 | 5.03720 | -0.28300 |
| H | 6.14260 | 5.86050 | 0.22410 |

| Marilzafurollene C_31 | | | |
|------------------------------|----------|----------|----------|
| C | 3.07980 | -0.66300 | -0.59010 |
| O | 2.30200 | -0.21920 | 0.52150 |
| C | 3.67290 | 0.53270 | -1.35860 |
| C | 2.16360 | -1.57480 | -1.41500 |
| C | 1.00690 | -0.81470 | 0.48340 |
| C | 4.67480 | 1.32820 | -0.50520 |
| Br | 2.20640 | 1.75280 | -1.95230 |
| C | 1.18320 | -2.07390 | -0.37450 |
| C | 0.45320 | -1.00830 | 1.90820 |
| C | 5.36620 | 2.42500 | -1.29190 |
| Cl | 1.91880 | -3.42320 | 0.54370 |
| C | -0.91050 | -1.72300 | 1.97720 |
| C | -1.36170 | -1.90260 | 3.41360 |
| O | -1.87740 | -0.96450 | 1.28080 |
| C | -1.59140 | -3.07500 | 3.96000 |
| C | 6.69070 | 2.49070 | -1.50680 |
| C | 7.37950 | 3.59060 | -2.29310 |
| C | 8.11330 | 3.01530 | -3.50700 |
| O | 8.34630 | 4.26230 | -1.49880 |
| C | -1.83640 | -4.24890 | 4.49240 |
| Br | -3.62500 | -5.09370 | 4.41930 |
| C | 7.79400 | 5.09290 | -0.48640 |
| H | 3.89140 | -1.27180 | -0.18840 |
| H | 4.17380 | 0.16910 | -2.25710 |
| H | 1.62470 | -1.00500 | -2.17220 |
| H | 2.70070 | -2.37630 | -1.92260 |
| H | 0.35890 | -0.12220 | -0.05720 |
| H | 4.16310 | 1.77560 | 0.34790 |
| H | 5.42730 | 0.65330 | -0.09540 |
| H | 0.24520 | -2.42490 | -0.80620 |
| H | 1.18040 | -1.56490 | 2.50020 |
| H | 0.37650 | -0.03010 | 2.38400 |
| H | 4.72410 | 3.19570 | -1.69490 |
| H | -0.83570 | -2.70210 | 1.49930 |
| H | -1.48730 | -0.99740 | 3.99050 |
| H | -2.70610 | -1.42230 | 1.31690 |
| H | 7.33890 | 1.72560 | -1.10430 |
| H | 6.63710 | 4.30810 | -2.64860 |
| H | 8.59550 | 3.80780 | -4.07940 |
| H | 8.88580 | 2.30820 | -3.20380 |
| H | 7.42450 | 2.49620 | -4.17400 |
| H | -1.10860 | -4.85720 | 5.00960 |
| H | 7.14960 | 5.86190 | -0.91410 |
| H | 8.59850 | 5.59370 | 0.05210 |
| H | 7.21740 | 4.51850 | 0.23940 |

| Marilzafurollene C_32 | | | |
|------------------------------|----------|----------|----------|
| C | 3.05640 | -1.30920 | -0.25520 |
| O | 1.87730 | -0.58270 | 0.10220 |
| C | 4.09000 | -0.35230 | -0.87840 |
| C | 2.59430 | -2.44280 | -1.18290 |
| C | 0.71460 | -1.36070 | -0.17470 |
| C | 4.56490 | 0.72170 | 0.11560 |
| Br | 3.29940 | 0.54130 | -2.47980 |
| C | 1.13910 | -2.10590 | -1.44200 |
| C | 0.38400 | -2.24940 | 1.04870 |
| C | 5.66820 | 1.59300 | -0.45280 |
| Cl | 0.15380 | -3.54850 | -1.81090 |
| C | 0.02370 | -1.44450 | 2.31020 |
| C | -0.48510 | -2.34430 | 3.41900 |
| O | 1.17730 | -0.76780 | 2.75920 |
| C | -1.68580 | -2.24080 | 3.94160 |
| C | 5.58800 | 2.92720 | -0.58720 |
| C | 6.68400 | 3.80100 | -1.16780 |
| C | 7.17180 | 4.82240 | -0.13740 |
| O | 6.21900 | 4.53140 | -2.29370 |
| C | -2.89180 | -2.13370 | 4.44670 |
| Br | -4.44300 | -3.11720 | 3.70810 |
| C | 5.95220 | 3.73310 | -3.43940 |
| H | 3.47480 | -1.75200 | 0.65030 |
| H | 4.94840 | -0.92920 | -1.22570 |
| H | 3.17070 | -2.51790 | -2.10550 |
| H | 2.67570 | -3.39850 | -0.66390 |
| H | -0.13080 | -0.70400 | -0.38360 |
| H | 3.72180 | 1.34280 | 0.42160 |
| H | 4.94550 | 0.24690 | 1.02050 |
| H | 1.06580 | -1.43140 | -2.29660 |
| H | -0.47160 | -2.87720 | 0.79640 |
| H | 1.20240 | -2.93680 | 1.26520 |
| H | 6.56760 | 1.08210 | -0.76530 |
| H | -0.73720 | -0.70150 | 2.06000 |
| H | 0.20250 | -3.09770 | 3.77460 |
| H | 1.59080 | -0.38770 | 1.98850 |
| H | 4.69030 | 3.44300 | -0.27720 |
| H | 7.53060 | 3.17850 | -1.46410 |
| H | 7.56160 | 4.32850 | 0.75300 |
| H | 7.96960 | 5.43930 | -0.55120 |
| H | 6.36510 | 5.48730 | 0.17220 |
| H | -3.15370 | -1.51570 | 5.29300 |
| H | 5.14580 | 3.02150 | -3.25950 |
| H | 5.64720 | 4.37450 | -4.26620 |
| H | 6.83970 | 3.18260 | -3.75370 |

| Marilzafurollene C_33 | | | |
|------------------------------|----------|----------|----------|
| C | 2.92210 | -0.60920 | -1.06190 |
| O | 2.01510 | -0.72670 | 0.03500 |
| C | 2.68090 | 0.70700 | -1.82940 |
| C | 2.75040 | -1.88560 | -1.89600 |
| C | 1.32220 | -1.97160 | -0.03630 |
| C | 2.95090 | 1.97260 | -0.99620 |
| Br | 0.78250 | 0.78060 | -2.44010 |
| C | 2.23240 | -2.87650 | -0.87430 |
| C | 0.94970 | -2.48680 | 1.36770 |
| C | 4.40630 | 2.13180 | -0.59770 |
| Cl | 3.60150 | -3.52550 | 0.07710 |
| C | -0.06140 | -1.58220 | 2.09410 |
| C | -0.54310 | -2.21100 | 3.38690 |
| O | 0.57000 | -0.35430 | 2.38380 |
| C | -1.79310 | -2.54930 | 3.60830 |
| C | 5.21310 | 3.11020 | -1.04080 |
| C | 6.66780 | 3.27360 | -0.64100 |
| C | 6.89610 | 4.62220 | 0.04610 |
| O | 7.51980 | 3.23310 | -1.77640 |
| C | -3.03760 | -2.90260 | 3.82810 |
| Br | -4.36880 | -1.67670 | 4.63100 |
| C | 7.65620 | 1.94440 | -2.35900 |
| H | 3.93030 | -0.61910 | -0.64700 |
| H | 3.30220 | 0.72990 | -2.72610 |
| H | 2.00100 | -1.74720 | -2.67550 |
| H | 3.67320 | -2.20750 | -2.37940 |
| H | 0.40690 | -1.79740 | -0.60530 |
| H | 2.64440 | 2.84890 | -1.56880 |
| H | 2.33780 | 1.96640 | -0.09420 |
| H | 1.70230 | -3.71730 | -1.32320 |
| H | 0.51960 | -3.48380 | 1.26280 |
| H | 1.84250 | -2.60530 | 1.98290 |
| H | 4.79540 | 1.39850 | 0.09440 |
| H | -0.91290 | -1.38700 | 1.43810 |
| H | 0.20880 | -2.37130 | 4.14580 |
| H | 1.11030 | -0.13410 | 1.62850 |
| H | 4.83180 | 3.84820 | -1.73210 |
| H | 6.94910 | 2.48110 | 0.05550 |
| H | 7.93840 | 4.73280 | 0.34590 |
| H | 6.65270 | 5.45130 | -0.61880 |
| H | 6.28130 | 4.71720 | 0.94150 |
| H | -3.45270 | -3.87320 | 3.59920 |
| H | 8.34600 | 1.99710 | -3.20130 |
| H | 8.05880 | 1.22750 | -1.64230 |
| H | 6.70430 | 1.56640 | -2.73340 |

| Marilzafurollene C_34 | | | |
|------------------------------|----------|----------|----------|
| C | 2.78140 | -0.67880 | -1.63550 |
| O | 2.03380 | -0.69180 | -0.41870 |
| C | 2.40280 | 0.54620 | -2.49310 |
| C | 2.53040 | -2.03660 | -2.30430 |
| C | 1.36590 | -1.94280 | -0.26820 |
| C | 2.77270 | 1.88710 | -1.83610 |
| Br | 0.43410 | 0.54940 | -2.81870 |
| C | 2.17290 | -2.92200 | -1.12840 |
| C | 1.20060 | -2.31150 | 1.21900 |
| C | 4.26980 | 2.08400 | -1.69350 |
| Cl | 3.66860 | -3.46680 | -0.31200 |
| C | 0.28320 | -1.34020 | 1.98260 |
| C | -0.00250 | -1.83230 | 3.38800 |
| O | 0.92530 | -0.08600 | 2.05300 |
| C | -1.20290 | -2.15240 | 3.81540 |
| C | 4.90770 | 2.21550 | -0.51860 |
| C | 6.40470 | 2.41030 | -0.36750 |
| C | 7.02260 | 1.26750 | 0.44200 |
| O | 6.70090 | 3.61770 | 0.31900 |
| C | -2.39770 | -2.48840 | 4.24130 |
| Br | -3.63090 | -1.19340 | 5.09080 |
| C | 6.44260 | 4.79610 | -0.43200 |
| H | 3.83660 | -0.62880 | -1.36270 |
| H | 2.88380 | 0.47530 | -3.46970 |
| H | 1.68190 | -1.98480 | -2.98680 |
| H | 3.38840 | -2.39860 | -2.87150 |
| H | 0.37790 | -1.83530 | -0.72000 |
| H | 2.38600 | 2.70870 | -2.43960 |
| H | 2.28990 | 1.96730 | -0.86090 |
| H | 1.60300 | -3.80620 | -1.41610 |
| H | 0.77920 | -3.31600 | 1.27760 |
| H | 2.17200 | -2.36110 | 1.71270 |
| H | 4.83720 | 2.11640 | -2.61270 |
| H | -0.65450 | -1.21850 | 1.43550 |
| H | 0.85020 | -1.90770 | 4.04690 |
| H | 1.35700 | 0.05280 | 1.21280 |
| H | 4.34290 | 2.18370 | 0.40260 |
| H | 6.87420 | 2.42700 | -1.35310 |
| H | 8.10070 | 1.39800 | 0.53700 |
| H | 6.60370 | 1.22430 | 1.44760 |
| H | 6.84500 | 0.30430 | -0.03720 |
| H | -2.82010 | -3.48020 | 4.17360 |
| H | 7.02060 | 4.80990 | -1.35690 |
| H | 5.38520 | 4.89530 | -0.67940 |
| H | 6.72880 | 5.67000 | 0.15320 |

| Marilzafurollene C_35 | | | |
|------------------------------|----------|----------|----------|
| C | 2.87200 | -0.55490 | -1.38500 |
| O | 2.02710 | -0.49470 | -0.23520 |
| C | 2.53020 | 0.58070 | -2.37130 |
| C | 2.71860 | -1.97190 | -1.95270 |
| C | 1.39200 | -1.75490 | -0.02890 |
| C | 2.79830 | 1.98380 | -1.80070 |
| Br | 0.59850 | 0.48080 | -2.86140 |
| C | 2.29870 | -2.76930 | -0.73510 |
| C | 1.11930 | -2.00330 | 1.46730 |
| C | 4.26780 | 2.24080 | -1.52940 |
| Cl | 3.74250 | -3.17970 | 0.23860 |
| C | 0.11450 | -1.00580 | 2.07000 |
| C | -0.26880 | -1.38790 | 3.48590 |
| O | 0.70880 | 0.27370 | 2.08130 |
| C | -1.49830 | -1.67060 | 3.85140 |
| C | 4.78100 | 2.50610 | -0.31560 |
| C | 6.24930 | 2.75890 | -0.01660 |
| C | 6.49370 | 4.23780 | 0.29290 |
| O | 7.09190 | 2.40720 | -1.10760 |
| C | -2.72890 | -1.96280 | 4.20000 |
| Br | -3.44820 | -3.80510 | 4.11020 |
| C | 7.38180 | 1.01770 | -1.18840 |
| H | 3.89890 | -0.44410 | -1.03380 |
| H | 3.09760 | 0.45050 | -3.29400 |
| H | 1.92520 | -2.01020 | -2.69930 |
| H | 3.62990 | -2.34600 | -2.41990 |
| H | 0.44070 | -1.72590 | -0.56380 |
| H | 2.45390 | 2.73830 | -2.50850 |
| H | 2.21850 | 2.12930 | -0.88810 |
| H | 1.78470 | -3.69760 | -0.98700 |
| H | 0.72440 | -3.01400 | 1.58020 |
| H | 2.04870 | -1.97550 | 2.03730 |
| H | 4.92580 | 2.20420 | -2.38620 |
| H | -0.77890 | -0.96610 | 1.44260 |
| H | 0.53640 | -1.41760 | 4.20540 |
| H | 1.20140 | 0.35680 | 1.26760 |
| H | 4.11950 | 2.54910 | 0.53830 |
| H | 6.52420 | 2.17540 | 0.86420 |
| H | 7.54190 | 4.41550 | 0.53360 |
| H | 6.23800 | 4.86530 | -0.56130 |
| H | 5.89700 | 4.56820 | 1.14340 |
| H | -3.45420 | -1.24830 | 4.56120 |
| H | 8.00340 | 0.82490 | -2.06260 |
| H | 7.93050 | 0.67990 | -0.30840 |
| H | 6.47630 | 0.41750 | -1.28300 |

| Marilzafurollene C_36 | | | |
|------------------------------|----------|----------|----------|
| C | 2.73330 | -1.38920 | -1.03770 |
| O | 2.20180 | -1.58330 | 0.27270 |
| C | 2.88400 | 0.11020 | -1.35310 |
| C | 1.81310 | -2.16380 | -1.98840 |
| C | 1.09170 | -2.47580 | 0.22640 |
| C | 3.90380 | 0.79640 | -0.42910 |
| Br | 1.11680 | 1.02080 | -1.16520 |
| C | 1.26110 | -3.24860 | -1.08780 |
| C | 1.01800 | -3.32930 | 1.50720 |
| C | 4.15670 | 2.24120 | -0.81430 |
| Cl | 2.45500 | -4.57470 | -0.94880 |
| C | 0.65360 | -2.51970 | 2.76470 |
| C | -0.78870 | -2.04900 | 2.75350 |
| O | 0.85130 | -3.33970 | 3.89850 |
| C | -1.14340 | -0.78500 | 2.79350 |
| C | 5.34760 | 2.73180 | -1.19640 |
| C | 5.59710 | 4.17850 | -1.57970 |
| C | 6.09610 | 4.28170 | -3.02320 |
| O | 6.58910 | 4.76620 | -0.75060 |
| C | -1.51780 | 0.47120 | 2.84420 |
| Br | -1.82310 | 1.55700 | 1.21870 |
| C | 6.16340 | 5.01230 | 0.58280 |
| H | 3.71660 | -1.86210 | -1.05660 |
| H | 3.19950 | 0.22940 | -2.39070 |
| H | 0.99400 | -1.53570 | -2.33890 |
| H | 2.33190 | -2.55210 | -2.86510 |
| H | 0.19140 | -1.86520 | 0.13770 |
| H | 3.55080 | 0.76430 | 0.60250 |
| H | 4.84740 | 0.24970 | -0.45090 |
| H | 0.32550 | -3.67330 | -1.45340 |
| H | 0.29500 | -4.13440 | 1.37020 |
| H | 1.98390 | -3.81160 | 1.65980 |
| H | 3.30130 | 2.90060 | -0.76730 |
| H | 1.32280 | -1.65990 | 2.84870 |
| H | -1.53980 | -2.82430 | 2.71510 |
| H | 1.78230 | -3.42600 | 4.04930 |
| H | 6.20760 | 2.07920 | -1.24260 |
| H | 4.66820 | 4.74630 | -1.49590 |
| H | 6.26110 | 5.32240 | -3.30240 |
| H | 7.03850 | 3.74960 | -3.15500 |
| H | 5.37150 | 3.86170 | -3.72120 |
| H | -1.69520 | 1.02530 | 3.75430 |
| H | 5.30000 | 5.67850 | 0.60540 |
| H | 5.90540 | 4.08920 | 1.10290 |
| H | 6.96890 | 5.49150 | 1.13920 |

| Marilzafurollene C_37 | | | |
|------------------------------|----------|----------|----------|
| C | 2.84560 | -1.69020 | -1.14340 |
| O | 2.20090 | -1.93010 | 0.10730 |
| C | 2.94570 | -0.17670 | -1.42230 |
| C | 2.06360 | -2.49400 | -2.19500 |
| C | 0.98980 | -2.64220 | -0.10700 |
| C | 3.75270 | 0.55530 | -0.33650 |
| Br | 1.11940 | 0.62790 | -1.53440 |
| C | 1.28000 | -3.48380 | -1.35520 |
| C | 0.53930 | -3.41160 | 1.15050 |
| C | 3.95000 | 2.02620 | -0.64680 |
| Cl | 2.31580 | -4.89800 | -0.99640 |
| C | 0.37360 | -2.53250 | 2.40450 |
| C | -0.58290 | -1.37090 | 2.20500 |
| O | -0.10740 | -3.35460 | 3.44890 |
| C | -0.28310 | -0.13170 | 2.52400 |
| C | 5.14300 | 2.61630 | -0.82710 |
| C | 5.33180 | 4.09050 | -1.13210 |
| C | 6.05630 | 4.28310 | -2.46660 |
| O | 6.11580 | 4.72570 | -0.13280 |
| C | 0.01480 | 1.09110 | 2.89700 |
| Br | 0.91710 | 2.39520 | 1.71270 |
| C | 5.45010 | 4.88770 | 1.11260 |
| H | 3.85040 | -2.10800 | -1.06330 |
| H | 3.42180 | -0.02190 | -2.39160 |
| H | 1.36780 | -1.85790 | -2.74140 |
| H | 2.71000 | -2.97380 | -2.93030 |
| H | 0.22180 | -1.91210 | -0.36670 |
| H | 3.24410 | 0.46990 | 0.62480 |
| H | 4.72610 | 0.07860 | -0.21530 |
| H | 0.37520 | -3.84180 | -1.84750 |
| H | -0.39910 | -3.92260 | 0.93230 |
| H | 1.26110 | -4.19370 | 1.38470 |
| H | 3.04850 | 2.61910 | -0.71710 |
| H | 1.35610 | -2.15220 | 2.69480 |
| H | -1.54430 | -1.60940 | 1.77390 |
| H | 0.01120 | -2.89930 | 4.27030 |
| H | 6.04860 | 2.03150 | -0.75330 |
| H | 4.35750 | 4.57940 | -1.19640 |
| H | 6.17760 | 5.34280 | -2.69180 |
| H | 7.04880 | 3.83260 | -2.44650 |
| H | 5.49750 | 3.83130 | -3.28660 |
| H | -0.19680 | 1.50210 | 3.87310 |
| H | 6.10500 | 5.41000 | 1.80990 |
| H | 4.54120 | 5.48020 | 1.00090 |
| H | 5.18760 | 3.92850 | 1.56020 |

| Marilzafurollene C_38 | | | |
|------------------------------|----------|----------|----------|
| C | 2.77370 | -1.42840 | -1.09550 |
| O | 2.22600 | -1.63330 | 0.20640 |
| C | 2.91750 | 0.07400 | -1.39970 |
| C | 1.87220 | -2.20380 | -2.06360 |
| C | 1.12120 | -2.53090 | 0.14000 |
| C | 3.90910 | 0.76420 | -0.44840 |
| Br | 1.13810 | 0.96760 | -1.24860 |
| C | 1.31230 | -3.29550 | -1.17640 |
| C | 1.02450 | -3.39340 | 1.41380 |
| C | 4.15860 | 2.21300 | -0.82020 |
| Cl | 2.50980 | -4.61760 | -1.03130 |
| C | 0.67450 | -2.59310 | 2.68100 |
| C | -0.73820 | -2.04050 | 2.64670 |
| O | 0.79510 | -3.46020 | 3.79060 |
| C | -1.02510 | -0.76490 | 2.77490 |
| C | 5.35410 | 2.71570 | -1.17080 |
| C | 5.60020 | 4.16660 | -1.54070 |
| C | 6.13460 | 4.28130 | -2.97060 |
| O | 6.56560 | 4.75900 | -0.68400 |
| C | -1.33180 | 0.50220 | 2.92240 |
| Br | -1.49460 | 1.74600 | 1.39260 |
| C | 6.10450 | 4.99340 | 0.63980 |
| H | 3.76060 | -1.89390 | -1.10270 |
| H | 3.25580 | 0.20140 | -2.42910 |
| H | 1.05490 | -1.57950 | -2.42450 |
| H | 2.40670 | -2.58560 | -2.93370 |
| H | 0.22090 | -1.92220 | 0.04010 |
| H | 3.53200 | 0.72370 | 0.57430 |
| H | 4.85750 | 0.22540 | -0.45020 |
| H | 0.38360 | -3.72190 | -1.55700 |
| H | 0.28660 | -4.18270 | 1.26530 |
| H | 1.97860 | -3.89700 | 1.57230 |
| H | 3.29650 | 2.86470 | -0.79080 |
| H | 1.39670 | -1.78180 | 2.80040 |
| H | -1.52790 | -2.76490 | 2.50860 |
| H | 0.84120 | -2.93780 | 4.57880 |
| H | 6.22060 | 2.07080 | -1.19920 |
| H | 4.66440 | 4.72560 | -1.47770 |
| H | 6.29720 | 5.32490 | -3.24060 |
| H | 7.08480 | 3.75830 | -3.08100 |
| H | 5.43170 | 3.85830 | -3.68870 |
| H | -1.52420 | 0.98370 | 3.87000 |
| H | 5.23400 | 5.65060 | 0.64440 |
| H | 5.84340 | 4.06480 | 1.14850 |
| H | 6.89100 | 5.47780 | 1.21840 |

| Marilzafurollene C_39 | | | |
|------------------------------|----------|----------|----------|
| C | 2.96130 | -0.97930 | -0.96510 |
| O | 1.54550 | -0.80900 | -0.86580 |
| C | 3.49310 | -0.21910 | -2.19660 |
| C | 3.20500 | -2.49600 | -0.99020 |
| C | 0.94440 | -2.00370 | -0.37340 |
| C | 3.23220 | 1.29760 | -2.15670 |
| Br | 2.63240 | -0.94260 | -3.84420 |
| C | 1.80290 | -3.07140 | -1.05500 |
| C | 0.97650 | -2.00320 | 1.17450 |
| C | 3.90860 | 1.99430 | -0.99100 |
| Cl | 1.68730 | -4.68960 | -0.30950 |
| C | 0.17750 | -0.84770 | 1.80400 |
| C | 0.07430 | -0.99590 | 3.30910 |
| O | 0.82950 | 0.36730 | 1.50400 |
| C | -1.06720 | -1.11520 | 3.94790 |
| C | 4.92260 | 2.86700 | -1.11070 |
| C | 5.59770 | 3.56520 | 0.05520 |
| C | 5.47250 | 5.08540 | -0.07270 |
| O | 6.98410 | 3.26130 | 0.10160 |
| C | -2.21390 | -1.24470 | 4.57200 |
| Br | -3.04540 | -3.00930 | 4.90910 |
| C | 7.27730 | 1.93390 | 0.51520 |
| H | 3.41850 | -0.58070 | -0.05850 |
| H | 4.56530 | -0.39380 | -2.29960 |
| H | 3.82410 | -2.82790 | -1.82410 |
| H | 3.70120 | -2.80400 | -0.06910 |
| H | -0.08960 | -2.06770 | -0.71470 |
| H | 3.57860 | 1.74490 | -3.08920 |
| H | 2.16040 | 1.49260 | -2.10360 |
| H | 1.49570 | -3.16660 | -2.09780 |
| H | 0.54620 | -2.94170 | 1.52670 |
| H | 2.00200 | -1.99130 | 1.54500 |
| H | 3.52780 | 1.75820 | -0.00700 |
| H | -0.82320 | -0.81990 | 1.36670 |
| H | 1.00760 | -0.99810 | 3.85290 |
| H | 1.04510 | 0.33810 | 0.57550 |
| H | 5.30940 | 3.10950 | -2.09020 |
| H | 5.12510 | 3.25910 | 0.99070 |
| H | 5.94510 | 5.58540 | 0.77290 |
| H | 5.95260 | 5.44690 | -0.98230 |
| H | 4.42700 | 5.39360 | -0.09840 |
| H | -2.80420 | -0.42490 | 4.95460 |
| H | 8.35770 | 1.79480 | 0.55240 |
| H | 6.88070 | 1.73390 | 1.51140 |
| H | 6.87160 | 1.19500 | -0.17670 |

| Marilzafurollene C_40 | | | |
|------------------------------|----------|----------|----------|
| C | 3.12920 | -0.93470 | -0.14720 |
| O | 2.07000 | -1.03180 | 0.80510 |
| C | 3.79880 | 0.44770 | -0.05190 |
| C | 2.47620 | -1.24410 | -1.49860 |
| C | 0.90200 | -1.59290 | 0.20610 |
| C | 4.98720 | 0.61170 | -1.01640 |
| Br | 4.45140 | 0.69720 | 1.81680 |
| C | 1.37800 | -2.21290 | -1.11360 |
| C | 0.17020 | -2.53420 | 1.18270 |
| C | 5.57160 | 2.01070 | -0.98250 |
| Cl | 2.07280 | -3.84680 | -0.89130 |
| C | -0.38920 | -1.80850 | 2.41890 |
| C | -1.27790 | -2.71940 | 3.24250 |
| O | 0.69160 | -1.37600 | 3.21640 |
| C | -2.54760 | -2.47580 | 3.47420 |
| C | 5.61260 | 2.84600 | -2.03390 |
| C | 6.19880 | 4.24510 | -1.99690 |
| C | 5.13570 | 5.29070 | -2.34310 |
| O | 7.24910 | 4.38690 | -2.94200 |
| C | -3.81760 | -2.22540 | 3.68770 |
| Br | -5.24410 | -2.86580 | 2.47340 |
| C | 8.44200 | 3.69600 | -2.59640 |
| H | 3.85450 | -1.71430 | 0.09180 |
| H | 3.05800 | 1.22750 | -0.23450 |
| H | 2.03540 | -0.34150 | -1.92400 |
| H | 3.17420 | -1.65500 | -2.22880 |
| H | 0.24470 | -0.75690 | -0.03940 |
| H | 5.77270 | -0.10270 | -0.76710 |
| H | 4.67550 | 0.38740 | -2.03700 |
| H | 0.58620 | -2.28320 | -1.86030 |
| H | -0.65520 | -3.00610 | 0.64740 |
| H | 0.82710 | -3.34450 | 1.50150 |
| H | 5.97790 | 2.33290 | -0.03370 |
| H | -0.95590 | -0.93080 | 2.09980 |
| H | -0.80830 | -3.60490 | 3.64540 |
| H | 1.38250 | -1.08020 | 2.62730 |
| H | 5.21150 | 2.53160 | -2.98680 |
| H | 6.57740 | 4.45880 | -0.99520 |
| H | 5.55420 | 6.29640 | -2.30220 |
| H | 4.74120 | 5.13640 | -3.34770 |
| H | 4.30070 | 5.25010 | -1.64320 |
| H | -4.20310 | -1.66050 | 4.52390 |
| H | 8.28500 | 2.61810 | -2.54270 |
| H | 9.20280 | 3.88230 | -3.35440 |
| H | 8.83420 | 4.03970 | -1.63840 |

| Marilzafurollene C_41 | | | |
|------------------------------|----------|----------|----------|
| C | 3.17430 | -1.84750 | -0.76670 |
| O | 2.39960 | -2.06540 | 0.41190 |
| C | 4.00660 | -0.55900 | -0.62380 |
| C | 2.18600 | -1.89540 | -1.94070 |
| C | 1.03040 | -2.25650 | 0.06590 |
| C | 3.18350 | 0.70020 | -0.29280 |
| Br | 5.04410 | -0.26420 | -2.30110 |
| C | 1.06200 | -2.74580 | -1.38580 |
| C | 0.32380 | -3.17530 | 1.08090 |
| C | 4.05700 | 1.90410 | -0.00170 |
| Cl | 1.49700 | -4.47730 | -1.50610 |
| C | 0.17330 | -2.53960 | 2.47520 |
| C | -0.79830 | -1.37370 | 2.47810 |
| O | -0.29810 | -3.52400 | 3.37210 |
| C | -0.45280 | -0.13770 | 2.75870 |
| C | 3.98900 | 3.06880 | -0.66710 |
| C | 4.86760 | 4.27240 | -0.38440 |
| C | 4.02190 | 5.48030 | 0.02610 |
| O | 5.60990 | 4.65030 | -1.53490 |
| C | -0.11850 | 1.10420 | 3.01770 |
| Br | 0.45250 | 2.36610 | 1.60320 |
| C | 6.62420 | 3.72560 | -1.90540 |
| H | 3.85450 | -2.69580 | -0.85810 |
| H | 4.73740 | -0.72180 | 0.16950 |
| H | 1.80530 | -0.90300 | -2.17830 |
| H | 2.62770 | -2.30370 | -2.85020 |
| H | 0.55560 | -1.27400 | 0.06930 |
| H | 2.49300 | 0.93930 | -1.10080 |
| H | 2.57520 | 0.51520 | 0.59280 |
| H | 0.11540 | -2.59760 | -1.90670 |
| H | -0.65940 | -3.45370 | 0.69920 |
| H | 0.88980 | -4.10310 | 1.16820 |
| H | 4.77310 | 1.79120 | 0.79940 |
| H | 1.15220 | -2.20440 | 2.82650 |
| H | -1.82360 | -1.61110 | 2.23470 |
| H | 0.40810 | -4.12710 | 3.55810 |
| H | 3.27370 | 3.18670 | -1.46820 |
| H | 5.55570 | 4.04010 | 0.43080 |
| H | 4.65470 | 6.33990 | 0.24700 |
| H | 3.33440 | 5.76950 | -0.76910 |
| H | 3.43230 | 5.26300 | 0.91720 |
| H | -0.12210 | 1.55230 | 4.00060 |
| H | 7.17270 | 4.11260 | -2.76410 |
| H | 7.33740 | 3.57420 | -1.09430 |
| H | 6.20820 | 2.75810 | -2.18900 |

| Marilzafurollene C_42 | | | |
|------------------------------|----------|----------|----------|
| C | 2.63480 | -0.55730 | -1.27560 |
| O | 2.22180 | -0.88720 | 0.05030 |
| C | 1.85120 | 0.66430 | -1.79990 |
| C | 2.46810 | -1.83760 | -2.10600 |
| C | 1.77290 | -2.23730 | 0.09570 |
| C | 2.13970 | 1.95310 | -1.01170 |
| Br | -0.10930 | 0.30600 | -1.68490 |
| C | 2.51950 | -2.92490 | -1.05140 |
| C | 1.94910 | -2.84830 | 1.50000 |
| C | 3.57170 | 2.42890 | -1.16050 |
| Cl | 4.22390 | -3.27850 | -0.63790 |
| C | 1.13780 | -2.12130 | 2.58810 |
| C | -0.35720 | -2.17280 | 2.33280 |
| O | 1.41530 | -2.73020 | 3.83260 |
| C | -1.08280 | -1.10360 | 2.09530 |
| C | 4.44580 | 2.53510 | -0.14470 |
| C | 5.88700 | 3.00110 | -0.26800 |
| C | 6.05700 | 4.40270 | 0.32310 |
| O | 6.32500 | 3.05350 | -1.62060 |
| C | -1.78450 | -0.02480 | 1.84070 |
| Br | -2.66110 | 1.03260 | 3.26640 |
| C | 6.72200 | 1.79420 | -2.14770 |
| H | 3.69930 | -0.32340 | -1.22980 |
| H | 2.08210 | 0.82520 | -2.85380 |
| H | 1.49540 | -1.85840 | -2.59810 |
| H | 3.23060 | -1.94900 | -2.87720 |
| H | 0.71330 | -2.23400 | -0.16410 |
| H | 1.48620 | 2.75170 | -1.36370 |
| H | 1.90310 | 1.80150 | 0.04250 |
| H | 2.04730 | -3.85470 | -1.37020 |
| H | 1.66760 | -3.90150 | 1.47340 |
| H | 3.00280 | -2.82130 | 1.77840 |
| H | 3.88560 | 2.69590 | -2.15970 |
| H | 1.47100 | -1.08160 | 2.63630 |
| H | -0.81260 | -3.15240 | 2.34940 |
| H | 1.09560 | -2.16430 | 4.52140 |
| H | 4.12620 | 2.27300 | 0.85410 |
| H | 6.51830 | 2.31280 | 0.29730 |
| H | 7.09570 | 4.72700 | 0.25910 |
| H | 5.44790 | 5.13130 | -0.21260 |
| H | 5.76520 | 4.42760 | 1.37320 |
| H | -1.94980 | 0.38390 | 0.85400 |
| H | 5.91480 | 1.06210 | -2.10550 |
| H | 7.01300 | 1.91090 | -3.19160 |
| H | 7.57990 | 1.39490 | -1.60530 |

| Marilzafurollene C_43 | | | |
|------------------------------|----------|----------|----------|
| C | 3.59340 | -1.73920 | -1.69670 |
| O | 3.06760 | -1.45850 | -0.40020 |
| C | 5.05260 | -1.25230 | -1.84130 |
| C | 2.57360 | -1.17620 | -2.69350 |
| C | 1.74030 | -0.93960 | -0.51080 |
| C | 5.29280 | 0.27230 | -1.83260 |
| Br | 5.78580 | -1.97600 | -3.54570 |
| C | 1.27450 | -1.30850 | -1.92490 |
| C | 0.85150 | -1.41600 | 0.65380 |
| C | 4.79610 | 0.95660 | -0.57440 |
| Cl | 0.67850 | -2.99250 | -2.02650 |
| C | 1.30760 | -0.87240 | 2.01900 |
| C | 0.31740 | -1.21580 | 3.11380 |
| O | 2.55760 | -1.44880 | 2.32990 |
| C | -0.32250 | -0.31280 | 3.82110 |
| C | 3.94860 | 2.00160 | -0.56660 |
| C | 3.39190 | 2.71180 | 0.66180 |
| C | 3.98410 | 2.22230 | 1.99070 |
| O | 1.98460 | 2.53400 | 0.75860 |
| C | -0.97170 | 0.59280 | 4.51360 |
| Br | -2.72650 | 1.30930 | 3.94240 |
| C | 1.22350 | 3.30100 | -0.16410 |
| H | 3.59070 | -2.82680 | -1.78550 |
| H | 5.64150 | -1.70790 | -1.04390 |
| H | 2.76100 | -0.12290 | -2.89710 |
| H | 2.57080 | -1.70660 | -3.64620 |
| H | 1.81760 | 0.14690 | -0.46750 |
| H | 6.36380 | 0.46160 | -1.91040 |
| H | 4.84420 | 0.73540 | -2.71130 |
| H | 0.48860 | -0.65060 | -2.29720 |
| H | -0.16900 | -1.07940 | 0.46520 |
| H | 0.81160 | -2.50550 | 0.68570 |
| H | 5.16110 | 0.54240 | 0.35380 |
| H | 1.42840 | 0.21130 | 1.95670 |
| H | 0.15600 | -2.26810 | 3.29600 |
| H | 3.04190 | -1.50960 | 1.51000 |
| H | 3.61190 | 2.39300 | -1.51500 |
| H | 3.62220 | 3.77450 | 0.56740 |
| H | 3.56770 | 2.78490 | 2.82630 |
| H | 3.76130 | 1.16950 | 2.16590 |
| H | 5.06620 | 2.35170 | 2.01670 |
| H | -0.62420 | 1.02740 | 5.43940 |
| H | 1.42410 | 3.01400 | -1.19620 |
| H | 0.16180 | 3.13820 | 0.02160 |
| H | 1.42090 | 4.36770 | -0.05110 |

| Marilzafurollene C_44 | | | |
|------------------------------|----------|----------|----------|
| C | 3.25410 | -1.49530 | -0.65400 |
| O | 2.37830 | -1.43800 | 0.47160 |
| C | 4.24350 | -0.31460 | -0.63120 |
| C | 2.34730 | -1.60580 | -1.88620 |
| C | 1.03050 | -1.66890 | 0.05680 |
| C | 3.58710 | 1.07950 | -0.62020 |
| Br | 5.46310 | -0.46470 | -2.20150 |
| C | 1.13640 | -2.32320 | -1.32710 |
| C | 0.24060 | -2.45170 | 1.12440 |
| C | 4.59880 | 2.18930 | -0.41190 |
| Cl | 1.46900 | -4.07850 | -1.22540 |
| C | 0.05510 | -1.67040 | 2.43690 |
| C | -0.87870 | -2.39330 | 3.38750 |
| O | 1.31640 | -1.52270 | 3.05150 |
| C | -2.00830 | -1.88190 | 3.82080 |
| C | 4.81300 | 3.19450 | -1.27700 |
| C | 5.83540 | 4.29750 | -1.07730 |
| C | 5.15700 | 5.66880 | -1.02750 |
| O | 6.77100 | 4.33150 | -2.14530 |
| C | -3.14000 | -1.36410 | 4.23590 |
| Br | -4.84410 | -1.61930 | 3.26120 |
| C | 7.66100 | 3.22330 | -2.17840 |
| H | 3.81990 | -2.42400 | -0.56320 |
| H | 4.86830 | -0.42090 | 0.25680 |
| H | 2.04860 | -0.62370 | -2.24950 |
| H | 2.81890 | -2.13550 | -2.71460 |
| H | 0.57020 | -0.68810 | -0.07580 |
| H | 3.04130 | 1.25690 | -1.54640 |
| H | 2.85900 | 1.13900 | 0.18960 |
| H | 0.24010 | -2.18560 | -1.93310 |
| H | -0.74250 | -2.69010 | 0.71540 |
| H | 0.72110 | -3.40850 | 1.33290 |
| H | 5.17550 | 2.14340 | 0.50090 |
| H | -0.34020 | -0.67640 | 2.21530 |
| H | -0.56660 | -3.37740 | 3.70520 |
| H | 1.95670 | -1.40850 | 2.35370 |
| H | 4.24040 | 3.24540 | -2.19200 |
| H | 6.36530 | 4.14040 | -0.13570 |
| H | 4.43270 | 5.72080 | -0.21430 |
| H | 5.89150 | 6.45870 | -0.86910 |
| H | 4.63350 | 5.88480 | -1.95910 |
| H | -3.25390 | -0.76300 | 5.12630 |
| H | 7.13320 | 2.28320 | -2.34310 |
| H | 8.36990 | 3.35070 | -2.99630 |
| H | 8.23090 | 3.14550 | -1.25170 |

| Marilzafurollene C_45 | | | |
|------------------------------|----------|----------|----------|
| C | 2.65410 | -0.61020 | -0.60260 |
| O | 2.63040 | -0.66130 | 0.82350 |
| C | 3.07830 | 0.78690 | -1.09320 |
| C | 1.26680 | -1.06670 | -1.06730 |
| C | 1.35990 | -1.11520 | 1.28250 |
| C | 4.52510 | 1.12380 | -0.69570 |
| Br | 1.85290 | 2.17190 | -0.33650 |
| C | 0.79680 | -1.91350 | 0.09650 |
| C | 1.50930 | -1.83330 | 2.64190 |
| C | 4.99940 | 2.43750 | -1.28660 |
| Cl | 1.51670 | -3.54730 | -0.02810 |
| C | 0.18820 | -2.10300 | 3.39160 |
| C | -0.63870 | -3.20210 | 2.75330 |
| O | 0.50800 | -2.48750 | 4.71270 |
| C | -1.87420 | -3.03290 | 2.34060 |
| C | 6.03040 | 2.56260 | -2.13880 |
| C | 6.50330 | 3.87900 | -2.72690 |
| C | 6.40170 | 3.86140 | -4.25420 |
| O | 7.86260 | 4.12920 | -2.40050 |
| C | -3.09070 | -2.84420 | 1.88790 |
| Br | -3.43760 | -2.22750 | 0.03980 |
| C | 8.08330 | 4.45970 | -1.03590 |
| H | 3.38500 | -1.34830 | -0.93680 |
| H | 2.98370 | 0.83020 | -2.17930 |
| H | 0.59510 | -0.21660 | -1.18780 |
| H | 1.28840 | -1.60780 | -2.01370 |
| H | 0.74550 | -0.22370 | 1.42150 |
| H | 4.60980 | 1.17520 | 0.39060 |
| H | 5.19220 | 0.32420 | -1.02040 |
| H | -0.28740 | -2.01870 | 0.12000 |
| H | 2.08700 | -2.75160 | 2.53660 |
| H | 2.12070 | -1.18530 | 3.27130 |
| H | 4.45240 | 3.31890 | -0.98230 |
| H | -0.38940 | -1.17730 | 3.44470 |
| H | -0.15120 | -4.16080 | 2.64310 |
| H | -0.28270 | -2.48390 | 5.23350 |
| H | 6.58370 | 1.68640 | -2.44490 |
| H | 5.88170 | 4.69400 | -2.35060 |
| H | 6.72790 | 4.81270 | -4.67500 |
| H | 7.02640 | 3.07750 | -4.68320 |
| H | 5.37510 | 3.68950 | -4.57870 |
| H | -3.99640 | -2.99850 | 2.45640 |
| H | 9.14170 | 4.66750 | -0.87870 |
| H | 7.52220 | 5.35000 | -0.74920 |
| H | 7.80420 | 3.64200 | -0.37050 |

| Marilzafurollene C_46 | | | |
|------------------------------|----------|----------|----------|
| C | 2.86230 | -1.82290 | -1.85700 |
| O | 2.56590 | -1.64530 | -0.47210 |
| C | 2.74690 | -0.49870 | -2.64090 |
| C | 1.92300 | -2.93290 | -2.34840 |
| C | 1.51790 | -2.52490 | -0.08030 |
| C | 3.87640 | 0.51260 | -2.35700 |
| Br | 0.97060 | 0.35690 | -2.31590 |
| C | 1.60420 | -3.68690 | -1.07380 |
| C | 1.61120 | -2.88780 | 1.41480 |
| C | 3.80540 | 1.15490 | -0.98350 |
| Cl | 2.94280 | -4.81070 | -0.69140 |
| C | 1.46430 | -1.67300 | 2.34860 |
| C | 0.11910 | -0.98760 | 2.20030 |
| O | 1.61310 | -2.11590 | 3.68190 |
| C | -0.01470 | 0.25270 | 1.78940 |
| C | 3.86600 | 2.47860 | -0.76280 |
| C | 3.77970 | 3.12740 | 0.60520 |
| C | 2.69390 | 4.20550 | 0.62400 |
| O | 5.00150 | 3.76180 | 0.95350 |
| C | -0.12820 | 1.49170 | 1.37470 |
| Br | -0.15020 | 3.02470 | 2.62660 |
| C | 6.05800 | 2.86220 | 1.25970 |
| H | 3.88670 | -2.19320 | -1.92150 |
| H | 2.78300 | -0.73560 | -3.70540 |
| H | 1.00450 | -2.50830 | -2.75510 |
| H | 2.36860 | -3.56040 | -3.12070 |
| H | 0.57620 | -2.00710 | -0.26890 |
| H | 4.84510 | 0.02270 | -2.46070 |
| H | 3.84920 | 1.29950 | -3.11160 |
| H | 0.68160 | -4.26490 | -1.13550 |
| H | 0.84800 | -3.62920 | 1.65400 |
| H | 2.57140 | -3.36420 | 1.61420 |
| H | 3.70390 | 0.48450 | -0.14260 |
| H | 2.26860 | -0.96520 | 2.13300 |
| H | -0.75000 | -1.58040 | 2.44640 |
| H | 1.71410 | -1.35890 | 4.24170 |
| H | 3.98100 | 3.15530 | -1.59710 |
| H | 3.53080 | 2.37250 | 1.35410 |
| H | 2.59460 | 4.63920 | 1.61920 |
| H | 2.92700 | 5.01380 | -0.06930 |
| H | 1.72510 | 3.79310 | 0.34280 |
| H | -0.21940 | 1.79050 | 0.34000 |
| H | 6.32730 | 2.24610 | 0.40120 |
| H | 6.94320 | 3.42710 | 1.55190 |
| H | 5.79120 | 2.20690 | 2.08980 |

| Marilzafurollene C_47 | | | |
|------------------------------|----------|----------|----------|
| C | 3.16910 | -1.82410 | -0.78770 |
| O | 2.39230 | -2.03630 | 0.39010 |
| C | 4.00940 | -0.54090 | -0.64860 |
| C | 2.18080 | -1.87160 | -1.96070 |
| C | 1.03330 | -2.28980 | 0.04070 |
| C | 3.19470 | 0.72850 | -0.33640 |
| Br | 5.06360 | -0.26960 | -2.31950 |
| C | 1.08070 | -2.75990 | -1.41770 |
| C | 0.36360 | -3.24760 | 1.04570 |
| C | 4.07870 | 1.92450 | -0.04310 |
| Cl | 1.56270 | -4.47710 | -1.56290 |
| C | 0.19500 | -2.64110 | 2.45060 |
| C | -0.79950 | -1.49490 | 2.46700 |
| O | -0.26540 | -3.65690 | 3.31800 |
| C | -0.47950 | -0.25720 | 2.76950 |
| C | 4.05020 | 3.07700 | -0.73250 |
| C | 4.94210 | 4.27070 | -0.44840 |
| C | 4.10740 | 5.50160 | -0.08680 |
| O | 5.72360 | 4.61220 | -1.58420 |
| C | -0.16720 | 0.98790 | 3.04060 |
| Br | 0.38860 | 2.26900 | 1.63780 |
| C | 6.73230 | 3.66360 | -1.90610 |
| H | 3.84480 | -2.67630 | -0.87660 |
| H | 4.73210 | -0.70310 | 0.15230 |
| H | 1.77480 | -0.88450 | -2.17700 |
| H | 2.62960 | -2.25210 | -2.87880 |
| H | 0.51670 | -1.32870 | 0.05360 |
| H | 2.51830 | 0.96900 | -1.15580 |
| H | 2.57250 | 0.55550 | 0.54190 |
| H | 0.13060 | -2.63120 | -1.93730 |
| H | -0.60930 | -3.55800 | 0.66290 |
| H | 0.96270 | -4.15550 | 1.12350 |
| H | 4.77000 | 1.81540 | 0.78000 |
| H | 1.17000 | -2.30200 | 2.80890 |
| H | -1.81820 | -1.74690 | 2.20910 |
| H | -0.11330 | -3.38470 | 4.21200 |
| H | 3.36030 | 3.19090 | -1.55630 |
| H | 5.60230 | 4.04300 | 0.39080 |
| H | 4.74950 | 6.35420 | 0.13480 |
| H | 3.44820 | 5.78670 | -0.90710 |
| H | 3.48900 | 5.31350 | 0.79140 |
| H | -0.18290 | 1.42930 | 4.02650 |
| H | 7.31140 | 4.02330 | -2.75640 |
| H | 7.41950 | 3.51800 | -1.07170 |
| H | 6.30820 | 2.69730 | -2.18130 |

| Marilzafurollene C_48 | | | |
|------------------------------|----------|----------|----------|
| C | 2.83930 | -1.67070 | -1.10430 |
| O | 2.19210 | -1.90090 | 0.14700 |
| C | 2.93590 | -0.15940 | -1.39790 |
| C | 2.06270 | -2.48750 | -2.15010 |
| C | 0.97570 | -2.60380 | -0.06530 |
| C | 3.72820 | 0.58780 | -0.31150 |
| Br | 1.10830 | 0.63790 | -1.53900 |
| C | 1.26600 | -3.46090 | -1.30310 |
| C | 0.51990 | -3.35730 | 1.19970 |
| C | 3.92310 | 2.05590 | -0.63580 |
| Cl | 2.28780 | -4.87960 | -0.92170 |
| C | 0.34650 | -2.45930 | 2.43950 |
| C | -0.62490 | -1.31260 | 2.22700 |
| O | -0.11530 | -3.26200 | 3.50750 |
| C | -0.33510 | -0.06470 | 2.52030 |
| C | 5.11560 | 2.64790 | -0.81350 |
| C | 5.30200 | 4.11940 | -1.13250 |
| C | 6.03310 | 4.30040 | -2.46510 |
| O | 6.07910 | 4.76690 | -0.13560 |
| C | -0.04380 | 1.16500 | 2.87430 |
| Br | 0.83250 | 2.46300 | 1.66360 |
| C | 5.40650 | 4.93960 | 1.10460 |
| H | 3.84530 | -2.08390 | -1.01690 |
| H | 3.42180 | -0.01290 | -2.36370 |
| H | 1.37540 | -1.85710 | -2.71340 |
| H | 2.71360 | -2.98180 | -2.87170 |
| H | 0.21340 | -1.87130 | -0.33440 |
| H | 3.20930 | 0.51130 | 0.64500 |
| H | 4.70200 | 0.11620 | -0.17440 |
| H | 0.36130 | -3.81690 | -1.79680 |
| H | -0.41780 | -3.87070 | 0.98340 |
| H | 1.24260 | -4.13530 | 1.44360 |
| H | 3.02030 | 2.64510 | -0.71920 |
| H | 1.32110 | -2.05270 | 2.72080 |
| H | -1.58880 | -1.56990 | 1.81390 |
| H | 0.60780 | -3.78180 | 3.82940 |
| H | 6.02240 | 2.06680 | -0.72700 |
| H | 4.32690 | 4.60510 | -1.20700 |
| H | 6.15300 | 5.35810 | -2.70020 |
| H | 7.02660 | 3.85260 | -2.43520 |
| H | 5.47980 | 3.83900 | -3.28340 |
| H | -0.24770 | 1.58480 | 3.84830 |
| H | 6.05630 | 5.47070 | 1.80000 |
| H | 4.49650 | 5.52840 | 0.98210 |
| H | 5.14420 | 3.98420 | 1.56050 |

| Marilzafurollene C_49 | | | |
|------------------------------|----------|----------|----------|
| C | 3.13200 | -1.20910 | -1.43660 |
| O | 1.78110 | -0.82330 | -1.17240 |
| C | 3.67030 | -0.42760 | -2.65220 |
| C | 3.10990 | -2.73530 | -1.61040 |
| C | 1.03420 | -1.94660 | -0.71410 |
| C | 3.68260 | 1.09670 | -2.44160 |
| Br | 2.54060 | -0.81960 | -4.24880 |
| C | 1.63030 | -3.06730 | -1.56840 |
| C | 1.21100 | -2.10180 | 0.81620 |
| C | 4.58130 | 1.52830 | -1.29870 |
| Cl | 1.30960 | -4.71040 | -0.94750 |
| C | 0.68670 | -0.89750 | 1.61890 |
| C | 0.68940 | -1.17730 | 3.10900 |
| O | 1.51800 | 0.21180 | 1.35730 |
| C | -0.40000 | -1.21510 | 3.84220 |
| C | 4.14540 | 2.14030 | -0.18490 |
| C | 5.03160 | 2.56420 | 0.97080 |
| C | 4.58820 | 1.88560 | 2.26920 |
| O | 4.96590 | 3.96690 | 1.18490 |
| C | -1.48930 | -1.26920 | 4.57190 |
| Br | -2.24560 | 0.31980 | 5.47890 |
| C | 5.60070 | 4.74280 | 0.17790 |
| H | 3.73090 | -0.97680 | -0.55460 |
| H | 4.67900 | -0.76880 | -2.88980 |
| H | 3.58170 | -3.07920 | -2.53130 |
| H | 3.63090 | -3.20760 | -0.77680 |
| H | -0.02280 | -1.80880 | -0.94490 |
| H | 4.02880 | 1.59080 | -3.34980 |
| H | 2.66610 | 1.45220 | -2.26650 |
| H | 1.21510 | -3.00900 | -2.57600 |
| H | 0.65990 | -2.98700 | 1.13610 |
| H | 2.25330 | -2.29410 | 1.07280 |
| H | 5.63470 | 1.31470 | -1.41070 |
| H | -0.32670 | -0.65580 | 1.29040 |
| H | 1.65670 | -1.34610 | 3.55900 |
| H | 1.66910 | 0.22690 | 0.41580 |
| H | 3.09280 | 2.35750 | -0.06830 |
| H | 6.06450 | 2.27540 | 0.76660 |
| H | 5.23020 | 2.17590 | 3.10060 |
| H | 3.56420 | 2.15860 | 2.52730 |
| H | 4.62690 | 0.79970 | 2.17950 |
| H | -2.06980 | -2.16290 | 4.74790 |
| H | 5.12570 | 4.61100 | -0.79480 |
| H | 5.53470 | 5.79930 | 0.43760 |
| H | 6.65710 | 4.48640 | 0.08860 |

| Marilzafurollene C_50 | | | |
|------------------------------|----------|----------|----------|
| C | 3.18690 | -1.51850 | -1.02500 |
| O | 2.36450 | -1.39490 | 0.13600 |
| C | 3.71270 | -0.14000 | -1.46600 |
| C | 2.34050 | -2.25400 | -2.07250 |
| C | 1.09050 | -1.98940 | -0.10450 |
| C | 4.65820 | 0.47960 | -0.42300 |
| Br | 2.17650 | 1.10120 | -1.76650 |
| C | 1.34460 | -3.01120 | -1.21820 |
| C | 0.47330 | -2.53380 | 1.19820 |
| C | 5.29620 | 1.76690 | -0.90740 |
| Cl | 2.10320 | -4.50890 | -0.60010 |
| C | 0.14280 | -1.42790 | 2.21580 |
| C | -0.62530 | -1.97460 | 3.40280 |
| O | 1.35300 | -0.86200 | 2.66940 |
| C | -1.83300 | -1.57470 | 3.72970 |
| C | 5.13740 | 2.96440 | -0.31760 |
| C | 5.76540 | 4.26670 | -0.78600 |
| C | 4.71010 | 5.18020 | -1.41410 |
| O | 6.78190 | 4.05970 | -1.75970 |
| C | -3.04400 | -1.17470 | 4.03750 |
| Br | -4.66610 | -2.04270 | 3.30640 |
| C | 8.03880 | 3.68330 | -1.21230 |
| H | 4.02850 | -2.15910 | -0.75600 |
| H | 4.23640 | -0.24150 | -2.41780 |
| H | 1.80610 | -1.54750 | -2.70800 |
| H | 2.93100 | -2.90080 | -2.72200 |
| H | 0.44110 | -1.20910 | -0.50630 |
| H | 4.11760 | 0.65720 | 0.50780 |
| H | 5.46050 | -0.22010 | -0.18700 |
| H | 0.43870 | -3.28750 | -1.75890 |
| H | -0.44470 | -3.06650 | 0.94560 |
| H | 1.13380 | -3.26970 | 1.65840 |
| H | 5.91300 | 1.69110 | -1.79160 |
| H | -0.44150 | -0.64580 | 1.72540 |
| H | -0.12190 | -2.72980 | 3.98850 |
| H | 1.93520 | -0.81140 | 1.91450 |
| H | 4.51140 | 3.03990 | 0.56020 |
| H | 6.18590 | 4.77650 | 0.08290 |
| H | 5.15240 | 6.12500 | -1.73040 |
| H | 4.25960 | 4.71340 | -2.29050 |
| H | 3.91140 | 5.40650 | -0.70740 |
| H | -3.27260 | -0.35450 | 4.70220 |
| H | 8.75230 | 3.51560 | -2.01890 |
| H | 8.43890 | 4.47040 | -0.57200 |
| H | 7.97090 | 2.76400 | -0.62980 |

| Marilzafurollene C_51 | | | |
|------------------------------|----------|----------|----------|
| C | 2.81520 | -0.55230 | -1.19740 |
| O | 1.98150 | -0.56540 | -0.03770 |
| C | 2.56790 | 0.72240 | -2.03030 |
| C | 2.54030 | -1.86930 | -1.93530 |
| C | 1.23650 | -1.78080 | 0.01350 |
| C | 2.95040 | 2.02390 | -1.30350 |
| Br | 0.63280 | 0.84040 | -2.50410 |
| C | 2.05270 | -2.77330 | -0.82190 |
| C | 0.93780 | -2.19250 | 1.46810 |
| C | 4.44010 | 2.14950 | -1.04610 |
| Cl | 3.45500 | -3.42260 | 0.07970 |
| C | 0.01600 | -1.20010 | 2.19810 |
| C | -0.40470 | -1.72620 | 3.55610 |
| O | 0.71350 | 0.01430 | 2.36900 |
| C | -1.65520 | -1.94930 | 3.89010 |
| C | 5.23390 | 3.08440 | -1.59700 |
| C | 6.72730 | 3.22900 | -1.35080 |
| C | 7.52290 | 2.84080 | -2.59960 |
| O | 7.18450 | 2.40440 | -0.28560 |
| C | -2.90780 | -2.17840 | 4.20590 |
| Br | -3.78000 | -3.92660 | 3.88650 |
| C | 6.96370 | 2.95290 | 1.00750 |
| H | 3.84870 | -0.57750 | -0.85060 |
| H | 3.12070 | 0.66170 | -2.96910 |
| H | 1.74730 | -1.74670 | -2.67310 |
| H | 3.41640 | -2.25880 | -2.45440 |
| H | 0.29310 | -1.60160 | -0.50590 |
| H | 2.62260 | 2.87620 | -1.89970 |
| H | 2.42100 | 2.09260 | -0.35240 |
| H | 1.46120 | -3.61580 | -1.18190 |
| H | 0.46000 | -3.17330 | 1.45470 |
| H | 1.86390 | -2.31430 | 2.03120 |
| H | 4.87030 | 1.42640 | -0.36770 |
| H | -0.86810 | -1.00750 | 1.58580 |
| H | 0.39190 | -1.91480 | 4.26100 |
| H | 1.21890 | 0.15820 | 1.57200 |
| H | 4.80590 | 3.80620 | -2.27800 |
| H | 6.93740 | 4.27610 | -1.12380 |
| H | 7.24380 | 3.45660 | -3.45480 |
| H | 8.59250 | 2.96940 | -2.43300 |
| H | 7.35150 | 1.79750 | -2.86580 |
| H | -3.57160 | -1.45700 | 4.65960 |
| H | 5.90740 | 3.15070 | 1.19230 |
| H | 7.30930 | 2.25020 | 1.76550 |
| H | 7.51800 | 3.88310 | 1.13820 |

| Marilzafurollene C_52 | | | |
|------------------------------|----------|----------|----------|
| C | 3.17180 | -1.08680 | -1.24670 |
| O | 1.78160 | -0.79180 | -1.09310 |
| C | 3.70300 | -0.43410 | -2.53880 |
| C | 3.28700 | -2.61790 | -1.20100 |
| C | 1.11100 | -1.90030 | -0.50080 |
| C | 3.56960 | 1.09880 | -2.54480 |
| Br | 2.69590 | -1.14700 | -4.10600 |
| C | 1.84050 | -3.07360 | -1.15840 |
| C | 1.22550 | -1.81430 | 1.04080 |
| C | 4.36740 | 1.76420 | -1.44020 |
| Cl | 1.63350 | -4.63110 | -0.31040 |
| C | 0.56920 | -0.55410 | 1.63370 |
| C | 0.52460 | -0.60780 | 3.14790 |
| O | 1.31760 | 0.57340 | 1.23410 |
| C | -0.59110 | -0.57940 | 3.84040 |
| C | 3.82310 | 2.45120 | -0.42080 |
| C | 4.59360 | 3.11590 | 0.70730 |
| C | 4.55530 | 4.63950 | 0.56680 |
| O | 5.96150 | 2.72500 | 0.73170 |
| C | -1.71380 | -0.56120 | 4.51890 |
| Br | -2.69240 | -2.21450 | 4.99630 |
| C | 6.19240 | 1.47680 | 1.37160 |
| H | 3.70290 | -0.68140 | -0.38410 |
| H | 4.74900 | -0.70740 | -2.68560 |
| H | 3.82600 | -3.04290 | -2.04810 |
| H | 3.80950 | -2.92000 | -0.29260 |
| H | 0.05850 | -1.89370 | -0.78700 |
| H | 3.91670 | 1.49580 | -3.49910 |
| H | 2.51820 | 1.37720 | -2.46000 |
| H | 1.46900 | -3.20080 | -2.17660 |
| H | 0.73120 | -2.68690 | 1.47000 |
| H | 2.26610 | -1.87740 | 1.36040 |
| H | 5.44200 | 1.66320 | -1.49810 |
| H | -0.44410 | -0.45410 | 1.23780 |
| H | 1.47850 | -0.67100 | 3.65080 |
| H | 1.51630 | 0.45230 | 0.30870 |
| H | 2.74840 | 2.55610 | -0.36690 |
| H | 4.11460 | 2.84720 | 1.65120 |
| H | 5.08540 | 5.11810 | 1.39040 |
| H | 5.02610 | 4.96030 | -0.36280 |
| H | 3.53040 | 5.01120 | 0.57100 |
| H | -2.20450 | 0.33240 | 4.87610 |
| H | 7.25300 | 1.23110 | 1.32090 |
| H | 5.63790 | 0.66720 | 0.89610 |
| H | 5.90940 | 1.51810 | 2.42420 |

| Marilzafurollene C_53 | | | |
|------------------------------|----------|----------|----------|
| C | 3.21590 | -1.59080 | -0.43800 |
| O | 1.95360 | -1.13700 | 0.05540 |
| C | 4.03440 | -0.39390 | -0.95810 |
| C | 2.90110 | -2.65720 | -1.49800 |
| C | 0.92730 | -2.06420 | -0.28330 |
| C | 4.37260 | 0.60980 | 0.15750 |
| Br | 3.01650 | 0.54510 | -2.39710 |
| C | 1.39720 | -2.55090 | -1.65570 |
| C | 0.82560 | -3.14950 | 0.81540 |
| C | 5.27980 | 1.72710 | -0.32010 |
| Cl | 0.64940 | -4.08200 | -2.18970 |
| C | 0.47270 | -2.58980 | 2.20550 |
| C | -0.90440 | -1.95390 | 2.24180 |
| O | 0.51410 | -3.65450 | 3.13320 |
| C | -1.10880 | -0.69080 | 2.53940 |
| C | 4.96530 | 3.03230 | -0.27290 |
| C | 5.86480 | 4.15220 | -0.76150 |
| C | 6.21840 | 5.10670 | 0.38170 |
| O | 5.22690 | 4.92370 | -1.76910 |
| C | -1.29390 | 0.57190 | 2.84350 |
| Br | -1.58670 | 1.18350 | 4.70310 |
| C | 5.04720 | 4.24050 | -3.00280 |
| H | 3.75410 | -2.06670 | 0.38340 |
| H | 4.95820 | -0.76090 | -1.40750 |
| H | 3.42640 | -2.50740 | -2.44160 |
| H | 3.17420 | -3.64310 | -1.12020 |
| H | -0.02630 | -1.54400 | -0.37640 |
| H | 3.45320 | 1.02750 | 0.57060 |
| H | 4.87580 | 0.09660 | 0.97750 |
| H | 1.16100 | -1.79290 | -2.40400 |
| H | 0.07480 | -3.88750 | 0.53110 |
| H | 1.76690 | -3.69510 | 0.88260 |
| H | 6.23630 | 1.42660 | -0.72290 |
| H | 1.23010 | -1.85860 | 2.49770 |
| H | -1.73570 | -2.60140 | 2.00220 |
| H | 0.45420 | -3.29480 | 4.00730 |
| H | 4.00930 | 3.33780 | 0.12750 |
| H | 6.79080 | 3.73170 | -1.15870 |
| H | 6.87700 | 5.90210 | 0.03250 |
| H | 5.32510 | 5.57400 | 0.79670 |
| H | 6.72990 | 4.58210 | 1.18900 |
| H | -1.30500 | 1.38350 | 2.13050 |
| H | 6.00020 | 3.89970 | -3.40910 |
| H | 4.38510 | 3.38030 | -2.89770 |
| H | 4.59670 | 4.91590 | -3.73000 |

| Marilzafurollene C_54 | | | |
|------------------------------|----------|----------|----------|
| C | 2.91050 | -1.47990 | -1.13510 |
| O | 2.25350 | -1.78540 | 0.09470 |
| C | 3.15560 | 0.03640 | -1.25590 |
| C | 2.04350 | -2.08750 | -2.24690 |
| C | 1.02800 | -2.46020 | -0.16730 |
| C | 4.13830 | 0.54900 | -0.18960 |
| Br | 1.42540 | 1.02100 | -1.07940 |
| C | 1.26200 | -3.15750 | -1.51100 |
| C | 0.61560 | -3.36020 | 1.01400 |
| C | 4.48710 | 2.01260 | -0.37680 |
| Cl | 2.26940 | -4.62680 | -1.34500 |
| C | 0.35450 | -2.57820 | 2.31490 |
| C | -0.79580 | -1.59620 | 2.18910 |
| O | 0.06220 | -3.50050 | 3.34490 |
| C | -0.64150 | -0.29330 | 2.25990 |
| C | 5.72030 | 2.47730 | -0.64340 |
| C | 6.08800 | 3.93980 | -0.83750 |
| C | 6.91290 | 4.45290 | 0.34540 |
| O | 4.94470 | 4.77880 | -0.95110 |
| C | -0.46260 | 1.00550 | 2.30930 |
| Br | -0.55830 | 2.03070 | 4.00030 |
| C | 4.35550 | 4.78590 | -2.24510 |
| H | 3.86830 | -2.00260 | -1.12470 |
| H | 3.55390 | 0.25850 | -2.24710 |
| H | 1.35080 | -1.34770 | -2.64860 |
| H | 2.62850 | -2.47780 | -3.08010 |
| H | 0.26310 | -1.69830 | -0.32440 |
| H | 3.71220 | 0.41410 | 0.80550 |
| H | 5.05370 | -0.04330 | -0.21710 |
| H | 0.33550 | -3.43520 | -2.01470 |
| H | -0.27600 | -3.92610 | 0.74130 |
| H | 1.39970 | -4.09490 | 1.19720 |
| H | 3.66740 | 2.71100 | -0.28010 |
| H | 1.26200 | -2.03710 | 2.59370 |
| H | -1.77480 | -2.02500 | 2.03390 |
| H | 0.87440 | -3.88060 | 3.64900 |
| H | 6.54050 | 1.77920 | -0.73110 |
| H | 6.69640 | 4.02300 | -1.74000 |
| H | 7.20000 | 5.49380 | 0.19540 |
| H | 6.34450 | 4.39590 | 1.27410 |
| H | 7.82630 | 3.87160 | 0.47380 |
| H | -0.25060 | 1.63030 | 1.45360 |
| H | 4.04070 | 3.78930 | -2.55600 |
| H | 3.47420 | 5.42720 | -2.24040 |
| H | 5.04920 | 5.17830 | -2.98970 |

| Marilzafurollene C_55 | | | |
|------------------------------|----------|----------|----------|
| C | 3.07290 | -1.15900 | -0.81580 |
| O | 2.19380 | -1.16960 | 0.30980 |
| C | 3.41690 | 0.28610 | -1.22140 |
| C | 2.38290 | -1.99020 | -1.90540 |
| C | 1.03130 | -1.94100 | 0.01220 |
| C | 4.22700 | 1.01580 | -0.13660 |
| Br | 1.73450 | 1.30360 | -1.57610 |
| C | 1.47460 | -2.89700 | -1.10080 |
| C | 0.45090 | -2.59100 | 1.28310 |
| C | 4.70470 | 2.38180 | -0.59050 |
| Cl | 2.41750 | -4.27960 | -0.46810 |
| C | -0.07740 | -1.56250 | 2.29830 |
| C | -0.80440 | -2.23520 | 3.44570 |
| O | 1.01850 | -0.83530 | 2.80860 |
| C | -2.06940 | -2.02000 | 3.72650 |
| C | 5.99810 | 2.74100 | -0.68600 |
| C | 6.53630 | 4.09610 | -1.13360 |
| C | 5.45090 | 5.15690 | -1.36540 |
| O | 7.25750 | 3.98780 | -2.35360 |
| C | -3.33680 | -1.80460 | 3.98810 |
| Br | -4.78560 | -2.88490 | 3.18000 |
| C | 8.53230 | 3.37000 | -2.24100 |
| H | 3.98430 | -1.67930 | -0.51680 |
| H | 3.98980 | 0.27350 | -2.15030 |
| H | 1.77710 | -1.35710 | -2.55410 |
| H | 3.08540 | -2.53410 | -2.53740 |
| H | 0.29040 | -1.25790 | -0.40760 |
| H | 3.62270 | 1.13470 | 0.76360 |
| H | 5.08970 | 0.41180 | 0.14720 |
| H | 0.64020 | -3.29250 | -1.68130 |
| H | -0.36850 | -3.24800 | 0.98760 |
| H | 1.19390 | -3.23000 | 1.76190 |
| H | 3.92380 | 3.08330 | -0.84560 |
| H | -0.74940 | -0.86510 | 1.79270 |
| H | -0.22030 | -2.91980 | 4.04320 |
| H | 1.61610 | -0.68600 | 2.07930 |
| H | 6.75160 | 2.01490 | -0.41900 |
| H | 7.19900 | 4.46640 | -0.34930 |
| H | 5.90010 | 6.11030 | -1.64360 |
| H | 4.77610 | 4.86740 | -2.17140 |
| H | 4.85870 | 5.32480 | -0.46540 |
| H | -3.70810 | -1.03770 | 4.65230 |
| H | 8.45490 | 2.32800 | -1.93070 |
| H | 9.02890 | 3.38710 | -3.21110 |
| H | 9.16920 | 3.90090 | -1.53240 |

| Marilzafurollene C_56 | | | |
|------------------------------|----------|----------|----------|
| C | 3.44010 | -1.86900 | -1.50710 |
| O | 2.82440 | -1.34190 | -0.33380 |
| C | 4.55750 | -0.94670 | -2.04270 |
| C | 2.28950 | -2.19430 | -2.46590 |
| C | 1.41000 | -1.54220 | -0.38720 |
| C | 4.14580 | 0.45800 | -2.53050 |
| Br | 5.45520 | -1.88190 | -3.55520 |
| C | 1.17790 | -2.56740 | -1.50570 |
| C | 0.84920 | -1.89490 | 1.00420 |
| C | 3.61210 | 1.35260 | -1.42790 |
| Cl | 1.40240 | -4.25120 | -0.94320 |
| C | 1.00110 | -0.75070 | 2.02230 |
| C | 0.30070 | -1.07020 | 3.32800 |
| O | 2.37600 | -0.55300 | 2.27000 |
| C | -0.67740 | -0.34490 | 3.82060 |
| C | 4.24570 | 2.43550 | -0.94910 |
| C | 3.70790 | 3.32620 | 0.15520 |
| C | 3.56650 | 4.77120 | -0.32950 |
| O | 4.58590 | 3.34150 | 1.27060 |
| C | -1.66100 | 0.38250 | 4.29450 |
| Br | -3.55530 | 0.02970 | 3.84040 |
| C | 4.55190 | 2.15280 | 2.04940 |
| H | 3.90170 | -2.81070 | -1.20480 |
| H | 5.31500 | -0.83720 | -1.26490 |
| H | 1.99210 | -1.31700 | -3.03840 |
| H | 2.53460 | -2.98780 | -3.17260 |
| H | 0.96960 | -0.59860 | -0.71380 |
| H | 5.01960 | 0.94130 | -2.96930 |
| H | 3.40910 | 0.39840 | -3.33040 |
| H | 0.18530 | -2.49300 | -1.95150 |
| H | -0.21000 | -2.13430 | 0.89780 |
| H | 1.32590 | -2.79620 | 1.39200 |
| H | 2.65380 | 1.08050 | -1.01230 |
| H | 0.59180 | 0.16920 | 1.59840 |
| H | 0.65050 | -1.94620 | 3.85460 |
| H | 2.83700 | -0.75820 | 1.45970 |
| H | 5.20740 | 2.71770 | -1.35310 |
| H | 2.72380 | 2.97120 | 0.46820 |
| H | 3.16720 | 5.40710 | 0.46080 |
| H | 4.52970 | 5.18310 | -0.63130 |
| H | 2.89010 | 4.83650 | -1.18200 |
| H | -1.54100 | 1.22380 | 4.96140 |
| H | 5.25090 | 2.24080 | 2.88090 |
| H | 3.55830 | 1.98600 | 2.46710 |
| H | 4.83650 | 1.27560 | 1.46720 |

| Marilzafurollene C_57 | | | |
|------------------------------|----------|----------|----------|
| C | 3.07980 | -1.44730 | -0.91600 |
| O | 2.32070 | -1.76660 | 0.24960 |
| C | 3.16010 | 0.07940 | -1.10610 |
| C | 2.42720 | -2.21300 | -2.07560 |
| C | 1.22640 | -2.60650 | -0.10200 |
| C | 3.94600 | 0.76090 | 0.02670 |
| Br | 1.31810 | 0.85190 | -1.17920 |
| C | 1.69990 | -3.33590 | -1.36300 |
| C | 0.78180 | -3.48860 | 1.08150 |
| C | 4.16270 | 2.24070 | -0.22560 |
| Cl | 2.85140 | -4.65410 | -0.99240 |
| C | 0.29340 | -2.67890 | 2.29670 |
| C | -0.91800 | -1.82210 | 1.97850 |
| O | -0.03880 | -3.58310 | 3.33040 |
| C | -0.90000 | -0.50910 | 2.01890 |
| C | 5.37050 | 2.82120 | -0.34810 |
| C | 5.64910 | 4.29950 | -0.60000 |
| C | 4.39650 | 5.18700 | -0.57460 |
| O | 6.25750 | 4.50150 | -1.86850 |
| C | -0.85360 | 0.80180 | 2.04570 |
| Br | -1.27640 | 1.84660 | 3.67310 |
| C | 7.61650 | 4.09420 | -1.95060 |
| H | 4.08340 | -1.84790 | -0.76470 |
| H | 3.64180 | 0.29900 | -2.06050 |
| H | 1.70210 | -1.58680 | -2.59600 |
| H | 3.14760 | -2.56640 | -2.81370 |
| H | 0.40040 | -1.95660 | -0.39480 |
| H | 3.41690 | 0.63760 | 0.97250 |
| H | 4.91390 | 0.27300 | 0.14810 |
| H | 0.87970 | -3.75480 | -1.94680 |
| H | -0.00560 | -4.16640 | 0.75050 |
| H | 1.61320 | -4.11880 | 1.39790 |
| H | 3.26290 | 2.83260 | -0.30680 |
| H | 1.11310 | -2.04730 | 2.64790 |
| H | -1.81990 | -2.35030 | 1.70480 |
| H | -0.12770 | -3.09630 | 4.13790 |
| H | 6.24850 | 2.19900 | -0.25760 |
| H | 6.31950 | 4.65040 | 0.18660 |
| H | 4.66550 | 6.23330 | -0.72010 |
| H | 3.70000 | 4.91660 | -1.36860 |
| H | 3.87480 | 5.11340 | 0.37990 |
| H | -0.58670 | 1.42590 | 1.20490 |
| H | 7.72920 | 3.01870 | -1.81440 |
| H | 8.00900 | 4.34270 | -2.93670 |
| H | 8.23010 | 4.60820 | -1.20970 |

| Marilzafurollene C_58 | | | |
|------------------------------|----------|----------|----------|
| C | 3.15280 | -1.75130 | -1.12350 |
| O | 2.41920 | -1.91390 | 0.08990 |
| C | 3.42950 | -0.25990 | -1.39310 |
| C | 2.34300 | -2.46800 | -2.21320 |
| C | 1.20380 | -2.60790 | -0.17050 |
| C | 4.35980 | 0.35480 | -0.33410 |
| Br | 1.70950 | 0.75740 | -1.41220 |
| C | 1.50780 | -3.44850 | -1.41430 |
| C | 0.70450 | -3.36930 | 1.07330 |
| C | 4.76250 | 1.77780 | -0.66880 |
| Cl | 2.48700 | -4.89620 | -1.03190 |
| C | 0.38830 | -2.44880 | 2.26640 |
| C | -0.71300 | -1.45150 | 1.95760 |
| O | -0.01000 | -3.25390 | 3.35720 |
| C | -0.52030 | -0.15210 | 1.93550 |
| C | 4.48910 | 2.84780 | 0.09740 |
| C | 4.88210 | 4.28120 | -0.22010 |
| C | 3.65700 | 5.09760 | -0.63850 |
| O | 5.82820 | 4.36250 | -1.27950 |
| C | -0.30130 | 1.14090 | 1.90060 |
| Br | -0.51060 | 2.29600 | 3.49470 |
| C | 7.16890 | 4.11290 | -0.87780 |
| H | 4.09950 | -2.27940 | -0.99900 |
| H | 3.88000 | -0.15090 | -2.38070 |
| H | 1.68370 | -1.77000 | -2.72980 |
| H | 2.96940 | -2.94830 | -2.96530 |
| H | 0.46030 | -1.86270 | -0.45730 |
| H | 3.87900 | 0.32090 | 0.64470 |
| H | 5.27160 | -0.23760 | -0.25220 |
| H | 0.60920 | -3.77440 | -1.93890 |
| H | -0.18170 | -3.94790 | 0.81040 |
| H | 1.45900 | -4.09210 | 1.38450 |
| H | 5.30260 | 1.91550 | -1.59470 |
| H | 1.30080 | -1.91870 | 2.55010 |
| H | -1.68820 | -1.86510 | 1.74550 |
| H | 0.00520 | -2.72450 | 4.14220 |
| H | 3.94000 | 2.70960 | 1.01800 |
| H | 5.30060 | 4.73010 | 0.68280 |
| H | 3.93130 | 6.13210 | -0.84480 |
| H | 3.20240 | 4.68730 | -1.54080 |
| H | 2.89920 | 5.10410 | 0.14520 |
| H | 0.00720 | 1.68990 | 1.02240 |
| H | 7.28340 | 3.12500 | -0.43080 |
| H | 7.82530 | 4.16460 | -1.74640 |
| H | 7.50820 | 4.85980 | -0.15910 |

| Marilzafurollene C_59 | | | |
|------------------------------|----------|----------|----------|
| C | 2.62370 | -1.22600 | -1.92390 |
| O | 2.50200 | -1.03820 | -0.51130 |
| C | 1.78500 | -0.19040 | -2.70590 |
| C | 2.22520 | -2.68560 | -2.18380 |
| C | 1.98090 | -2.21540 | 0.09400 |
| C | 2.38360 | 1.23010 | -2.73490 |
| Br | -0.06780 | -0.10840 | -1.96620 |
| C | 2.44230 | -3.34050 | -0.83440 |
| C | 2.40250 | -2.32260 | 1.57170 |
| C | 2.68750 | 1.78850 | -1.35850 |
| Cl | 4.17750 | -3.72040 | -0.62110 |
| C | 1.81980 | -1.20200 | 2.45300 |
| C | 0.30490 | -1.24150 | 2.52970 |
| O | 2.34770 | -1.33340 | 3.75730 |
| C | -0.46600 | -0.28900 | 2.05570 |
| C | 3.87950 | 2.28500 | -0.98910 |
| C | 4.20270 | 2.80070 | 0.39940 |
| C | 4.52570 | 4.29630 | 0.36610 |
| O | 5.33890 | 2.13810 | 0.93660 |
| C | -1.21960 | 0.66340 | 1.55950 |
| Br | -1.79040 | 2.23280 | 2.62260 |
| C | 5.12070 | 0.77100 | 1.25830 |
| H | 3.67790 | -1.10800 | -2.17980 |
| H | 1.68750 | -0.52670 | -3.73930 |
| H | 1.16970 | -2.75190 | -2.45050 |
| H | 2.79990 | -3.15000 | -2.98560 |
| H | 0.89290 | -2.16530 | 0.03140 |
| H | 3.30160 | 1.22410 | -3.32390 |
| H | 1.69600 | 1.90740 | -3.24210 |
| H | 1.87250 | -4.26150 | -0.70670 |
| H | 2.09640 | -3.29280 | 1.96490 |
| H | 3.49040 | -2.29610 | 1.63590 |
| H | 1.87580 | 1.76050 | -0.64510 |
| H | 2.13210 | -0.23410 | 2.05440 |
| H | -0.12640 | -2.10990 | 3.00560 |
| H | 3.23680 | -1.00910 | 3.76240 |
| H | 4.69060 | 2.32030 | -1.70180 |
| H | 3.34510 | 2.64520 | 1.05730 |
| H | 4.74600 | 4.66740 | 1.36710 |
| H | 5.39350 | 4.49930 | -0.26180 |
| H | 3.68570 | 4.87160 | -0.02400 |
| H | -1.59480 | 0.68710 | 0.54660 |
| H | 6.03360 | 0.34510 | 1.67410 |
| H | 4.33500 | 0.66710 | 2.00620 |
| H | 4.85010 | 0.17970 | 0.38270 |

| Marilzafurollene C_60 | | | |
|------------------------------|----------|----------|----------|
| C | 2.87300 | -1.33870 | -0.58140 |
| O | 1.66190 | -1.08830 | 0.13460 |
| C | 3.31260 | -0.06450 | -1.32700 |
| C | 2.58940 | -2.54500 | -1.48920 |
| C | 0.80590 | -2.22470 | 0.07330 |
| C | 3.62530 | 1.09400 | -0.36500 |
| Br | 1.88020 | 0.50320 | -2.59800 |
| C | 1.09420 | -2.74430 | -1.33670 |
| C | 1.15100 | -3.19360 | 1.23010 |
| C | 4.19110 | 2.30580 | -1.07980 |
| Cl | 0.59150 | -4.43480 | -1.61680 |
| C | 0.92310 | -2.58840 | 2.62700 |
| C | -0.54430 | -2.32320 | 2.90670 |
| O | 1.41750 | -3.49900 | 3.58790 |
| C | -1.03110 | -1.12800 | 3.15170 |
| C | 5.41030 | 2.82360 | -0.85540 |
| C | 5.97260 | 4.03750 | -1.57130 |
| C | 7.24810 | 3.67660 | -2.33670 |
| O | 6.31260 | 5.06480 | -0.65150 |
| C | -1.52280 | 0.06860 | 3.36930 |
| Br | -2.17840 | 1.22620 | 1.90420 |
| C | 5.19370 | 5.71490 | -0.06380 |
| H | 3.64390 | -1.61950 | 0.13810 |
| H | 4.19990 | -0.28560 | -1.92230 |
| H | 2.88170 | -2.39140 | -2.52830 |
| H | 3.12820 | -3.41820 | -1.11960 |
| H | -0.23530 | -1.91050 | 0.15250 |
| H | 2.72040 | 1.39090 | 0.16690 |
| H | 4.33520 | 0.76160 | 0.39330 |
| H | 0.56670 | -2.12180 | -2.06090 |
| H | 0.55590 | -4.10270 | 1.13890 |
| H | 2.19050 | -3.51060 | 1.14540 |
| H | 3.54580 | 2.76630 | -1.81480 |
| H | 1.49630 | -1.66210 | 2.71220 |
| H | -1.19520 | -3.18560 | 2.89180 |
| H | 1.46570 | -3.05940 | 4.42500 |
| H | 6.05940 | 2.37050 | -0.11990 |
| H | 5.23850 | 4.41560 | -2.28570 |
| H | 7.64330 | 4.54600 | -2.86250 |
| H | 8.02520 | 3.31530 | -1.66270 |
| H | 7.05650 | 2.89980 | -3.07730 |
| H | -1.61840 | 0.53120 | 4.34080 |
| H | 5.54050 | 6.50650 | 0.60030 |
| H | 4.55790 | 6.17130 | -0.82350 |
| H | 4.59000 | 5.02650 | 0.52870 |

| Marilzafurollene C_61 | | | |
|------------------------------|----------|----------|----------|
| C | 3.04920 | -0.70770 | -0.53300 |
| O | 2.15600 | -0.21290 | 0.46440 |
| C | 3.68770 | 0.45010 | -1.32280 |
| C | 2.23960 | -1.70010 | -1.37630 |
| C | 0.88550 | -0.84890 | 0.34380 |
| C | 4.58200 | 1.33100 | -0.43450 |
| Br | 2.25930 | 1.58310 | -2.14010 |
| C | 1.17450 | -2.15740 | -0.40180 |
| C | 0.19660 | -0.96010 | 1.71780 |
| C | 5.32260 | 2.39180 | -1.22580 |
| Cl | 1.85010 | -3.41760 | 0.67480 |
| C | -1.15140 | -1.70770 | 1.70530 |
| C | -1.75220 | -1.77360 | 3.09610 |
| O | -2.05290 | -1.04210 | 0.84490 |
| C | -2.03240 | -2.89780 | 3.71550 |
| C | 6.66000 | 2.48220 | -1.31520 |
| C | 7.39770 | 3.54600 | -2.10660 |
| C | 8.26140 | 2.91140 | -3.19960 |
| O | 8.26540 | 4.29890 | -1.27150 |
| C | -2.30300 | -4.01440 | 4.34940 |
| Br | -0.98320 | -4.92270 | 5.51160 |
| C | 7.59640 | 5.17940 | -0.37870 |
| H | 3.83110 | -1.26370 | -0.01300 |
| H | 4.28290 | 0.04130 | -2.14070 |
| H | 1.76380 | -1.19910 | -2.21950 |
| H | 2.84240 | -2.51740 | -1.77290 |
| H | 0.27870 | -0.21460 | -0.30520 |
| H | 3.97850 | 1.81990 | 0.33140 |
| H | 5.30560 | 0.70800 | 0.09280 |
| H | 0.29180 | -2.56580 | -0.89510 |
| H | 0.87280 | -1.45240 | 2.41760 |
| H | 0.05110 | 0.04660 | 2.11100 |
| H | 4.70600 | 3.11390 | -1.74270 |
| H | -1.00310 | -2.72190 | 1.32820 |
| H | -1.94330 | -0.82460 | 3.57680 |
| H | -2.86580 | -1.52740 | 0.81960 |
| H | 7.28240 | 1.76580 | -0.79860 |
| H | 6.67800 | 4.21510 | -2.58250 |
| H | 8.77950 | 3.67720 | -3.77700 |
| H | 9.01620 | 2.25020 | -2.77330 |
| H | 7.65420 | 2.32770 | -3.89190 |
| H | -3.24660 | -4.53840 | 4.30320 |
| H | 8.33180 | 5.73970 | 0.19860 |
| H | 6.97970 | 5.89780 | -0.92020 |
| H | 6.96430 | 4.63860 | 0.32650 |

| Marilzafurollene C_62 | | | |
|------------------------------|----------|----------|----------|
| C | 3.08900 | -1.76840 | -1.31150 |
| O | 2.35250 | -1.59260 | -0.10160 |
| C | 4.15430 | -0.66590 | -1.46250 |
| C | 2.04230 | -1.86560 | -2.42830 |
| C | 0.95390 | -1.74570 | -0.35070 |
| C | 3.60070 | 0.77140 | -1.47020 |
| Br | 5.18730 | -0.99260 | -3.13660 |
| C | 0.85680 | -2.46620 | -1.70210 |
| C | 0.24290 | -2.42240 | 0.83820 |
| C | 4.70290 | 1.81080 | -1.41140 |
| Cl | 1.07720 | -4.23520 | -1.54680 |
| C | 0.25900 | -1.57120 | 2.12010 |
| C | -0.60120 | -2.18580 | 3.20710 |
| O | 1.59030 | -1.48260 | 2.57870 |
| C | -1.66760 | -1.60270 | 3.70600 |
| C | 4.85140 | 2.70880 | -0.42330 |
| C | 5.95510 | 3.74850 | -0.36570 |
| C | 6.81200 | 3.56450 | 0.88920 |
| O | 5.42070 | 5.06350 | -0.31900 |
| C | -2.74190 | -1.03140 | 4.19730 |
| Br | -2.68480 | 0.18080 | 5.76150 |
| C | 4.83900 | 5.50060 | -1.53970 |
| H | 3.59490 | -2.73210 | -1.23230 |
| H | 4.86040 | -0.76700 | -0.63650 |
| H | 1.77240 | -0.88040 | -2.80580 |
| H | 2.37890 | -2.46430 | -3.27540 |
| H | 0.54670 | -0.74140 | -0.48180 |
| H | 3.00840 | 0.95440 | -2.36600 |
| H | 2.93420 | 0.91360 | -0.61840 |
| H | -0.09110 | -2.28940 | -2.21180 |
| H | -0.79330 | -2.61110 | 0.55390 |
| H | 0.68290 | -3.39940 | 1.04250 |
| H | 5.40330 | 1.80700 | -2.23500 |
| H | -0.09680 | -0.56370 | 1.89310 |
| H | -0.28830 | -3.15410 | 3.56980 |
| H | 2.15120 | -1.43720 | 1.80860 |
| H | 4.15360 | 2.71970 | 0.40180 |
| H | 6.60080 | 3.64780 | -1.24050 |
| H | 7.61360 | 4.30250 | 0.92270 |
| H | 6.21660 | 3.68030 | 1.79520 |
| H | 7.27020 | 2.57540 | 0.91170 |
| H | -3.74140 | -1.16020 | 3.80860 |
| H | 5.56710 | 5.48660 | -2.35170 |
| H | 4.48460 | 6.52510 | -1.42730 |
| H | 3.98570 | 4.88450 | -1.82550 |

| Marilzafurollene C_63 | | | |
|------------------------------|----------|----------|----------|
| C | 2.72440 | -0.70000 | -1.10440 |
| O | 2.22680 | -1.06120 | 0.18370 |
| C | 2.08390 | 0.62070 | -1.58120 |
| C | 2.46990 | -1.90910 | -2.01540 |
| C | 1.64820 | -2.36100 | 0.13170 |
| C | 2.44890 | 1.83550 | -0.70990 |
| Br | 0.09540 | 0.44290 | -1.56690 |
| C | 2.37370 | -3.05330 | -1.02610 |
| C | 1.70430 | -3.06460 | 1.50210 |
| C | 3.91820 | 2.20530 | -0.78410 |
| Cl | 4.01790 | -3.59230 | -0.57150 |
| C | 0.91740 | -2.32570 | 2.60020 |
| C | -0.56330 | -2.22020 | 2.28540 |
| O | 1.08250 | -3.02720 | 3.81560 |
| C | -1.17550 | -1.07540 | 2.08360 |
| C | 4.39130 | 3.35440 | -1.29760 |
| C | 5.85830 | 3.74540 | -1.38030 |
| C | 6.34200 | 3.73170 | -2.83260 |
| O | 6.69820 | 2.86170 | -0.64740 |
| C | -1.76240 | 0.07740 | 1.86540 |
| Br | -2.59890 | 1.13450 | 3.31520 |
| C | 6.75050 | 3.13530 | 0.74700 |
| H | 3.80380 | -0.57930 | -1.00890 |
| H | 2.37700 | 0.82000 | -2.61310 |
| H | 1.52120 | -1.80750 | -2.54270 |
| H | 3.24970 | -2.05140 | -2.76400 |
| H | 0.60600 | -2.23900 | -0.16680 |
| H | 1.85330 | 2.69330 | -1.02410 |
| H | 2.18560 | 1.64250 | 0.33080 |
| H | 1.82950 | -3.91390 | -1.41650 |
| H | 1.32660 | -4.08260 | 1.40100 |
| H | 2.74260 | -3.15510 | 1.82180 |
| H | 4.61380 | 1.47850 | -0.38900 |
| H | 1.34350 | -1.32690 | 2.72330 |
| H | -1.10820 | -3.15140 | 2.22720 |
| H | 0.79150 | -2.47130 | 4.52490 |
| H | 3.69660 | 4.08030 | -1.69580 |
| H | 5.96450 | 4.76110 | -0.99450 |
| H | 7.38650 | 4.03730 | -2.89590 |
| H | 6.26160 | 2.73350 | -3.26390 |
| H | 5.75850 | 4.41390 | -3.45130 |
| H | -1.84580 | 0.55280 | 0.89850 |
| H | 5.76410 | 3.08960 | 1.20940 |
| H | 7.38460 | 2.39810 | 1.23960 |
| H | 7.17660 | 4.12120 | 0.93690 |

| Marilzafurollene C_64 | | | |
|------------------------------|----------|----------|----------|
| C | 2.61480 | -0.65670 | -0.60850 |
| O | 2.59010 | -0.72530 | 0.81700 |
| C | 3.03360 | 0.74810 | -1.08120 |
| C | 1.22940 | -1.11250 | -1.08030 |
| C | 1.31790 | -1.18070 | 1.26840 |
| C | 4.48040 | 1.08430 | -0.68280 |
| Br | 1.80570 | 2.11860 | -0.30230 |
| C | 0.75770 | -1.96990 | 0.07500 |
| C | 1.46630 | -1.90820 | 2.62290 |
| C | 4.94880 | 2.40760 | -1.25690 |
| Cl | 1.48010 | -3.60150 | -0.06160 |
| C | 0.14500 | -2.16280 | 3.37760 |
| C | -0.71240 | -3.23140 | 2.72790 |
| O | 0.45220 | -2.57570 | 4.69330 |
| C | -1.94100 | -3.02210 | 2.31340 |
| C | 5.97740 | 2.54790 | -2.10950 |
| C | 6.44440 | 3.87380 | -2.68090 |
| C | 6.33930 | 3.87650 | -4.20800 |
| O | 7.80370 | 4.12410 | -2.35430 |
| C | -3.15150 | -2.79160 | 1.86430 |
| Br | -3.48250 | -2.15320 | 0.02040 |
| C | 8.02650 | 4.43720 | -0.98600 |
| H | 3.34870 | -1.38790 | -0.95140 |
| H | 2.93620 | 0.80600 | -2.16650 |
| H | 0.55640 | -0.26260 | -1.19550 |
| H | 1.25450 | -1.64550 | -2.03110 |
| H | 0.70400 | -0.28970 | 1.41240 |
| H | 4.56800 | 1.12100 | 0.40380 |
| H | 5.14930 | 0.29150 | -1.02040 |
| H | -0.32640 | -2.07690 | 0.09480 |
| H | 2.02760 | -2.83560 | 2.50710 |
| H | 2.09420 | -1.27300 | 3.24850 |
| H | 4.39950 | 3.28290 | -0.93940 |
| H | -0.41870 | -1.22950 | 3.44700 |
| H | -0.25510 | -4.20420 | 2.61620 |
| H | 0.81720 | -1.84300 | 5.16940 |
| H | 6.53300 | 1.67790 | -2.42890 |
| H | 5.82100 | 4.68140 | -2.29200 |
| H | 6.66110 | 4.83460 | -4.61660 |
| H | 6.96550 | 3.10070 | -4.64910 |
| H | 5.31250 | 3.70560 | -4.53230 |
| H | -4.05990 | -2.92030 | 2.43480 |
| H | 9.08460 | 4.64640 | -0.82850 |
| H | 7.46330 | 5.32190 | -0.68620 |
| H | 7.75160 | 3.60990 | -0.33080 |

| Marilzafurollene C_65 | | | |
|------------------------------|----------|----------|----------|
| C | 2.54570 | 0.24970 | -0.77330 |
| O | 1.41350 | -0.10080 | 0.02100 |
| C | 2.10580 | 1.11320 | -1.97080 |
| C | 3.19790 | -1.08570 | -1.14250 |
| C | 1.47400 | -1.47530 | 0.40340 |
| C | 3.24810 | 1.50780 | -2.92760 |
| Br | 1.24340 | 2.77300 | -1.28000 |
| C | 2.90210 | -1.93310 | 0.07690 |
| C | 1.00530 | -1.67090 | 1.85870 |
| C | 4.38830 | 2.22780 | -2.23220 |
| Cl | 4.06450 | -1.53600 | 1.37840 |
| C | -0.47610 | -1.31290 | 2.07150 |
| C | -0.95220 | -1.71810 | 3.45250 |
| O | -0.62960 | 0.08180 | 1.92280 |
| C | -1.92260 | -2.57870 | 3.66010 |
| C | 5.65720 | 1.78800 | -2.19990 |
| C | 6.79370 | 2.49510 | -1.48640 |
| C | 7.88930 | 2.90210 | -2.47480 |
| O | 7.39620 | 1.64800 | -0.51880 |
| C | -2.88560 | -3.44860 | 3.85230 |
| Br | -2.54320 | -5.39160 | 4.01630 |
| C | 6.58480 | 1.39000 | 0.61960 |
| H | 3.22270 | 0.81640 | -0.13250 |
| H | 1.33680 | 0.58310 | -2.53410 |
| H | 2.71140 | -1.51780 | -2.01780 |
| H | 4.26350 | -0.99640 | -1.35670 |
| H | 0.79540 | -2.01240 | -0.26170 |
| H | 3.63450 | 0.61870 | -3.42710 |
| H | 2.85990 | 2.15530 | -3.71450 |
| H | 2.97040 | -3.00400 | -0.11840 |
| H | 1.15740 | -2.71720 | 2.12810 |
| H | 1.62300 | -1.08860 | 2.54360 |
| H | 4.13220 | 3.15180 | -1.73270 |
| H | -1.08320 | -1.81030 | 1.31180 |
| H | -0.44520 | -1.25380 | 4.28570 |
| H | -0.05750 | 0.35860 | 1.21010 |
| H | 5.91990 | 0.86660 | -2.69930 |
| H | 6.41720 | 3.39620 | -0.99820 |
| H | 8.69900 | 3.42210 | -1.96260 |
| H | 8.31680 | 2.03120 | -2.97220 |
| H | 7.49870 | 3.57050 | -3.24250 |
| H | -3.93340 | -3.20030 | 3.93820 |
| H | 6.31300 | 2.31460 | 1.13030 |
| H | 5.67160 | 0.85790 | 0.35290 |
| H | 7.13420 | 0.76730 | 1.32550 |

| Marilzafurollene C_66 | | | |
|------------------------------|----------|----------|----------|
| C | 2.94620 | -1.76560 | -1.65930 |
| O | 2.71950 | -1.46150 | -0.28460 |
| C | 3.60900 | -0.59620 | -2.41950 |
| C | 1.60030 | -2.26300 | -2.19500 |
| C | 1.46020 | -1.98820 | 0.13500 |
| C | 2.83550 | 0.73680 | -2.47430 |
| Br | 3.95620 | -1.18910 | -4.28960 |
| C | 1.01920 | -2.95040 | -0.97680 |
| C | 1.56380 | -2.58340 | 1.55240 |
| C | 2.73130 | 1.41860 | -1.12460 |
| Cl | 1.74030 | -4.57870 | -0.79510 |
| C | 1.71750 | -1.51430 | 2.64950 |
| C | 0.42910 | -0.74590 | 2.87690 |
| O | 2.08100 | -2.15130 | 3.85660 |
| C | 0.29460 | 0.54230 | 2.65910 |
| C | 3.40070 | 2.53010 | -0.77820 |
| C | 3.30500 | 3.19650 | 0.58060 |
| C | 2.83470 | 4.64670 | 0.44880 |
| O | 4.56550 | 3.21540 | 1.23400 |
| C | 0.12700 | 1.82120 | 2.42220 |
| Br | -0.46580 | 2.49680 | 0.65900 |
| C | 5.00500 | 1.94120 | 1.68550 |
| H | 3.64230 | -2.60610 | -1.67210 |
| H | 4.58830 | -0.41050 | -1.97570 |
| H | 0.95920 | -1.43080 | -2.48300 |
| H | 1.70060 | -2.92380 | -3.05660 |
| H | 0.75460 | -1.15610 | 0.13720 |
| H | 3.35480 | 1.41120 | -3.15610 |
| H | 1.83760 | 0.60340 | -2.89000 |
| H | -0.06370 | -3.06820 | -1.02920 |
| H | 0.68390 | -3.19340 | 1.76170 |
| H | 2.41670 | -3.26250 | 1.58090 |
| H | 2.07120 | 0.95540 | -0.40580 |
| H | 2.52010 | -0.82480 | 2.37620 |
| H | -0.40700 | -1.32480 | 3.24160 |
| H | 2.96730 | -2.47470 | 3.77500 |
| H | 4.06510 | 3.00130 | -1.48820 |
| H | 2.58830 | 2.65770 | 1.20150 |
| H | 1.85680 | 4.70000 | -0.03080 |
| H | 2.74950 | 5.11700 | 1.42840 |
| H | 3.53350 | 5.23730 | -0.14400 |
| H | 0.29240 | 2.61110 | 3.14050 |
| H | 5.95770 | 2.04750 | 2.20410 |
| H | 4.29170 | 1.50170 | 2.38400 |
| H | 5.15410 | 1.24630 | 0.85820 |

| Marilzafurollene C_67 | | | |
|------------------------------|----------|----------|----------|
| C | 2.80240 | -1.46450 | -1.15850 |
| O | 2.11830 | -1.15930 | 0.05740 |
| C | 3.62170 | -0.25220 | -1.63880 |
| C | 1.72990 | -1.95190 | -2.14170 |
| C | 0.72280 | -1.41350 | -0.09210 |
| C | 4.76110 | 0.09820 | -0.66640 |
| Br | 2.42430 | 1.33470 | -1.83620 |
| C | 0.63890 | -2.45130 | -1.21680 |
| C | 0.07500 | -1.80310 | 1.25110 |
| C | 5.64110 | 1.22100 | -1.18060 |
| Cl | 1.04600 | -4.09810 | -0.64840 |
| C | 0.10400 | -0.65910 | 2.29120 |
| C | -0.68000 | -0.91970 | 3.57050 |
| O | 1.44970 | -0.40320 | 2.62860 |
| C | -1.35940 | -2.01030 | 3.84930 |
| C | 5.84260 | 2.38250 | -0.53640 |
| C | 6.71150 | 3.51360 | -1.05360 |
| C | 7.86660 | 3.79930 | -0.09060 |
| O | 5.96830 | 4.71680 | -1.18460 |
| C | -2.04830 | -3.09540 | 4.11260 |
| Br | -3.95520 | -3.28650 | 3.61670 |
| C | 5.00010 | 4.69600 | -2.22540 |
| H | 3.47580 | -2.29700 | -0.94780 |
| H | 4.03690 | -0.46710 | -2.62450 |
| H | 1.34460 | -1.12600 | -2.74000 |
| H | 2.09510 | -2.71530 | -2.82920 |
| H | 0.26390 | -0.49050 | -0.45190 |
| H | 4.34800 | 0.36600 | 0.30730 |
| H | 5.39320 | -0.77570 | -0.50540 |
| H | -0.34240 | -2.48860 | -1.69140 |
| H | -0.96020 | -2.08350 | 1.05150 |
| H | 0.55900 | -2.68840 | 1.66540 |
| H | 6.12510 | 1.05140 | -2.13170 |
| H | -0.30920 | 0.24330 | 1.83740 |
| H | -0.65090 | -0.11450 | 4.29020 |
| H | 1.96170 | -0.51090 | 1.82970 |
| H | 5.35980 | 2.55740 | 0.41450 |
| H | 7.13090 | 3.23940 | -2.02360 |
| H | 8.49860 | 4.60190 | -0.47090 |
| H | 7.49770 | 4.10360 | 0.88920 |
| H | 8.49400 | 2.91800 | 0.04480 |
| H | -1.65630 | -3.96970 | 4.61130 |
| H | 4.22600 | 3.94950 | -2.04480 |
| H | 4.51180 | 5.66850 | -2.28700 |
| H | 5.46230 | 4.49250 | -3.19210 |

| Marilzafurollene C_68 | | | |
|------------------------------|----------|----------|----------|
| C | 2.94350 | -1.52870 | -1.07720 |
| O | 2.29970 | -1.76860 | 0.17330 |
| C | 3.02730 | -0.01620 | -1.35830 |
| C | 2.16700 | -2.34270 | -2.12190 |
| C | 1.16240 | -2.60220 | -0.01840 |
| C | 3.92180 | 0.70990 | -0.33950 |
| Br | 1.19770 | 0.78690 | -1.30880 |
| C | 1.49290 | -3.40730 | -1.27940 |
| C | 0.83150 | -3.41100 | 1.25260 |
| C | 4.11770 | 2.17530 | -0.67710 |
| Cl | 2.64800 | -4.73380 | -0.95310 |
| C | 0.48240 | -2.52720 | 2.46560 |
| C | -0.74310 | -1.66010 | 2.23400 |
| O | 0.27260 | -3.35110 | 3.59620 |
| C | -0.69060 | -0.34870 | 2.17110 |
| C | 5.30420 | 2.74290 | -0.95040 |
| C | 5.49750 | 4.21010 | -1.28550 |
| C | 6.10250 | 4.37520 | -2.68190 |
| O | 6.38410 | 4.83440 | -0.36840 |
| C | -0.61150 | 0.95790 | 2.08110 |
| Br | -0.80380 | 2.14990 | 3.64960 |
| C | 5.84110 | 5.02340 | 0.93130 |
| H | 3.95120 | -1.94080 | -1.00270 |
| H | 3.42340 | 0.14190 | -2.36270 |
| H | 1.40570 | -1.73020 | -2.60530 |
| H | 2.80550 | -2.75310 | -2.90460 |
| H | 0.32080 | -1.95140 | -0.26020 |
| H | 3.48680 | 0.63420 | 0.65800 |
| H | 4.89560 | 0.22110 | -0.28980 |
| H | 0.61030 | -3.83520 | -1.75610 |
| H | 0.00860 | -4.09310 | 1.03720 |
| H | 1.68680 | -4.03410 | 1.51560 |
| H | 3.22380 | 2.78300 | -0.68970 |
| H | 1.33960 | -1.88630 | 2.68590 |
| H | -1.68650 | -2.17170 | 2.11400 |
| H | -0.40170 | -3.98490 | 3.40230 |
| H | 6.20270 | 2.14280 | -0.93680 |
| H | 4.53300 | 4.72160 | -1.26610 |
| H | 6.22750 | 5.43000 | -2.92740 |
| H | 7.08210 | 3.90130 | -2.74710 |
| H | 5.46170 | 3.93080 | -3.44380 |
| H | -0.43750 | 1.50150 | 1.16380 |
| H | 5.59900 | 4.07470 | 1.41150 |
| H | 6.57030 | 5.53520 | 1.55920 |
| H | 4.94030 | 5.63750 | 0.89780 |

| Marilzafurollene C_69 | | | |
|------------------------------|----------|----------|----------|
| C | 3.26720 | -1.52910 | -0.78610 |
| O | 2.39640 | -1.83590 | 0.30210 |
| C | 3.51100 | -0.00980 | -0.87150 |
| C | 2.63210 | -2.15850 | -2.03450 |
| C | 1.25010 | -2.52990 | -0.17800 |
| C | 4.25640 | 0.51790 | 0.37230 |
| Br | 1.75930 | 0.93990 | -1.04110 |
| C | 1.74050 | -3.23450 | -1.44670 |
| C | 0.62540 | -3.42220 | 0.91300 |
| C | 4.73410 | 1.96310 | 0.31110 |
| Cl | 2.71900 | -4.68700 | -1.08120 |
| C | 0.15710 | -2.63540 | 2.15110 |
| C | -0.90780 | -1.60560 | 1.82220 |
| O | -0.36100 | -3.55240 | 3.09290 |
| C | -0.71960 | -0.31210 | 1.95420 |
| C | 4.63390 | 2.80870 | -0.73100 |
| C | 5.13690 | 4.23990 | -0.72460 |
| C | 3.98870 | 5.22110 | -0.97330 |
| O | 6.09780 | 4.45040 | -1.74910 |
| C | -0.49910 | 0.97550 | 2.07520 |
| Br | -0.88010 | 1.96620 | 3.74600 |
| C | 7.35110 | 3.82410 | -1.51190 |
| H | 4.21260 | -2.03820 | -0.59170 |
| H | 4.09190 | 0.19980 | -1.77040 |
| H | 2.01750 | -1.43290 | -2.56750 |
| H | 3.36830 | -2.54690 | -2.73870 |
| H | 0.52140 | -1.77840 | -0.48540 |
| H | 3.61920 | 0.40260 | 1.25010 |
| H | 5.13710 | -0.09880 | 0.55410 |
| H | 0.92830 | -3.52990 | -2.11160 |
| H | -0.21310 | -3.97580 | 0.48920 |
| H | 1.35200 | -4.16860 | 1.23440 |
| H | 5.20400 | 2.31960 | 1.21680 |
| H | 1.02360 | -2.14230 | 2.59860 |
| H | -1.85100 | -1.98930 | 1.46090 |
| H | -0.44620 | -3.11070 | 3.92620 |
| H | 4.17140 | 2.49370 | -1.65400 |
| H | 5.58180 | 4.47010 | 0.24550 |
| H | 4.34670 | 6.25050 | -0.95430 |
| H | 3.52480 | 5.04850 | -1.94480 |
| H | 3.21580 | 5.12340 | -0.21040 |
| H | -0.09720 | 1.60740 | 1.29630 |
| H | 7.25930 | 2.73840 | -1.46460 |
| H | 8.03650 | 4.06290 | -2.32510 |
| H | 7.79990 | 4.17740 | -0.58270 |

| Marilzafurollene C_70 | | | |
|------------------------------|----------|----------|----------|
| C | 3.05780 | -1.28980 | -1.09520 |
| O | 2.22280 | -1.33590 | 0.06240 |
| C | 3.50750 | 0.15470 | -1.38270 |
| C | 2.26070 | -1.95600 | -2.22430 |
| C | 0.98990 | -1.98100 | -0.25120 |
| C | 4.41570 | 0.71120 | -0.27310 |
| Br | 1.90560 | 1.33330 | -1.57190 |
| C | 1.30950 | -2.85900 | -1.46640 |
| C | 0.40580 | -2.70130 | 0.97980 |
| C | 4.97130 | 2.08100 | -0.61080 |
| Cl | 2.15490 | -4.36730 | -1.00680 |
| C | 0.00360 | -1.73640 | 2.10910 |
| C | -0.73330 | -2.45690 | 3.22120 |
| O | 1.17640 | -1.15300 | 2.63320 |
| C | -1.97970 | -2.20310 | 3.54980 |
| C | 6.27710 | 2.35890 | -0.77030 |
| C | 6.85260 | 3.72420 | -1.11180 |
| C | 7.59520 | 4.31520 | 0.08900 |
| O | 5.84970 | 4.65930 | -1.49070 |
| C | -3.22940 | -1.96390 | 3.87100 |
| Br | -3.74360 | -0.61270 | 5.22350 |
| C | 5.41990 | 4.53580 | -2.84040 |
| H | 3.93250 | -1.90760 | -0.88540 |
| H | 4.04330 | 0.18280 | -2.33280 |
| H | 1.68670 | -1.21790 | -2.78490 |
| H | 2.89110 | -2.49230 | -2.93410 |
| H | 0.29320 | -1.20430 | -0.57230 |
| H | 3.86260 | 0.77840 | 0.66460 |
| H | 5.24380 | 0.02390 | -0.09560 |
| H | 0.42390 | -3.12870 | -2.04290 |
| H | -0.47540 | -3.26050 | 0.66230 |
| H | 1.11100 | -3.43970 | 1.36340 |
| H | 4.24350 | 2.87280 | -0.72210 |
| H | -0.62610 | -0.94170 | 1.70250 |
| H | -0.17080 | -3.21050 | 3.75270 |
| H | 1.75290 | -0.97410 | 1.89380 |
| H | 7.00410 | 1.56840 | -0.65010 |
| H | 7.56690 | 3.60020 | -1.92800 |
| H | 8.03100 | 5.28230 | -0.16220 |
| H | 6.92070 | 4.46430 | 0.93270 |
| H | 8.40380 | 3.66140 | 0.41630 |
| H | -4.08350 | -2.46660 | 3.44140 |
| H | 5.01570 | 3.54530 | -3.05120 |
| H | 4.63530 | 5.26530 | -3.04090 |
| H | 6.24030 | 4.72990 | -3.53240 |

| Marilzafurollene C_71 | | | |
|------------------------------|----------|----------|----------|
| C | 2.76660 | -1.01860 | -1.56530 |
| O | 1.60370 | -0.93140 | -0.73840 |
| C | 2.66460 | -0.00460 | -2.72320 |
| C | 2.86220 | -2.48590 | -2.01020 |
| C | 1.22570 | -2.22640 | -0.28380 |
| C | 2.62020 | 1.45830 | -2.25020 |
| Br | 1.01090 | -0.36360 | -3.77970 |
| C | 1.56360 | -3.08350 | -1.50540 |
| C | 1.99950 | -2.56750 | 1.01250 |
| C | 3.90240 | 1.89730 | -1.56900 |
| Cl | 1.69410 | -4.83160 | -1.16500 |
| C | 1.70170 | -1.60680 | 2.17830 |
| C | 0.26090 | -1.69680 | 2.64620 |
| O | 2.55620 | -1.94040 | 3.25280 |
| C | -0.57150 | -0.68050 | 2.63110 |
| C | 3.98650 | 2.25800 | -0.27770 |
| C | 5.26330 | 2.69470 | 0.41550 |
| C | 5.60630 | 1.74790 | 1.56870 |
| O | 5.12950 | 3.99610 | 0.96790 |
| C | -1.39800 | 0.33880 | 2.63220 |
| Br | -1.58070 | 1.55630 | 4.18310 |
| C | 5.08860 | 5.03920 | 0.00320 |
| H | 3.63980 | -0.79110 | -0.95200 |
| H | 3.50650 | -0.13840 | -3.40400 |
| H | 2.98200 | -2.61170 | -3.08660 |
| H | 3.71450 | -2.96280 | -1.52470 |
| H | 0.15280 | -2.25420 | -0.09120 |
| H | 2.45360 | 2.11530 | -3.10420 |
| H | 1.77180 | 1.60330 | -1.57940 |
| H | 0.78520 | -2.95360 | -2.25890 |
| H | 1.76140 | -3.58500 | 1.32430 |
| H | 3.07150 | -2.56190 | 0.81380 |
| H | 4.79120 | 1.90930 | -2.18410 |
| H | 1.93320 | -0.58490 | 1.86770 |
| H | -0.06520 | -2.66440 | 3.00030 |
| H | 2.48670 | -1.26560 | 3.91370 |
| H | 3.09830 | 2.24540 | 0.33840 |
| H | 6.09080 | 2.68370 | -0.29700 |
| H | 6.53180 | 2.05190 | 2.05830 |
| H | 4.81850 | 1.74170 | 2.32270 |
| H | 5.73860 | 0.72550 | 1.21350 |
| H | -2.04410 | 0.61040 | 1.81000 |
| H | 4.22400 | 4.94880 | -0.65550 |
| H | 5.01860 | 6.00120 | 0.51090 |
| H | 5.99300 | 5.04860 | -0.60690 |

| Marilzafurollene C_72 | | | |
|------------------------------|----------|----------|----------|
| C | 3.07250 | -1.34250 | -0.07040 |
| O | 2.08500 | -0.52820 | 0.56770 |
| C | 4.31420 | -0.48530 | -0.38020 |
| C | 2.37890 | -1.97770 | -1.28650 |
| C | 0.78030 | -0.89410 | 0.12040 |
| C | 4.05070 | 0.69770 | -1.33080 |
| Br | 5.72810 | -1.66210 | -1.15050 |
| C | 1.05000 | -1.25240 | -1.34300 |
| C | 0.22930 | -2.04070 | 1.00230 |
| C | 5.25990 | 1.60070 | -1.47640 |
| Cl | -0.23470 | -2.22540 | -2.11060 |
| C | 0.02100 | -1.63720 | 2.47300 |
| C | -0.71320 | -2.71440 | 3.24690 |
| O | 1.28230 | -1.42270 | 3.06740 |
| C | -1.87520 | -2.52320 | 3.82860 |
| C | 5.28810 | 2.89810 | -1.12890 |
| C | 6.49900 | 3.80070 | -1.27580 |
| C | 6.93770 | 4.34940 | 0.08420 |
| O | 6.21000 | 4.91720 | -2.10450 |
| C | -3.04100 | -2.32110 | 4.39550 |
| Br | -4.75060 | -2.63040 | 3.44650 |
| C | 6.06840 | 4.59990 | -3.48250 |
| H | 3.35530 | -2.13410 | 0.62560 |
| H | 4.70880 | -0.10300 | 0.56280 |
| H | 2.94230 | -1.89310 | -2.21570 |
| H | 2.22230 | -3.04080 | -1.09980 |
| H | 0.11040 | -0.03570 | 0.18490 |
| H | 3.76730 | 0.34020 | -2.32050 |
| H | 3.21160 | 1.28730 | -0.95900 |
| H | 1.15730 | -0.33580 | -1.92470 |
| H | -0.73710 | -2.34860 | 0.60090 |
| H | 0.86850 | -2.92230 | 0.94370 |
| H | 6.14690 | 1.14340 | -1.89230 |
| H | -0.54430 | -0.70330 | 2.51540 |
| H | -0.22530 | -3.67650 | 3.30360 |
| H | 1.80260 | -0.92290 | 2.44480 |
| H | 4.40480 | 3.36260 | -0.71460 |
| H | 7.32980 | 3.23480 | -1.70220 |
| H | 7.19270 | 3.54190 | 0.77100 |
| H | 7.81630 | 4.98620 | -0.02020 |
| H | 6.14890 | 4.94560 | 0.54350 |
| H | -3.18260 | -1.97530 | 5.40910 |
| H | 6.97630 | 4.14290 | -3.87800 |
| H | 5.23170 | 3.92290 | -3.65860 |
| H | 5.88050 | 5.51230 | -4.04830 |

| Marilzafurollene C_73 | | | |
|------------------------------|----------|----------|----------|
| C | 2.97320 | -0.99810 | -1.07340 |
| O | 2.63010 | -0.69480 | 0.27860 |
| C | 3.82520 | 0.12640 | -1.69160 |
| C | 1.65070 | -1.28210 | -1.79560 |
| C | 1.22170 | -0.81350 | 0.46620 |
| C | 5.18570 | 0.27270 | -0.98920 |
| Br | 2.84460 | 1.86310 | -1.57730 |
| C | 0.75640 | -1.74120 | -0.66310 |
| C | 0.89820 | -1.24760 | 1.90880 |
| C | 6.08100 | 1.29610 | -1.66070 |
| Cl | 1.08180 | -3.46450 | -0.30340 |
| C | -0.59840 | -1.48680 | 2.18890 |
| C | -0.82120 | -1.94290 | 3.61770 |
| O | -1.31780 | -0.29160 | 1.96810 |
| C | -1.37190 | -3.09280 | 3.93410 |
| C | 6.57890 | 2.38480 | -1.05100 |
| C | 7.46350 | 3.41810 | -1.72310 |
| C | 8.83000 | 3.49600 | -1.03790 |
| O | 6.88650 | 4.71420 | -1.65510 |
| C | -1.93960 | -4.23520 | 4.24120 |
| Br | -3.89670 | -4.41730 | 4.47550 |
| C | 5.71840 | 4.87680 | -2.44900 |
| H | 3.55460 | -1.92140 | -1.05460 |
| H | 3.98170 | -0.08480 | -2.75010 |
| H | 1.23980 | -0.37080 | -2.23050 |
| H | 1.74760 | -2.01710 | -2.59490 |
| H | 0.79680 | 0.17660 | 0.29070 |
| H | 5.03350 | 0.53980 | 0.05780 |
| H | 5.70920 | -0.68390 | -0.99220 |
| H | -0.30530 | -1.63290 | -0.88750 |
| H | 1.45620 | -2.15510 | 2.14110 |
| H | 1.27960 | -0.48710 | 2.59110 |
| H | 6.31710 | 1.11560 | -2.69950 |
| H | -0.98200 | -2.24730 | 1.50550 |
| H | -0.49420 | -1.26290 | 4.39160 |
| H | -2.23700 | -0.45630 | 2.12840 |
| H | 6.34420 | 2.56990 | -0.01260 |
| H | 7.61690 | 3.14430 | -2.76880 |
| H | 9.46970 | 4.22770 | -1.53150 |
| H | 8.73160 | 3.79240 | 0.00670 |
| H | 9.34130 | 2.53350 | -1.06790 |
| H | -1.41290 | -5.16620 | 4.39270 |
| H | 5.37090 | 5.90730 | -2.37730 |
| H | 5.92090 | 4.66490 | -3.49950 |
| H | 4.90610 | 4.23120 | -2.11320 |

| Marilzafurollene C_74 | | | |
|------------------------------|----------|----------|----------|
| C | 3.22620 | -1.21530 | -0.71740 |
| O | 2.32190 | -1.23710 | 0.38780 |
| C | 3.72630 | 0.21730 | -0.98250 |
| C | 2.48450 | -1.87050 | -1.89010 |
| C | 1.09620 | -1.85640 | 0.00180 |
| C | 4.57350 | 0.75500 | 0.18980 |
| Br | 2.15750 | 1.42250 | -1.26960 |
| C | 1.46980 | -2.74860 | -1.18720 |
| C | 0.42180 | -2.55550 | 1.19810 |
| C | 5.29370 | 2.07610 | -0.04810 |
| Cl | 2.25340 | -4.27130 | -0.66920 |
| C | -0.02660 | -1.57390 | 2.29500 |
| C | -0.84540 | -2.26960 | 3.36430 |
| O | 1.12330 | -1.01040 | 2.88690 |
| C | -2.08920 | -1.95330 | 3.64360 |
| C | 5.32430 | 2.79150 | -1.18760 |
| C | 6.06800 | 4.10300 | -1.35610 |
| C | 5.10480 | 5.22930 | -1.73930 |
| O | 7.03960 | 4.01290 | -2.38810 |
| C | -3.33510 | -1.63490 | 3.90370 |
| Br | -4.86360 | -2.48620 | 2.97720 |
| C | 8.16850 | 3.21490 | -2.05910 |
| H | 4.07190 | -1.85220 | -0.45270 |
| H | 4.31770 | 0.21590 | -1.89900 |
| H | 1.96170 | -1.12360 | -2.48790 |
| H | 3.14500 | -2.42430 | -2.55780 |
| H | 0.43800 | -1.06650 | -0.36520 |
| H | 3.94220 | 0.86150 | 1.07290 |
| H | 5.33760 | 0.02170 | 0.44960 |
| H | 0.61510 | -3.00320 | -1.81500 |
| H | -0.45140 | -3.09640 | 0.83040 |
| H | 1.08490 | -3.30720 | 1.62800 |
| H | 5.83330 | 2.45430 | 0.80860 |
| H | -0.61290 | -0.76940 | 1.84500 |
| H | -0.34730 | -3.06070 | 3.90560 |
| H | 1.74980 | -0.85620 | 2.18340 |
| H | 4.79870 | 2.45100 | -2.06670 |
| H | 6.55660 | 4.37300 | -0.41780 |
| H | 5.63610 | 6.17510 | -1.84560 |
| H | 4.60770 | 5.01900 | -2.68660 |
| H | 4.33470 | 5.36360 | -0.97920 |
| H | -3.64480 | -0.89690 | 4.62930 |
| H | 8.68140 | 3.60060 | -1.17710 |
| H | 7.89110 | 2.17640 | -1.87540 |
| H | 8.87600 | 3.22670 | -2.88800 |

| Marilzafurollene C_75 | | | |
|------------------------------|----------|----------|----------|
| C | 3.16660 | -1.40920 | -1.75320 |
| O | 2.37670 | -0.78370 | -0.73920 |
| C | 3.26880 | -0.51050 | -3.00410 |
| C | 2.51280 | -2.77520 | -2.00020 |
| C | 1.28780 | -1.62640 | -0.37370 |
| C | 4.23590 | 0.68170 | -2.85690 |
| Br | 1.45870 | 0.16790 | -3.50160 |
| C | 1.78330 | -3.03710 | -0.69730 |
| C | 0.85080 | -1.35440 | 1.07730 |
| C | 3.97170 | 1.53960 | -1.63350 |
| Cl | 2.93610 | -3.63950 | 0.53050 |
| C | 0.19710 | 0.03660 | 1.25080 |
| C | -0.35670 | 0.32830 | 2.63860 |
| O | 1.15250 | 1.02180 | 0.92550 |
| C | -0.33670 | -0.49440 | 3.66410 |
| C | 4.90020 | 1.84220 | -0.71100 |
| C | 4.64740 | 2.66630 | 0.53660 |
| C | 5.38630 | 4.00470 | 0.46260 |
| O | 5.12860 | 1.99070 | 1.68950 |
| C | -0.33280 | -1.32570 | 4.67910 |
| Br | -1.81070 | -2.59980 | 5.01110 |
| C | 4.31450 | 0.90330 | 2.10660 |
| H | 4.16290 | -1.57630 | -1.34050 |
| H | 3.61340 | -1.11320 | -3.84590 |
| H | 1.78860 | -2.71040 | -2.81350 |
| H | 3.23160 | -3.55410 | -2.25610 |
| H | 0.45580 | -1.40050 | -1.04340 |
| H | 5.26010 | 0.30970 | -2.80980 |
| H | 4.17870 | 1.31220 | -3.74460 |
| H | 0.97590 | -3.76380 | -0.79430 |
| H | 0.13560 | -2.12580 | 1.36650 |
| H | 1.70260 | -1.45420 | 1.75150 |
| H | 2.96270 | 1.91100 | -1.51940 |
| H | -0.63150 | 0.12800 | 0.54650 |
| H | -0.79680 | 1.30820 | 2.75310 |
| H | 1.70430 | 0.65620 | 0.23590 |
| H | 5.91050 | 1.47860 | -0.82950 |
| H | 3.57830 | 2.86460 | 0.63970 |
| H | 5.19910 | 4.59940 | 1.35680 |
| H | 6.46340 | 3.85780 | 0.38050 |
| H | 5.05880 | 4.58750 | -0.39860 |
| H | 0.45480 | -1.39830 | 5.41480 |
| H | 4.78200 | 0.40230 | 2.95390 |
| H | 3.33520 | 1.25480 | 2.43150 |
| H | 4.17720 | 0.16330 | 1.31690 |

| Marilzafurollene C_76 | | | |
|------------------------------|----------|----------|----------|
| C | 2.78860 | -1.86920 | -1.44090 |
| O | 2.24870 | -1.99970 | -0.12590 |
| C | 3.25930 | -0.42410 | -1.69740 |
| C | 1.70690 | -2.37830 | -2.40590 |
| C | 0.89450 | -2.42820 | -0.19900 |
| C | 4.36540 | 0.00500 | -0.71800 |
| Br | 1.71930 | 0.83780 | -1.53320 |
| C | 0.82690 | -3.22410 | -1.50820 |
| C | 0.46070 | -3.17960 | 1.07510 |
| C | 4.90000 | 1.39280 | -1.01320 |
| Cl | 1.54290 | -4.85660 | -1.35180 |
| C | 0.56580 | -2.34800 | 2.36670 |
| C | -0.29590 | -1.09900 | 2.34450 |
| O | 0.15630 | -3.16900 | 3.44200 |
| C | 0.15870 | 0.09600 | 2.64810 |
| C | 4.90450 | 2.40600 | -0.13100 |
| C | 5.41930 | 3.80200 | -0.42700 |
| C | 6.62390 | 4.13860 | 0.45520 |
| O | 4.42700 | 4.78570 | -0.17180 |
| C | 0.60810 | 1.27720 | 3.00210 |
| Br | 1.41360 | 2.55360 | 1.72340 |
| C | 3.30920 | 4.73360 | -1.04880 |
| H | 3.64570 | -2.54210 | -1.49660 |
| H | 3.62700 | -0.34520 | -2.72120 |
| H | 1.11850 | -1.55480 | -2.80980 |
| H | 2.11630 | -2.93180 | -3.25130 |
| H | 0.27720 | -1.53630 | -0.31750 |
| H | 3.98750 | -0.03440 | 0.30500 |
| H | 5.19830 | -0.69670 | -0.76930 |
| H | -0.18980 | -3.33490 | -1.88640 |
| H | -0.56330 | -3.53280 | 0.94870 |
| H | 1.07490 | -4.07160 | 1.19820 |
| H | 5.29510 | 1.55210 | -2.00610 |
| H | 1.61190 | -2.07450 | 2.52460 |
| H | -1.32890 | -1.23530 | 2.05890 |
| H | 0.43950 | -2.76900 | 4.25200 |
| H | 4.50980 | 2.25140 | 0.86330 |
| H | 5.72750 | 3.86360 | -1.47250 |
| H | 7.00210 | 5.13590 | 0.23040 |
| H | 6.35710 | 4.11520 | 1.51200 |
| H | 7.43790 | 3.43060 | 0.29750 |
| H | 0.58470 | 1.66570 | 4.00970 |
| H | 3.61700 | 4.83810 | -2.08980 |
| H | 2.75110 | 3.80280 | -0.94180 |
| H | 2.62790 | 5.55220 | -0.81740 |

| Marilzafurollene C_77 | | | |
|------------------------------|----------|----------|----------|
| C | 3.39380 | -1.80060 | -1.83550 |
| O | 2.72630 | -1.40060 | -0.63750 |
| C | 3.68850 | -0.58640 | -2.74160 |
| C | 2.49480 | -2.86830 | -2.47400 |
| C | 1.49530 | -2.10370 | -0.49730 |
| C | 4.80190 | 0.35080 | -2.22820 |
| Br | 2.01970 | 0.47060 | -3.03300 |
| C | 1.70710 | -3.39570 | -1.29130 |
| C | 1.11750 | -2.25580 | 0.98860 |
| C | 4.51850 | 0.95630 | -0.86590 |
| Cl | 2.69680 | -4.58390 | -0.39210 |
| C | 0.79430 | -0.91200 | 1.66720 |
| C | 0.29550 | -1.11030 | 3.08500 |
| O | 1.96870 | -0.13050 | 1.69390 |
| C | -0.91000 | -0.77420 | 3.48450 |
| C | 4.26400 | 2.25570 | -0.64270 |
| C | 3.96650 | 2.84680 | 0.72250 |
| C | 2.57300 | 3.47830 | 0.74800 |
| O | 4.89940 | 3.86540 | 1.05450 |
| C | -2.11800 | -0.45560 | 3.88600 |
| Br | -2.56180 | 1.32690 | 4.62380 |
| C | 6.19980 | 3.38270 | 1.36220 |
| H | 4.33310 | -2.27300 | -1.54370 |
| H | 3.99350 | -0.95320 | -3.72290 |
| H | 1.80840 | -2.41510 | -3.19020 |
| H | 3.05590 | -3.64250 | -2.99800 |
| H | 0.72500 | -1.51840 | -1.00330 |
| H | 5.74390 | -0.19460 | -2.16350 |
| H | 4.96020 | 1.15100 | -2.95210 |
| H | 0.77280 | -3.87910 | -1.57890 |
| H | 0.24370 | -2.90520 | 1.05720 |
| H | 1.91480 | -2.76100 | 1.53530 |
| H | 4.52150 | 0.27010 | -0.03110 |
| H | 0.04130 | -0.38050 | 1.08080 |
| H | 0.99740 | -1.55110 | 3.77770 |
| H | 2.41130 | -0.27250 | 0.86010 |
| H | 4.25720 | 2.95070 | -1.46980 |
| H | 3.99860 | 2.06000 | 1.47920 |
| H | 2.35280 | 3.89030 | 1.73280 |
| H | 2.48900 | 4.28570 | 0.02060 |
| H | 1.80560 | 2.73700 | 0.52130 |
| H | -2.97200 | -1.11630 | 3.85570 |
| H | 6.65680 | 2.87800 | 0.51040 |
| H | 6.84290 | 4.21920 | 1.63550 |
| H | 6.17510 | 2.69140 | 2.20550 |

| Marilzafurollene C_78 | | | |
|------------------------------|----------|----------|----------|
| C | 2.98720 | -1.42420 | -0.95950 |
| O | 1.85290 | -1.24550 | -0.11050 |
| C | 3.48180 | -0.06780 | -1.49500 |
| C | 2.56020 | -2.42880 | -2.03760 |
| C | 0.77270 | -2.06100 | -0.56120 |
| C | 4.02000 | 0.83660 | -0.37350 |
| Br | 1.98730 | 0.87070 | -2.43170 |
| C | 1.44280 | -3.18920 | -1.35360 |
| C | -0.13140 | -2.49060 | 0.61090 |
| C | 4.62930 | 2.11980 | -0.90420 |
| Cl | 2.13950 | -4.44370 | -0.28530 |
| C | -0.86540 | -1.31220 | 1.27590 |
| C | -1.91140 | -1.79930 | 2.27290 |
| O | 0.09750 | -0.46820 | 1.88210 |
| C | -1.89730 | -1.57740 | 3.56940 |
| C | 5.91450 | 2.47700 | -0.74470 |
| C | 6.52060 | 3.76280 | -1.27570 |
| C | 7.65420 | 3.46510 | -2.26040 |
| O | 7.07260 | 4.54300 | -0.22520 |
| C | -1.86300 | -1.35380 | 4.86180 |
| Br | -0.99660 | -2.59680 | 6.13750 |
| C | 6.10530 | 5.14560 | 0.62410 |
| H | 3.77130 | -1.88470 | -0.35610 |
| H | 4.27000 | -0.23660 | -2.23070 |
| H | 2.16300 | -1.91590 | -2.91380 |
| H | 3.37630 | -3.06990 | -2.37210 |
| H | 0.18700 | -1.46140 | -1.26070 |
| H | 3.21670 | 1.08970 | 0.31970 |
| H | 4.77080 | 0.29790 | 0.20620 |
| H | 0.76590 | -3.67870 | -2.05480 |
| H | -0.86800 | -3.20010 | 0.23160 |
| H | 0.44620 | -3.02840 | 1.36400 |
| H | 3.95950 | 2.77530 | -1.44330 |
| H | -1.38620 | -0.73270 | 0.51180 |
| H | -2.72330 | -2.36790 | 1.84330 |
| H | 0.86990 | -0.47870 | 1.32100 |
| H | 6.58940 | 1.82870 | -0.20450 |
| H | 5.75570 | 4.34180 | -1.79710 |
| H | 8.07940 | 4.38930 | -2.65210 |
| H | 8.45870 | 2.90710 | -1.78070 |
| H | 7.29640 | 2.87930 | -3.10750 |
| H | -2.29550 | -0.49220 | 5.34830 |
| H | 5.50280 | 4.40060 | 1.14490 |
| H | 6.60960 | 5.74940 | 1.37850 |
| H | 5.43970 | 5.80170 | 0.06180 |

| Marilzafurollene C_79 | | | |
|------------------------------|----------|----------|----------|
| C | 2.66780 | -1.63830 | -1.37520 |
| O | 2.27390 | -1.75360 | -0.00830 |
| C | 3.14720 | -0.20960 | -1.69030 |
| C | 1.47140 | -2.12100 | -2.20340 |
| C | 0.98240 | -2.34900 | 0.08360 |
| C | 4.41350 | 0.16220 | -0.90040 |
| Br | 1.70330 | 1.09930 | -1.25590 |
| C | 0.78830 | -3.07980 | -1.25100 |
| C | 0.86820 | -3.21520 | 1.35270 |
| C | 4.95680 | 1.52640 | -1.27930 |
| Cl | 1.62680 | -4.66050 | -1.28990 |
| C | 0.86980 | -2.39430 | 2.65490 |
| C | -0.41580 | -1.61190 | 2.84690 |
| O | 1.02500 | -3.28040 | 3.74470 |
| C | -0.46930 | -0.30140 | 2.91670 |
| C | 5.12520 | 2.54220 | -0.41660 |
| C | 5.65440 | 3.91290 | -0.79480 |
| C | 6.95680 | 4.21990 | -0.05160 |
| O | 4.72850 | 4.93560 | -0.45650 |
| C | -0.54750 | 1.00610 | 2.98800 |
| Br | -0.84800 | 2.14060 | 1.39510 |
| C | 3.54050 | 4.93110 | -1.23740 |
| H | 3.49190 | -2.33680 | -1.52980 |
| H | 3.34530 | -0.12570 | -2.75970 |
| H | 0.79520 | -1.29680 | -2.43110 |
| H | 1.76180 | -2.58270 | -3.14740 |
| H | 0.25530 | -1.53620 | 0.12460 |
| H | 4.20360 | 0.12950 | 0.16990 |
| H | 5.19570 | -0.57440 | -1.08610 |
| H | -0.26160 | -3.24810 | -1.49310 |
| H | -0.03780 | -3.82070 | 1.30460 |
| H | 1.70200 | -3.91740 | 1.37030 |
| H | 5.21580 | 1.66530 | -2.31910 |
| H | 1.72230 | -1.71050 | 2.65150 |
| H | -1.31850 | -2.19870 | 2.93270 |
| H | 1.92380 | -3.57790 | 3.76520 |
| H | 4.86650 | 2.40840 | 0.62400 |
| H | 5.85330 | 3.94540 | -1.86780 |
| H | 7.34370 | 5.19850 | -0.33600 |
| H | 6.80380 | 4.22470 | 1.02790 |
| H | 7.72440 | 3.47990 | -0.27950 |
| H | -0.46110 | 1.58070 | 3.89850 |
| H | 2.91250 | 5.77380 | -0.94840 |
| H | 3.76440 | 5.03020 | -2.30020 |
| H | 2.95900 | 4.02080 | -1.08670 |

| Marilzafurollene C_80 | | | |
|------------------------------|----------|----------|----------|
| C | 2.80870 | -1.21060 | -0.85780 |
| O | 1.81980 | -0.92190 | 0.13120 |
| C | 3.37350 | 0.09150 | -1.45520 |
| C | 2.13990 | -2.15050 | -1.86930 |
| C | 0.60830 | -1.60980 | -0.17530 |
| C | 4.14730 | 0.91840 | -0.41460 |
| Br | 1.88080 | 1.19730 | -2.19060 |
| C | 1.04490 | -2.79470 | -1.04420 |
| C | -0.18330 | -1.95000 | 1.10290 |
| C | 4.81820 | 2.13530 | -1.02180 |
| Cl | 1.73560 | -4.12790 | -0.07190 |
| C | -0.69460 | -0.69630 | 1.85000 |
| C | -1.62310 | -0.97010 | 3.02600 |
| O | 0.42340 | 0.02860 | 2.31390 |
| C | -2.05210 | -2.15120 | 3.41400 |
| C | 6.14440 | 2.34920 | -1.03260 |
| C | 6.81250 | 3.56910 | -1.63920 |
| C | 7.76770 | 3.16430 | -2.76480 |
| O | 7.57950 | 4.26990 | -0.67100 |
| C | -2.49280 | -3.32160 | 3.81130 |
| Br | -1.52940 | -4.42850 | 5.13990 |
| C | 6.80380 | 4.96080 | 0.29910 |
| H | 3.61000 | -1.75980 | -0.36060 |
| H | 4.03670 | -0.15170 | -2.28700 |
| H | 1.69040 | -1.58730 | -2.68750 |
| H | 2.83180 | -2.87130 | -2.30570 |
| H | 0.00810 | -0.94230 | -0.79660 |
| H | 3.47290 | 1.24760 | 0.37700 |
| H | 4.90410 | 0.29470 | 0.06310 |
| H | 0.23460 | -3.20140 | -1.65020 |
| H | -1.03290 | -2.56930 | 0.81230 |
| H | 0.42300 | -2.55710 | 1.77680 |
| H | 4.15920 | 2.86650 | -1.46880 |
| H | -1.23930 | -0.06200 | 1.14860 |
| H | -1.93450 | -0.08950 | 3.56890 |
| H | 1.11010 | -0.06790 | 1.65720 |
| H | 6.80930 | 1.62440 | -0.58520 |
| H | 6.05370 | 4.23500 | -2.05510 |
| H | 8.23620 | 4.04240 | -3.20950 |
| H | 8.56240 | 2.51580 | -2.39520 |
| H | 7.23990 | 2.63270 | -3.55700 |
| H | -3.40180 | -3.78940 | 3.46230 |
| H | 6.19810 | 4.27750 | 0.89530 |
| H | 7.46570 | 5.49610 | 0.97990 |
| H | 6.14490 | 5.69260 | -0.16990 |

| Marilzafurollene C_81 | | | |
|------------------------------|----------|----------|----------|
| C | 2.95530 | -1.77820 | -1.70450 |
| O | 2.72520 | -1.48590 | -0.32810 |
| C | 3.61960 | -0.60240 | -2.45360 |
| C | 1.60970 | -2.26970 | -2.24610 |
| C | 1.47390 | -2.03380 | 0.08950 |
| C | 2.84930 | 0.73290 | -2.49140 |
| Br | 3.96040 | -1.17540 | -4.33120 |
| C | 1.03340 | -2.97830 | -1.03780 |
| C | 1.58390 | -2.65400 | 1.49630 |
| C | 2.76220 | 1.40540 | -1.13580 |
| Cl | 1.75760 | -4.60840 | -0.88680 |
| C | 1.73240 | -1.60840 | 2.61620 |
| C | 0.44620 | -0.83580 | 2.84260 |
| O | 2.07160 | -2.28410 | 3.80960 |
| C | 0.32540 | 0.45880 | 2.65760 |
| C | 3.42970 | 2.51900 | -0.79280 |
| C | 3.35240 | 3.17530 | 0.57220 |
| C | 2.86540 | 4.62170 | 0.45880 |
| O | 4.62450 | 3.20370 | 1.20270 |
| C | 0.16770 | 1.74390 | 2.44760 |
| Br | -0.39720 | 2.46110 | 0.69190 |
| C | 5.09360 | 1.93010 | 1.62540 |
| H | 3.65100 | -2.61880 | -1.72380 |
| H | 4.60050 | -0.42460 | -2.01010 |
| H | 0.96630 | -1.43430 | -2.51910 |
| H | 1.70990 | -2.91630 | -3.11830 |
| H | 0.76180 | -1.20750 | 0.10900 |
| H | 3.36350 | 1.41080 | -3.17380 |
| H | 1.84670 | 0.60500 | -2.89730 |
| H | -0.04930 | -3.09790 | -1.08960 |
| H | 0.71000 | -3.27580 | 1.69500 |
| H | 2.44300 | -3.32580 | 1.51550 |
| H | 2.11660 | 0.93290 | -0.40980 |
| H | 2.54910 | -0.92750 | 2.36410 |
| H | -0.40220 | -1.41810 | 3.17320 |
| H | 2.40080 | -1.65410 | 4.43490 |
| H | 4.07910 | 2.99960 | -1.51030 |
| H | 2.65290 | 2.62480 | 1.20280 |
| H | 2.79290 | 5.08460 | 1.44300 |
| H | 3.54790 | 5.22310 | -0.14200 |
| H | 1.87890 | 4.66860 | -0.00340 |
| H | 0.32520 | 2.51730 | 3.18540 |
| H | 6.05210 | 2.04490 | 2.13140 |
| H | 4.39900 | 1.46580 | 2.32670 |
| H | 5.24270 | 1.25220 | 0.78410 |

| Marilzafurollene C_82 | | | |
|------------------------------|----------|----------|----------|
| C | 3.12110 | -1.48920 | -0.17580 |
| O | 2.13580 | -1.93020 | 0.75770 |
| C | 3.51540 | -0.03510 | 0.14130 |
| C | 2.49250 | -1.69690 | -1.56230 |
| C | 0.94540 | -2.30940 | 0.07900 |
| C | 4.62060 | 0.50780 | -0.78180 |
| Br | 4.16120 | 0.04270 | 2.02780 |
| C | 1.43190 | -2.74810 | -1.30380 |
| C | 0.14240 | -3.34280 | 0.89400 |
| C | 4.91300 | 1.97440 | -0.53100 |
| Cl | 2.18740 | -4.36940 | -1.27470 |
| C | -0.32930 | -2.80120 | 2.25670 |
| C | -1.29230 | -1.63660 | 2.11970 |
| O | -0.96510 | -3.84270 | 2.96920 |
| C | -0.97750 | -0.40400 | 2.44720 |
| C | 4.76800 | 2.94830 | -1.44490 |
| C | 5.05950 | 4.41530 | -1.18930 |
| C | 3.80260 | 5.26430 | -1.39570 |
| O | 6.04830 | 4.90600 | -2.08280 |
| C | -0.61840 | 0.82600 | 2.72710 |
| Br | 0.22020 | 2.00570 | 1.37610 |
| C | 7.36000 | 4.42520 | -1.82180 |
| H | 3.98740 | -2.14310 | -0.06430 |
| H | 2.63250 | 0.60350 | 0.08560 |
| H | 2.01230 | -0.77850 | -1.90290 |
| H | 3.21780 | -1.99450 | -2.32020 |
| H | 0.34680 | -1.40700 | -0.05550 |
| H | 5.53910 | -0.06300 | -0.64070 |
| H | 4.33320 | 0.38130 | -1.82590 |
| H | 0.64010 | -2.75480 | -2.05370 |
| H | -0.71770 | -3.67500 | 0.31140 |
| H | 0.75910 | -4.22590 | 1.06080 |
| H | 5.26110 | 2.22630 | 0.46110 |
| H | 0.54310 | -2.48300 | 2.83310 |
| H | -2.27190 | -1.86880 | 1.72840 |
| H | -0.29970 | -4.42680 | 3.30540 |
| H | 4.42330 | 2.70560 | -2.43970 |
| H | 5.39870 | 4.54860 | -0.16000 |
| H | 4.00850 | 6.31600 | -1.19640 |
| H | 3.43590 | 5.18620 | -2.41950 |
| H | 3.00130 | 4.95010 | -0.72620 |
| H | -0.73680 | 1.30390 | 3.68860 |
| H | 7.42440 | 3.34230 | -1.93350 |
| H | 8.05870 | 4.87290 | -2.52830 |
| H | 7.68580 | 4.69220 | -0.81570 |

| Marilzafurollene C_83 | | | |
|------------------------------|----------|----------|----------|
| C | 2.62140 | -0.59780 | -0.56050 |
| O | 2.56330 | -0.60920 | 0.86560 |
| C | 3.04350 | 0.78930 | -1.08040 |
| C | 1.25050 | -1.08210 | -1.04550 |
| C | 1.28500 | -1.05860 | 1.30640 |
| C | 4.47690 | 1.15270 | -0.65840 |
| Br | 1.78670 | 2.18210 | -0.39280 |
| C | 0.75820 | -1.89700 | 0.13170 |
| C | 1.41280 | -1.73640 | 2.68840 |
| C | 4.95230 | 2.45390 | -1.27550 |
| Cl | 1.49500 | -3.52740 | 0.07740 |
| C | 0.07670 | -2.01840 | 3.40660 |
| C | -0.71790 | -3.14760 | 2.77720 |
| O | 0.34620 | -2.34340 | 4.75510 |
| C | -1.94820 | -3.00620 | 2.33950 |
| C | 6.00250 | 2.56560 | -2.10570 |
| C | 6.47670 | 3.86950 | -2.72010 |
| C | 6.41300 | 3.80690 | -4.24820 |
| O | 7.82490 | 4.14340 | -2.36800 |
| C | -3.16040 | -2.84180 | 1.86670 |
| Br | -3.48940 | -2.27130 | 0.00030 |
| C | 8.00860 | 4.51560 | -1.00870 |
| H | 3.36750 | -1.33720 | -0.85590 |
| H | 2.97460 | 0.80110 | -2.16930 |
| H | 0.57460 | -0.24260 | -1.20920 |
| H | 1.30100 | -1.65170 | -1.97380 |
| H | 0.65960 | -0.16940 | 1.40530 |
| H | 4.53500 | 1.23610 | 0.42760 |
| H | 5.15960 | 0.35140 | -0.94400 |
| H | -0.32570 | -2.01080 | 0.13140 |
| H | 2.01720 | -2.64070 | 2.61960 |
| H | 1.98860 | -1.05360 | 3.31500 |
| H | 4.38930 | 3.33780 | -1.01000 |
| H | -0.52400 | -1.10590 | 3.41280 |
| H | -0.21880 | -4.10230 | 2.69320 |
| H | 0.96510 | -3.05850 | 4.78610 |
| H | 6.57190 | 1.68690 | -2.37300 |
| H | 5.83790 | 4.68830 | -2.38270 |
| H | 7.05580 | 3.01780 | -4.63900 |
| H | 5.39640 | 3.61480 | -4.59250 |
| H | 6.73990 | 4.74920 | -4.68830 |
| H | -4.07130 | -2.99420 | 2.42730 |
| H | 7.72120 | 3.71470 | -0.32670 |
| H | 9.06060 | 4.73910 | -0.83180 |
| H | 7.43190 | 5.40790 | -0.76190 |

| Marilzafurollene C_84 | | | |
|------------------------------|----------|----------|----------|
| C | 2.85140 | -0.21040 | -1.12610 |
| O | 1.94040 | -0.29020 | -0.02920 |
| C | 2.46880 | 0.94900 | -2.07050 |
| C | 2.85430 | -1.59860 | -1.77810 |
| C | 1.42280 | -1.61490 | 0.08100 |
| C | 2.59820 | 2.34010 | -1.41690 |
| Br | 0.56910 | 0.72590 | -2.63960 |
| C | 2.45500 | -2.49940 | -0.62770 |
| C | 1.10600 | -1.96990 | 1.54680 |
| C | 4.01230 | 2.80510 | -1.09540 |
| Cl | 3.88330 | -2.82790 | 0.39860 |
| C | -0.01820 | -1.10710 | 2.14630 |
| C | -0.42950 | -1.60290 | 3.51850 |
| O | 0.44800 | 0.22010 | 2.25510 |
| C | -1.64200 | -2.01950 | 3.80390 |
| C | 5.16270 | 2.25640 | -1.52740 |
| C | 6.54400 | 2.76160 | -1.15630 |
| C | 7.31870 | 3.19740 | -2.40250 |
| O | 7.30630 | 1.74400 | -0.52390 |
| C | -2.85400 | -2.44420 | 4.07170 |
| Br | -3.38850 | -4.33730 | 3.84880 |
| C | 6.86520 | 1.41080 | 0.78590 |
| H | 3.84060 | -0.03910 | -0.70100 |
| H | 3.06810 | 0.91040 | -2.98070 |
| H | 2.10200 | -1.66220 | -2.56460 |
| H | 3.81660 | -1.86180 | -2.21820 |
| H | 0.49900 | -1.64670 | -0.49990 |
| H | 2.15400 | 3.09030 | -2.07160 |
| H | 2.01450 | 2.35830 | -0.49560 |
| H | 2.04480 | -3.45570 | -0.95430 |
| H | 0.80670 | -3.01830 | 1.58790 |
| H | 2.00070 | -1.88570 | 2.16490 |
| H | 4.06600 | 3.67340 | -0.45370 |
| H | -0.88050 | -1.11650 | 1.47560 |
| H | 0.33990 | -1.59790 | 4.27660 |
| H | 0.96890 | 0.39530 | 1.47430 |
| H | 5.15500 | 1.39510 | -2.17760 |
| H | 6.45580 | 3.61990 | -0.48720 |
| H | 6.79540 | 3.99300 | -2.93360 |
| H | 8.30620 | 3.57230 | -2.13290 |
| H | 7.45740 | 2.36560 | -3.09350 |
| H | -3.66060 | -1.82190 | 4.43100 |
| H | 5.85470 | 1.00020 | 0.78200 |
| H | 7.52610 | 0.65530 | 1.21070 |
| H | 6.88610 | 2.28060 | 1.44370 |

| Marilzafurollene C_85 | | | |
|------------------------------|----------|----------|----------|
| C | 2.66030 | -1.61480 | -1.40230 |
| O | 2.27120 | -1.73190 | -0.03460 |
| C | 3.14940 | -0.18940 | -1.71680 |
| C | 1.45620 | -2.08660 | -2.22410 |
| C | 0.99940 | -2.36940 | 0.06380 |
| C | 4.43170 | 0.16470 | -0.94480 |
| Br | 1.72570 | 1.13170 | -1.25370 |
| C | 0.79880 | -3.07480 | -1.28380 |
| C | 0.92440 | -3.26570 | 1.31560 |
| C | 4.99080 | 1.51970 | -1.33370 |
| Cl | 1.65660 | -4.64330 | -1.36840 |
| C | 0.91120 | -2.47470 | 2.63580 |
| C | -0.39420 | -1.73030 | 2.84500 |
| O | 1.08650 | -3.38890 | 3.69930 |
| C | -0.48400 | -0.42270 | 2.93140 |
| C | 5.19240 | 2.53250 | -0.47450 |
| C | 5.73810 | 3.89380 | -0.86260 |
| C | 7.05580 | 4.18090 | -0.13840 |
| O | 4.83360 | 4.93160 | -0.51310 |
| C | -0.60150 | 0.88200 | 3.00050 |
| Br | -0.94380 | 2.00010 | 1.40470 |
| C | 3.63600 | 4.94640 | -1.27910 |
| H | 3.47790 | -2.31920 | -1.56410 |
| H | 3.33230 | -0.10220 | -2.78860 |
| H | 0.76970 | -1.26250 | -2.41960 |
| H | 1.73570 | -2.52260 | -3.18350 |
| H | 0.25170 | -1.57760 | 0.13280 |
| H | 4.23660 | 0.13510 | 0.12830 |
| H | 5.20040 | -0.58340 | -1.14120 |
| H | -0.25190 | -3.25230 | -1.51580 |
| H | 0.03960 | -3.90100 | 1.26220 |
| H | 1.78180 | -3.93960 | 1.31550 |
| H | 5.23310 | 1.65430 | -2.37800 |
| H | 1.75280 | -1.77770 | 2.64140 |
| H | -1.28100 | -2.34250 | 2.92430 |
| H | 1.34880 | -2.90760 | 4.47130 |
| H | 4.95050 | 2.40290 | 0.57070 |
| H | 5.92250 | 3.92140 | -1.93840 |
| H | 7.80800 | 3.42820 | -0.37590 |
| H | 7.45440 | 5.15270 | -0.43010 |
| H | 6.91810 | 4.18980 | 0.94310 |
| H | -0.52940 | 1.46270 | 3.90840 |
| H | 3.84840 | 5.04310 | -2.34450 |
| H | 3.04240 | 4.04510 | -1.12220 |
| H | 3.02500 | 5.79850 | -0.98190 |

| Marilzafurollene C_86 | | | |
|------------------------------|----------|----------|----------|
| C | 3.38410 | -1.47810 | -1.81560 |
| O | 2.40830 | -1.08400 | -0.84940 |
| C | 3.46050 | -0.45370 | -2.96680 |
| C | 2.98700 | -2.89560 | -2.24710 |
| C | 1.45390 | -2.12380 | -0.65680 |
| C | 4.19050 | 0.85650 | -2.60840 |
| Br | 1.62260 | -0.02770 | -3.61910 |
| C | 2.20100 | -3.39930 | -1.05270 |
| C | 0.87710 | -2.06670 | 0.76940 |
| C | 3.64500 | 1.54960 | -1.37310 |
| Cl | 3.32610 | -3.94160 | 0.22780 |
| C | -0.02030 | -0.83800 | 1.00630 |
| C | -0.64500 | -0.87200 | 2.39630 |
| O | 0.74630 | 0.33450 | 0.79540 |
| C | -0.40970 | -0.00880 | 3.36050 |
| C | 4.39710 | 1.92390 | -0.32450 |
| C | 3.86760 | 2.59380 | 0.92880 |
| C | 4.35590 | 4.04180 | 1.01730 |
| O | 4.33950 | 1.92830 | 2.09090 |
| C | -0.14420 | 0.85210 | 4.31390 |
| Br | 1.31300 | 0.56860 | 5.62470 |
| C | 3.67010 | 0.70620 | 2.37000 |
| H | 4.34900 | -1.53180 | -1.30860 |
| H | 3.98810 | -0.90640 | -3.80780 |
| H | 2.33450 | -2.86050 | -3.12050 |
| H | 3.84310 | -3.52320 | -2.49620 |
| H | 0.64710 | -1.96860 | -1.37580 |
| H | 5.25010 | 0.64810 | -2.45520 |
| H | 4.13230 | 1.54880 | -3.44880 |
| H | 1.53500 | -4.22820 | -1.29500 |
| H | 0.29360 | -2.97120 | 0.94600 |
| H | 1.68470 | -2.07780 | 1.50290 |
| H | 2.58050 | 1.73860 | -1.36170 |
| H | -0.83300 | -0.83850 | 0.27790 |
| H | -1.33620 | -1.68400 | 2.56940 |
| H | 1.41670 | 0.11730 | 0.14960 |
| H | 5.46190 | 1.74230 | -0.33810 |
| H | 2.77540 | 2.59620 | 0.91580 |
| H | 3.96990 | 4.52520 | 1.91500 |
| H | 5.44430 | 4.09060 | 1.05520 |
| H | 4.02180 | 4.62260 | 0.15730 |
| H | -0.67910 | 1.77590 | 4.47640 |
| H | 2.62180 | 0.88560 | 2.60890 |
| H | 3.72500 | 0.00660 | 1.53480 |
| H | 4.12650 | 0.22870 | 3.23670 |

| Marilzafurollene C_87 | | | |
|------------------------------|----------|----------|----------|
| C | 3.12860 | -1.50360 | -0.21040 |
| O | 2.13440 | -1.94420 | 0.71350 |
| C | 3.52640 | -0.05210 | 0.11370 |
| C | 2.51050 | -1.70510 | -1.60230 |
| C | 0.95600 | -2.34120 | 0.02320 |
| C | 4.64230 | 0.48760 | -0.79840 |
| Br | 4.15510 | 0.01970 | 2.00610 |
| C | 1.45850 | -2.76830 | -1.35780 |
| C | 0.15500 | -3.38610 | 0.82630 |
| C | 4.93940 | 1.95240 | -0.54220 |
| Cl | 2.23120 | -4.38150 | -1.33300 |
| C | -0.31090 | -2.86730 | 2.19950 |
| C | -1.25090 | -1.68180 | 2.08370 |
| O | -0.97170 | -3.91740 | 2.87590 |
| C | -0.91960 | -0.46530 | 2.45270 |
| C | 4.80650 | 2.92880 | -1.45530 |
| C | 5.10310 | 4.39380 | -1.19450 |
| C | 3.85180 | 5.24920 | -1.40770 |
| O | 6.10030 | 4.88170 | -2.08030 |
| C | -0.54760 | 0.75150 | 2.77100 |
| Br | 0.32300 | 1.95710 | 1.46430 |
| C | 7.40770 | 4.39330 | -1.81220 |
| H | 3.99130 | -2.16140 | -0.09410 |
| H | 2.64700 | 0.59040 | 0.05090 |
| H | 2.02400 | -0.78830 | -1.93810 |
| H | 3.24300 | -1.99020 | -2.35810 |
| H | 0.34690 | -1.44620 | -0.11400 |
| H | 5.55680 | -0.08780 | -0.65050 |
| H | 4.36340 | 0.36460 | -1.84530 |
| H | 0.67280 | -2.77910 | -2.11390 |
| H | -0.70630 | -3.71130 | 0.24190 |
| H | 0.76970 | -4.27260 | 0.98340 |
| H | 5.28060 | 2.20060 | 0.45330 |
| H | 0.57050 | -2.58820 | 2.78230 |
| H | -2.22750 | -1.88300 | 1.66760 |
| H | -0.98600 | -3.71770 | 3.80140 |
| H | 4.46870 | 2.68960 | -2.45330 |
| H | 5.43600 | 4.52340 | -0.16270 |
| H | 4.06140 | 6.29960 | -1.20490 |
| H | 3.49160 | 5.17480 | -2.43400 |
| H | 3.04460 | 4.93760 | -0.74410 |
| H | -0.67200 | 1.20510 | 3.74350 |
| H | 7.46720 | 3.31030 | -1.92630 |
| H | 8.11330 | 4.83900 | -2.51320 |
| H | 7.72850 | 4.65610 | -0.80340 |

| Marilzafurollene C_88 | | | |
|------------------------------|----------|----------|----------|
| C | 3.10590 | -1.47190 | -1.01890 |
| O | 2.00830 | -1.39360 | -0.10870 |
| C | 3.49160 | -0.06940 | -1.52460 |
| C | 2.68410 | -2.46120 | -2.11300 |
| C | 0.95610 | -2.25580 | -0.53770 |
| C | 4.03200 | 0.82500 | -0.39610 |
| Br | 1.89850 | 0.80990 | -2.34970 |
| C | 1.64980 | -3.31210 | -1.40520 |
| C | 0.13830 | -2.78160 | 0.65870 |
| C | 4.53740 | 2.16100 | -0.90530 |
| Cl | 2.47270 | -4.55950 | -0.42150 |
| C | -0.62660 | -1.67380 | 1.40540 |
| C | -1.59860 | -2.25810 | 2.42530 |
| O | 0.32290 | -0.81120 | 2.00680 |
| C | -1.62180 | -1.98010 | 3.71080 |
| C | 5.80570 | 2.58960 | -0.79360 |
| C | 6.30780 | 3.92810 | -1.30250 |
| C | 7.40760 | 3.73530 | -2.34960 |
| O | 6.86300 | 4.70290 | -0.24980 |
| C | -1.62950 | -1.69370 | 4.99120 |
| Br | -2.72120 | -0.22590 | 5.75070 |
| C | 5.90420 | 5.21450 | 0.66610 |
| H | 3.94590 | -1.90510 | -0.47340 |
| H | 4.24970 | -0.16310 | -2.30390 |
| H | 2.21310 | -1.94220 | -2.94810 |
| H | 3.51830 | -3.03910 | -2.51180 |
| H | 0.30180 | -1.66770 | -1.18410 |
| H | 3.25150 | 1.00400 | 0.34450 |
| H | 4.84150 | 0.31220 | 0.12510 |
| H | 0.96800 | -3.81630 | -2.09100 |
| H | -0.57510 | -3.51750 | 0.28530 |
| H | 0.78230 | -3.31380 | 1.36000 |
| H | 3.80410 | 2.79350 | -1.38600 |
| H | -1.21120 | -1.09290 | 0.69000 |
| H | -2.31970 | -2.95530 | 2.02410 |
| H | 1.05480 | -0.73480 | 1.39870 |
| H | 6.54370 | 1.96460 | -0.31160 |
| H | 5.48520 | 4.47730 | -1.76520 |
| H | 7.75750 | 4.69700 | -2.72520 |
| H | 8.26630 | 3.21120 | -1.92950 |
| H | 7.04440 | 3.15880 | -3.20080 |
| H | -1.05790 | -2.21880 | 5.74200 |
| H | 6.40770 | 5.82110 | 1.41870 |
| H | 5.17390 | 5.84790 | 0.16100 |
| H | 5.37330 | 4.41600 | 1.18550 |

| Marilzafurollene C_89 | | | |
|------------------------------|----------|----------|----------|
| C | 2.79070 | -1.85290 | -1.40060 |
| O | 2.25380 | -1.97440 | -0.08340 |
| C | 3.25790 | -0.40860 | -1.66910 |
| C | 1.70800 | -2.37210 | -2.35930 |
| C | 0.89560 | -2.38970 | -0.15080 |
| C | 4.35840 | 0.03360 | -0.68910 |
| Br | 1.71390 | 0.85060 | -1.52340 |
| C | 0.82140 | -3.19980 | -1.45090 |
| C | 0.46390 | -3.12570 | 1.13260 |
| C | 4.88630 | 1.42230 | -0.99230 |
| Cl | 1.52410 | -4.83600 | -1.27380 |
| C | 0.56460 | -2.27300 | 2.41110 |
| C | -0.32580 | -1.04450 | 2.38440 |
| O | 0.19400 | -3.08070 | 3.51040 |
| C | 0.10810 | 0.16540 | 2.65760 |
| C | 4.87580 | 2.44340 | -0.11930 |
| C | 5.38410 | 3.84010 | -0.42310 |
| C | 6.58040 | 4.19130 | 0.46480 |
| O | 4.38410 | 4.81980 | -0.18300 |
| C | 0.54010 | 1.35980 | 2.98750 |
| Br | 1.28720 | 2.63920 | 1.67650 |
| C | 3.27300 | 4.75430 | -1.06770 |
| H | 3.64950 | -2.52400 | -1.45240 |
| H | 3.62960 | -0.33810 | -2.69210 |
| H | 1.12460 | -1.55250 | -2.77780 |
| H | 2.11640 | -2.94080 | -3.19500 |
| H | 0.28440 | -1.49440 | -0.27630 |
| H | 3.97710 | 0.00010 | 0.33280 |
| H | 5.19520 | -0.66400 | -0.73200 |
| H | -0.19620 | -3.30690 | -1.82800 |
| H | -0.55930 | -3.48350 | 1.01080 |
| H | 1.08250 | -4.01340 | 1.26320 |
| H | 5.28930 | 1.57530 | -1.98290 |
| H | 1.60280 | -1.96370 | 2.55430 |
| H | -1.36160 | -1.20950 | 2.12740 |
| H | 0.90360 | -3.67890 | 3.69810 |
| H | 4.47270 | 2.29530 | 0.87270 |
| H | 5.69940 | 3.89510 | -1.46690 |
| H | 6.95400 | 5.18910 | 0.23450 |
| H | 6.30610 | 4.17490 | 1.51990 |
| H | 7.39970 | 3.48710 | 0.31880 |
| H | 0.53150 | 1.75770 | 3.99160 |
| H | 2.58480 | 5.57000 | -0.84700 |
| H | 3.58790 | 4.85340 | -2.10710 |
| H | 2.72030 | 3.82060 | -0.95810 |

| Marilzafurollene C_90 | | | |
|------------------------------|----------|----------|----------|
| C | 2.97090 | -0.62510 | -1.39170 |
| O | 2.10580 | -0.63980 | -0.25540 |
| C | 2.56350 | 0.49460 | -2.37140 |
| C | 2.92770 | -2.04210 | -1.97890 |
| C | 1.54460 | -1.93980 | -0.08490 |
| C | 2.72340 | 1.90730 | -1.78420 |
| Br | 0.65080 | 0.26370 | -2.89110 |
| C | 2.53020 | -2.88330 | -0.78340 |
| C | 1.25090 | -2.23130 | 1.39980 |
| C | 4.16830 | 2.27110 | -1.50240 |
| Cl | 3.97310 | -3.21850 | 0.21960 |
| C | 0.17300 | -1.30750 | 1.99390 |
| C | -0.21950 | -1.73750 | 3.39380 |
| O | 0.69030 | 0.00430 | 2.04040 |
| C | -1.42670 | -2.14250 | 3.71750 |
| C | 4.65160 | 2.57760 | -0.28600 |
| C | 6.09500 | 2.93920 | 0.02240 |
| C | 6.22730 | 4.43320 | 0.32750 |
| O | 6.96930 | 2.64670 | -1.06120 |
| C | -2.62680 | -2.56250 | 4.04180 |
| Br | -4.05240 | -1.33940 | 4.66730 |
| C | 7.36120 | 1.28200 | -1.13420 |
| H | 3.98160 | -0.44490 | -1.02240 |
| H | 3.15120 | 0.41480 | -3.28700 |
| H | 2.15870 | -2.12310 | -2.74730 |
| H | 3.87390 | -2.34820 | -2.42590 |
| H | 0.60680 | -1.96050 | -0.64340 |
| H | 2.32820 | 2.64130 | -2.48700 |
| H | 2.12900 | 2.00020 | -0.87410 |
| H | 2.08210 | -3.83780 | -1.06180 |
| H | 0.91660 | -3.26610 | 1.48570 |
| H | 2.16280 | -2.15720 | 1.99350 |
| H | 4.83370 | 2.28040 | -2.35410 |
| H | -0.70650 | -1.30980 | 1.34580 |
| H | 0.55990 | -1.69190 | 4.14040 |
| H | 1.19170 | 0.13300 | 1.23820 |
| H | 3.98230 | 2.57480 | 0.56300 |
| H | 6.40570 | 2.38070 | 0.90750 |
| H | 7.25770 | 4.68870 | 0.57490 |
| H | 5.93230 | 5.03700 | -0.53110 |
| H | 5.60150 | 4.72170 | 1.17230 |
| H | -2.95160 | -3.59190 | 4.00170 |
| H | 6.50300 | 0.61650 | -1.23310 |
| H | 8.00190 | 1.13240 | -2.00320 |
| H | 7.92670 | 0.98850 | -0.24900 |

| Marilzafurollene C_91 | | | |
|------------------------------|----------|----------|----------|
| C | 2.48610 | -1.20020 | -2.19820 |
| O | 2.54530 | -1.13960 | -0.77500 |
| C | 1.78920 | 0.05350 | -2.77430 |
| C | 1.79930 | -2.53530 | -2.52440 |
| C | 1.85750 | -2.24000 | -0.20180 |
| C | 2.60130 | 1.35770 | -2.62320 |
| Br | -0.00490 | 0.30020 | -1.93180 |
| C | 2.00120 | -3.34190 | -1.25380 |
| C | 2.38760 | -2.53300 | 1.21450 |
| C | 2.97100 | 1.67850 | -1.18640 |
| Cl | 3.63660 | -4.06660 | -1.25530 |
| C | 2.16510 | -1.35920 | 2.18820 |
| C | 0.69350 | -1.07100 | 2.41790 |
| O | 2.77120 | -1.67890 | 3.42360 |
| C | 0.12100 | 0.06650 | 2.09540 |
| C | 4.22570 | 1.88340 | -0.74910 |
| C | 4.63080 | 2.15430 | 0.69080 |
| C | 5.47570 | 0.99990 | 1.23560 |
| O | 3.51270 | 2.30210 | 1.55830 |
| C | -0.46020 | 1.19040 | 1.74900 |
| Br | -0.63970 | 2.72380 | 2.98790 |
| C | 2.95280 | 3.60830 | 1.55770 |
| H | 3.51400 | -1.24190 | -2.56180 |
| H | 1.60840 | -0.10690 | -3.83810 |
| H | 0.73190 | -2.38770 | -2.69120 |
| H | 2.20800 | -3.02040 | -3.41110 |
| H | 0.80040 | -1.97690 | -0.14430 |
| H | 3.51230 | 1.28970 | -3.21890 |
| H | 2.02940 | 2.19350 | -3.02690 |
| H | 1.27280 | -4.14430 | -1.13340 |
| H | 1.91350 | -3.43410 | 1.60430 |
| H | 3.45570 | -2.74550 | 1.16380 |
| H | 2.15050 | 1.71700 | -0.48430 |
| H | 2.65710 | -0.46900 | 1.78830 |
| H | 0.11600 | -1.86720 | 2.86460 |
| H | 2.92430 | -0.86960 | 3.89160 |
| H | 5.04130 | 1.84100 | -1.45610 |
| H | 5.24070 | 3.05940 | 0.71120 |
| H | 5.77030 | 1.18630 | 2.26830 |
| H | 4.92220 | 0.06080 | 1.21050 |
| H | 6.38480 | 0.86480 | 0.64960 |
| H | -0.89180 | 1.38560 | 0.77810 |
| H | 2.60880 | 3.90430 | 0.56640 |
| H | 2.09750 | 3.63850 | 2.23150 |
| H | 3.67600 | 4.34550 | 1.90830 |

| Marilzafurollene C_92 | | | |
|------------------------------|----------|----------|----------|
| C | 2.67100 | -1.13800 | -1.31390 |
| O | 2.63740 | -1.08680 | 0.11140 |
| C | 3.86040 | -0.32110 | -1.85350 |
| C | 1.27600 | -0.70810 | -1.78600 |
| C | 1.32220 | -0.76310 | 0.55990 |
| C | 3.86360 | 1.16360 | -1.44260 |
| Br | 3.89560 | -0.46670 | -3.84220 |
| C | 0.40370 | -1.11500 | -0.61710 |
| C | 1.02130 | -1.43520 | 1.91330 |
| C | 5.15090 | 1.86410 | -1.83190 |
| Cl | 0.05460 | -2.86830 | -0.70610 |
| C | -0.40220 | -1.18870 | 2.45080 |
| C | -0.61100 | -1.88160 | 3.78350 |
| O | -0.60930 | 0.19940 | 2.61480 |
| C | -1.53930 | -2.78680 | 3.99560 |
| C | 6.00450 | 2.42840 | -0.96150 |
| C | 7.29210 | 3.12940 | -1.35270 |
| C | 8.50240 | 2.44030 | -0.71750 |
| O | 7.29820 | 4.47880 | -0.91000 |
| C | -2.45340 | -3.70230 | 4.21510 |
| Br | -2.11490 | -5.63120 | 3.92840 |
| C | 6.41290 | 5.33100 | -1.62400 |
| H | 2.81610 | -2.18510 | -1.58460 |
| H | 4.77690 | -0.78810 | -1.48920 |
| H | 1.21720 | 0.37120 | -1.91900 |
| H | 0.98320 | -1.17410 | -2.72730 |
| H | 1.29980 | 0.32010 | 0.69280 |
| H | 3.03360 | 1.69650 | -1.90480 |
| H | 3.72690 | 1.24610 | -0.36340 |
| H | -0.54600 | -0.57980 | -0.58660 |
| H | 1.19140 | -2.50890 | 1.82630 |
| H | 1.75120 | -1.08180 | 2.64240 |
| H | 5.37140 | 1.89770 | -2.88970 |
| H | -1.13430 | -1.56200 | 1.73150 |
| H | 0.06140 | -1.59440 | 4.57950 |
| H | -1.49360 | 0.34120 | 2.92340 |
| H | 5.78830 | 2.39980 | 0.09690 |
| H | 7.41070 | 3.10090 | -2.43780 |
| H | 9.42820 | 2.93530 | -1.01100 |
| H | 8.44450 | 2.46340 | 0.37090 |
| H | 8.57010 | 1.39760 | -1.02900 |
| H | -3.45610 | -3.50340 | 4.56440 |
| H | 5.37280 | 5.02550 | -1.50570 |
| H | 6.50380 | 6.34900 | -1.24530 |
| H | 6.65290 | 5.34800 | -2.68780 |

| Marilzafurollene C_93 | | | |
|------------------------------|----------|----------|----------|
| C | 2.59930 | -0.55670 | -1.24580 |
| O | 2.18530 | -0.87120 | 0.08380 |
| C | 1.82010 | 0.66140 | -1.78470 |
| C | 2.42890 | -1.84530 | -2.06250 |
| C | 1.72260 | -2.21600 | 0.14140 |
| C | 2.10880 | 1.95780 | -1.00930 |
| Br | -0.14150 | 0.30870 | -1.67340 |
| C | 2.46720 | -2.92150 | -0.99620 |
| C | 1.89620 | -2.81120 | 1.55240 |
| C | 3.54200 | 2.42970 | -1.15920 |
| Cl | 4.16690 | -3.28470 | -0.57150 |
| C | 1.07240 | -2.07930 | 2.62830 |
| C | -0.42280 | -2.17060 | 2.38530 |
| O | 1.36960 | -2.64690 | 3.88800 |
| C | -1.17060 | -1.12980 | 2.09590 |
| C | 4.41190 | 2.55090 | -0.14160 |
| C | 5.85400 | 3.01380 | -0.26630 |
| C | 6.02270 | 4.42430 | 0.30370 |
| O | 6.29750 | 3.04510 | -1.61780 |
| C | -1.89580 | -0.08210 | 1.78300 |
| Br | -2.79190 | 1.03960 | 3.14650 |
| C | 6.69590 | 1.77770 | -2.12400 |
| H | 3.66450 | -0.32530 | -1.20200 |
| H | 2.05480 | 0.81100 | -2.83950 |
| H | 1.45910 | -1.86550 | -2.56000 |
| H | 3.19490 | -1.97020 | -2.82830 |
| H | 0.66320 | -2.20710 | -0.11920 |
| H | 1.45780 | 2.75370 | -1.37180 |
| H | 1.86850 | 1.81820 | 0.04580 |
| H | 1.98850 | -3.85070 | -1.30720 |
| H | 1.62080 | -3.86640 | 1.53480 |
| H | 2.94950 | -2.77470 | 1.83030 |
| H | 3.86030 | 2.68080 | -2.16110 |
| H | 1.37110 | -1.02840 | 2.65250 |
| H | -0.85960 | -3.15550 | 2.46160 |
| H | 2.20450 | -2.31010 | 4.18130 |
| H | 4.08790 | 2.30510 | 0.85990 |
| H | 6.48260 | 2.33390 | 0.31210 |
| H | 7.06200 | 4.74690 | 0.23900 |
| H | 5.41640 | 5.14500 | -0.24570 |
| H | 5.72680 | 4.46580 | 1.35220 |
| H | -2.07230 | 0.26490 | 0.77510 |
| H | 5.88810 | 1.04680 | -2.07380 |
| H | 6.99110 | 1.87830 | -3.16830 |
| H | 7.55150 | 1.38640 | -1.57220 |

| Marilzafurollene C_94 | | | |
|------------------------------|----------|----------|----------|
| C | 2.98370 | -1.87440 | -1.38670 |
| O | 2.31620 | -1.88500 | -0.12610 |
| C | 3.93440 | -0.66700 | -1.49260 |
| C | 1.87640 | -1.96660 | -2.44300 |
| C | 0.93510 | -2.20270 | -0.30200 |
| C | 3.25830 | 0.70530 | -1.31280 |
| Br | 4.86110 | -0.73140 | -3.25750 |
| C | 0.82200 | -2.77890 | -1.72120 |
| C | 0.40670 | -3.09860 | 0.83690 |
| C | 4.26400 | 1.83930 | -1.26090 |
| Cl | 1.24760 | -4.51610 | -1.79350 |
| C | 0.40350 | -2.41850 | 2.21850 |
| C | -0.54860 | -1.23730 | 2.28500 |
| O | 0.00650 | -3.37870 | 3.17670 |
| C | -0.17030 | -0.01710 | 2.59700 |
| C | 4.45110 | 2.64670 | -0.20350 |
| C | 5.45640 | 3.78290 | -0.15780 |
| C | 6.48670 | 3.55650 | 0.95240 |
| O | 4.81680 | 5.02230 | 0.10960 |
| C | 0.19920 | 1.19700 | 2.93570 |
| Br | 0.19070 | 1.82060 | 4.81610 |
| C | 4.04510 | 5.52600 | -0.97290 |
| H | 3.57810 | -2.78860 | -1.43430 |
| H | 4.70660 | -0.78160 | -0.73000 |
| H | 1.47340 | -0.98370 | -2.68220 |
| H | 2.21280 | -2.42440 | -3.37390 |
| H | 0.39510 | -1.25450 | -0.29690 |
| H | 2.56470 | 0.90600 | -2.12870 |
| H | 2.67080 | 0.70660 | -0.39350 |
| H | -0.17460 | -2.66110 | -2.14780 |
| H | -0.60300 | -3.43420 | 0.59490 |
| H | 1.01910 | -3.99950 | 0.89520 |
| H | 4.85860 | 1.98680 | -2.15200 |
| H | 1.42100 | -2.09730 | 2.45830 |
| H | -1.58510 | -1.44690 | 2.05720 |
| H | 0.20070 | -3.04080 | 4.04020 |
| H | 3.86100 | 2.50620 | 0.69100 |
| H | 5.98680 | 3.84360 | -1.11080 |
| H | 7.21540 | 4.36710 | 0.97640 |
| H | 6.00920 | 3.51070 | 1.93190 |
| H | 7.03190 | 2.62480 | 0.79980 |
| H | 0.53520 | 1.95800 | 2.24500 |
| H | 3.22380 | 4.85670 | -1.23200 |
| H | 3.61340 | 6.48740 | -0.69520 |
| H | 4.66230 | 5.68090 | -1.85910 |

| Marilzafurollene C_95 | | | |
|------------------------------|----------|----------|----------|
| C | 3.24850 | -1.63400 | -0.10120 |
| O | 2.02810 | -1.05880 | 0.36890 |
| C | 4.31840 | -0.53130 | -0.20720 |
| C | 2.89910 | -2.35600 | -1.41300 |
| C | 0.91430 | -1.68570 | -0.26020 |
| C | 3.96650 | 0.60500 | -1.18550 |
| Br | 6.04890 | -1.36620 | -0.74220 |
| C | 1.46550 | -1.93440 | -1.66600 |
| C | 0.50590 | -2.95030 | 0.53380 |
| C | 4.96900 | 1.74130 | -1.13390 |
| Cl | 0.54790 | -3.13720 | -2.61380 |
| C | 0.09380 | -2.66240 | 1.98890 |
| C | -1.14390 | -1.78970 | 2.08020 |
| O | -0.16390 | -3.89670 | 2.62580 |
| C | -1.15640 | -0.61400 | 2.66610 |
| C | 4.67210 | 3.00390 | -0.78400 |
| C | 5.67630 | 4.14030 | -0.73330 |
| C | 5.77350 | 4.71890 | 0.68050 |
| O | 5.29430 | 5.20240 | -1.59520 |
| C | -1.15130 | 0.55490 | 3.26200 |
| Br | -1.55180 | 0.76530 | 5.18890 |
| C | 5.43860 | 4.91150 | -2.97880 |
| H | 3.57450 | -2.37370 | 0.63170 |
| H | 4.47060 | -0.11000 | 0.78800 |
| H | 3.55960 | -2.11330 | -2.24520 |
| H | 2.95610 | -3.43420 | -1.25940 |
| H | 0.07400 | -0.99220 | -0.30360 |
| H | 3.92150 | 0.23200 | -2.20840 |
| H | 2.97550 | 0.99640 | -0.95150 |
| H | 1.45370 | -0.99890 | -2.22670 |
| H | -0.31980 | -3.44850 | 0.02470 |
| H | 1.32750 | -3.66690 | 0.53570 |
| H | 5.98550 | 1.49040 | -1.40320 |
| H | 0.92830 | -2.18360 | 2.50700 |
| H | -2.04160 | -2.18560 | 1.62730 |
| H | -0.25050 | -3.74350 | 3.55650 |
| H | 3.65770 | 3.26240 | -0.51570 |
| H | 6.66280 | 3.77220 | -1.02250 |
| H | 6.50580 | 5.52550 | 0.71940 |
| H | 4.81610 | 5.12420 | 1.00890 |
| H | 6.08050 | 3.95710 | 1.39760 |
| H | -0.93450 | 1.49500 | 2.77600 |
| H | 6.47220 | 4.66460 | -3.22490 |
| H | 4.79910 | 4.08410 | -3.28780 |
| H | 5.15580 | 5.78550 | -3.56550 |

| Marilzafurollene C_96 | | | |
|------------------------------|----------|----------|----------|
| C | 2.88170 | -0.90920 | -0.57080 |
| O | 1.92170 | -0.93440 | 0.48540 |
| C | 3.37560 | 0.53030 | -0.79890 |
| C | 2.16860 | -1.54540 | -1.76870 |
| C | 0.79400 | -1.73180 | 0.12450 |
| C | 4.44970 | 0.63340 | -1.89720 |
| Br | 4.14650 | 1.20270 | 0.91360 |
| C | 1.23910 | -2.53800 | -1.10220 |
| C | 0.27510 | -2.54230 | 1.32840 |
| C | 4.88120 | 2.06410 | -2.15440 |
| Cl | 2.15370 | -4.01080 | -0.65920 |
| C | -0.27240 | -1.65840 | 2.46280 |
| C | -0.96260 | -2.48730 | 3.52800 |
| O | 0.80290 | -0.95820 | 3.04980 |
| C | -2.23050 | -2.35090 | 3.84300 |
| C | 6.14470 | 2.50740 | -2.04540 |
| C | 6.57690 | 3.94140 | -2.28780 |
| C | 7.58490 | 4.02130 | -3.43700 |
| O | 7.20660 | 4.49110 | -1.13960 |
| C | -3.50100 | -2.21200 | 4.13900 |
| Br | -4.92300 | -3.23680 | 3.21870 |
| C | 6.33040 | 4.71440 | -0.04240 |
| H | 3.71660 | -1.54330 | -0.26790 |
| H | 2.52830 | 1.17450 | -1.03650 |
| H | 1.58210 | -0.79740 | -2.30380 |
| H | 2.85360 | -2.00900 | -2.47940 |
| H | 0.01400 | -1.04050 | -0.19940 |
| H | 5.31570 | 0.02690 | -1.62790 |
| H | 4.06740 | 0.23210 | -2.83600 |
| H | 0.40560 | -2.83910 | -1.73800 |
| H | -0.52150 | -3.20050 | 0.97850 |
| H | 1.05720 | -3.19440 | 1.71930 |
| H | 4.10060 | 2.75430 | -2.44080 |
| H | -0.97450 | -0.93040 | 2.05010 |
| H | -0.34850 | -3.21740 | 4.03480 |
| H | 1.39920 | -0.70710 | 2.34760 |
| H | 6.92980 | 1.82260 | -1.75840 |
| H | 5.70710 | 4.54730 | -2.54920 |
| H | 7.88310 | 5.05380 | -3.61950 |
| H | 8.48630 | 3.45070 | -3.21220 |
| H | 7.16040 | 3.62970 | -4.36170 |
| H | -3.88930 | -1.54340 | 4.89350 |
| H | 5.90540 | 3.78330 | 0.33400 |
| H | 6.88230 | 5.17840 | 0.77480 |
| H | 5.51470 | 5.38420 | -0.31710 |

| Marilzafurollene C_97 | | | |
|------------------------------|----------|----------|----------|
| C | 3.03190 | -1.83240 | -1.06190 |
| O | 2.43480 | -1.90520 | 0.23190 |
| C | 3.77460 | -0.49420 | -1.23470 |
| C | 1.90720 | -2.12440 | -2.06390 |
| C | 1.06900 | -2.29820 | 0.11960 |
| C | 2.89880 | 0.75750 | -1.04050 |
| Br | 4.62070 | -0.45160 | -3.03990 |
| C | 0.96520 | -2.98470 | -1.24750 |
| C | 0.63000 | -3.13380 | 1.33780 |
| C | 3.71630 | 2.03360 | -1.01990 |
| Cl | 1.56590 | -4.67000 | -1.20830 |
| C | 0.59890 | -2.32930 | 2.65010 |
| C | -0.49390 | -1.27660 | 2.65800 |
| O | 0.37620 | -3.22170 | 3.72250 |
| C | -0.26020 | 0.01440 | 2.72490 |
| C | 3.80120 | 2.86710 | 0.03140 |
| C | 4.61180 | 4.15190 | 0.07670 |
| C | 3.68880 | 5.37280 | 0.07290 |
| O | 5.49120 | 4.28140 | -1.03400 |
| C | -0.03610 | 1.30620 | 2.76740 |
| Br | 0.18320 | 2.39700 | 1.13040 |
| C | 6.70000 | 3.54380 | -0.90620 |
| H | 3.75860 | -2.64460 | -1.11700 |
| H | 4.58820 | -0.46780 | -0.50820 |
| H | 1.39450 | -1.21060 | -2.36120 |
| H | 2.26300 | -2.61350 | -2.97130 |
| H | 0.47590 | -1.38350 | 0.07020 |
| H | 2.15550 | 0.84230 | -1.83220 |
| H | 2.34860 | 0.67520 | -0.10260 |
| H | -0.05180 | -2.99800 | -1.64090 |
| H | -0.35470 | -3.56380 | 1.15000 |
| H | 1.31320 | -3.97600 | 1.45070 |
| H | 4.25420 | 2.26760 | -1.92800 |
| H | 1.57020 | -1.85300 | 2.80410 |
| H | -1.50800 | -1.64550 | 2.60790 |
| H | 1.16770 | -3.72030 | 3.87050 |
| H | 3.25460 | 2.63350 | 0.93400 |
| H | 5.18700 | 4.16100 | 1.00450 |
| H | 4.26540 | 6.29580 | 0.13490 |
| H | 3.09500 | 5.41210 | -0.84070 |
| H | 3.00120 | 5.35200 | 0.91880 |
| H | 0.04720 | 1.88920 | 3.67300 |
| H | 6.51580 | 2.47660 | -0.77870 |
| H | 7.30210 | 3.67280 | -1.80550 |
| H | 7.28740 | 3.89780 | -0.05810 |

| Marilzafurollene C_98 | | | |
|------------------------------|----------|----------|----------|
| C | 2.94610 | -1.34240 | -0.56370 |
| O | 1.65810 | -1.09960 | 0.00710 |
| C | 3.43530 | -0.08370 | -1.30530 |
| C | 2.79330 | -2.58680 | -1.45080 |
| C | 0.82900 | -2.25010 | -0.12680 |
| C | 3.62920 | 1.11250 | -0.35830 |
| Br | 2.12840 | 0.41150 | -2.73220 |
| C | 1.29450 | -2.81140 | -1.47240 |
| C | 1.03450 | -3.17700 | 1.09540 |
| C | 4.24240 | 2.31150 | -1.05550 |
| Cl | 0.85850 | -4.52090 | -1.74810 |
| C | 0.63640 | -2.52920 | 2.43480 |
| C | -0.84800 | -2.22490 | 2.51760 |
| O | 0.98090 | -3.41420 | 3.48140 |
| C | -1.33340 | -1.01060 | 2.64390 |
| C | 5.42470 | 2.86060 | -0.73080 |
| C | 6.03470 | 4.06160 | -1.42950 |
| C | 7.38320 | 3.70000 | -2.05730 |
| O | 6.26930 | 5.12320 | -0.51590 |
| C | -1.80620 | 0.20810 | 2.75700 |
| Br | -2.13230 | 1.06640 | 4.51080 |
| C | 5.08970 | 5.77130 | -0.05920 |
| H | 3.64060 | -1.57670 | 0.24460 |
| H | 4.38220 | -0.30450 | -1.80070 |
| H | 3.20740 | -2.46580 | -2.45220 |
| H | 3.29680 | -3.43470 | -0.98530 |
| H | -0.21710 | -1.94890 | -0.18910 |
| H | 2.67080 | 1.40780 | 0.07050 |
| H | 4.26590 | 0.82090 | 0.47790 |
| H | 0.84830 | -2.22630 | -2.27790 |
| H | 0.45310 | -4.09000 | 0.96240 |
| H | 2.07660 | -3.49240 | 1.14310 |
| H | 3.66540 | 2.73490 | -1.86580 |
| H | 1.20490 | -1.60660 | 2.57410 |
| H | -1.51080 | -3.07650 | 2.46860 |
| H | 1.89500 | -3.29260 | 3.69510 |
| H | 6.00580 | 2.44500 | 0.07990 |
| H | 5.36680 | 4.40350 | -2.22280 |
| H | 7.81370 | 4.55950 | -2.57140 |
| H | 8.09730 | 3.37430 | -1.30060 |
| H | 7.27530 | 2.89690 | -2.78680 |
| H | -2.05890 | 0.85040 | 1.92600 |
| H | 4.44240 | 5.09120 | 0.49560 |
| H | 5.35960 | 6.58950 | 0.60850 |
| H | 4.52290 | 6.19220 | -0.89060 |

| Marilzafurollene C_99 | | | |
|------------------------------|----------|----------|----------|
| C | 2.84940 | -1.83550 | -1.79820 |
| O | 2.53540 | -1.63670 | -0.41990 |
| C | 2.76960 | -0.52010 | -2.60120 |
| C | 1.89990 | -2.93580 | -2.29210 |
| C | 1.46250 | -2.48930 | -0.03620 |
| C | 3.89930 | 0.48460 | -2.29510 |
| Br | 0.99140 | 0.35500 | -2.34540 |
| C | 1.54200 | -3.66540 | -1.01400 |
| C | 1.52840 | -2.83760 | 1.46380 |
| C | 3.77030 | 1.17460 | -0.94910 |
| Cl | 2.84950 | -4.81200 | -0.59290 |
| C | 1.39930 | -1.60910 | 2.38280 |
| C | 0.07260 | -0.89260 | 2.21600 |
| O | 1.52900 | -2.03310 | 3.72450 |
| C | -0.02990 | 0.33660 | 1.76420 |
| C | 3.86330 | 2.50260 | -0.76890 |
| C | 3.71860 | 3.20290 | 0.56840 |
| C | 2.68110 | 4.32430 | 0.48070 |
| O | 4.94220 | 3.80020 | 0.97220 |
| C | -0.11300 | 1.56140 | 1.30260 |
| Br | -0.09720 | 3.14270 | 2.49310 |
| C | 5.93630 | 2.87070 | 1.38070 |
| H | 3.86840 | -2.22320 | -1.84130 |
| H | 2.83720 | -0.77200 | -3.66070 |
| H | 0.99720 | -2.50200 | -2.72340 |
| H | 2.34920 | -3.58240 | -3.04630 |
| H | 0.53460 | -1.95430 | -0.24470 |
| H | 4.86480 | -0.02040 | -2.33670 |
| H | 3.91910 | 1.24700 | -3.07480 |
| H | 0.60860 | -4.22480 | -1.08570 |
| H | 0.74250 | -3.55600 | 1.69990 |
| H | 2.47330 | -3.33730 | 1.67700 |
| H | 3.59660 | 0.53720 | -0.09450 |
| H | 2.21510 | -0.91470 | 2.16730 |
| H | -0.81000 | -1.45210 | 2.48870 |
| H | 2.44310 | -2.20500 | 3.90150 |
| H | 4.05090 | 3.14520 | -1.61690 |
| H | 3.39110 | 2.48650 | 1.32480 |
| H | 2.54190 | 4.80050 | 1.45140 |
| H | 2.98930 | 5.09460 | -0.22640 |
| H | 1.71350 | 3.94070 | 0.15700 |
| H | -0.19820 | 1.82210 | 0.25730 |
| H | 6.23210 | 2.20940 | 0.56560 |
| H | 6.82510 | 3.40980 | 1.70830 |
| H | 5.58850 | 2.26160 | 2.21590 |

| Marilzafurollene C_100 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.52010 | -1.08050 | -1.71520 |
| O | 1.46660 | -0.89910 | -0.77310 |
| C | 2.35750 | -0.12390 | -2.91200 |
| C | 2.51810 | -2.58280 | -2.03500 |
| C | 1.35740 | -2.07370 | 0.02110 |
| C | 2.31970 | 1.36120 | -2.50000 |
| Br | 0.66760 | -0.53890 | -3.88650 |
| C | 1.48530 | -3.14390 | -1.06720 |
| C | 2.46140 | -2.08090 | 1.10900 |
| C | 3.48700 | 1.76290 | -1.61530 |
| Cl | 1.92190 | -4.76140 | -0.44950 |
| C | 2.41580 | -0.83730 | 2.01520 |
| C | 1.28620 | -0.90280 | 3.02440 |
| O | 3.64500 | -0.71910 | 2.70000 |
| C | 0.29190 | -0.04560 | 3.05970 |
| C | 3.34730 | 2.23220 | -0.36130 |
| C | 4.46260 | 2.60020 | 0.60960 |
| C | 5.86660 | 2.22150 | 0.11840 |
| O | 4.27990 | 1.93620 | 1.85590 |
| C | -0.71860 | 0.79050 | 3.09140 |
| Br | -2.38800 | 0.47340 | 2.07700 |
| C | 3.35440 | 2.58140 | 2.72370 |
| H | 3.46130 | -0.85360 | -1.21310 |
| H | 3.17550 | -0.28610 | -3.61510 |
| H | 2.25480 | -2.80770 | -3.06860 |
| H | 3.50650 | -3.00310 | -1.84700 |
| H | 0.37490 | -2.11440 | 0.49290 |
| H | 2.31160 | 1.99430 | -3.38750 |
| H | 1.38680 | 1.55990 | -1.97020 |
| H | 0.52770 | -3.23660 | -1.58220 |
| H | 2.37670 | -2.98000 | 1.72030 |
| H | 3.44290 | -2.14760 | 0.64070 |
| H | 4.46810 | 1.63500 | -2.04780 |
| H | 2.30720 | 0.05580 | 1.39670 |
| H | 1.33560 | -1.71240 | 3.73780 |
| H | 4.03770 | 0.11390 | 2.44680 |
| H | 2.34490 | 2.35580 | 0.02160 |
| H | 4.43950 | 3.68160 | 0.75710 |
| H | 6.61810 | 2.49110 | 0.86070 |
| H | 5.95020 | 1.14870 | -0.05810 |
| H | 6.12230 | 2.74290 | -0.80420 |
| H | -0.74280 | 1.71000 | 3.65750 |
| H | 3.27900 | 2.02330 | 3.65720 |
| H | 3.68090 | 3.59280 | 2.96890 |
| H | 2.35570 | 2.63250 | 2.28970 |

| Marilzafurollene C_101 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.25790 | -1.12180 | -1.26600 |
| O | 1.84910 | -0.93280 | -1.11540 |
| C | 3.74510 | -0.41020 | -2.54430 |
| C | 3.48570 | -2.64090 | -1.24480 |
| C | 1.25900 | -2.09820 | -0.54720 |
| C | 3.49660 | 1.10830 | -2.52770 |
| Br | 2.80350 | -1.17170 | -4.12930 |
| C | 2.07650 | -3.20250 | -1.22080 |
| C | 1.35860 | -2.03310 | 0.99650 |
| C | 4.23200 | 1.81380 | -1.40500 |
| Cl | 1.97960 | -4.78640 | -0.40210 |
| C | 0.60890 | -0.83560 | 1.60830 |
| C | 0.55570 | -0.92430 | 3.12100 |
| O | 1.28030 | 0.34890 | 1.23790 |
| C | -0.56190 | -1.03730 | 3.80220 |
| C | 3.62840 | 2.44680 | -0.38400 |
| C | 4.33700 | 3.14850 | 0.76200 |
| C | 4.20190 | 4.66780 | 0.63500 |
| O | 5.72690 | 2.84680 | 0.80400 |
| C | -1.67750 | -1.16590 | 4.48110 |
| Br | -2.71470 | 0.38960 | 5.13230 |
| C | 6.02800 | 1.60840 | 1.43350 |
| H | 3.75380 | -0.69280 | -0.39400 |
| H | 4.80960 | -0.60150 | -2.68830 |
| H | 4.06010 | -3.01040 | -2.09470 |
| H | 4.02310 | -2.91910 | -0.33760 |
| H | 0.21050 | -2.16380 | -0.84040 |
| H | 3.82100 | 1.54560 | -3.47230 |
| H | 2.42650 | 1.30530 | -2.44900 |
| H | 1.72120 | -3.33790 | -2.24370 |
| H | 0.92770 | -2.94770 | 1.40570 |
| H | 2.39940 | -2.02580 | 1.32190 |
| H | 5.31170 | 1.79010 | -1.45030 |
| H | -0.40580 | -0.79890 | 1.20510 |
| H | 1.50580 | -0.88590 | 3.63320 |
| H | 1.48660 | 0.26540 | 0.31020 |
| H | 2.54850 | 2.47490 | -0.34230 |
| H | 3.86270 | 2.83960 | 1.69570 |
| H | 4.68790 | 5.17130 | 1.47070 |
| H | 4.66400 | 5.02790 | -0.28450 |
| H | 3.15500 | 4.97200 | 0.62720 |
| H | -2.13220 | -2.10880 | 4.74730 |
| H | 5.53490 | 0.77060 | 0.93950 |
| H | 7.10300 | 1.43240 | 1.39790 |
| H | 5.72610 | 1.61810 | 2.48160 |

| Marilzafurollene C_102 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.95250 | -0.99320 | -0.21440 |
| O | 1.62130 | -0.50670 | -0.02270 |
| C | 3.78710 | 0.05680 | -0.97120 |
| C | 2.81430 | -2.34160 | -0.93690 |
| C | 0.68040 | -1.56610 | -0.18420 |
| C | 3.94940 | 1.36080 | -0.17170 |
| Br | 2.92630 | 0.46150 | -2.72720 |
| C | 1.34030 | -2.39630 | -1.28740 |
| C | 0.47710 | -2.28800 | 1.16970 |
| C | 4.88470 | 2.34320 | -0.84890 |
| Cl | 0.72520 | -4.06760 | -1.41670 |
| C | -0.13210 | -1.38660 | 2.25850 |
| C | -0.49980 | -2.17950 | 3.49710 |
| O | 0.81260 | -0.39860 | 2.60780 |
| C | -1.72460 | -2.26680 | 3.96340 |
| C | 6.04800 | 2.77400 | -0.33040 |
| C | 6.99970 | 3.75580 | -0.99550 |
| C | 6.98840 | 5.10090 | -0.26520 |
| O | 6.66010 | 4.00930 | -2.35350 |
| C | -2.95430 | -2.35440 | 4.41200 |
| Br | -4.20020 | -3.77560 | 3.82330 |
| C | 7.10700 | 3.00990 | -3.26060 |
| H | 3.39820 | -1.17040 | 0.76590 |
| H | 4.77450 | -0.35530 | -1.18590 |
| H | 3.45120 | -2.43560 | -1.81690 |
| H | 3.07220 | -3.15220 | -0.25440 |
| H | -0.27430 | -1.16590 | -0.52760 |
| H | 2.97890 | 1.83920 | -0.03430 |
| H | 4.32840 | 1.13620 | 0.82610 |
| H | 1.17460 | -1.91050 | -2.25030 |
| H | -0.20060 | -3.12830 | 1.01290 |
| H | 1.41170 | -2.72330 | 1.52490 |
| H | 4.56690 | 2.71010 | -1.81510 |
| H | -1.02050 | -0.89000 | 1.86140 |
| H | 0.31300 | -2.68500 | 3.99770 |
| H | 1.17970 | -0.06800 | 1.79210 |
| H | 6.36020 | 2.41330 | 0.63920 |
| H | 8.00960 | 3.34520 | -0.93940 |
| H | 7.27150 | 4.98640 | 0.78130 |
| H | 7.68970 | 5.79750 | -0.72480 |
| H | 5.99840 | 5.55670 | -0.29790 |
| H | -3.39940 | -1.67910 | 5.12810 |
| H | 6.70180 | 2.02720 | -3.01760 |
| H | 6.78340 | 3.26340 | -4.27010 |
| H | 8.19570 | 2.94420 | -3.26630 |

| Marilzafurollene C_103 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.44210 | -0.88050 | -1.14950 |
| O | 2.75080 | -1.08590 | 0.22870 |
| C | 3.06640 | 0.43120 | -1.66180 |
| C | 0.91510 | -0.95720 | -1.25900 |
| C | 1.55650 | -1.28380 | 0.98040 |
| C | 4.60370 | 0.38830 | -1.63410 |
| Br | 2.43870 | 1.96360 | -0.54410 |
| C | 0.54440 | -1.79750 | -0.05530 |
| C | 1.84470 | -2.16160 | 2.21830 |
| C | 5.23210 | 1.62690 | -2.24320 |
| Cl | 0.78450 | -3.52830 | -0.44190 |
| C | 0.71900 | -2.20120 | 3.27250 |
| C | -0.48560 | -3.00300 | 2.81950 |
| O | 1.24060 | -2.79250 | 4.44440 |
| C | -1.70080 | -2.50930 | 2.75080 |
| C | 6.06530 | 2.45410 | -1.59030 |
| C | 6.68520 | 3.70140 | -2.19180 |
| C | 8.21270 | 3.60230 | -2.20090 |
| O | 6.34520 | 4.85940 | -1.44270 |
| C | -2.90300 | -1.99660 | 2.63950 |
| Br | -3.51790 | -1.11750 | 0.97660 |
| C | 4.97640 | 5.23290 | -1.53250 |
| H | 2.86600 | -1.72180 | -1.70020 |
| H | 2.72490 | 0.61560 | -2.68120 |
| H | 0.46560 | 0.03090 | -1.15960 |
| H | 0.57400 | -1.38210 | -2.20330 |
| H | 1.23590 | -0.29610 | 1.31660 |
| H | 4.95100 | 0.25990 | -0.60770 |
| H | 4.96040 | -0.47770 | -2.19260 |
| H | -0.49340 | -1.65500 | 0.24450 |
| H | 2.13160 | -3.17070 | 1.92290 |
| H | 2.73170 | -1.74410 | 2.69680 |
| H | 4.97450 | 1.83670 | -3.27130 |
| H | 0.42230 | -1.17900 | 3.51870 |
| H | -0.29540 | -4.03020 | 2.54070 |
| H | 0.62690 | -2.66180 | 5.15350 |
| H | 6.32460 | 2.24880 | -0.56150 |
| H | 6.34120 | 3.82180 | -3.22090 |
| H | 8.65600 | 4.49250 | -2.64720 |
| H | 8.60830 | 3.50620 | -1.18950 |
| H | 8.54810 | 2.73950 | -2.77690 |
| H | -3.65430 | -1.99940 | 3.41590 |
| H | 4.68320 | 5.41670 | -2.56680 |
| H | 4.31910 | 4.47000 | -1.11390 |
| H | 4.81310 | 6.15240 | -0.97080 |

| Marilzafurollene C_104 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.82110 | -0.60130 | -0.93780 |
| O | 1.72670 | -0.46250 | -0.03080 |
| C | 2.83550 | 0.55770 | -1.95570 |
| C | 2.69080 | -2.00130 | -1.55240 |
| C | 0.94790 | -1.65770 | -0.02030 |
| C | 3.06140 | 1.94160 | -1.32110 |
| Br | 1.09010 | 0.61470 | -2.92150 |
| C | 1.91190 | -2.75210 | -0.49220 |
| C | 0.27570 | -1.88020 | 1.34870 |
| C | 4.43040 | 2.09620 | -0.68560 |
| Cl | 3.02540 | -3.27780 | 0.80580 |
| C | -0.76840 | -0.79330 | 1.69450 |
| C | -1.59510 | -1.05660 | 2.94600 |
| O | -0.09200 | 0.43510 | 1.84840 |
| C | -1.49200 | -2.10650 | 3.73090 |
| C | 5.38520 | 2.93000 | -1.13030 |
| C | 6.75380 | 3.08900 | -0.49440 |
| C | 6.97170 | 4.52880 | -0.02280 |
| O | 7.78800 | 2.79140 | -1.42100 |
| C | -1.39430 | -3.16520 | 4.49960 |
| Br | -2.45340 | -4.80710 | 4.18180 |
| C | 7.91410 | 1.41080 | -1.73240 |
| H | 3.73470 | -0.58560 | -0.34280 |
| H | 3.60630 | 0.37870 | -2.70700 |
| H | 2.10940 | -1.97290 | -2.47400 |
| H | 3.65360 | -2.45770 | -1.78390 |
| H | 0.17310 | -1.54290 | -0.78080 |
| H | 2.93910 | 2.70920 | -2.08620 |
| H | 2.29890 | 2.13750 | -0.56610 |
| H | 1.40050 | -3.63420 | -0.87920 |
| H | -0.21330 | -2.85520 | 1.32370 |
| H | 1.02640 | -1.93290 | 2.13820 |
| H | 4.62470 | 1.48690 | 0.18570 |
| H | -1.46640 | -0.69410 | 0.86140 |
| H | -2.31960 | -0.28980 | 3.17870 |
| H | 0.60870 | 0.44980 | 1.19990 |
| H | 5.19890 | 3.54370 | -2.00020 |
| H | 6.83660 | 2.42780 | 0.37050 |
| H | 7.94930 | 4.63890 | 0.44680 |
| H | 6.92350 | 5.22990 | -0.85640 |
| H | 6.21760 | 4.82240 | 0.70780 |
| H | -0.74420 | -3.24660 | 5.35840 |
| H | 7.01520 | 1.01960 | -2.21010 |
| H | 8.74510 | 1.26820 | -2.42320 |
| H | 8.11880 | 0.82120 | -0.83790 |

| Marilzafurollene C_105 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.57210 | -1.94140 | -1.43270 |
| O | 2.95960 | -1.50650 | -0.22100 |
| C | 5.00430 | -1.38710 | -1.58290 |
| C | 2.57640 | -1.59750 | -2.54490 |
| C | 1.58420 | -1.19360 | -0.45180 |
| C | 5.15560 | 0.13730 | -1.76370 |
| Br | 5.85210 | -2.27480 | -3.15130 |
| C | 1.24910 | -1.76930 | -1.83550 |
| C | 0.70570 | -1.66820 | 0.72250 |
| C | 4.62800 | 0.95250 | -0.59850 |
| Cl | 0.81880 | -3.50500 | -1.76710 |
| C | 0.98570 | -0.91710 | 2.03630 |
| C | 0.02120 | -1.33260 | 3.12930 |
| O | 2.30340 | -1.20670 | 2.44860 |
| C | -0.80750 | -0.50230 | 3.72030 |
| C | 3.85670 | 2.04550 | -0.72440 |
| C | 3.33600 | 2.87060 | 0.43820 |
| C | 1.81440 | 3.02200 | 0.36900 |
| O | 3.87710 | 4.18330 | 0.41720 |
| C | -1.64840 | 0.32120 | 4.30000 |
| Br | -3.47460 | 0.63680 | 3.60400 |
| C | 5.25230 | 4.25460 | 0.76830 |
| H | 3.63880 | -3.02830 | -1.36000 |
| H | 5.58350 | -1.70010 | -0.71290 |
| H | 2.68230 | -0.56090 | -2.86210 |
| H | 2.68320 | -2.23180 | -3.42540 |
| H | 1.52090 | -0.10760 | -0.52760 |
| H | 6.21620 | 0.36990 | -1.86440 |
| H | 4.69000 | 0.46650 | -2.69250 |
| H | 0.43120 | -1.24140 | -2.32750 |
| H | -0.34100 | -1.52200 | 0.45130 |
| H | 0.83060 | -2.74040 | 0.88040 |
| H | 4.91350 | 0.61570 | 0.38820 |
| H | 0.90770 | 0.15820 | 1.86420 |
| H | 0.04500 | -2.37450 | 3.41370 |
| H | 2.82100 | -1.33840 | 1.65760 |
| H | 3.57600 | 2.39140 | -1.70880 |
| H | 3.59310 | 2.38250 | 1.38050 |
| H | 1.44670 | 3.60960 | 1.21040 |
| H | 1.50860 | 3.52860 | -0.54670 |
| H | 1.31650 | 2.05440 | 0.40070 |
| H | -1.43570 | 0.89510 | 5.19010 |
| H | 5.42570 | 3.85750 | 1.76930 |
| H | 5.87950 | 3.70900 | 0.06260 |
| H | 5.57560 | 5.29550 | 0.76190 |

| Marilzafurollene C_106 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.70670 | -0.71180 | -1.52590 |
| O | 1.79060 | -0.45860 | -0.45980 |
| C | 2.62280 | 0.40090 | -2.59090 |
| C | 2.38430 | -2.12150 | -2.03900 |
| C | 0.94580 | -1.59050 | -0.26240 |
| C | 3.06060 | 1.77940 | -2.06690 |
| Br | 0.74250 | 0.56420 | -3.23860 |
| C | 1.73980 | -2.77150 | -0.83200 |
| C | 0.50030 | -1.70810 | 1.20840 |
| C | 4.53190 | 1.83510 | -1.70300 |
| Cl | 3.01130 | -3.33800 | 0.29180 |
| C | -0.38850 | -0.52910 | 1.66750 |
| C | -1.00790 | -0.67820 | 3.05070 |
| O | 0.39120 | 0.64640 | 1.64460 |
| C | -0.85000 | -1.70290 | 3.85930 |
| C | 4.99730 | 2.07620 | -0.46610 |
| C | 6.46690 | 2.13110 | -0.09340 |
| C | 6.80240 | 1.06660 | 0.95410 |
| O | 6.81060 | 3.39090 | 0.46490 |
| C | -0.70020 | -2.73670 | 4.65310 |
| Br | -1.91440 | -4.29920 | 4.59930 |
| C | 6.82400 | 4.46100 | -0.47010 |
| H | 3.70680 | -0.73350 | -1.09050 |
| H | 3.23150 | 0.13070 | -3.45500 |
| H | 1.66330 | -2.08450 | -2.85580 |
| H | 3.26340 | -2.65670 | -2.39880 |
| H | 0.06380 | -1.44600 | -0.88930 |
| H | 2.87890 | 2.53550 | -2.83130 |
| H | 2.45110 | 2.05890 | -1.20620 |
| H | 1.11040 | -3.62420 | -1.08930 |
| H | -0.05460 | -2.64150 | 1.31380 |
| H | 1.36810 | -1.79040 | 1.86410 |
| H | 5.23060 | 1.66570 | -2.50990 |
| H | -1.20850 | -0.40580 | 0.95790 |
| H | -1.62450 | 0.15260 | 3.36160 |
| H | 0.97510 | 0.57760 | 0.89170 |
| H | 4.30090 | 2.24620 | 0.34310 |
| H | 7.07760 | 1.94650 | -0.97940 |
| H | 7.86150 | 1.09450 | 1.21030 |
| H | 6.23470 | 1.22280 | 1.87180 |
| H | 6.57530 | 0.06590 | 0.58550 |
| H | 0.07890 | -2.83780 | 5.39460 |
| H | 5.83800 | 4.63320 | -0.90300 |
| H | 7.12950 | 5.37880 | 0.03220 |
| H | 7.53180 | 4.27110 | -1.27790 |

| Marilzafurollene C_107 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.35790 | -1.53850 | -0.60290 |
| O | 2.37130 | -1.47890 | 0.42680 |
| C | 4.28710 | -0.31150 | -0.53440 |
| C | 2.58560 | -1.74120 | -1.91250 |
| C | 1.08440 | -1.79610 | -0.10720 |
| C | 3.57230 | 1.04870 | -0.65020 |
| Br | 5.66450 | -0.46480 | -1.96790 |
| C | 1.35900 | -2.49630 | -1.44490 |
| C | 0.23090 | -2.57790 | 0.91130 |
| C | 4.50800 | 2.21340 | -0.39160 |
| Cl | 1.75930 | -4.22780 | -1.23610 |
| C | -0.12470 | -1.75690 | 2.16340 |
| C | -1.10930 | -2.49320 | 3.05090 |
| O | 1.06120 | -1.51600 | 2.88860 |
| C | -2.31970 | -2.05460 | 3.31250 |
| C | 4.76480 | 3.19260 | -1.27470 |
| C | 5.71230 | 4.35050 | -1.02320 |
| C | 4.97290 | 5.68850 | -1.10200 |
| O | 6.74920 | 4.38690 | -1.99310 |
| C | -3.53480 | -1.62770 | 3.56410 |
| Br | -3.95460 | -0.44740 | 5.09710 |
| C | 7.68560 | 3.32240 | -1.88820 |
| H | 3.95200 | -2.43450 | -0.41560 |
| H | 4.82310 | -0.35220 | 0.41500 |
| H | 2.28010 | -0.78970 | -2.34510 |
| H | 3.16190 | -2.27800 | -2.66680 |
| H | 0.59280 | -0.84650 | -0.32630 |
| H | 3.11600 | 1.16300 | -1.63300 |
| H | 2.76410 | 1.10510 | 0.07980 |
| H | 0.52280 | -2.42660 | -2.14160 |
| H | -0.69240 | -2.88570 | 0.41830 |
| H | 0.73570 | -3.49810 | 1.20870 |
| H | 4.99030 | 2.23150 | 0.57530 |
| H | -0.54700 | -0.79590 | 1.86110 |
| H | -0.76150 | -3.42290 | 3.47710 |
| H | 1.76000 | -1.39060 | 2.25160 |
| H | 4.28660 | 3.17940 | -2.24360 |
| H | 6.15010 | 4.25650 | -0.02750 |
| H | 5.65220 | 6.51830 | -0.90640 |
| H | 4.53770 | 5.84190 | -2.08980 |
| H | 4.16820 | 5.73780 | -0.36810 |
| H | -4.40780 | -1.86990 | 2.97580 |
| H | 7.21900 | 2.35220 | -2.06280 |
| H | 8.46760 | 3.45120 | -2.63630 |
| H | 8.16130 | 3.30900 | -0.90680 |

| Marilzafurollene C_108 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.71270 | -1.76940 | -1.62070 |
| O | 3.03150 | -1.47600 | -0.40170 |
| C | 5.19350 | -1.33160 | -1.56920 |
| C | 2.85120 | -1.16820 | -2.73730 |
| C | 1.74730 | -0.91320 | -0.67970 |
| C | 5.48100 | 0.18420 | -1.52300 |
| Br | 6.12160 | -2.08020 | -3.16440 |
| C | 1.45900 | -1.25920 | -2.14600 |
| C | 0.69870 | -1.36590 | 0.35460 |
| C | 4.83710 | 0.88690 | -0.34410 |
| Cl | 0.82490 | -2.92110 | -2.34030 |
| C | 0.98890 | -0.84620 | 1.77380 |
| C | -0.14580 | -1.16820 | 2.72620 |
| O | 2.16990 | -1.46520 | 2.23580 |
| C | -0.86490 | -0.25400 | 3.33700 |
| C | 4.03070 | 1.95870 | -0.45170 |
| C | 3.33040 | 2.68770 | 0.68910 |
| C | 3.71420 | 2.18030 | 2.08610 |
| O | 1.91830 | 2.55630 | 0.58530 |
| C | -1.59940 | 0.64730 | 3.94540 |
| Br | -1.13410 | 1.38030 | 5.72480 |
| C | 1.32100 | 3.35320 | -0.42820 |
| H | 3.68540 | -2.85600 | -1.71780 |
| H | 5.65610 | -1.80610 | -0.70260 |
| H | 3.09840 | -0.12110 | -2.90580 |
| H | 2.95540 | -1.69430 | -3.68670 |
| H | 1.85290 | 0.16980 | -0.61650 |
| H | 6.55810 | 0.33780 | -1.45150 |
| H | 5.17350 | 0.66020 | -2.45390 |
| H | 0.75120 | -0.57280 | -2.61200 |
| H | -0.27680 | -0.99520 | 0.03710 |
| H | 0.62050 | -2.45370 | 0.37020 |
| H | 5.05600 | 0.46290 | 0.62470 |
| H | 1.14920 | 0.23380 | 1.74090 |
| H | -0.34390 | -2.21740 | 2.88980 |
| H | 2.75540 | -1.53320 | 1.48550 |
| H | 3.84230 | 2.35910 | -1.43660 |
| H | 3.60660 | 3.74220 | 0.63220 |
| H | 3.20130 | 2.75530 | 2.85710 |
| H | 3.43710 | 1.13490 | 2.22410 |
| H | 4.78520 | 2.27640 | 2.26490 |
| H | -2.50970 | 1.07100 | 3.54750 |
| H | 0.23910 | 3.22430 | -0.39760 |
| H | 1.53380 | 4.41220 | -0.27700 |
| H | 1.65790 | 3.06620 | -1.42430 |

| Marilzafurollene C_109 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.13030 | -1.73670 | -1.07470 |
| O | 2.38870 | -1.88370 | 0.13590 |
| C | 3.41120 | -0.24920 | -1.36170 |
| C | 2.32740 | -2.46650 | -2.16100 |
| C | 1.17080 | -2.57290 | -0.12450 |
| C | 4.32030 | 0.38320 | -0.29450 |
| Br | 1.69220 | 0.76730 | -1.43030 |
| C | 1.47920 | -3.43060 | -1.35580 |
| C | 0.66560 | -3.31830 | 1.12650 |
| C | 4.72640 | 1.80170 | -0.64340 |
| Cl | 2.44580 | -4.87980 | -0.94730 |
| C | 0.34930 | -2.38250 | 2.30810 |
| C | -0.76090 | -1.39590 | 1.99640 |
| O | -0.03150 | -3.16930 | 3.41850 |
| C | -0.56800 | -0.09900 | 1.91250 |
| C | 4.42850 | 2.88360 | 0.09660 |
| C | 4.82340 | 4.31300 | -0.23570 |
| C | 3.60620 | 5.11570 | -0.70130 |
| O | 5.79730 | 4.38040 | -1.27080 |
| C | -0.34710 | 1.19010 | 1.80920 |
| Br | -0.48850 | 2.42250 | 3.35210 |
| C | 7.12780 | 4.14440 | -0.82880 |
| H | 4.07570 | -2.26380 | -0.93630 |
| H | 3.88050 | -0.15510 | -2.34210 |
| H | 1.67660 | -1.77420 | -2.69540 |
| H | 2.95880 | -2.96150 | -2.89930 |
| H | 0.43210 | -1.82750 | -0.42290 |
| H | 3.82050 | 0.36380 | 0.67510 |
| H | 5.23110 | -0.20630 | -0.18570 |
| H | 0.58260 | -3.75720 | -1.88370 |
| H | -0.22290 | -3.89530 | 0.86720 |
| H | 1.41760 | -4.04080 | 1.44340 |
| H | 5.28980 | 1.92580 | -1.55730 |
| H | 1.25430 | -1.83290 | 2.57880 |
| H | -1.74390 | -1.81590 | 1.84180 |
| H | 0.74870 | -3.53420 | 3.81160 |
| H | 3.85590 | 2.75900 | 1.00480 |
| H | 5.21540 | 4.77990 | 0.66990 |
| H | 3.88120 | 6.14790 | -0.91840 |
| H | 3.17790 | 4.68730 | -1.60800 |
| H | 2.82750 | 5.13210 | 0.06160 |
| H | -0.07220 | 1.69570 | 0.89470 |
| H | 7.23460 | 3.16500 | -0.36160 |
| H | 7.80720 | 4.18420 | -1.68020 |
| H | 7.44430 | 4.90550 | -0.11440 |

| Marilzafurollene C_110 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.21340 | -0.29190 | -0.73240 |
| O | 1.88150 | 0.07660 | -0.37520 |
| C | 3.59290 | 0.28100 | -2.11380 |
| C | 3.27620 | -1.82020 | -0.62230 |
| C | 1.13710 | -1.07890 | 0.00410 |
| C | 3.59050 | 1.81900 | -2.17010 |
| Br | 2.30320 | -0.37400 | -3.48850 |
| C | 2.19820 | -2.11330 | 0.39980 |
| C | 0.07650 | -0.72130 | 1.06300 |
| C | 4.64450 | 2.45580 | -1.28380 |
| Cl | 2.84130 | -1.83030 | 2.04660 |
| C | -0.72790 | -1.92180 | 1.59900 |
| C | -1.72090 | -1.48540 | 2.65850 |
| O | -1.42670 | -2.53510 | 0.53580 |
| C | -1.70720 | -1.93360 | 3.89340 |
| C | 5.70310 | 3.14740 | -1.73740 |
| C | 6.75640 | 3.78720 | -0.85210 |
| C | 6.80700 | 5.30120 | -1.07200 |
| O | 8.05000 | 3.27880 | -1.14360 |
| C | -1.69780 | -2.40030 | 5.11960 |
| Br | -2.70770 | -4.01940 | 5.64550 |
| C | 8.26300 | 1.94180 | -0.71210 |
| H | 3.87290 | 0.11980 | 0.03200 |
| H | 4.57760 | -0.08680 | -2.40560 |
| H | 3.01220 | -2.29350 | -1.56800 |
| H | 4.25990 | -2.18870 | -0.33060 |
| H | 0.63260 | -1.43590 | -0.89580 |
| H | 3.75400 | 2.13920 | -3.19970 |
| H | 2.61070 | 2.20180 | -1.88150 |
| H | 1.82860 | -3.13800 | 0.34800 |
| H | 0.56270 | -0.21400 | 1.89690 |
| H | -0.60640 | 0.01200 | 0.63280 |
| H | 4.50880 | 2.33380 | -0.21850 |
| H | -0.04510 | -2.65800 | 2.02840 |
| H | -2.46300 | -0.76360 | 2.34790 |
| H | -1.90370 | -3.27990 | 0.87540 |
| H | 5.84490 | 3.27440 | -2.80120 |
| H | 6.51820 | 3.60000 | 0.19690 |
| H | 7.55380 | 5.76190 | -0.42510 |
| H | 7.06700 | 5.54280 | -2.10290 |
| H | 5.84490 | 5.76370 | -0.85030 |
| H | -1.15350 | -1.96220 | 5.94360 |
| H | 7.59010 | 1.24320 | -1.21050 |
| H | 9.28440 | 1.64230 | -0.94670 |
| H | 8.12710 | 1.84830 | 0.36610 |

| Marilzafurollene C_111 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.04700 | -1.83820 | -1.09170 |
| O | 2.42750 | -1.90360 | 0.19170 |
| C | 3.80240 | -0.50640 | -1.25720 |
| C | 1.93660 | -2.12580 | -2.11010 |
| C | 1.07410 | -2.33490 | 0.06260 |
| C | 2.93190 | 0.75240 | -1.08830 |
| Br | 4.68470 | -0.48040 | -3.04530 |
| C | 0.99580 | -3.00630 | -1.31440 |
| C | 0.64050 | -3.19560 | 1.26590 |
| C | 3.75830 | 2.02270 | -1.05530 |
| Cl | 1.61520 | -4.68520 | -1.29160 |
| C | 0.59210 | -2.41850 | 2.59390 |
| C | -0.49210 | -1.35680 | 2.60210 |
| O | 0.33640 | -3.33970 | 3.63420 |
| C | -0.25120 | -0.07200 | 2.73200 |
| C | 3.83530 | 2.85400 | -0.00170 |
| C | 4.65330 | 4.13350 | 0.05720 |
| C | 3.73810 | 5.36020 | 0.04650 |
| O | 5.54660 | 4.26130 | -1.04250 |
| C | -0.02180 | 1.21550 | 2.83650 |
| Br | 0.27360 | 2.37000 | 1.25660 |
| C | 6.74900 | 3.51540 | -0.90300 |
| H | 3.76870 | -2.65570 | -1.13250 |
| H | 4.60130 | -0.48190 | -0.51450 |
| H | 1.41800 | -1.21270 | -2.39900 |
| H | 2.30640 | -2.59900 | -3.02020 |
| H | 0.45890 | -1.43480 | 0.01840 |
| H | 2.20720 | 0.83860 | -1.89690 |
| H | 2.36020 | 0.67830 | -0.16260 |
| H | -0.01640 | -3.02690 | -1.71960 |
| H | -0.33630 | -3.63730 | 1.06550 |
| H | 1.33420 | -4.03000 | 1.37410 |
| H | 4.30990 | 2.25380 | -1.95600 |
| H | 1.56910 | -1.96320 | 2.77310 |
| H | -1.50630 | -1.71310 | 2.49180 |
| H | 0.56990 | -2.93830 | 4.45930 |
| H | 3.27600 | 2.62230 | 0.89350 |
| H | 5.21740 | 4.13610 | 0.99180 |
| H | 4.31960 | 6.27940 | 0.11870 |
| H | 3.15570 | 5.40640 | -0.87410 |
| H | 3.04020 | 5.34080 | 0.88400 |
| H | 0.02630 | 1.76170 | 3.76730 |
| H | 6.55660 | 2.44890 | -0.78170 |
| H | 7.36270 | 3.64380 | -1.79450 |
| H | 7.32850 | 3.86240 | -0.04670 |

| Marilzafurollene C_112 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.42250 | 0.20690 | -0.06380 |
| O | 1.82500 | -0.50190 | 1.02030 |
| C | 1.51010 | 1.37160 | -0.49490 |
| C | 2.68280 | -0.84800 | -1.14690 |
| C | 1.74530 | -1.89120 | 0.72080 |
| C | 2.02700 | 2.17040 | -1.70730 |
| Br | 1.29140 | 2.61770 | 1.04680 |
| C | 2.82690 | -2.12060 | -0.33850 |
| C | 1.83160 | -2.74690 | 2.00070 |
| C | 3.43380 | 2.70340 | -1.51150 |
| Cl | 4.46900 | -2.20020 | 0.36800 |
| C | 0.68290 | -2.47190 | 2.98970 |
| C | -0.67820 | -2.81260 | 2.41210 |
| O | 0.89120 | -3.23490 | 4.16060 |
| C | -1.56360 | -1.90000 | 2.08270 |
| C | 4.48160 | 2.38540 | -2.28960 |
| C | 5.89440 | 2.89480 | -2.07850 |
| C | 6.36770 | 3.70790 | -3.28580 |
| O | 6.80720 | 1.81900 | -1.91390 |
| C | -2.39920 | -0.96270 | 1.70430 |
| Br | -2.34640 | -0.18840 | -0.11730 |
| C | 6.66390 | 1.11000 | -0.68990 |
| H | 3.37610 | 0.59270 | 0.29900 |
| H | 0.51390 | 0.98590 | -0.71720 |
| H | 1.82030 | -0.93360 | -1.80910 |
| H | 3.55640 | -0.62420 | -1.75990 |
| H | 0.78130 | -2.05800 | 0.23760 |
| H | 2.00040 | 1.54410 | -2.59970 |
| H | 1.36080 | 3.01090 | -1.90460 |
| H | 2.66480 | -3.02500 | -0.92600 |
| H | 1.83960 | -3.80340 | 1.72980 |
| H | 2.78020 | -2.55120 | 2.50050 |
| H | 3.57440 | 3.37640 | -0.67700 |
| H | 0.70200 | -1.41550 | 3.26920 |
| H | -0.89200 | -3.86240 | 2.27500 |
| H | 1.57650 | -2.82450 | 4.66930 |
| H | 4.34590 | 1.71580 | -3.12670 |
| H | 5.92540 | 3.53690 | -1.19600 |
| H | 7.37810 | 4.08470 | -3.12670 |
| H | 6.37880 | 3.10120 | -4.19160 |
| H | 5.71770 | 4.56520 | -3.46250 |
| H | -3.17080 | -0.53060 | 2.32450 |
| H | 5.69460 | 0.61600 | -0.61890 |
| H | 7.43100 | 0.33870 | -0.62400 |
| H | 6.78160 | 1.77260 | 0.16850 |

| Marilzafurollene C_113 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.20980 | -0.97650 | -0.12250 |
| O | 2.06590 | -1.09420 | 0.72350 |
| C | 3.77700 | 0.45190 | -0.04370 |
| C | 2.72100 | -1.40190 | -1.51130 |
| C | 1.00180 | -1.76130 | 0.04530 |
| C | 5.04840 | 0.64600 | -0.88950 |
| Br | 4.20990 | 0.84550 | 1.86360 |
| C | 1.64820 | -2.41830 | -1.18070 |
| C | 0.23030 | -2.69500 | 0.99870 |
| C | 5.53580 | 2.08210 | -0.88100 |
| Cl | 2.41060 | -3.98990 | -0.79290 |
| C | -0.49810 | -1.94250 | 2.12630 |
| C | -1.40880 | -2.86580 | 2.91210 |
| O | 0.46720 | -1.39580 | 2.99840 |
| C | -2.71460 | -2.72980 | 2.96080 |
| C | 5.63660 | 2.85990 | -1.97170 |
| C | 6.12550 | 4.29630 | -1.95990 |
| C | 5.04210 | 5.24510 | -2.47880 |
| O | 7.26080 | 4.45920 | -2.79730 |
| C | -4.02060 | -2.60740 | 2.99900 |
| Br | -4.95030 | -1.51350 | 4.36230 |
| C | 8.45070 | 3.87290 | -2.28720 |
| H | 3.95370 | -1.69070 | 0.23450 |
| H | 3.01210 | 1.16770 | -0.34790 |
| H | 2.27390 | -0.55480 | -2.03320 |
| H | 3.51480 | -1.80510 | -2.14100 |
| H | 0.32480 | -0.98420 | -0.31410 |
| H | 5.84670 | 0.00250 | -0.51790 |
| H | 4.86180 | 0.34580 | -1.92100 |
| H | 0.94370 | -2.57930 | -1.99760 |
| H | -0.50390 | -3.24960 | 0.41260 |
| H | 0.89870 | -3.44090 | 1.43080 |
| H | 5.81660 | 2.48270 | 0.08320 |
| H | -1.08260 | -1.12400 | 1.70020 |
| H | -0.92230 | -3.66500 | 3.45210 |
| H | 1.19390 | -1.08340 | 2.46370 |
| H | 5.36110 | 2.46720 | -2.93990 |
| H | 6.37930 | 4.59000 | -0.93930 |
| H | 5.38910 | 6.27820 | -2.45630 |
| H | 4.76910 | 5.00930 | -3.50760 |
| H | 4.14050 | 5.18460 | -1.86860 |
| H | -4.70450 | -3.07850 | 2.30840 |
| H | 8.71430 | 4.29470 | -1.31650 |
| H | 9.27570 | 4.07010 | -2.97160 |
| H | 8.35760 | 2.79120 | -2.18390 |

| Marilzafurollene C_114 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.74380 | -0.29970 | -0.93560 |
| O | 2.20920 | -0.74020 | 0.31250 |
| C | 1.94550 | 0.90710 | -1.47450 |
| C | 2.75190 | -1.52910 | -1.85360 |
| C | 1.86870 | -2.12040 | 0.23400 |
| C | 2.08510 | 2.16940 | -0.59960 |
| Br | 0.00740 | 0.43330 | -1.54550 |
| C | 2.77990 | -2.67680 | -0.86450 |
| C | 1.94970 | -2.80610 | 1.61220 |
| C | 3.45530 | 2.83410 | -0.58960 |
| Cl | 4.45550 | -2.93360 | -0.29210 |
| C | 0.97330 | -2.21620 | 2.64630 |
| C | -0.47810 | -2.36810 | 2.23030 |
| O | 1.17300 | -2.88060 | 3.87730 |
| C | -1.26440 | -1.34610 | 1.97900 |
| C | 4.47820 | 2.59260 | -1.43030 |
| C | 5.82750 | 3.28180 | -1.35690 |
| C | 6.10950 | 4.06700 | -2.64030 |
| O | 6.87610 | 2.33620 | -1.20620 |
| C | -2.02630 | -0.31160 | 1.71390 |
| Br | -3.13050 | 0.57610 | 3.09670 |
| C | 6.91270 | 1.70020 | 0.06470 |
| H | 3.77940 | -0.01390 | -0.75050 |
| H | 2.24360 | 1.13200 | -2.49890 |
| H | 1.83510 | -1.58080 | -2.44140 |
| H | 3.59200 | -1.53790 | -2.54840 |
| H | 0.84410 | -2.17850 | -0.13640 |
| H | 1.36610 | 2.91990 | -0.92910 |
| H | 1.81650 | 1.92230 | 0.42840 |
| H | 2.41670 | -3.61510 | -1.28490 |
| H | 1.76110 | -3.87390 | 1.49590 |
| H | 2.96340 | -2.71660 | 2.00330 |
| H | 3.58950 | 3.57820 | 0.18290 |
| H | 1.21090 | -1.15900 | 2.78790 |
| H | -0.84770 | -3.37940 | 2.14170 |
| H | 0.74010 | -2.38580 | 4.55890 |
| H | 4.38390 | 1.86510 | -2.22170 |
| H | 5.84110 | 3.97820 | -0.51620 |
| H | 7.07370 | 4.57220 | -2.58090 |
| H | 6.13300 | 3.40940 | -3.50960 |
| H | 5.34680 | 4.82680 | -2.81310 |
| H | -2.12470 | 0.14760 | 0.74070 |
| H | 6.01490 | 1.10900 | 0.24920 |
| H | 7.76680 | 1.02450 | 0.10840 |
| H | 7.02220 | 2.42900 | 0.86870 |

| Marilzafurollene C_115 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.73950 | -1.63990 | -1.93950 |
| O | 2.59140 | -1.49670 | -0.52570 |
| C | 2.43120 | -0.31630 | -2.67270 |
| C | 1.83080 | -2.81220 | -2.33610 |
| C | 1.61010 | -2.40730 | -0.04480 |
| C | 3.53220 | 0.75740 | -2.55600 |
| Br | 0.69670 | 0.44040 | -2.03450 |
| C | 1.67340 | -3.57220 | -1.03390 |
| C | 1.84400 | -2.74280 | 1.43980 |
| C | 3.85470 | 1.16530 | -1.13040 |
| Cl | 3.10550 | -4.60900 | -0.76110 |
| C | 1.60760 | -1.53930 | 2.37180 |
| C | 0.15470 | -1.10000 | 2.38970 |
| O | 1.99310 | -1.90040 | 3.68230 |
| C | -0.25960 | 0.06220 | 1.93790 |
| C | 3.67980 | 2.39790 | -0.62690 |
| C | 4.01350 | 2.79310 | 0.79900 |
| C | 2.75610 | 3.22960 | 1.55170 |
| O | 4.92580 | 3.88110 | 0.83180 |
| C | -0.67990 | 1.20910 | 1.45900 |
| Br | -0.84300 | 2.83580 | 2.57570 |
| C | 6.24670 | 3.54630 | 0.42890 |
| H | 3.77350 | -1.92990 | -2.13250 |
| H | 2.29830 | -0.53230 | -3.73390 |
| H | 0.85550 | -2.44690 | -2.66030 |
| H | 2.24250 | -3.41970 | -3.14240 |
| H | 0.63390 | -1.93460 | -0.16090 |
| H | 4.45200 | 0.38790 | -3.01050 |
| H | 3.24040 | 1.63870 | -3.12840 |
| H | 0.78450 | -4.20350 | -1.00900 |
| H | 1.19160 | -3.56590 | 1.73420 |
| H | 2.86540 | -3.10270 | 1.56590 |
| H | 4.25320 | 0.38840 | -0.49360 |
| H | 2.23700 | -0.70550 | 2.05040 |
| H | -0.54980 | -1.80770 | 2.80140 |
| H | 2.93870 | -1.89850 | 3.73120 |
| H | 3.27710 | 3.18130 | -1.25240 |
| H | 4.44580 | 1.93910 | 1.32440 |
| H | 2.99220 | 3.50670 | 2.57910 |
| H | 2.28380 | 4.08860 | 1.07480 |
| H | 2.02650 | 2.42110 | 1.58670 |
| H | -0.97200 | 1.37710 | 0.43240 |
| H | 6.28120 | 3.21060 | -0.60810 |
| H | 6.88640 | 4.42460 | 0.51390 |
| H | 6.66700 | 2.76470 | 1.06300 |

| Marilzafurollene C_116 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.05150 | -1.42330 | -0.87400 |
| O | 2.29280 | -1.73120 | 0.29520 |
| C | 3.13100 | 0.10120 | -1.08180 |
| C | 2.39990 | -2.20200 | -2.02550 |
| C | 1.19770 | -2.57360 | -0.04760 |
| C | 3.91210 | 0.79720 | 0.04550 |
| Br | 1.28880 | 0.87110 | -1.17150 |
| C | 1.67080 | -3.31600 | -1.30130 |
| C | 0.76120 | -3.44510 | 1.14640 |
| C | 4.12890 | 2.27380 | -0.22450 |
| Cl | 2.82010 | -4.63200 | -0.91590 |
| C | 0.25720 | -2.62470 | 2.34840 |
| C | -0.98180 | -1.80990 | 2.02550 |
| O | -0.03810 | -3.51130 | 3.40850 |
| C | -0.99440 | -0.49620 | 2.00470 |
| C | 5.33690 | 2.85360 | -0.35000 |
| C | 5.61550 | 4.32870 | -0.61940 |
| C | 4.36220 | 5.21560 | -0.61070 |
| O | 6.22930 | 4.51500 | -1.88770 |
| C | -0.97910 | 0.81510 | 1.96370 |
| Br | -1.38240 | 1.93610 | 3.54500 |
| C | 7.58900 | 4.10820 | -1.95870 |
| H | 4.05550 | -1.82130 | -0.71830 |
| H | 3.61600 | 0.30990 | -2.03690 |
| H | 1.67590 | -1.58170 | -2.55430 |
| H | 3.12110 | -2.56440 | -2.75850 |
| H | 0.37020 | -1.92750 | -0.34440 |
| H | 3.37930 | 0.68570 | 0.99070 |
| H | 4.87980 | 0.31150 | 0.17680 |
| H | 0.85030 | -3.73990 | -1.88130 |
| H | -0.01750 | -4.13640 | 0.82200 |
| H | 1.60120 | -4.06030 | 1.46860 |
| H | 3.22900 | 2.86410 | -0.31620 |
| H | 1.05340 | -1.95420 | 2.68120 |
| H | -1.87850 | -2.37070 | 1.80670 |
| H | 0.77390 | -3.76690 | 3.82310 |
| H | 6.21490 | 2.23310 | -0.24860 |
| H | 6.28220 | 4.69010 | 0.16560 |
| H | 4.63100 | 6.26010 | -0.76850 |
| H | 3.66920 | 4.93440 | -1.40410 |
| H | 3.83650 | 5.15380 | 0.34250 |
| H | -0.75060 | 1.40030 | 1.08460 |
| H | 7.70230 | 3.03470 | -1.80800 |
| H | 7.98550 | 4.34430 | -2.94620 |
| H | 8.19890 | 4.63250 | -1.22190 |

| Marilzafurollene C_117 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.87320 | -1.30400 | -0.52900 |
| O | 1.67390 | -1.04710 | 0.20570 |
| C | 3.30610 | -0.03600 | -1.28970 |
| C | 2.57430 | -2.51500 | -1.42490 |
| C | 0.80020 | -2.17070 | 0.14340 |
| C | 3.64380 | 1.12620 | -0.34080 |
| Br | 1.85480 | 0.53380 | -2.53790 |
| C | 1.07790 | -2.69700 | -1.26670 |
| C | 1.13510 | -3.13970 | 1.30280 |
| C | 4.20450 | 2.32970 | -1.07340 |
| Cl | 0.55680 | -4.38260 | -1.54190 |
| C | 0.85220 | -2.54680 | 2.69560 |
| C | -0.63140 | -2.36300 | 2.95430 |
| O | 1.37790 | -3.42060 | 3.67410 |
| C | -1.19120 | -1.19780 | 3.18630 |
| C | 5.43120 | 2.84010 | -0.87510 |
| C | 5.98860 | 4.04580 | -1.60870 |
| C | 7.24670 | 3.67110 | -2.39620 |
| O | 6.35360 | 5.07570 | -0.70150 |
| C | -1.76390 | -0.03760 | 3.40140 |
| Br | -2.48700 | 1.07570 | 1.93350 |
| C | 5.25080 | 5.73780 | -0.09690 |
| H | 3.65540 | -1.58210 | 0.17920 |
| H | 4.18120 | -0.26520 | -1.89990 |
| H | 2.86580 | -2.37400 | -2.46600 |
| H | 3.10390 | -3.39090 | -1.04880 |
| H | -0.23670 | -1.84230 | 0.22320 |
| H | 2.75080 | 1.43240 | 0.20570 |
| H | 4.36550 | 0.79400 | 0.40640 |
| H | 0.55420 | -2.07100 | -1.99070 |
| H | 0.56050 | -4.06000 | 1.19360 |
| H | 2.18230 | -3.43460 | 1.23800 |
| H | 3.54880 | 2.79050 | -1.79910 |
| H | 1.36390 | -1.58640 | 2.79300 |
| H | -1.22950 | -3.26230 | 2.94110 |
| H | 2.31490 | -3.29440 | 3.72310 |
| H | 6.09100 | 2.38690 | -0.14920 |
| H | 5.24370 | 4.42520 | -2.31120 |
| H | 7.63810 | 4.53460 | -2.93430 |
| H | 8.03390 | 3.30790 | -1.73500 |
| H | 7.03540 | 2.89150 | -3.12860 |
| H | -1.89580 | 0.41520 | 4.37310 |
| H | 5.61610 | 6.53040 | 0.55610 |
| H | 4.60470 | 6.19500 | -0.84740 |
| H | 4.65290 | 5.05760 | 0.51060 |

| Marilzafurollene C_118 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.45640 | 0.19650 | -0.09210 |
| O | 1.85930 | -0.51990 | 0.98690 |
| C | 1.54000 | 1.35880 | -0.52100 |
| C | 2.72420 | -0.85270 | -1.17880 |
| C | 1.80370 | -1.91120 | 0.68950 |
| C | 2.05830 | 2.16700 | -1.72650 |
| Br | 1.30600 | 2.59520 | 1.02620 |
| C | 2.88540 | -2.12510 | -0.37340 |
| C | 1.90300 | -2.76900 | 1.96750 |
| C | 3.46100 | 2.70730 | -1.52050 |
| Cl | 4.53130 | -2.18690 | 0.32600 |
| C | 0.76890 | -2.49370 | 2.97260 |
| C | -0.60160 | -2.80570 | 2.40070 |
| O | 0.98340 | -3.28720 | 4.12200 |
| C | -1.48510 | -1.87700 | 2.11350 |
| C | 4.51450 | 2.40000 | -2.29520 |
| C | 5.92330 | 2.91630 | -2.07370 |
| C | 6.39800 | 3.73960 | -3.27350 |
| O | 6.84150 | 1.84490 | -1.91100 |
| C | -2.32270 | -0.92650 | 1.77410 |
| Br | -2.29130 | -0.09770 | -0.02370 |
| C | 6.69520 | 1.12670 | -0.69260 |
| H | 3.40730 | 0.58480 | 0.27510 |
| H | 0.54720 | 0.96880 | -0.75040 |
| H | 1.86020 | -0.94610 | -1.83810 |
| H | 3.59320 | -0.61780 | -1.79430 |
| H | 0.84150 | -2.09270 | 0.20820 |
| H | 2.04010 | 1.54520 | -2.62230 |
| H | 1.38820 | 3.00460 | -1.92280 |
| H | 2.73220 | -3.03020 | -0.96210 |
| H | 1.90820 | -3.82510 | 1.69580 |
| H | 2.85540 | -2.57600 | 2.46170 |
| H | 3.59330 | 3.37600 | -0.68140 |
| H | 0.81720 | -1.44320 | 3.27020 |
| H | -0.82330 | -3.84880 | 2.22650 |
| H | 0.49040 | -2.91650 | 4.84050 |
| H | 4.38710 | 1.73460 | -3.13690 |
| H | 5.94600 | 3.55310 | -1.18700 |
| H | 7.40550 | 4.12130 | -3.10690 |
| H | 6.41730 | 3.13860 | -4.18300 |
| H | 5.74390 | 4.59420 | -3.44830 |
| H | -3.08580 | -0.51110 | 2.41610 |
| H | 6.80380 | 1.78410 | 0.17090 |
| H | 5.72860 | 0.62650 | -0.63080 |
| H | 7.46660 | 0.35950 | -0.62730 |

| Marilzafurollene C_119 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.93210 | -0.72970 | -1.30450 |
| O | 1.52550 | -0.63630 | -1.06810 |
| C | 3.29920 | 0.01700 | -2.60450 |
| C | 3.26050 | -2.23060 | -1.31000 |
| C | 1.05680 | -1.83530 | -0.45790 |
| C | 2.95770 | 1.52130 | -2.57160 |
| Br | 2.29630 | -0.79650 | -4.12490 |
| C | 1.89670 | -2.88440 | -1.18940 |
| C | 1.26420 | -1.75880 | 1.07460 |
| C | 3.72170 | 2.36340 | -1.55930 |
| Cl | 1.96240 | -4.46980 | -0.37100 |
| C | 0.48100 | -0.61510 | 1.74390 |
| C | 0.54730 | -0.70520 | 3.25560 |
| O | 1.03640 | 0.61490 | 1.33190 |
| C | -0.51220 | -0.84470 | 4.01940 |
| C | 4.85330 | 2.02320 | -0.91580 |
| C | 5.55110 | 2.89950 | 0.10680 |
| C | 6.97970 | 3.22510 | -0.33590 |
| O | 5.63920 | 2.24360 | 1.36360 |
| C | -1.57790 | -0.99490 | 4.76960 |
| Br | -2.28780 | -2.77650 | 5.26040 |
| C | 4.39410 | 2.09810 | 2.03560 |
| H | 3.44230 | -0.27740 | -0.45400 |
| H | 4.35810 | -0.11630 | -2.82910 |
| H | 3.79470 | -2.55980 | -2.20170 |
| H | 3.88000 | -2.47430 | -0.44610 |
| H | -0.00330 | -1.97260 | -0.67440 |
| H | 3.12870 | 1.95680 | -3.55650 |
| H | 1.89210 | 1.63880 | -2.37050 |
| H | 1.48090 | -3.04470 | -2.18560 |
| H | 0.92750 | -2.69970 | 1.51210 |
| H | 2.32290 | -1.68010 | 1.32400 |
| H | 3.28670 | 3.33230 | -1.35760 |
| H | -0.56090 | -0.65070 | 1.41730 |
| H | 1.53290 | -0.64690 | 3.69360 |
| H | 1.16580 | 0.55500 | 0.38870 |
| H | 5.32830 | 1.07170 | -1.09900 |
| H | 5.00380 | 3.83700 | 0.22400 |
| H | 6.98640 | 3.74660 | -1.29330 |
| H | 7.47440 | 3.86580 | 0.39430 |
| H | 7.57770 | 2.31960 | -0.44110 |
| H | -2.15990 | -0.18480 | 5.18420 |
| H | 3.91820 | 3.06480 | 2.20460 |
| H | 3.70460 | 1.46360 | 1.47840 |
| H | 4.55650 | 1.63200 | 3.00730 |

| Marilzafurollene C_120 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.03530 | -1.63250 | -1.25060 |
| O | 2.31200 | -1.46560 | -0.03050 |
| C | 3.56510 | -0.27740 | -1.75550 |
| C | 2.08620 | -2.35660 | -2.21470 |
| C | 1.00520 | -2.02240 | -0.15920 |
| C | 4.61000 | 0.32640 | -0.80160 |
| Br | 2.04750 | 1.00660 | -1.95250 |
| C | 1.13870 | -3.06860 | -1.27100 |
| C | 0.47680 | -2.52640 | 1.19770 |
| C | 5.23090 | 1.59910 | -1.34480 |
| Cl | 1.89820 | -4.58000 | -0.68820 |
| C | 0.26290 | -1.39460 | 2.21820 |
| C | -0.42600 | -1.89720 | 3.47150 |
| O | 1.52240 | -0.86190 | 2.56510 |
| C | -1.58960 | -1.45070 | 3.88610 |
| C | 5.16330 | 2.79450 | -0.73070 |
| C | 5.75670 | 4.10930 | -1.22500 |
| C | 6.35190 | 4.03590 | -2.63830 |
| O | 6.80060 | 4.56030 | -0.37240 |
| C | -2.75760 | -1.00340 | 4.28210 |
| Br | -4.46180 | -1.82360 | 3.69730 |
| C | 6.36950 | 5.05560 | 0.88800 |
| H | 3.87600 | -2.29480 | -1.03790 |
| H | 4.00700 | -0.40950 | -2.74420 |
| H | 1.52460 | -1.64330 | -2.81840 |
| H | 2.60310 | -3.03180 | -2.89720 |
| H | 0.35030 | -1.22800 | -0.52240 |
| H | 4.15540 | 0.51810 | 0.17140 |
| H | 5.41450 | -0.38980 | -0.63120 |
| H | 0.18460 | -3.32440 | -1.73340 |
| H | -0.47450 | -3.03280 | 1.02790 |
| H | 1.14850 | -3.27620 | 1.61750 |
| H | 5.75270 | 1.49870 | -2.28450 |
| H | -0.33330 | -0.60140 | 1.76110 |
| H | 0.09700 | -2.66090 | 4.02830 |
| H | 2.04500 | -0.84360 | 1.76640 |
| H | 4.62970 | 2.85540 | 0.20650 |
| H | 4.95430 | 4.84910 | -1.24210 |
| H | 6.71620 | 5.01450 | -2.95130 |
| H | 7.19500 | 3.34600 | -2.68090 |
| H | 5.60730 | 3.71550 | -3.36750 |
| H | -2.90400 | -0.16610 | 4.94880 |
| H | 5.90620 | 4.27790 | 1.49510 |
| H | 7.22940 | 5.43400 | 1.44070 |
| H | 5.66200 | 5.87740 | 0.77050 |

| Marilzafurollene C_121 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.45960 | -1.19220 | -1.88950 |
| O | 2.38630 | -0.88790 | -0.49500 |
| C | 1.77030 | -0.10830 | -2.74430 |
| C | 1.85290 | -2.59200 | -2.03570 |
| C | 1.87700 | -2.00260 | 0.23140 |
| C | 2.57210 | 1.20030 | -2.88900 |
| Br | -0.03450 | 0.30000 | -1.99740 |
| C | 2.12700 | -3.20790 | -0.67980 |
| C | 2.49770 | -2.07210 | 1.63920 |
| C | 2.94850 | 1.83390 | -1.56380 |
| Cl | 3.82300 | -3.77380 | -0.60560 |
| C | 1.98560 | -0.96750 | 2.58050 |
| C | 0.55680 | -1.21500 | 3.02650 |
| O | 2.81930 | -0.93660 | 3.72100 |
| C | -0.44040 | -0.40000 | 2.76850 |
| C | 4.19930 | 2.17760 | -1.21490 |
| C | 4.58320 | 2.78090 | 0.12220 |
| C | 5.14920 | 4.19160 | -0.05770 |
| O | 5.58660 | 2.00670 | 0.76360 |
| C | -1.45460 | 0.38950 | 2.50590 |
| Br | -2.57390 | 0.17330 | 0.88900 |
| C | 5.13360 | 0.74560 | 1.23850 |
| H | 3.51570 | -1.24930 | -2.15820 |
| H | 1.60440 | -0.50570 | -3.74660 |
| H | 0.77550 | -2.52750 | -2.19340 |
| H | 2.27900 | -3.16020 | -2.86290 |
| H | 0.79680 | -1.86950 | 0.31160 |
| H | 3.48070 | 1.00800 | -3.46100 |
| H | 1.99180 | 1.92180 | -3.46470 |
| H | 1.47690 | -4.05360 | -0.45330 |
| H | 2.30310 | -3.04900 | 2.08320 |
| H | 3.58150 | -1.99340 | 1.54670 |
| H | 2.13590 | 1.99900 | -0.87030 |
| H | 2.06130 | -0.00230 | 2.07420 |
| H | 0.38550 | -2.12330 | 3.58640 |
| H | 2.61840 | -0.15990 | 4.22360 |
| H | 5.01300 | 2.01610 | -1.90670 |
| H | 3.70210 | 2.84050 | 0.76430 |
| H | 4.42190 | 4.84960 | -0.53380 |
| H | 5.41270 | 4.62880 | 0.90540 |
| H | 6.04810 | 4.18080 | -0.67440 |
| H | -1.77540 | 1.21260 | 3.12750 |
| H | 4.33150 | 0.86740 | 1.96610 |
| H | 4.77730 | 0.10690 | 0.42950 |
| H | 5.95320 | 0.22470 | 1.73300 |

| Marilzafurollene C_122 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.07460 | -1.23280 | -0.15300 |
| O | 2.11420 | -1.59310 | 0.83910 |
| C | 3.57280 | 0.20400 | 0.08610 |
| C | 2.36140 | -1.45750 | -1.49010 |
| C | 0.99260 | -2.24490 | 0.24650 |
| C | 4.63600 | 0.65210 | -0.93370 |
| Br | 4.36630 | 0.29200 | 1.91470 |
| C | 1.44150 | -2.61720 | -1.17200 |
| C | 0.49560 | -3.40580 | 1.13130 |
| C | 5.05040 | 2.09920 | -0.74620 |
| Cl | 2.36770 | -4.14780 | -1.22000 |
| C | -0.11860 | -2.93990 | 2.46430 |
| C | -1.43880 | -2.21490 | 2.27190 |
| O | -0.33900 | -4.07290 | 3.28020 |
| C | -1.62370 | -0.94910 | 2.57460 |
| C | 4.91710 | 3.05790 | -1.67790 |
| C | 5.33420 | 4.50460 | -1.48750 |
| C | 4.13550 | 5.44370 | -1.64790 |
| O | 6.30100 | 4.89150 | -2.45350 |
| C | -1.79870 | 0.32320 | 2.84690 |
| Br | -1.48250 | 1.74330 | 1.50440 |
| C | 7.58690 | 4.31890 | -2.25400 |
| H | 3.90900 | -1.93100 | -0.06760 |
| H | 2.72570 | 0.89150 | 0.07480 |
| H | 1.76830 | -0.58150 | -1.75630 |
| H | 3.04580 | -1.66570 | -2.31290 |
| H | 0.20660 | -1.49410 | 0.15140 |
| H | 5.52140 | 0.02100 | -0.85020 |
| H | 4.25880 | 0.52540 | -1.94880 |
| H | 0.60810 | -2.70710 | -1.86960 |
| H | -0.23630 | -3.99900 | 0.58100 |
| H | 1.33440 | -4.07180 | 1.33780 |
| H | 5.48300 | 2.34950 | 0.21250 |
| H | 0.59070 | -2.28570 | 2.97900 |
| H | -2.24920 | -2.80310 | 1.86530 |
| H | 0.49650 | -4.37120 | 3.61330 |
| H | 4.48960 | 2.81660 | -2.64060 |
| H | 5.74500 | 4.63990 | -0.48450 |
| H | 4.43350 | 6.48120 | -1.49550 |
| H | 3.70260 | 5.36610 | -2.64590 |
| H | 3.35410 | 5.21310 | -0.92280 |
| H | -2.12410 | 0.71360 | 3.80050 |
| H | 7.56290 | 3.23130 | -2.33260 |
| H | 8.27300 | 4.69060 | -3.01530 |
| H | 7.99280 | 4.58950 | -1.27810 |

| Marilzafurollene C_123 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.99910 | -0.75090 | -0.57950 |
| O | 2.17330 | -0.29430 | 0.49200 |
| C | 3.62430 | 0.43730 | -1.33410 |
| C | 2.11980 | -1.67180 | -1.43500 |
| C | 0.87500 | -0.87160 | 0.38680 |
| C | 4.59330 | 1.23870 | -0.44890 |
| Br | 2.18370 | 1.65400 | -1.99480 |
| C | 1.08240 | -2.14680 | -0.43930 |
| C | 0.23310 | -1.03090 | 1.77890 |
| C | 5.31680 | 2.32780 | -1.21710 |
| Cl | 1.76000 | -3.48460 | 0.53760 |
| C | -1.16040 | -1.68850 | 1.76560 |
| C | -1.71240 | -1.85800 | 3.16890 |
| O | -2.05720 | -0.90930 | 0.99940 |
| C | -2.06240 | -3.01940 | 3.67330 |
| C | 6.64880 | 2.39010 | -1.38020 |
| C | 7.36970 | 3.48230 | -2.14820 |
| C | 8.14980 | 2.89550 | -3.32740 |
| O | 8.30580 | 4.15950 | -1.32230 |
| C | -2.42300 | -4.18060 | 4.16630 |
| Br | -1.17020 | -5.35030 | 5.15670 |
| C | 7.71570 | 4.99950 | -0.33950 |
| H | 3.79230 | -1.35510 | -0.13610 |
| H | 4.15960 | 0.06530 | -2.20910 |
| H | 1.62550 | -1.11230 | -2.22950 |
| H | 2.67670 | -2.48560 | -1.90000 |
| H | 0.27280 | -0.17870 | -0.20370 |
| H | 4.04950 | 1.69400 | 0.37990 |
| H | 5.32820 | 0.56630 | -0.00440 |
| H | 0.16450 | -2.49870 | -0.91230 |
| H | 0.89910 | -1.61670 | 2.41370 |
| H | 0.17500 | -0.04900 | 2.24930 |
| H | 4.69230 | 3.09580 | -1.65190 |
| H | -1.09070 | -2.67110 | 1.29400 |
| H | -1.80650 | -0.96090 | 3.76330 |
| H | -2.12180 | -0.04420 | 1.37810 |
| H | 7.27940 | 1.62770 | -0.94580 |
| H | 6.64320 | 4.19770 | -2.53880 |
| H | 8.65550 | 3.68240 | -3.88710 |
| H | 8.90850 | 2.19000 | -2.98790 |
| H | 7.48680 | 2.37160 | -4.01640 |
| H | -3.41320 | -4.60470 | 4.08510 |
| H | 8.49930 | 5.50390 | 0.22580 |
| H | 7.08970 | 5.76570 | -0.79870 |
| H | 7.11010 | 4.43210 | 0.36810 |

| Marilzafurollene C_124 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.57120 | -1.89830 | -1.48060 |
| O | 2.84550 | -1.39400 | -0.36150 |
| C | 4.68950 | -0.93300 | -1.93170 |
| C | 2.51250 | -2.27020 | -2.52450 |
| C | 1.44860 | -1.65080 | -0.52330 |
| C | 4.26200 | 0.45500 | -2.45260 |
| Br | 5.73580 | -1.83160 | -3.36880 |
| C | 1.34490 | -2.68560 | -1.65220 |
| C | 0.79670 | -2.02420 | 0.82250 |
| C | 3.61270 | 1.32790 | -1.39550 |
| Cl | 1.59000 | -4.35860 | -1.06650 |
| C | 0.81930 | -0.87200 | 1.84280 |
| C | 0.03920 | -1.22090 | 3.09510 |
| O | 2.16210 | -0.61290 | 2.18990 |
| C | -1.04160 | -0.58030 | 3.47950 |
| C | 4.16920 | 2.43070 | -0.86870 |
| C | 3.51660 | 3.30010 | 0.18980 |
| C | 3.36870 | 4.74160 | -0.30300 |
| O | 4.30210 | 3.33880 | 1.37150 |
| C | -2.13150 | 0.04420 | 3.85910 |
| Br | -2.09630 | 1.62530 | 5.05000 |
| C | 4.23490 | 2.15050 | 2.14880 |
| H | 4.04450 | -2.82050 | -1.13910 |
| H | 5.38050 | -0.79440 | -1.09850 |
| H | 2.22660 | -1.40610 | -3.12250 |
| H | 2.84300 | -3.05440 | -3.20640 |
| H | 0.99780 | -0.72590 | -0.88680 |
| H | 5.14720 | 0.97190 | -2.82530 |
| H | 3.59060 | 0.36750 | -3.30580 |
| H | 0.38810 | -2.65070 | -2.17450 |
| H | -0.23930 | -2.31040 | 0.63540 |
| H | 1.28090 | -2.90280 | 1.25120 |
| H | 2.63480 | 1.02180 | -1.05610 |
| H | 0.40130 | 0.02760 | 1.38530 |
| H | 0.42330 | -2.04360 | 3.68050 |
| H | 2.69090 | -0.79840 | 1.41710 |
| H | 5.14940 | 2.74650 | -1.19600 |
| H | 2.52220 | 2.91330 | 0.42250 |
| H | 2.88780 | 5.36170 | 0.45360 |
| H | 4.33950 | 5.18480 | -0.52650 |
| H | 2.76070 | 4.78890 | -1.20680 |
| H | -3.13410 | -0.23330 | 3.56810 |
| H | 4.58280 | 1.27930 | 1.59260 |
| H | 4.86560 | 2.25510 | 3.03140 |
| H | 3.21600 | 1.96230 | 2.48940 |

| Marilzafurollene C_125 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.91050 | -0.64260 | -1.24120 |
| O | 2.04500 | -0.70960 | -0.10720 |
| C | 2.60400 | 0.61250 | -2.08420 |
| C | 2.74660 | -1.97600 | -1.98250 |
| C | 1.38150 | -1.97170 | -0.07310 |
| C | 2.86640 | 1.93680 | -1.34540 |
| Br | 0.68400 | 0.59480 | -2.62830 |
| C | 2.28600 | -2.90890 | -0.88130 |
| C | 1.06910 | -2.39950 | 1.37420 |
| C | 4.33170 | 2.16250 | -1.02470 |
| Cl | 3.70020 | -3.46430 | 0.06330 |
| C | 0.06660 | -1.46640 | 2.07600 |
| C | -0.35620 | -2.01590 | 3.42440 |
| O | 0.68340 | -0.21090 | 2.26050 |
| C | -1.59050 | -2.36080 | 3.71340 |
| C | 5.08480 | 3.14620 | -1.54690 |
| C | 6.55330 | 3.39010 | -1.23810 |
| C | 7.42520 | 3.04790 | -2.44880 |
| O | 7.01710 | 2.60280 | -0.14790 |
| C | -2.81890 | -2.72130 | 4.00120 |
| Br | -4.14610 | -1.46910 | 4.76960 |
| C | 6.70380 | 3.14140 | 1.13030 |
| H | 3.93230 | -0.59830 | -0.86310 |
| H | 3.19360 | 0.59210 | -3.00220 |
| H | 1.97040 | -1.90800 | -2.74480 |
| H | 3.66230 | -2.30710 | -2.47300 |
| H | 0.44380 | -1.85630 | -0.62000 |
| H | 2.50720 | 2.76520 | -1.95700 |
| H | 2.29380 | 1.96930 | -0.41760 |
| H | 1.76230 | -3.78880 | -1.25660 |
| H | 0.65600 | -3.40890 | 1.35070 |
| H | 1.98520 | -2.46080 | 1.96300 |
| H | 4.77900 | 1.47190 | -0.32390 |
| H | -0.81130 | -1.33040 | 1.44020 |
| H | 0.42530 | -2.11170 | 4.16400 |
| H | 1.19540 | -0.03460 | 1.47430 |
| H | 4.63960 | 3.83570 | -2.25010 |
| H | 6.68460 | 4.44980 | -1.01090 |
| H | 8.47610 | 3.24690 | -2.23800 |
| H | 7.33370 | 1.99420 | -2.71350 |
| H | 7.14370 | 3.63970 | -3.32010 |
| H | -3.22170 | -3.71240 | 3.85210 |
| H | 5.62970 | 3.26880 | 1.26760 |
| H | 7.06210 | 2.46680 | 1.90790 |
| H | 7.18860 | 4.10720 | 1.27780 |

| Marilzafurollene C_126 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.68520 | -0.69180 | -1.07830 |
| O | 2.18940 | -1.03890 | 0.21460 |
| C | 2.04680 | 0.62500 | -1.56860 |
| C | 2.42700 | -1.90990 | -1.97640 |
| C | 1.60090 | -2.33440 | 0.17520 |
| C | 2.41040 | 1.84790 | -0.70800 |
| Br | 0.05810 | 0.44920 | -1.55850 |
| C | 2.32240 | -3.04280 | -0.97530 |
| C | 1.65970 | -3.02200 | 1.55330 |
| C | 3.88090 | 2.21350 | -0.77880 |
| Cl | 3.96270 | -3.58760 | -0.51270 |
| C | 0.86120 | -2.27820 | 2.64010 |
| C | -0.62480 | -2.21780 | 2.33790 |
| O | 1.05350 | -2.93970 | 3.87400 |
| C | -1.26310 | -1.09830 | 2.08170 |
| C | 4.35930 | 3.35470 | -1.30470 |
| C | 5.82760 | 3.74130 | -1.38400 |
| C | 6.32070 | 3.70410 | -2.83270 |
| O | 6.66080 | 2.86740 | -0.63180 |
| C | -1.87750 | 0.02680 | 1.80260 |
| Br | -2.72560 | 1.15180 | 3.19370 |
| C | 6.70430 | 3.16260 | 0.75840 |
| H | 3.76490 | -0.57190 | -0.98580 |
| H | 2.34270 | 0.81450 | -2.60150 |
| H | 1.48030 | -1.80970 | -2.50750 |
| H | 3.20790 | -2.06420 | -2.72140 |
| H | 0.55860 | -2.20960 | -0.12210 |
| H | 1.81820 | 2.70370 | -1.03370 |
| H | 2.14160 | 1.66610 | 0.33340 |
| H | 1.77310 | -3.90390 | -1.35750 |
| H | 1.29020 | -4.04410 | 1.46220 |
| H | 2.69930 | -3.09990 | 1.87140 |
| H | 4.57270 | 1.49050 | -0.37040 |
| H | 1.25200 | -1.26220 | 2.73710 |
| H | -1.15130 | -3.16080 | 2.34150 |
| H | 1.90340 | -2.69980 | 4.21560 |
| H | 3.66850 | 4.07690 | -1.71620 |
| H | 5.93360 | 4.76270 | -1.01340 |
| H | 7.36620 | 4.00650 | -2.89400 |
| H | 6.24080 | 2.69950 | -3.24900 |
| H | 5.74270 | 4.37780 | -3.46560 |
| H | -1.97980 | 0.44190 | 0.81020 |
| H | 5.71470 | 3.12600 | 1.21470 |
| H | 7.33360 | 2.43220 | 1.26660 |
| H | 7.13100 | 4.15060 | 0.93570 |

| Marilzafurollene C_127 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.70450 | -1.88470 | -1.46150 |
| O | 2.36890 | -2.00690 | -0.08030 |
| C | 3.56710 | -0.62910 | -1.68950 |
| C | 1.37590 | -1.94920 | -2.22680 |
| C | 0.96440 | -2.19650 | 0.06870 |
| C | 2.92960 | 0.68360 | -1.19850 |
| Br | 4.00430 | -0.48220 | -3.62970 |
| C | 0.49770 | -2.74580 | -1.28400 |
| C | 0.64650 | -3.06150 | 1.30490 |
| C | 3.89280 | 1.85210 | -1.26260 |
| Cl | 0.84410 | -4.49230 | -1.46060 |
| C | 0.96010 | -2.35670 | 2.63820 |
| C | 0.03720 | -1.18140 | 2.90890 |
| O | 0.84720 | -3.28910 | 3.69550 |
| C | 0.45260 | 0.06220 | 2.99110 |
| C | 4.33630 | 2.52880 | -0.19040 |
| C | 5.29000 | 3.70670 | -0.25000 |
| C | 6.59630 | 3.38750 | 0.48120 |
| O | 4.73180 | 4.85450 | 0.37320 |
| C | 0.85320 | 1.31020 | 3.04600 |
| Br | 0.90040 | 2.47630 | 1.44710 |
| C | 3.63180 | 5.42310 | -0.32480 |
| H | 3.29250 | -2.76630 | -1.72180 |
| H | 4.51310 | -0.77520 | -1.16550 |
| H | 0.95100 | -0.95570 | -2.36400 |
| H | 1.47570 | -2.40410 | -3.21280 |
| H | 0.51810 | -1.20800 | 0.18880 |
| H | 2.04670 | 0.93480 | -1.78500 |
| H | 2.59460 | 0.56160 | -0.16780 |
| H | -0.56750 | -2.59350 | -1.46130 |
| H | -0.40280 | -3.35730 | 1.28030 |
| H | 1.22710 | -3.98310 | 1.24580 |
| H | 4.22660 | 2.13920 | -2.24980 |
| H | 1.99670 | -2.01140 | 2.61940 |
| H | -1.01090 | -1.40960 | 3.03620 |
| H | 0.01040 | -3.72630 | 3.64120 |
| H | 4.00460 | 2.24340 | 0.79790 |
| H | 5.52400 | 3.93650 | -1.29140 |
| H | 7.28690 | 4.22900 | 0.42560 |
| H | 6.41700 | 3.17420 | 1.53520 |
| H | 7.09180 | 2.52140 | 0.04180 |
| H | 1.18560 | 1.81440 | 3.94180 |
| H | 3.91120 | 5.70660 | -1.34020 |
| H | 2.78450 | 4.73810 | -0.37360 |
| H | 3.29880 | 6.32230 | 0.19340 |

| Marilzafurollene C_128 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.30720 | -1.58540 | -1.02190 |
| O | 2.40090 | -1.48990 | 0.07780 |
| C | 3.79360 | -0.18720 | -1.44600 |
| C | 2.57300 | -2.37450 | -2.11400 |
| C | 1.17720 | -2.14960 | -0.24080 |
| C | 4.63040 | 0.49200 | -0.34870 |
| Br | 2.22260 | 0.97060 | -1.87300 |
| C | 1.55750 | -3.16980 | -1.31950 |
| C | 0.49850 | -2.70970 | 1.02450 |
| C | 5.23600 | 1.80440 | -0.80670 |
| Cl | 2.34220 | -4.62180 | -0.62900 |
| C | 0.04500 | -1.61090 | 2.00190 |
| C | -0.77510 | -2.18290 | 3.14170 |
| O | 1.19370 | -0.98280 | 2.52770 |
| C | -2.03420 | -1.87520 | 3.35610 |
| C | 4.97520 | 2.99910 | -0.24840 |
| C | 5.56890 | 4.32620 | -0.69130 |
| C | 4.51680 | 5.17670 | -1.40720 |
| O | 6.66200 | 4.16000 | -1.58670 |
| C | -3.29640 | -1.58270 | 3.56430 |
| Br | -3.86650 | -0.07180 | 4.70960 |
| C | 7.89350 | 3.85520 | -0.94520 |
| H | 4.15860 | -2.17960 | -0.68580 |
| H | 4.38800 | -0.27330 | -2.35690 |
| H | 2.05070 | -1.70310 | -2.79600 |
| H | 3.23830 | -2.99880 | -2.71100 |
| H | 0.52000 | -1.40700 | -0.69750 |
| H | 4.01680 | 0.65270 | 0.53890 |
| H | 5.44800 | -0.16310 | -0.04610 |
| H | 0.70610 | -3.49630 | -1.91770 |
| H | -0.37220 | -3.29040 | 0.71690 |
| H | 1.16100 | -3.40670 | 1.53930 |
| H | 5.91760 | 1.74980 | -1.64350 |
| H | -0.54160 | -0.86330 | 1.46290 |
| H | -0.26280 | -2.87440 | 3.79460 |
| H | 1.82080 | -0.90650 | 1.81210 |
| H | 4.28490 | 3.05290 | 0.58150 |
| H | 5.89960 | 4.86740 | 0.19730 |
| H | 4.93250 | 6.13900 | -1.70590 |
| H | 4.15470 | 4.67670 | -2.30610 |
| H | 3.65890 | 5.37000 | -0.76290 |
| H | -4.13190 | -2.12210 | 3.14300 |
| H | 7.83020 | 2.94070 | -0.35470 |
| H | 8.67080 | 3.71480 | -1.69620 |
| H | 8.20640 | 4.66940 | -0.29030 |

| Marilzafurollene C_129 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.04180 | -0.66850 | 0.63020 |
| O | 1.69980 | -0.18630 | 0.73830 |
| C | 3.98270 | 0.51490 | 0.33550 |
| C | 3.01080 | -1.77920 | -0.43230 |
| C | 0.79130 | -1.12500 | 0.16370 |
| C | 3.67820 | 1.25860 | -0.97900 |
| Br | 5.86160 | -0.15270 | 0.30590 |
| C | 1.61390 | -1.66620 | -1.00800 |
| C | 0.37440 | -2.16690 | 1.23000 |
| C | 4.53840 | 2.49440 | -1.15570 |
| Cl | 1.01590 | -3.21030 | -1.67510 |
| C | -0.41060 | -1.55990 | 2.40660 |
| C | -0.97680 | -2.63600 | 3.31190 |
| O | 0.45820 | -0.73900 | 3.15580 |
| C | -2.26190 | -2.79240 | 3.53440 |
| C | 5.36880 | 2.70020 | -2.19140 |
| C | 6.24140 | 3.92940 | -2.36280 |
| C | 5.88330 | 4.67870 | -3.64860 |
| O | 7.61450 | 3.57760 | -2.45160 |
| C | -3.54890 | -2.94440 | 3.73870 |
| Br | -4.67480 | -4.10550 | 2.59710 |
| C | 8.17350 | 3.09190 | -1.23810 |
| H | 3.31890 | -1.10880 | 1.58960 |
| H | 3.91780 | 1.21580 | 1.16920 |
| H | 3.78620 | -1.69040 | -1.19320 |
| H | 3.14340 | -2.74740 | 0.05180 |
| H | -0.09680 | -0.60780 | -0.20150 |
| H | 3.81180 | 0.59540 | -1.83360 |
| H | 2.63510 | 1.57690 | -0.98970 |
| H | 1.60970 | -0.93660 | -1.81900 |
| H | -0.26400 | -2.91100 | 0.75180 |
| H | 1.24050 | -2.71530 | 1.60190 |
| H | 4.46170 | 3.24360 | -0.38060 |
| H | -1.22250 | -0.94040 | 2.01860 |
| H | -0.25710 | -3.28940 | 3.78310 |
| H | 0.96760 | -0.22980 | 2.53180 |
| H | 5.45100 | 1.95440 | -2.96900 |
| H | 6.09390 | 4.60470 | -1.51760 |
| H | 4.84030 | 4.99640 | -3.64220 |
| H | 6.50110 | 5.56960 | -3.76260 |
| H | 6.03920 | 4.05250 | -4.52740 |
| H | -4.10920 | -2.46530 | 4.52820 |
| H | 7.70160 | 2.16270 | -0.91690 |
| H | 9.23470 | 2.88980 | -1.38200 |
| H | 8.07900 | 3.82600 | -0.43700 |

| Marilzafurollene C_130 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.11730 | -1.57010 | -0.48320 |
| O | 1.95390 | -1.12110 | 0.21560 |
| C | 3.88410 | -0.36500 | -1.06000 |
| C | 2.62080 | -2.57300 | -1.53550 |
| C | 0.86790 | -2.01570 | -0.00580 |
| C | 4.40000 | 0.57930 | 0.03920 |
| Br | 2.70130 | 0.65890 | -2.30130 |
| C | 1.11340 | -2.43240 | -1.45750 |
| C | 0.91930 | -3.15680 | 1.03900 |
| C | 5.26540 | 1.69560 | -0.51270 |
| Cl | 0.25530 | -3.91750 | -1.95450 |
| C | 0.72230 | -2.67210 | 2.48660 |
| C | -0.68600 | -2.16480 | 2.73560 |
| O | 0.97830 | -3.75880 | 3.35300 |
| C | -0.96150 | -0.93330 | 3.10100 |
| C | 5.00190 | 3.00450 | -0.36430 |
| C | 5.85770 | 4.12360 | -0.92740 |
| C | 6.40640 | 5.00890 | 0.19430 |
| O | 5.10650 | 4.96230 | -1.79330 |
| C | -1.24940 | 0.30060 | 3.44220 |
| Br | -1.60810 | 1.71360 | 2.10370 |
| C | 4.71990 | 4.34600 | -3.01470 |
| H | 3.75800 | -2.09870 | 0.22460 |
| H | 4.72660 | -0.72840 | -1.65010 |
| H | 3.00150 | -2.38190 | -2.53910 |
| H | 2.92280 | -3.58230 | -1.25350 |
| H | -0.07860 | -1.48040 | 0.07690 |
| H | 3.55780 | 0.99860 | 0.59200 |
| H | 4.99580 | 0.01830 | 0.75980 |
| H | 0.78650 | -1.62870 | -2.11900 |
| H | 0.15630 | -3.90170 | 0.81140 |
| H | 1.87330 | -3.67870 | 0.96450 |
| H | 6.14580 | 1.39120 | -1.06020 |
| H | 1.45090 | -1.88700 | 2.70350 |
| H | -1.48170 | -2.88210 | 2.59240 |
| H | 1.05630 | -3.42920 | 4.23720 |
| H | 4.12190 | 3.31400 | 0.18140 |
| H | 6.70100 | 3.69930 | -1.47590 |
| H | 7.01220 | 4.43050 | 0.89220 |
| H | 7.03350 | 5.80330 | -0.21080 |
| H | 5.59940 | 5.47800 | 0.75770 |
| H | -1.31960 | 0.66130 | 4.45800 |
| H | 4.04780 | 3.50320 | -2.84940 |
| H | 4.19320 | 5.07000 | -3.63620 |
| H | 5.58840 | 3.99520 | -3.57350 |

| Marilzafurollene C_131 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.84080 | -1.40780 | -0.56250 |
| O | 2.11790 | -1.80720 | 0.60130 |
| C | 3.05720 | 0.11610 | -0.53340 |
| C | 2.01380 | -1.91830 | -1.75250 |
| C | 0.89840 | -2.43900 | 0.23370 |
| C | 3.86410 | 0.63710 | -1.73600 |
| Br | 4.03700 | 0.57840 | 1.14190 |
| C | 1.19240 | -3.03720 | -1.14350 |
| C | 0.42150 | -3.41360 | 1.32890 |
| C | 4.00220 | 2.14700 | -1.72760 |
| Cl | 2.18280 | -4.52330 | -1.04070 |
| C | 0.12260 | -2.71440 | 2.66860 |
| C | -1.01520 | -1.71580 | 2.56420 |
| O | -0.21040 | -3.69240 | 3.63260 |
| C | -0.83750 | -0.41640 | 2.63960 |
| C | 5.17460 | 2.80280 | -1.73670 |
| C | 5.31470 | 4.31330 | -1.71210 |
| C | 6.03100 | 4.81590 | -2.96800 |
| O | 6.07890 | 4.74200 | -0.59440 |
| C | -0.62490 | 0.87760 | 2.65890 |
| Br | -0.23470 | 1.89980 | 1.00850 |
| C | 5.43110 | 4.56540 | 0.65880 |
| H | 3.80310 | -1.92140 | -0.53850 |
| H | 2.09120 | 0.61970 | -0.47910 |
| H | 1.34380 | -1.13660 | -2.11290 |
| H | 2.62880 | -2.24360 | -2.59210 |
| H | 0.15390 | -1.65310 | 0.09670 |
| H | 4.85110 | 0.17280 | -1.75110 |
| H | 3.37300 | 0.35770 | -2.66830 |
| H | 0.29020 | -3.26770 | -1.71130 |
| H | -0.46750 | -3.94200 | 0.98230 |
| H | 1.18600 | -4.17340 | 1.49110 |
| H | 3.07980 | 2.71010 | -1.70960 |
| H | 1.02480 | -2.20000 | 3.00910 |
| H | -2.00260 | -2.12860 | 2.41810 |
| H | 0.58520 | -4.12660 | 3.90760 |
| H | 6.10000 | 2.24520 | -1.75340 |
| H | 4.32490 | 4.77250 | -1.67220 |
| H | 6.11760 | 5.90250 | -2.95570 |
| H | 7.03780 | 4.40380 | -3.04010 |
| H | 5.48710 | 4.53610 | -3.87060 |
| H | -0.63810 | 1.49590 | 3.54450 |
| H | 6.06270 | 4.96180 | 1.45360 |
| H | 4.47970 | 5.09780 | 0.69130 |
| H | 5.24870 | 3.51260 | 0.87700 |

| Marilzafurollene C_132 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.85590 | -0.56330 | -1.49200 |
| O | 2.03780 | -0.47010 | -0.32460 |
| C | 2.43760 | 0.49580 | -2.53260 |
| C | 2.74840 | -2.01630 | -1.97280 |
| C | 1.45110 | -1.73760 | -0.03670 |
| C | 2.67420 | 1.93910 | -2.05650 |
| Br | 0.49420 | 0.29770 | -2.94060 |
| C | 2.38030 | -2.75760 | -0.70390 |
| C | 1.21470 | -1.91120 | 1.47610 |
| C | 4.14520 | 2.27760 | -1.90970 |
| Cl | 3.85480 | -3.06260 | 0.26190 |
| C | 0.18220 | -0.92030 | 2.04160 |
| C | -0.15890 | -1.23390 | 3.48480 |
| O | 0.72460 | 0.37990 | 1.96680 |
| C | -1.36940 | -1.54040 | 3.89210 |
| C | 4.74200 | 2.55940 | -0.73740 |
| C | 6.21020 | 2.91150 | -0.52340 |
| C | 6.99400 | 3.14220 | -1.82310 |
| O | 6.89440 | 1.88300 | 0.17920 |
| C | -2.58140 | -1.85630 | 4.28270 |
| Br | -3.23290 | -3.72540 | 4.31360 |
| C | 6.54280 | 1.75900 | 1.55060 |
| H | 3.88600 | -0.38830 | -1.17760 |
| H | 2.97550 | 0.32830 | -3.46690 |
| H | 1.94460 | -2.12770 | -2.70080 |
| H | 3.66570 | -2.38200 | -2.43500 |
| H | 0.48980 | -1.77160 | -0.55290 |
| H | 2.24460 | 2.63720 | -2.77540 |
| H | 2.15220 | 2.10830 | -1.11350 |
| H | 1.89540 | -3.71590 | -0.89320 |
| H | 0.86180 | -2.92820 | 1.65320 |
| H | 2.15240 | -1.81570 | 2.02500 |
| H | 4.71640 | 2.27850 | -2.82620 |
| H | -0.72360 | -0.95210 | 1.43180 |
| H | 0.66050 | -1.19220 | 4.18750 |
| H | 1.20130 | 0.43300 | 1.14110 |
| H | 4.13830 | 2.54450 | 0.15860 |
| H | 6.24860 | 3.83580 | 0.05580 |
| H | 8.01880 | 3.44190 | -1.60320 |
| H | 7.04360 | 2.23530 | -2.42600 |
| H | 6.54430 | 3.93220 | -2.42500 |
| H | -3.32570 | -1.14880 | 4.61770 |
| H | 5.50430 | 1.45300 | 1.67840 |
| H | 7.16770 | 0.99690 | 2.01610 |
| H | 6.70260 | 2.69450 | 2.08810 |

| Marilzafurollene C_133 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.96050 | -1.83310 | -1.32120 |
| O | 2.36210 | -1.94000 | -0.02990 |
| C | 3.22100 | -0.35730 | -1.67790 |
| C | 2.02920 | -2.57790 | -2.28750 |
| C | 1.12640 | -2.64080 | -0.12710 |
| C | 4.28510 | 0.27750 | -0.76670 |
| Br | 1.52450 | 0.68730 | -1.52150 |
| C | 1.28850 | -3.52620 | -1.36620 |
| C | 0.77210 | -3.35710 | 1.19100 |
| C | 4.65350 | 1.68590 | -1.19250 |
| Cl | 2.30290 | -4.96440 | -1.04420 |
| C | 0.55970 | -2.39210 | 2.37180 |
| C | -0.59960 | -1.44000 | 2.14240 |
| O | 0.30580 | -3.15720 | 3.53210 |
| C | -0.45380 | -0.13790 | 2.04750 |
| C | 4.53640 | 2.77040 | -0.40460 |
| C | 4.88140 | 4.20860 | -0.77600 |
| C | 5.23570 | 4.40550 | -2.25680 |
| O | 5.99410 | 4.68410 | -0.03050 |
| C | -0.28650 | 1.15840 | 1.93500 |
| Br | -0.37370 | 2.37870 | 3.49150 |
| C | 5.72660 | 4.94440 | 1.34060 |
| H | 3.90950 | -2.37030 | -1.28120 |
| H | 3.54630 | -0.29200 | -2.71710 |
| H | 1.31750 | -1.89150 | -2.74690 |
| H | 2.56360 | -3.08640 | -3.09040 |
| H | 0.35420 | -1.90470 | -0.35540 |
| H | 3.93550 | 0.27590 | 0.26680 |
| H | 5.19480 | -0.32340 | -0.78640 |
| H | 0.33640 | -3.86610 | -1.77510 |
| H | -0.12440 | -3.96050 | 1.04470 |
| H | 1.56940 | -4.05410 | 1.45040 |
| H | 5.03320 | 1.78340 | -2.19840 |
| H | 1.48080 | -1.82610 | 2.53160 |
| H | -1.57770 | -1.89010 | 2.05220 |
| H | 0.39100 | -2.59340 | 4.28820 |
| H | 4.15190 | 2.63420 | 0.59540 |
| H | 4.00690 | 4.82520 | -0.56050 |
| H | 5.42250 | 5.45830 | -2.46880 |
| H | 6.13630 | 3.85440 | -2.52860 |
| H | 4.42320 | 4.08000 | -2.90710 |
| H | -0.08980 | 1.67590 | 1.00680 |
| H | 6.61810 | 5.36020 | 1.81010 |
| H | 4.92050 | 5.67000 | 1.45670 |
| H | 5.46270 | 4.03700 | 1.88390 |

| Marilzafurollene C_134 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.24640 | -1.49830 | -0.75010 |
| O | 2.38510 | -1.79800 | 0.34790 |
| C | 3.48820 | 0.02050 | -0.85060 |
| C | 2.60150 | -2.13790 | -1.98820 |
| C | 1.23370 | -2.49320 | -0.11760 |
| C | 4.24530 | 0.55970 | 0.38100 |
| Br | 1.73410 | 0.96720 | -1.01150 |
| C | 1.71310 | -3.20760 | -1.38500 |
| C | 0.62520 | -3.37980 | 0.98660 |
| C | 4.71790 | 2.00580 | 0.30380 |
| Cl | 2.69160 | -4.65910 | -1.01480 |
| C | 0.13640 | -2.58150 | 2.20980 |
| C | -0.97540 | -1.60610 | 1.86970 |
| O | -0.33090 | -3.49100 | 3.18530 |
| C | -0.83610 | -0.30160 | 1.94340 |
| C | 4.61100 | 2.84080 | -0.74600 |
| C | 5.10840 | 4.27400 | -0.75510 |
| C | 3.95630 | 5.24790 | -1.01480 |
| O | 6.06880 | 4.47720 | -1.78140 |
| C | -0.66780 | 0.99840 | 1.99980 |
| Br | -1.05040 | 2.05320 | 3.63100 |
| C | 7.32490 | 3.85950 | -1.53610 |
| H | 4.19400 | -2.00480 | -0.56000 |
| H | 4.06010 | 0.22290 | -1.75690 |
| H | 1.98370 | -1.41610 | -2.52290 |
| H | 3.33200 | -2.53300 | -2.69460 |
| H | 0.50110 | -1.74440 | -0.42260 |
| H | 3.61720 | 0.45000 | 1.26610 |
| H | 5.12950 | -0.05330 | 0.55890 |
| H | 0.89530 | -3.50680 | -2.04150 |
| H | -0.20200 | -3.95610 | 0.57030 |
| H | 1.36840 | -4.10590 | 1.31580 |
| H | 5.18990 | 2.37280 | 1.20420 |
| H | 0.97950 | -2.03260 | 2.63670 |
| H | -1.91260 | -2.04090 | 1.55520 |
| H | 0.41590 | -3.86660 | 3.63010 |
| H | 4.14640 | 2.51520 | -1.66430 |
| H | 5.55190 | 4.51640 | 0.21270 |
| H | 4.31020 | 6.27880 | -1.00650 |
| H | 3.49360 | 5.06310 | -1.98460 |
| H | 3.18340 | 5.15520 | -0.25130 |
| H | -0.31220 | 1.60860 | 1.18210 |
| H | 7.23800 | 2.77410 | -1.47600 |
| H | 8.00970 | 4.09190 | -2.35160 |
| H | 7.77130 | 4.22590 | -0.61090 |

| Marilzafurollene C_135 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.26220 | -1.67930 | -1.85490 |
| O | 3.35290 | -1.37080 | -0.46590 |
| C | 4.51680 | -1.22290 | -2.63000 |
| C | 1.91670 | -1.11480 | -2.32540 |
| C | 2.11810 | -0.82230 | -0.00580 |
| C | 4.79360 | 0.29400 | -2.68880 |
| Br | 4.36740 | -1.89270 | -4.50020 |
| C | 1.07990 | -1.20890 | -1.06720 |
| C | 1.83470 | -1.25150 | 1.44630 |
| C | 5.11600 | 0.91060 | -1.34120 |
| Cl | 0.48190 | -2.88350 | -0.85930 |
| C | 0.50470 | -0.72620 | 2.01990 |
| C | 0.28150 | -1.22870 | 3.43290 |
| O | 0.52240 | 0.68630 | 2.02880 |
| C | -0.75020 | -1.96090 | 3.78700 |
| C | 4.49170 | 1.98170 | -0.82350 |
| C | 4.82580 | 2.60640 | 0.51860 |
| C | 3.61800 | 2.57950 | 1.45800 |
| O | 5.20650 | 3.96670 | 0.36850 |
| C | -1.79320 | -2.67630 | 4.13600 |
| Br | -3.47980 | -1.85390 | 4.76610 |
| C | 6.48080 | 4.15350 | -0.23190 |
| H | 3.20920 | -2.76770 | -1.91360 |
| H | 5.38400 | -1.72480 | -2.19870 |
| H | 2.00560 | -0.06930 | -2.61630 |
| H | 1.49500 | -1.66230 | -3.16880 |
| H | 2.23210 | 0.26180 | -0.03710 |
| H | 5.66010 | 0.46380 | -3.32850 |
| H | 3.96890 | 0.82640 | -3.16120 |
| H | 0.21900 | -0.53960 | -1.07740 |
| H | 1.84940 | -2.34020 | 1.50660 |
| H | 2.65980 | -0.91380 | 2.07420 |
| H | 5.90990 | 0.43850 | -0.78030 |
| H | -0.32270 | -1.05390 | 1.38680 |
| H | 1.03200 | -0.95480 | 4.16070 |
| H | -0.30540 | 0.99760 | 2.36930 |
| H | 3.69540 | 2.45750 | -1.37720 |
| H | 5.63870 | 2.05070 | 0.99050 |
| H | 3.85700 | 3.04990 | 2.41160 |
| H | 2.76730 | 3.11000 | 1.02990 |
| H | 3.30320 | 1.55740 | 1.66760 |
| H | -1.83760 | -3.75550 | 4.11540 |
| H | 6.70820 | 5.21840 | -0.27840 |
| H | 7.26640 | 3.66970 | 0.34990 |
| H | 6.51030 | 3.76400 | -1.25000 |

| Marilzafurollene C_136 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.40460 | -0.91730 | -1.13910 |
| O | 2.70100 | -1.12080 | 0.24220 |
| C | 3.02500 | 0.39860 | -1.64520 |
| C | 0.87930 | -1.00410 | -1.26400 |
| C | 1.50020 | -1.32520 | 0.98120 |
| C | 4.56240 | 0.36510 | -1.60560 |
| Br | 2.37920 | 1.92600 | -0.53080 |
| C | 0.50170 | -1.84630 | -0.06380 |
| C | 1.78480 | -2.20000 | 2.22220 |
| C | 5.18790 | 1.60870 | -2.20740 |
| Cl | 0.75740 | -3.57560 | -0.44700 |
| C | 0.65800 | -2.22790 | 3.27560 |
| C | -0.56060 | -3.00660 | 2.81970 |
| O | 1.15810 | -2.82980 | 4.45180 |
| C | -1.76420 | -2.48700 | 2.73870 |
| C | 6.01120 | 2.43950 | -1.54660 |
| C | 6.62810 | 3.69180 | -2.14070 |
| C | 8.15610 | 3.60200 | -2.13830 |
| O | 6.27520 | 4.84590 | -1.39180 |
| C | -2.95360 | -1.94730 | 2.62030 |
| Br | -3.54540 | -1.06890 | 0.94840 |
| C | 4.90520 | 5.21210 | -1.49250 |
| H | 2.83940 | -1.75560 | -1.68590 |
| H | 2.69050 | 0.58200 | -2.66710 |
| H | 0.42240 | -0.01880 | -1.16960 |
| H | 0.55050 | -1.43150 | -2.21160 |
| H | 1.17040 | -0.33900 | 1.31310 |
| H | 4.90250 | 0.23680 | -0.57690 |
| H | 4.92870 | -0.49760 | -2.16300 |
| H | -0.54010 | -1.71080 | 0.22500 |
| H | 2.06230 | -3.21260 | 1.92920 |
| H | 2.67670 | -1.78680 | 2.69440 |
| H | 4.93670 | 1.81910 | -3.23700 |
| H | 0.36930 | -1.20410 | 3.52500 |
| H | -0.39160 | -4.04070 | 2.55520 |
| H | 1.79150 | -2.24940 | 4.85010 |
| H | 6.26410 | 2.23360 | -0.51630 |
| H | 6.29120 | 3.81220 | -3.17220 |
| H | 8.59740 | 4.49590 | -2.57940 |
| H | 8.54450 | 3.50620 | -1.12410 |
| H | 8.50120 | 2.74250 | -2.71350 |
| H | -3.70530 | -1.92620 | 3.39600 |
| H | 4.73190 | 6.12910 | -0.92960 |
| H | 4.62000 | 5.39730 | -2.52870 |
| H | 4.24860 | 4.44440 | -1.08180 |

| Marilzafurollene C_137 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.18390 | -1.23410 | -0.82240 |
| O | 2.23130 | -1.27530 | 0.24080 |
| C | 3.47460 | 0.22110 | -1.23380 |
| C | 2.61750 | -2.12120 | -1.93890 |
| C | 1.13620 | -2.11570 | -0.11850 |
| C | 4.16500 | 1.01430 | -0.11140 |
| Br | 1.76710 | 1.13490 | -1.72490 |
| C | 1.70640 | -3.06360 | -1.17950 |
| C | 0.50670 | -2.77640 | 1.12350 |
| C | 4.59660 | 2.39720 | -0.56010 |
| Cl | 2.67680 | -4.38130 | -0.45660 |
| C | -0.14550 | -1.76300 | 2.08060 |
| C | -0.91020 | -2.45750 | 3.19050 |
| O | 0.87330 | -0.96860 | 2.64740 |
| C | -2.20870 | -2.34690 | 3.35720 |
| C | 5.87160 | 2.82760 | -0.57420 |
| C | 6.36360 | 4.20320 | -1.01240 |
| C | 5.23970 | 5.19650 | -1.34000 |
| O | 7.17270 | 4.11510 | -2.17760 |
| C | -3.50750 | -2.25210 | 3.51850 |
| Br | -4.34400 | -0.85030 | 4.63870 |
| C | 8.46900 | 3.57300 | -1.96500 |
| H | 4.09990 | -1.69690 | -0.45160 |
| H | 4.11090 | 0.22510 | -2.12050 |
| H | 2.02450 | -1.53440 | -2.64060 |
| H | 3.39080 | -2.63570 | -2.51000 |
| H | 0.38930 | -1.48220 | -0.60100 |
| H | 3.49360 | 1.11400 | 0.74240 |
| H | 5.03790 | 0.46520 | 0.24390 |
| H | 0.93690 | -3.51410 | -1.80740 |
| H | -0.25270 | -3.48340 | 0.78660 |
| H | 1.24950 | -3.36430 | 1.66400 |
| H | 3.79760 | 3.04870 | -0.88260 |
| H | -0.81920 | -1.11220 | 1.51850 |
| H | -0.32280 | -3.06460 | 3.86380 |
| H | 1.50680 | -0.79330 | 1.95520 |
| H | 6.64380 | 2.15010 | -0.24110 |
| H | 6.94870 | 4.62390 | -0.19250 |
| H | 5.65360 | 6.16900 | -1.60680 |
| H | 4.63960 | 4.85550 | -2.18410 |
| H | 4.57810 | 5.34590 | -0.48640 |
| H | -4.23460 | -2.91180 | 3.06810 |
| H | 8.42840 | 2.53390 | -1.63850 |
| H | 9.03010 | 3.60150 | -2.89900 |
| H | 9.02460 | 4.15170 | -1.22600 |

| Marilzafurollene C_138 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.85100 | -1.42490 | -0.60190 |
| O | 2.11950 | -1.82720 | 0.55540 |
| C | 3.07150 | 0.09820 | -0.56590 |
| C | 2.03080 | -1.92890 | -1.79910 |
| C | 0.91150 | -2.47610 | 0.17800 |
| C | 3.88980 | 0.62090 | -1.76000 |
| Br | 4.03810 | 0.55290 | 1.11930 |
| C | 1.21760 | -3.06030 | -1.20280 |
| C | 0.43730 | -3.46370 | 1.26320 |
| C | 4.03260 | 2.13030 | -1.74500 |
| Cl | 2.22230 | -4.53750 | -1.11020 |
| C | 0.14640 | -2.78420 | 2.61430 |
| C | -0.97260 | -1.76340 | 2.52140 |
| O | -0.21260 | -3.78030 | 3.55010 |
| C | -0.77590 | -0.47010 | 2.64140 |
| C | 5.20700 | 2.78250 | -1.74270 |
| C | 5.35140 | 4.29240 | -1.71120 |
| C | 6.07810 | 4.79780 | -2.96000 |
| O | 6.10890 | 4.71450 | -0.58640 |
| C | -0.54930 | 0.82040 | 2.70350 |
| Br | -0.12080 | 1.88790 | 1.09190 |
| C | 5.45200 | 4.53440 | 0.66160 |
| H | 3.81170 | -1.94150 | -0.57350 |
| H | 2.10640 | 0.60390 | -0.51820 |
| H | 1.35560 | -1.14850 | -2.15260 |
| H | 2.65020 | -2.24070 | -2.64060 |
| H | 0.15760 | -1.69890 | 0.04260 |
| H | 4.87550 | 0.15340 | -1.76860 |
| H | 3.40540 | 0.34610 | -2.69710 |
| H | 0.32010 | -3.29490 | -1.77610 |
| H | -0.45260 | -3.98800 | 0.91350 |
| H | 1.20030 | -4.22690 | 1.41790 |
| H | 3.11190 | 2.69610 | -1.73200 |
| H | 1.06250 | -2.30180 | 2.96460 |
| H | -1.96370 | -2.15390 | 2.34020 |
| H | -0.09140 | -3.43210 | 4.42230 |
| H | 6.13090 | 2.22220 | -1.75440 |
| H | 4.36270 | 4.75450 | -1.67650 |
| H | 6.16770 | 5.88410 | -2.94290 |
| H | 7.08410 | 4.38310 | -3.02660 |
| H | 5.53980 | 4.52310 | -3.86740 |
| H | -0.57080 | 1.41250 | 3.60670 |
| H | 5.26540 | 3.48110 | 0.87410 |
| H | 6.07900 | 4.92590 | 1.46240 |
| H | 4.50170 | 5.06900 | 0.68970 |

| Marilzafurollene C_139 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.09650 | -1.26230 | -0.18370 |
| O | 2.12470 | -1.63300 | 0.79270 |
| C | 3.58340 | 0.17580 | 0.07060 |
| C | 2.40190 | -1.48110 | -1.53200 |
| C | 1.01350 | -2.28520 | 0.18060 |
| C | 4.66710 | 0.62990 | -0.92460 |
| Br | 4.33650 | 0.26460 | 1.91640 |
| C | 1.48250 | -2.64690 | -1.23440 |
| C | 0.49820 | -3.45030 | 1.05030 |
| C | 5.06230 | 2.08170 | -0.73280 |
| Cl | 2.41620 | -4.17310 | -1.28170 |
| C | -0.09910 | -2.99610 | 2.39460 |
| C | -1.37860 | -2.19850 | 2.21660 |
| O | -0.38250 | -4.14700 | 3.16520 |
| C | -1.50080 | -0.93630 | 2.56160 |
| C | 4.94680 | 3.03400 | -1.67380 |
| C | 5.34390 | 4.48570 | -1.48080 |
| C | 4.14130 | 5.41190 | -1.68460 |
| O | 6.33560 | 4.87600 | -2.42020 |
| C | -1.61070 | 0.33490 | 2.86970 |
| Br | -1.19580 | 1.77350 | 1.57400 |
| C | 7.62010 | 4.31570 | -2.17970 |
| H | 3.93300 | -1.95720 | -0.09090 |
| H | 2.73340 | 0.85950 | 0.04240 |
| H | 1.80830 | -0.60580 | -1.79980 |
| H | 3.09790 | -1.68070 | -2.34740 |
| H | 0.22930 | -1.53340 | 0.07720 |
| H | 5.55640 | 0.00780 | -0.81670 |
| H | 4.31670 | 0.49560 | -1.94840 |
| H | 0.65860 | -2.73560 | -1.94350 |
| H | -0.24600 | -4.02180 | 0.49400 |
| H | 1.32290 | -4.13620 | 1.24880 |
| H | 5.46450 | 2.34080 | 0.23690 |
| H | 0.64720 | -2.40170 | 2.92860 |
| H | -2.21250 | -2.72790 | 1.77760 |
| H | -0.45980 | -3.89040 | 4.07330 |
| H | 4.54950 | 2.78300 | -2.64690 |
| H | 5.72290 | 4.63150 | -0.46680 |
| H | 4.42390 | 6.45340 | -1.53000 |
| H | 3.74060 | 5.32370 | -2.69530 |
| H | 3.34000 | 5.17780 | -0.98240 |
| H | -1.92880 | 0.71520 | 3.82950 |
| H | 7.60850 | 3.22770 | -2.25450 |
| H | 8.32530 | 4.69080 | -2.92180 |
| H | 7.99430 | 4.59380 | -1.19320 |

| Marilzafurollene C_140 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.94140 | -1.78220 | -1.37800 |
| O | 2.34790 | -1.92830 | -0.08860 |
| C | 3.39160 | -0.32640 | -1.60530 |
| C | 1.90990 | -2.30660 | -2.38670 |
| C | 1.02440 | -2.43470 | -0.21890 |
| C | 4.51400 | 0.08860 | -0.63910 |
| Br | 1.84110 | 0.91120 | -1.36410 |
| C | 1.04690 | -3.21680 | -1.53620 |
| C | 0.58700 | -3.21370 | 1.03850 |
| C | 5.06560 | 1.46730 | -0.94640 |
| Cl | 1.84320 | -4.80970 | -1.36530 |
| C | 0.55270 | -2.34950 | 2.31360 |
| C | -0.42100 | -1.18790 | 2.21500 |
| O | 0.20730 | -3.16460 | 3.41700 |
| C | -0.04150 | 0.06950 | 2.24870 |
| C | 5.02650 | 2.50780 | -0.09770 |
| C | 5.57040 | 3.89020 | -0.40620 |
| C | 6.65520 | 4.28690 | 0.59810 |
| O | 4.54940 | 4.87450 | -0.33140 |
| C | 0.36000 | 1.31840 | 2.26310 |
| Br | 0.50550 | 2.37040 | 3.93410 |
| C | 3.59020 | 4.80150 | -1.37790 |
| H | 3.81170 | -2.43980 | -1.40580 |
| H | 3.73640 | -0.21540 | -2.63430 |
| H | 1.29880 | -1.49270 | -2.77730 |
| H | 2.36420 | -2.81520 | -3.23750 |
| H | 0.36290 | -1.57880 | -0.36080 |
| H | 4.14890 | 0.05160 | 0.38850 |
| H | 5.33880 | -0.62210 | -0.70020 |
| H | 0.05260 | -3.37740 | -1.95420 |
| H | -0.39390 | -3.65520 | 0.86010 |
| H | 1.27280 | -4.04500 | 1.20420 |
| H | 5.51290 | 1.59550 | -1.92150 |
| H | 1.55780 | -1.96220 | 2.49760 |
| H | -1.46620 | -1.43630 | 2.10610 |
| H | -0.62450 | -3.58230 | 3.25080 |
| H | 4.57670 | 2.38570 | 0.87740 |
| H | 6.00810 | 3.89700 | -1.40640 |
| H | 7.05590 | 5.27370 | 0.36590 |
| H | 6.26010 | 4.32000 | 1.61380 |
| H | 7.48450 | 3.57930 | 0.58250 |
| H | 0.64350 | 1.88390 | 1.38690 |
| H | 3.03460 | 3.86340 | -1.35410 |
| H | 2.87110 | 5.61320 | -1.26900 |
| H | 4.06260 | 4.90270 | -2.35570 |

| Marilzafurollene C_141 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.90270 | -1.01180 | -1.01710 |
| O | 2.49400 | -0.64660 | 0.30090 |
| C | 3.80930 | 0.07030 | -1.63300 |
| C | 1.61500 | -1.30120 | -1.79800 |
| C | 1.07540 | -0.73190 | 0.41590 |
| C | 5.13290 | 0.22110 | -0.86390 |
| Br | 2.85960 | 1.82780 | -1.64310 |
| C | 0.65260 | -1.69730 | -0.69810 |
| C | 0.66410 | -1.09630 | 1.85560 |
| C | 6.08360 | 1.19920 | -1.52680 |
| Cl | 0.92500 | -3.40930 | -0.25270 |
| C | -0.85050 | -1.29370 | 2.06390 |
| C | -1.16140 | -1.65360 | 3.50390 |
| O | -1.53290 | -0.10280 | 1.72890 |
| C | -1.76690 | -2.76300 | 3.86250 |
| C | 6.57000 | 2.30320 | -0.93590 |
| C | 7.51000 | 3.29140 | -1.60040 |
| C | 8.83940 | 3.37290 | -0.84580 |
| O | 6.95680 | 4.59950 | -1.61650 |
| C | -2.35820 | -3.87410 | 4.23340 |
| Br | -1.35000 | -5.52520 | 4.65200 |
| C | 5.83640 | 4.75020 | -2.47840 |
| H | 3.46310 | -1.94400 | -0.92950 |
| H | 4.01830 | -0.18770 | -2.67200 |
| H | 1.24650 | -0.40140 | -2.29080 |
| H | 1.73970 | -2.07010 | -2.56090 |
| H | 0.68200 | 0.25770 | 0.17580 |
| H | 4.93000 | 0.53430 | 0.16140 |
| H | 5.63610 | -0.74420 | -0.79950 |
| H | -0.39340 | -1.58000 | -0.98340 |
| H | 1.18840 | -2.00340 | 2.15810 |
| H | 1.02460 | -0.31350 | 2.52380 |
| H | 6.37140 | 0.97100 | -2.54290 |
| H | -1.20870 | -2.09000 | 1.40790 |
| H | -0.84950 | -0.93730 | 4.25070 |
| H | -2.46370 | -0.24510 | 1.83020 |
| H | 6.28360 | 2.53590 | 0.07990 |
| H | 7.71350 | 2.97160 | -2.62430 |
| H | 9.51930 | 4.07180 | -1.33330 |
| H | 8.69140 | 3.71420 | 0.17900 |
| H | 9.33180 | 2.40090 | -0.80920 |
| H | -3.42540 | -3.99900 | 4.34490 |
| H | 5.50650 | 5.78890 | -2.46750 |
| H | 6.09040 | 4.49120 | -3.50700 |
| H | 4.99440 | 4.13380 | -2.16140 |

| Marilzafurollene C_142 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.10960 | -0.47980 | -1.39920 |
| O | 2.03980 | 0.11130 | -0.66150 |
| C | 3.31240 | 0.23890 | -2.74920 |
| C | 2.77800 | -1.97300 | -1.50610 |
| C | 1.11130 | -0.89030 | -0.25280 |
| C | 3.74660 | 1.70650 | -2.59580 |
| Br | 1.60840 | 0.21210 | -3.78730 |
| C | 1.90920 | -2.19980 | -0.28680 |
| C | 0.44920 | -0.50620 | 1.08440 |
| C | 5.12930 | 1.85540 | -1.98990 |
| Cl | 2.94540 | -2.40300 | 1.15890 |
| C | -0.51500 | -1.56550 | 1.65310 |
| C | -1.09060 | -1.12250 | 2.98410 |
| O | -1.57230 | -1.78080 | 0.74150 |
| C | -0.92850 | -1.79200 | 4.10270 |
| C | 5.38050 | 2.46030 | -0.81710 |
| C | 6.75950 | 2.61210 | -0.20310 |
| C | 6.82830 | 1.91620 | 1.15850 |
| O | 7.08230 | 3.97890 | 0.00820 |
| C | -0.77740 | -2.47640 | 5.21190 |
| Br | -2.05160 | -3.88420 | 5.77090 |
| C | 7.33630 | 4.71060 | -1.18330 |
| H | 4.00930 | -0.37970 | -0.79030 |
| H | 4.05130 | -0.29880 | -3.34460 |
| H | 2.19660 | -2.18060 | -2.40450 |
| H | 3.66380 | -2.60810 | -1.52980 |
| H | 0.34310 | -0.93970 | -1.02680 |
| H | 3.75980 | 2.18800 | -3.57390 |
| H | 3.01340 | 2.24720 | -1.99540 |
| H | 1.27110 | -3.07960 | -0.37610 |
| H | 1.22710 | -0.29700 | 1.81940 |
| H | -0.08370 | 0.43530 | 0.94700 |
| H | 5.94770 | 1.43820 | -2.55910 |
| H | 0.01660 | -2.50980 | 1.78840 |
| H | -1.65520 | -0.20100 | 2.97620 |
| H | -2.14760 | -2.44530 | 1.09520 |
| H | 4.56280 | 2.87740 | -0.24630 |
| H | 7.50530 | 2.15880 | -0.85920 |
| H | 7.82390 | 2.00980 | 1.59230 |
| H | 6.11760 | 2.35200 | 1.86110 |
| H | 6.60270 | 0.85320 | 1.06920 |
| H | 0.03420 | -2.34610 | 5.91300 |
| H | 7.60840 | 5.73510 | -0.92970 |
| H | 8.16310 | 4.27520 | -1.74580 |
| H | 6.45820 | 4.75160 | -1.82860 |

| Marilzafurollene C_143 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.24300 | -1.63900 | -0.96370 |
| O | 2.44510 | -1.43800 | 0.20280 |
| C | 4.17690 | -0.43590 | -1.19470 |
| C | 2.25930 | -1.96740 | -2.09380 |
| C | 1.08210 | -1.76590 | -0.07270 |
| C | 3.45950 | 0.91800 | -1.35360 |
| Br | 5.30140 | -0.79180 | -2.80250 |
| C | 1.11950 | -2.62460 | -1.34360 |
| C | 0.39680 | -2.39350 | 1.15720 |
| C | 4.43040 | 2.08190 | -1.37180 |
| Cl | 1.52940 | -4.33180 | -0.99810 |
| C | 0.27020 | -1.42130 | 2.34310 |
| C | -0.56620 | -2.01280 | 3.46050 |
| O | 1.56360 | -1.14140 | 2.83260 |
| C | -1.68320 | -1.47290 | 3.89200 |
| C | 4.46590 | 3.06200 | -0.45200 |
| C | 5.43360 | 4.23470 | -0.45040 |
| C | 4.70540 | 5.53890 | -0.78490 |
| O | 6.48000 | 4.07880 | -1.40130 |
| C | -2.80370 | -0.92950 | 4.30470 |
| Br | -4.55900 | -1.38400 | 3.51000 |
| C | 7.54270 | 3.24180 | -0.96310 |
| H | 3.85480 | -2.52290 | -0.77550 |
| H | 4.86000 | -0.37390 | -0.34590 |
| H | 1.89700 | -1.06250 | -2.57960 |
| H | 2.69440 | -2.60520 | -2.86400 |
| H | 0.57720 | -0.83040 | -0.32050 |
| H | 2.87920 | 0.94530 | -2.27510 |
| H | 2.75390 | 1.05850 | -0.53380 |
| H | 0.17900 | -2.60970 | -1.89580 |
| H | -0.60160 | -2.72030 | 0.86250 |
| H | 0.92710 | -3.29210 | 1.47530 |
| H | 5.13090 | 2.10150 | -2.19520 |
| H | -0.17930 | -0.48660 | 2.00020 |
| H | -0.19350 | -2.92530 | 3.90260 |
| H | 2.15030 | -1.12310 | 2.08070 |
| H | 3.76010 | 3.04430 | 0.36630 |
| H | 5.85740 | 4.32740 | 0.55140 |
| H | 5.39280 | 6.38450 | -0.75800 |
| H | 4.26730 | 5.49890 | -1.78260 |
| H | 3.90410 | 5.73940 | -0.07340 |
| H | -2.88040 | -0.19960 | 5.09740 |
| H | 8.28540 | 3.15110 | -1.75570 |
| H | 8.03880 | 3.66370 | -0.08820 |
| H | 7.19620 | 2.23820 | -0.71460 |

| Marilzafurollene C_144 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.64840 | -1.25090 | -1.95770 |
| O | 2.53820 | -1.03500 | -0.55060 |
| C | 1.82800 | -0.20670 | -2.74530 |
| C | 2.21620 | -2.70570 | -2.18840 |
| C | 2.01270 | -2.19240 | 0.08540 |
| C | 2.44930 | 1.20440 | -2.77420 |
| Br | -0.02730 | -0.09570 | -2.01430 |
| C | 2.43680 | -3.34270 | -0.83030 |
| C | 2.46500 | -2.26710 | 1.55620 |
| C | 2.71520 | 1.78700 | -1.39870 |
| Cl | 4.16490 | -3.76040 | -0.63300 |
| C | 1.92290 | -1.10390 | 2.40780 |
| C | 0.41050 | -1.12380 | 2.54270 |
| O | 2.51570 | -1.15040 | 3.69090 |
| C | -0.36270 | -0.17790 | 2.05910 |
| C | 3.89940 | 2.28080 | -1.00070 |
| C | 4.18070 | 2.84180 | 0.37980 |
| C | 4.50580 | 4.33550 | 0.30410 |
| O | 5.30330 | 2.20110 | 0.96780 |
| C | -1.11590 | 0.76760 | 1.54910 |
| Br | -1.63520 | 2.38240 | 2.56950 |
| C | 5.04330 | 0.88050 | 1.42420 |
| H | 3.70350 | -1.15980 | -2.22100 |
| H | 1.73120 | -0.54520 | -3.77790 |
| H | 1.15630 | -2.75430 | -2.44120 |
| H | 2.77100 | -3.19520 | -2.98920 |
| H | 0.92460 | -2.12500 | 0.04400 |
| H | 3.38490 | 1.17710 | -3.33420 |
| H | 1.78740 | 1.88250 | -3.31330 |
| H | 1.84800 | -4.24820 | -0.68040 |
| H | 2.15580 | -3.22140 | 1.98320 |
| H | 3.55480 | -2.25010 | 1.59430 |
| H | 1.88050 | 1.78560 | -0.71190 |
| H | 2.22440 | -0.16250 | 1.94370 |
| H | -0.02210 | -1.96730 | 3.05990 |
| H | 2.32790 | -1.98500 | 4.09390 |
| H | 4.73500 | 2.28570 | -1.68520 |
| H | 3.30380 | 2.71040 | 1.01730 |
| H | 4.69830 | 4.74020 | 1.29780 |
| H | 5.39110 | 4.51700 | -0.30570 |
| H | 3.67740 | 4.89690 | -0.12860 |
| H | -1.51840 | 0.76040 | 0.54640 |
| H | 4.69030 | 0.23020 | 0.62280 |
| H | 5.95860 | 0.44580 | 1.82510 |
| H | 4.30270 | 0.88530 | 2.22410 |

| Marilzafurollene C_145 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.94400 | -1.77660 | -1.36700 |
| O | 2.34310 | -1.92460 | -0.08120 |
| C | 3.39480 | -0.32050 | -1.59150 |
| C | 1.91890 | -2.30080 | -2.38240 |
| C | 1.02200 | -2.43510 | -0.21960 |
| C | 4.51170 | 0.09620 | -0.61970 |
| Br | 1.84280 | 0.91690 | -1.35920 |
| C | 1.05330 | -3.21450 | -1.53840 |
| C | 0.57950 | -3.21830 | 1.03340 |
| C | 5.07280 | 1.46940 | -0.93450 |
| Cl | 1.85220 | -4.80600 | -1.36670 |
| C | 0.53780 | -2.35860 | 2.31120 |
| C | -0.43370 | -1.19540 | 2.21050 |
| O | 0.18440 | -3.17720 | 3.40950 |
| C | -0.05240 | 0.06120 | 2.25210 |
| C | 5.03180 | 2.51840 | -0.09640 |
| C | 5.58710 | 3.89420 | -0.41370 |
| C | 6.66380 | 4.29510 | 0.59770 |
| O | 4.57180 | 4.88580 | -0.36020 |
| C | 0.35260 | 1.30880 | 2.27650 |
| Br | 0.49000 | 2.34950 | 3.95510 |
| C | 3.62280 | 4.80730 | -1.41560 |
| H | 3.81480 | -2.43370 | -1.39050 |
| H | 3.74500 | -0.20990 | -2.61870 |
| H | 1.30800 | -1.48720 | -2.77420 |
| H | 2.37860 | -2.80650 | -3.23190 |
| H | 0.35880 | -1.58070 | -0.36320 |
| H | 4.13890 | 0.06860 | 0.40540 |
| H | 5.33360 | -0.61870 | -0.66960 |
| H | 0.06160 | -3.37640 | -1.96210 |
| H | -0.39990 | -3.66050 | 0.84870 |
| H | 1.26540 | -4.04940 | 1.20010 |
| H | 5.52980 | 1.58610 | -1.90660 |
| H | 1.54220 | -1.97320 | 2.50300 |
| H | -1.47850 | -1.44180 | 2.09340 |
| H | -0.64780 | -3.59180 | 3.23730 |
| H | 4.57240 | 2.40850 | 0.87570 |
| H | 6.03530 | 3.88780 | -1.40930 |
| H | 7.07240 | 5.27730 | 0.35980 |
| H | 6.25840 | 4.34060 | 1.60880 |
| H | 7.48920 | 3.58280 | 0.59770 |
| H | 0.64350 | 1.87870 | 1.40560 |
| H | 3.06090 | 3.87310 | -1.38700 |
| H | 2.90800 | 5.62490 | -1.32320 |
| H | 4.10580 | 4.89440 | -2.38960 |

| Marilzafurollene C_146 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.11440 | -1.37840 | -1.21590 |
| O | 2.43450 | -1.53140 | 0.03000 |
| C | 3.30040 | 0.11370 | -1.55030 |
| C | 2.30480 | -2.17680 | -2.24740 |
| C | 1.25290 | -2.30290 | -0.15630 |
| C | 4.23630 | 0.81700 | -0.55300 |
| Br | 1.52670 | 1.03480 | -1.54240 |
| C | 1.55670 | -3.17100 | -1.38220 |
| C | 0.84630 | -3.04670 | 1.13120 |
| C | 4.53330 | 2.25100 | -0.94700 |
| Cl | 2.63050 | -4.54830 | -0.99320 |
| C | 0.56560 | -2.12530 | 2.33430 |
| C | -0.54200 | -1.10950 | 2.06630 |
| O | 0.26960 | -2.95050 | 3.45000 |
| C | -1.70820 | -1.06680 | 2.67310 |
| C | 5.75720 | 2.72570 | -1.23240 |
| C | 6.05140 | 4.16160 | -1.62510 |
| C | 6.67540 | 4.22770 | -3.02140 |
| O | 6.97230 | 4.76200 | -0.72610 |
| C | -2.86190 | -1.03380 | 3.29660 |
| Br | -3.13640 | -0.00380 | 4.96480 |
| C | 6.43450 | 5.04160 | 0.55940 |
| H | 4.09180 | -1.85160 | -1.10860 |
| H | 3.71050 | 0.20860 | -2.55700 |
| H | 1.58840 | -1.53530 | -2.76110 |
| H | 2.92790 | -2.64970 | -3.00680 |
| H | 0.45620 | -1.61470 | -0.44120 |
| H | 3.79170 | 0.81020 | 0.44300 |
| H | 5.17450 | 0.26590 | -0.47670 |
| H | 0.65850 | -3.56460 | -1.85910 |
| H | -0.03400 | -3.65740 | 0.92780 |
| H | 1.63770 | -3.74120 | 1.41330 |
| H | 3.68240 | 2.91640 | -0.99200 |
| H | 1.47320 | -1.56520 | 2.56700 |
| H | -0.31180 | -0.36740 | 1.31450 |
| H | 0.22900 | -2.40670 | 4.22410 |
| H | 6.61290 | 2.06740 | -1.18650 |
| H | 5.12360 | 4.73710 | -1.63570 |
| H | 6.87320 | 5.26060 | -3.30850 |
| H | 7.62110 | 3.68650 | -3.05820 |
| H | 6.01090 | 3.79640 | -3.77050 |
| H | -3.75370 | -1.55010 | 2.97280 |
| H | 7.19280 | 5.52840 | 1.17280 |
| H | 5.57810 | 5.71370 | 0.49180 |
| H | 6.12480 | 4.13240 | 1.07580 |

| Marilzafurollene C_147 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.35880 | -1.72500 | -0.66140 |
| O | 2.38960 | -1.85490 | 0.37690 |
| C | 4.16250 | -0.42220 | -0.49230 |
| C | 2.58610 | -1.88930 | -1.97540 |
| C | 1.14270 | -2.28940 | -0.16470 |
| C | 3.31410 | 0.86360 | -0.47990 |
| Br | 5.52370 | -0.30950 | -1.94530 |
| C | 1.46800 | -2.82510 | -1.56640 |
| C | 0.42020 | -3.26620 | 0.78500 |
| C | 4.13610 | 2.09070 | -0.13680 |
| Cl | 2.07450 | -4.50880 | -1.53420 |
| C | -0.00240 | -2.63740 | 2.12520 |
| C | -1.03800 | -1.54160 | 1.95400 |
| O | -0.54800 | -3.65850 | 2.93460 |
| C | -0.85660 | -0.30450 | 2.35690 |
| C | 4.26310 | 3.16690 | -0.93080 |
| C | 5.09810 | 4.38850 | -0.59590 |
| C | 4.22580 | 5.64450 | -0.52740 |
| O | 6.09010 | 4.62070 | -1.58540 |
| C | -0.68170 | 0.92430 | 2.78200 |
| Br | -1.19810 | 1.49950 | 4.60420 |
| C | 7.13140 | 3.65290 | -1.60790 |
| H | 4.04230 | -2.56970 | -0.55970 |
| H | 4.71510 | -0.49340 | 0.44570 |
| H | 2.16150 | -0.94340 | -2.30810 |
| H | 3.20260 | -2.28030 | -2.78550 |
| H | 0.53210 | -1.39510 | -0.29690 |
| H | 2.82590 | 1.01320 | -1.44240 |
| H | 2.52180 | 0.77500 | 0.26410 |
| H | 0.61290 | -2.79050 | -2.24220 |
| H | -0.45660 | -3.67720 | 0.28310 |
| H | 1.07530 | -4.11310 | 0.99180 |
| H | 4.64680 | 2.07100 | 0.81530 |
| H | 0.88450 | -2.24270 | 2.62690 |
| H | -1.96090 | -1.82950 | 1.47130 |
| H | -0.61700 | -3.33560 | 3.82230 |
| H | 3.75590 | 3.19220 | -1.88460 |
| H | 5.57910 | 4.24920 | 0.37430 |
| H | 4.82510 | 6.51860 | -0.27240 |
| H | 3.74170 | 5.84210 | -1.48410 |
| H | 3.44760 | 5.54310 | 0.22940 |
| H | -0.25040 | 1.72490 | 2.19900 |
| H | 6.75800 | 2.66020 | -1.86190 |
| H | 7.86890 | 3.93010 | -2.36100 |
| H | 7.64150 | 3.59780 | -0.64550 |

| Marilzafurollene C_148 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.35790 | -1.72030 | -0.66110 |
| O | 2.38990 | -1.84890 | 0.37840 |
| C | 4.16290 | -0.41790 | -0.49380 |
| C | 2.58330 | -1.88500 | -1.97380 |
| C | 1.14340 | -2.28830 | -0.16070 |
| C | 3.31550 | 0.86860 | -0.48280 |
| Br | 5.52340 | -0.30810 | -1.94760 |
| C | 1.46770 | -2.82290 | -1.56310 |
| C | 0.42680 | -3.26790 | 0.79060 |
| C | 4.13840 | 2.09540 | -0.14100 |
| Cl | 2.07710 | -4.50550 | -1.53260 |
| C | 0.00140 | -2.63990 | 2.13030 |
| C | -1.04240 | -1.55200 | 1.95850 |
| O | -0.53610 | -3.66370 | 2.94190 |
| C | -0.86990 | -0.31280 | 2.35910 |
| C | 4.26740 | 3.16990 | -0.93700 |
| C | 5.10270 | 4.39160 | -0.60330 |
| C | 4.23160 | 5.64870 | -0.54080 |
| O | 6.09770 | 4.62010 | -1.59080 |
| C | -0.70440 | 0.91820 | 2.78180 |
| Br | -1.22370 | 1.49270 | 4.60330 |
| C | 7.13830 | 3.65150 | -1.60730 |
| H | 4.04110 | -2.56530 | -0.55970 |
| H | 4.71580 | -0.48840 | 0.44400 |
| H | 2.15650 | -0.93960 | -2.30520 |
| H | 3.19890 | -2.27460 | -2.78520 |
| H | 0.52920 | -1.39630 | -0.29160 |
| H | 2.82740 | 1.01750 | -1.44540 |
| H | 2.52310 | 0.78130 | 0.26140 |
| H | 0.61130 | -2.78970 | -2.23750 |
| H | -0.44800 | -3.68420 | 0.28970 |
| H | 1.08670 | -4.11090 | 0.99790 |
| H | 4.64780 | 2.07720 | 0.81190 |
| H | 0.88600 | -2.23790 | 2.63030 |
| H | -1.96360 | -1.84750 | 1.47710 |
| H | -0.60590 | -3.34010 | 3.82920 |
| H | 3.76160 | 3.19370 | -1.89160 |
| H | 5.58100 | 4.25470 | 0.36860 |
| H | 4.83100 | 6.52300 | -0.28670 |
| H | 3.75030 | 5.84410 | -1.49940 |
| H | 3.45110 | 5.55030 | 0.21410 |
| H | -0.27990 | 1.72110 | 2.19690 |
| H | 6.76490 | 2.65830 | -1.85940 |
| H | 7.87820 | 3.92580 | -2.35910 |
| H | 7.64550 | 3.59900 | -0.64320 |

| Marilzafurollene C_149 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.35780 | -1.71920 | -0.66060 |
| O | 2.38960 | -1.84750 | 0.37880 |
| C | 4.16300 | -0.41700 | -0.49360 |
| C | 2.58310 | -1.88400 | -1.97330 |
| C | 1.14350 | -2.28800 | -0.16010 |
| C | 3.31590 | 0.86970 | -0.48300 |
| Br | 5.52380 | -0.30790 | -1.94710 |
| C | 1.46790 | -2.82240 | -1.56260 |
| C | 0.42770 | -3.26810 | 0.79120 |
| C | 4.13900 | 2.09650 | -0.14170 |
| Cl | 2.07790 | -4.50470 | -1.53230 |
| C | 0.00170 | -2.64040 | 2.13080 |
| C | -1.04340 | -1.55370 | 1.95890 |
| O | -0.53460 | -3.66470 | 2.94260 |
| C | -0.87230 | -0.31440 | 2.35970 |
| C | 4.26850 | 3.17060 | -0.93810 |
| C | 5.10410 | 4.39220 | -0.60490 |
| C | 4.23320 | 5.64960 | -0.54310 |
| O | 6.09920 | 4.61990 | -1.59230 |
| C | -0.70840 | 0.91680 | 2.78250 |
| Br | -1.22880 | 1.49040 | 4.60400 |
| C | 7.13960 | 3.65110 | -1.60830 |
| H | 4.04080 | -2.56430 | -0.55900 |
| H | 4.71570 | -0.48740 | 0.44430 |
| H | 2.15600 | -0.93870 | -2.30450 |
| H | 3.19880 | -2.27330 | -2.78480 |
| H | 0.52850 | -1.39640 | -0.29090 |
| H | 2.82780 | 1.01840 | -1.44570 |
| H | 2.52350 | 0.78290 | 0.26120 |
| H | 0.61150 | -2.78940 | -2.23700 |
| H | -0.44670 | -3.68540 | 0.29030 |
| H | 1.08840 | -4.11050 | 0.99860 |
| H | 4.64830 | 2.07860 | 0.81130 |
| H | 0.88580 | -2.23740 | 2.63080 |
| H | -1.96410 | -1.85030 | 1.47740 |
| H | -0.60490 | -3.34110 | 3.82990 |
| H | 3.76280 | 3.19400 | -1.89280 |
| H | 5.58220 | 4.25560 | 0.36710 |
| H | 4.83290 | 6.52380 | -0.28930 |
| H | 3.75220 | 5.84460 | -1.50190 |
| H | 3.45270 | 5.55170 | 0.21170 |
| H | -0.28480 | 1.72020 | 2.19770 |
| H | 6.76590 | 2.65790 | -1.85990 |
| H | 7.87960 | 3.92480 | -2.36010 |
| H | 7.64670 | 3.59890 | -0.64410 |

| Marilzafurollene C_150 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.90620 | -2.04680 | -1.37760 |
| O | 2.27310 | -2.08540 | -0.10030 |
| C | 3.25450 | -0.59050 | -1.75000 |
| C | 1.95890 | -2.77370 | -2.34630 |
| C | 0.95640 | -2.60490 | -0.22750 |
| C | 4.19890 | 0.04510 | -0.71300 |
| Br | 1.58750 | 0.50600 | -1.87010 |
| C | 1.06180 | -3.56850 | -1.41420 |
| C | 0.44620 | -3.18170 | 1.10870 |
| C | 4.55410 | 1.48410 | -1.03390 |
| Cl | 1.87610 | -5.09940 | -0.97390 |
| C | 0.52020 | -2.17590 | 2.27400 |
| C | -0.27780 | -0.90960 | 2.02180 |
| O | 0.03470 | -2.80580 | 3.44190 |
| C | 0.28270 | 0.26590 | 1.84550 |
| C | 4.25070 | 2.52470 | -0.23590 |
| C | 4.56280 | 3.99530 | -0.48790 |
| C | 5.23820 | 4.26910 | -1.83890 |
| O | 5.42890 | 4.51820 | 0.51030 |
| C | 0.87160 | 1.41950 | 1.63530 |
| Br | 1.34540 | 2.66620 | 3.09700 |
| C | 4.82240 | 4.71780 | 1.78080 |
| H | 3.82670 | -2.62610 | -1.29030 |
| H | 3.72160 | -0.56950 | -2.73570 |
| H | 1.35290 | -2.06540 | -2.91070 |
| H | 2.48610 | -3.39790 | -3.06820 |
| H | 0.30570 | -1.78160 | -0.52560 |
| H | 3.74110 | -0.00020 | 0.27630 |
| H | 5.12310 | -0.53000 | -0.64950 |
| H | 0.09390 | -3.81210 | -1.85360 |
| H | -0.57850 | -3.53220 | 0.98190 |
| H | 1.03530 | -4.05690 | 1.38210 |
| H | 5.07910 | 1.64160 | -1.96410 |
| H | 1.56920 | -1.91960 | 2.44200 |
| H | -1.35240 | -1.01650 | 1.99250 |
| H | 0.28990 | -2.28630 | 4.19140 |
| H | 3.72200 | 2.32140 | 0.68340 |
| H | 3.61810 | 4.54190 | -0.47190 |
| H | 5.40640 | 5.33770 | -1.97310 |
| H | 6.20780 | 3.77510 | -1.90670 |
| H | 4.61950 | 3.92910 | -2.66980 |
| H | 1.15560 | 1.79570 | 0.66370 |
| H | 3.95840 | 5.37970 | 1.70930 |
| H | 4.50660 | 3.77930 | 2.23630 |
| H | 5.54150 | 5.18260 | 2.45510 |

| Marilzafurollene C_151 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.50350 | -0.53400 | -0.91380 |
| O | 2.03290 | -0.88030 | 0.38830 |
| C | 2.06620 | 0.89450 | -1.29720 |
| C | 2.00760 | -1.64130 | -1.85100 |
| C | 1.39100 | -2.15270 | 0.35780 |
| C | 2.63380 | 1.98730 | -0.37430 |
| Br | 0.07700 | 1.02430 | -1.23030 |
| C | 1.91080 | -2.82920 | -0.91710 |
| C | 1.62690 | -2.91830 | 1.67410 |
| C | 4.14470 | 2.10780 | -0.44230 |
| Cl | 3.53480 | -3.54770 | -0.69320 |
| C | 0.90640 | -2.29420 | 2.88280 |
| C | -0.59800 | -2.47930 | 2.81810 |
| O | 1.38640 | -2.91100 | 4.06010 |
| C | -1.45330 | -1.48420 | 2.75930 |
| C | 4.80150 | 3.17400 | -0.92860 |
| C | 6.31240 | 3.29720 | -0.99510 |
| C | 6.79810 | 4.49690 | -0.17770 |
| O | 6.75320 | 3.49500 | -2.33050 |
| C | -2.32400 | -0.50520 | 2.69480 |
| Br | -2.97340 | 0.22630 | 0.97480 |
| C | 6.64610 | 2.34460 | -3.15760 |
| H | 3.59200 | -0.59100 | -0.88490 |
| H | 2.36070 | 1.10510 | -2.32630 |
| H | 1.01730 | -1.41060 | -2.24370 |
| H | 2.66970 | -1.81200 | -2.70020 |
| H | 0.32340 | -1.97040 | 0.22290 |
| H | 2.18990 | 2.94690 | -0.64180 |
| H | 2.34280 | 1.79220 | 0.65870 |
| H | 1.24370 | -3.60960 | -1.28490 |
| H | 1.31050 | -3.95570 | 1.55750 |
| H | 2.69870 | -2.94830 | 1.87160 |
| H | 4.70790 | 1.26690 | -0.06330 |
| H | 1.14630 | -1.22940 | 2.93740 |
| H | -0.95050 | -3.50030 | 2.82800 |
| H | 2.25880 | -2.58720 | 4.23580 |
| H | 4.24520 | 4.01910 | -1.30850 |
| H | 6.77320 | 2.39480 | -0.58810 |
| H | 7.88470 | 4.57620 | -0.21410 |
| H | 6.38460 | 5.43010 | -0.56080 |
| H | 6.50680 | 4.40430 | 0.86890 |
| H | -2.76470 | -0.01380 | 3.54980 |
| H | 7.03140 | 2.57370 | -4.15110 |
| H | 7.22900 | 1.51430 | -2.75690 |
| H | 5.61050 | 2.02170 | -3.27020 |

| Marilzafurollene C_152 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.54920 | -0.54990 | -0.96260 |
| O | 2.06670 | -0.90480 | 0.33240 |
| C | 2.09440 | 0.87180 | -1.35100 |
| C | 2.08350 | -1.66370 | -1.90770 |
| C | 1.45510 | -2.19180 | 0.29530 |
| C | 2.62520 | 1.97250 | -0.41550 |
| Br | 0.10230 | 0.96800 | -1.32380 |
| C | 1.99740 | -2.85530 | -0.97760 |
| C | 1.69140 | -2.95980 | 1.61070 |
| C | 4.13540 | 2.11180 | -0.44780 |
| Cl | 3.63050 | -3.55000 | -0.74500 |
| C | 0.97610 | -2.34200 | 2.82530 |
| C | -0.53260 | -2.47880 | 2.73860 |
| O | 1.42620 | -3.01200 | 3.98550 |
| C | -1.35860 | -1.45740 | 2.74750 |
| C | 4.79110 | 3.17750 | -0.93630 |
| C | 6.30170 | 3.31710 | -0.96840 |
| C | 6.75320 | 4.54440 | -0.17270 |
| O | 6.77360 | 3.48260 | -2.29760 |
| C | -2.20200 | -0.45250 | 2.75830 |
| Br | -2.81990 | 0.43500 | 1.10170 |
| C | 6.69810 | 2.30830 | -3.09430 |
| H | 3.63800 | -0.58980 | -0.91880 |
| H | 2.40570 | 1.08960 | -2.37370 |
| H | 1.09370 | -1.45030 | -2.31100 |
| H | 2.75790 | -1.82050 | -2.74980 |
| H | 0.38530 | -2.03090 | 0.15120 |
| H | 2.17530 | 2.92610 | -0.69420 |
| H | 2.31260 | 1.77370 | 0.61050 |
| H | 1.34590 | -3.64490 | -1.35340 |
| H | 1.37690 | -3.99720 | 1.49090 |
| H | 2.76250 | -2.98950 | 1.81350 |
| H | 4.69880 | 1.28390 | -0.04100 |
| H | 1.25810 | -1.28940 | 2.90670 |
| H | -0.91430 | -3.48710 | 2.66730 |
| H | 1.20500 | -2.48770 | 4.74220 |
| H | 4.23440 | 4.00910 | -1.34430 |
| H | 6.76210 | 2.43180 | -0.52520 |
| H | 7.83950 | 4.63530 | -0.18400 |
| H | 6.33930 | 5.46180 | -0.59180 |
| H | 6.43650 | 4.47710 | 0.86840 |
| H | -2.63550 | -0.01960 | 3.64790 |
| H | 7.10660 | 2.51340 | -4.08380 |
| H | 7.27810 | 1.49540 | -2.65580 |
| H | 5.66880 | 1.97210 | -3.22400 |

| Marilzafurollene C_153 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.42980 | -1.14070 | -1.38150 |
| O | 2.86000 | -1.44620 | -0.05650 |
| C | 3.31270 | -0.03760 | -1.99520 |
| C | 0.93120 | -0.83750 | -1.27530 |
| C | 1.74610 | -1.48340 | 0.83440 |
| C | 3.34030 | 1.28340 | -1.20340 |
| Br | 2.70440 | 0.31290 | -3.86180 |
| C | 0.52330 | -1.67070 | -0.07900 |
| C | 1.98970 | -2.52060 | 1.95350 |
| C | 4.37340 | 2.25380 | -1.74180 |
| Cl | 0.29960 | -3.37330 | -0.58400 |
| C | 1.03420 | -2.42220 | 3.16100 |
| C | -0.37780 | -2.86870 | 2.83580 |
| O | 1.54520 | -3.24490 | 4.18890 |
| C | -1.43160 | -2.09890 | 2.98470 |
| C | 5.42060 | 2.71880 | -1.04040 |
| C | 6.45340 | 3.69020 | -1.58060 |
| C | 7.85280 | 3.07050 | -1.55010 |
| O | 6.50290 | 4.87520 | -0.79940 |
| C | -2.46930 | -1.30350 | 3.08930 |
| Br | -3.03780 | -0.12450 | 1.60500 |
| C | 5.37320 | 5.72350 | -0.95420 |
| H | 2.55410 | -2.05250 | -1.96800 |
| H | 4.32990 | -0.42650 | -2.06560 |
| H | 0.75260 | 0.21460 | -1.05850 |
| H | 0.38130 | -1.08650 | -2.18340 |
| H | 1.68690 | -0.49080 | 1.28440 |
| H | 2.36760 | 1.77300 | -1.23100 |
| H | 3.55900 | 1.07820 | -0.15460 |
| H | -0.40840 | -1.32430 | 0.36730 |
| H | 1.99930 | -3.53370 | 1.55140 |
| H | 3.00300 | -2.35380 | 2.32120 |
| H | 4.23250 | 2.57820 | -2.76340 |
| H | 1.02870 | -1.39400 | 3.53010 |
| H | -0.48370 | -3.87600 | 2.45740 |
| H | 1.06690 | -3.07210 | 4.98770 |
| H | 5.56580 | 2.40000 | -0.01810 |
| H | 6.21280 | 3.94470 | -2.61480 |
| H | 8.59210 | 3.76340 | -1.95210 |
| H | 8.15220 | 2.81970 | -0.53220 |
| H | 7.89280 | 2.15910 | -2.14710 |
| H | -3.09650 | -1.21070 | 3.96430 |
| H | 5.50590 | 6.61990 | -0.34860 |
| H | 5.25350 | 6.03670 | -1.99210 |
| H | 4.45330 | 5.23690 | -0.62820 |

| Marilzafurollene C_154 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.23150 | -0.53690 | -1.38160 |
| O | 1.96840 | -0.73810 | 0.00670 |
| C | 1.58170 | 0.76880 | -1.88290 |
| C | 1.75640 | -1.81070 | -2.08940 |
| C | 1.49570 | -2.06340 | 0.23300 |
| C | 2.15460 | 2.02860 | -1.21180 |
| Br | -0.37880 | 0.72320 | -1.51930 |
| C | 1.92210 | -2.85780 | -1.00830 |
| C | 1.99970 | -2.59960 | 1.58680 |
| C | 3.60920 | 2.27770 | -1.56220 |
| Cl | 3.63380 | -3.37560 | -0.93320 |
| C | 1.37610 | -1.88320 | 2.79820 |
| C | -0.08860 | -2.23170 | 2.98490 |
| O | 2.08260 | -2.26680 | 3.96040 |
| C | -1.06160 | -1.35160 | 2.92130 |
| C | 4.61360 | 2.27480 | -0.67010 |
| C | 6.07110 | 2.52140 | -1.01180 |
| C | 6.92890 | 1.30800 | -0.64460 |
| O | 6.58790 | 3.63220 | -0.29350 |
| C | -2.04870 | -0.49020 | 2.85530 |
| Br | -3.00730 | -0.10160 | 1.16870 |
| C | 6.08950 | 4.89100 | -0.72560 |
| H | 3.31480 | -0.47540 | -1.49540 |
| H | 1.69890 | 0.84660 | -2.96450 |
| H | 0.70350 | -1.73770 | -2.36180 |
| H | 2.31980 | -2.03240 | -2.99610 |
| H | 0.40530 | -2.01770 | 0.23650 |
| H | 1.58270 | 2.90230 | -1.52560 |
| H | 2.03680 | 1.95540 | -0.12960 |
| H | 1.30900 | -3.74420 | -1.17430 |
| H | 1.80220 | -3.67020 | 1.65480 |
| H | 3.08360 | -2.48760 | 1.62310 |
| H | 3.82400 | 2.46620 | -2.60440 |
| H | 1.48700 | -0.80280 | 2.67660 |
| H | -0.30640 | -3.27050 | 3.18490 |
| H | 2.92550 | -1.83510 | 3.95650 |
| H | 4.40050 | 2.08560 | 0.37250 |
| H | 6.17140 | 2.70190 | -2.08390 |
| H | 7.97350 | 1.47790 | -0.90570 |
| H | 6.88340 | 1.10100 | 0.42480 |
| H | 6.59470 | 0.41500 | -1.17370 |
| H | -2.42970 | 0.07710 | 3.69170 |
| H | 6.56060 | 5.68620 | -0.14810 |
| H | 6.31460 | 5.06480 | -1.77850 |
| H | 5.01160 | 4.97120 | -0.58110 |

| Marilzafurollene C_155 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.50880 | 0.24380 | -0.47400 |
| O | 2.18390 | 0.38970 | 0.90790 |
| C | 2.41800 | 1.59950 | -1.20510 |
| C | 1.57990 | -0.84870 | -1.01600 |
| C | 1.14450 | -0.51470 | 1.27150 |
| C | 3.41310 | 2.65270 | -0.68610 |
| Br | 0.58110 | 2.35130 | -0.99540 |
| C | 1.24820 | -1.64060 | 0.23100 |
| C | 1.26040 | -0.88800 | 2.76600 |
| C | 4.86410 | 2.28030 | -0.92660 |
| Cl | 2.58490 | -2.77620 | 0.58680 |
| C | 0.02710 | -1.59650 | 3.36340 |
| C | -0.13460 | -3.01980 | 2.86610 |
| O | 0.17650 | -1.62190 | 4.76770 |
| C | -1.21040 | -3.45290 | 2.24920 |
| C | 5.69080 | 2.93810 | -1.75640 |
| C | 7.14290 | 2.56860 | -1.99570 |
| C | 8.07050 | 3.72190 | -1.60490 |
| O | 7.38160 | 2.28600 | -3.36680 |
| C | -2.26790 | -3.86130 | 1.58960 |
| Br | -2.40090 | -3.70090 | -0.37840 |
| C | 6.82480 | 1.05810 | -3.81560 |
| H | 3.52950 | -0.13650 | -0.52290 |
| H | 2.57790 | 1.45170 | -2.27410 |
| H | 0.66400 | -0.42070 | -1.42340 |
| H | 2.03940 | -1.45120 | -1.79980 |
| H | 0.20420 | 0.01670 | 1.11350 |
| H | 3.20820 | 3.60770 | -1.17130 |
| H | 3.26420 | 2.81300 | 0.38250 |
| H | 0.33020 | -2.21700 | 0.12170 |
| H | 2.16560 | -1.46480 | 2.95540 |
| H | 1.40110 | 0.04600 | 3.31170 |
| H | 5.23460 | 1.42640 | -0.37720 |
| H | -0.86710 | -1.01230 | 3.13400 |
| H | 0.70170 | -3.68260 | 3.04000 |
| H | -0.64440 | -1.88520 | 5.15910 |
| H | 5.32780 | 3.79340 | -2.30830 |
| H | 7.40490 | 1.69720 | -1.39200 |
| H | 9.11430 | 3.45030 | -1.76340 |
| H | 7.86580 | 4.61290 | -2.19900 |
| H | 7.95160 | 3.98390 | -0.55330 |
| H | -3.14440 | -4.30920 | 2.03530 |
| H | 5.73740 | 1.05260 | -3.73360 |
| H | 7.07860 | 0.90550 | -4.86450 |
| H | 7.22180 | 0.21420 | -3.24990 |

| Marilzafurollene C_156 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.94120 | -1.04060 | -0.80770 |
| O | 2.71720 | -1.14270 | 0.59750 |
| C | 4.22470 | -0.23680 | -1.08890 |
| C | 1.64100 | -0.48700 | -1.40530 |
| C | 1.36840 | -0.79400 | 0.90550 |
| C | 4.23640 | 1.18800 | -0.50200 |
| Br | 4.51620 | -0.15080 | -3.05990 |
| C | 0.60320 | -0.96690 | -0.41250 |
| C | 0.85950 | -1.58760 | 2.12440 |
| C | 5.58760 | 1.85960 | -0.65060 |
| Cl | 0.19770 | -2.67860 | -0.74310 |
| C | -0.61180 | -1.31900 | 2.49730 |
| C | -1.02770 | -2.13650 | 3.70490 |
| O | -0.78000 | 0.05340 | 2.78880 |
| C | -2.01310 | -3.00540 | 3.69130 |
| C | 5.79640 | 3.00900 | -1.31400 |
| C | 7.15020 | 3.67410 | -1.47630 |
| C | 7.15110 | 5.07110 | -0.85060 |
| O | 7.48680 | 3.82880 | -2.84750 |
| C | -2.98570 | -3.88620 | 3.68550 |
| Br | -2.69180 | -5.78980 | 3.22970 |
| C | 7.76720 | 2.60900 | -3.52170 |
| H | 3.07980 | -2.05840 | -1.17620 |
| H | 5.06330 | -0.79820 | -0.67480 |
| H | 1.64390 | 0.60170 | -1.42370 |
| H | 1.45930 | -0.83430 | -2.42290 |
| H | 1.37390 | 0.26850 | 1.15530 |
| H | 3.47150 | 1.80610 | -0.97090 |
| H | 3.99990 | 1.15070 | 0.56210 |
| H | -0.31920 | -0.38590 | -0.44510 |
| H | 0.99420 | -2.65390 | 1.93980 |
| H | 1.49860 | -1.35550 | 2.97690 |
| H | 6.42280 | 1.35690 | -0.18420 |
| H | -1.25520 | -1.57140 | 1.65160 |
| H | -0.45790 | -1.97370 | 4.60880 |
| H | -1.69140 | 0.21220 | 2.99270 |
| H | 4.96500 | 3.51520 | -1.78320 |
| H | 7.91550 | 3.07360 | -0.98060 |
| H | 8.12900 | 5.54150 | -0.95480 |
| H | 6.41820 | 5.71970 | -1.33090 |
| H | 6.91560 | 5.02650 | 0.21300 |
| H | -4.01730 | -3.66960 | 3.92160 |
| H | 6.89610 | 1.95370 | -3.55490 |
| H | 8.05930 | 2.82100 | -4.55010 |
| H | 8.58880 | 2.07310 | -3.04500 |

| Marilzafurollene C_157 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.05460 | -1.70850 | -1.10280 |
| O | 2.02060 | -1.35810 | -0.18230 |
| C | 3.89640 | -0.47190 | -1.46840 |
| C | 2.35880 | -2.39170 | -2.28730 |
| C | 0.75400 | -1.77340 | -0.68970 |
| C | 4.66690 | 0.08220 | -0.25760 |
| Br | 2.70840 | 0.96080 | -2.19440 |
| C | 1.08110 | -2.91260 | -1.66180 |
| C | -0.22470 | -2.10760 | 0.45320 |
| C | 5.58310 | 1.23260 | -0.62720 |
| Cl | 1.41520 | -4.45090 | -0.81180 |
| C | -0.59790 | -0.88460 | 1.31030 |
| C | -1.73140 | -1.20780 | 2.27790 |
| O | 0.56560 | -0.43550 | 1.98220 |
| C | -1.64730 | -1.19200 | 3.59050 |
| C | 5.50420 | 2.46510 | -0.09850 |
| C | 6.41030 | 3.62220 | -0.47500 |
| C | 7.20170 | 4.11390 | 0.73950 |
| O | 5.66170 | 4.72670 | -0.96200 |
| C | -1.54330 | -1.17920 | 4.89830 |
| Br | -1.04830 | -2.78580 | 5.94570 |
| C | 5.05350 | 4.50840 | -2.22830 |
| H | 3.68870 | -2.44600 | -0.60790 |
| H | 4.60060 | -0.73760 | -2.25820 |
| H | 2.11040 | -1.66840 | -3.06420 |
| H | 2.96430 | -3.17390 | -2.74590 |
| H | 0.35130 | -0.94140 | -1.27060 |
| H | 3.96450 | 0.39960 | 0.51470 |
| H | 5.27890 | -0.70480 | 0.18420 |
| H | 0.28980 | -3.09260 | -2.39030 |
| H | -1.13190 | -2.52510 | 0.01460 |
| H | 0.18700 | -2.88730 | 1.09540 |
| H | 6.34000 | 1.02130 | -1.36890 |
| H | -0.94230 | -0.07860 | 0.66020 |
| H | -2.67220 | -1.46230 | 1.81200 |
| H | 1.30000 | -0.56870 | 1.38700 |
| H | 4.74810 | 2.68160 | 0.64270 |
| H | 7.11860 | 3.29900 | -1.24040 |
| H | 7.86340 | 4.93520 | 0.46410 |
| H | 6.53660 | 4.47300 | 1.52520 |
| H | 7.81720 | 3.31700 | 1.15760 |
| H | -1.71570 | -0.31340 | 5.52020 |
| H | 4.31250 | 3.70910 | -2.19030 |
| H | 4.54210 | 5.41650 | -2.54720 |
| H | 5.79650 | 4.25950 | -2.98680 |

| Marilzafurollene C_158 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.60680 | 0.17430 | -0.78120 |
| O | 1.50150 | -0.24720 | 0.01630 |
| C | 2.10970 | 1.00660 | -1.97840 |
| C | 3.34170 | -1.11720 | -1.15070 |
| C | 1.65370 | -1.61290 | 0.40530 |
| C | 3.22160 | 1.47070 | -2.93970 |
| Br | 1.14720 | 2.61020 | -1.28690 |
| C | 3.10650 | -1.97900 | 0.07180 |
| C | 1.20770 | -1.83060 | 1.86480 |
| C | 4.31640 | 2.26250 | -2.24950 |
| Cl | 4.24800 | -1.50640 | 1.36660 |
| C | -0.29350 | -1.57340 | 2.08520 |
| C | -0.73170 | -1.99750 | 3.47350 |
| O | -0.54090 | -0.19350 | 1.92540 |
| C | -1.60150 | -2.95580 | 3.69980 |
| C | 5.61060 | 1.90370 | -2.22060 |
| C | 6.70260 | 2.68280 | -1.51260 |
| C | 7.76760 | 3.15500 | -2.50550 |
| O | 7.36000 | 1.87790 | -0.54470 |
| C | -2.45760 | -3.92300 | 3.93120 |
| Br | -4.40820 | -3.61240 | 4.06450 |
| C | 6.57000 | 1.57370 | 0.59730 |
| H | 3.24810 | 0.78370 | -0.14280 |
| H | 1.37350 | 0.42840 | -2.53830 |
| H | 2.87980 | -1.58170 | -2.02290 |
| H | 4.39830 | -0.96030 | -1.37030 |
| H | 1.00740 | -2.19640 | -0.25270 |
| H | 3.66180 | 0.60680 | -3.43910 |
| H | 2.79070 | 2.09090 | -3.72630 |
| H | 3.24210 | -3.04360 | -0.12220 |
| H | 1.43320 | -2.86200 | 2.13980 |
| H | 1.78810 | -1.20260 | 2.54190 |
| H | 4.00420 | 3.16960 | -1.75080 |
| H | -0.87080 | -2.11780 | 1.33450 |
| H | -0.28690 | -1.45790 | 4.29690 |
| H | 0.00480 | 0.11490 | 1.20530 |
| H | 5.92930 | 0.99970 | -2.71920 |
| H | 6.27170 | 3.55990 | -1.02550 |
| H | 8.54450 | 3.72620 | -1.99720 |
| H | 8.24740 | 2.31130 | -3.00190 |
| H | 7.33350 | 3.79540 | -3.27370 |
| H | -2.19260 | -4.96110 | 4.06890 |
| H | 7.15920 | 0.98810 | 1.30290 |
| H | 6.24360 | 2.48120 | 1.10660 |
| H | 5.69040 | 0.98560 | 0.33540 |

| Marilzafurollene C_159 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.58300 | -0.97410 | -1.51980 |
| O | 1.53760 | -0.83320 | -0.55520 |
| C | 2.38960 | 0.04660 | -2.66010 |
| C | 2.55240 | -2.44430 | -1.96460 |
| C | 1.17380 | -2.10780 | -0.03620 |
| C | 2.43850 | 1.50790 | -2.18230 |
| Br | 0.62420 | -0.25780 | -3.53750 |
| C | 1.30850 | -2.98270 | -1.28400 |
| C | 2.10720 | -2.47030 | 1.14480 |
| C | 3.79080 | 1.89910 | -1.61720 |
| Cl | 1.40750 | -4.73400 | -0.94840 |
| C | 1.98520 | -1.50620 | 2.33910 |
| C | 0.64030 | -1.62120 | 3.03300 |
| O | 3.00710 | -1.81900 | 3.26400 |
| C | -0.21770 | -0.63040 | 3.12600 |
| C | 4.00420 | 2.22990 | -0.33270 |
| C | 5.35110 | 2.61690 | 0.24830 |
| C | 5.77170 | 1.63370 | 1.34360 |
| O | 5.30540 | 3.90750 | 0.83940 |
| C | -1.09320 | 0.34410 | 3.20310 |
| Br | -2.48760 | 0.62640 | 1.82670 |
| C | 5.20090 | 4.97400 | -0.09440 |
| H | 3.53470 | -0.78930 | -1.01920 |
| H | 3.15070 | -0.11010 | -3.42570 |
| H | 2.51900 | -2.57550 | -3.04660 |
| H | 3.44090 | -2.95860 | -1.59630 |
| H | 0.13730 | -2.09060 | 0.30260 |
| H | 2.21630 | 2.17550 | -3.01520 |
| H | 1.66030 | 1.67690 | -1.43610 |
| H | 0.44210 | -2.82030 | -1.92750 |
| H | 1.89480 | -3.48410 | 1.48610 |
| H | 3.14260 | -2.48440 | 0.80350 |
| H | 4.61840 | 1.89970 | -2.31240 |
| H | 2.14600 | -0.48260 | 1.99070 |
| H | 0.40670 | -2.58660 | 3.46000 |
| H | 3.06260 | -1.12130 | 3.90180 |
| H | 3.17600 | 2.22710 | 0.36220 |
| H | 6.10860 | 2.60200 | -0.53810 |
| H | 6.74700 | 1.90090 | 1.75130 |
| H | 5.05710 | 1.62990 | 2.16730 |
| H | 5.84040 | 0.61710 | 0.95500 |
| H | -1.14260 | 1.07020 | 4.00180 |
| H | 6.04250 | 4.97560 | -0.78860 |
| H | 4.27480 | 4.92100 | -0.66840 |
| H | 5.20630 | 5.92500 | 0.43840 |

| Marilzafurollene C_160 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.58030 | -0.96570 | -1.51170 |
| O | 1.53240 | -0.83210 | -0.54890 |
| C | 2.38340 | 0.05670 | -2.64960 |
| C | 2.55800 | -2.43470 | -1.96040 |
| C | 1.17260 | -2.10960 | -0.03500 |
| C | 2.43590 | 1.51700 | -2.16940 |
| Br | 0.61450 | -0.24570 | -3.52070 |
| C | 1.31550 | -2.98110 | -1.28440 |
| C | 2.10300 | -2.47030 | 1.14830 |
| C | 3.79460 | 1.90780 | -1.62000 |
| Cl | 1.42330 | -4.73250 | -0.95280 |
| C | 1.96950 | -1.51120 | 2.34460 |
| C | 0.62410 | -1.63880 | 3.03380 |
| O | 2.99080 | -1.81890 | 3.27180 |
| C | -0.24010 | -0.65450 | 3.13160 |
| C | 4.02350 | 2.23980 | -0.33860 |
| C | 5.37780 | 2.62530 | 0.22500 |
| C | 5.80870 | 1.64450 | 1.31900 |
| O | 5.34220 | 3.91860 | 0.81180 |
| C | -1.12250 | 0.31270 | 3.21570 |
| Br | -2.51720 | 0.59680 | 1.84020 |
| C | 5.23440 | 4.98260 | -0.12490 |
| H | 3.53000 | -0.77750 | -1.00880 |
| H | 3.14130 | -0.09940 | -3.41840 |
| H | 2.52750 | -2.56330 | -3.04260 |
| H | 3.44790 | -2.94550 | -1.59130 |
| H | 0.13500 | -2.09790 | 0.29990 |
| H | 2.20400 | 2.18580 | -2.99860 |
| H | 1.66620 | 1.68410 | -1.41440 |
| H | 0.45020 | -2.82230 | -1.92980 |
| H | 1.89590 | -3.48630 | 1.48540 |
| H | 3.13960 | -2.47670 | 0.81140 |
| H | 4.61390 | 1.90740 | -2.32490 |
| H | 2.12290 | -0.48550 | 2.00030 |
| H | 0.39590 | -2.60830 | 3.45340 |
| H | 3.03840 | -1.12320 | 3.91210 |
| H | 3.20400 | 2.23900 | 0.36630 |
| H | 6.12610 | 2.60520 | -0.57030 |
| H | 6.78930 | 1.91060 | 1.71370 |
| H | 5.10410 | 1.64580 | 2.15160 |
| H | 5.87020 | 0.62580 | 0.93350 |
| H | -1.17770 | 1.03130 | 4.02030 |
| H | 5.24690 | 5.93590 | 0.40450 |
| H | 6.07070 | 4.97900 | -0.82550 |
| H | 4.30420 | 4.93100 | -0.69150 |

| Marilzafurollene C_161 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.22040 | -1.04930 | 0.52350 |
| O | 1.81040 | -0.85860 | 0.65360 |
| C | 3.90200 | 0.32290 | 0.36850 |
| C | 3.40980 | -2.02800 | -0.64720 |
| C | 1.10940 | -1.90890 | -0.00610 |
| C | 3.44790 | 1.12270 | -0.86750 |
| Br | 5.87720 | 0.05500 | 0.30420 |
| C | 2.01150 | -2.15650 | -1.21720 |
| C | 0.93410 | -3.10870 | 0.95620 |
| C | 4.03960 | 2.51810 | -0.90130 |
| Cl | 1.73730 | -3.72160 | -2.03100 |
| C | 0.13540 | -2.77150 | 2.22850 |
| C | -1.29610 | -2.37010 | 1.92610 |
| O | 0.12840 | -3.91390 | 3.05940 |
| C | -1.79870 | -1.19760 | 2.23990 |
| C | 4.80630 | 2.99430 | -1.89630 |
| C | 5.41140 | 4.38530 | -1.92510 |
| C | 4.90340 | 5.17720 | -3.13250 |
| O | 6.82690 | 4.32900 | -2.02660 |
| C | -2.28540 | -0.02410 | 2.56750 |
| Br | -3.15630 | 0.31390 | 4.31250 |
| C | 7.47780 | 3.84080 | -0.86080 |
| H | 3.58110 | -1.52190 | 1.43860 |
| H | 3.69770 | 0.90430 | 1.26880 |
| H | 4.13620 | -1.69940 | -1.39040 |
| H | 3.75310 | -2.98950 | -0.26390 |
| H | 0.13140 | -1.55420 | -0.33260 |
| H | 3.70910 | 0.59280 | -1.78350 |
| H | 2.36200 | 1.22310 | -0.86290 |
| H | 1.84460 | -1.37110 | -1.95560 |
| H | 0.43590 | -3.92540 | 0.43260 |
| H | 1.91100 | -3.49590 | 1.24600 |
| H | 3.81640 | 3.15100 | -0.05420 |
| H | 0.64420 | -1.96740 | 2.76550 |
| H | -1.90350 | -3.10970 | 1.42430 |
| H | -0.20980 | -3.66700 | 3.90890 |
| H | 5.03400 | 2.36590 | -2.74530 |
| H | 5.13410 | 4.92480 | -1.01730 |
| H | 5.32760 | 6.18130 | -3.14330 |
| H | 5.17890 | 4.69070 | -4.06850 |
| H | 3.81780 | 5.27550 | -3.11080 |
| H | -2.26150 | 0.85250 | 1.93670 |
| H | 8.55740 | 3.87350 | -1.00660 |
| H | 7.24000 | 4.45210 | 0.01070 |
| H | 7.20530 | 2.80690 | -0.64630 |

| Marilzafurollene C_162 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.62480 | -0.58090 | -1.34810 |
| O | 2.23500 | -0.81780 | 0.00470 |
| C | 1.73830 | 0.51120 | -1.98320 |
| C | 2.57450 | -1.94410 | -2.05200 |
| C | 1.90390 | -2.19090 | 0.18020 |
| C | 1.91530 | 1.88950 | -1.32420 |
| Br | -0.18360 | -0.00230 | -1.81630 |
| C | 2.71160 | -2.91820 | -0.89900 |
| C | 2.12640 | -2.64710 | 1.63580 |
| C | 3.28950 | 2.48510 | -1.56220 |
| Cl | 4.43710 | -3.08740 | -0.45790 |
| C | 1.24860 | -1.89410 | 2.65220 |
| C | -0.23460 | -2.10490 | 2.41020 |
| O | 1.57480 | -2.35180 | 3.94860 |
| C | -1.05320 | -1.13370 | 2.07510 |
| C | 4.20180 | 2.68580 | -0.59420 |
| C | 5.59510 | 3.28170 | -0.76320 |
| C | 5.85380 | 3.88250 | -2.15210 |
| O | 6.60730 | 2.30620 | -0.55420 |
| C | -1.84900 | -0.15240 | 1.72180 |
| Br | -2.82330 | 0.95300 | 3.04390 |
| C | 6.74950 | 1.86880 | 0.79050 |
| H | 3.66450 | -0.25070 | -1.32890 |
| H | 1.95440 | 0.58760 | -3.04970 |
| H | 1.61070 | -2.09490 | -2.53870 |
| H | 3.34930 | -2.06190 | -2.81000 |
| H | 0.84910 | -2.30380 | -0.07450 |
| H | 1.17840 | 2.58600 | -1.72490 |
| H | 1.71790 | 1.81380 | -0.25370 |
| H | 2.32090 | -3.91040 | -1.12700 |
| H | 1.93940 | -3.71890 | 1.71100 |
| H | 3.17220 | -2.50040 | 1.90650 |
| H | 3.51340 | 2.74670 | -2.58570 |
| H | 1.48640 | -0.82890 | 2.59780 |
| H | -0.59940 | -3.11560 | 2.52290 |
| H | 1.19960 | -1.75490 | 4.58080 |
| H | 3.94160 | 2.40580 | 0.41650 |
| H | 5.70450 | 4.08220 | -0.02940 |
| H | 6.84230 | 4.34040 | -2.19240 |
| H | 5.81770 | 3.11980 | -2.93030 |
| H | 5.12470 | 4.65620 | -2.39390 |
| H | -2.04700 | 0.14310 | 0.70130 |
| H | 5.86630 | 1.33350 | 1.13980 |
| H | 7.59480 | 1.18430 | 0.86010 |
| H | 6.94250 | 2.70580 | 1.46270 |

| Marilzafurollene C_163 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.01310 | -1.63920 | -2.15430 |
| O | 3.17270 | -1.49170 | -0.74400 |
| C | 4.27540 | -1.17770 | -2.91920 |
| C | 1.69240 | -0.94100 | -2.51140 |
| C | 2.09460 | -0.72130 | -0.22160 |
| C | 4.69090 | 0.30470 | -2.78250 |
| Br | 4.01630 | -1.57220 | -4.85440 |
| C | 0.94000 | -0.96700 | -1.19430 |
| C | 1.86330 | -1.02470 | 1.26850 |
| C | 5.00830 | 0.71180 | -1.35610 |
| Cl | 0.18650 | -2.57070 | -0.94890 |
| C | 0.72000 | -0.21620 | 1.90890 |
| C | 0.60240 | -0.49640 | 3.39510 |
| O | 0.91870 | 1.16970 | 1.70980 |
| C | -0.47990 | -0.98360 | 3.95810 |
| C | 4.54330 | 1.82540 | -0.76010 |
| C | 4.77780 | 2.24620 | 0.68670 |
| C | 5.59080 | 1.23600 | 1.50830 |
| O | 3.54090 | 2.41350 | 1.37270 |
| C | -1.56400 | -1.45570 | 4.52660 |
| Br | -1.88800 | -3.39550 | 4.75200 |
| C | 2.88520 | 3.64470 | 1.08690 |
| H | 2.88500 | -2.70890 | -2.32730 |
| H | 5.10820 | -1.80300 | -2.59450 |
| H | 1.86450 | 0.09330 | -2.80650 |
| H | 1.15780 | -1.43240 | -3.32470 |
| H | 2.37570 | 0.32650 | -0.31420 |
| H | 5.58960 | 0.47200 | -3.37680 |
| H | 3.92750 | 0.96180 | -3.19840 |
| H | 0.16040 | -0.20680 | -1.12960 |
| H | 1.67070 | -2.09030 | 1.39810 |
| H | 2.79240 | -0.82790 | 1.80420 |
| H | 5.64040 | 0.02580 | -0.81210 |
| H | -0.22140 | -0.48350 | 1.42390 |
| H | 1.47250 | -0.27440 | 3.99540 |
| H | 1.84240 | 1.38430 | 1.81050 |
| H | 3.92890 | 2.49550 | -1.34250 |
| H | 5.32870 | 3.18850 | 0.67850 |
| H | 5.71920 | 1.58800 | 2.53190 |
| H | 5.09270 | 0.26710 | 1.55420 |
| H | 6.58620 | 1.08950 | 1.08840 |
| H | -2.36810 | -0.85040 | 4.91890 |
| H | 2.58550 | 3.71260 | 0.04110 |
| H | 1.98310 | 3.73010 | 1.69270 |
| H | 3.52070 | 4.49860 | 1.32500 |

| Marilzafurollene C_164 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.87490 | -0.93430 | -1.18050 |
| O | 1.50310 | -0.63830 | -0.90580 |
| C | 3.34550 | -0.12710 | -2.40750 |
| C | 2.95530 | -2.45940 | -1.34620 |
| C | 0.82960 | -1.81120 | -0.45610 |
| C | 3.27000 | 1.39840 | -2.21610 |
| Br | 2.21850 | -0.60240 | -3.98340 |
| C | 1.50160 | -2.88960 | -1.30880 |
| C | 1.00710 | -1.95460 | 1.07490 |
| C | 4.19980 | 1.91150 | -1.13290 |
| Cl | 1.29030 | -4.55100 | -0.69000 |
| C | 0.37290 | -0.80200 | 1.87440 |
| C | 0.40090 | -1.07650 | 3.36500 |
| O | 1.09330 | 0.38210 | 1.61060 |
| C | -0.68060 | -1.16580 | 4.10500 |
| C | 5.23530 | 2.74220 | -1.34530 |
| C | 6.17890 | 3.26760 | -0.27480 |
| C | 7.58000 | 2.67660 | -0.45040 |
| O | 5.74620 | 2.93960 | 1.03990 |
| C | -1.76980 | -1.26270 | 4.82980 |
| Br | -2.71230 | -2.98170 | 5.10510 |
| C | 4.75460 | 3.81590 | 1.56060 |
| H | 3.46690 | -0.66030 | -0.30640 |
| H | 4.37060 | -0.40460 | -2.65840 |
| H | 3.45450 | -2.77570 | -2.26250 |
| H | 3.50180 | -2.89160 | -0.50720 |
| H | -0.23290 | -1.74390 | -0.69280 |
| H | 3.51580 | 1.89060 | -3.15780 |
| H | 2.24960 | 1.69590 | -1.97180 |
| H | 1.08620 | -2.85930 | -2.31740 |
| H | 0.53140 | -2.88400 | 1.39070 |
| H | 2.06020 | -2.05670 | 1.33890 |
| H | 3.99400 | 1.57300 | -0.12700 |
| H | -0.65880 | -0.65880 | 1.54500 |
| H | 1.37830 | -1.19800 | 3.80860 |
| H | 1.24780 | 0.40590 | 0.66980 |
| H | 5.44290 | 3.08080 | -2.35050 |
| H | 6.24970 | 4.35170 | -0.38190 |
| H | 7.56450 | 1.59130 | -0.34650 |
| H | 7.99100 | 2.91500 | -1.43170 |
| H | 8.26410 | 3.07190 | 0.30070 |
| H | -2.24950 | -0.43780 | 5.33610 |
| H | 3.86440 | 3.84610 | 0.93160 |
| H | 4.45160 | 3.47600 | 2.55090 |
| H | 5.14230 | 4.83040 | 1.66040 |

| Marilzafurollene C_165 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.03290 | -2.10940 | -1.17300 |
| O | 2.30560 | -1.34750 | -0.21340 |
| C | 4.51570 | -2.27660 | -0.77530 |
| C | 2.74720 | -1.44490 | -2.52260 |
| C | 1.38300 | -0.47160 | -0.86510 |
| C | 5.39580 | -1.01010 | -0.79450 |
| Br | 5.34100 | -3.60930 | -2.00420 |
| C | 1.33070 | -0.94710 | -2.32480 |
| C | 0.02420 | -0.41010 | -0.13560 |
| C | 4.93200 | 0.06780 | 0.16530 |
| Cl | 0.17780 | -2.29610 | -2.56200 |
| C | -0.01190 | 0.40020 | 1.17690 |
| C | 0.98370 | -0.08060 | 2.21600 |
| O | 0.17440 | 1.77720 | 0.91660 |
| C | 0.64300 | -0.46770 | 3.42370 |
| C | 4.59940 | 1.31680 | -0.20710 |
| C | 4.12380 | 2.44040 | 0.70370 |
| C | 4.29380 | 2.15420 | 2.20230 |
| O | 2.74660 | 2.71700 | 0.48280 |
| C | 0.29100 | -0.84250 | 4.63060 |
| Br | -0.18260 | -2.71440 | 5.06700 |
| C | 2.48920 | 3.47090 | -0.69690 |
| H | 2.57290 | -3.09900 | -1.17520 |
| H | 4.55180 | -2.72150 | 0.22000 |
| H | 3.40400 | -0.59300 | -2.69140 |
| H | 2.85440 | -2.12710 | -3.36640 |
| H | 1.83420 | 0.52050 | -0.86510 |
| H | 6.41260 | -1.28270 | -0.51030 |
| H | 5.46910 | -0.60850 | -1.80490 |
| H | 1.05790 | -0.14980 | -3.01690 |
| H | -0.72000 | 0.01300 | -0.81150 |
| H | -0.31110 | -1.42710 | 0.07190 |
| H | 4.87260 | -0.22750 | 1.20220 |
| H | -1.01880 | 0.30530 | 1.58920 |
| H | 2.01950 | -0.10300 | 1.91400 |
| H | 1.10680 | 1.96670 | 0.82720 |
| H | 4.66950 | 1.57500 | -1.25350 |
| H | 4.72090 | 3.32530 | 0.47530 |
| H | 3.98310 | 3.01600 | 2.79320 |
| H | 3.69360 | 1.30630 | 2.52740 |
| H | 5.33540 | 1.94770 | 2.44950 |
| H | 0.22610 | -0.18590 | 5.48580 |
| H | 2.79010 | 2.93320 | -1.59620 |
| H | 1.42100 | 3.67310 | -0.77700 |
| H | 3.00550 | 4.43150 | -0.67410 |

| Marilzafurollene C_166 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.26620 | -0.55530 | -1.43630 |
| O | 1.99450 | -0.76670 | -0.05140 |
| C | 1.60970 | 0.74780 | -1.93530 |
| C | 1.80690 | -1.82900 | -2.15420 |
| C | 1.54980 | -2.10310 | 0.16720 |
| C | 2.16220 | 2.00760 | -1.24760 |
| Br | -0.35470 | 0.68050 | -1.59640 |
| C | 1.98620 | -2.88190 | -1.08100 |
| C | 2.06120 | -2.64540 | 1.51640 |
| C | 3.61860 | 2.27290 | -1.57800 |
| Cl | 3.70410 | -3.37950 | -1.01360 |
| C | 1.45140 | -1.93630 | 2.73870 |
| C | -0.02540 | -2.24120 | 2.90600 |
| O | 2.13930 | -2.38000 | 3.89090 |
| C | -0.96410 | -1.32230 | 2.90470 |
| C | 4.61190 | 2.27150 | -0.67360 |
| C | 6.07120 | 2.53370 | -0.99510 |
| C | 6.93580 | 1.32680 | -0.62230 |
| O | 6.56810 | 3.64630 | -0.26550 |
| C | -1.91820 | -0.42180 | 2.90680 |
| Br | -2.86400 | 0.12870 | 1.25870 |
| C | 6.06260 | 4.90200 | -0.69830 |
| H | 3.34990 | -0.48420 | -1.54130 |
| H | 1.73930 | 0.83490 | -3.01480 |
| H | 0.75310 | -1.76750 | -2.42590 |
| H | 2.37300 | -2.03660 | -3.06250 |
| H | 0.45880 | -2.07650 | 0.17190 |
| H | 1.58600 | 2.87830 | -1.56150 |
| H | 2.03200 | 1.92470 | -0.16750 |
| H | 1.38420 | -3.77460 | -1.25360 |
| H | 1.86450 | -3.71620 | 1.57960 |
| H | 3.14540 | -2.53360 | 1.55220 |
| H | 3.84450 | 2.47220 | -2.61580 |
| H | 1.60850 | -0.85940 | 2.63970 |
| H | -0.28350 | -3.28290 | 3.03160 |
| H | 1.96980 | -1.77220 | 4.59660 |
| H | 4.38770 | 2.07120 | 0.36470 |
| H | 6.18360 | 2.72000 | -2.06510 |
| H | 7.98200 | 1.50770 | -0.86910 |
| H | 6.87830 | 1.11450 | 0.44560 |
| H | 6.61680 | 0.43300 | -1.15940 |
| H | -2.27720 | 0.09570 | 3.78440 |
| H | 4.98220 | 4.97100 | -0.56680 |
| H | 6.51870 | 5.69930 | -0.11140 |
| H | 6.29910 | 5.08280 | -1.74760 |

| Marilzafurollene C_167 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.79850 | -1.48590 | -1.11350 |
| O | 2.01650 | -1.10790 | 0.02010 |
| C | 3.67920 | -0.31190 | -1.58010 |
| C | 1.80700 | -2.00830 | -2.16150 |
| C | 0.63550 | -1.35620 | -0.23540 |
| C | 4.73450 | 0.07310 | -0.52910 |
| Br | 2.53320 | 1.27880 | -1.96400 |
| C | 0.63190 | -2.44710 | -1.31200 |
| C | -0.12830 | -1.67220 | 1.06580 |
| C | 5.67730 | 1.15490 | -1.01950 |
| Cl | 0.95910 | -4.06900 | -0.63230 |
| C | -0.18100 | -0.47460 | 2.04270 |
| C | -1.06320 | -0.67010 | 3.26900 |
| O | 1.13400 | -0.19450 | 2.47010 |
| C | -1.80210 | -1.72640 | 3.52960 |
| C | 5.84220 | 2.34590 | -0.42030 |
| C | 6.77450 | 3.43600 | -0.91500 |
| C | 7.84420 | 3.75650 | 0.13190 |
| O | 6.06820 | 4.64060 | -1.17440 |
| C | -2.54850 | -2.77060 | 3.80230 |
| Br | -1.87590 | -4.32250 | 4.83080 |
| C | 5.19630 | 4.57780 | -2.29540 |
| H | 3.43500 | -2.31590 | -0.80230 |
| H | 4.17570 | -0.58400 | -2.51270 |
| H | 1.48880 | -1.20860 | -2.83070 |
| H | 2.21740 | -2.80960 | -2.77650 |
| H | 0.22170 | -0.44780 | -0.67740 |
| H | 4.24190 | 0.39750 | 0.38890 |
| H | 5.33340 | -0.79990 | -0.26790 |
| H | -0.30490 | -2.49510 | -1.86840 |
| H | -1.14410 | -1.96100 | 0.79260 |
| H | 0.31210 | -2.53530 | 1.56690 |
| H | 6.24060 | 0.92860 | -1.91330 |
| H | -0.55570 | 0.40170 | 1.51110 |
| H | -1.05310 | 0.15390 | 3.96750 |
| H | 1.71030 | -0.36310 | 1.72740 |
| H | 5.28020 | 2.57750 | 0.47320 |
| H | 7.27350 | 3.10480 | -1.82790 |
| H | 8.52230 | 4.52900 | -0.23100 |
| H | 7.39520 | 4.11750 | 1.05760 |
| H | 8.44060 | 2.87510 | 0.36850 |
| H | -3.57900 | -2.88800 | 3.50030 |
| H | 4.73340 | 5.55220 | -2.45090 |
| H | 5.73880 | 4.31680 | -3.20490 |
| H | 4.39540 | 3.85270 | -2.14670 |

| Marilzafurollene C_168 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.25220 | -0.94860 | -0.78480 |
| O | 2.47820 | -0.75030 | 0.39840 |
| C | 3.65580 | 0.40060 | -1.40840 |
| C | 2.41790 | -1.85940 | -1.69420 |
| C | 1.25730 | -1.47980 | 0.31110 |
| C | 4.59500 | 1.20280 | -0.49230 |
| Br | 2.02290 | 1.48870 | -1.78470 |
| C | 1.54260 | -2.59550 | -0.70160 |
| C | 0.77720 | -1.90940 | 1.71110 |
| C | 5.10650 | 2.46970 | -1.15040 |
| Cl | 2.46440 | -3.94810 | 0.02320 |
| C | -0.50680 | -2.76170 | 1.71110 |
| C | -0.85800 | -3.23850 | 3.11600 |
| O | -1.56640 | -2.03310 | 1.11250 |
| C | -1.98480 | -2.99770 | 3.75050 |
| C | 6.40050 | 2.73060 | -1.40020 |
| C | 6.90910 | 4.00010 | -2.05760 |
| C | 7.64470 | 3.68160 | -3.36170 |
| O | 7.82630 | 4.68310 | -1.21550 |
| C | -3.10950 | -2.73680 | 4.37370 |
| Br | -3.34490 | -1.13220 | 5.50870 |
| C | 7.22950 | 5.30170 | -0.08370 |
| H | 4.15060 | -1.49380 | -0.49080 |
| H | 4.15140 | 0.22070 | -2.36370 |
| H | 1.78770 | -1.27240 | -2.36250 |
| H | 3.02540 | -2.52320 | -2.30980 |
| H | 0.51960 | -0.80410 | -0.12580 |
| H | 4.07660 | 1.46940 | 0.42970 |
| H | 5.44420 | 0.58300 | -0.20150 |
| H | 0.63470 | -3.00100 | -1.15020 |
| H | 1.57720 | -2.46180 | 2.20520 |
| H | 0.62550 | -1.01600 | 2.31760 |
| H | 4.35560 | 3.19700 | -1.42580 |
| H | -0.34460 | -3.65860 | 1.11160 |
| H | -0.09280 | -3.82740 | 3.60190 |
| H | -1.76660 | -1.28410 | 1.65640 |
| H | 7.15680 | 2.00960 | -1.12490 |
| H | 6.06780 | 4.65650 | -2.28900 |
| H | 7.99700 | 4.59530 | -3.84060 |
| H | 8.51190 | 3.04590 | -3.18170 |
| H | 6.99100 | 3.16800 | -4.06720 |
| H | -3.99590 | -3.35280 | 4.33170 |
| H | 6.76450 | 4.57130 | 0.57940 |
| H | 7.99360 | 5.82820 | 0.48810 |
| H | 6.47550 | 6.03060 | -0.38340 |

| Marilzafurollene C_169 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.95870 | -1.89330 | -1.36570 |
| O | 2.31660 | -1.92040 | -0.09190 |
| C | 3.88350 | -0.66690 | -1.47990 |
| C | 1.83510 | -2.00120 | -2.40420 |
| C | 0.92440 | -2.18860 | -0.24880 |
| C | 3.18540 | 0.68960 | -1.26830 |
| Br | 4.77210 | -0.69350 | -3.26520 |
| C | 0.78420 | -2.79130 | -1.65290 |
| C | 0.38190 | -3.04230 | 0.91430 |
| C | 4.17130 | 1.84010 | -1.21580 |
| Cl | 1.19600 | -4.53260 | -1.69280 |
| C | 0.41590 | -2.32670 | 2.27730 |
| C | -0.51260 | -1.12740 | 2.33120 |
| O | 0.02660 | -3.24870 | 3.27440 |
| C | -0.09990 | 0.10210 | 2.54160 |
| C | 4.36470 | 2.63140 | -0.14770 |
| C | 5.35030 | 3.78400 | -0.10030 |
| C | 6.39880 | 3.56120 | 0.99260 |
| O | 4.69310 | 5.00860 | 0.19180 |
| C | 0.30580 | 1.32890 | 2.76940 |
| Br | 0.43840 | 2.08380 | 4.59440 |
| C | 3.89660 | 5.51130 | -0.87250 |
| H | 3.56890 | -2.79590 | -1.42810 |
| H | 4.67470 | -0.77460 | -0.73590 |
| H | 1.43570 | -1.02080 | -2.65980 |
| H | 2.15610 | -2.48000 | -3.32980 |
| H | 0.41620 | -1.22320 | -0.25950 |
| H | 2.47350 | 0.88920 | -2.06840 |
| H | 2.61500 | 0.66740 | -0.33870 |
| H | -0.21750 | -2.67350 | -2.06780 |
| H | -0.64050 | -3.34990 | 0.69090 |
| H | 0.96710 | -3.95970 | 0.98250 |
| H | 4.74530 | 2.01380 | -2.11550 |
| H | 1.43880 | -2.00800 | 2.49250 |
| H | -1.56310 | -1.33360 | 2.18720 |
| H | 0.75610 | -3.82460 | 3.45620 |
| H | 3.79510 | 2.46440 | 0.75530 |
| H | 5.86620 | 3.86610 | -1.05910 |
| H | 7.11460 | 4.38310 | 1.01590 |
| H | 5.93590 | 3.49670 | 1.97770 |
| H | 6.95650 | 2.64010 | 0.82150 |
| H | 0.60090 | 2.03370 | 2.00590 |
| H | 3.08070 | 4.83280 | -1.12380 |
| H | 3.45620 | 6.46390 | -0.57840 |
| H | 4.49600 | 5.68300 | -1.76750 |

| Marilzafurollene C_170 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.24650 | -1.50700 | -1.69610 |
| O | 2.30240 | -0.86950 | -0.83520 |
| C | 3.54170 | -0.62380 | -2.92580 |
| C | 2.64420 | -2.88040 | -2.01440 |
| C | 1.21620 | -1.74450 | -0.54800 |
| C | 4.45600 | 0.58410 | -2.63390 |
| Br | 1.82740 | 0.02240 | -3.71820 |
| C | 1.77640 | -3.14670 | -0.79970 |
| C | 0.66520 | -1.44800 | 0.85850 |
| C | 3.98050 | 1.44980 | -1.48120 |
| Cl | 2.79210 | -3.71780 | 0.55740 |
| C | -0.09010 | -0.09920 | 0.93530 |
| C | -0.65690 | 0.24810 | 2.30490 |
| O | 0.77990 | 0.93620 | 0.53320 |
| C | -0.50810 | -0.46300 | 3.40090 |
| C | 4.72680 | 1.75140 | -0.40530 |
| C | 4.25540 | 2.58340 | 0.77200 |
| C | 4.99270 | 3.92390 | 0.81870 |
| O | 4.52780 | 1.91990 | 1.99810 |
| C | -0.32560 | -1.16190 | 4.49610 |
| Br | 1.22330 | -0.86660 | 5.69260 |
| C | 3.64490 | 0.84370 | 2.28500 |
| H | 4.16490 | -1.66020 | -1.12670 |
| H | 4.02620 | -1.23120 | -3.69180 |
| H | 2.01640 | -2.82520 | -2.90470 |
| H | 3.39780 | -3.64990 | -2.18380 |
| H | 0.43680 | -1.55590 | -1.28880 |
| H | 5.46240 | 0.22690 | -2.41190 |
| H | 4.54050 | 1.20530 | -3.52600 |
| H | 1.00030 | -3.89110 | -0.98080 |
| H | -0.01420 | -2.25280 | 1.14240 |
| H | 1.48150 | -1.46370 | 1.58210 |
| H | 2.96990 | 1.82720 | -1.55320 |
| H | -0.92470 | -0.12430 | 0.23270 |
| H | -1.21920 | 1.16980 | 2.34180 |
| H | 1.42440 | 0.54890 | -0.05740 |
| H | 5.73920 | 1.38130 | -0.33560 |
| H | 3.18450 | 2.77890 | 0.68300 |
| H | 6.06770 | 3.78030 | 0.92900 |
| H | 4.82080 | 4.49900 | -0.09140 |
| H | 4.64940 | 4.52450 | 1.66110 |
| H | -0.97990 | -1.94700 | 4.84590 |
| H | 3.95560 | 0.35130 | 3.20620 |
| H | 2.62730 | 1.20500 | 2.43380 |
| H | 3.63940 | 0.09440 | 1.49240 |

| Marilzafurollene C_171 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.43060 | -1.38480 | -1.91770 |
| O | 2.53460 | -1.11580 | -0.83790 |
| C | 3.25770 | -0.34380 | -3.04390 |
| C | 3.14780 | -2.83390 | -2.33430 |
| C | 1.72920 | -2.25840 | -0.56480 |
| C | 3.87200 | 1.03710 | -2.73620 |
| Br | 1.32010 | -0.12240 | -3.46960 |
| C | 2.56490 | -3.43600 | -1.07070 |
| C | 1.31340 | -2.28060 | 0.91780 |
| C | 3.41130 | 1.63590 | -1.41990 |
| Cl | 3.88220 | -3.85760 | 0.06360 |
| C | 0.31470 | -1.16440 | 1.27730 |
| C | -0.15080 | -1.28210 | 2.72450 |
| O | 0.92510 | 0.08650 | 1.01430 |
| C | -0.03860 | -0.34770 | 3.64370 |
| C | 4.24170 | 2.06020 | -0.45270 |
| C | 3.80030 | 2.62710 | 0.88290 |
| C | 4.14420 | 4.11520 | 0.98190 |
| O | 4.47260 | 1.97540 | 1.95100 |
| C | 0.08430 | 0.59590 | 4.54700 |
| Br | -1.32260 | 1.95060 | 4.87430 |
| C | 3.98860 | 0.66880 | 2.22900 |
| H | 4.44740 | -1.33340 | -1.52490 |
| H | 3.73080 | -0.72210 | -3.95150 |
| H | 2.40000 | -2.86420 | -3.12790 |
| H | 4.03470 | -3.35740 | -2.69230 |
| H | 0.83450 | -2.18820 | -1.18650 |
| H | 4.95920 | 0.95160 | -2.72120 |
| H | 3.62990 | 1.73330 | -3.53970 |
| H | 1.97330 | -4.33340 | -1.25540 |
| H | 0.85830 | -3.24750 | 1.13650 |
| H | 2.19400 | -2.20700 | 1.55750 |
| H | 2.34210 | 1.70710 | -1.27570 |
| H | -0.56580 | -1.25020 | 0.63850 |
| H | -0.60950 | -2.22510 | 2.98370 |
| H | 1.52000 | -0.04180 | 0.27750 |
| H | 5.31010 | 1.99760 | -0.59950 |
| H | 2.72010 | 2.51190 | 0.99620 |
| H | 5.21850 | 4.27960 | 0.89590 |
| H | 3.65150 | 4.68560 | 0.19410 |
| H | 3.82080 | 4.52360 | 1.93940 |
| H | 0.94280 | 0.72420 | 5.18940 |
| H | 4.02710 | 0.01900 | 1.35360 |
| H | 4.59780 | 0.21270 | 3.00890 |
| H | 2.96210 | 0.70640 | 2.59340 |

| Marilzafurollene C_172 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.33350 | -1.27500 | -0.70670 |
| O | 2.34720 | -1.32250 | 0.32500 |
| C | 3.77560 | 0.17690 | -0.96990 |
| C | 2.72300 | -1.99600 | -1.91580 |
| C | 1.19070 | -2.01730 | -0.13800 |
| C | 4.49570 | 0.78720 | 0.25080 |
| Br | 2.17240 | 1.28600 | -1.41240 |
| C | 1.70380 | -2.91290 | -1.27130 |
| C | 0.46310 | -2.72710 | 1.02060 |
| C | 5.16070 | 2.14070 | 0.03500 |
| Cl | 2.52320 | -4.37920 | -0.65530 |
| C | -0.12210 | -1.74920 | 2.05470 |
| C | -0.98230 | -2.46730 | 3.07610 |
| O | 0.94780 | -1.11130 | 2.71710 |
| C | -2.26940 | -2.24900 | 3.22370 |
| C | 5.24460 | 2.83060 | -1.11740 |
| C | 5.92780 | 4.17740 | -1.26190 |
| C | 4.93960 | 5.23910 | -1.75090 |
| O | 6.98300 | 4.11800 | -2.21070 |
| C | -3.55810 | -2.04550 | 3.36400 |
| Br | -4.29490 | -0.67990 | 4.59350 |
| C | 8.12300 | 3.39220 | -1.77130 |
| H | 4.18850 | -1.85810 | -0.36030 |
| H | 4.43800 | 0.18780 | -1.83640 |
| H | 2.21030 | -1.29270 | -2.57220 |
| H | 3.46280 | -2.52730 | -2.51520 |
| H | 0.52170 | -1.27330 | -0.57500 |
| H | 3.79070 | 0.87830 | 1.07810 |
| H | 5.27470 | 0.10360 | 0.58980 |
| H | 0.91620 | -3.22720 | -1.95700 |
| H | -0.34760 | -3.32410 | 0.60050 |
| H | 1.13040 | -3.43100 | 1.51950 |
| H | 5.60840 | 2.56770 | 0.92120 |
| H | -0.71460 | -0.98790 | 1.54200 |
| H | -0.47520 | -3.18760 | 3.70140 |
| H | 1.61530 | -0.93250 | 2.05870 |
| H | 4.81060 | 2.44150 | -2.02590 |
| H | 6.32380 | 4.49550 | -0.29540 |
| H | 5.42610 | 6.21050 | -1.84040 |
| H | 4.53260 | 4.97980 | -2.72860 |
| H | 4.10450 | 5.34770 | -1.05820 |
| H | -4.32910 | -2.58790 | 2.83660 |
| H | 8.89350 | 3.42430 | -2.54160 |
| H | 8.54160 | 3.82630 | -0.86240 |
| H | 7.88810 | 2.34430 | -1.58160 |

| Marilzafurollene C_173 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.55260 | -0.94820 | -1.67510 |
| O | 2.51940 | -0.09370 | -0.53050 |
| C | 2.41810 | -0.15020 | -2.98930 |
| C | 1.44250 | -1.98000 | -1.44960 |
| C | 1.51830 | -0.52090 | 0.38830 |
| C | 3.67540 | 0.64930 | -3.38610 |
| Br | 0.84970 | 1.08140 | -2.88790 |
| C | 1.32090 | -2.00720 | 0.05900 |
| C | 1.92180 | -0.13740 | 1.82860 |
| C | 4.10840 | 1.66360 | -2.34510 |
| Cl | 2.61730 | -3.03440 | 0.74270 |
| C | 0.80720 | -0.27550 | 2.88540 |
| C | 0.48780 | -1.71910 | 3.22170 |
| O | 1.24260 | 0.37730 | 4.05990 |
| C | -0.70980 | -2.24410 | 3.09810 |
| C | 5.33930 | 1.72930 | -1.81110 |
| C | 5.76020 | 2.73030 | -0.75200 |
| C | 6.87980 | 3.63590 | -1.27080 |
| O | 6.25390 | 2.07770 | 0.40930 |
| C | -1.89750 | -2.77400 | 2.92750 |
| Br | -2.44110 | -3.59840 | 1.21260 |
| C | 5.26390 | 1.36910 | 1.14370 |
| H | 3.51110 | -1.46960 | -1.66420 |
| H | 2.20550 | -0.85000 | -3.79880 |
| H | 0.50230 | -1.63410 | -1.88060 |
| H | 1.66840 | -2.95490 | -1.88230 |
| H | 0.60600 | 0.01660 | 0.12300 |
| H | 4.49930 | -0.03870 | -3.57980 |
| H | 3.48900 | 1.17840 | -4.32100 |
| H | 0.36080 | -2.40160 | 0.39040 |
| H | 2.81680 | -0.67630 | 2.13940 |
| H | 2.21740 | 0.91170 | 1.79850 |
| H | 3.35150 | 2.36500 | -2.02360 |
| H | -0.08950 | 0.23810 | 2.53090 |
| H | 1.31520 | -2.31980 | 3.57320 |
| H | 0.51240 | 0.45250 | 4.65810 |
| H | 6.10070 | 1.03160 | -2.12760 |
| H | 4.90750 | 3.35600 | -0.48080 |
| H | 7.16990 | 4.36480 | -0.51400 |
| H | 7.76640 | 3.05770 | -1.53190 |
| H | 6.56250 | 4.18540 | -2.15740 |
| H | -2.67450 | -2.81260 | 3.67720 |
| H | 4.44380 | 2.02450 | 1.43910 |
| H | 4.85580 | 0.53510 | 0.57220 |
| H | 5.70620 | 0.95900 | 2.05130 |

| Marilzafurollene C_174 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.66560 | -0.81150 | -1.07860 |
| O | 2.18560 | -1.26010 | 0.18860 |
| C | 2.06300 | 0.56480 | -1.43770 |
| C | 2.36020 | -1.93610 | -2.08130 |
| C | 1.45980 | -2.47120 | 0.02470 |
| C | 2.35960 | 1.66240 | -0.40040 |
| Br | 0.07930 | 0.42220 | -1.60930 |
| C | 2.12770 | -3.13600 | -1.18490 |
| C | 1.41400 | -3.30160 | 1.32280 |
| C | 3.83740 | 1.97380 | -0.26150 |
| Cl | 3.70510 | -3.87310 | -0.77220 |
| C | 0.83900 | -2.54870 | 2.53710 |
| C | -0.55110 | -1.98910 | 2.29600 |
| O | 0.79360 | -3.45040 | 3.62460 |
| C | -0.87340 | -0.73970 | 2.54520 |
| C | 4.40700 | 3.13650 | -0.61930 |
| C | 5.88530 | 3.44830 | -0.47990 |
| C | 6.10350 | 4.66490 | 0.42310 |
| O | 6.46690 | 3.75160 | -1.73960 |
| C | -1.18450 | 0.49950 | 2.84530 |
| Br | -0.98270 | 2.00180 | 1.57330 |
| C | 6.61220 | 2.63050 | -2.60060 |
| H | 3.74900 | -0.72600 | -0.98970 |
| H | 2.43730 | 0.88230 | -2.41200 |
| H | 1.45160 | -1.73010 | -2.64600 |
| H | 3.16210 | -2.09040 | -2.80380 |
| H | 0.44100 | -2.20410 | -0.26010 |
| H | 1.82750 | 2.57280 | -0.67900 |
| H | 1.97090 | 1.36880 | 0.57560 |
| H | 1.50510 | -3.90250 | -1.64750 |
| H | 0.83180 | -4.20570 | 1.14090 |
| H | 2.41740 | -3.63680 | 1.58390 |
| H | 4.45060 | 1.18990 | 0.16000 |
| H | 1.52130 | -1.73550 | 2.79670 |
| H | -1.28270 | -2.67570 | 1.89560 |
| H | 0.67000 | -2.95550 | 4.42200 |
| H | 3.79870 | 3.92410 | -1.04070 |
| H | 6.40080 | 2.59420 | -0.03630 |
| H | 7.16650 | 4.87890 | 0.53470 |
| H | 5.62770 | 5.55460 | 0.00990 |
| H | 5.69260 | 4.49510 | 1.41860 |
| H | -1.57280 | 0.82000 | 3.80090 |
| H | 7.09210 | 2.94380 | -3.52770 |
| H | 7.23660 | 1.86090 | -2.14510 |
| H | 5.64850 | 2.19030 | -2.85880 |

| Marilzafurollene C_175 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.90820 | -1.27690 | -1.02520 |
| O | 2.11980 | -1.26720 | 0.16570 |
| C | 3.28120 | 0.15830 | -1.44060 |
| C | 2.10000 | -2.06210 | -2.06650 |
| C | 0.90610 | -1.98550 | -0.04800 |
| C | 4.20820 | 0.83590 | -0.41730 |
| Br | 1.62180 | 1.25190 | -1.64630 |
| C | 1.21960 | -2.94240 | -1.20350 |
| C | 0.40000 | -2.62970 | 1.25710 |
| C | 4.68770 | 2.19790 | -0.88070 |
| Cl | 2.14930 | -4.37230 | -0.66340 |
| C | -0.00350 | -1.59540 | 2.32250 |
| C | -0.66750 | -2.25450 | 3.51520 |
| O | 1.15870 | -0.92230 | 2.75440 |
| C | -1.89660 | -1.99100 | 3.89620 |
| C | 5.97280 | 2.51730 | -1.10750 |
| C | 6.45190 | 3.87800 | -1.56760 |
| C | 7.15650 | 3.77360 | -2.92690 |
| O | 7.35190 | 4.39900 | -0.60090 |
| C | -3.12960 | -1.72690 | 4.25840 |
| Br | -4.68150 | -2.73340 | 3.55300 |
| C | 7.42380 | 5.81740 | -0.57350 |
| H | 3.81710 | -1.83920 | -0.80480 |
| H | 3.77600 | 0.13470 | -2.41290 |
| H | 1.47280 | -1.39460 | -2.65780 |
| H | 2.72690 | -2.62520 | -2.75850 |
| H | 0.16410 | -1.26610 | -0.40000 |
| H | 3.69160 | 0.95130 | 0.53640 |
| H | 5.07320 | 0.19970 | -0.22570 |
| H | 0.32630 | -3.29400 | -1.72090 |
| H | -0.46700 | -3.24790 | 1.01960 |
| H | 1.15050 | -3.30580 | 1.66860 |
| H | 3.92050 | 2.94500 | -1.02880 |
| H | -0.68210 | -0.86310 | 1.87920 |
| H | -0.06860 | -2.97170 | 4.05720 |
| H | 1.70400 | -0.78640 | 1.98270 |
| H | 6.74430 | 1.77590 | -0.95740 |
| H | 5.57890 | 4.52790 | -1.65800 |
| H | 7.46020 | 4.75120 | -3.29940 |
| H | 8.04930 | 3.15140 | -2.86020 |
| H | 6.49700 | 3.33210 | -3.67460 |
| H | -3.41520 | -0.95530 | 4.95840 |
| H | 7.76300 | 6.22500 | -1.52590 |
| H | 6.45570 | 6.25700 | -0.32990 |
| H | 8.13290 | 6.13050 | 0.19290 |

| Marilzafurollene C_176 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.43200 | -0.86950 | -1.09130 |
| O | 2.71640 | -1.03760 | 0.29730 |
| C | 3.05580 | 0.43360 | -1.62550 |
| C | 0.90790 | -0.96120 | -1.22690 |
| C | 1.50970 | -1.22120 | 1.03220 |
| C | 4.59270 | 0.40340 | -1.57010 |
| Br | 2.39750 | 1.98870 | -0.55780 |
| C | 0.52020 | -1.77000 | -0.00700 |
| C | 1.78570 | -2.06590 | 2.29540 |
| C | 5.22260 | 1.63170 | -2.19810 |
| Cl | 0.77990 | -3.50960 | -0.33860 |
| C | 0.63400 | -2.10780 | 3.32100 |
| C | -0.55060 | -2.93750 | 2.86190 |
| O | 1.12520 | -2.64160 | 4.53360 |
| C | -1.77100 | -2.46100 | 2.76790 |
| C | 6.03870 | 2.48040 | -1.55140 |
| C | 6.65990 | 3.71770 | -2.17200 |
| C | 8.18790 | 3.62940 | -2.15410 |
| O | 6.29980 | 4.89040 | -1.45600 |
| C | -2.97700 | -1.96260 | 2.63640 |
| Br | -3.58480 | -1.11830 | 0.95270 |
| C | 4.93020 | 5.25190 | -1.57650 |
| H | 2.87220 | -1.72100 | -1.61270 |
| H | 2.73100 | 0.59000 | -2.65500 |
| H | 0.44960 | 0.02590 | -1.16380 |
| H | 0.58760 | -1.41500 | -2.16510 |
| H | 1.17630 | -0.22750 | 1.33720 |
| H | 4.92280 | 0.30270 | -0.53500 |
| H | 4.96550 | -0.47310 | -2.10110 |
| H | -0.52400 | -1.62610 | 0.26950 |
| H | 2.10300 | -3.07260 | 2.02390 |
| H | 2.65020 | -1.61510 | 2.78520 |
| H | 4.98090 | 1.81510 | -3.23510 |
| H | 0.30730 | -1.08680 | 3.53170 |
| H | -0.34850 | -3.96640 | 2.60070 |
| H | 1.53040 | -3.47980 | 4.36410 |
| H | 6.28220 | 2.30160 | -0.51380 |
| H | 6.33180 | 3.81140 | -3.20910 |
| H | 8.56760 | 3.56000 | -1.13440 |
| H | 8.53860 | 2.75580 | -2.70410 |
| H | 8.63240 | 4.51210 | -2.61410 |
| H | -3.73510 | -1.96060 | 3.40620 |
| H | 4.27130 | 4.49430 | -1.15080 |
| H | 4.75150 | 6.18310 | -1.03920 |
| H | 4.65260 | 5.40940 | -2.61940 |

| Marilzafurollene C_177 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.20310 | -1.76510 | -1.17110 |
| O | 2.17030 | -1.52490 | -0.21460 |
| C | 3.93900 | -0.45670 | -1.51440 |
| C | 2.52990 | -2.46100 | -2.36130 |
| C | 0.92520 | -2.01670 | -0.70670 |
| C | 4.69710 | 0.11570 | -0.30430 |
| Br | 2.62740 | 0.90360 | -2.16270 |
| C | 1.31090 | -3.09610 | -1.72440 |
| C | 0.00220 | -2.46030 | 0.44560 |
| C | 5.51400 | 1.34370 | -0.65660 |
| Cl | 1.77980 | -4.63170 | -0.93520 |
| C | -0.43690 | -1.29750 | 1.35400 |
| C | -1.52580 | -1.73290 | 2.32910 |
| O | 0.71040 | -0.80240 | 2.02170 |
| C | -1.46920 | -1.62990 | 3.63940 |
| C | 5.35630 | 2.54930 | -0.08510 |
| C | 6.16250 | 3.78340 | -0.44390 |
| C | 6.94640 | 4.29500 | 0.76720 |
| O | 5.32040 | 4.84270 | -0.87530 |
| C | -1.39550 | -1.52310 | 4.94490 |
| Br | -2.05350 | 0.06710 | 5.92540 |
| C | 4.69650 | 4.61900 | -2.13300 |
| H | 3.90410 | -2.46750 | -0.71720 |
| H | 4.64020 | -0.64220 | -2.32940 |
| H | 2.20850 | -1.73410 | -3.10760 |
| H | 3.18010 | -3.18040 | -2.85990 |
| H | 0.44780 | -1.19860 | -1.24940 |
| H | 3.99340 | 0.35400 | 0.49470 |
| H | 5.37810 | -0.63600 | 0.09610 |
| H | 0.51670 | -3.31130 | -2.44020 |
| H | -0.88290 | -2.92700 | 0.01130 |
| H | 0.48440 | -3.23010 | 1.04950 |
| H | 6.26480 | 1.21450 | -1.42280 |
| H | -0.84810 | -0.49440 | 0.74000 |
| H | -2.40820 | -2.15620 | 1.87170 |
| H | 1.43270 | -0.83770 | 1.39870 |
| H | 4.60590 | 2.68400 | 0.68090 |
| H | 6.87260 | 3.53950 | -1.23650 |
| H | 7.53700 | 5.17260 | 0.50400 |
| H | 6.27720 | 4.57720 | 1.58030 |
| H | 7.63100 | 3.53430 | 1.14340 |
| H | -0.98180 | -2.27470 | 5.60070 |
| H | 4.11030 | 5.49540 | -2.40880 |
| H | 5.43560 | 4.45120 | -2.91730 |
| H | 4.01880 | 3.76520 | -2.10380 |

| Marilzafurollene C_178 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.88880 | -1.58040 | -1.11370 |
| O | 2.22380 | -1.85600 | 0.11850 |
| C | 3.00140 | -0.06030 | -1.33820 |
| C | 2.11390 | -2.34180 | -2.19850 |
| C | 1.07680 | -2.66420 | -0.12160 |
| C | 3.90080 | 0.61270 | -0.28770 |
| Br | 1.18570 | 0.77270 | -1.27410 |
| C | 1.41490 | -3.42820 | -1.40560 |
| C | 0.70880 | -3.51240 | 1.11200 |
| C | 4.12660 | 2.08500 | -0.57240 |
| Cl | 2.55060 | -4.77920 | -1.11270 |
| C | 0.36740 | -2.66840 | 2.35380 |
| C | -0.82900 | -1.76140 | 2.13310 |
| O | 0.09120 | -3.54520 | 3.42680 |
| C | -0.74780 | -0.45020 | 2.14620 |
| C | 5.32450 | 2.63680 | -0.82870 |
| C | 5.55100 | 4.10730 | -1.11040 |
| C | 6.14650 | 4.30550 | -2.51080 |
| O | 6.43930 | 4.63040 | -0.13410 |
| C | -0.63760 | 0.85700 | 2.14290 |
| Br | -0.85250 | 1.94560 | 3.78200 |
| C | 6.29740 | 6.02450 | 0.09860 |
| H | 3.88850 | -2.01190 | -1.04160 |
| H | 3.40870 | 0.12700 | -2.33310 |
| H | 1.36720 | -1.70000 | -2.66650 |
| H | 2.75620 | -2.73100 | -2.98900 |
| H | 0.24980 | -1.99120 | -0.35320 |
| H | 3.45700 | 0.51020 | 0.70350 |
| H | 4.86520 | 0.10460 | -0.24840 |
| H | 0.53380 | -3.82770 | -1.90870 |
| H | -0.13190 | -4.16170 | 0.86550 |
| H | 1.54010 | -4.17190 | 1.36170 |
| H | 3.24550 | 2.71090 | -0.55980 |
| H | 1.24230 | -2.07030 | 2.62030 |
| H | -1.77550 | -2.25100 | 1.95530 |
| H | 0.10060 | -3.04640 | 4.23190 |
| H | 6.20940 | 2.01690 | -0.83870 |
| H | 4.58490 | 4.61290 | -1.04970 |
| H | 6.26580 | 5.36110 | -2.75220 |
| H | 7.12590 | 3.83340 | -2.59190 |
| H | 5.50140 | 3.86920 | -3.27380 |
| H | -0.42340 | 1.45470 | 1.26850 |
| H | 5.29760 | 6.26400 | 0.46310 |
| H | 7.01230 | 6.34060 | 0.85820 |
| H | 6.49020 | 6.60780 | -0.80190 |

| Marilzafurollene C_179 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.68020 | -0.59020 | -1.24370 |
| O | 1.91610 | -0.65820 | -0.03900 |
| C | 2.52960 | 0.79430 | -1.90710 |
| C | 2.22260 | -1.77340 | -2.10660 |
| C | 1.05010 | -1.79130 | -0.07470 |
| C | 3.09290 | 1.95340 | -1.06560 |
| Br | 0.59630 | 1.16680 | -2.23270 |
| C | 1.70670 | -2.75210 | -1.07220 |
| C | 0.79240 | -2.34410 | 1.34040 |
| C | 4.59810 | 1.88780 | -0.88520 |
| Cl | 3.08200 | -3.63990 | -0.35020 |
| C | 0.02090 | -1.36240 | 2.23970 |
| C | -0.37680 | -2.00560 | 3.55340 |
| O | 0.84930 | -0.25100 | 2.50160 |
| C | -1.62350 | -2.14590 | 3.94230 |
| C | 5.46390 | 2.77650 | -1.40620 |
| C | 6.98240 | 2.76100 | -1.26250 |
| C | 7.53380 | 1.50720 | -0.56870 |
| O | 7.44280 | 3.87290 | -0.50670 |
| C | -2.87380 | -2.29050 | 4.31270 |
| Br | -3.93750 | -3.89580 | 3.85360 |
| C | 7.37410 | 5.12290 | -1.17930 |
| H | 3.72230 | -0.76280 | -0.97310 |
| H | 3.01900 | 0.78990 | -2.88240 |
| H | 1.40540 | -1.48350 | -2.76730 |
| H | 3.01960 | -2.18290 | -2.72780 |
| H | 0.10310 | -1.45830 | -0.50390 |
| H | 2.83490 | 2.89940 | -1.54310 |
| H | 2.62080 | 1.96830 | -0.08240 |
| H | 1.00920 | -3.48290 | -1.48330 |
| H | 0.21510 | -3.26520 | 1.24770 |
| H | 1.73100 | -2.62180 | 1.82160 |
| H | 4.96000 | 1.06350 | -0.28880 |
| H | -0.87070 | -1.01240 | 1.71440 |
| H | 0.43340 | -2.35360 | 4.17740 |
| H | 1.32050 | -0.05890 | 1.69400 |
| H | 5.06830 | 3.59040 | -1.99580 |
| H | 7.41120 | 2.79970 | -2.26550 |
| H | 8.62310 | 1.53510 | -0.53740 |
| H | 7.18110 | 1.43300 | 0.46030 |
| H | 7.24520 | 0.59860 | -1.09760 |
| H | -3.43390 | -1.56900 | 4.88940 |
| H | 6.34640 | 5.41210 | -1.39890 |
| H | 7.80440 | 5.89820 | -0.54540 |
| H | 7.94040 | 5.10360 | -2.11140 |

| Marilzafurollene C_180 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.71520 | -0.89290 | -0.95250 |
| O | 1.50130 | -0.90850 | -0.19860 |
| C | 2.62310 | 0.16150 | -2.07510 |
| C | 2.92900 | -2.33260 | -1.44400 |
| C | 1.16620 | -2.24200 | 0.17170 |
| C | 2.40330 | 1.59770 | -1.56760 |
| Br | 1.11150 | -0.29190 | -3.29560 |
| C | 1.63540 | -3.02270 | -1.05770 |
| C | 1.86900 | -2.59940 | 1.50380 |
| C | 3.55590 | 2.12100 | -0.73160 |
| Cl | 1.84350 | -4.77490 | -0.78330 |
| C | 1.41570 | -1.72870 | 2.68940 |
| C | -0.03240 | -1.97910 | 3.06620 |
| O | 2.23860 | -2.03030 | 3.79790 |
| C | -0.96350 | -1.05350 | 3.02230 |
| C | 4.37050 | 3.12310 | -1.10140 |
| C | 5.52330 | 3.64750 | -0.26580 |
| C | 5.33160 | 5.13130 | 0.05810 |
| O | 6.75660 | 3.52630 | -0.95930 |
| C | -1.90020 | -0.13770 | 2.95270 |
| Br | -2.97130 | 0.15840 | 1.31530 |
| C | 7.23130 | 2.19220 | -1.07870 |
| H | 3.53360 | -0.64190 | -0.27680 |
| H | 3.53130 | 0.13260 | -2.67910 |
| H | 3.13370 | -2.40690 | -2.51230 |
| H | 3.77060 | -2.78090 | -0.91470 |
| H | 0.08580 | -2.33570 | 0.28680 |
| H | 2.25440 | 2.26000 | -2.42130 |
| H | 1.48840 | 1.65020 | -0.97580 |
| H | 0.90350 | -2.90140 | -1.85770 |
| H | 1.68770 | -3.64680 | 1.74680 |
| H | 2.94850 | -2.50580 | 1.38570 |
| H | 3.70830 | 1.63940 | 0.22380 |
| H | 1.56230 | -0.67600 | 2.43600 |
| H | -0.27610 | -2.98440 | 3.37850 |
| H | 2.08970 | -1.38160 | 4.47130 |
| H | 4.22350 | 3.60970 | -2.05520 |
| H | 5.57730 | 3.09470 | 0.67430 |
| H | 6.15290 | 5.50340 | 0.67070 |
| H | 5.29650 | 5.73320 | -0.85030 |
| H | 4.40510 | 5.29790 | 0.60820 |
| H | -2.17570 | 0.52840 | 3.75730 |
| H | 8.19200 | 2.19280 | -1.59360 |
| H | 7.37800 | 1.73600 | -0.09890 |
| H | 6.54690 | 1.56870 | -1.65510 |

| Marilzafurollene C_181 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.83860 | -1.68860 | -2.09200 |
| O | 2.59630 | -1.62580 | -0.68560 |
| C | 2.89710 | -0.28450 | -2.73070 |
| C | 1.73890 | -2.59140 | -2.66950 |
| C | 1.40760 | -2.33960 | -0.36550 |
| C | 4.15840 | 0.53150 | -2.38360 |
| Br | 1.26480 | 0.76820 | -2.26230 |
| C | 1.29960 | -3.39870 | -1.46600 |
| C | 1.41940 | -2.86300 | 1.08410 |
| C | 4.23470 | 0.96430 | -0.93100 |
| Cl | 2.43370 | -4.75940 | -1.21380 |
| C | 1.47720 | -1.75210 | 2.14820 |
| C | 0.30730 | -0.79080 | 2.05530 |
| O | 1.47250 | -2.36370 | 3.42200 |
| C | 0.45240 | 0.50990 | 1.94440 |
| C | 4.29910 | 2.24640 | -0.52770 |
| C | 4.37250 | 2.74700 | 0.90970 |
| C | 4.49140 | 1.63110 | 1.95670 |
| O | 3.21400 | 3.49340 | 1.25330 |
| C | 0.61060 | 1.80980 | 1.87000 |
| Br | 0.65110 | 2.95870 | 3.48240 |
| C | 3.13470 | 4.78460 | 0.66680 |
| H | 3.79820 | -2.18900 | -2.23050 |
| H | 2.87970 | -0.40790 | -3.81460 |
| H | 0.89890 | -1.99500 | -3.02720 |
| H | 2.08350 | -3.20830 | -3.49980 |
| H | 0.57170 | -1.65000 | -0.49290 |
| H | 5.05130 | -0.04920 | -2.61710 |
| H | 4.19450 | 1.41700 | -3.01910 |
| H | 0.29390 | -3.80790 | -1.56710 |
| H | 0.53290 | -3.47690 | 1.24700 |
| H | 2.27540 | -3.52260 | 1.22760 |
| H | 4.23230 | 0.16450 | -0.20580 |
| H | 2.41660 | -1.20600 | 2.03470 |
| H | -0.67850 | -1.23210 | 2.07490 |
| H | 1.67090 | -1.70400 | 4.07190 |
| H | 4.30130 | 3.01820 | -1.28270 |
| H | 5.25560 | 3.38230 | 0.99810 |
| H | 4.56590 | 2.05270 | 2.95920 |
| H | 3.61830 | 0.97920 | 1.94250 |
| H | 5.37870 | 1.01990 | 1.79010 |
| H | 0.73310 | 2.36790 | 0.95240 |
| H | 3.05050 | 4.73500 | -0.41870 |
| H | 2.24760 | 5.29510 | 1.04180 |
| H | 4.00270 | 5.39220 | 0.92560 |

| Marilzafurollene C_182 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.18460 | -1.56530 | -1.90680 |
| O | 2.55990 | -1.09320 | -0.71240 |
| C | 3.28790 | -0.45960 | -2.97710 |
| C | 2.37380 | -2.79080 | -2.34860 |
| C | 1.46430 | -1.93760 | -0.36340 |
| C | 4.31700 | 0.64470 | -2.66160 |
| Br | 1.49510 | 0.35380 | -3.31470 |
| C | 1.76670 | -3.27430 | -1.04890 |
| C | 1.25410 | -1.98600 | 1.16250 |
| C | 3.94280 | 1.53480 | -1.49040 |
| Cl | 2.97370 | -4.24190 | -0.15010 |
| C | 0.87730 | -0.62060 | 1.76090 |
| C | 0.48820 | -0.73780 | 3.22100 |
| O | 1.99530 | 0.23020 | 1.64860 |
| C | -0.69230 | -0.39630 | 3.68450 |
| C | 4.66440 | 1.65070 | -0.36050 |
| C | 4.34710 | 2.54400 | 0.83520 |
| C | 3.06750 | 3.37770 | 0.67420 |
| O | 5.39550 | 3.47520 | 1.07100 |
| C | -1.87940 | -0.06090 | 4.13100 |
| Br | -3.38470 | -1.34440 | 4.21110 |
| C | 6.55570 | 2.92260 | 1.67720 |
| H | 4.18690 | -1.90010 | -1.63490 |
| H | 3.59150 | -0.92710 | -3.91510 |
| H | 1.57500 | -2.50030 | -3.03180 |
| H | 2.97910 | -3.54670 | -2.84960 |
| H | 0.57390 | -1.51320 | -0.83140 |
| H | 5.29530 | 0.19610 | -2.48460 |
| H | 4.43070 | 1.28830 | -3.53440 |
| H | 0.87820 | -3.89010 | -1.19360 |
| H | 0.45620 | -2.69890 | 1.37560 |
| H | 2.14430 | -2.36900 | 1.66280 |
| H | 3.03230 | 2.10190 | -1.61380 |
| H | 0.05270 | -0.18700 | 1.19040 |
| H | 1.24650 | -1.12430 | 3.88610 |
| H | 2.38860 | 0.05850 | 0.79450 |
| H | 5.56200 | 1.05860 | -0.26740 |
| H | 4.22300 | 1.90420 | 1.71070 |
| H | 2.88670 | 3.97580 | 1.56720 |
| H | 3.14140 | 4.06230 | -0.17080 |
| H | 2.19270 | 2.74390 | 0.52750 |
| H | -2.14860 | 0.92160 | 4.49030 |
| H | 7.27830 | 3.71670 | 1.86470 |
| H | 6.31860 | 2.45670 | 2.63450 |
| H | 7.03880 | 2.18350 | 1.03830 |

Table S11. Calculated Energies (Hartrees) for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,14*R** of **3**.

| Entry ID | Gas Phase Energy |
|-----------------|-------------------------|
| 143 | -1335,69167 |
| 144 | -1335,686622 |
| 145 | -1335,688013 |
| 146 | -1335,690842 |
| 147 | -1335,691849 |
| 148 | -1335,691951 |
| 149 | -1335,689106 |
| 150 | -1335,686557 |
| 151 | -1335,688437 |
| 152 | -1335,690532 |
| 153 | -1335,689517 |
| 154 | -1335,689371 |
| 155 | -1335,68772 |
| 156 | -1335,686384 |
| 157 | -1335,679403 |
| 158 | -1335,688972 |
| 159 | -1335,690139 |
| 160 | -1335,690955 |
| 161 | -1335,68773 |
| 162 | -1335,688286 |
| 163 | -1335,687563 |
| 164 | -1335,68634 |
| 165 | -1335,685297 |
| 166 | -1335,686988 |
| 167 | -1335,690233 |
| 168 | -1335,690051 |
| 169 | -1335,688278 |
| 170 | -1335,689638 |
| 171 | -1335,689451 |
| 172 | -1335,689709 |
| 173 | -1335,689253 |
| 174 | -1335,683545 |
| 175 | -1335,686713 |
| 176 | -1335,684604 |
| 177 | -1335,684408 |
| 178 | -1335,68635 |
| 179 | -1335,682776 |
| 180 | -1335,681469 |
| 181 | -1335,687188 |
| 182 | -1335,687735 |
| 183 | -1335,686522 |
| 184 | -1335,686052 |
| 185 | -1335,689022 |

| | |
|-----|--------------|
| 186 | -1335,689024 |
| 187 | -1335,687393 |
| 188 | -1335,687453 |
| 189 | -1335,686534 |
| 190 | -1335,689686 |
| 191 | -1335,688534 |
| 192 | -1335,688622 |
| 193 | -1335,684539 |
| 194 | -1335,68199 |
| 195 | -1335,68405 |
| 196 | -1335,688334 |
| 197 | -1335,687957 |
| 198 | -1335,687629 |
| 199 | -1335,686071 |
| 200 | -1335,687074 |
| 201 | -1335,689343 |
| 202 | -1335,6847 |
| 203 | -1335,684909 |
| 204 | -1335,69019 |

Table S12. Coordinates (Angstroms) of calculated geometries for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,14*R** of **3**.

| Marilzafurollene C_143 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.44890 | -0.59010 | 1.12620 |
| O | 4.77200 | -1.10180 | 1.29210 |
| C | 2.41640 | -1.54130 | 1.75900 |
| C | 3.26930 | -0.34860 | -0.37830 |
| C | 5.42410 | -1.18490 | 0.02610 |
| C | 2.56760 | -1.62720 | 3.28710 |
| Br | 2.61810 | -3.36900 | 0.97760 |
| C | 4.69560 | -0.16270 | -0.85350 |
| C | 6.94780 | -1.00400 | 0.16830 |
| C | 1.47550 | -2.45740 | 3.93310 |
| Cl | 5.22360 | 1.51380 | -0.51990 |
| C | 7.61700 | -2.13620 | 0.96710 |
| C | 9.12840 | -2.02680 | 0.92900 |
| O | 7.18160 | -2.05520 | 2.30660 |
| C | 9.90890 | -2.95750 | 0.42900 |
| C | 0.58240 | -1.98570 | 4.81890 |
| C | -0.51060 | -2.81790 | 5.46310 |
| C | -0.36250 | -2.82760 | 6.98660 |
| O | -1.79640 | -2.29080 | 5.17050 |
| C | 10.67560 | -3.89050 | -0.08380 |
| Br | 11.19310 | -3.90700 | -1.99470 |
| C | -2.21350 | -2.48390 | 3.82570 |
| H | 3.41170 | 0.37570 | 1.63290 |
| H | 1.41070 | -1.19420 | 1.51620 |

| | | | |
|-------------------------------|----------|----------|----------|
| H | 2.83860 | -1.22380 | -0.86530 |
| H | 2.62610 | 0.50320 | -0.60100 |
| H | 5.22050 | -2.17920 | -0.37620 |
| H | 3.53560 | -2.05990 | 3.54290 |
| H | 2.55400 | -0.62410 | 3.71540 |
| H | 4.82020 | -0.35180 | -1.92040 |
| H | 7.38330 | -0.97280 | -0.83150 |
| H | 7.17970 | -0.04340 | 0.62980 |
| H | 1.43670 | -3.49820 | 3.64330 |
| H | 7.30550 | -3.10110 | 0.56040 |
| H | 9.55090 | -1.12370 | 1.34460 |
| H | 6.25670 | -1.82040 | 2.28400 |
| H | 0.61490 | -0.94640 | 5.11290 |
| H | -0.44780 | -3.84760 | 5.10520 |
| H | 0.60250 | -3.23740 | 7.28590 |
| H | -0.44330 | -1.82130 | 7.39850 |
| H | -1.13950 | -3.43770 | 7.44740 |
| H | 11.09070 | -4.72080 | 0.46860 |
| H | -2.24520 | -3.54380 | 3.57030 |
| H | -3.21690 | -2.07910 | 3.69440 |
| H | -1.55580 | -1.97480 | 3.12030 |
| Marilzafurollene C_144 | | | |
| C | 2.84550 | -1.20500 | 0.46430 |
| O | 4.10400 | -1.87570 | 0.46670 |
| C | 1.70900 | -2.16210 | 0.05370 |
| C | 3.04610 | 0.03750 | -0.41390 |
| C | 5.14110 | -0.91100 | 0.33860 |
| C | 1.60790 | -3.39930 | 0.96760 |
| Br | 2.00540 | -2.79480 | -1.81420 |
| C | 4.53400 | 0.00520 | -0.72960 |
| C | 5.42890 | -0.26470 | 1.71810 |
| C | 1.48280 | -3.04390 | 2.43880 |
| Cl | 5.26130 | 1.63460 | -0.79540 |
| C | 5.93110 | -1.28100 | 2.76180 |
| C | 7.37320 | -1.68370 | 2.52120 |
| O | 5.81830 | -0.71990 | 4.05300 |
| C | 7.74660 | -2.90560 | 2.21670 |
| C | 2.50270 | -3.14310 | 3.30790 |
| C | 2.45390 | -2.76830 | 4.77520 |
| C | 2.97660 | -3.91100 | 5.64870 |
| O | 3.27770 | -1.63490 | 5.02370 |
| C | 8.12490 | -4.11770 | 1.88730 |
| Br | 8.25410 | -4.71160 | 0.00380 |
| C | 2.63770 | -0.39630 | 4.74150 |
| H | 2.65350 | -0.85410 | 1.47680 |
| H | 0.76030 | -1.62390 | 0.05910 |
| H | 2.44810 | 0.02670 | -1.32520 |

| | | | |
|-------------------------------|----------|----------|----------|
| H | 2.77980 | 0.93460 | 0.14590 |
| H | 6.04730 | -1.38620 | -0.03900 |
| H | 0.75880 | -4.01840 | 0.67730 |
| H | 2.49770 | -4.01520 | 0.82750 |
| H | 4.67810 | -0.45680 | -1.70770 |
| H | 6.16930 | 0.52860 | 1.61050 |
| H | 4.53310 | 0.22970 | 2.09160 |
| H | 0.52210 | -2.67730 | 2.77150 |
| H | 5.29750 | -2.16860 | 2.74000 |
| H | 8.10640 | -0.89600 | 2.61470 |
| H | 5.02460 | -1.06280 | 4.45910 |
| H | 3.45460 | -3.50890 | 2.95120 |
| H | 1.42260 | -2.55940 | 5.06720 |
| H | 2.38360 | -4.81540 | 5.51030 |
| H | 4.01380 | -4.14940 | 5.41130 |
| H | 2.93160 | -3.64350 | 6.70460 |
| H | 8.39650 | -4.89240 | 2.58940 |
| H | 1.76430 | -0.25120 | 5.37850 |
| H | 3.32650 | 0.42680 | 4.93190 |
| H | 2.32180 | -0.33230 | 3.70100 |
| Marilzafurollene C_145 | | | |
| C | 2.80090 | 0.26420 | 0.61520 |
| O | 3.85070 | -0.55830 | 1.12760 |
| C | 1.41420 | -0.35570 | 0.88640 |
| C | 3.12120 | 0.46930 | -0.87150 |
| C | 4.78220 | -0.87140 | 0.09460 |
| C | 0.95700 | -0.30360 | 2.35910 |
| Br | 1.36710 | -2.24430 | 0.23990 |
| C | 4.62100 | 0.26240 | -0.92230 |
| C | 6.19530 | -1.08470 | 0.67080 |
| C | 1.83030 | -1.10490 | 3.30700 |
| Cl | 5.45030 | 1.75950 | -0.40140 |
| C | 6.29030 | -2.31490 | 1.59030 |
| C | 7.71840 | -2.57600 | 2.02570 |
| O | 5.49400 | -2.07880 | 2.73020 |
| C | 8.36970 | -3.68220 | 1.74730 |
| C | 1.41820 | -2.18050 | 3.99760 |
| C | 2.29800 | -2.99240 | 4.92920 |
| C | 1.76380 | -2.94480 | 6.36280 |
| O | 2.32660 | -4.35730 | 4.53880 |
| C | 9.01920 | -4.78270 | 1.45020 |
| Br | 10.08620 | -4.97050 | -0.20670 |
| C | 3.08830 | -4.60470 | 3.36450 |
| H | 2.87080 | 1.23100 | 1.11630 |
| H | 0.67540 | 0.18830 | 0.29580 |
| H | 2.63210 | -0.29240 | -1.47980 |
| H | 2.80740 | 1.44400 | -1.24640 |

| | | | |
|-------------------------------|----------|----------|----------|
| H | 4.44520 | -1.79730 | -0.37570 |
| H | 0.93900 | 0.73030 | 2.70520 |
| H | -0.06900 | -0.66710 | 2.42720 |
| H | 4.98500 | 0.00020 | -1.91640 |
| H | 6.89100 | -1.21050 | -0.16020 |
| H | 6.52600 | -0.19700 | 1.21140 |
| H | 2.85120 | -0.76920 | 3.41550 |
| H | 5.89490 | -3.18970 | 1.06890 |
| H | 8.19380 | -1.79000 | 2.59410 |
| H | 4.72060 | -1.60690 | 2.42850 |
| H | 0.39880 | -2.52370 | 3.89650 |
| H | 3.31240 | -2.58760 | 4.92490 |
| H | 1.72730 | -1.92080 | 6.73520 |
| H | 0.75850 | -3.36210 | 6.42410 |
| H | 2.40340 | -3.51940 | 7.03280 |
| H | 9.03710 | -5.67300 | 2.06170 |
| H | 3.04890 | -5.66640 | 3.12190 |
| H | 2.70660 | -4.05340 | 2.50440 |
| H | 4.13490 | -4.33710 | 3.51320 |
| Marilzafurollene C_146 | | | |
| C | 3.29370 | -0.23440 | 0.61960 |
| O | 4.54440 | -0.79580 | 1.01970 |
| C | 2.12380 | -1.00800 | 1.25550 |
| C | 3.30260 | -0.22030 | -0.91470 |
| C | 5.32170 | -1.12260 | -0.13070 |
| C | 2.10250 | -0.86900 | 2.78740 |
| Br | 2.26030 | -2.94380 | 0.78130 |
| C | 4.78320 | -0.20620 | -1.23490 |
| C | 6.83030 | -1.02370 | 0.16740 |
| C | 0.88780 | -1.52410 | 3.41610 |
| Cl | 5.41010 | 1.46330 | -1.09250 |
| C | 7.30860 | -2.05690 | 1.20260 |
| C | 8.81870 | -2.05540 | 1.33440 |
| O | 6.73550 | -1.73650 | 2.45120 |
| C | 9.56870 | -3.10250 | 1.07680 |
| C | 0.94380 | -2.51700 | 4.31930 |
| C | -0.26790 | -3.17830 | 4.94880 |
| C | -0.29980 | -4.67420 | 4.62640 |
| O | -0.24620 | -3.05460 | 6.36350 |
| C | 10.30650 | -4.15250 | 0.80450 |
| Br | 11.02950 | -4.50090 | -1.00520 |
| C | -0.49500 | -1.73870 | 6.83890 |
| H | 3.27870 | 0.79900 | 0.97000 |
| H | 1.18330 | -0.64040 | 0.84260 |
| H | 2.85620 | -1.13050 | -1.31580 |
| H | 2.76190 | 0.62670 | -1.33790 |
| H | 5.07990 | -2.15230 | -0.40120 |

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| H | 3.01470 | -1.29280 | 3.21020 |
| H | 2.09370 | 0.18570 | 3.06400 |
| H | 5.00850 | -0.56900 | -2.23840 |
| H | 7.37440 | -1.18090 | -0.76510 |
| H | 7.09070 | -0.01970 | 0.50460 |
| H | -0.07490 | -1.14950 | 3.09900 |
| H | 6.96390 | -3.05130 | 0.90940 |
| H | 9.26700 | -1.12830 | 1.66080 |
| H | 5.84110 | -1.44960 | 2.28050 |
| H | 1.90450 | -2.89480 | 4.63900 |
| H | -1.17950 | -2.72270 | 4.55700 |
| H | -0.33000 | -4.84360 | 3.54960 |
| H | 0.58020 | -5.18230 | 5.02140 |
| H | -1.18000 | -5.14670 | 5.06260 |
| H | 10.58660 | -4.91210 | 1.51970 |
| H | -0.49450 | -1.73980 | 7.92880 |
| H | 0.27130 | -1.03680 | 6.50840 |
| H | -1.46820 | -1.37570 | 6.50600 |
| Marilzafurollene C_147 | | | |
| C | 2.68350 | -1.46650 | 0.74910 |
| O | 4.00120 | -1.92310 | 1.05590 |
| C | 1.73410 | -2.65820 | 0.51240 |
| C | 2.83100 | -0.50960 | -0.44040 |
| C | 4.94860 | -1.29480 | 0.19450 |
| C | 1.52140 | -3.52460 | 1.76580 |
| Br | 2.47960 | -3.82890 | -0.92100 |
| C | 4.25400 | -0.01470 | -0.28390 |
| C | 6.30870 | -1.11620 | 0.89650 |
| C | 0.81040 | -2.78570 | 2.88370 |
| Cl | 4.30360 | 1.28320 | 0.94690 |
| C | 6.99020 | -2.45280 | 1.23810 |
| C | 8.39880 | -2.24290 | 1.75740 |
| O | 6.22510 | -3.10420 | 2.22830 |
| C | 9.46750 | -2.72700 | 1.16680 |
| C | 1.33600 | -2.56450 | 4.10010 |
| C | 0.63290 | -1.82080 | 5.22040 |
| C | 0.41020 | -2.73660 | 6.42650 |
| O | 1.40360 | -0.71680 | 5.67270 |
| C | 10.52700 | -3.20660 | 0.55980 |
| Br | 11.49730 | -2.19580 | -0.83870 |
| C | 1.49820 | 0.35500 | 4.74430 |
| H | 2.33880 | -0.88420 | 1.60400 |
| H | 0.76980 | -2.29560 | 0.15380 |
| H | 2.73670 | -1.04420 | -1.38580 |
| H | 2.09250 | 0.29240 | -0.43830 |
| H | 5.07800 | -1.94880 | -0.67000 |
| H | 0.92020 | -4.39700 | 1.50850 |

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| H | 2.48090 | -3.90460 | 2.12010 |
| H | 4.67550 | 0.37900 | -1.20950 |
| H | 6.96260 | -0.54520 | 0.23580 |
| H | 6.19780 | -0.51970 | 1.80290 |
| H | -0.18340 | -2.42400 | 2.66080 |
| H | 7.01440 | -3.08600 | 0.34830 |
| H | 8.49020 | -1.66130 | 2.66320 |
| H | 5.30710 | -2.94630 | 2.01830 |
| H | 2.32990 | -2.92430 | 4.32690 |
| H | -0.33930 | -1.46670 | 4.87200 |
| H | -0.19350 | -3.60360 | 6.15690 |
| H | 1.35710 | -3.09780 | 6.82840 |
| H | -0.10830 | -2.20620 | 7.22540 |
| H | 10.96530 | -4.17430 | 0.75590 |
| H | 2.05590 | 1.17660 | 5.19370 |
| H | 2.02430 | 0.05840 | 3.83670 |
| H | 0.51170 | 0.73110 | 4.47050 |
| Marilzafurollene C_148 | | | |
| C | 3.13600 | -1.07890 | 0.95810 |
| O | 4.43930 | -1.63050 | 1.14850 |
| C | 2.07500 | -2.19740 | 0.90420 |
| C | 3.22170 | -0.20520 | -0.30040 |
| C | 5.32300 | -1.15440 | 0.13500 |
| C | 1.94960 | -3.00080 | 2.21110 |
| Br | 2.53740 | -3.48250 | -0.55090 |
| C | 4.69200 | 0.15650 | -0.34740 |
| C | 6.77200 | -1.06800 | 0.65250 |
| C | 1.45440 | -2.17240 | 3.38190 |
| Cl | 5.01020 | 1.51300 | 0.77500 |
| C | 7.36810 | -2.44150 | 1.00730 |
| C | 8.84470 | -2.34020 | 1.33450 |
| O | 6.68000 | -2.95030 | 2.12900 |
| C | 9.78070 | -2.96410 | 0.65630 |
| C | 0.27080 | -2.34910 | 3.99230 |
| C | -0.22260 | -1.52480 | 5.16700 |
| C | -1.52320 | -0.79780 | 4.81560 |
| O | -0.49390 | -2.34610 | 6.29330 |
| C | 10.70610 | -3.58310 | -0.03760 |
| Br | 11.57650 | -2.76240 | -1.61500 |
| C | 0.66530 | -2.87220 | 6.92530 |
| H | 2.94000 | -0.41970 | 1.80420 |
| H | 1.10300 | -1.77050 | 0.65170 |
| H | 2.96250 | -0.77530 | -1.19250 |
| H | 2.56490 | 0.66430 | -0.26250 |
| H | 5.28190 | -1.86960 | -0.68880 |
| H | 1.26450 | -3.83470 | 2.05350 |
| H | 2.91210 | -3.44080 | 2.47480 |

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| H | 5.02930 | 0.45220 | -1.34150 |
| H | 7.38530 | -0.60700 | -0.12310 |
| H | 6.83240 | -0.40800 | 1.51870 |
| H | 2.11960 | -1.39660 | 3.73360 |
| H | 7.22080 | -3.12860 | 0.17090 |
| H | 9.10380 | -1.71500 | 2.17640 |
| H | 5.75980 | -2.72300 | 2.01610 |
| H | -0.39910 | -3.12510 | 3.65010 |
| H | 0.52790 | -0.77760 | 5.43290 |
| H | -1.38460 | -0.13160 | 3.96380 |
| H | -2.31570 | -1.50360 | 4.56570 |
| H | -1.86890 | -0.19510 | 5.65550 |
| H | 11.07680 | -4.57520 | 0.17510 |
| H | 0.37040 | -3.46000 | 7.79450 |
| H | 1.22870 | -3.52650 | 6.25900 |
| H | 1.32410 | -2.07420 | 7.27000 |
| Marilzafurollene C_149 | | | |
| C | 2.68710 | -0.14210 | 0.43220 |
| O | 3.74480 | -0.93230 | 0.97810 |
| C | 1.42480 | -0.99440 | 0.18420 |
| C | 3.26630 | 0.51330 | -0.82900 |
| C | 4.90510 | -0.83870 | 0.15630 |
| C | 0.66460 | -1.40250 | 1.46230 |
| Br | 1.89650 | -2.63120 | -0.85760 |
| C | 4.75700 | 0.50800 | -0.55650 |
| C | 6.18520 | -1.04680 | 0.98700 |
| C | 1.49690 | -2.20420 | 2.44600 |
| Cl | 5.17880 | 1.88340 | 0.50670 |
| C | 6.30190 | -2.47240 | 1.55500 |
| C | 7.63280 | -2.68970 | 2.24690 |
| O | 5.25960 | -2.67030 | 2.48460 |
| C | 8.50520 | -3.59590 | 1.86900 |
| C | 1.64800 | -1.89240 | 3.74400 |
| C | 2.48900 | -2.68480 | 4.72750 |
| C | 3.52350 | -1.78540 | 5.40890 |
| O | 1.68350 | -3.24400 | 5.75550 |
| C | 9.37160 | -4.49810 | 1.47330 |
| Br | 10.77400 | -4.10620 | 0.13190 |
| C | 0.86640 | -4.32560 | 5.32930 |
| H | 2.46000 | 0.64400 | 1.15410 |
| H | 0.73630 | -0.42200 | -0.43940 |
| H | 3.05920 | -0.09730 | -1.70870 |
| H | 2.86580 | 1.51000 | -1.01590 |
| H | 4.83690 | -1.62730 | -0.59560 |
| H | 0.28310 | -0.51030 | 1.96040 |
| H | -0.20670 | -1.99880 | 1.18990 |
| H | 5.35960 | 0.58090 | -1.46260 |

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| H | 7.04750 | -0.84900 | 0.34850 |
| H | 6.23590 | -0.32110 | 1.79980 |
| H | 1.99120 | -3.07990 | 2.04930 |
| H | 6.18230 | -3.19610 | 0.74550 |
| H | 7.84020 | -2.04940 | 3.09180 |
| H | 4.49990 | -2.19510 | 2.15220 |
| H | 1.15080 | -1.02240 | 4.14760 |
| H | 3.01790 | -3.48200 | 4.20100 |
| H | 4.18470 | -1.32160 | 4.67630 |
| H | 3.04380 | -0.99070 | 5.98030 |
| H | 4.14440 | -2.36170 | 6.09460 |
| H | 9.40700 | -5.51740 | 1.82910 |
| H | 0.14240 | -4.01430 | 4.57560 |
| H | 1.46840 | -5.13820 | 4.92050 |
| H | 0.31010 | -4.71830 | 6.18030 |
| Marilzafurollene C_150 | | | |
| C | 3.53720 | -0.15920 | 0.27650 |
| O | 4.82200 | -0.29410 | 0.88210 |
| C | 2.46140 | -0.82400 | 1.15560 |
| C | 3.68380 | -0.70000 | -1.15220 |
| C | 5.75670 | -0.80910 | -0.06290 |
| C | 2.70660 | -2.31450 | 1.45470 |
| Br | 0.68090 | -0.59590 | 0.28710 |
| C | 5.15540 | -0.47510 | -1.43260 |
| C | 7.17430 | -0.27140 | 0.21200 |
| C | 1.74070 | -2.86100 | 2.48720 |
| Cl | 5.42990 | 1.23170 | -1.89500 |
| C | 7.77770 | -0.79570 | 1.52800 |
| C | 8.09270 | -2.27900 | 1.46900 |
| O | 8.97220 | -0.08920 | 1.79210 |
| C | 7.48840 | -3.18200 | 2.20730 |
| C | 2.10690 | -3.36010 | 3.67940 |
| C | 1.14470 | -3.90950 | 4.71520 |
| C | 1.45560 | -5.37670 | 5.02100 |
| O | 1.24400 | -3.19570 | 5.93910 |
| C | 6.87010 | -4.09540 | 2.91730 |
| Br | 5.24570 | -5.01910 | 2.26520 |
| C | 0.71610 | -1.87720 | 5.88960 |
| H | 3.32920 | 0.91040 | 0.21800 |
| H | 2.42060 | -0.27980 | 2.10050 |
| H | 3.46720 | -1.76650 | -1.19570 |
| H | 3.02660 | -0.20060 | -1.86480 |
| H | 5.75120 | -1.89560 | 0.03880 |
| H | 2.61660 | -2.91520 | 0.55040 |
| H | 3.72540 | -2.44970 | 1.81950 |
| H | 5.54070 | -1.10810 | -2.23270 |
| H | 7.83170 | -0.52930 | -0.61940 |

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| H | 7.13640 | 0.81790 | 0.24320 |
| H | 0.69390 | -2.83680 | 2.21890 |
| H | 7.08190 | -0.59930 | 2.34730 |
| H | 8.86460 | -2.57200 | 0.77230 |
| H | 8.74930 | 0.78760 | 2.07230 |
| H | 3.15270 | -3.38580 | 3.95050 |
| H | 0.12230 | -3.84550 | 4.33740 |
| H | 1.38270 | -5.98980 | 4.12230 |
| H | 2.46200 | -5.49150 | 5.42440 |
| H | 0.75570 | -5.77710 | 5.75460 |
| H | 7.17600 | -4.42810 | 3.89840 |
| H | 0.80090 | -1.41440 | 6.87280 |
| H | 1.25780 | -1.25010 | 5.18070 |
| H | -0.33910 | -1.88420 | 5.61380 |
| Marilzafurollene C_151 | | | |
| C | 3.85810 | -0.96730 | 1.43160 |
| O | 4.54630 | -2.10320 | 0.90060 |
| C | 2.44620 | -1.38030 | 1.88750 |
| C | 3.88680 | 0.10260 | 0.32990 |
| C | 5.32800 | -1.72270 | -0.22990 |
| C | 2.47940 | -2.40080 | 3.03770 |
| Br | 1.44240 | -2.15740 | 0.34570 |
| C | 4.44480 | -0.64610 | -0.86450 |
| C | 6.72540 | -1.25350 | 0.24200 |
| C | 1.09770 | -2.70570 | 3.58300 |
| Cl | 5.29960 | 0.42430 | -2.00980 |
| C | 7.54420 | -2.36250 | 0.92700 |
| C | 8.97030 | -1.92080 | 1.18990 |
| O | 6.92850 | -2.68590 | 2.15450 |
| C | 10.02010 | -2.52200 | 0.67830 |
| C | 0.70320 | -2.45610 | 4.84270 |
| C | -0.68050 | -2.76070 | 5.38590 |
| C | -0.60150 | -3.73310 | 6.56550 |
| O | -1.31760 | -1.58200 | 5.85660 |
| C | 11.05940 | -3.12540 | 0.15190 |
| Br | 11.81890 | -2.59810 | -1.59860 |
| C | -1.73690 | -0.69550 | 4.82820 |
| H | 4.42030 | -0.59500 | 2.28980 |
| H | 1.89970 | -0.49320 | 2.21240 |
| H | 2.91200 | 0.54420 | 0.12110 |
| H | 4.56010 | 0.91020 | 0.61960 |
| H | 5.44060 | -2.57090 | -0.90620 |
| H | 2.93570 | -3.33170 | 2.69880 |
| H | 3.10740 | -2.02410 | 3.84620 |
| H | 3.63000 | -1.12540 | -1.40950 |
| H | 7.28630 | -0.91320 | -0.62950 |
| H | 6.64570 | -0.38750 | 0.89990 |

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| H | 0.40240 | -3.15580 | 2.88820 |
| H | 7.54480 | -3.25390 | 0.29550 |
| H | 9.09220 | -1.06470 | 1.83720 |
| H | 5.99200 | -2.74630 | 1.98540 |
| H | 1.39270 | -2.00610 | 5.54250 |
| H | -1.29000 | -3.21800 | 4.60380 |
| H | -0.13400 | -4.67290 | 6.27050 |
| H | -0.02170 | -3.31210 | 7.38730 |
| H | -1.59700 | -3.96260 | 6.94560 |
| H | 11.59150 | -3.94780 | 0.60730 |
| H | -0.89360 | -0.32200 | 4.24630 |
| H | -2.44040 | -1.18100 | 4.15060 |
| H | -2.23990 | 0.16390 | 5.27150 |
| Marilzafurollene C_152 | | | |
| C | 3.28820 | -0.16060 | 0.65590 |
| O | 4.51530 | -0.73500 | 1.10510 |
| C | 2.13290 | -0.54270 | 1.60060 |
| C | 3.14010 | -0.58280 | -0.81120 |
| C | 5.21120 | -1.32740 | 0.00680 |
| C | 1.89870 | -2.05720 | 1.75610 |
| Br | 0.45930 | 0.33020 | 0.95770 |
| C | 4.58300 | -0.71450 | -1.25190 |
| C | 6.73700 | -1.16740 | 0.15690 |
| C | 0.89300 | -2.37320 | 2.84570 |
| Cl | 5.24960 | 0.90360 | -1.62540 |
| C | 7.31130 | -1.92890 | 1.36430 |
| C | 8.82700 | -1.90140 | 1.36970 |
| O | 6.83430 | -1.32130 | 2.54490 |
| C | 9.57070 | -2.98240 | 1.30980 |
| C | 1.16610 | -3.08630 | 3.95100 |
| C | 0.15930 | -3.39930 | 5.04220 |
| C | -0.02360 | -4.91100 | 5.19830 |
| O | 0.59110 | -2.89790 | 6.29870 |
| C | 10.30110 | -4.06980 | 1.23720 |
| Br | 10.88170 | -4.84450 | -0.48960 |
| C | 0.53570 | -1.48240 | 6.41270 |
| H | 3.41980 | 0.92230 | 0.68830 |
| H | 2.34840 | -0.11740 | 2.58230 |
| H | 2.64710 | -1.55000 | -0.89790 |
| H | 2.57070 | 0.13370 | -1.40420 |
| H | 4.96420 | -2.39060 | 0.01510 |
| H | 1.53840 | -2.49210 | 0.82450 |
| H | 2.84180 | -2.55290 | 1.99010 |
| H | 4.70460 | -1.34050 | -2.13670 |
| H | 7.21060 | -1.54140 | -0.75210 |
| H | 7.00760 | -0.11300 | 0.22680 |
| H | -0.10530 | -1.98590 | 2.69680 |

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| H | 6.96080 | -2.96330 | 1.34190 |
| H | 9.28540 | -0.92490 | 1.42790 |
| H | 5.94120 | -1.03410 | 2.37190 |
| H | 2.16220 | -3.47550 | 4.10650 |
| H | -0.80740 | -2.96050 | 4.78700 |
| H | -0.37200 | -5.36370 | 4.26970 |
| H | 0.91190 | -5.39570 | 5.47890 |
| H | -0.75780 | -5.13440 | 5.97250 |
| H | 10.64990 | -4.63690 | 2.08790 |
| H | 0.85130 | -1.18550 | 7.41290 |
| H | 1.19710 | -0.99190 | 5.69770 |
| H | -0.47910 | -1.11310 | 6.25950 |
| Marilzafurollene C_153 | | | |
| C | 3.46490 | -0.33940 | 1.13500 |
| O | 4.73970 | -0.96040 | 1.30560 |
| C | 2.34830 | -1.22350 | 1.72050 |
| C | 3.33300 | -0.03790 | -0.36360 |
| C | 5.40500 | -1.05960 | 0.04770 |
| C | 2.46610 | -1.37140 | 3.24690 |
| Br | 2.41560 | -3.03500 | 0.88080 |
| C | 4.77810 | 0.04470 | -0.81060 |
| C | 6.93560 | -1.00880 | 0.21900 |
| C | 1.28260 | -2.09940 | 3.85440 |
| Cl | 5.43470 | 1.66150 | -0.41640 |
| C | 7.49530 | -2.21490 | 0.99340 |
| C | 9.01110 | -2.22880 | 0.98290 |
| O | 7.04320 | -2.13770 | 2.32760 |
| C | 9.72220 | -3.20450 | 0.46560 |
| C | 0.44920 | -1.57180 | 4.76840 |
| C | -0.74050 | -2.28320 | 5.39340 |
| C | -2.05630 | -1.69770 | 4.87460 |
| O | -0.75520 | -3.67610 | 5.10590 |
| C | 10.41970 | -4.18060 | -0.06550 |
| Br | 10.96920 | -4.17930 | -1.96750 |
| C | 0.10150 | -4.44850 | 5.93730 |
| H | 3.49560 | 0.61020 | 1.67170 |
| H | 1.37780 | -0.78880 | 1.47510 |
| H | 2.84110 | -0.85930 | -0.88510 |
| H | 2.76550 | 0.87020 | -0.56880 |
| H | 5.12800 | -2.02140 | -0.38810 |
| H | 3.37950 | -1.91130 | 3.49960 |
| H | 2.55160 | -0.38610 | 3.70680 |
| H | 4.90600 | -0.12200 | -1.88080 |
| H | 7.39010 | -0.98460 | -0.77250 |
| H | 7.23690 | -0.08440 | 0.71310 |
| H | 1.12030 | -3.11160 | 3.51060 |
| H | 7.11380 | -3.13870 | 0.55240 |

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| H | 9.49800 | -1.37660 | 1.43410 |
| H | 6.14050 | -1.82870 | 2.29700 |
| H | 0.60980 | -0.55810 | 5.10670 |
| H | -0.70140 | -2.13080 | 6.47370 |
| H | -2.12780 | -0.63120 | 5.08940 |
| H | -2.14670 | -1.83080 | 3.79620 |
| H | -2.90990 | -2.18850 | 5.34230 |
| H | 10.75570 | -5.05900 | 0.46590 |
| H | -0.20860 | -4.39010 | 6.98140 |
| H | 0.05670 | -5.49460 | 5.63470 |
| H | 1.14020 | -4.12460 | 5.86590 |
| Marilzafurollene C_154 | | | |
| C | 3.38080 | -0.15140 | 0.97880 |
| O | 4.64040 | -0.77340 | 1.23630 |
| C | 2.24280 | -0.92600 | 1.66890 |
| C | 3.25990 | -0.04640 | -0.54720 |
| C | 5.30480 | -1.05530 | 0.00610 |
| C | 2.35440 | -0.87500 | 3.20210 |
| Br | 2.27150 | -2.83430 | 1.07800 |
| C | 4.70750 | -0.05880 | -0.99350 |
| C | 6.83570 | -1.02090 | 0.17750 |
| C | 1.18170 | -1.54470 | 3.89080 |
| Cl | 5.40360 | 1.57920 | -0.81190 |
| C | 7.36260 | -2.12870 | 1.10650 |
| C | 8.87750 | -2.17990 | 1.10880 |
| O | 6.90690 | -1.86790 | 2.41600 |
| C | 9.56670 | -3.23140 | 0.72820 |
| C | 1.28820 | -2.57990 | 4.74180 |
| C | 0.12520 | -3.27510 | 5.43000 |
| C | 0.07390 | -2.90800 | 6.91500 |
| O | -1.13010 | -2.92400 | 4.85970 |
| C | 10.24250 | -4.28440 | 0.33380 |
| Br | 10.79930 | -4.54410 | -1.54810 |
| C | -1.43270 | -3.62200 | 3.65810 |
| H | 3.43180 | 0.85930 | 1.38730 |
| H | 1.28370 | -0.50740 | 1.36030 |
| H | 2.74880 | -0.91710 | -0.95860 |
| H | 2.71570 | 0.84040 | -0.87320 |
| H | 5.00400 | -2.05910 | -0.30020 |
| H | 3.28850 | -1.33910 | 3.52190 |
| H | 2.39170 | 0.16190 | 3.53740 |
| H | 4.83360 | -0.36800 | -2.03170 |
| H | 7.29300 | -1.13820 | -0.80610 |
| H | 7.15930 | -0.04740 | 0.54790 |
| H | 0.20330 | -1.14440 | 3.66600 |
| H | 6.96030 | -3.09270 | 0.78660 |
| H | 9.38330 | -1.28800 | 1.44870 |

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| H | 6.01360 | -1.54030 | 2.33850 |
| H | 2.26760 | -2.97430 | 4.97220 |
| H | 0.27570 | -4.35330 | 5.34900 |
| H | 0.99990 | -3.17960 | 7.42230 |
| H | -0.08170 | -1.83720 | 7.04950 |
| H | -0.74360 | -3.42780 | 7.41480 |
| H | 10.55490 | -5.09370 | 0.97740 |
| H | -0.67990 | -3.45410 | 2.88700 |
| H | -1.51070 | -4.69510 | 3.83700 |
| H | -2.39120 | -3.27910 | 3.26870 |
| Marilzafurollene C_155 | | | |
| C | 2.84070 | -0.68950 | 0.86550 |
| O | 3.57110 | -1.80410 | 0.34690 |
| C | 1.32760 | -0.93030 | 0.69180 |
| C | 3.37800 | 0.54900 | 0.13270 |
| C | 4.76080 | -1.35540 | -0.29760 |
| C | 0.80700 | -2.15010 | 1.47150 |
| Br | 0.91620 | -1.21140 | -1.23960 |
| C | 4.28890 | -0.04240 | -0.92530 |
| C | 5.89850 | -1.23210 | 0.74430 |
| C | 0.93010 | -1.98920 | 2.97480 |
| Cl | 5.60990 | 1.06410 | -1.39280 |
| C | 6.28190 | -2.57500 | 1.39090 |
| C | 7.52390 | -2.44530 | 2.25020 |
| O | 5.20980 | -3.01010 | 2.19700 |
| C | 8.63260 | -3.11240 | 2.02490 |
| C | 1.61790 | -2.82160 | 3.77420 |
| C | 1.74690 | -2.65860 | 5.27760 |
| C | 1.06480 | -3.81590 | 6.01120 |
| O | 3.10680 | -2.65350 | 5.68580 |
| C | 9.73650 | -3.77850 | 1.78200 |
| Br | 11.16560 | -3.07270 | 0.60790 |
| C | 3.84750 | -1.51740 | 5.26160 |
| H | 3.07770 | -0.58730 | 1.92540 |
| H | 0.77610 | -0.04170 | 1.00260 |
| H | 2.59800 | 1.17610 | -0.29990 |
| H | 3.95110 | 1.16600 | 0.82570 |
| H | 5.05440 | -2.06520 | -1.07200 |
| H | -0.24670 | -2.30700 | 1.23910 |
| H | 1.33140 | -3.05020 | 1.14750 |
| H | 3.71070 | -0.26200 | -1.82430 |
| H | 6.78270 | -0.83660 | 0.24280 |
| H | 5.64530 | -0.50490 | 1.51640 |
| H | 0.41860 | -1.14130 | 3.40750 |
| H | 6.45010 | -3.31860 | 0.60860 |
| H | 7.45720 | -1.76150 | 3.08360 |
| H | 4.41000 | -2.86930 | 1.69690 |

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| H | 2.13120 | -3.67320 | 3.34990 |
| H | 1.27290 | -1.72510 | 5.58700 |
| H | 0.00540 | -3.87220 | 5.76020 |
| H | 1.52310 | -4.77100 | 5.75330 |
| H | 1.14450 | -3.69080 | 7.09120 |
| H | 9.97130 | -4.75210 | 2.18680 |
| H | 4.86300 | -1.57970 | 5.65240 |
| H | 3.91780 | -1.46010 | 4.17510 |
| H | 3.40150 | -0.59380 | 5.63210 |
| Marilzafurollene C_156 | | | |
| C | 3.70530 | -0.48040 | 0.94900 |
| O | 5.09210 | -0.66720 | 1.23070 |
| C | 2.86170 | -1.60930 | 1.56880 |
| C | 3.59520 | -0.34870 | -0.57460 |
| C | 5.85480 | -0.57640 | 0.03030 |
| C | 2.93600 | -1.61090 | 3.10470 |
| Br | 3.48910 | -3.37640 | 0.88230 |
| C | 4.95880 | 0.19220 | -0.94950 |
| C | 7.24040 | 0.03970 | 0.30400 |
| C | 2.00940 | -2.63540 | 3.73020 |
| Cl | 4.99900 | 1.95900 | -0.66660 |
| C | 8.16210 | -0.86740 | 1.13890 |
| C | 8.62970 | -2.08710 | 0.36720 |
| O | 9.29550 | -0.11820 | 1.52760 |
| C | 8.38730 | -3.32300 | 0.74020 |
| C | 0.98610 | -2.33900 | 4.54860 |
| C | 0.05920 | -3.36620 | 5.17140 |
| C | 0.11690 | -3.29730 | 6.69950 |
| O | -1.29000 | -3.13640 | 4.79220 |
| C | 8.16700 | -4.56400 | 1.10400 |
| Br | 6.58400 | -5.58550 | 0.49950 |
| C | -1.57670 | -3.45420 | 3.43700 |
| H | 3.41480 | 0.47270 | 1.39410 |
| H | 1.82230 | -1.49330 | 1.25810 |
| H | 3.45340 | -1.32280 | -1.04280 |
| H | 2.77330 | 0.29410 | -0.89080 |
| H | 5.97170 | -1.59110 | -0.35420 |
| H | 3.95740 | -1.81740 | 3.42720 |
| H | 2.68470 | -0.62060 | 3.48660 |
| H | 5.21890 | 0.01110 | -1.99290 |
| H | 7.72710 | 0.28190 | -0.64160 |
| H | 7.10310 | 0.98700 | 0.82600 |
| H | 2.21020 | -3.66870 | 3.48350 |
| H | 7.63770 | -1.18160 | 2.04480 |
| H | 9.19520 | -1.89080 | -0.53180 |
| H | 9.03770 | 0.48650 | 2.20920 |
| H | 0.77980 | -1.30830 | 4.79880 |

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| H | 0.36010 | -4.36880 | 4.86090 |
| H | 1.12780 | -3.48140 | 7.06410 |
| H | -0.19960 | -2.31970 | 7.06380 |
| H | -0.53830 | -4.04560 | 7.14590 |
| H | 8.81160 | -5.14010 | 1.75160 |
| H | -2.63390 | -3.27870 | 3.23810 |
| H | -1.00250 | -2.83660 | 2.74560 |
| H | -1.36670 | -4.50320 | 3.22440 |
| Marilzafurollene C_157 | | | |
| C | 3.03700 | -0.38610 | 0.07160 |
| O | 4.08880 | -0.54920 | 1.02050 |
| C | 1.72100 | -1.04450 | 0.54050 |
| C | 3.60580 | -0.86670 | -1.26950 |
| C | 5.29040 | -0.94080 | 0.35770 |
| C | 1.77350 | -2.55220 | 0.86280 |
| Br | 0.34750 | -0.75500 | -0.87420 |
| C | 5.08190 | -0.56620 | -1.11370 |
| C | 6.52370 | -0.33070 | 1.05150 |
| C | 2.45350 | -2.85830 | 2.18400 |
| Cl | 5.38630 | 1.17030 | -1.42140 |
| C | 6.79380 | -0.94410 | 2.43690 |
| C | 7.34760 | -2.35330 | 2.34250 |
| O | 7.72640 | -0.13510 | 3.12400 |
| C | 6.64880 | -3.42890 | 2.62430 |
| C | 1.83690 | -3.40130 | 3.24840 |
| C | 2.48820 | -3.72040 | 4.58430 |
| C | 2.61930 | -5.23320 | 4.77580 |
| O | 3.79040 | -3.16110 | 4.70910 |
| C | 5.92900 | -4.50240 | 2.84480 |
| Br | 4.92950 | -5.40820 | 1.39550 |
| C | 3.79560 | -1.78410 | 5.06290 |
| H | 2.86410 | 0.68840 | -0.00830 |
| H | 1.36110 | -0.51220 | 1.42230 |
| H | 3.46500 | -1.93920 | -1.39660 |
| H | 3.15340 | -0.36840 | -2.12740 |
| H | 5.34110 | -2.02950 | 0.40690 |
| H | 0.75240 | -2.93090 | 0.91730 |
| H | 2.25860 | -3.11710 | 0.06820 |
| H | 5.71020 | -1.14430 | -1.79220 |
| H | 7.40430 | -0.45320 | 0.41940 |
| H | 6.36840 | 0.74380 | 1.15220 |
| H | 3.50540 | -2.62130 | 2.24790 |
| H | 5.86550 | -0.95090 | 3.01190 |
| H | 8.37710 | -2.43900 | 2.02690 |
| H | 7.30450 | 0.67870 | 3.36120 |
| H | 0.78670 | -3.64660 | 3.17940 |
| H | 1.84530 | -3.33310 | 5.37700 |

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| H | 3.24490 | -5.67610 | 4.00100 |
| H | 3.06970 | -5.46510 | 5.74100 |
| H | 1.64550 | -5.72190 | 4.73800 |
| H | 5.80910 | -4.98200 | 3.80540 |
| H | 4.82440 | -1.43630 | 5.15270 |
| H | 3.29900 | -1.16900 | 4.31170 |
| H | 3.30700 | -1.62160 | 6.02430 |
| Marilzafurollene C_158 | | | |
| C | 3.24430 | -0.78600 | 0.91740 |
| O | 3.91590 | -1.84840 | 0.23640 |
| C | 1.72210 | -1.03000 | 0.89070 |
| C | 3.70150 | 0.51150 | 0.23340 |
| C | 5.05520 | -1.34100 | -0.45320 |
| C | 1.28680 | -2.34080 | 1.57100 |
| Br | 1.09450 | -1.08820 | -1.00190 |
| C | 4.53150 | 0.01370 | -0.93490 |
| C | 6.26640 | -1.28990 | 0.51000 |
| C | 1.62650 | -2.39520 | 3.04880 |
| Cl | 5.81000 | 1.16510 | -1.41190 |
| C | 6.68580 | -2.67240 | 1.04160 |
| C | 7.98300 | -2.59960 | 1.82260 |
| O | 5.66570 | -3.15940 | 1.88650 |
| C | 9.07080 | -3.25200 | 1.48140 |
| C | 0.71890 | -2.41530 | 4.03880 |
| C | 1.06040 | -2.47590 | 5.51620 |
| C | 0.50810 | -1.25400 | 6.25470 |
| O | 0.49420 | -3.62570 | 6.12750 |
| C | 10.15360 | -3.90000 | 1.12250 |
| Br | 11.50290 | -3.11870 | -0.09740 |
| C | 1.11660 | -4.84890 | 5.75800 |
| H | 3.59750 | -0.76360 | 1.94910 |
| H | 1.20880 | -0.19280 | 1.36660 |
| H | 2.87960 | 1.15100 | -0.08980 |
| H | 4.31910 | 1.09130 | 0.92030 |
| H | 5.29330 | -1.98390 | -1.30150 |
| H | 0.21080 | -2.46860 | 1.44730 |
| H | 1.75470 | -3.19260 | 1.07600 |
| H | 3.88600 | -0.13910 | -1.80140 |
| H | 7.11450 | -0.86400 | -0.02790 |
| H | 6.07570 | -0.61310 | 1.34340 |
| H | 2.67850 | -2.42510 | 3.29680 |
| H | 6.79850 | -3.36320 | 0.20280 |
| H | 7.97610 | -1.97020 | 2.70040 |
| H | 4.84120 | -3.00950 | 1.43110 |
| H | -0.33520 | -2.39080 | 3.80160 |
| H | 2.14490 | -2.49250 | 5.64230 |
| H | 0.91600 | -0.32900 | 5.84650 |

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| H | -0.57850 | -1.20470 | 6.18040 |
| H | 0.76650 | -1.29200 | 7.31310 |
| H | 10.41200 | -4.89750 | 1.44700 |
| H | 0.64580 | -5.67290 | 6.29410 |
| H | 1.01660 | -5.04840 | 4.69060 |
| H | 2.17670 | -4.84630 | 6.01460 |
| Marilzafurollene C_159 | | | |
| C | 3.43350 | -1.15630 | 0.93780 |
| O | 4.83340 | -1.19040 | 1.21580 |
| C | 2.63570 | -1.41280 | 2.22850 |
| C | 3.22320 | -2.19530 | -0.16910 |
| C | 5.52250 | -1.97640 | 0.24390 |
| C | 1.11190 | -1.33870 | 2.02340 |
| Br | 3.16950 | -0.03980 | 3.57390 |
| C | 4.53720 | -2.14060 | -0.91990 |
| C | 6.89470 | -1.36390 | -0.09850 |
| C | 0.34090 | -1.69180 | 3.28050 |
| Cl | 4.53900 | -0.73120 | -2.02230 |
| C | 7.86720 | -1.35260 | 1.09390 |
| C | 9.26330 | -0.94380 | 0.66770 |
| O | 7.39270 | -0.43540 | 2.05560 |
| C | 10.31640 | -1.71760 | 0.80010 |
| C | -0.50010 | -2.73350 | 3.39170 |
| C | -1.26820 | -3.08660 | 4.65180 |
| C | -2.77720 | -3.06080 | 4.39610 |
| O | -0.94170 | -4.39350 | 5.10140 |
| C | 11.35730 | -2.50580 | 0.92790 |
| Br | 11.90650 | -3.77620 | -0.48770 |
| C | 0.35750 | -4.50810 | 5.66580 |
| H | 3.20250 | -0.16240 | 0.55080 |
| H | 2.91050 | -2.38390 | 2.64250 |
| H | 3.08920 | -3.18850 | 0.26170 |
| H | 2.35940 | -1.98200 | -0.79960 |
| H | 5.67540 | -2.96100 | 0.68960 |
| H | 0.82510 | -0.33560 | 1.70580 |
| H | 0.80840 | -2.01630 | 1.22470 |
| H | 4.72840 | -3.03370 | -1.51600 |
| H | 7.33600 | -1.94720 | -0.90810 |
| H | 6.77850 | -0.35020 | -0.48390 |
| H | 0.49740 | -1.04350 | 4.13150 |
| H | 7.89670 | -2.34540 | 1.54860 |
| H | 9.35980 | 0.04260 | 0.23800 |
| H | 6.44100 | -0.50990 | 2.07780 |
| H | -0.66190 | -3.38680 | 2.54640 |
| H | -1.04020 | -2.36250 | 5.43660 |
| H | -3.10310 | -2.07580 | 4.06070 |
| H | -3.06220 | -3.78720 | 3.63470 |

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| H | -3.32820 | -3.30050 | 5.30570 |
| H | 12.00220 | -2.54080 | 1.79390 |
| H | 1.13710 | -4.27920 | 4.93840 |
| H | 0.47550 | -3.84480 | 6.52360 |
| H | 0.51570 | -5.53000 | 6.01030 |
| Marilzafurollene C_160 | | | |
| C | 2.95950 | -0.96440 | 1.03970 |
| O | 4.12930 | -1.78040 | 1.11500 |
| C | 1.72410 | -1.81800 | 0.68630 |
| C | 3.28160 | 0.15090 | 0.03650 |
| C | 5.14700 | -1.25540 | 0.26510 |
| C | 1.36950 | -2.85120 | 1.76910 |
| Br | 2.05950 | -2.80700 | -1.01400 |
| C | 4.79320 | 0.22710 | 0.10240 |
| C | 6.55080 | -1.56950 | 0.81780 |
| C | 0.92680 | -2.21190 | 3.07060 |
| Cl | 5.28300 | 1.19980 | 1.52180 |
| C | 6.86390 | -3.07580 | 0.84560 |
| C | 8.30910 | -3.33770 | 1.22010 |
| O | 6.02140 | -3.68870 | 1.79690 |
| C | 9.16000 | -3.95560 | 0.43300 |
| C | 1.58070 | -2.33530 | 4.23860 |
| C | 1.16220 | -1.70050 | 5.55430 |
| C | 2.11450 | -0.56330 | 5.93230 |
| O | -0.15020 | -1.15380 | 5.49910 |
| C | 10.00220 | -4.56360 | -0.36840 |
| Br | 11.11070 | -3.58390 | -1.68390 |
| C | -1.18380 | -2.11310 | 5.68040 |
| H | 2.82510 | -0.50520 | 2.02020 |
| H | 0.86560 | -1.16800 | 0.51050 |
| H | 2.97910 | -0.13160 | -0.97200 |
| H | 2.79150 | 1.09500 | 0.27580 |
| H | 5.03220 | -1.73660 | -0.70810 |
| H | 0.55590 | -3.48600 | 1.41720 |
| H | 2.22100 | -3.51000 | 1.94570 |
| H | 5.23840 | 0.67650 | -0.78590 |
| H | 7.28690 | -1.06710 | 0.18850 |
| H | 6.67220 | -1.15240 | 1.81830 |
| H | 0.02480 | -1.61770 | 3.02810 |
| H | 6.65100 | -3.50920 | -0.13440 |
| H | 8.62010 | -2.98540 | 2.19270 |
| H | 5.16850 | -3.26570 | 1.72330 |
| H | 2.48720 | -2.92320 | 4.27480 |
| H | 1.21280 | -2.46250 | 6.33440 |
| H | 3.14110 | -0.91970 | 6.02120 |
| H | 2.09820 | 0.22810 | 5.18250 |
| H | 1.83200 | -0.12180 | 6.88810 |

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| H | 10.17180 | -5.63020 | -0.39110 |
| H | -1.12730 | -2.56740 | 6.67040 |
| H | -2.15420 | -1.62460 | 5.59330 |
| H | -1.14020 | -2.90570 | 4.93280 |
| Marilzafurollene C_161 | | | |
| C | 3.09620 | -0.59470 | 0.89660 |
| O | 3.64610 | -1.74020 | 0.24120 |
| C | 1.56020 | -0.60420 | 0.76180 |
| C | 3.79220 | 0.62430 | 0.27280 |
| C | 4.90070 | -1.40810 | -0.34640 |
| C | 0.90170 | -1.83150 | 1.41580 |
| Br | 1.06280 | -0.58960 | -1.16980 |
| C | 4.62940 | 0.01590 | -0.83650 |
| C | 6.02310 | -1.55690 | 0.70950 |
| C | 1.13830 | -1.89320 | 2.91210 |
| Cl | 6.10230 | 0.96220 | -1.18690 |
| C | 6.18540 | -2.99660 | 1.23050 |
| C | 7.40380 | -3.13260 | 2.12180 |
| O | 5.03420 | -3.34200 | 1.96920 |
| C | 8.40900 | -3.93510 | 1.85590 |
| C | 1.87120 | -2.83890 | 3.52510 |
| C | 2.14290 | -2.91540 | 5.01770 |
| C | 3.60060 | -2.55800 | 5.31750 |
| O | 1.32420 | -2.02230 | 5.76380 |
| C | 9.41040 | -4.73370 | 1.57230 |
| Br | 10.96540 | -4.14600 | 0.49730 |
| C | 0.01480 | -2.51480 | 6.01680 |
| H | 3.37410 | -0.63920 | 1.95090 |
| H | 1.14740 | 0.30520 | 1.20110 |
| H | 3.10100 | 1.37930 | -0.10260 |
| H | 4.43150 | 1.10230 | 1.01590 |
| H | 5.10440 | -2.07090 | -1.18830 |
| H | -0.17460 | -1.81020 | 1.24310 |
| H | 1.27170 | -2.74320 | 0.94460 |
| H | 4.03990 | -0.02800 | -1.75380 |
| H | 6.96670 | -1.25510 | 0.25300 |
| H | 5.86740 | -0.87370 | 1.54510 |
| H | 0.68660 | -1.10720 | 3.50070 |
| H | 6.26910 | -3.68010 | 0.38240 |
| H | 7.41120 | -2.52420 | 3.01440 |
| H | 4.28690 | -3.00420 | 1.48120 |
| H | 2.32970 | -3.61950 | 2.93410 |
| H | 1.96760 | -3.94150 | 5.34660 |
| H | 4.28640 | -3.22320 | 4.79110 |
| H | 3.82610 | -1.53690 | 5.00930 |
| H | 3.81050 | -2.63920 | 6.38390 |
| H | 9.48640 | -5.76400 | 1.88790 |

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| H | -0.55760 | -1.76500 | 6.56290 |
| H | -0.52190 | -2.73860 | 5.09440 |
| H | 0.04710 | -3.41840 | 6.62670 |
| Marilzafurollene C_162 | | | |
| C | 3.65350 | -1.59850 | 1.26170 |
| O | 4.76810 | -1.02590 | 1.94480 |
| C | 2.80350 | -2.45250 | 2.22100 |
| C | 4.23370 | -2.35500 | 0.06160 |
| C | 5.98220 | -1.35160 | 1.27350 |
| C | 2.15210 | -1.60440 | 3.32610 |
| Br | 3.94190 | -3.86230 | 3.06310 |
| C | 5.54570 | -1.63640 | -0.17190 |
| C | 7.03730 | -0.24970 | 1.51480 |
| C | 1.20740 | -2.41030 | 4.19660 |
| Cl | 5.24480 | -0.13640 | -1.10070 |
| C | 8.47820 | -0.61800 | 1.10450 |
| C | 8.67160 | -0.65830 | -0.39900 |
| O | 9.34730 | 0.35490 | 1.64590 |
| C | 9.10250 | -1.71690 | -1.04620 |
| C | -0.11110 | -2.17850 | 4.30850 |
| C | -1.05470 | -2.98740 | 5.17880 |
| C | -1.72870 | -2.09770 | 6.22630 |
| O | -2.08780 | -3.57850 | 4.40390 |
| C | 9.48790 | -2.79220 | -1.69100 |
| Br | 8.19660 | -4.14150 | -2.34530 |
| C | -1.65670 | -4.65420 | 3.58130 |
| H | 3.05100 | -0.77100 | 0.88350 |
| H | 2.02440 | -2.96290 | 1.65270 |
| H | 4.43420 | -3.39610 | 0.31510 |
| H | 3.57650 | -2.34710 | -0.80830 |
| H | 6.33920 | -2.28320 | 1.71630 |
| H | 2.92280 | -1.16170 | 3.95840 |
| H | 1.60480 | -0.77390 | 2.87840 |
| H | 6.25750 | -2.24560 | -0.72810 |
| H | 6.73340 | 0.68950 | 1.05270 |
| H | 7.03960 | -0.04950 | 2.58710 |
| H | 1.65330 | -3.22110 | 4.75550 |
| H | 8.74130 | -1.58220 | 1.54570 |
| H | 8.42630 | 0.24840 | -0.93430 |
| H | 10.24010 | 0.05210 | 1.55810 |
| H | -0.56330 | -1.36990 | 3.75240 |
| H | -0.49630 | -3.76830 | 5.69920 |
| H | -0.99050 | -1.62060 | 6.87140 |
| H | -2.32210 | -1.31310 | 5.75620 |
| H | -2.39510 | -2.68260 | 6.86040 |
| H | 10.51270 | -3.04460 | -1.92220 |
| H | -0.92700 | -4.32940 | 2.83880 |

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|-------------------------------|----------|----------|----------|
| H | -1.21570 | -5.45470 | 4.17670 |
| H | -2.51140 | -5.06840 | 3.04660 |
| Marilzafurollene C_163 | | | |
| C | 3.78720 | -0.64880 | 1.19860 |
| O | 4.45100 | -1.90360 | 1.02360 |
| C | 2.39010 | -0.87770 | 1.80540 |
| C | 3.78190 | 0.02720 | -0.18060 |
| C | 5.19180 | -1.90480 | -0.19500 |
| C | 2.45880 | -1.49800 | 3.21150 |
| Br | 1.32770 | -2.07700 | 0.61360 |
| C | 4.29110 | -1.06360 | -1.10210 |
| C | 6.60820 | -1.33540 | 0.06050 |
| C | 1.09600 | -1.60510 | 3.86820 |
| Cl | 5.10820 | -0.41470 | -2.55100 |
| C | 7.44620 | -2.19050 | 1.02780 |
| C | 8.88310 | -1.71180 | 1.09300 |
| O | 6.87450 | -2.10800 | 2.31500 |
| C | 9.91050 | -2.45810 | 0.75740 |
| C | 0.53390 | -2.75900 | 4.26500 |
| C | -0.83060 | -2.87260 | 4.91840 |
| C | -1.76740 | -3.73970 | 4.07380 |
| O | -0.73970 | -3.47860 | 6.19970 |
| C | 10.92670 | -3.21080 | 0.40800 |
| Br | 11.62260 | -3.26140 | -1.44460 |
| C | -0.13660 | -2.65940 | 7.19200 |
| H | 4.38120 | -0.03830 | 1.88090 |
| H | 1.86040 | 0.07490 | 1.85480 |
| H | 2.80270 | 0.39920 | -0.48360 |
| H | 4.47020 | 0.87320 | -0.17770 |
| H | 5.27500 | -2.92260 | -0.57830 |
| H | 2.92500 | -2.48300 | 3.15980 |
| H | 3.09310 | -0.88810 | 3.85560 |
| H | 3.45420 | -1.67480 | -1.44360 |
| H | 7.13800 | -1.29100 | -0.89190 |
| H | 6.55720 | -0.30690 | 0.41950 |
| H | 0.56150 | -0.67740 | 4.01410 |
| H | 7.41940 | -3.23360 | 0.70420 |
| H | 9.03280 | -0.69970 | 1.43930 |
| H | 5.93210 | -2.20350 | 2.20410 |
| H | 1.06460 | -3.68920 | 4.12060 |
| H | -1.27490 | -1.87990 | 5.01510 |
| H | -1.89320 | -3.32350 | 3.07380 |
| H | -1.38020 | -4.75350 | 3.96900 |
| H | -2.75380 | -3.80660 | 4.53300 |
| H | 11.47170 | -3.86100 | 1.07670 |
| H | -0.13780 | -3.18470 | 8.14700 |
| H | 0.89900 | -2.42160 | 6.94650 |

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|-------------------------------|----------|----------|----------|
| H | -0.68740 | -1.72720 | 7.32310 |
| Marilzafurollene C_164 | | | |
| C | 3.41960 | -0.26550 | 0.31030 |
| O | 4.75720 | -0.14560 | 0.79310 |
| C | 2.51120 | -0.85760 | 1.40440 |
| C | 3.51070 | -1.05440 | -1.00360 |
| C | 5.66210 | -0.76210 | -0.11930 |
| C | 2.97290 | -2.22150 | 1.95090 |
| Br | 0.65490 | -1.01390 | 0.69370 |
| C | 4.92380 | -0.75930 | -1.46240 |
| C | 7.03680 | -0.06640 | -0.09480 |
| C | 2.16900 | -2.66740 | 3.15610 |
| Cl | 4.97810 | 0.84090 | -2.26160 |
| C | 7.78970 | -0.24920 | 1.23580 |
| C | 8.22300 | -1.68540 | 1.46520 |
| O | 8.93820 | 0.57350 | 1.22090 |
| C | 7.79800 | -2.42350 | 2.46540 |
| C | 1.45200 | -3.80190 | 3.21270 |
| C | 0.65210 | -4.25400 | 4.41960 |
| C | -0.83370 | -4.37720 | 4.07310 |
| O | 1.08350 | -5.52780 | 4.87660 |
| C | 7.37330 | -3.17730 | 3.45160 |
| Br | 5.77000 | -4.32790 | 3.29530 |
| C | 2.37270 | -5.52790 | 5.47510 |
| H | 3.07740 | 0.74470 | 0.07960 |
| H | 2.47070 | -0.14130 | 2.22620 |
| H | 3.40320 | -2.12440 | -0.83200 |
| H | 2.75090 | -0.76010 | -1.72830 |
| H | 5.77340 | -1.80260 | 0.19040 |
| H | 2.92460 | -2.98780 | 1.17810 |
| H | 4.01610 | -2.15620 | 2.26060 |
| H | 5.31020 | -1.50040 | -2.16290 |
| H | 7.64990 | -0.44130 | -0.91530 |
| H | 6.89560 | 0.99830 | -0.28250 |
| H | 2.19390 | -2.01160 | 4.01440 |
| H | 7.15090 | 0.07860 | 2.05960 |
| H | 8.92330 | -2.08920 | 0.74870 |
| H | 8.66640 | 1.47460 | 1.32610 |
| H | 1.42430 | -4.46050 | 2.35670 |
| H | 0.75880 | -3.52400 | 5.22440 |
| H | -1.23620 | -3.42540 | 3.72510 |
| H | -0.99650 | -5.11720 | 3.28930 |
| H | -1.41140 | -4.68400 | 4.94510 |
| H | 7.84310 | -3.24600 | 4.42190 |
| H | 2.60670 | -6.52980 | 5.83450 |
| H | 3.14930 | -5.24260 | 4.76490 |
| H | 2.41340 | -4.84910 | 6.32780 |

| Marilzafurollene C_165 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.54000 | -0.73690 | 0.44400 |
| O | 4.86720 | -0.26980 | 0.68190 |
| C | 3.00550 | -1.40810 | 1.72210 |
| C | 3.64700 | -1.67040 | -0.77340 |
| C | 5.78590 | -0.95750 | -0.15550 |
| C | 1.55430 | -1.90260 | 1.59380 |
| Br | 3.10220 | -0.08800 | 3.21520 |
| C | 4.96420 | -1.26820 | -1.40760 |
| C | 7.07800 | -0.14130 | -0.35440 |
| C | 1.11270 | -2.68490 | 2.81480 |
| Cl | 4.72030 | 0.17760 | -2.43220 |
| C | 7.84410 | 0.10080 | 0.95980 |
| C | 8.33960 | -1.18610 | 1.59330 |
| O | 8.95070 | 0.93910 | 0.69650 |
| C | 7.85820 | -1.66600 | 2.71760 |
| C | 0.76030 | -3.98100 | 2.80360 |
| C | 0.33940 | -4.76500 | 4.03230 |
| C | -1.07760 | -5.32000 | 3.86810 |
| O | 1.20160 | -5.87180 | 4.25420 |
| C | 7.33150 | -2.15250 | 3.81600 |
| Br | 5.78040 | -3.38310 | 3.78510 |
| C | 2.50960 | -5.51580 | 4.68320 |
| H | 2.92880 | 0.13130 | 0.19300 |
| H | 3.65820 | -2.23800 | 1.99600 |
| H | 3.70890 | -2.71060 | -0.45060 |
| H | 2.79880 | -1.58410 | -1.45310 |
| H | 6.02520 | -1.90630 | 0.32780 |
| H | 0.88000 | -1.05780 | 1.44950 |
| H | 1.45020 | -2.53820 | 0.71400 |
| H | 5.40300 | -2.05320 | -2.02450 |
| H | 7.72390 | -0.65250 | -1.06930 |
| H | 6.82940 | 0.82180 | -0.80020 |
| H | 1.09550 | -2.13850 | 3.74760 |
| H | 7.18810 | 0.62070 | 1.66260 |
| H | 9.12560 | -1.70640 | 1.06590 |
| H | 8.63650 | 1.82560 | 0.58490 |
| H | 0.77430 | -4.53490 | 1.87600 |
| H | 0.35440 | -4.11200 | 4.90730 |
| H | -1.79890 | -4.51790 | 3.70960 |
| H | -1.13970 | -6.00140 | 3.01930 |
| H | -1.38340 | -5.87030 | 4.75810 |
| H | 7.67780 | -1.93840 | 4.81650 |
| H | 3.03940 | -4.93430 | 3.92810 |
| H | 2.48030 | -4.93960 | 5.60890 |
| H | 3.09010 | -6.41900 | 4.87070 |

| Marilzafurollene C_166 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.98400 | -0.65390 | 1.41840 |
| O | 5.00230 | -1.54090 | 0.95080 |
| C | 2.71970 | -1.45490 | 1.78220 |
| C | 3.78350 | 0.38760 | 0.30720 |
| C | 5.72340 | -0.94540 | -0.12310 |
| C | 2.96970 | -2.44760 | 2.92980 |
| Br | 2.06580 | -2.45110 | 0.17930 |
| C | 4.61620 | -0.16390 | -0.83350 |
| C | 6.88680 | -0.09670 | 0.44460 |
| C | 1.70000 | -3.13970 | 3.38620 |
| Cl | 5.20470 | 1.11070 | -1.93710 |
| C | 7.92680 | -0.92280 | 1.22280 |
| C | 8.68740 | -1.88180 | 0.32640 |
| O | 8.84230 | -0.02800 | 1.82110 |
| C | 8.66730 | -3.18640 | 0.47800 |
| C | 1.17540 | -3.03520 | 4.61850 |
| C | -0.09640 | -3.72730 | 5.07220 |
| C | 0.18200 | -4.66060 | 6.25320 |
| O | -1.06750 | -2.78480 | 5.50300 |
| C | 8.62590 | -4.49090 | 0.61130 |
| Br | 7.27150 | -5.60600 | -0.30420 |
| C | -1.65580 | -2.03180 | 4.45100 |
| H | 4.35660 | -0.14430 | 2.30850 |
| H | 1.92840 | -0.76240 | 2.07380 |
| H | 2.74070 | 0.53320 | 0.02430 |
| H | 4.17610 | 1.35190 | 0.63170 |
| H | 6.11800 | -1.72050 | -0.78090 |
| H | 3.68970 | -3.20520 | 2.61720 |
| H | 3.41730 | -1.92590 | 3.77660 |
| H | 4.01420 | -0.85590 | -1.42430 |
| H | 7.39050 | 0.42800 | -0.36770 |
| H | 6.48940 | 0.68040 | 1.09760 |
| H | 1.20390 | -3.75420 | 2.64790 |
| H | 7.42120 | -1.47290 | 2.02000 |
| H | 9.26250 | -1.43340 | -0.47100 |
| H | 9.35950 | -0.50330 | 2.45590 |
| H | 1.66600 | -2.42230 | 5.36090 |
| H | -0.50350 | -4.32250 | 4.25230 |
| H | 0.91260 | -5.42490 | 5.98720 |
| H | 0.56840 | -4.10920 | 7.11070 |
| H | -0.72950 | -5.16830 | 6.56880 |
| H | 9.30640 | -5.07320 | 1.21530 |
| H | -2.40680 | -1.35750 | 4.86230 |
| H | -0.91790 | -1.42490 | 3.92520 |
| H | -2.15090 | -2.68220 | 3.72880 |

| Marilzafurollene C_167 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.84860 | -1.17020 | 2.15230 |
| O | 4.60050 | -2.21350 | 1.53300 |
| C | 2.35690 | -1.54400 | 2.23780 |
| C | 4.15390 | 0.10530 | 1.35760 |
| C | 5.37880 | -1.68700 | 0.46070 |
| C | 2.11760 | -2.75900 | 3.14960 |
| Br | 1.65220 | -1.94660 | 0.41220 |
| C | 5.52160 | -0.19390 | 0.78040 |
| C | 6.67860 | -2.49480 | 0.27990 |
| C | 0.64380 | -3.05570 | 3.34810 |
| Cl | 6.77520 | 0.11840 | 2.01920 |
| C | 7.62950 | -1.95300 | -0.80560 |
| C | 8.88020 | -2.80430 | -0.91010 |
| O | 6.96850 | -1.95000 | -2.05420 |
| C | 10.09510 | -2.33830 | -0.72930 |
| C | 0.01000 | -3.01240 | 4.53180 |
| C | -1.46530 | -3.30820 | 4.72760 |
| C | -1.66320 | -4.48200 | 5.69000 |
| O | -2.14320 | -2.19130 | 5.28410 |
| C | 11.31230 | -1.88740 | -0.53700 |
| Br | 12.17310 | -1.88010 | 1.24540 |
| C | -2.30980 | -1.10340 | 4.38490 |
| H | 4.24740 | -1.04510 | 3.16030 |
| H | 1.79470 | -0.69070 | 2.62000 |
| H | 3.44160 | 0.23800 | 0.54310 |
| H | 4.13080 | 1.00740 | 1.96920 |
| H | 4.77360 | -1.78490 | -0.44250 |
| H | 2.60090 | -3.64130 | 2.72780 |
| H | 2.58180 | -2.58700 | 4.12150 |
| H | 5.75380 | 0.40590 | -0.10030 |
| H | 7.20870 | -2.53650 | 1.23210 |
| H | 6.41180 | -3.52650 | 0.04840 |
| H | 0.08930 | -3.31840 | 2.45810 |
| H | 7.91160 | -0.92580 | -0.56470 |
| H | 8.72640 | -3.84840 | -1.14310 |
| H | 7.55010 | -1.58570 | -2.70690 |
| H | 0.55830 | -2.75000 | 5.42520 |
| H | -1.91800 | -3.56970 | 3.76900 |
| H | -1.17860 | -5.38410 | 5.31560 |
| H | -1.24900 | -4.26110 | 6.67400 |
| H | -2.72280 | -4.70330 | 5.81830 |
| H | 11.95160 | -1.48480 | -1.30920 |
| H | -1.35190 | -0.69340 | 4.06290 |
| H | -2.87510 | -1.40380 | 3.50180 |
| H | -2.86270 | -0.30450 | 4.87900 |

| Marilzafurollene C_168 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.36020 | -0.46200 | 0.60050 |
| O | 4.67760 | -0.78910 | 1.04210 |
| C | 2.34450 | -0.64360 | 1.74460 |
| C | 3.12320 | -1.29540 | -0.66510 |
| C | 5.32980 | -1.61210 | 0.07300 |
| C | 2.29390 | -2.06130 | 2.34580 |
| Br | 0.53280 | -0.13630 | 1.08450 |
| C | 4.52490 | -1.43460 | -1.22140 |
| C | 6.83620 | -1.29570 | -0.00990 |
| C | 1.42920 | -2.12920 | 3.58970 |
| Cl | 4.97490 | 0.05640 | -2.10260 |
| C | 7.60020 | -1.63580 | 1.28170 |
| C | 9.09740 | -1.48450 | 1.09860 |
| O | 7.16860 | -0.76030 | 2.30040 |
| C | 9.94830 | -2.47420 | 1.24580 |
| C | 0.34240 | -2.90830 | 3.71830 |
| C | -0.52700 | -2.97510 | 4.95990 |
| C | -1.96480 | -2.55860 | 4.64020 |
| O | -0.57890 | -4.29510 | 5.48140 |
| C | 10.78600 | -3.47440 | 1.38320 |
| Br | 11.28750 | -4.65320 | -0.12610 |
| C | 0.62790 | -4.72890 | 6.09360 |
| H | 3.37800 | 0.59150 | 0.31640 |
| H | 2.59780 | 0.06860 | 2.53130 |
| H | 2.73160 | -2.28240 | -0.42340 |
| H | 2.42740 | -0.82420 | -1.36010 |
| H | 5.20270 | -2.64520 | 0.40180 |
| H | 1.92930 | -2.77920 | 1.61170 |
| H | 3.29860 | -2.38080 | 2.62490 |
| H | 4.63120 | -2.27550 | -1.90770 |
| H | 7.26180 | -1.87300 | -0.83210 |
| H | 6.99480 | -0.24670 | -0.26350 |
| H | 1.72890 | -1.49710 | 4.41350 |
| H | 7.36640 | -2.65930 | 1.58340 |
| H | 9.44760 | -0.49720 | 0.83460 |
| H | 6.23860 | -0.60230 | 2.15910 |
| H | 0.03790 | -3.54220 | 2.89790 |
| H | -0.13400 | -2.29740 | 5.72030 |
| H | -2.00100 | -1.54320 | 4.24420 |
| H | -2.41400 | -3.22300 | 3.90170 |
| H | -2.58580 | -2.58880 | 5.53560 |
| H | 11.27340 | -3.74880 | 2.30740 |
| H | 1.45330 | -4.76480 | 5.38170 |
| H | 0.90840 | -4.07560 | 6.92070 |
| H | 0.49200 | -5.73370 | 6.49350 |

| Marilzafurollene C_169 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.78780 | -0.71440 | 1.23630 |
| O | 4.62570 | -1.83250 | 1.54180 |
| C | 2.50340 | -0.79670 | 2.08270 |
| C | 3.58620 | -0.73770 | -0.28760 |
| C | 5.27510 | -2.29920 | 0.35990 |
| C | 1.65290 | -2.05560 | 1.82920 |
| Br | 1.40710 | 0.83390 | 1.74180 |
| C | 4.19080 | -2.06590 | -0.69490 |
| C | 6.59630 | -1.52080 | 0.14900 |
| C | 0.48970 | -2.16950 | 2.79480 |
| Cl | 4.78940 | -2.06430 | -2.37670 |
| C | 7.63170 | -1.75680 | 1.26330 |
| C | 8.97570 | -1.15010 | 0.91160 |
| O | 7.15850 | -1.16690 | 2.45420 |
| C | 10.07870 | -1.85340 | 0.79320 |
| C | 0.32200 | -3.17470 | 3.67010 |
| C | -0.84100 | -3.28620 | 4.63820 |
| C | -1.63760 | -4.56930 | 4.38840 |
| O | -0.38690 | -3.33050 | 5.98300 |
| C | 11.17040 | -2.57000 | 0.66740 |
| Br | 11.71860 | -3.37570 | -1.05580 |
| C | 0.12070 | -2.09490 | 6.46840 |
| H | 4.32950 | 0.19410 | 1.50500 |
| H | 2.78680 | -0.76530 | 3.13620 |
| H | 2.54740 | -0.63640 | -0.60160 |
| H | 4.14150 | 0.08530 | -0.73900 |
| H | 5.49430 | -3.36370 | 0.45150 |
| H | 1.25790 | -2.05510 | 0.81340 |
| H | 2.27760 | -2.94500 | 1.92150 |
| H | 3.43730 | -2.85080 | -0.61700 |
| H | 7.04000 | -1.84630 | -0.79280 |
| H | 6.40820 | -0.45280 | 0.03390 |
| H | -0.24080 | -1.37350 | 2.75470 |
| H | 7.74480 | -2.83040 | 1.43070 |
| H | 8.99030 | -0.08080 | 0.75880 |
| H | 6.23480 | -1.38960 | 2.52780 |
| H | 1.04860 | -3.97330 | 3.71650 |
| H | -1.51140 | -2.43440 | 4.50710 |
| H | -2.03290 | -4.59620 | 3.37270 |
| H | -1.01720 | -5.45430 | 4.53190 |
| H | -2.48130 | -4.64110 | 5.07490 |
| H | 11.86170 | -2.78710 | 1.46850 |
| H | 0.41620 | -2.20770 | 7.51140 |
| H | 0.99830 | -1.76940 | 5.90890 |
| H | -0.63540 | -1.31040 | 6.41870 |

| Marilzafurollene C_170 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.08840 | -1.09580 | 1.20370 |
| O | 4.32710 | -1.80650 | 1.21610 |
| C | 1.90970 | -2.06360 | 0.97190 |
| C | 3.23870 | 0.00490 | 0.14490 |
| C | 5.22770 | -1.23390 | 0.26990 |
| C | 1.72280 | -3.09730 | 2.09670 |
| Br | 2.19950 | -3.06770 | -0.72830 |
| C | 4.73900 | 0.20770 | 0.09150 |
| C | 6.69250 | -1.41110 | 0.71460 |
| C | 1.31290 | -2.47750 | 3.41930 |
| Cl | 5.24840 | 1.26610 | 1.44090 |
| C | 7.13490 | -2.88430 | 0.75690 |
| C | 8.62310 | -3.01150 | 1.01520 |
| O | 6.42930 | -3.53310 | 1.79200 |
| C | 9.45700 | -3.58250 | 0.17620 |
| C | 0.12710 | -2.67850 | 4.02020 |
| C | -0.30400 | -2.06980 | 5.34490 |
| C | -0.33910 | -3.13390 | 6.44460 |
| O | 0.57450 | -1.03920 | 5.78030 |
| C | 10.28040 | -4.14480 | -0.67640 |
| Br | 11.18930 | -3.12120 | -2.10660 |
| C | 0.33580 | 0.22210 | 5.16960 |
| H | 2.98690 | -0.61020 | 2.17480 |
| H | 0.98560 | -1.49640 | 0.85010 |
| H | 2.88710 | -0.33710 | -0.82860 |
| H | 2.68970 | 0.91380 | 0.39280 |
| H | 5.07750 | -1.75860 | -0.67560 |
| H | 0.96280 | -3.81920 | 1.79560 |
| H | 2.64290 | -3.66420 | 2.24340 |
| H | 5.07740 | 0.66060 | -0.84110 |
| H | 7.33050 | -0.87110 | 0.01350 |
| H | 6.85670 | -0.95130 | 1.68980 |
| H | 2.04440 | -1.84030 | 3.89620 |
| H | 6.88100 | -3.36730 | -0.18950 |
| H | 8.98090 | -2.60160 | 1.94840 |
| H | 5.53990 | -3.18620 | 1.78180 |
| H | -0.60100 | -3.32390 | 3.54970 |
| H | -1.31230 | -1.66870 | 5.22560 |
| H | -1.02070 | -3.94560 | 6.18930 |
| H | 0.64980 | -3.56360 | 6.60670 |
| H | -0.67320 | -2.70440 | 7.38920 |
| H | 10.53890 | -5.19370 | -0.68440 |
| H | -0.65790 | 0.59650 | 5.41820 |
| H | 1.06500 | 0.94650 | 5.53240 |
| H | 0.42640 | 0.17220 | 4.08410 |

| Marilzafurollene C_171 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.63370 | -0.77240 | 1.36380 |
| O | 4.76380 | -1.63010 | 1.20020 |
| C | 2.39800 | -1.58150 | 1.79940 |
| C | 3.47720 | -0.01430 | 0.03910 |
| C | 5.32300 | -1.45700 | -0.10060 |
| C | 2.57390 | -2.20090 | 3.19610 |
| Br | 2.04660 | -3.03740 | 0.47700 |
| C | 4.88110 | -0.05300 | -0.52870 |
| C | 6.84030 | -1.72940 | -0.10060 |
| C | 1.31580 | -2.88930 | 3.68890 |
| Cl | 5.86920 | 1.22860 | 0.23340 |
| C | 7.19110 | -3.20150 | 0.21730 |
| C | 8.66150 | -3.56970 | 0.06730 |
| O | 6.78750 | -3.47640 | 1.54090 |
| C | 9.62040 | -2.77060 | -0.34690 |
| C | 0.62480 | -2.52360 | 4.78130 |
| C | -0.63480 | -3.21310 | 5.27180 |
| C | -0.44060 | -3.76100 | 6.68790 |
| O | -1.72920 | -2.30930 | 5.31860 |
| C | 10.58840 | -1.98790 | -0.76220 |
| Br | 11.65530 | -0.86580 | 0.47130 |
| C | -2.23190 | -1.93580 | 4.04290 |
| H | 3.88790 | -0.05030 | 2.14160 |
| H | 1.52330 | -0.92900 | 1.80300 |
| H | 2.80140 | -0.54130 | -0.63470 |
| H | 3.09210 | 0.99750 | 0.16830 |
| H | 4.83370 | -2.17730 | -0.75910 |
| H | 3.38890 | -2.92570 | 3.18340 |
| H | 2.85960 | -1.42640 | 3.90910 |
| H | 4.91070 | 0.09310 | -1.60900 |
| H | 7.22380 | -1.47160 | -1.08870 |
| H | 7.34620 | -1.07060 | 0.60670 |
| H | 0.97440 | -3.73040 | 3.10170 |
| H | 6.62470 | -3.85390 | -0.44950 |
| H | 8.90120 | -4.58770 | 0.33800 |
| H | 5.98640 | -2.98020 | 1.69680 |
| H | 0.95990 | -1.68370 | 5.37280 |
| H | -0.87820 | -4.04750 | 4.61090 |
| H | 0.37960 | -4.47840 | 6.72350 |
| H | -0.21900 | -2.96100 | 7.39470 |
| H | -1.34110 | -4.26890 | 7.03350 |
| H | 10.89330 | -1.87750 | -1.79250 |
| H | -2.57050 | -2.80720 | 3.48110 |
| H | -3.08440 | -1.26850 | 4.16900 |
| H | -1.48310 | -1.40850 | 3.45080 |

| Marilzafurollene C_172 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.27850 | -0.84200 | 0.88550 |
| O | 4.37500 | -1.26680 | 1.69340 |
| C | 1.94340 | -1.12360 | 1.60030 |
| C | 3.47630 | -1.50950 | -0.48170 |
| C | 5.27960 | -2.05250 | 0.91890 |
| C | 1.70510 | -2.60110 | 1.96520 |
| Br | 0.44710 | -0.46440 | 0.45840 |
| C | 4.97970 | -1.68140 | -0.53890 |
| C | 6.72860 | -1.86670 | 1.40900 |
| C | 0.47880 | -2.78630 | 2.83750 |
| Cl | 5.74600 | -0.13640 | -1.01820 |
| C | 7.78670 | -2.63440 | 0.59240 |
| C | 9.17970 | -2.39800 | 1.14320 |
| O | 7.50180 | -4.01770 | 0.63580 |
| C | 10.16120 | -1.87790 | 0.44170 |
| C | 0.49950 | -3.28550 | 4.08450 |
| C | -0.72790 | -3.46730 | 4.95790 |
| C | -0.91450 | -4.93850 | 5.33720 |
| O | -0.61010 | -2.73440 | 6.16860 |
| C | 11.14510 | -1.34630 | -0.24470 |
| Br | 11.47000 | 0.60550 | -0.29800 |
| C | -0.71440 | -1.32590 | 6.01040 |
| H | 3.38510 | 0.23650 | 0.75830 |
| H | 1.92450 | -0.52900 | 2.51500 |
| H | 3.00160 | -2.48890 | -0.51740 |
| H | 3.07670 | -0.91770 | -1.30560 |
| H | 4.98910 | -3.09410 | 1.06820 |
| H | 1.57960 | -3.20770 | 1.06910 |
| H | 2.57670 | -2.99440 | 2.49030 |
| H | 5.29480 | -2.45110 | -1.24430 |
| H | 6.97450 | -0.80420 | 1.40660 |
| H | 6.78050 | -2.17630 | 2.45330 |
| H | -0.46380 | -2.48800 | 2.40020 |
| H | 7.75080 | -2.30940 | -0.44970 |
| H | 9.33770 | -2.68030 | 2.17450 |
| H | 8.14380 | -4.47770 | 0.11280 |
| H | 1.43900 | -3.58450 | 4.52700 |
| H | -1.61630 | -3.13640 | 4.41620 |
| H | -1.02850 | -5.56240 | 4.45040 |
| H | -0.06150 | -5.31190 | 5.90420 |
| H | -1.80480 | -5.06990 | 5.95240 |
| H | 11.85850 | -1.90280 | -0.83500 |
| H | -0.64690 | -0.84440 | 6.98580 |
| H | 0.08780 | -0.92740 | 5.38820 |
| H | -1.67100 | -1.04790 | 5.56640 |

| Marilzafurollene C_173 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.58570 | -0.35670 | 1.26620 |
| O | 4.75380 | -1.13640 | 1.00730 |
| C | 2.40810 | -1.26280 | 1.67070 |
| C | 3.34910 | 0.48950 | 0.00850 |
| C | 5.26420 | -0.83470 | -0.29010 |
| C | 2.65920 | -1.97630 | 3.00980 |
| Br | 2.09260 | -2.63090 | 0.24930 |
| C | 4.73490 | 0.57060 | -0.59790 |
| C | 6.79380 | -1.01820 | -0.34820 |
| C | 1.45440 | -2.76690 | 3.48170 |
| Cl | 5.67780 | 1.84430 | 0.23240 |
| C | 7.23820 | -2.47880 | -0.15010 |
| C | 8.72410 | -2.65400 | -0.44610 |
| O | 6.90880 | -2.86410 | 1.17290 |
| C | 9.61870 | -3.14940 | 0.38140 |
| C | 0.78060 | -2.52400 | 4.61820 |
| C | -0.42570 | -3.31550 | 5.08780 |
| C | -0.15840 | -3.96050 | 6.45000 |
| O | -1.56260 | -2.47760 | 5.23680 |
| C | 10.49880 | -3.64320 | 1.21990 |
| Br | 10.94360 | -5.57200 | 1.28840 |
| C | -2.12460 | -2.03370 | 4.00940 |
| H | 3.82510 | 0.31740 | 2.09030 |
| H | 1.50100 | -0.66130 | 1.74840 |
| H | 2.68160 | -0.02140 | -0.68580 |
| H | 2.91540 | 1.46600 | 0.22540 |
| H | 4.79620 | -1.53020 | -0.98950 |
| H | 3.50980 | -2.65310 | 2.91880 |
| H | 2.92670 | -1.24400 | 3.77280 |
| H | 4.72310 | 0.79830 | -1.66440 |
| H | 7.14100 | -0.66910 | -1.32150 |
| H | 7.28490 | -0.38600 | 0.39260 |
| H | 1.13810 | -3.57750 | 2.84000 |
| H | 6.68800 | -3.12080 | -0.84010 |
| H | 9.03600 | -2.33650 | -1.43040 |
| H | 6.07250 | -2.45440 | 1.38280 |
| H | 1.09100 | -1.71550 | 5.26440 |
| H | -0.64760 | -4.10790 | 4.37000 |
| H | 0.69780 | -4.63410 | 6.40550 |
| H | 0.04500 | -3.20730 | 7.21140 |
| H | -1.02040 | -4.54080 | 6.77960 |
| H | 11.05800 | -3.06130 | 1.93740 |
| H | -2.43670 | -2.87580 | 3.39040 |
| H | -3.00530 | -1.42430 | 4.21190 |
| H | -1.42310 | -1.42320 | 3.43980 |

| Marilzafurollene C_174 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.46820 | 0.26420 | 1.12800 |
| O | 3.70090 | -1.14080 | 1.00280 |
| C | 1.99230 | 0.54890 | 1.47350 |
| C | 3.93630 | 0.88290 | -0.19890 |
| C | 4.64870 | -1.39320 | -0.02960 |
| C | 1.55340 | 0.05020 | 2.86610 |
| Br | 0.79150 | -0.20430 | 0.06680 |
| C | 4.25500 | -0.32870 | -1.05430 |
| C | 6.08600 | -1.27720 | 0.53370 |
| C | 1.50020 | -1.46150 | 2.99460 |
| Cl | 5.50870 | 0.00400 | -2.28120 |
| C | 6.38180 | -2.26800 | 1.67310 |
| C | 7.85570 | -2.28890 | 2.02630 |
| O | 5.64280 | -1.87760 | 2.80950 |
| C | 8.60530 | -3.36380 | 1.93850 |
| C | 2.23300 | -2.18680 | 3.85600 |
| C | 2.15910 | -3.69770 | 3.97740 |
| C | 3.50530 | -4.34390 | 3.64390 |
| O | 1.81900 | -4.09130 | 5.29910 |
| C | 9.34210 | -4.44460 | 1.83810 |
| Br | 10.31310 | -4.91700 | 0.17890 |
| C | 0.47230 | -3.81780 | 5.66070 |
| H | 4.10330 | 0.64440 | 1.93010 |
| H | 1.84350 | 1.62970 | 1.45150 |
| H | 3.19470 | 1.53030 | -0.66770 |
| H | 4.83400 | 1.47880 | -0.03070 |
| H | 4.49690 | -2.39450 | -0.43460 |
| H | 2.21370 | 0.46100 | 3.63100 |
| H | 0.55570 | 0.43110 | 3.08570 |
| H | 3.35500 | -0.65160 | -1.58030 |
| H | 6.78620 | -1.47430 | -0.27930 |
| H | 6.29780 | -0.26000 | 0.86470 |
| H | 0.81300 | -1.96810 | 2.33210 |
| H | 6.05950 | -3.26890 | 1.37670 |
| H | 8.27750 | -1.35410 | 2.36550 |
| H | 4.74870 | -1.71960 | 2.51640 |
| H | 2.92830 | -1.69450 | 4.52090 |
| H | 1.41350 | -4.08500 | 3.28020 |
| H | 3.80950 | -4.11040 | 2.62330 |
| H | 4.29010 | -3.99410 | 4.31540 |
| H | 3.44910 | -5.42860 | 3.73370 |
| H | 9.49000 | -5.16610 | 2.62840 |
| H | 0.28680 | -4.17930 | 6.67210 |
| H | 0.25800 | -2.74860 | 5.64690 |
| H | -0.22660 | -4.32250 | 4.99250 |

| Marilzafurollene C_175 | | | |
|-------------------------------|---------|----------|----------|
| C | 3.08580 | -0.51210 | 0.75440 |
| O | 4.15540 | -1.40570 | 0.45230 |
| C | 1.75400 | -1.03910 | 0.18470 |
| C | 3.54880 | 0.86090 | 0.24730 |
| C | 5.38330 | -0.69110 | 0.51340 |
| C | 1.38180 | -2.43220 | 0.72850 |
| Br | 1.87140 | -1.15720 | -1.80270 |
| C | 4.97980 | 0.60290 | -0.20100 |
| C | 5.83130 | -0.54810 | 1.99000 |
| C | 1.35550 | -2.48200 | 2.24550 |
| Cl | 6.06490 | 1.98440 | 0.11990 |
| C | 6.08290 | -1.90700 | 2.67110 |
| C | 7.41170 | -2.51440 | 2.26440 |
| O | 6.06410 | -1.73440 | 4.07220 |
| C | 7.52610 | -3.64590 | 1.60750 |
| C | 2.29360 | -3.09850 | 2.98430 |
| C | 2.33600 | -3.12550 | 4.49620 |
| C | 2.34630 | -4.57070 | 5.01170 |
| O | 3.51070 | -2.44880 | 4.92930 |
| C | 7.65640 | -4.76390 | 0.93360 |
| Br | 7.71160 | -4.80870 | -1.04450 |
| C | 3.41960 | -1.91590 | 6.24500 |
| H | 2.99990 | -0.44500 | 1.83940 |
| H | 0.95590 | -0.33170 | 0.41380 |
| H | 2.94160 | 1.24940 | -0.57040 |
| H | 3.51380 | 1.58720 | 1.05990 |
| H | 6.15140 | -1.21870 | -0.05350 |
| H | 0.40940 | -2.74180 | 0.34510 |
| H | 2.10470 | -3.16220 | 0.36090 |
| H | 4.98730 | 0.42420 | -1.27750 |
| H | 6.73740 | 0.05540 | 2.04910 |
| H | 5.08250 | 0.00810 | 2.55290 |
| H | 0.53960 | -1.96660 | 2.73170 |
| H | 5.27390 | -2.59690 | 2.42360 |
| H | 8.29230 | -1.95770 | 2.54950 |
| H | 5.19040 | -1.96910 | 4.38330 |
| H | 3.10400 | -3.60920 | 2.48410 |
| H | 1.44670 | -2.61010 | 4.86510 |
| H | 2.31700 | -4.61230 | 6.09990 |
| H | 1.48000 | -5.12140 | 4.64370 |
| H | 3.24120 | -5.09960 | 4.68280 |
| H | 7.74500 | -5.74520 | 1.37640 |
| H | 2.61360 | -1.18480 | 6.32000 |
| H | 3.25440 | -2.69540 | 6.98890 |
| H | 4.35070 | -1.40910 | 6.49930 |

| Marilzafurollene C_176 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.54050 | -0.00630 | 0.67060 |
| O | 4.91180 | -0.23200 | 0.99300 |
| C | 2.62520 | -0.68180 | 1.70880 |
| C | 3.37030 | -0.45590 | -0.78630 |
| C | 5.62180 | -0.67250 | -0.16250 |
| C | 2.82420 | -2.20220 | 1.85140 |
| Br | 0.72550 | -0.29410 | 1.24250 |
| C | 4.75790 | -0.23660 | -1.35230 |
| C | 7.07470 | -0.15850 | -0.15060 |
| C | 2.07310 | -2.77230 | 3.03870 |
| Cl | 4.97970 | 1.49270 | -1.75630 |
| C | 7.93090 | -0.77180 | 0.97260 |
| C | 8.18750 | -2.25230 | 0.76190 |
| O | 9.17200 | -0.09810 | 1.01420 |
| C | 7.75940 | -3.18760 | 1.57880 |
| C | 2.65320 | -3.40490 | 4.07360 |
| C | 1.92590 | -3.98950 | 5.27340 |
| C | 2.20310 | -3.16190 | 6.53080 |
| O | 0.51540 | -4.02500 | 5.09220 |
| C | 7.31140 | -4.12720 | 2.37680 |
| Br | 5.54870 | -4.98700 | 2.11120 |
| C | 0.05850 | -5.12830 | 4.32070 |
| H | 3.38270 | 1.07250 | 0.71650 |
| H | 2.81200 | -0.21140 | 2.67550 |
| H | 3.11950 | -1.51400 | -0.84710 |
| H | 2.59460 | 0.09920 | -1.31460 |
| H | 5.61910 | -1.76350 | -0.14150 |
| H | 2.49260 | -2.72420 | 0.95460 |
| H | 3.88600 | -2.42250 | 1.96710 |
| H | 4.94950 | -0.82030 | -2.25330 |
| H | 7.54120 | -0.36000 | -1.11590 |
| H | 7.06270 | 0.92600 | -0.03900 |
| H | 0.99930 | -2.64730 | 3.02680 |
| H | 7.43110 | -0.61730 | 1.93200 |
| H | 8.75900 | -2.51450 | -0.11650 |
| H | 9.03640 | 0.76330 | 1.38380 |
| H | 3.72740 | -3.52250 | 4.08330 |
| H | 2.30140 | -5.00090 | 5.44050 |
| H | 3.27040 | -3.11770 | 6.74880 |
| H | 1.84050 | -2.14010 | 6.41540 |
| H | 1.70440 | -3.59520 | 7.39790 |
| H | 7.84280 | -4.51630 | 3.23320 |
| H | -1.02300 | -5.06610 | 4.20060 |
| H | 0.50480 | -5.14330 | 3.32590 |
| H | 0.28510 | -6.07330 | 4.81600 |

| Marilzafurollene C_177 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.41670 | 0.01020 | 0.54620 |
| O | 4.78940 | -0.18790 | 0.88480 |
| C | 2.54560 | -1.12540 | 1.11870 |
| C | 3.36480 | 0.15890 | -0.98220 |
| C | 5.56690 | -0.30920 | -0.29970 |
| C | 2.62410 | -1.19340 | 2.65350 |
| Br | 3.12420 | -2.88080 | 0.36030 |
| C | 4.79430 | 0.51760 | -1.33470 |
| C | 7.03560 | 0.09540 | -0.06550 |
| C | 1.71510 | -2.25630 | 3.23930 |
| Cl | 5.03060 | 2.27760 | -1.11460 |
| C | 7.76180 | -0.74820 | 0.99850 |
| C | 7.81970 | -2.22490 | 0.65300 |
| O | 9.08030 | -0.25210 | 1.11470 |
| C | 7.47160 | -3.17600 | 1.49040 |
| C | 2.14330 | -3.28410 | 3.99090 |
| C | 1.24820 | -4.36190 | 4.57150 |
| C | 1.66920 | -5.74370 | 4.06530 |
| O | 1.32690 | -4.39150 | 5.98950 |
| C | 7.17340 | -4.12240 | 2.34950 |
| Br | 5.35330 | -4.87380 | 2.54200 |
| C | 0.71590 | -3.28100 | 6.63170 |
| H | 3.11540 | 0.95720 | 0.99660 |
| H | 1.51030 | -0.97210 | 0.81160 |
| H | 3.10400 | -0.78400 | -1.46210 |
| H | 2.64110 | 0.90400 | -1.31330 |
| H | 5.52830 | -1.35470 | -0.61000 |
| H | 3.65430 | -1.38130 | 2.96070 |
| H | 2.34260 | -0.23150 | 3.08310 |
| H | 5.05800 | 0.26620 | -2.36250 |
| H | 7.57580 | 0.03730 | -1.01110 |
| H | 7.08030 | 1.13950 | 0.24430 |
| H | 0.66150 | -2.16000 | 3.02080 |
| H | 7.25920 | -0.61130 | 1.95910 |
| H | 8.16800 | -2.47050 | -0.33980 |
| H | 9.45880 | -0.58570 | 1.91570 |
| H | 3.19710 | -3.38140 | 4.21040 |
| H | 0.21490 | -4.18340 | 4.26750 |
| H | 1.62250 | -5.79390 | 2.97690 |
| H | 2.69050 | -5.97940 | 4.36570 |
| H | 1.01670 | -6.52030 | 4.46410 |
| H | 7.87930 | -4.57940 | 3.02730 |
| H | 1.20470 | -2.34220 | 6.36950 |
| H | -0.34140 | -3.20830 | 6.37430 |
| H | 0.78860 | -3.40110 | 7.71260 |

| Marilzafurollene C_178 | | | |
|-------------------------------|----------|----------|----------|
| C | 4.04450 | -0.76510 | 1.52310 |
| O | 4.59990 | -1.96520 | 0.97820 |
| C | 2.60930 | -1.03130 | 2.01420 |
| C | 4.15580 | 0.29680 | 0.41890 |
| C | 5.38810 | -1.66630 | -0.17200 |
| C | 2.56550 | -2.05290 | 3.16320 |
| Br | 1.49380 | -1.69760 | 0.49770 |
| C | 4.60450 | -0.50470 | -0.78720 |
| C | 6.83750 | -1.34300 | 0.26440 |
| C | 1.18150 | -2.18950 | 3.76760 |
| Cl | 5.53630 | 0.47280 | -1.95530 |
| C | 7.55470 | -2.53010 | 0.93200 |
| C | 9.02440 | -2.23650 | 1.15980 |
| O | 6.93880 | -2.78910 | 2.17460 |
| C | 9.99480 | -2.94150 | 0.62440 |
| C | 0.87990 | -1.92730 | 5.05160 |
| C | -0.49850 | -2.06010 | 5.67970 |
| C | -1.09040 | -0.68190 | 5.98490 |
| O | -1.41970 | -2.73810 | 4.83420 |
| C | 10.95390 | -3.64770 | 0.07440 |
| Br | 11.72070 | -3.20000 | -1.69490 |
| C | -1.30440 | -4.15470 | 4.86960 |
| H | 4.66250 | -0.45250 | 2.36660 |
| H | 2.16460 | -0.09370 | 2.35220 |
| H | 3.22650 | 0.83610 | 0.23320 |
| H | 4.91520 | 1.03100 | 0.69040 |
| H | 5.39650 | -2.52140 | -0.84910 |
| H | 2.89160 | -3.03050 | 2.80610 |
| H | 3.26740 | -1.75850 | 3.94450 |
| H | 3.73170 | -0.89770 | -1.31100 |
| H | 7.40870 | -1.06190 | -0.62140 |
| H | 6.86300 | -0.47340 | 0.92180 |
| H | 0.40130 | -2.52220 | 3.09680 |
| H | 7.44900 | -3.41670 | 0.30260 |
| H | 9.24860 | -1.39760 | 1.80230 |
| H | 5.99720 | -2.75230 | 2.02800 |
| H | 1.66000 | -1.58980 | 5.71900 |
| H | -0.39460 | -2.60310 | 6.62110 |
| H | -0.44730 | -0.11410 | 6.65770 |
| H | -1.22030 | -0.09980 | 5.07210 |
| H | -2.06700 | -0.77620 | 6.46010 |
| H | 11.41000 | -4.52050 | 0.51840 |
| H | -0.30800 | -4.49040 | 4.58060 |
| H | -1.52480 | -4.54110 | 5.86540 |
| H | -2.01950 | -4.59590 | 4.17540 |

| Marilzafurollene C_179 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.36230 | 0.24540 | 1.17120 |
| O | 3.60380 | -1.16160 | 1.09730 |
| C | 1.88020 | 0.51540 | 1.50360 |
| C | 3.82560 | 0.81840 | -0.17690 |
| C | 4.52110 | -1.45980 | 0.05080 |
| C | 1.47860 | 0.17460 | 2.95360 |
| Br | 0.70210 | -0.46520 | 0.22510 |
| C | 4.13010 | -0.41870 | -0.99860 |
| C | 5.96410 | -1.36760 | 0.59940 |
| C | 1.63700 | -1.29120 | 3.31410 |
| Cl | 5.37770 | -0.13050 | -2.24270 |
| C | 6.25450 | -2.39070 | 1.71300 |
| C | 7.72560 | -2.41760 | 2.07650 |
| O | 5.50480 | -2.04370 | 2.85690 |
| C | 8.47950 | -3.48700 | 1.96150 |
| C | 2.46190 | -1.75550 | 4.26920 |
| C | 2.64710 | -3.21540 | 4.65160 |
| C | 2.08890 | -3.48190 | 6.05150 |
| O | 1.98570 | -4.10560 | 3.76030 |
| C | 9.22240 | -4.56050 | 1.83180 |
| Br | 10.20580 | -4.97540 | 0.16460 |
| C | 2.71210 | -4.37900 | 2.56940 |
| H | 3.99110 | 0.66570 | 1.95800 |
| H | 1.67890 | 1.57700 | 1.35160 |
| H | 3.08600 | 1.45790 | -0.65950 |
| H | 4.73030 | 1.41000 | -0.03240 |
| H | 4.34020 | -2.46770 | -0.32480 |
| H | 2.06530 | 0.78060 | 3.64510 |
| H | 0.43570 | 0.44850 | 3.11600 |
| H | 3.22400 | -0.74810 | -1.50990 |
| H | 6.65670 | -1.55530 | -0.22210 |
| H | 6.18590 | -0.35910 | 0.95030 |
| H | 1.03410 | -1.98680 | 2.74750 |
| H | 5.93840 | -3.38290 | 1.38290 |
| H | 8.14200 | -1.49230 | 2.44710 |
| H | 4.63310 | -1.79760 | 2.55410 |
| H | 3.06240 | -1.05570 | 4.83260 |
| H | 3.71710 | -3.43200 | 4.66510 |
| H | 2.57580 | -2.85400 | 6.79790 |
| H | 1.01750 | -3.28350 | 6.09090 |
| H | 2.24520 | -4.52160 | 6.33920 |
| H | 9.36900 | -5.30600 | 2.59960 |
| H | 2.14140 | -5.06490 | 1.94370 |
| H | 2.89550 | -3.47620 | 1.98880 |
| H | 3.67150 | -4.84810 | 2.79100 |

| Marilzafurollene C_180 | | | |
|-------------------------------|---------|----------|----------|
| C | 3.24960 | 0.08330 | 0.42010 |
| O | 4.39670 | -0.33440 | 1.15630 |
| C | 1.92970 | -0.36690 | 1.08290 |
| C | 3.49450 | -0.38360 | -1.01830 |
| C | 5.42580 | -0.76100 | 0.26320 |
| C | 1.73040 | -1.88160 | 1.29370 |
| Br | 0.41740 | 0.31180 | -0.02290 |
| C | 5.00110 | -0.27020 | -1.12710 |
| C | 6.80850 | -0.29690 | 0.76200 |
| C | 2.62600 | -2.45600 | 2.37450 |
| Cl | 5.46500 | 1.43380 | -1.41910 |
| C | 7.28000 | -1.05180 | 2.01830 |
| C | 7.67360 | -2.48280 | 1.70410 |
| O | 8.39940 | -0.38370 | 2.56230 |
| C | 6.99020 | -3.53150 | 2.10100 |
| C | 2.19850 | -2.84290 | 3.58790 |
| C | 3.08900 | -3.41570 | 4.67400 |
| C | 3.16000 | -2.46770 | 5.87370 |
| O | 2.58330 | -4.65290 | 5.15350 |
| C | 6.28000 | -4.58040 | 2.43950 |
| Br | 4.84250 | -5.28470 | 1.27600 |
| C | 2.72960 | -5.73730 | 4.24780 |
| H | 3.26680 | 1.17450 | 0.42310 |
| H | 1.84300 | 0.13180 | 2.04950 |
| H | 3.19650 | -1.42290 | -1.15070 |
| H | 2.96290 | 0.21490 | -1.75870 |
| H | 5.38970 | -1.85100 | 0.23990 |
| H | 0.69490 | -2.05600 | 1.58820 |
| H | 1.87470 | -2.43840 | 0.36870 |
| H | 5.41750 | -0.87380 | -1.93430 |
| H | 7.54710 | -0.41620 | -0.03190 |
| H | 6.76020 | 0.77180 | 0.97350 |
| H | 3.67420 | -2.54450 | 2.12810 |
| H | 6.48430 | -1.04120 | 2.76710 |
| H | 8.57200 | -2.60840 | 1.11740 |
| H | 8.10780 | 0.42940 | 2.95070 |
| H | 1.15190 | -2.75280 | 3.84110 |
| H | 4.09930 | -3.55640 | 4.28530 |
| H | 2.17450 | -2.31190 | 6.31330 |
| H | 3.80950 | -2.87250 | 6.64990 |
| H | 3.55640 | -1.49450 | 5.58270 |
| H | 6.40070 | -5.14500 | 3.35260 |
| H | 3.78180 | -5.93350 | 4.04070 |
| H | 2.30430 | -6.63910 | 4.68790 |
| H | 2.21500 | -5.55380 | 3.30390 |

| Marilzafurollene C_181 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.99770 | -0.10610 | 1.34600 |
| O | 5.03690 | -1.08670 | 1.32720 |
| C | 2.83730 | -0.61210 | 2.22320 |
| C | 3.65120 | 0.17210 | -0.12580 |
| C | 5.64600 | -1.13510 | 0.03980 |
| C | 2.19080 | -1.92070 | 1.73120 |
| Br | 1.45350 | 0.81950 | 2.34220 |
| C | 4.44000 | -0.88690 | -0.86890 |
| C | 6.77710 | -0.08090 | -0.03950 |
| C | 1.15460 | -2.45280 | 2.70170 |
| Cl | 4.85900 | -0.39640 | -2.53350 |
| C | 7.93770 | -0.35080 | 0.93490 |
| C | 8.71500 | -1.60130 | 0.56860 |
| O | 8.81080 | 0.75950 | 0.89720 |
| C | 8.82060 | -2.64780 | 1.35530 |
| C | 1.23890 | -3.63480 | 3.33440 |
| C | 0.20170 | -4.16410 | 4.30730 |
| C | -0.38430 | -5.48880 | 3.81250 |
| O | 0.77290 | -4.40890 | 5.58450 |
| C | 8.90700 | -3.70740 | 2.12370 |
| Br | 7.59950 | -5.18950 | 2.03140 |
| C | 1.10700 | -3.23310 | 6.30960 |
| H | 4.40410 | 0.80420 | 1.78980 |
| H | 3.21800 | -0.76260 | 3.23480 |
| H | 2.58500 | 0.13310 | -0.34830 |
| H | 4.00250 | 1.16760 | -0.39940 |
| H | 6.05470 | -2.12950 | -0.14230 |
| H | 1.71120 | -1.77360 | 0.76370 |
| H | 2.96270 | -2.67780 | 1.58570 |
| H | 3.84950 | -1.80140 | -0.93720 |
| H | 7.17360 | -0.04010 | -1.05440 |
| H | 6.36960 | 0.91070 | 0.15810 |
| H | 0.29850 | -1.81660 | 2.87810 |
| H | 7.54060 | -0.43560 | 1.94940 |
| H | 9.19230 | -1.59740 | -0.40100 |
| H | 9.40260 | 0.70490 | 1.63440 |
| H | 2.09250 | -4.27550 | 3.16400 |
| H | -0.61260 | -3.44300 | 4.40440 |
| H | -0.85670 | -5.37060 | 2.83690 |
| H | 0.38760 | -6.25360 | 3.72220 |
| H | -1.14010 | -5.86050 | 4.50450 |
| H | 9.67680 | -3.87540 | 2.86240 |
| H | 1.50690 | -3.50870 | 7.28540 |
| H | 1.86580 | -2.64200 | 5.79560 |
| H | 0.22900 | -2.60680 | 6.47330 |

| Marilzafurollene C_182 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.12760 | -0.53680 | 0.99140 |
| O | 4.23340 | -1.43580 | 1.08380 |
| C | 1.87910 | -1.26480 | 0.45210 |
| C | 3.60770 | 0.64330 | 0.13650 |
| C | 5.35610 | -0.90340 | 0.38400 |
| C | 1.37040 | -2.37500 | 1.38760 |
| Br | 2.30310 | -2.10110 | -1.30940 |
| C | 5.10830 | 0.60880 | 0.34140 |
| C | 6.68050 | -1.36420 | 1.02330 |
| C | 0.86180 | -1.84620 | 2.71520 |
| Cl | 5.51970 | 1.40650 | 1.88910 |
| C | 6.89810 | -2.88450 | 0.92860 |
| C | 8.28380 | -3.27950 | 1.39920 |
| O | 5.93530 | -3.52370 | 1.73800 |
| C | 9.16530 | -3.87860 | 0.63150 |
| C | 1.40840 | -2.14970 | 3.90660 |
| C | 0.95400 | -1.64980 | 5.27360 |
| C | -0.14470 | -0.57900 | 5.21510 |
| O | 0.44040 | -2.70970 | 6.06890 |
| C | 10.04010 | -4.46600 | -0.15010 |
| Br | 11.32310 | -3.44670 | -1.26100 |
| C | 1.41900 | -3.61700 | 6.55770 |
| H | 2.93300 | -0.16420 | 1.99810 |
| H | 1.07960 | -0.54390 | 0.27530 |
| H | 3.38470 | 0.47860 | -0.91780 |
| H | 3.15490 | 1.59220 | 0.42520 |
| H | 5.30480 | -1.28080 | -0.63910 |
| H | 0.55080 | -2.91060 | 0.90780 |
| H | 2.16080 | -3.10840 | 1.55440 |
| H | 5.66100 | 1.10890 | -0.45480 |
| H | 7.50130 | -0.85730 | 0.51360 |
| H | 6.73290 | -1.05190 | 2.06690 |
| H | 0.00600 | -1.19010 | 2.65870 |
| H | 6.75140 | -3.20900 | -0.10420 |
| H | 8.52380 | -3.04170 | 2.42520 |
| H | 5.11910 | -3.04040 | 1.62940 |
| H | 2.26530 | -2.80750 | 3.92060 |
| H | 1.82030 | -1.20840 | 5.76980 |
| H | 0.17470 | 0.28870 | 4.63730 |
| H | -1.06040 | -0.97050 | 4.77160 |
| H | -0.39260 | -0.23040 | 6.21780 |
| H | 10.14630 | -5.53500 | -0.26360 |
| H | 0.93940 | -4.35190 | 7.20430 |
| H | 1.91000 | -4.16140 | 5.75100 |
| H | 2.17890 | -3.10180 | 7.14670 |

| Marilzafurollene C_183 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.31320 | -1.16760 | 0.86140 |
| O | 4.58370 | -1.55360 | 1.38410 |
| C | 2.60410 | -2.35860 | 0.18670 |
| C | 3.58190 | 0.03380 | -0.05040 |
| C | 5.58070 | -0.60820 | 1.00450 |
| C | 2.27100 | -3.49890 | 1.16390 |
| Br | 3.76860 | -3.10540 | -1.24970 |
| C | 4.80440 | 0.65060 | 0.59580 |
| C | 6.62170 | -0.42810 | 2.12640 |
| C | 1.26980 | -3.09340 | 2.22920 |
| Cl | 4.30330 | 1.63160 | 2.00710 |
| C | 7.49940 | -1.67240 | 2.35150 |
| C | 8.47480 | -1.90540 | 1.21310 |
| O | 8.23360 | -1.49550 | 3.54590 |
| C | 8.46360 | -2.97550 | 0.45160 |
| C | 1.52520 | -3.09770 | 3.54820 |
| C | 0.53380 | -2.68500 | 4.62000 |
| C | 0.21140 | -3.86060 | 5.54580 |
| O | 1.05540 | -1.64450 | 5.43430 |
| C | 8.45790 | -4.03100 | -0.32710 |
| Br | 7.42970 | -4.09680 | -2.01630 |
| C | 1.18330 | -0.39090 | 4.77710 |
| H | 2.71530 | -0.81670 | 1.70290 |
| H | 1.68910 | -2.01500 | -0.29740 |
| H | 3.83130 | -0.28960 | -1.06110 |
| H | 2.73620 | 0.71850 | -0.11810 |
| H | 6.06710 | -0.99990 | 0.10950 |
| H | 1.85130 | -4.34120 | 0.61340 |
| H | 3.18760 | -3.86130 | 1.63180 |
| H | 5.36740 | 1.29450 | -0.08060 |
| H | 7.25650 | 0.43080 | 1.90470 |
| H | 6.09730 | -0.18780 | 3.05160 |
| H | 0.29600 | -2.78440 | 1.87710 |
| H | 6.85920 | -2.54930 | 2.47540 |
| H | 9.20870 | -1.12950 | 1.05160 |
| H | 7.64460 | -1.60160 | 4.27970 |
| H | 2.49880 | -3.40590 | 3.90220 |
| H | -0.39390 | -2.34980 | 4.15200 |
| H | -0.21220 | -4.69640 | 4.98840 |
| H | 1.10550 | -4.21660 | 6.05820 |
| H | -0.51230 | -3.56770 | 6.30650 |
| H | 8.99980 | -4.94490 | -0.13250 |
| H | 0.22650 | -0.05240 | 4.37770 |
| H | 1.53210 | 0.35810 | 5.48800 |
| H | 1.90730 | -0.43310 | 3.96310 |

| Marilzafurollene C_184 | | | |
|-------------------------------|----------|----------|----------|
| C | 4.05170 | -0.61490 | 1.60150 |
| O | 4.63370 | -1.85120 | 1.17860 |
| C | 2.66060 | -0.87400 | 2.20950 |
| C | 4.04900 | 0.29970 | 0.36750 |
| C | 5.33790 | -1.67170 | -0.04840 |
| C | 2.73010 | -1.73810 | 3.48020 |
| Br | 1.49600 | -1.78090 | 0.86420 |
| C | 4.46460 | -0.63190 | -0.75390 |
| C | 6.79300 | -1.23640 | 0.24990 |
| C | 1.37800 | -1.89480 | 4.14770 |
| Cl | 5.27800 | 0.22340 | -2.09370 |
| C | 7.60490 | -2.29830 | 1.01310 |
| C | 9.06950 | -1.91840 | 1.10730 |
| O | 7.07640 | -2.42140 | 2.31540 |
| C | 10.03970 | -2.64550 | 0.60190 |
| C | 0.77110 | -3.07310 | 4.37220 |
| C | -0.58980 | -3.25020 | 5.02500 |
| C | -0.44390 | -3.79970 | 6.44610 |
| O | -1.31220 | -2.02750 | 5.11200 |
| C | 10.99790 | -3.37570 | 0.08250 |
| Br | 11.63580 | -3.12440 | -1.77470 |
| C | -1.95120 | -1.64810 | 3.89940 |
| H | 4.69970 | -0.17140 | 2.35950 |
| H | 2.18960 | 0.08090 | 2.44790 |
| H | 3.08630 | 0.77380 | 0.17440 |
| H | 4.78760 | 1.09180 | 0.49570 |
| H | 5.34810 | -2.60600 | -0.61110 |
| H | 3.14280 | -2.71910 | 3.24070 |
| H | 3.40880 | -1.28280 | 4.20210 |
| H | 3.58270 | -1.12430 | -1.16670 |
| H | 7.29690 | -1.04790 | -0.69890 |
| H | 6.81480 | -0.28960 | 0.79050 |
| H | 0.88820 | -0.98180 | 4.45500 |
| H | 7.50570 | -3.26160 | 0.50750 |
| H | 9.29010 | -0.99630 | 1.62490 |
| H | 6.12710 | -2.44020 | 2.22660 |
| H | 1.26500 | -3.98620 | 4.07200 |
| H | -1.15960 | -3.97140 | 4.43590 |
| H | 0.07800 | -4.75680 | 6.44900 |
| H | 0.11540 | -3.10960 | 7.07830 |
| H | -1.42100 | -3.95270 | 6.90470 |
| H | 11.52160 | -4.16580 | 0.60060 |
| H | -2.45650 | -0.69220 | 4.03710 |
| H | -1.23990 | -1.53460 | 3.08040 |
| H | -2.70220 | -2.38240 | 3.60560 |

| Marilzafurollene C_185 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.40170 | -0.42900 | 1.03910 |
| O | 4.80210 | -0.66380 | 1.18690 |
| C | 2.59160 | -1.54590 | 1.72420 |
| C | 3.14900 | -0.27670 | -0.46750 |
| C | 5.41910 | -0.72600 | -0.09430 |
| C | 2.78670 | -1.54820 | 3.24960 |
| Br | 3.13770 | -3.32370 | 0.99250 |
| C | 4.51320 | 0.12320 | -0.99250 |
| C | 6.90520 | -0.32080 | -0.03390 |
| C | 1.89510 | -2.55650 | 3.94830 |
| Cl | 4.75670 | 1.87800 | -0.74250 |
| C | 7.76540 | -1.20040 | 0.89440 |
| C | 7.74580 | -2.67740 | 0.50880 |
| O | 9.08130 | -0.66980 | 0.89430 |
| C | 8.77580 | -3.37220 | 0.07720 |
| C | 0.94550 | -2.24180 | 4.84490 |
| C | 0.05310 | -3.25210 | 5.54170 |
| C | 0.23350 | -3.18360 | 7.06020 |
| O | -1.31770 | -2.99850 | 5.27080 |
| C | 9.81690 | -4.05170 | -0.34180 |
| Br | 11.03090 | -5.00360 | 0.89900 |
| C | -1.71760 | -3.31250 | 3.94370 |
| H | 3.18370 | 0.52580 | 1.52020 |
| H | 1.53260 | -1.41320 | 1.49730 |
| H | 2.85660 | -1.22850 | -0.91150 |
| H | 2.36860 | 0.44870 | -0.69890 |
| H | 5.34110 | -1.75620 | -0.44370 |
| H | 3.82680 | -1.77040 | 3.49170 |
| H | 2.58210 | -0.55370 | 3.64830 |
| H | 4.64430 | -0.09020 | -2.05390 |
| H | 7.32160 | -0.34000 | -1.04160 |
| H | 6.98530 | 0.71150 | 0.30700 |
| H | 2.05740 | -3.59330 | 3.68870 |
| H | 7.37610 | -1.12320 | 1.91130 |
| H | 6.78930 | -3.16850 | 0.62250 |
| H | 9.58500 | -1.11430 | 1.56160 |
| H | 0.77760 | -1.20750 | 5.10890 |
| H | 0.31050 | -4.26010 | 5.21010 |
| H | 1.26690 | -3.38520 | 7.34350 |
| H | -0.03580 | -2.20040 | 7.44670 |
| H | -0.39700 | -3.91990 | 7.55870 |
| H | 10.10910 | -4.15810 | -1.37610 |
| H | -2.78400 | -3.11790 | 3.82950 |
| H | -1.18940 | -2.70610 | 3.20710 |
| H | -1.54440 | -4.36530 | 3.71760 |

| Marilzafurollene C_186 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.78360 | -1.07500 | 1.29480 |
| O | 5.14900 | -1.48620 | 1.36200 |
| C | 2.93960 | -1.88930 | 2.29130 |
| C | 3.38980 | -1.24610 | -0.17630 |
| C | 5.68680 | -1.66840 | 0.05240 |
| C | 1.45900 | -1.46840 | 2.31430 |
| Br | 3.70460 | -1.62720 | 4.11480 |
| C | 4.69610 | -0.98000 | -0.89480 |
| C | 7.15120 | -1.19360 | -0.02110 |
| C | 0.62430 | -2.32940 | 3.24280 |
| Cl | 4.96940 | 0.78480 | -1.00680 |
| C | 8.10060 | -2.01920 | 0.86490 |
| C | 9.55140 | -1.66550 | 0.60390 |
| O | 7.79930 | -1.75620 | 2.21820 |
| C | 10.44070 | -2.52990 | 0.17120 |
| C | -0.07510 | -1.86000 | 4.28930 |
| C | -0.90730 | -2.71810 | 5.22360 |
| C | -0.39300 | -2.61300 | 6.66140 |
| O | -2.26520 | -2.30220 | 5.23240 |
| C | 11.31540 | -3.40150 | -0.27200 |
| Br | 11.62750 | -3.70340 | -2.20350 |
| C | -2.97680 | -2.60510 | 4.04020 |
| H | 3.74880 | -0.01650 | 1.55840 |
| H | 3.02810 | -2.95210 | 2.06310 |
| H | 3.06950 | -2.27110 | -0.36790 |
| H | 2.58560 | -0.57790 | -0.48590 |
| H | 5.65130 | -2.73980 | -0.15340 |
| H | 1.37540 | -0.41990 | 2.60390 |
| H | 1.02850 | -1.55130 | 1.31610 |
| H | 4.72090 | -1.38850 | -1.90580 |
| H | 7.48220 | -1.26840 | -1.05800 |
| H | 7.22800 | -0.13890 | 0.24620 |
| H | 0.60890 | -3.38820 | 3.02740 |
| H | 7.94110 | -3.08320 | 0.67600 |
| H | 9.83310 | -0.64050 | 0.79610 |
| H | 6.85020 | -1.68090 | 2.29140 |
| H | -0.06300 | -0.80210 | 4.50980 |
| H | -0.84770 | -3.76310 | 4.91300 |
| H | 0.64790 | -2.93050 | 6.73060 |
| H | -0.45650 | -1.58890 | 7.03010 |
| H | -0.97850 | -3.24380 | 7.33030 |
| H | 11.93640 | -4.02530 | 0.35420 |
| H | -4.01310 | -2.28350 | 4.14370 |
| H | -2.55560 | -2.09150 | 3.17540 |
| H | -2.97850 | -3.67790 | 3.84280 |

| Marilzafurollene C_187 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.72320 | -1.04770 | 0.86990 |
| O | 4.73440 | -0.98650 | 1.87520 |
| C | 2.52120 | -1.88230 | 1.35060 |
| C | 4.41230 | -1.57280 | -0.39450 |
| C | 5.98480 | -1.42180 | 1.34820 |
| C | 1.80830 | -1.23140 | 2.54810 |
| Br | 3.13120 | -3.71100 | 1.87510 |
| C | 5.85680 | -1.18190 | -0.16390 |
| C | 7.14760 | -0.73820 | 2.10080 |
| C | 0.54910 | -1.97420 | 2.95160 |
| Cl | 6.08410 | 0.53840 | -0.60230 |
| C | 8.54380 | -1.34080 | 1.84050 |
| C | 9.07650 | -1.01960 | 0.45760 |
| O | 9.43290 | -0.81070 | 2.80150 |
| C | 9.43330 | -1.93630 | -0.41280 |
| C | 0.34610 | -2.52150 | 4.16160 |
| C | -0.90940 | -3.26930 | 4.56920 |
| C | -0.58080 | -4.71330 | 4.95600 |
| O | -1.52780 | -2.66380 | 5.69530 |
| C | 9.74310 | -2.85730 | -1.29380 |
| Br | 8.40630 | -3.59680 | -2.55160 |
| C | -2.14620 | -1.41420 | 5.42060 |
| H | 3.39910 | -0.02300 | 0.68060 |
| H | 1.81620 | -2.00210 | 0.52690 |
| H | 4.33960 | -2.65870 | -0.45740 |
| H | 3.99490 | -1.15980 | -1.31310 |
| H | 6.03630 | -2.49780 | 1.52420 |
| H | 2.49300 | -1.16890 | 3.39540 |
| H | 1.52760 | -0.20720 | 2.30080 |
| H | 6.54680 | -1.78000 | -0.75820 |
| H | 7.15190 | 0.33650 | 1.91890 |
| H | 6.93480 | -0.84390 | 3.16550 |
| H | -0.21990 | -2.05560 | 2.19700 |
| H | 8.50050 | -2.42250 | 1.98750 |
| H | 9.14740 | 0.02980 | 0.20750 |
| H | 10.24300 | -1.30000 | 2.77310 |
| H | 1.11320 | -2.44250 | 4.91870 |
| H | -1.61220 | -3.28870 | 3.73390 |
| H | -0.11120 | -5.24480 | 4.12770 |
| H | 0.10030 | -4.74920 | 5.80670 |
| H | -1.48470 | -5.25700 | 5.23080 |
| H | 10.72380 | -3.29300 | -1.41890 |
| H | -1.42230 | -0.66710 | 5.09330 |
| H | -2.91590 | -1.51410 | 4.65430 |
| H | -2.62350 | -1.03810 | 6.32550 |

| Marilzafurollene C_188 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.60320 | -0.65910 | 0.84320 |
| O | 4.58110 | -0.57650 | 1.87810 |
| C | 2.27240 | -1.19930 | 1.39980 |
| C | 4.25350 | -1.47020 | -0.28290 |
| C | 5.81450 | -1.14990 | 1.44700 |
| C | 2.36380 | -2.58840 | 2.05910 |
| Br | 0.92710 | -1.24290 | -0.07180 |
| C | 5.72270 | -1.16180 | -0.08810 |
| C | 7.00500 | -0.41550 | 2.10340 |
| C | 1.07660 | -2.97690 | 2.76000 |
| Cl | 6.10020 | 0.43220 | -0.80950 |
| C | 8.36380 | -1.13870 | 1.99680 |
| C | 8.92930 | -1.13060 | 0.59010 |
| O | 9.27400 | -0.48450 | 2.85590 |
| C | 9.22490 | -2.22310 | -0.07650 |
| C | 0.96850 | -3.21440 | 4.07780 |
| C | -0.32100 | -3.59960 | 4.77850 |
| C | -0.18700 | -4.96610 | 5.45530 |
| O | -0.65530 | -2.66180 | 5.79120 |
| C | 9.46760 | -3.32200 | -0.75030 |
| Br | 8.07950 | -4.20130 | -1.85310 |
| C | -1.09360 | -1.40270 | 5.29890 |
| H | 3.44260 | 0.35860 | 0.48370 |
| H | 1.90580 | -0.48380 | 2.13770 |
| H | 4.08950 | -2.53850 | -0.14970 |
| H | 3.88210 | -1.19900 | -1.27170 |
| H | 5.80500 | -2.18350 | 1.79730 |
| H | 2.59280 | -3.35500 | 1.31980 |
| H | 3.17900 | -2.59750 | 2.78390 |
| H | 6.36660 | -1.90640 | -0.55510 |
| H | 7.08330 | 0.60760 | 1.73570 |
| H | 6.76710 | -0.31650 | 3.16330 |
| H | 0.20110 | -3.06150 | 2.13140 |
| H | 8.25130 | -2.16580 | 2.35180 |
| H | 9.07700 | -0.15790 | 0.14160 |
| H | 10.05960 | -1.00810 | 2.92810 |
| H | 1.83980 | -3.13040 | 4.71150 |
| H | -1.13260 | -3.65470 | 4.05020 |
| H | 0.05470 | -5.74300 | 4.72950 |
| H | 0.59720 | -4.95710 | 6.21270 |
| H | -1.11860 | -5.24830 | 5.94590 |
| H | 10.41380 | -3.84310 | -0.77060 |
| H | -0.31480 | -0.89790 | 4.72630 |
| H | -1.97620 | -1.51100 | 4.66730 |
| H | -1.35960 | -0.75750 | 6.13610 |

| Marilzafurollene C_189 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.43330 | -1.25420 | 0.82370 |
| O | 4.77980 | -1.36340 | 1.28410 |
| C | 2.73190 | -2.62780 | 0.83750 |
| C | 3.50910 | -0.57560 | -0.54900 |
| C | 5.66560 | -0.71790 | 0.37290 |
| C | 2.61080 | -3.25020 | 2.23970 |
| Br | 3.74940 | -3.90860 | -0.30380 |
| C | 4.77850 | 0.24130 | -0.43100 |
| C | 6.85080 | -0.07680 | 1.12050 |
| C | 1.72470 | -2.45140 | 3.17710 |
| Cl | 4.43430 | 1.75660 | 0.45740 |
| C | 7.81570 | -1.10640 | 1.73560 |
| C | 8.62410 | -1.84210 | 0.68340 |
| O | 8.70760 | -0.42820 | 2.59660 |
| C | 8.56970 | -3.14130 | 0.49820 |
| C | 0.54560 | -2.87890 | 3.65830 |
| C | -0.33930 | -2.08200 | 4.59880 |
| C | -1.70530 | -1.81100 | 3.96320 |
| O | -0.57320 | -2.78920 | 5.80780 |
| C | 8.52880 | -4.43650 | 0.29450 |
| Br | 7.27880 | -5.27010 | -0.99290 |
| C | 0.55850 | -2.87370 | 6.66330 |
| H | 2.91940 | -0.57060 | 1.50000 |
| H | 1.73740 | -2.53650 | 0.39830 |
| H | 3.62670 | -1.31050 | -1.34540 |
| H | 2.62860 | 0.02470 | -0.77910 |
| H | 6.03250 | -1.48240 | -0.31420 |
| H | 2.21020 | -4.26050 | 2.14910 |
| H | 3.59900 | -3.35120 | 2.69040 |
| H | 5.20820 | 0.50630 | -1.39760 |
| H | 7.40060 | 0.57870 | 0.44380 |
| H | 6.45810 | 0.56350 | 1.91080 |
| H | 2.09180 | -1.47660 | 3.46530 |
| H | 7.24770 | -1.82310 | 2.33390 |
| H | 9.27420 | -1.23210 | 0.07350 |
| H | 8.24050 | -0.18510 | 3.38370 |
| H | 0.17330 | -3.85390 | 3.37780 |
| H | 0.13210 | -1.12290 | 4.82260 |
| H | -1.60310 | -1.25240 | 3.03250 |
| H | -2.23010 | -2.74070 | 3.74210 |
| H | -2.33520 | -1.22630 | 4.63370 |
| H | 9.15730 | -5.15970 | 0.79320 |
| H | 1.37820 | -3.42230 | 6.19820 |
| H | 0.91670 | -1.88230 | 6.94370 |
| H | 0.28470 | -3.40020 | 7.57760 |

| Marilzafurollene C_190 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.37120 | -2.44550 | 1.63620 |
| O | 4.73800 | -2.66970 | 1.29270 |
| C | 2.60330 | -3.78090 | 1.65020 |
| C | 2.87010 | -1.42390 | 0.61130 |
| C | 5.18980 | -1.68740 | 0.35980 |
| C | 1.10370 | -3.64940 | 1.98060 |
| Br | 3.45280 | -4.99770 | 2.98230 |
| C | 4.11100 | -0.59570 | 0.35330 |
| C | 6.62680 | -1.23200 | 0.68100 |
| C | 0.84230 | -2.98170 | 3.31790 |
| Cl | 4.32470 | 0.58920 | 1.67720 |
| C | 7.66600 | -2.35740 | 0.53490 |
| C | 9.08070 | -1.82500 | 0.64950 |
| O | 7.44840 | -3.30850 | 1.55430 |
| C | 9.97070 | -1.92170 | -0.31170 |
| C | 0.16700 | -1.83120 | 3.47530 |
| C | -0.08340 | -1.15880 | 4.81170 |
| C | 0.54530 | 0.23640 | 4.84320 |
| O | -1.47360 | -0.99890 | 5.05370 |
| C | 10.84570 | -2.01540 | -1.28470 |
| Br | 11.03590 | -0.62240 | -2.67850 |
| C | -2.15750 | -2.21000 | 5.34530 |
| H | 3.35910 | -1.99490 | 2.63000 |
| H | 2.71300 | -4.26860 | 0.68080 |
| H | 2.56460 | -1.92500 | -0.30810 |
| H | 2.02650 | -0.83470 | 0.97220 |
| H | 5.18150 | -2.16490 | -0.62150 |
| H | 0.59880 | -3.09000 | 1.19220 |
| H | 0.64390 | -4.63810 | 1.99520 |
| H | 4.07080 | -0.04430 | -0.58680 |
| H | 6.88770 | -0.42060 | -0.00010 |
| H | 6.68200 | -0.81310 | 1.68670 |
| H | 1.24220 | -3.48640 | 4.18640 |
| H | 7.53490 | -2.85030 | -0.43110 |
| H | 9.33540 | -1.34880 | 1.58510 |
| H | 6.50440 | -3.39350 | 1.67000 |
| H | -0.23770 | -1.32280 | 2.61220 |
| H | 0.36110 | -1.75410 | 5.61190 |
| H | 1.62160 | 0.18700 | 4.67450 |
| H | 0.11480 | 0.88210 | 4.07740 |
| H | 0.38220 | 0.71360 | 5.80970 |
| H | 11.53170 | -2.83870 | -1.42040 |
| H | -3.20670 | -1.99540 | 5.54810 |
| H | -2.11810 | -2.90910 | 4.50930 |
| H | -1.74000 | -2.69700 | 6.22750 |

| Marilzafurollene C_191 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.35890 | -0.17730 | 0.75940 |
| O | 4.58640 | -0.79730 | 1.14260 |
| C | 2.24820 | -0.49900 | 1.77720 |
| C | 3.10420 | -0.61170 | -0.68940 |
| C | 5.18580 | -1.43770 | 0.01490 |
| C | 1.96270 | -2.00050 | 1.96850 |
| Br | 0.57620 | 0.43430 | 1.22100 |
| C | 4.51060 | -0.81420 | -1.21360 |
| C | 6.72360 | -1.34670 | 0.07050 |
| C | 1.03650 | -2.26510 | 3.13930 |
| Cl | 5.22460 | 0.76690 | -1.65220 |
| C | 7.33460 | -2.11900 | 1.25280 |
| C | 8.84770 | -2.15810 | 1.16900 |
| O | 6.95480 | -1.47800 | 2.45090 |
| C | 9.53900 | -3.27150 | 1.08000 |
| C | 1.36670 | -2.98590 | 4.22530 |
| C | 0.45500 | -3.26620 | 5.40930 |
| C | 0.90930 | -2.47990 | 6.64160 |
| O | -0.89710 | -2.90640 | 5.15260 |
| C | 10.21590 | -4.39070 | 0.97860 |
| Br | 10.65830 | -5.20830 | -0.76930 |
| C | -1.62280 | -3.87510 | 4.40670 |
| H | 3.53670 | 0.89940 | 0.76730 |
| H | 2.53850 | -0.07060 | 2.73810 |
| H | 2.56440 | -1.55680 | -0.73050 |
| H | 2.53210 | 0.12160 | -1.25870 |
| H | 4.89150 | -2.48800 | 0.05640 |
| H | 1.51140 | -2.42640 | 1.07310 |
| H | 2.89940 | -2.53470 | 2.13260 |
| H | 4.55060 | -1.45680 | -2.09390 |
| H | 7.12380 | -1.75350 | -0.85940 |
| H | 7.04540 | -0.30520 | 0.10800 |
| H | 0.04860 | -1.83070 | 3.07090 |
| H | 6.93890 | -3.13710 | 1.26510 |
| H | 9.35060 | -1.20220 | 1.18720 |
| H | 6.06920 | -1.14670 | 2.32370 |
| H | 2.35720 | -3.41270 | 4.29460 |
| H | 0.51450 | -4.33100 | 5.64250 |
| H | 1.93430 | -2.73020 | 6.91590 |
| H | 0.86210 | -1.40570 | 6.46080 |
| H | 0.27280 | -2.70050 | 7.49860 |
| H | 10.59000 | -4.96370 | 1.81450 |
| H | -1.16210 | -4.07320 | 3.43860 |
| H | -1.69780 | -4.81560 | 4.95390 |
| H | -2.63500 | -3.51290 | 4.22690 |

| Marilzafurollene C_192 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.56280 | -2.25620 | 1.44010 |
| O | 4.75570 | -2.29190 | 2.22250 |
| C | 2.67150 | -3.47890 | 1.74220 |
| C | 4.01560 | -2.12780 | -0.01870 |
| C | 5.90260 | -2.18050 | 1.38410 |
| C | 2.16830 | -3.53650 | 3.19560 |
| Br | 3.69470 | -5.15630 | 1.39180 |
| C | 5.37720 | -1.48080 | 0.12110 |
| C | 7.06530 | -1.51890 | 2.15630 |
| C | 1.23850 | -2.39290 | 3.55540 |
| Cl | 5.17640 | 0.28260 | 0.35290 |
| C | 8.44590 | -1.61430 | 1.47430 |
| C | 8.56710 | -0.71550 | 0.25910 |
| O | 9.42490 | -1.23240 | 2.41820 |
| C | 8.86830 | -1.15600 | -0.94110 |
| C | -0.06640 | -2.53420 | 3.84170 |
| C | -0.99550 | -1.39090 | 4.20570 |
| C | -2.14160 | -1.27800 | 3.19730 |
| O | -1.58080 | -1.59100 | 5.48390 |
| C | 9.12280 | -1.60890 | -2.14550 |
| Br | 7.68360 | -2.19420 | -3.37120 |
| C | -0.67800 | -1.43400 | 6.57040 |
| H | 3.03600 | -1.33870 | 1.70360 |
| H | 1.81520 | -3.48480 | 1.06610 |
| H | 4.12920 | -3.10730 | -0.48310 |
| H | 3.32420 | -1.54970 | -0.63220 |
| H | 6.19110 | -3.19950 | 1.11960 |
| H | 1.64640 | -4.48050 | 3.35630 |
| H | 3.01400 | -3.53190 | 3.88450 |
| H | 6.00330 | -1.64110 | -0.75610 |
| H | 6.82950 | -0.48440 | 2.40560 |
| H | 7.13430 | -2.03240 | 3.11620 |
| H | 1.68210 | -1.40760 | 3.58010 |
| H | 8.63780 | -2.65340 | 1.19710 |
| H | 8.38360 | 0.33680 | 0.42590 |
| H | 10.28080 | -1.45460 | 2.07970 |
| H | -0.51660 | -3.51650 | 3.82310 |
| H | -0.44030 | -0.45070 | 4.20180 |
| H | -1.76400 | -1.10550 | 2.18910 |
| H | -2.74440 | -2.18630 | 3.18030 |
| H | -2.80050 | -0.44760 | 3.45140 |
| H | 10.10830 | -1.70730 | -2.57730 |
| H | 0.12720 | -2.16870 | 6.53770 |
| H | -0.23940 | -0.43550 | 6.57860 |
| H | -1.21280 | -1.57100 | 7.51020 |

| Marilzafurollene C_193 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.91440 | -0.71900 | 0.54450 |
| O | 3.64620 | -1.89200 | 0.18090 |
| C | 1.40590 | -0.95860 | 0.33290 |
| C | 3.51070 | 0.42660 | -0.28720 |
| C | 4.89600 | -1.52580 | -0.39650 |
| C | 0.84810 | -2.11030 | 1.18780 |
| Br | 1.06500 | -1.39160 | -1.58410 |
| C | 4.49960 | -0.28150 | -1.19410 |
| C | 5.94090 | -1.30460 | 0.72440 |
| C | 0.97450 | -1.85370 | 2.67750 |
| Cl | 5.87470 | 0.75800 | -1.65930 |
| C | 6.22420 | -2.56960 | 1.55510 |
| C | 7.38160 | -2.36140 | 2.51160 |
| O | 5.06670 | -2.89130 | 2.29500 |
| C | 8.48700 | -3.06990 | 2.47500 |
| C | 1.77380 | -2.56160 | 3.49650 |
| C | 1.96710 | -2.35120 | 4.99380 |
| C | 1.23640 | -1.12210 | 5.55260 |
| O | 1.50270 | -3.46930 | 5.73810 |
| C | 9.59010 | -3.77790 | 2.41990 |
| Br | 11.14320 | -3.23890 | 1.31710 |
| C | 2.33000 | -4.62210 | 5.65440 |
| H | 3.10960 | -0.50900 | 1.59730 |
| H | 0.85380 | -0.04330 | 0.55210 |
| H | 2.76840 | 0.99120 | -0.85200 |
| H | 4.02820 | 1.12670 | 0.36960 |
| H | 5.24260 | -2.31520 | -1.06460 |
| H | -0.20680 | -2.26390 | 0.95870 |
| H | 1.35670 | -3.03980 | 0.92820 |
| H | 3.99490 | -0.59020 | -2.11120 |
| H | 6.87710 | -0.98720 | 0.26310 |
| H | 5.64330 | -0.48650 | 1.38120 |
| H | 0.37470 | -1.04360 | 3.06490 |
| H | 6.44590 | -3.40120 | 0.88220 |
| H | 7.25590 | -1.58230 | 3.24920 |
| H | 4.32710 | -2.77470 | 1.70340 |
| H | 2.36130 | -3.36180 | 3.07060 |
| H | 3.03510 | -2.21160 | 5.17210 |
| H | 1.55620 | -0.20720 | 5.05340 |
| H | 0.15600 | -1.21610 | 5.44150 |
| H | 1.44540 | -1.00410 | 6.61590 |
| H | 9.75860 | -4.70070 | 2.95560 |
| H | 1.93030 | -5.40180 | 6.30280 |
| H | 2.36820 | -5.02500 | 4.64240 |
| H | 3.34720 | -4.40540 | 5.98320 |

| Marilzafurollene C_194 | | | |
|-------------------------------|---------|----------|----------|
| C | 2.99570 | -0.78530 | -0.27320 |
| O | 3.98740 | -0.84810 | 0.75250 |
| C | 2.31860 | -2.15510 | -0.50160 |
| C | 3.70600 | -0.22000 | -1.51300 |
| C | 5.25900 | -0.48900 | 0.23090 |
| C | 1.47270 | -2.66160 | 0.68470 |
| Br | 3.67960 | -3.53780 | -0.97880 |
| C | 4.92770 | 0.45860 | -0.92790 |
| C | 6.18420 | 0.07300 | 1.32770 |
| C | 2.28120 | -2.89760 | 1.94570 |
| Cl | 4.47760 | 2.09660 | -0.36560 |
| C | 6.45250 | -0.90080 | 2.49000 |
| C | 7.12640 | -2.18720 | 2.05070 |
| O | 7.28800 | -0.23960 | 3.41880 |
| C | 6.72580 | -3.37880 | 2.43330 |
| C | 1.94790 | -2.46150 | 3.17080 |
| C | 2.79370 | -2.69090 | 4.40860 |
| C | 3.07790 | -1.37020 | 5.12830 |
| O | 2.13690 | -3.54370 | 5.33460 |
| C | 6.36190 | -4.56410 | 2.86340 |
| Br | 5.01900 | -5.68370 | 1.93830 |
| C | 2.05950 | -4.90050 | 4.91750 |
| H | 2.24590 | -0.06440 | 0.05610 |
| H | 1.65870 | -2.06890 | -1.36590 |
| H | 4.02790 | -1.02110 | -2.17820 |
| H | 3.07670 | 0.45430 | -2.09440 |
| H | 5.70500 | -1.39200 | -0.18920 |
| H | 0.66690 | -1.95770 | 0.89590 |
| H | 0.99870 | -3.60430 | 0.40990 |
| H | 5.74540 | 0.55870 | -1.64230 |
| H | 7.12940 | 0.37620 | 0.87600 |
| H | 5.74430 | 0.97880 | 1.74480 |
| H | 3.19500 | -3.45900 | 1.82060 |
| H | 5.50540 | -1.13010 | 2.98350 |
| H | 7.97440 | -2.08130 | 1.38970 |
| H | 7.28470 | -0.72620 | 4.23060 |
| H | 1.03210 | -1.90720 | 3.31510 |
| H | 3.74810 | -3.13590 | 4.11960 |
| H | 3.58420 | -0.66390 | 4.46980 |
| H | 2.15540 | -0.90300 | 5.47370 |
| H | 3.71440 | -1.53120 | 5.99830 |
| H | 6.75130 | -5.04000 | 3.75150 |
| H | 1.58230 | -5.49420 | 5.69710 |
| H | 1.46820 | -5.01220 | 4.00810 |
| H | 3.05180 | -5.31750 | 4.74030 |

| Marilzafurollene C_195 | | | |
|-------------------------------|----------|----------|----------|
| C | 2.68100 | -0.48820 | 0.64760 |
| O | 3.60900 | -1.43690 | 0.12580 |
| C | 1.23600 | -0.86110 | 0.26200 |
| C | 3.18280 | 0.88040 | 0.16720 |
| C | 4.89080 | -0.82770 | 0.04220 |
| C | 0.82080 | -2.25640 | 0.76810 |
| Br | 1.04790 | -0.84060 | -1.72330 |
| C | 4.50640 | 0.55070 | -0.50660 |
| C | 5.57400 | -0.84380 | 1.43380 |
| C | 1.00050 | -2.42270 | 2.26680 |
| Cl | 5.74560 | 1.81020 | -0.24920 |
| C | 5.75110 | -2.25970 | 2.01820 |
| C | 6.80650 | -3.07150 | 1.27280 |
| O | 6.03980 | -2.14800 | 3.40200 |
| C | 7.90080 | -3.57550 | 1.80050 |
| C | 1.99640 | -3.13910 | 2.81480 |
| C | 2.24840 | -3.30880 | 4.29940 |
| C | 2.39520 | -4.78810 | 4.66310 |
| O | 3.45660 | -2.65740 | 4.67500 |
| C | 8.99750 | -4.06100 | 2.33250 |
| Br | 9.09260 | -5.87920 | 3.11210 |
| C | 3.29930 | -1.26350 | 4.91110 |
| H | 2.76780 | -0.49990 | 1.73300 |
| H | 0.54870 | -0.11000 | 0.65370 |
| H | 2.50000 | 1.37470 | -0.52400 |
| H | 3.32710 | 1.54370 | 1.02070 |
| H | 5.51010 | -1.36130 | -0.67890 |
| H | -0.21930 | -2.45850 | 0.51140 |
| H | 1.41590 | -3.01190 | 0.25280 |
| H | 4.34430 | 0.46660 | -1.58250 |
| H | 6.55040 | -0.36210 | 1.37170 |
| H | 4.99930 | -0.23610 | 2.13220 |
| H | 0.28920 | -1.91340 | 2.90140 |
| H | 4.81130 | -2.80450 | 1.93600 |
| H | 6.60530 | -3.23430 | 0.22430 |
| H | 5.27430 | -2.44190 | 3.89000 |
| H | 2.69780 | -3.63900 | 2.16270 |
| H | 1.40690 | -2.90100 | 4.86360 |
| H | 1.49620 | -5.34840 | 4.40510 |
| H | 3.23690 | -5.24350 | 4.14060 |
| H | 2.56540 | -4.90900 | 5.73310 |
| H | 9.93680 | -3.53190 | 2.39470 |
| H | 2.93390 | -0.74310 | 4.02660 |
| H | 2.60650 | -1.07920 | 5.73320 |
| H | 4.25910 | -0.82430 | 5.18330 |

| Marilzafurollene C_196 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.14600 | -2.46630 | 1.04130 |
| O | 4.20130 | -2.83880 | 1.92660 |
| C | 2.18380 | -3.64720 | 0.80060 |
| C | 3.82520 | -1.91520 | -0.21640 |
| C | 5.46630 | -2.50670 | 1.36050 |
| C | 1.44720 | -4.09950 | 2.07320 |
| Br | 3.20340 | -5.21110 | 0.09600 |
| C | 5.14570 | -1.41420 | 0.32810 |
| C | 6.48150 | -2.18150 | 2.47820 |
| C | 0.51980 | -3.03670 | 2.63150 |
| Cl | 4.90580 | 0.19090 | 1.08350 |
| C | 7.95530 | -2.11150 | 2.02750 |
| C | 8.26310 | -0.87520 | 1.20520 |
| O | 8.76470 | -2.09730 | 3.18500 |
| C | 8.75840 | -0.91790 | -0.01060 |
| C | 0.63360 | -2.50250 | 3.85900 |
| C | -0.28120 | -1.43030 | 4.42080 |
| C | -1.05070 | -1.95240 | 5.63660 |
| O | 0.45510 | -0.29420 | 4.85070 |
| C | 9.20890 | -0.96890 | -1.24140 |
| Br | 7.99300 | -1.06420 | -2.79980 |
| C | 1.05280 | 0.45310 | 3.79980 |
| H | 2.60760 | -1.64480 | 1.51480 |
| H | 1.45470 | -3.37630 | 0.03590 |
| H | 4.01150 | -2.70810 | -0.94100 |
| H | 3.24150 | -1.14070 | -0.71440 |
| H | 5.80450 | -3.39640 | 0.82620 |
| H | 0.84880 | -4.98410 | 1.85410 |
| H | 2.17280 | -4.39690 | 2.83200 |
| H | 5.90350 | -1.31640 | -0.44870 |
| H | 6.19760 | -1.27410 | 3.01120 |
| H | 6.39880 | -2.98020 | 3.21650 |
| H | -0.27480 | -2.70450 | 1.97870 |
| H | 8.20000 | -3.01310 | 1.46110 |
| H | 8.04510 | 0.07410 | 1.67440 |
| H | 9.66630 | -2.23570 | 2.93100 |
| H | 1.42720 | -2.83370 | 4.51390 |
| H | -1.00250 | -1.12810 | 3.65910 |
| H | -1.65700 | -2.82030 | 5.37620 |
| H | -0.37170 | -2.24460 | 6.43800 |
| H | -1.71880 | -1.18650 | 6.03070 |
| H | 10.25230 | -0.96590 | -1.52210 |
| H | 1.81200 | -0.12550 | 3.27280 |
| H | 0.30720 | 0.79110 | 3.07910 |
| H | 1.54110 | 1.33520 | 4.21360 |

| Marilzafurollene C_197 | | | |
|-------------------------------|---------|----------|----------|
| C | 2.95660 | 0.07420 | 0.18980 |
| O | 4.00500 | -0.55340 | 0.92630 |
| C | 1.62140 | 0.07840 | 0.96760 |
| C | 2.95140 | -0.60040 | -1.18790 |
| C | 4.73340 | -1.44430 | 0.07990 |
| C | 1.02580 | -1.29170 | 1.35550 |
| Br | 0.27220 | 1.05050 | -0.12950 |
| C | 4.40290 | -1.00410 | -1.35090 |
| C | 6.22370 | -1.48050 | 0.46770 |
| C | 1.83330 | -2.02560 | 2.41020 |
| Cl | 5.37340 | 0.40840 | -1.86480 |
| C | 6.46730 | -2.09170 | 1.85920 |
| C | 7.94700 | -2.25510 | 2.14430 |
| O | 5.89980 | -1.24140 | 2.83190 |
| C | 8.51340 | -3.41550 | 2.38520 |
| C | 1.41130 | -2.27600 | 3.66030 |
| C | 2.22950 | -3.00550 | 4.70980 |
| C | 2.46550 | -2.11580 | 5.93270 |
| O | 1.56000 | -4.17300 | 5.16300 |
| C | 9.06760 | -4.58270 | 2.61250 |
| Br | 9.79500 | -5.71270 | 1.15890 |
| C | 1.52350 | -5.22990 | 4.21400 |
| H | 3.26630 | 1.11140 | 0.05100 |
| H | 1.75270 | 0.66980 | 1.87530 |
| H | 2.32550 | -1.49150 | -1.18920 |
| H | 2.59510 | 0.05670 | -1.98200 |
| H | 4.30860 | -2.43960 | 0.22160 |
| H | 0.90430 | -1.93350 | 0.48420 |
| H | 0.02100 | -1.13290 | 1.74920 |
| H | 4.54700 | -1.79710 | -2.08570 |
| H | 6.75840 | -2.07380 | -0.27560 |
| H | 6.65510 | -0.47950 | 0.42330 |
| H | 2.81530 | -2.36310 | 2.11600 |
| H | 5.97050 | -3.06270 | 1.92030 |
| H | 8.53560 | -1.34920 | 2.14260 |
| H | 5.13940 | -0.82410 | 2.43390 |
| H | 0.42960 | -1.94970 | 3.97270 |
| H | 3.20120 | -3.27960 | 4.29340 |
| H | 3.06410 | -2.63640 | 6.68030 |
| H | 1.52420 | -1.82860 | 6.40180 |
| H | 2.99800 | -1.20470 | 5.65830 |
| H | 9.18000 | -5.03310 | 3.58800 |
| H | 0.97340 | -4.94870 | 3.31540 |
| H | 2.52960 | -5.53690 | 3.92580 |
| H | 1.02350 | -6.09410 | 4.65130 |

| Marilzafurollene C_198 | | | |
|-------------------------------|----------|----------|----------|
| C | 4.22500 | -0.78850 | 1.75910 |
| O | 4.98340 | -2.00060 | 1.79020 |
| C | 3.17090 | -0.82190 | 2.88180 |
| C | 3.67510 | -0.66710 | 0.32860 |
| C | 5.28660 | -2.42620 | 0.46220 |
| C | 2.15550 | -1.97490 | 2.76780 |
| Br | 2.20180 | 0.92070 | 2.90200 |
| C | 4.01990 | -2.00740 | -0.28790 |
| C | 6.60020 | -1.75870 | -0.01220 |
| C | 1.23480 | -2.05610 | 3.96970 |
| Cl | 4.20940 | -1.92270 | -2.06090 |
| C | 7.83340 | -2.18170 | 0.80600 |
| C | 9.11750 | -1.67390 | 0.18030 |
| O | 7.71630 | -1.65300 | 2.10870 |
| C | 10.07930 | -2.46340 | -0.24020 |
| C | -0.10320 | -1.95150 | 3.90990 |
| C | -1.02720 | -2.02770 | 5.11080 |
| C | -1.82640 | -0.73140 | 5.26510 |
| O | -1.96540 | -3.08480 | 4.97200 |
| C | 11.02730 | -3.26400 | -0.66630 |
| Br | 11.06980 | -3.96870 | -2.51570 |
| C | -1.40510 | -4.38400 | 5.10470 |
| H | 4.90980 | 0.04110 | 1.94320 |
| H | 3.69380 | -0.89510 | 3.83670 |
| H | 2.60940 | -0.44410 | 0.27780 |
| H | 4.19770 | 0.13530 | -0.19340 |
| H | 5.40330 | -3.51040 | 0.43640 |
| H | 1.56230 | -1.87340 | 1.85890 |
| H | 2.68390 | -2.92590 | 2.69180 |
| H | 3.22350 | -2.72280 | -0.07830 |
| H | 6.77500 | -2.04410 | -1.05030 |
| H | 6.50880 | -0.67200 | -0.01550 |
| H | 1.71280 | -2.20730 | 4.92710 |
| H | 7.86410 | -3.27140 | 0.87690 |
| H | 9.21310 | -0.60150 | 0.09260 |
| H | 6.81530 | -1.79190 | 2.38590 |
| H | -0.58640 | -1.80000 | 2.95540 |
| H | -0.43870 | -2.17860 | 6.01800 |
| H | -1.16440 | 0.12610 | 5.38920 |
| H | -2.45390 | -0.54750 | 4.39270 |
| H | -2.47720 | -0.77830 | 6.13840 |
| H | 11.85770 | -3.61010 | -0.06840 |
| H | -2.19420 | -5.13090 | 5.01770 |
| H | -0.66820 | -4.58890 | 4.32740 |
| H | -0.93050 | -4.51200 | 6.07840 |

| Marilzafurollene C_199 | | | |
|-------------------------------|----------|----------|----------|
| C | 4.07390 | -0.11160 | 1.39090 |
| O | 4.92020 | -1.22370 | 1.09060 |
| C | 2.68290 | -0.61010 | 1.82640 |
| C | 4.07040 | 0.77190 | 0.13420 |
| C | 5.74510 | -0.92850 | -0.03240 |
| C | 2.74080 | -1.45010 | 3.11360 |
| Br | 1.86890 | -1.70460 | 0.36790 |
| C | 4.79870 | -0.08130 | -0.88550 |
| C | 7.03430 | -0.21880 | 0.44800 |
| C | 1.36370 | -1.82440 | 3.62750 |
| Cl | 5.61040 | 0.89060 | -2.14470 |
| C | 7.91870 | -1.09860 | 1.34990 |
| C | 8.53570 | -2.25990 | 0.59200 |
| O | 8.95350 | -0.29070 | 1.87370 |
| C | 8.31420 | -3.52100 | 0.88750 |
| C | 0.92970 | -3.08600 | 3.78500 |
| C | -0.44790 | -3.46580 | 4.29440 |
| C | -1.20910 | -4.28220 | 3.24690 |
| O | -0.36260 | -4.26320 | 5.46680 |
| C | 8.07890 | -4.78360 | 1.15870 |
| Br | 6.59340 | -5.78880 | 0.32100 |
| C | 0.06530 | -3.55720 | 6.62350 |
| H | 4.52670 | 0.45100 | 2.20900 |
| H | 2.02920 | 0.24920 | 1.98290 |
| H | 3.07240 | 1.05470 | -0.20170 |
| H | 4.62680 | 1.68960 | 0.32790 |
| H | 6.00290 | -1.84870 | -0.55760 |
| H | 3.33250 | -2.35050 | 2.94110 |
| H | 3.24990 | -0.89040 | 3.89890 |
| H | 4.08680 | -0.73840 | -1.38750 |
| H | 7.62150 | 0.10420 | -0.41210 |
| H | 6.77190 | 0.69240 | 0.98580 |
| H | 0.70670 | -1.00310 | 3.87500 |
| H | 7.32060 | -1.46820 | 2.18680 |
| H | 9.18550 | -1.99850 | -0.23150 |
| H | 9.37950 | -0.76220 | 2.57560 |
| H | 1.58360 | -3.91030 | 3.53790 |
| H | -1.02170 | -2.56210 | 4.50910 |
| H | -1.32260 | -3.72170 | 2.31840 |
| H | -0.68840 | -5.21190 | 3.01590 |
| H | -2.20610 | -4.53970 | 3.60450 |
| H | 8.65490 | -5.38690 | 1.84530 |
| H | 0.07040 | -4.23150 | 7.47980 |
| H | 1.07520 | -3.16270 | 6.50690 |
| H | -0.60820 | -2.73060 | 6.85360 |

| Marilzafurollene C_200 | | | |
|-------------------------------|----------|----------|----------|
| C | 4.19260 | -1.14040 | 1.66720 |
| O | 4.32980 | -1.79690 | 0.40390 |
| C | 2.71920 | -1.17400 | 2.11390 |
| C | 4.77170 | 0.26990 | 1.47910 |
| C | 5.28160 | -1.11100 | -0.40650 |
| C | 2.21430 | -2.60710 | 2.35240 |
| Br | 1.57790 | -0.29430 | 0.73110 |
| C | 5.01780 | 0.34480 | -0.01490 |
| C | 6.70260 | -1.64470 | -0.10110 |
| C | 0.81050 | -2.63990 | 2.92470 |
| Cl | 6.33490 | 1.47220 | -0.44200 |
| C | 6.89630 | -3.13290 | -0.47640 |
| C | 8.32070 | -3.65700 | -0.34650 |
| O | 6.05160 | -3.91540 | 0.33880 |
| C | 9.36870 | -2.95940 | 0.03380 |
| C | 0.48820 | -3.15120 | 4.12450 |
| C | -0.91710 | -3.18160 | 4.69600 |
| C | -1.36220 | -4.61970 | 4.97330 |
| O | -0.98540 | -2.47710 | 5.92720 |
| C | 10.41340 | -2.27040 | 0.42860 |
| Br | 10.94290 | -2.13620 | 2.33150 |
| C | -0.89080 | -1.06520 | 5.79720 |
| H | 4.80430 | -1.67090 | 2.39900 |
| H | 2.60960 | -0.59860 | 3.03480 |
| H | 4.11320 | 1.06550 | 1.82890 |
| H | 5.71270 | 0.35640 | 2.02370 |
| H | 5.05460 | -1.26890 | -1.46160 |
| H | 2.22470 | -3.16790 | 1.41690 |
| H | 2.88990 | -3.12710 | 3.03290 |
| H | 4.11370 | 0.69270 | -0.51710 |
| H | 7.41400 | -1.05160 | -0.67650 |
| H | 6.95840 | -1.48750 | 0.94740 |
| H | 0.03450 | -2.21660 | 2.30220 |
| H | 6.59190 | -3.27760 | -1.51440 |
| H | 8.44200 | -4.70130 | -0.59530 |
| H | 5.22700 | -3.44190 | 0.41880 |
| H | 1.25860 | -3.57580 | 4.75200 |
| H | -1.61390 | -2.73780 | 3.98220 |
| H | -1.34920 | -5.21860 | 4.06230 |
| H | -0.71070 | -5.10190 | 5.70250 |
| H | -2.37730 | -4.64130 | 5.37020 |
| H | 11.07310 | -1.72010 | -0.22620 |
| H | 0.06740 | -0.76030 | 5.37520 |
| H | -1.69000 | -0.67200 | 5.16770 |
| H | -0.98210 | -0.60250 | 6.77990 |

| Marilzafurollene C_201 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.61860 | -0.54180 | 1.43550 |
| O | 4.47670 | -1.66270 | 1.64750 |
| C | 2.16330 | -0.88350 | 1.80670 |
| C | 3.83290 | -0.10980 | -0.02010 |
| C | 5.23500 | -1.92950 | 0.47000 |
| C | 2.00690 | -1.19300 | 3.30510 |
| Br | 1.54550 | -2.46260 | 0.75060 |
| C | 5.23710 | -0.60300 | -0.29970 |
| C | 6.60540 | -2.53680 | 0.82760 |
| C | 0.56050 | -1.40500 | 3.70940 |
| Cl | 6.42340 | 0.56340 | 0.36060 |
| C | 7.53530 | -2.78560 | -0.37640 |
| C | 8.85870 | -3.37720 | 0.06890 |
| O | 6.91240 | -3.67670 | -1.27850 |
| C | 10.02210 | -2.80960 | -0.15590 |
| C | 0.08290 | -2.53710 | 4.25260 |
| C | -1.36340 | -2.75610 | 4.65470 |
| C | -1.97230 | -3.92660 | 3.87870 |
| O | -1.47330 | -3.06640 | 6.03640 |
| C | 11.18850 | -2.24500 | -0.36220 |
| Br | 11.99380 | -0.97110 | 0.92090 |
| C | -1.21090 | -1.97170 | 6.90360 |
| H | 3.97660 | 0.25990 | 2.08350 |
| H | 1.51950 | -0.04520 | 1.53750 |
| H | 3.13470 | -0.61830 | -0.68530 |
| H | 3.71360 | 0.96330 | -0.17110 |
| H | 4.66600 | -2.65840 | -0.11010 |
| H | 2.59980 | -2.07180 | 3.56370 |
| H | 2.40220 | -0.36750 | 3.89770 |
| H | 5.44010 | -0.73280 | -1.36330 |
| H | 7.11000 | -1.88450 | 1.54110 |
| H | 6.43690 | -3.47490 | 1.35760 |
| H | -0.10990 | -0.57530 | 3.53730 |
| H | 7.71860 | -1.84330 | -0.89710 |
| H | 8.80450 | -4.31590 | 0.60180 |
| H | 7.47790 | -3.79720 | -2.02860 |
| H | 0.75050 | -3.36910 | 4.42540 |
| H | -1.94510 | -1.85860 | 4.43530 |
| H | -1.93190 | -3.74860 | 2.80370 |
| H | -1.44130 | -4.85620 | 4.08490 |
| H | -3.01710 | -4.07280 | 4.15300 |
| H | 11.81130 | -2.41190 | -1.22900 |
| H | -1.35040 | -2.28580 | 7.93790 |
| H | -0.18670 | -1.61110 | 6.80250 |
| H | -1.89360 | -1.14290 | 6.71150 |

| Marilzafurollene C_202 | | | |
|-------------------------------|----------|----------|----------|
| C | 4.08130 | -0.38230 | 1.29690 |
| O | 5.49840 | -0.54580 | 1.25580 |
| C | 3.45130 | -1.58150 | 2.02820 |
| C | 3.64570 | -0.22130 | -0.16820 |
| C | 5.94860 | -0.61080 | -0.09080 |
| C | 1.92230 | -1.47500 | 2.16590 |
| Br | 4.24870 | -1.69280 | 3.85360 |
| C | 4.92010 | 0.22000 | -0.86040 |
| C | 7.42320 | -0.17710 | -0.20780 |
| C | 1.31360 | -2.70950 | 2.80220 |
| Cl | 5.15470 | 1.97750 | -0.62420 |
| C | 8.38250 | -1.08800 | 0.58160 |
| C | 8.39270 | -2.51410 | 0.06300 |
| O | 9.68990 | -0.55880 | 0.49860 |
| C | 7.88790 | -3.52510 | 0.73290 |
| C | 0.58960 | -2.70300 | 3.93370 |
| C | -0.01390 | -3.93780 | 4.57600 |
| C | 0.54110 | -4.14260 | 5.98770 |
| O | -1.42460 | -3.82070 | 4.69230 |
| C | 7.32880 | -4.50910 | 1.39590 |
| Br | 5.41880 | -4.97880 | 1.16580 |
| C | -2.12170 | -3.91090 | 3.45720 |
| H | 3.87660 | 0.53880 | 1.84460 |
| H | 3.72140 | -2.50410 | 1.51320 |
| H | 3.32940 | -1.18140 | -0.57830 |
| H | 2.82200 | 0.48200 | -0.29400 |
| H | 5.84670 | -1.64640 | -0.41930 |
| H | 1.66200 | -0.58860 | 2.74620 |
| H | 1.46300 | -1.35190 | 1.18500 |
| H | 4.92100 | 0.01700 | -1.93190 |
| H | 7.71370 | -0.15810 | -1.25890 |
| H | 7.52730 | 0.84460 | 0.15750 |
| H | 1.49170 | -3.64560 | 2.29230 |
| H | 8.08600 | -1.08830 | 1.63360 |
| H | 8.84210 | -2.66700 | -0.90720 |
| H | 9.74870 | 0.18940 | 1.07630 |
| H | 0.40910 | -1.77000 | 4.44810 |
| H | 0.23130 | -4.81880 | 3.97940 |
| H | 1.62590 | -4.25280 | 5.97090 |
| H | 0.29960 | -3.29830 | 6.63370 |
| H | 0.12230 | -5.04010 | 6.44300 |
| H | 7.83430 | -5.14110 | 2.11140 |
| H | -1.85050 | -3.10130 | 2.77880 |
| H | -1.92560 | -4.86250 | 2.96150 |
| H | -3.19420 | -3.84460 | 3.63950 |

| Marilzafurollene C_203 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.18870 | -1.15730 | 0.57750 |
| O | 4.46440 | -1.24500 | 1.21230 |
| C | 2.75450 | -2.53070 | 0.02140 |
| C | 3.30380 | -0.04150 | -0.47310 |
| C | 5.39240 | -0.40060 | 0.54470 |
| C | 2.64930 | -3.61890 | 1.10370 |
| Br | 4.06260 | -3.15970 | -1.34860 |
| C | 4.52180 | 0.73280 | -0.01110 |
| C | 6.56000 | 0.01940 | 1.45970 |
| C | 1.56940 | -3.33310 | 2.12980 |
| Cl | 4.02920 | 1.89790 | 1.25460 |
| C | 7.32500 | -1.15800 | 2.09240 |
| C | 7.86300 | -2.14530 | 1.07310 |
| O | 8.40290 | -0.62520 | 2.83560 |
| C | 7.67000 | -3.44220 | 1.16130 |
| C | 1.79820 | -3.16840 | 3.44320 |
| C | 0.72540 | -2.87530 | 4.47520 |
| C | 0.62990 | -4.00920 | 5.49900 |
| O | 1.01130 | -1.68570 | 5.19690 |
| C | 7.50570 | -4.73740 | 1.29560 |
| Br | 5.94700 | -5.71070 | 0.56150 |
| C | 0.90450 | -0.49320 | 4.43130 |
| H | 2.48130 | -0.83260 | 1.34100 |
| H | 1.79540 | -2.43080 | -0.48810 |
| H | 3.49450 | -0.44970 | -1.46520 |
| H | 2.40560 | 0.57270 | -0.54140 |
| H | 5.79130 | -0.96230 | -0.30140 |
| H | 2.42330 | -4.57810 | 0.63710 |
| H | 3.61370 | -3.73940 | 1.59980 |
| H | 5.00710 | 1.28820 | -0.81430 |
| H | 7.24880 | 0.64130 | 0.88690 |
| H | 6.18900 | 0.64750 | 2.26930 |
| H | 0.55910 | -3.26230 | 1.75300 |
| H | 6.65570 | -1.67460 | 2.78480 |
| H | 8.42110 | -1.72780 | 0.24780 |
| H | 8.72820 | -1.29640 | 3.41850 |
| H | 2.80850 | -3.23810 | 3.82120 |
| H | -0.24220 | -2.77540 | 3.97960 |
| H | 0.39340 | -4.95750 | 5.01570 |
| H | 1.56820 | -4.13240 | 6.04050 |
| H | -0.15150 | -3.80550 | 6.23130 |
| H | 8.19130 | -5.39180 | 1.81370 |
| H | 1.64180 | -0.46070 | 3.62870 |
| H | -0.09060 | -0.38790 | 3.99730 |
| H | 1.08120 | 0.36860 | 5.07470 |

| Marilzafurollene C_204 | | | |
|-------------------------------|----------|----------|----------|
| C | 3.44010 | -0.87130 | 1.64350 |
| O | 4.62140 | -1.63800 | 1.87650 |
| C | 2.18160 | -1.66590 | 2.03980 |
| C | 3.49690 | -0.43570 | 0.17440 |
| C | 5.42530 | -1.67060 | 0.69920 |
| C | 2.13500 | -1.95920 | 3.54870 |
| Br | 2.12450 | -3.39210 | 1.03560 |
| C | 4.98480 | -0.44250 | -0.10670 |
| C | 6.91970 | -1.77160 | 1.06110 |
| C | 0.83860 | -2.62220 | 3.97220 |
| Cl | 5.71820 | 1.07060 | 0.50810 |
| C | 7.88050 | -1.71950 | -0.14320 |
| C | 9.33440 | -1.74680 | 0.31500 |
| O | 7.58060 | -2.78360 | -1.03170 |
| C | 10.22820 | -2.65350 | -0.01580 |
| C | -0.04600 | -2.08820 | 4.83080 |
| C | -1.34340 | -2.75290 | 5.25150 |
| C | -1.37710 | -2.97400 | 6.76580 |
| O | -2.46410 | -1.94570 | 4.92080 |
| C | 11.10810 | -3.56220 | -0.36420 |
| Br | 12.24230 | -3.37500 | -1.97570 |
| C | -2.75050 | -1.88750 | 3.53010 |
| H | 3.51260 | 0.02260 | 2.26510 |
| H | 1.29450 | -1.09780 | 1.75590 |
| H | 3.00670 | -1.16660 | -0.46890 |
| H | 3.02750 | 0.53180 | -0.00450 |
| H | 5.13340 | -2.56460 | 0.14470 |
| H | 2.96870 | -2.60490 | 3.82780 |
| H | 2.26140 | -1.03140 | 4.10820 |
| H | 5.21820 | -0.52940 | -1.16850 |
| H | 7.17040 | -0.97180 | 1.75850 |
| H | 7.07960 | -2.69970 | 1.61100 |
| H | 0.63850 | -3.59180 | 3.53800 |
| H | 7.73930 | -0.78180 | -0.68250 |
| H | 9.62210 | -0.93350 | 0.96640 |
| H | 8.19620 | -2.76030 | -1.75140 |
| H | 0.14790 | -1.11930 | 5.26810 |
| H | -1.43510 | -3.72380 | 4.76030 |
| H | -0.54800 | -3.60320 | 7.09030 |
| H | -1.31360 | -2.02870 | 7.30520 |
| H | -2.30330 | -3.46500 | 7.06500 |
| H | 11.29720 | -4.47810 | 0.17650 |
| H | -3.63780 | -1.27590 | 3.36660 |
| H | -1.93130 | -1.44020 | 2.96590 |
| H | -2.95070 | -2.88060 | 3.12600 |

Table S13. Calculated Energies (Hartrees) for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,12*S** of 5.

| Entry ID | Gas Phase Energy |
|-----------|------------------|
| 128.00000 | -1360,038652 |
| 129.00000 | -1360,036526 |
| 130.00000 | -1360,03812 |
| 131.00000 | -1360,037303 |
| 132.00000 | -1360,0373 |
| 133.00000 | -1360,037053 |
| 134.00000 | -1360,040298 |
| 135.00000 | -1360,034155 |
| 136.00000 | -1360,034866 |
| 137.00000 | -1360,037188 |
| 138.00000 | -1360,037237 |
| 139.00000 | -1360,039209 |
| 140.00000 | -1360,036278 |
| 141.00000 | -1360,036456 |
| 142.00000 | -1360,040141 |

Table S14. Coordinates (Angstroms) of calculated geometries for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,12*S** of 5.

| 12-Acetoxy-marilzafurenyne_128 | | | |
|--------------------------------|----------|----------|----------|
| C | 0.67890 | 0.89490 | -1.54770 |
| O | 1.37750 | 0.07050 | -0.61860 |
| C | -0.80300 | 0.48390 | -1.68790 |
| C | 1.52610 | 0.88920 | -2.82610 |
| C | 2.68170 | -0.23400 | -1.11610 |
| C | -1.08370 | -0.89030 | -2.33240 |
| Br | -1.72640 | 1.87200 | -2.77910 |
| C | 2.92730 | 0.74690 | -2.27100 |
| C | 3.72540 | -0.22940 | 0.01230 |
| C | -0.58650 | -2.10320 | -1.51650 |
| Cl | 3.51790 | 2.33870 | -1.70380 |
| C | 3.47800 | -1.33750 | 1.01550 |
| C | -1.36890 | -2.26450 | -0.22730 |
| O | -0.70600 | -3.28890 | -2.29100 |
| C | 4.35200 | -2.31770 | 1.29830 |
| C | -0.83460 | -2.15160 | 0.99920 |
| C | 4.06460 | -3.33640 | 2.25140 |
| C | 3.85490 | -4.21810 | 3.06970 |
| C | -1.61020 | -2.31020 | 2.28920 |
| C | 0.27020 | -3.63130 | -3.15000 |
| C | -0.00580 | -4.95110 | -3.85200 |
| O | 1.28460 | -2.97520 | -3.38720 |
| H | 0.70800 | 1.90160 | -1.12740 |
| H | -1.26460 | 0.51840 | -0.69990 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 1.30930 | 0.02340 | -3.44970 |
| H | 1.38940 | 1.78390 | -3.43410 |
| H | 2.63290 | -1.23680 | -1.54430 |
| H | -2.15920 | -0.99410 | -2.47880 |
| H | -0.66210 | -0.91150 | -3.33560 |
| H | 3.63970 | 0.36510 | -3.00320 |
| H | 4.72560 | -0.33590 | -0.40930 |
| H | 3.70640 | 0.72080 | 0.54640 |
| H | 0.46100 | -1.97810 | -1.25000 |
| H | 2.52140 | -1.30370 | 1.51870 |
| H | -2.42130 | -2.48410 | -0.33500 |
| H | 5.31180 | -2.36370 | 0.80410 |
| H | 0.21930 | -1.93020 | 1.09970 |
| H | 3.66920 | -4.98680 | 3.78650 |
| H | -2.66090 | -2.53270 | 2.09970 |
| H | -1.18980 | -3.12270 | 2.88250 |
| H | -1.55430 | -1.39340 | 2.87650 |
| H | 0.81880 | -5.20630 | -4.51720 |
| H | -0.91960 | -4.88100 | -4.44120 |
| H | -0.12190 | -5.74980 | -3.11990 |
| 12-Acetoxy-marilzafurenyne_129 | | | |
| C | 0.87100 | 0.50210 | -0.91300 |
| O | 1.42880 | -0.73050 | -0.46260 |
| C | -0.64600 | 0.35510 | -1.14820 |
| C | 1.71060 | 0.93170 | -2.12730 |
| C | 2.76180 | -0.86810 | -0.94550 |
| C | -1.07510 | -0.64260 | -2.24700 |
| Br | -1.37410 | 2.14960 | -1.61800 |
| C | 2.65200 | -0.23860 | -2.33680 |
| C | 3.73440 | -0.17350 | 0.03080 |
| C | -0.80700 | -2.13100 | -1.92950 |
| Cl | 4.21560 | 0.25570 | -3.04390 |
| C | 3.68620 | -0.79650 | 1.41180 |
| C | -1.52870 | -2.58170 | -0.67320 |
| O | -1.23760 | -2.93430 | -3.02070 |
| C | 4.74630 | -1.31990 | 2.04980 |
| C | -0.91140 | -3.00210 | 0.44300 |
| C | 4.63800 | -1.89430 | 3.34880 |
| C | 4.50780 | -2.39060 | 4.45680 |
| C | -1.62600 | -3.45420 | 1.69820 |
| C | -0.41450 | -3.17430 | -4.05420 |
| C | -1.04010 | -4.08220 | -5.10060 |
| O | 0.72190 | -2.72310 | -4.18990 |
| H | 1.02350 | 1.23220 | -0.11630 |
| H | -1.11720 | 0.07860 | -0.20390 |
| H | 1.12610 | 1.15720 | -3.01870 |
| H | 2.27350 | 1.83120 | -1.87540 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 3.02170 | -1.92480 | -1.02340 |
| H | -2.14510 | -0.52220 | -2.41910 |
| H | -0.59730 | -0.37400 | -3.18830 |
| H | 2.19830 | -0.95560 | -3.02070 |
| H | 4.75410 | -0.23550 | -0.35040 |
| H | 3.50350 | 0.88750 | 0.12460 |
| H | 0.25910 | -2.29500 | -1.77450 |
| H | 2.71410 | -0.80250 | 1.88670 |
| H | -2.60820 | -2.55260 | -0.70980 |
| H | 5.72450 | -1.32150 | 1.59080 |
| H | 0.16990 | -3.02640 | 0.47510 |
| H | 4.39070 | -2.82370 | 5.42530 |
| H | -1.33810 | -2.82570 | 2.54140 |
| H | -2.70920 | -3.39950 | 1.58390 |
| H | -1.35810 | -4.48470 | 1.93260 |
| H | -0.33270 | -4.27530 | -5.90680 |
| H | -1.92930 | -3.61470 | -5.52250 |
| H | -1.32450 | -5.03380 | -4.65230 |
| 12-Acetoxy-marilzafurenyne_130 | | | |
| C | 0.73150 | 0.65000 | -1.36910 |
| O | 0.83640 | -0.25320 | -0.27140 |
| C | -0.65700 | 0.58650 | -2.04170 |
| C | 1.95070 | 0.36810 | -2.25630 |
| C | 2.11020 | -0.89650 | -0.28600 |
| C | -1.01710 | -0.72590 | -2.76990 |
| Br | -0.77020 | 2.07230 | -3.36460 |
| C | 2.98320 | -0.06170 | -1.23540 |
| C | 2.63500 | -1.11000 | 1.14320 |
| C | -1.13760 | -1.96470 | -1.85650 |
| Cl | 3.67870 | 1.38410 | -0.43990 |
| C | 3.93420 | -1.89100 | 1.17070 |
| C | -2.30730 | -1.84560 | -0.89850 |
| O | -1.29340 | -3.13440 | -2.64860 |
| C | 5.09220 | -1.41820 | 1.66040 |
| C | -2.18330 | -1.77810 | 0.43710 |
| C | 6.28690 | -2.19360 | 1.65920 |
| C | 7.30280 | -2.87000 | 1.62250 |
| C | -3.34470 | -1.66050 | 1.40040 |
| C | -0.20980 | -3.76990 | -3.12800 |
| C | -0.56640 | -5.02070 | -3.91500 |
| O | 0.95890 | -3.41070 | -2.98360 |
| H | 0.84830 | 1.64730 | -0.94160 |
| H | -1.41460 | 0.79630 | -1.28520 |
| H | 1.76820 | -0.45930 | -2.94030 |
| H | 2.25850 | 1.23130 | -2.84710 |
| H | 1.95820 | -1.87370 | -0.74760 |
| H | -1.96700 | -0.58820 | -3.28710 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | -0.29090 | -0.91090 | -3.55970 |
| H | 3.80340 | -0.63540 | -1.66840 |
| H | 2.75500 | -0.15570 | 1.65680 |
| H | 1.89620 | -1.67010 | 1.71670 |
| H | -0.23770 | -2.08000 | -1.25640 |
| H | 3.89240 | -2.89100 | 0.76010 |
| H | -3.28920 | -1.81650 | -1.34830 |
| H | 5.15160 | -0.42070 | 2.07250 |
| H | -1.19670 | -1.80440 | 0.88060 |
| H | 8.19210 | -3.45960 | 1.59330 |
| H | -3.25620 | -0.74470 | 1.98560 |
| H | -4.30000 | -1.64060 | 0.87490 |
| H | -3.34980 | -2.50660 | 2.08800 |
| H | -1.17180 | -4.76030 | -4.78270 |
| H | -1.13080 | -5.71140 | -3.28920 |
| H | 0.33760 | -5.52260 | -4.25920 |
| 12-Acetoxy-marilzafurenyne_131 | | | |
| C | 0.73380 | 0.15060 | -0.99520 |
| O | 1.90630 | -0.55960 | -0.60260 |
| C | 0.34400 | -0.20430 | -2.44340 |
| C | 1.02880 | 1.63510 | -0.74610 |
| C | 2.87510 | 0.34570 | -0.08180 |
| C | -0.00600 | -1.69320 | -2.63650 |
| Br | 1.85770 | 0.22390 | -3.67220 |
| C | 2.07070 | 1.57720 | 0.35160 |
| C | 3.73200 | -0.32280 | 1.00510 |
| C | -1.24360 | -2.18160 | -1.85350 |
| Cl | 1.26410 | 1.34020 | 1.93140 |
| C | 4.58850 | -1.43690 | 0.43810 |
| C | -2.48250 | -1.37120 | -2.18710 |
| O | -1.48850 | -3.54620 | -2.16770 |
| C | 5.92630 | -1.50060 | 0.54530 |
| C | -3.18780 | -0.66110 | -1.29130 |
| C | 6.67890 | -2.57440 | -0.01100 |
| C | 7.29450 | -3.50390 | -0.50920 |
| C | -4.42240 | 0.14890 | -1.62360 |
| C | -0.93680 | -4.52570 | -1.43260 |
| C | -1.33000 | -5.91100 | -1.92030 |
| O | -0.18920 | -4.37270 | -0.46850 |
| H | -0.06290 | -0.14590 | -0.31240 |
| H | -0.49680 | 0.41550 | -2.75710 |
| H | 1.46310 | 2.10370 | -1.62910 |
| H | 0.14260 | 2.20710 | -0.47010 |
| H | 3.51900 | 0.64060 | -0.91280 |
| H | -0.16840 | -1.87750 | -3.69880 |
| H | 0.85920 | -2.29590 | -2.35690 |
| H | 2.67910 | 2.48000 | 0.41410 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 4.36900 | 0.42010 | 1.48620 |
| H | 3.09670 | -0.74780 | 1.78240 |
| H | -1.06280 | -2.07960 | -0.78230 |
| H | 4.04850 | -2.21720 | -0.08230 |
| H | -2.79400 | -1.38780 | -3.22180 |
| H | 6.47810 | -0.72940 | 1.06300 |
| H | -2.87720 | -0.64900 | -0.25530 |
| H | 7.82860 | -4.31810 | -0.94630 |
| H | -5.27620 | -0.21570 | -1.05180 |
| H | -4.26480 | 1.19780 | -1.37090 |
| H | -4.66950 | 0.08540 | -2.68400 |
| H | -0.98420 | -6.06290 | -2.94230 |
| H | -2.41330 | -6.02550 | -1.89650 |
| H | -0.88510 | -6.67650 | -1.28490 |
| 12-Acetoxy-marilzafurenyne_132 | | | |
| C | 0.73390 | 0.15040 | -0.99510 |
| O | 1.90640 | -0.55980 | -0.60250 |
| C | 0.34420 | -0.20430 | -2.44340 |
| C | 1.02890 | 1.63490 | -0.74590 |
| C | 2.87510 | 0.34550 | -0.08150 |
| C | -0.00600 | -1.69320 | -2.63670 |
| Br | 1.85800 | 0.22380 | -3.67200 |
| C | 2.07070 | 1.57700 | 0.35180 |
| C | 3.73200 | -0.32300 | 1.00550 |
| C | -1.24360 | -2.18160 | -1.85390 |
| Cl | 1.26390 | 1.33990 | 1.93160 |
| C | 4.58880 | -1.43680 | 0.43860 |
| C | -2.48250 | -1.37090 | -2.18720 |
| O | -1.48870 | -3.54610 | -2.16860 |
| C | 5.92650 | -1.50030 | 0.54620 |
| C | -3.18770 | -0.66120 | -1.29110 |
| C | 6.67960 | -2.57390 | -0.01010 |
| C | 7.29540 | -3.50280 | -0.50900 |
| C | -4.42230 | 0.14900 | -1.62320 |
| C | -0.93750 | -4.52590 | -1.43360 |
| C | -1.33080 | -5.91090 | -1.92180 |
| O | -0.19020 | -4.37340 | -0.46920 |
| H | -0.06280 | -0.14620 | -0.31240 |
| H | -0.49660 | 0.41560 | -2.75710 |
| H | 1.46320 | 2.10360 | -1.62880 |
| H | 0.14260 | 2.20680 | -0.47000 |
| H | 3.51910 | 0.64050 | -0.91240 |
| H | -0.16830 | -1.87730 | -3.69900 |
| H | 0.85920 | -2.29600 | -2.35710 |
| H | 2.67900 | 2.47980 | 0.41440 |
| H | 4.36870 | 0.42000 | 1.48680 |
| H | 3.09660 | -0.74810 | 1.78260 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | -1.06290 | -2.07990 | -0.78260 |
| H | 4.04910 | -2.21720 | -0.08210 |
| H | -2.79390 | -1.38700 | -3.22200 |
| H | 6.47810 | -0.72890 | 1.06400 |
| H | -2.87730 | -0.64970 | -0.25520 |
| H | 7.82970 | -4.31650 | -0.94670 |
| H | -4.26460 | 1.19780 | -1.37000 |
| H | -4.66930 | 0.08610 | -2.68360 |
| H | -5.27620 | -0.21580 | -1.05160 |
| H | -0.88460 | -6.67680 | -1.28770 |
| H | -0.98660 | -6.06190 | -2.94450 |
| H | -2.41400 | -6.02600 | -1.89640 |
| 12-Acetoxy-marilzafurenyne_133 | | | |
| C | 0.82630 | 0.95160 | -1.55130 |
| O | 1.53420 | 0.13560 | -0.62290 |
| C | -0.67520 | 0.59900 | -1.59440 |
| C | 1.60340 | 0.84510 | -2.86820 |
| C | 2.81530 | -0.21280 | -1.15260 |
| C | -1.04390 | -0.78820 | -2.16180 |
| Br | -1.60190 | 1.97590 | -2.69660 |
| C | 3.02690 | 0.69300 | -2.37490 |
| C | 3.89850 | -0.15270 | -0.06410 |
| C | -0.49110 | -2.00060 | -1.37920 |
| Cl | 3.68900 | 2.29670 | -1.93370 |
| C | 3.68680 | -1.20820 | 1.00290 |
| C | -1.06070 | -2.07280 | 0.03120 |
| O | -0.76130 | -3.19510 | -2.10750 |
| C | 4.59510 | -2.13870 | 1.34290 |
| C | -1.89880 | -3.01600 | 0.49790 |
| C | 4.34420 | -3.10810 | 2.35640 |
| C | 4.11550 | -3.96430 | 3.19770 |
| C | -2.43880 | -3.05370 | 1.91190 |
| C | 0.08760 | -3.60370 | -3.06710 |
| C | -0.33890 | -4.91650 | -3.70410 |
| O | 1.10160 | -3.00890 | -3.43350 |
| H | 0.92080 | 1.97410 | -1.18180 |
| H | -1.08250 | 0.69930 | -0.58800 |
| H | 1.32760 | -0.04900 | -3.42550 |
| H | 1.46050 | 1.70670 | -3.52080 |
| H | 2.74130 | -1.23880 | -1.51780 |
| H | -2.13070 | -0.87120 | -2.19480 |
| H | -0.72590 | -0.84150 | -3.20190 |
| H | 3.69050 | 0.24880 | -3.11770 |
| H | 4.88390 | -0.28120 | -0.51390 |
| H | 3.89650 | 0.82400 | 0.42040 |
| H | 0.58790 | -1.91760 | -1.26510 |
| H | 2.72800 | -1.17850 | 1.50390 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | -0.73610 | -1.28530 | 0.69660 |
| H | 5.55670 | -2.17960 | 0.85130 |
| H | -2.22960 | -3.81380 | -0.15270 |
| H | 3.91140 | -4.70910 | 3.93560 |
| H | -2.14570 | -3.98290 | 2.40170 |
| H | -2.06220 | -2.22050 | 2.50660 |
| H | -3.52810 | -3.00180 | 1.90020 |
| H | 0.37540 | -5.21570 | -4.47100 |
| H | -1.32050 | -4.81050 | -4.16520 |
| H | -0.38940 | -5.70210 | -2.95050 |
| 12-Acetoxy-marilzafurenyne_134 | | | |
| C | 1.54030 | 0.23950 | -1.80740 |
| O | 2.26070 | -0.01950 | -0.60330 |
| C | 0.72650 | -0.99650 | -2.22900 |
| C | 2.57590 | 0.71820 | -2.83250 |
| C | 3.63740 | 0.30180 | -0.77990 |
| C | -0.35990 | -1.34570 | -1.19550 |
| Br | 1.94420 | -2.56430 | -2.45070 |
| C | 3.66240 | 1.29440 | -1.94840 |
| C | 4.26730 | 0.78590 | 0.53610 |
| C | -1.32210 | -2.45390 | -1.65470 |
| Cl | 3.20740 | 2.94950 | -1.44220 |
| C | 4.31820 | -0.31750 | 1.57340 |
| C | -2.28140 | -2.84000 | -0.54330 |
| O | -2.04790 | -1.98140 | -2.78390 |
| C | 5.43710 | -0.73400 | 2.18970 |
| C | -2.40430 | -4.08270 | -0.04920 |
| C | 5.42290 | -1.77930 | 3.15710 |
| C | 5.37990 | -2.68950 | 3.97000 |
| C | -3.35840 | -4.47300 | 1.05910 |
| C | -2.36600 | -2.81780 | -3.78720 |
| C | -3.14610 | -2.12560 | -4.89360 |
| O | -2.08020 | -4.01200 | -3.85570 |
| H | 0.86040 | 1.06760 | -1.60060 |
| H | 0.26320 | -0.80650 | -3.19790 |
| H | 2.98110 | -0.11930 | -3.40060 |
| H | 2.17240 | 1.43780 | -3.54520 |
| H | 4.14270 | -0.61060 | -1.10320 |
| H | 0.12440 | -1.64460 | -0.26480 |
| H | -0.93870 | -0.45170 | -0.96080 |
| H | 4.63420 | 1.34560 | -2.44050 |
| H | 5.27450 | 1.16040 | 0.35060 |
| H | 3.69240 | 1.61400 | 0.95100 |
| H | -0.73360 | -3.33450 | -1.91750 |
| H | 3.36750 | -0.77810 | 1.80780 |
| H | -2.89300 | -2.04320 | -0.14510 |
| H | 6.39330 | -0.28300 | 1.96670 |

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|---------------------------------------|----------|----------|----------|
| H | -1.79360 | -4.87830 | -0.45420 |
| H | 5.33870 | -3.48630 | 4.67900 |
| H | -4.05570 | -5.23240 | 0.70430 |
| H | -2.80570 | -4.88390 | 1.90430 |
| H | -3.93490 | -3.61660 | 1.41060 |
| H | -3.42350 | -2.84250 | -5.66610 |
| H | -4.05510 | -1.67940 | -4.49140 |
| H | -2.54180 | -1.34110 | -5.34800 |
| 12-Acetoxy-marilzafurenyne_135 | | | |
| C | 0.75830 | 0.23310 | -1.05720 |
| O | 2.01530 | -0.29450 | -1.47970 |
| C | -0.26550 | 0.10350 | -2.20180 |
| C | 1.03230 | 1.67260 | -0.59640 |
| C | 3.08000 | 0.48190 | -0.94230 |
| C | -0.48780 | -1.35120 | -2.66130 |
| Br | 0.35610 | 1.15460 | -3.78010 |
| C | 2.48110 | 1.88960 | -0.98890 |
| C | 3.44010 | -0.05000 | 0.46130 |
| C | -1.05420 | -2.29420 | -1.57870 |
| Cl | 3.30830 | 3.07580 | 0.05900 |
| C | 3.93800 | -1.48110 | 0.41180 |
| C | -2.38510 | -1.80340 | -1.03980 |
| O | -1.22710 | -3.59320 | -2.12900 |
| C | 5.12390 | -1.89060 | 0.89270 |
| C | -2.61260 | -1.48980 | 0.24620 |
| C | 5.54210 | -3.25020 | 0.81940 |
| C | 5.88880 | -4.41700 | 0.72170 |
| C | -3.93840 | -0.99640 | 0.78420 |
| C | -0.23590 | -4.49760 | -2.06080 |
| C | -0.61640 | -5.82740 | -2.69190 |
| O | 0.87260 | -4.31830 | -1.55940 |
| H | 0.42140 | -0.33820 | -0.19170 |
| H | -1.21600 | 0.54000 | -1.89200 |
| H | 0.36800 | 2.41240 | -1.04380 |
| H | 0.91900 | 1.73920 | 0.48620 |
| H | 3.95470 | 0.41550 | -1.59070 |
| H | -1.16220 | -1.35000 | -3.51800 |
| H | 0.45890 | -1.75100 | -3.02690 |
| H | 2.53080 | 2.26450 | -2.01230 |
| H | 4.21000 | 0.57670 | 0.91220 |
| H | 2.57900 | -0.01000 | 1.12780 |
| H | -0.35970 | -2.34530 | -0.73870 |
| H | 3.26600 | -2.19440 | -0.04850 |
| H | -3.18340 | -1.71160 | -1.76260 |
| H | 5.80530 | -1.19110 | 1.35530 |
| H | -1.81430 | -1.58710 | 0.96940 |
| H | 6.18610 | -5.43810 | 0.63250 |

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|---------------------------------------|----------|----------|----------|
| H | -3.82000 | -0.00990 | 1.23330 |
| H | -4.68900 | -0.92600 | -0.00390 |
| H | -4.31050 | -1.67790 | 1.54980 |
| H | -1.49690 | -6.23970 | -2.20020 |
| H | 0.20210 | -6.54040 | -2.59510 |
| H | -0.83720 | -5.69280 | -3.75040 |
| 12-Acetoxy-marilzafurenyne_136 | | | |
| C | 1.02140 | 0.52730 | -0.87620 |
| O | 1.57830 | -0.69450 | -0.39640 |
| C | -0.50890 | 0.40270 | -1.01460 |
| C | 1.79740 | 0.87600 | -2.15700 |
| C | 2.88570 | -0.87490 | -0.93390 |
| C | -1.02400 | -0.62240 | -2.04890 |
| Br | -1.23210 | 2.19320 | -1.50540 |
| C | 2.71530 | -0.31610 | -2.34950 |
| C | 3.91360 | -0.14410 | -0.04400 |
| C | -0.68800 | -2.10550 | -1.76580 |
| Cl | 4.24810 | 0.12040 | -3.15520 |
| C | 3.93080 | -0.69490 | 1.36810 |
| C | -1.18850 | -2.56060 | -0.40120 |
| O | -1.23590 | -2.91340 | -2.80430 |
| C | 5.01910 | -1.19230 | 1.97900 |
| C | -2.18240 | -3.43800 | -0.17500 |
| C | 4.97420 | -1.69760 | 3.31000 |
| C | 4.89820 | -2.13120 | 4.44890 |
| C | -2.64290 | -3.86820 | 1.20130 |
| C | -0.54450 | -3.12500 | -3.93630 |
| C | -1.27610 | -4.03910 | -4.90590 |
| O | 0.55510 | -2.64510 | -4.20860 |
| H | 1.23530 | 1.29160 | -0.12720 |
| H | -0.92980 | 0.17310 | -0.03520 |
| H | 1.16720 | 1.05660 | -3.02740 |
| H | 2.38080 | 1.78190 | -1.98870 |
| H | 3.13000 | -1.93750 | -0.96910 |
| H | -2.10890 | -0.52880 | -2.10610 |
| H | -0.65720 | -0.34910 | -3.03750 |
| H | 2.22190 | -1.06140 | -2.97360 |
| H | 4.91200 | -0.23860 | -0.47230 |
| H | 3.69940 | 0.92330 | 0.00630 |
| H | 0.39230 | -2.24830 | -1.75530 |
| H | 2.98370 | -0.66910 | 1.89050 |
| H | -0.67050 | -2.12920 | 0.44360 |
| H | 5.97300 | -1.22480 | 1.47230 |
| H | -2.70900 | -3.88410 | -1.00720 |
| H | 4.82850 | -2.50990 | 5.44440 |
| H | -2.53030 | -4.94670 | 1.31510 |
| H | -2.06640 | -3.37950 | 1.98750 |

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|---------------------------------------|----------|----------|----------|
| H | -3.69470 | -3.61740 | 1.34170 |
| H | -0.67960 | -4.19330 | -5.80490 |
| H | -2.23040 | -3.59830 | -5.19290 |
| H | -1.46310 | -5.00740 | -4.44260 |
| 12-Acetoxy-marilzafurenyne_137 | | | |
| C | 0.66330 | -0.46580 | -0.69760 |
| O | 1.88490 | -1.01110 | -1.19280 |
| C | -0.18370 | 0.10480 | -1.85200 |
| C | 1.05360 | 0.54840 | 0.38570 |
| C | 2.98820 | -0.44500 | -0.49470 |
| C | -0.60830 | -0.95900 | -2.88400 |
| Br | 0.85620 | 1.50570 | -2.82200 |
| C | 2.40110 | 0.02920 | 0.84180 |
| C | 4.16360 | -1.43360 | -0.42500 |
| C | -1.53430 | -2.06720 | -2.33830 |
| Cl | 2.15920 | -1.31690 | 1.99720 |
| C | 5.38340 | -0.83350 | 0.24630 |
| C | -2.79820 | -1.49770 | -1.72090 |
| O | -1.89460 | -2.94190 | -3.39940 |
| C | 5.93150 | -1.30270 | 1.37940 |
| C | -3.16060 | -1.67130 | -0.43930 |
| C | 7.07680 | -0.69890 | 1.97270 |
| C | 8.04370 | -0.14680 | 2.47390 |
| C | -4.42020 | -1.10210 | 0.17760 |
| C | -1.15270 | -4.02850 | -3.67000 |
| C | -1.71030 | -4.83980 | -4.82870 |
| O | -0.12880 | -4.37010 | -3.08110 |
| H | 0.12570 | -1.27890 | -0.20920 |
| H | -1.06790 | 0.59800 | -1.44630 |
| H | 1.17640 | 1.54660 | -0.03440 |
| H | 0.32230 | 0.61650 | 1.19150 |
| H | 3.29990 | 0.43330 | -1.06350 |
| H | -1.11080 | -0.45910 | -3.71240 |
| H | 0.28810 | -1.41360 | -3.30800 |
| H | 3.01380 | 0.78830 | 1.32920 |
| H | 3.86510 | -2.35090 | 0.08300 |
| H | 4.44600 | -1.72750 | -1.43610 |
| H | -1.01400 | -2.62970 | -1.56150 |
| H | 5.81540 | 0.02880 | -0.24350 |
| H | -3.42890 | -0.92040 | -2.38210 |
| H | 5.51090 | -2.16250 | 1.88160 |
| H | -2.53070 | -2.25290 | 0.21990 |
| H | 8.89090 | 0.33240 | 2.91220 |
| H | -4.16850 | -0.44330 | 1.00920 |
| H | -4.99900 | -0.53070 | -0.54900 |
| H | -5.04940 | -1.90730 | 0.55800 |
| H | -1.09550 | -5.72250 | -5.00330 |

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|---------------------------------------|----------|----------|----------|
| H | -1.72300 | -4.23930 | -5.73770 |
| H | -2.72730 | -5.16240 | -4.60780 |
| 12-Acetoxy-marilzafurenyne_138 | | | |
| C | 1.52740 | 0.02960 | -1.20660 |
| O | 2.60470 | -0.78600 | -0.74290 |
| C | 0.53620 | -0.83040 | -2.01090 |
| C | 2.16970 | 1.17820 | -1.99890 |
| C | 3.83410 | -0.07110 | -0.81930 |
| C | -0.09600 | -1.93930 | -1.14990 |
| Br | 1.47190 | -1.66010 | -3.56760 |
| C | 3.62610 | 0.76480 | -2.08430 |
| C | 4.04030 | 0.72710 | 0.48570 |
| C | -1.23360 | -2.69930 | -1.85220 |
| Cl | 4.73010 | 2.16060 | -2.23390 |
| C | 4.14710 | -0.18320 | 1.69320 |
| C | -1.72170 | -3.85940 | -1.00340 |
| O | -2.30050 | -1.78980 | -2.09580 |
| C | 5.18470 | -0.19850 | 2.54660 |
| C | -1.73130 | -5.13990 | -1.40800 |
| C | 5.22990 | -1.07810 | 3.66610 |
| C | 5.24060 | -1.85180 | 4.61070 |
| C | -2.21610 | -6.30030 | -0.56570 |
| C | -3.03130 | -1.88330 | -3.22040 |
| C | -4.12560 | -0.83010 | -3.29020 |
| O | -2.87290 | -2.70320 | -4.12340 |
| H | 1.01840 | 0.45030 | -0.33780 |
| H | -0.24890 | -0.18850 | -2.41270 |
| H | 1.72660 | 1.33600 | -2.98260 |
| H | 2.07300 | 2.10910 | -1.43920 |
| H | 4.66300 | -0.76760 | -0.95250 |
| H | 0.68370 | -2.64230 | -0.85350 |
| H | -0.47940 | -1.50650 | -0.22520 |
| H | 3.77730 | 0.13180 | -2.95990 |
| H | 4.94630 | 1.32990 | 0.41660 |
| H | 3.21770 | 1.42210 | 0.65260 |
| H | -0.85040 | -3.10230 | -2.79120 |
| H | 3.31150 | -0.85270 | 1.84750 |
| H | -2.08040 | -3.60790 | -0.01570 |
| H | 6.02690 | 0.46400 | 2.40710 |
| H | -1.37600 | -5.38670 | -2.39930 |
| H | 5.24910 | -2.53070 | 5.43430 |
| H | -1.41270 | -7.02340 | -0.42280 |
| H | -2.55620 | -5.96770 | 0.41570 |
| H | -3.04570 | -6.80400 | -1.06250 |
| H | -4.77930 | -0.90770 | -2.42190 |
| H | -4.72540 | -0.96710 | -4.18970 |
| H | -3.68870 | 0.16770 | -3.31210 |

| 12-Acetoxy-marilzafurenyne_139 | | | |
|---------------------------------------|----------|----------|----------|
| C | 1.27840 | 0.78160 | -1.45010 |
| O | 2.04540 | 0.19190 | -0.40280 |
| C | 0.03500 | -0.07490 | -1.74800 |
| C | 2.25520 | 1.00350 | -2.61170 |
| C | 3.42890 | 0.18640 | -0.74980 |
| C | 0.34040 | -1.53110 | -2.15350 |
| Br | -1.02980 | 0.81110 | -3.18180 |
| C | 3.56830 | 1.20920 | -1.88510 |
| C | 4.31220 | 0.41520 | 0.48700 |
| C | -0.90350 | -2.43520 | -2.18460 |
| Cl | 3.66660 | 2.89030 | -1.27880 |
| C | 4.20090 | -0.72800 | 1.47550 |
| C | -0.56550 | -3.80940 | -2.73350 |
| O | -1.41400 | -2.55160 | -0.86180 |
| C | 5.23800 | -1.46180 | 1.91280 |
| C | -1.15000 | -4.35740 | -3.81120 |
| C | 5.07100 | -2.52750 | 2.84290 |
| C | 4.89120 | -3.44200 | 3.63200 |
| C | -0.81600 | -5.72680 | -4.36260 |
| C | -2.73950 | -2.57680 | -0.64200 |
| C | -3.07980 | -2.70970 | 0.83390 |
| O | -3.61930 | -2.50050 | -1.49810 |
| H | 0.95080 | 1.75730 | -1.08710 |
| H | -0.58670 | -0.07640 | -0.85170 |
| H | 2.32870 | 0.11990 | -3.24400 |
| H | 1.97660 | 1.84470 | -3.24720 |
| H | 3.64740 | -0.80000 | -1.16360 |
| H | 0.81360 | -1.54450 | -3.13470 |
| H | 1.06420 | -1.95820 | -1.45820 |
| H | 4.43990 | 1.02750 | -2.51470 |
| H | 5.35260 | 0.53720 | 0.18370 |
| H | 4.02140 | 1.33320 | 0.99820 |
| H | -1.64290 | -1.97790 | -2.84430 |
| H | 3.20110 | -0.93810 | 1.83200 |
| H | 0.19660 | -4.35930 | -2.20020 |
| H | 6.24250 | -1.26320 | 1.56750 |
| H | -1.91650 | -3.80580 | -4.33860 |
| H | 4.73210 | -4.23900 | 4.32380 |
| H | -0.03700 | -6.21520 | -3.77610 |
| H | -1.70180 | -6.36250 | -4.35110 |
| H | -0.46790 | -5.64360 | -5.39250 |
| H | -4.16050 | -2.70990 | 0.97470 |
| H | -2.65580 | -1.87790 | 1.39560 |
| H | -2.67730 | -3.64130 | 1.23040 |
| 12-Acetoxy-marilzafurenyne_140 | | | |
| C | 1.51820 | -0.95370 | -2.02560 |

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|---------------------------------------|----------|----------|----------|
| O | 2.30720 | -1.01150 | -0.83850 |
| C | 0.88650 | -2.32600 | -2.33390 |
| C | 2.43910 | -0.40750 | -3.12190 |
| C | 3.59400 | -0.44780 | -1.07840 |
| C | -0.15090 | -2.76950 | -1.28270 |
| Br | 2.33540 | -3.69920 | -2.39500 |
| C | 3.42040 | 0.42720 | -2.32630 |
| C | 4.13250 | 0.25760 | 0.17660 |
| C | -1.60340 | -2.33330 | -1.56860 |
| Cl | 2.68620 | 2.01500 | -1.94700 |
| C | 4.40500 | -0.72350 | 1.29890 |
| C | -2.55810 | -2.97230 | -0.57870 |
| O | -1.75450 | -0.92020 | -1.50440 |
| C | 5.58850 | -0.86320 | 1.91930 |
| C | -3.56090 | -3.79980 | -0.91610 |
| C | 5.78530 | -1.80580 | 2.96900 |
| C | 5.92460 | -2.63360 | 3.85580 |
| C | -4.51320 | -4.43680 | 0.07320 |
| C | -1.90370 | -0.19520 | -2.62690 |
| C | -2.12390 | 1.28160 | -2.34220 |
| O | -1.84030 | -0.62590 | -3.77770 |
| H | 0.74570 | -0.20990 | -1.84170 |
| H | 0.42310 | -2.31320 | -3.32210 |
| H | 2.97330 | -1.21580 | -3.62180 |
| H | 1.90540 | 0.16060 | -3.88440 |
| H | 4.26080 | -1.27240 | -1.33820 |
| H | -0.15320 | -3.85970 | -1.26270 |
| H | 0.16360 | -2.46070 | -0.28500 |
| H | 4.35850 | 0.60500 | -2.85290 |
| H | 5.04710 | 0.80020 | -0.06510 |
| H | 3.41310 | 0.99280 | 0.53750 |
| H | -1.88470 | -2.70440 | -2.55570 |
| H | 3.56350 | -1.33670 | 1.59340 |
| H | -2.39630 | -2.72420 | 0.46070 |
| H | 6.43730 | -0.25720 | 1.63680 |
| H | -3.72430 | -4.04530 | -1.95650 |
| H | 6.04300 | -3.35900 | 4.62970 |
| H | -5.53880 | -4.13910 | -0.14670 |
| H | -4.45130 | -5.52360 | 0.00950 |
| H | -4.28340 | -4.14040 | 1.09720 |
| H | -2.36140 | 1.81410 | -3.26280 |
| H | -1.22440 | 1.71890 | -1.90940 |
| H | -2.94840 | 1.41270 | -1.64180 |
| 12-Acetoxy-marilzafurenyne_141 | | | |
| C | 0.86200 | 0.70380 | -1.35280 |
| O | 1.00570 | -0.13400 | -0.20890 |
| C | -0.56920 | 0.65350 | -1.92810 |

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|---------------------------------------|----------|----------|----------|
| C | 2.00680 | 0.31610 | -2.29690 |
| C | 2.26070 | -0.81370 | -0.25520 |
| C | -1.02030 | -0.68560 | -2.54900 |
| Br | -0.71830 | 2.05860 | -3.33290 |
| C | 3.09250 | -0.07880 | -1.31800 |
| C | 2.87260 | -0.93970 | 1.14950 |
| C | -1.08310 | -1.88680 | -1.57880 |
| Cl | 3.88630 | 1.39290 | -0.67680 |
| C | 4.14780 | -1.76000 | 1.15170 |
| C | -2.13820 | -1.69200 | -0.49850 |
| O | -1.31690 | -3.08010 | -2.32130 |
| C | 5.34910 | -1.29200 | 1.52910 |
| C | -3.26620 | -2.41040 | -0.35670 |
| C | 6.51820 | -2.10510 | 1.50910 |
| C | 7.51020 | -2.81520 | 1.45710 |
| C | -4.28730 | -2.18720 | 0.73820 |
| C | -0.28200 | -3.75330 | -2.85440 |
| C | -0.71720 | -5.01860 | -3.57600 |
| O | 0.90090 | -3.41600 | -2.80160 |
| H | 1.04370 | 1.72040 | -0.99970 |
| H | -1.26770 | 0.94240 | -1.14230 |
| H | 1.75030 | -0.54970 | -2.90560 |
| H | 2.30090 | 1.12400 | -2.96750 |
| H | 2.05520 | -1.81710 | -0.63200 |
| H | -2.01040 | -0.54960 | -2.98530 |
| H | -0.37210 | -0.92190 | -3.39130 |
| H | 3.86260 | -0.71070 | -1.76200 |
| H | 3.05350 | 0.04470 | 1.58190 |
| H | 2.15800 | -1.43210 | 1.80930 |
| H | -0.13680 | -2.00090 | -1.05530 |
| H | 4.05000 | -2.78520 | 0.82080 |
| H | -1.92860 | -0.90310 | 0.20960 |
| H | 5.46450 | -0.26960 | 1.86070 |
| H | -3.49030 | -3.20660 | -1.05280 |
| H | 8.37880 | -3.43410 | 1.41440 |
| H | -3.99360 | -1.37160 | 1.39990 |
| H | -5.25730 | -1.94340 | 0.30410 |
| H | -4.39850 | -3.09080 | 1.33820 |
| H | 0.14980 | -5.54470 | -3.97500 |
| H | -1.38440 | -4.77140 | -4.40130 |
| H | -1.24120 | -5.68270 | -2.88920 |
| 12-Acetoxy-marilzafurenyne_142 | | | |
| C | 1.64370 | -0.53600 | -1.42960 |
| O | 1.84750 | -0.77880 | -0.03780 |
| C | 0.57230 | -1.48490 | -1.99500 |
| C | 3.02360 | -0.64380 | -2.09190 |
| C | 3.22850 | -1.00970 | 0.21680 |

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|----|----------|----------|----------|
| C | -0.80520 | -1.23970 | -1.35260 |
| Br | 1.11230 | -3.38160 | -1.67720 |
| C | 3.95740 | -0.31970 | -0.94440 |
| C | 3.60980 | -0.56470 | 1.63820 |
| C | -1.94880 | -2.02760 | -2.01320 |
| Cl | 4.04620 | 1.45600 | -0.73430 |
| C | 5.05840 | -0.86680 | 1.96810 |
| C | -3.24980 | -1.84410 | -1.25280 |
| O | -2.09720 | -1.56950 | -3.35220 |
| C | 5.97790 | 0.06650 | 2.26450 |
| C | -3.96770 | -2.85140 | -0.72980 |
| C | 7.32900 | -0.27040 | 2.56340 |
| C | 8.48620 | -0.58600 | 2.79200 |
| C | -5.26480 | -2.67400 | 0.02970 |
| C | -2.41530 | -2.43010 | -4.33490 |
| C | -2.53540 | -1.74670 | -5.68770 |
| O | -2.59490 | -3.64050 | -4.21050 |
| H | 1.30080 | 0.49540 | -1.52630 |
| H | 0.50350 | -1.34410 | -3.07440 |
| H | 3.21560 | -1.66010 | -2.43610 |
| H | 3.14210 | 0.02320 | -2.94610 |
| H | 3.38690 | -2.08650 | 0.13040 |
| H | -0.74920 | -1.49540 | -0.29350 |
| H | -1.04100 | -0.17570 | -1.39380 |
| H | 4.97050 | -0.69490 | -1.09300 |
| H | 3.40400 | 0.49680 | 1.77760 |
| H | 2.98380 | -1.09060 | 2.35940 |
| H | -1.69160 | -3.08800 | -1.99620 |
| H | 5.33780 | -1.91170 | 1.95350 |
| H | -3.59660 | -0.82670 | -1.14280 |
| H | 5.71530 | 1.11490 | 2.28200 |
| H | -3.61940 | -3.86870 | -0.84650 |
| H | 9.49750 | -0.86010 | 2.99570 |
| H | -6.07080 | -3.20880 | -0.47350 |
| H | -5.16740 | -3.07320 | 1.03960 |
| H | -5.54510 | -1.62260 | 0.10260 |
| H | -2.83550 | -2.46600 | -6.44940 |
| H | -3.28230 | -0.95450 | -5.64470 |
| H | -1.57940 | -1.31180 | -5.97740 |

Table S15. Calculated Energies (Hartrees) for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,12*R** of 5.

| Entry ID | Gas Phase Energy |
|-----------|------------------|
| 253.00000 | -1360,03979 |
| 254.00000 | -1360,037257 |
| 255.00000 | -1360,037251 |
| 256.00000 | -1360,03904 |
| 257.00000 | -1360,039494 |
| 258.00000 | -1360,039494 |
| 259.00000 | -1360,038818 |
| 260.00000 | -1360,038822 |
| 261.00000 | -1360,036139 |
| 262.00000 | -1360,035976 |
| 263.00000 | -1360,038559 |
| 264.00000 | -1360,03859 |
| 265.00000 | -1360,03438 |
| 266.00000 | -1360,031558 |
| 267.00000 | -1360,038532 |
| 268.00000 | -1360,034039 |
| 269.00000 | -1360,037011 |
| 270.00000 | -1360,035359 |

Table S16. Coordinates (Angstroms) of calculated geometries for diastereoisomer 4*S**,6*R**,7*R**,9*S**,10*S**,12*R** of 5.

| 12-Acetoxy-marilzafurenyne_253 | | | |
|--------------------------------|----------|----------|----------|
| C | 1.75270 | 2.49080 | -1.34450 |
| O | 1.90870 | 1.24240 | -0.67160 |
| C | 0.27890 | 2.71040 | -1.74160 |
| C | 2.74520 | 2.47640 | -2.51330 |
| C | 2.93590 | 0.47770 | -1.29540 |
| C | -0.67110 | 2.79190 | -0.53150 |
| Br | -0.33620 | 1.19910 | -2.89150 |
| C | 3.80400 | 1.50850 | -2.02670 |
| C | 3.65740 | -0.41690 | -0.27470 |
| C | -0.47000 | 4.01720 | 0.38470 |
| Cl | 4.92870 | 2.35340 | -0.92040 |
| C | 2.73960 | -1.48670 | 0.28160 |
| C | -1.26920 | 3.86520 | 1.66440 |
| O | -0.89080 | 5.20520 | -0.27800 |
| C | 2.99030 | -2.80590 | 0.23580 |
| C | -0.73280 | 3.84320 | 2.89570 |
| C | 2.08700 | -3.76620 | 0.77530 |
| C | 1.28500 | -4.56410 | 1.23470 |
| C | -1.53040 | 3.69200 | 4.17330 |
| C | 0.00260 | 6.04100 | -0.83200 |
| C | -0.64750 | 7.28300 | -1.42020 |

| | | | |
|---------------------------------------|----------|----------|----------|
| O | 1.21590 | 5.85520 | -0.90530 |
| H | 2.07620 | 3.26670 | -0.65110 |
| H | 0.19130 | 3.61510 | -2.34290 |
| H | 2.28260 | 2.08010 | -3.41710 |
| H | 3.13900 | 3.46560 | -2.74890 |
| H | 2.45740 | -0.15270 | -2.04750 |
| H | -1.70240 | 2.78470 | -0.88550 |
| H | -0.55250 | 1.88060 | 0.05650 |
| H | 4.38980 | 1.07170 | -2.83600 |
| H | 4.52610 | -0.88490 | -0.73890 |
| H | 4.02620 | 0.17940 | 0.56000 |
| H | 0.57660 | 4.09060 | 0.68150 |
| H | 1.82890 | -1.12410 | 0.73980 |
| H | -2.33920 | 3.77200 | 1.54600 |
| H | 3.89580 | -3.18260 | -0.21760 |
| H | 0.33800 | 3.93780 | 3.01330 |
| H | 0.58110 | -5.25860 | 1.63650 |
| H | -2.59820 | 3.60330 | 3.97020 |
| H | -1.20980 | 2.80100 | 4.71390 |
| H | -1.37570 | 4.55760 | 4.81800 |
| H | -1.18670 | 7.82810 | -0.64600 |
| H | -1.34950 | 7.00590 | -2.20610 |
| H | 0.10940 | 7.94170 | -1.84570 |
| 12-Acetoxy-marilzafurenyne_254 | | | |
| C | 1.70970 | 2.40500 | -1.53540 |
| O | 1.39530 | 1.01770 | -1.40830 |
| C | 0.46840 | 3.17380 | -2.03110 |
| C | 2.92760 | 2.48390 | -2.46820 |
| C | 2.51160 | 0.22460 | -1.79730 |
| C | -0.73970 | 3.06390 | -1.08120 |
| Br | -0.08810 | 2.46260 | -3.81050 |
| C | 3.08810 | 1.05400 | -2.94710 |
| C | 3.44260 | 0.02310 | -0.58260 |
| C | -0.54730 | 3.71360 | 0.30470 |
| Cl | 4.77660 | 0.65290 | -3.36820 |
| C | 2.74700 | -0.71410 | 0.54450 |
| C | -1.68510 | 3.33980 | 1.23460 |
| O | -0.50230 | 5.13150 | 0.18210 |
| C | 3.19100 | -1.85450 | 1.09880 |
| C | -1.53090 | 2.68160 | 2.39520 |
| C | 2.49190 | -2.50190 | 2.15770 |
| C | 1.86410 | -3.03220 | 3.06080 |
| C | -2.66620 | 2.30820 | 3.32410 |
| C | 0.66470 | 5.79390 | 0.24110 |
| C | 0.48420 | 7.30120 | 0.16090 |
| O | 1.78080 | 5.28420 | 0.32410 |
| H | 2.01420 | 2.77240 | -0.55580 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 0.72310 | 4.22300 | -2.18180 |
| H | 2.80470 | 3.18520 | -3.29380 |
| H | 3.80420 | 2.79550 | -1.89900 |
| H | 2.17110 | -0.74690 | -2.15800 |
| H | -1.61240 | 3.50880 | -1.56010 |
| H | -0.97880 | 2.00750 | -0.95150 |
| H | 2.48080 | 0.89690 | -3.83970 |
| H | 4.32900 | -0.53820 | -0.87970 |
| H | 3.79640 | 0.97960 | -0.19830 |
| H | 0.36530 | 3.33450 | 0.76560 |
| H | 1.83250 | -0.26050 | 0.90290 |
| H | -2.67400 | 3.63730 | 0.91630 |
| H | 4.10270 | -2.32050 | 0.75340 |
| H | -0.54080 | 2.38550 | 2.71380 |
| H | 1.31260 | -3.49570 | 3.84840 |
| H | -3.62860 | 2.64110 | 2.93360 |
| H | -2.70560 | 1.22640 | 3.45440 |
| H | -2.51770 | 2.76550 | 4.30260 |
| H | 0.00870 | 7.57540 | -0.78030 |
| H | -0.14070 | 7.64960 | 0.98280 |
| H | 1.44990 | 7.80260 | 0.22220 |
| 12-Acetoxy-marilzafurenyne_255 | | | |
| C | 1.70880 | 2.40560 | -1.53310 |
| O | 1.39410 | 1.01850 | -1.40430 |
| C | 0.46820 | 3.17480 | -2.03020 |
| C | 2.92700 | 2.48310 | -2.46560 |
| C | 2.50920 | 0.22430 | -1.79500 |
| C | -0.74070 | 3.06720 | -1.08110 |
| Br | -0.08810 | 2.46220 | -3.80910 |
| C | 3.08510 | 1.05330 | -2.94540 |
| C | 3.44180 | 0.02120 | -0.58180 |
| C | -0.54830 | 3.71740 | 0.30450 |
| Cl | 4.77260 | 0.65050 | -3.36900 |
| C | 2.74860 | -0.71920 | 0.54470 |
| C | -1.68640 | 3.34450 | 1.23440 |
| O | -0.50250 | 5.13520 | 0.18130 |
| C | 3.19480 | -1.86010 | 1.09610 |
| C | -1.53280 | 2.68630 | 2.39510 |
| C | 2.49780 | -2.51050 | 2.15450 |
| C | 1.87190 | -3.04300 | 3.05770 |
| C | -2.66840 | 2.31390 | 3.32390 |
| C | 0.66490 | 5.79690 | 0.23970 |
| C | 0.48530 | 7.30430 | 0.15870 |
| O | 1.78080 | 5.28660 | 0.32270 |
| H | 2.01320 | 2.77410 | -0.55380 |
| H | 0.72380 | 4.22360 | -2.18200 |
| H | 2.80540 | 3.18520 | -3.29070 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 3.80410 | 2.79270 | -1.89610 |
| H | 2.16720 | -0.74670 | -2.15570 |
| H | -1.61260 | 3.51280 | -1.56080 |
| H | -0.98110 | 2.01110 | -0.95090 |
| H | 2.47660 | 0.89720 | -3.83720 |
| H | 4.32830 | -0.53860 | -0.88100 |
| H | 3.79500 | 0.97730 | -0.19600 |
| H | 0.36410 | 3.33800 | 0.76590 |
| H | 1.83400 | -0.26740 | 0.90520 |
| H | -2.67510 | 3.64280 | 0.91600 |
| H | 4.10660 | -2.32420 | 0.74860 |
| H | -0.54290 | 2.38940 | 2.71370 |
| H | 1.32210 | -3.50820 | 3.84540 |
| H | -2.51960 | 2.77120 | 4.30240 |
| H | -3.63050 | 2.64740 | 2.93330 |
| H | -2.70860 | 1.23210 | 3.45440 |
| H | 1.45120 | 7.80520 | 0.22100 |
| H | 0.01110 | 7.57840 | -0.78320 |
| H | -0.14040 | 7.65330 | 0.97970 |
| 12-Acetoxy-marilzafurenyne_256 | | | |
| C | 1.79860 | 2.47060 | -1.46600 |
| O | 1.96410 | 1.16100 | -0.92440 |
| C | 0.31850 | 2.72930 | -1.81280 |
| C | 2.76860 | 2.57240 | -2.64950 |
| C | 2.96170 | 0.45410 | -1.65440 |
| C | -0.60870 | 2.70000 | -0.58270 |
| Br | -0.32360 | 1.33470 | -3.08860 |
| C | 3.82610 | 1.54870 | -2.29160 |
| C | 3.69820 | -0.55730 | -0.76020 |
| C | -0.39070 | 3.83980 | 0.43460 |
| Cl | 4.98330 | 2.26140 | -1.12730 |
| C | 2.79410 | -1.69080 | -0.31640 |
| C | -1.17680 | 3.58150 | 1.70530 |
| O | -0.81280 | 5.08250 | -0.11770 |
| C | 2.56410 | -2.02080 | 0.96540 |
| C | -0.62860 | 3.46100 | 2.92560 |
| C | 1.70320 | -3.09620 | 1.32780 |
| C | 0.95840 | -4.02440 | 1.60160 |
| C | -1.41330 | 3.20380 | 4.19420 |
| C | 0.07930 | 5.96370 | -0.59900 |
| C | -0.57170 | 7.25400 | -1.07050 |
| O | 1.29200 | 5.78380 | -0.69480 |
| H | 2.13630 | 3.17320 | -0.70450 |
| H | 0.22330 | 3.68660 | -2.32480 |
| H | 2.28390 | 2.27980 | -3.58080 |
| H | 3.16860 | 3.57770 | -2.78590 |
| H | 2.45400 | -0.08190 | -2.45870 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | -1.64620 | 2.72320 | -0.91710 |
| H | -0.47930 | 1.74000 | -0.08060 |
| H | 4.38970 | 1.19510 | -3.15540 |
| H | 4.53590 | -0.98950 | -1.30780 |
| H | 4.11600 | -0.06050 | 0.11580 |
| H | 0.65970 | 3.88200 | 0.72390 |
| H | 2.31670 | -2.25130 | -1.10850 |
| H | -2.24780 | 3.49520 | 1.59010 |
| H | 3.03070 | -1.47000 | 1.76950 |
| H | 0.44320 | 3.54880 | 3.04020 |
| H | 0.30470 | -4.83410 | 1.83870 |
| H | -1.25390 | 4.01420 | 4.90600 |
| H | -2.48290 | 3.12910 | 3.99470 |
| H | -1.08570 | 2.27250 | 4.65690 |
| H | -1.10560 | 7.72860 | -0.24760 |
| H | -1.27860 | 7.04900 | -1.87390 |
| H | 0.18400 | 7.94700 | -1.43980 |
| 12-Acetoxy-marilzafurenyne_257 | | | |
| C | 1.40610 | 2.34150 | -0.94110 |
| O | 0.93870 | 1.07600 | -0.47420 |
| C | 0.32840 | 3.03320 | -1.80030 |
| C | 2.73450 | 2.07230 | -1.65940 |
| C | 1.86380 | 0.05600 | -0.83310 |
| C | -0.95930 | 3.35460 | -1.01790 |
| Br | -0.17190 | 1.84900 | -3.32760 |
| C | 3.20130 | 0.78880 | -1.00450 |
| C | 1.82990 | -1.10030 | 0.17950 |
| C | -0.80870 | 4.41240 | 0.09550 |
| Cl | 3.97590 | 1.16680 | 0.56470 |
| C | 2.74960 | -2.23940 | -0.21480 |
| C | -2.05570 | 4.46410 | 0.95670 |
| O | -0.59190 | 5.70050 | -0.47150 |
| C | 3.79650 | -2.65510 | 0.51700 |
| C | -2.07610 | 4.22170 | 2.27770 |
| C | 4.63330 | -3.72900 | 0.09890 |
| C | 5.35010 | -4.63560 | -0.29520 |
| C | -3.32060 | 4.27390 | 3.13770 |
| C | 0.63870 | 6.23620 | -0.51960 |
| C | 0.63980 | 7.64440 | -1.09210 |
| O | 1.68140 | 5.68100 | -0.17770 |
| H | 1.62730 | 2.94200 | -0.05910 |
| H | 0.73520 | 3.94630 | -2.23460 |
| H | 2.57820 | 1.89810 | -2.72390 |
| H | 3.44600 | 2.89250 | -1.55880 |
| H | 1.55130 | -0.32100 | -1.80880 |
| H | -1.72770 | 3.68810 | -1.71590 |
| H | -1.33480 | 2.42690 | -0.58370 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 3.91660 | 0.23130 | -1.60990 |
| H | 2.07730 | -0.74370 | 1.17960 |
| H | 0.81510 | -1.49360 | 0.24190 |
| H | 0.01290 | 4.13890 | 0.75820 |
| H | 2.52150 | -2.72690 | -1.15310 |
| H | -2.97370 | 4.71710 | 0.44580 |
| H | 4.03860 | -2.17750 | 1.45600 |
| H | -1.15670 | 3.96990 | 2.78850 |
| H | 5.97660 | -5.42970 | -0.63620 |
| H | -4.20200 | 4.53400 | 2.55050 |
| H | -3.49530 | 3.30490 | 3.60620 |
| H | -3.20260 | 5.01840 | 3.92540 |
| H | 0.00810 | 8.29620 | -0.48920 |
| H | 0.26070 | 7.63740 | -2.11360 |
| H | 1.65130 | 8.05020 | -1.09880 |
| 12-Acetoxy-marilzafurenyne_258 | | | |
| C | 1.21930 | 2.24600 | -1.01800 |
| O | 0.86630 | 1.07530 | -0.28150 |
| C | -0.03590 | 2.89890 | -1.63140 |
| C | 2.28620 | 1.81250 | -2.03150 |
| C | 1.62570 | -0.03530 | -0.74490 |
| C | -1.04440 | 3.38900 | -0.57470 |
| Br | -0.97550 | 1.57840 | -2.79700 |
| C | 2.88180 | 0.58760 | -1.36910 |
| C | 1.84430 | -1.06140 | 0.37900 |
| C | -0.55960 | 4.55780 | 0.30860 |
| Cl | 4.07410 | 1.09670 | -0.13450 |
| C | 2.58530 | -2.29380 | -0.10120 |
| C | -1.51440 | 4.78720 | 1.46400 |
| O | -0.47420 | 5.75490 | -0.45750 |
| C | 3.78310 | -2.68600 | 0.36350 |
| C | -1.17170 | 4.70180 | 2.76000 |
| C | 4.43980 | -3.85150 | -0.12520 |
| C | 4.99230 | -4.84090 | -0.57980 |
| C | -2.12460 | 4.93140 | 3.91350 |
| C | 0.70830 | 6.20350 | -0.90940 |
| C | 0.58840 | 7.53270 | -1.63730 |
| O | 1.78920 | 5.62790 | -0.79700 |
| H | 1.69470 | 2.93020 | -0.31550 |
| H | 0.25840 | 3.72800 | -2.27460 |
| H | 1.83400 | 1.52560 | -2.98070 |
| H | 3.01980 | 2.59290 | -2.23640 |
| H | 1.04280 | -0.50340 | -1.54050 |
| H | -1.96760 | 3.68630 | -1.07270 |
| H | -1.30920 | 2.54340 | 0.06180 |
| H | 3.38380 | -0.08030 | -2.06980 |
| H | 2.37100 | -0.60670 | 1.21830 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 0.87680 | -1.38050 | 0.76720 |
| H | 0.40650 | 4.31240 | 0.75070 |
| H | 2.09080 | -2.87220 | -0.87000 |
| H | -2.53120 | 5.03590 | 1.19560 |
| H | 4.29100 | -2.11820 | 1.13040 |
| H | -0.15370 | 4.45410 | 3.02780 |
| H | 5.47630 | -5.70690 | -0.97370 |
| H | -3.12740 | 5.17600 | 3.56130 |
| H | -2.18840 | 4.03640 | 4.53290 |
| H | -1.77070 | 5.75370 | 4.53580 |
| H | 0.17030 | 8.28890 | -0.97340 |
| H | -0.06240 | 7.43090 | -2.50510 |
| H | 1.56830 | 7.87010 | -1.97440 |
| 12-Acetoxy-marilzafurenyne_259 | | | |
| C | 1.75440 | 2.40910 | -1.36380 |
| O | 1.98320 | 1.16610 | -0.70150 |
| C | 0.24400 | 2.64050 | -1.57150 |
| C | 2.58880 | 2.37180 | -2.64990 |
| C | 2.91090 | 0.38180 | -1.44550 |
| C | -0.54160 | 2.74260 | -0.25020 |
| Br | -0.52720 | 1.12450 | -2.61640 |
| C | 3.68980 | 1.39450 | -2.29340 |
| C | 3.74750 | -0.51440 | -0.51840 |
| C | -0.21600 | 3.97450 | 0.62120 |
| Cl | 4.95750 | 2.23410 | -1.34980 |
| C | 2.89660 | -1.56790 | 0.16160 |
| C | -0.81080 | 3.81380 | 2.01370 |
| O | -0.70340 | 5.16100 | -0.00500 |
| C | 3.12360 | -2.89050 | 0.09610 |
| C | -1.71690 | 4.62490 | 2.58900 |
| C | 2.28620 | -3.83490 | 0.75640 |
| C | 1.54060 | -4.61900 | 1.32230 |
| C | -2.27850 | 4.42510 | 3.98050 |
| C | 0.12270 | 5.97830 | -0.67820 |
| C | -0.58310 | 7.21950 | -1.19980 |
| O | 1.31560 | 5.77740 | -0.89850 |
| H | 2.17130 | 3.18850 | -0.72650 |
| H | 0.08780 | 3.54000 | -2.16670 |
| H | 2.00960 | 1.97400 | -3.48310 |
| H | 2.96080 | 3.35380 | -2.94390 |
| H | 2.33100 | -0.24810 | -2.12310 |
| H | -1.61020 | 2.74350 | -0.46740 |
| H | -0.35730 | 1.83330 | 0.32340 |
| H | 4.16130 | 0.94270 | -3.16660 |
| H | 4.54310 | -0.99730 | -1.08660 |
| H | 4.22850 | 0.08340 | 0.25600 |
| H | 0.86060 | 4.04150 | 0.77950 |

| | | | |
|---------------------------------------|----------|----------|----------|
| H | 2.05710 | -1.19020 | 0.73020 |
| H | -0.44910 | 2.96000 | 2.56910 |
| H | 3.95830 | -3.28240 | -0.46700 |
| H | -2.09180 | 5.48530 | 2.05240 |
| H | 0.88610 | -5.30170 | 1.81700 |
| H | -1.85650 | 3.54120 | 4.45990 |
| H | -2.05560 | 5.29150 | 4.60390 |
| H | -3.36130 | 4.30570 | 3.93550 |
| H | 0.11490 | 7.84870 | -1.75180 |
| H | -0.99020 | 7.79730 | -0.37050 |
| H | -1.39940 | 6.93900 | -1.86460 |
| 12-Acetoxy-marilzafurenyne_260 | | | |
| C | 1.78160 | 2.42550 | -1.34300 |
| O | 1.99460 | 1.17300 | -0.69330 |
| C | 0.27680 | 2.65890 | -1.58600 |
| C | 2.64890 | 2.40750 | -2.60760 |
| C | 2.94220 | 0.40040 | -1.42440 |
| C | -0.54250 | 2.74090 | -0.28390 |
| Br | -0.46570 | 1.15800 | -2.67270 |
| C | 3.74140 | 1.42600 | -2.23710 |
| C | 3.75560 | -0.50840 | -0.48900 |
| C | -0.24060 | 3.95990 | 0.61380 |
| Cl | 4.98350 | 2.25280 | -1.24900 |
| C | 2.88870 | -1.57230 | 0.15360 |
| C | -0.87020 | 3.77790 | 1.98820 |
| O | -0.71340 | 5.15520 | -0.00680 |
| C | 3.11880 | -2.89360 | 0.07510 |
| C | -1.79100 | 4.58000 | 2.55280 |
| C | 2.26570 | -3.84790 | 0.70010 |
| C | 1.50690 | -4.64050 | 1.23580 |
| C | -2.38740 | 4.35880 | 3.92650 |
| C | 0.12850 | 5.98300 | -0.64670 |
| C | -0.56530 | 7.23140 | -1.16740 |
| O | 1.32680 | 5.78620 | -0.84000 |
| H | 2.18130 | 3.19570 | -0.68380 |
| H | 0.13500 | 3.56700 | -2.17160 |
| H | 2.09170 | 2.02150 | -3.46110 |
| H | 3.02720 | 3.39400 | -2.87770 |
| H | 2.38070 | -0.22010 | -2.12580 |
| H | -1.60520 | 2.74440 | -0.52840 |
| H | -0.37200 | 1.82320 | 0.28060 |
| H | 4.23580 | 0.98730 | -3.10440 |
| H | 4.56620 | -0.98250 | -1.04340 |
| H | 4.21580 | 0.07850 | 0.30600 |
| H | 0.83150 | 4.02530 | 0.80030 |
| H | 2.03440 | -1.20330 | 0.70570 |
| H | -0.52210 | 2.91580 | 2.53950 |

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|---------------------------------------|----------|----------|----------|
| H | 3.96820 | -3.27680 | -0.47180 |
| H | -2.15280 | 5.44840 | 2.02010 |
| H | 0.84080 | -5.33050 | 1.70420 |
| H | -1.97710 | 3.46780 | 4.40290 |
| H | -2.18080 | 5.21560 | 4.56840 |
| H | -3.46870 | 4.23990 | 3.85230 |
| H | -1.36040 | 6.96040 | -1.86130 |
| H | 0.14690 | 7.87210 | -1.68700 |
| H | -0.99900 | 7.79340 | -0.34070 |
| 12-Acetoxy-marilzafurenyne_261 | | | |
| C | 2.15510 | 2.82530 | -2.16110 |
| O | 2.03540 | 1.79740 | -1.18740 |
| C | 2.07560 | 4.21960 | -1.50880 |
| C | 1.11390 | 2.48670 | -3.23100 |
| C | 1.33530 | 0.67730 | -1.72750 |
| C | 0.70240 | 4.67110 | -0.96950 |
| Br | 2.68000 | 5.56870 | -2.84440 |
| C | 1.15930 | 0.97090 | -3.22790 |
| C | 2.04220 | -0.63790 | -1.35880 |
| C | 0.05530 | 3.73530 | 0.06720 |
| Cl | 2.54800 | 0.41160 | -4.20970 |
| C | 2.05080 | -0.87600 | 0.13860 |
| C | -1.26810 | 4.30280 | 0.55050 |
| O | 0.94710 | 3.55240 | 1.15880 |
| C | 3.16190 | -1.06220 | 0.87040 |
| C | -2.44530 | 3.66330 | 0.45610 |
| C | 3.11440 | -1.27740 | 2.27760 |
| C | 3.03830 | -1.47230 | 3.48060 |
| C | -3.76630 | 4.22650 | 0.93410 |
| C | 0.92160 | 2.40360 | 1.85960 |
| C | 1.99060 | 2.35620 | 2.93900 |
| O | 0.13650 | 1.46990 | 1.69240 |
| H | 3.15000 | 2.71010 | -2.59480 |
| H | 2.80060 | 4.25140 | -0.69410 |
| H | 0.11870 | 2.81570 | -2.93520 |
| H | 1.34100 | 2.92610 | -4.20280 |
| H | 0.34370 | 0.68220 | -1.27180 |
| H | 0.82210 | 5.65940 | -0.52440 |
| H | 0.01320 | 4.80900 | -1.80250 |
| H | 0.25800 | 0.51640 | -3.64080 |
| H | 1.53390 | -1.47670 | -1.83470 |
| H | 3.06840 | -0.63760 | -1.72730 |
| H | -0.14580 | 2.77780 | -0.41340 |
| H | 1.08260 | -0.88630 | 0.62130 |
| H | -1.22840 | 5.28600 | 0.99690 |
| H | 4.13730 | -1.05120 | 0.40590 |
| H | -2.48000 | 2.67580 | 0.01660 |

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|---------------------------------------|----------|----------|----------|
| H | 2.96590 | -1.64400 | 4.53140 |
| H | -4.46990 | 4.29410 | 0.10400 |
| H | -4.19730 | 3.57660 | 1.69610 |
| H | -3.64510 | 5.22200 | 1.36260 |
| H | 2.05340 | 3.31220 | 3.45780 |
| H | 1.75740 | 1.57830 | 3.66560 |
| H | 2.95890 | 2.13250 | 2.49210 |
| 12-Acetoxy-marilzafurenyne_262 | | | |
| C | 1.13000 | 2.68570 | -1.71280 |
| O | 1.58600 | 1.52810 | -1.01710 |
| C | -0.41160 | 2.73840 | -1.72840 |
| C | 1.81790 | 2.65710 | -3.08290 |
| C | 2.59670 | 0.86740 | -1.77160 |
| C | -1.06090 | 2.69220 | -0.32670 |
| Br | -1.12790 | 1.17800 | -2.74700 |
| C | 3.10210 | 1.91570 | -2.77220 |
| C | 3.65220 | 0.24470 | -0.84360 |
| C | -0.72760 | 3.84500 | 0.65150 |
| Cl | 4.28200 | 3.04420 | -2.03810 |
| C | 3.05990 | -0.84270 | 0.02970 |
| C | -0.99750 | 5.21190 | 0.04960 |
| O | 0.61780 | 3.77940 | 1.10440 |
| C | 3.51270 | -2.10610 | 0.08810 |
| C | -1.94910 | 6.05600 | 0.48020 |
| C | 2.91210 | -3.08530 | 0.93030 |
| C | 2.37060 | -3.89880 | 1.66240 |
| C | -2.21540 | 7.42060 | -0.11830 |
| C | 0.96800 | 2.93130 | 2.08470 |
| C | 2.46180 | 2.95160 | 2.36420 |
| O | 0.20400 | 2.19860 | 2.71220 |
| H | 1.52140 | 3.55480 | -1.18540 |
| H | -0.74020 | 3.63200 | -2.25930 |
| H | 1.24160 | 2.08540 | -3.80930 |
| H | 1.98350 | 3.65090 | -3.49950 |
| H | 2.10350 | 0.07400 | -2.33650 |
| H | -2.14240 | 2.68000 | -0.46320 |
| H | -0.82370 | 1.73750 | 0.14410 |
| H | 3.56430 | 1.47040 | -3.65380 |
| H | 4.47350 | -0.16330 | -1.43360 |
| H | 4.07860 | 1.00380 | -0.18790 |
| H | -1.38430 | 3.74920 | 1.51840 |
| H | 2.21450 | -0.54210 | 0.63520 |
| H | -0.36220 | 5.50380 | -0.77380 |
| H | 4.35610 | -2.42110 | -0.50930 |
| H | -2.58290 | 5.76980 | 1.30840 |
| H | 1.89370 | -4.60640 | 2.30360 |
| H | -1.53650 | 7.63510 | -0.94440 |

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|---------------------------------------|----------|----------|----------|
| H | -3.23800 | 7.47490 | -0.49280 |
| H | -2.08710 | 8.19470 | 0.63880 |
| H | 2.71120 | 2.23700 | 3.14800 |
| H | 3.01160 | 2.68410 | 1.46180 |
| H | 2.77360 | 3.94550 | 2.68320 |
| 12-Acetoxy-marilzafurenyne_263 | | | |
| C | 2.22660 | 2.55120 | -1.75330 |
| O | 2.48840 | 1.37090 | -0.99600 |
| C | 0.85910 | 3.14730 | -1.37510 |
| C | 2.38050 | 2.15790 | -3.22790 |
| C | 2.83070 | 0.29760 | -1.86790 |
| C | 0.82400 | 3.61020 | 0.09430 |
| Br | -0.57540 | 1.78810 | -1.66500 |
| C | 3.32590 | 0.97700 | -3.15020 |
| C | 3.81090 | -0.67440 | -1.19180 |
| C | -0.46800 | 4.35060 | 0.49730 |
| Cl | 5.00890 | 1.56640 | -2.99870 |
| C | 3.17010 | -1.39460 | -0.02260 |
| C | -0.67080 | 5.61710 | -0.31420 |
| O | -0.40710 | 4.69340 | 1.87580 |
| C | 3.10360 | -2.73030 | 0.10670 |
| C | -1.71450 | 5.83280 | -1.13150 |
| C | 2.48540 | -3.35090 | 1.23000 |
| C | 1.93390 | -3.85160 | 2.19750 |
| C | -1.91980 | 7.09410 | -1.94260 |
| C | -0.85750 | 3.84030 | 2.81070 |
| C | -0.72520 | 4.39770 | 4.21900 |
| O | -1.32610 | 2.72220 | 2.60430 |
| H | 3.01330 | 3.26710 | -1.50950 |
| H | 0.64440 | 3.98790 | -2.03600 |
| H | 1.42930 | 1.82990 | -3.64730 |
| H | 2.75490 | 2.97020 | -3.85130 |
| H | 1.90650 | -0.23380 | -2.10420 |
| H | 0.96020 | 2.73840 | 0.73560 |
| H | 1.67700 | 4.26130 | 0.28830 |
| H | 3.27210 | 0.32570 | -4.02310 |
| H | 4.17160 | -1.40390 | -1.91770 |
| H | 4.68400 | -0.13730 | -0.82090 |
| H | -1.32850 | 3.70380 | 0.31740 |
| H | 2.74740 | -0.75490 | 0.74110 |
| H | 0.08970 | 6.37690 | -0.20460 |
| H | 3.52190 | -3.38170 | -0.64700 |
| H | -2.47470 | 5.07050 | -1.23700 |
| H | 1.44910 | -4.28480 | 3.04400 |
| H | -1.11320 | 7.81000 | -1.78040 |
| H | -1.95820 | 6.85630 | -3.00590 |
| H | -2.86030 | 7.57060 | -1.66470 |

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|---------------------------------------|----------|----------|----------|
| H | -1.26400 | 5.34100 | 4.30320 |
| H | 0.32350 | 4.57080 | 4.45870 |
| H | -1.13680 | 3.69600 | 4.94410 |
| 12-Acetoxy-marilzafurenyne_264 | | | |
| C | 1.25750 | 2.16450 | -0.93830 |
| O | 0.97790 | 0.97700 | -0.19690 |
| C | -0.05070 | 2.81360 | -1.43400 |
| C | 2.24180 | 1.76150 | -2.04380 |
| C | 1.70530 | -0.11700 | -0.74370 |
| C | -0.97450 | 3.26840 | -0.28800 |
| Br | -1.06780 | 1.50440 | -2.54600 |
| C | 2.90030 | 0.53030 | -1.45680 |
| C | 2.02460 | -1.16250 | 0.33730 |
| C | -0.43430 | 4.42550 | 0.57960 |
| Cl | 4.18580 | 1.02810 | -0.31460 |
| C | 2.73360 | -2.37790 | -0.22730 |
| C | -1.27250 | 4.58120 | 1.84120 |
| O | -0.42050 | 5.63810 | -0.17340 |
| C | 3.96890 | -2.76710 | 0.12890 |
| C | -1.96610 | 5.67520 | 2.20420 |
| C | 4.59260 | -3.91630 | -0.43580 |
| C | 5.11390 | -4.89100 | -0.95440 |
| C | -2.78520 | 5.78370 | 3.47270 |
| C | 0.71740 | 6.10630 | -0.71140 |
| C | 0.52630 | 7.44570 | -1.40450 |
| O | 1.80920 | 5.54090 | -0.69630 |
| H | 1.78210 | 2.84150 | -0.26450 |
| H | 0.18040 | 3.65890 | -2.08190 |
| H | 1.71610 | 1.48810 | -2.95860 |
| H | 2.94930 | 2.55310 | -2.29230 |
| H | 1.06250 | -0.57530 | -1.49780 |
| H | -1.93880 | 3.56540 | -0.70120 |
| H | -1.17780 | 2.40400 | 0.34550 |
| H | 3.34860 | -0.11910 | -2.20950 |
| H | 2.61530 | -0.71910 | 1.13930 |
| H | 1.09540 | -1.49870 | 0.79750 |
| H | 0.56830 | 4.18510 | 0.93390 |
| H | 2.18200 | -2.94600 | -0.96410 |
| H | -1.28990 | 3.71510 | 2.48770 |
| H | 4.53390 | -2.20940 | 0.86260 |
| H | -1.96220 | 6.55320 | 1.57350 |
| H | 5.57060 | -5.74440 | -1.40450 |
| H | -2.74280 | 4.86390 | 4.05710 |
| H | -2.41250 | 6.59990 | 4.09220 |
| H | -3.82860 | 5.98720 | 3.23050 |
| H | -0.21550 | 7.35840 | -2.19790 |
| H | 1.46560 | 7.78370 | -1.84170 |

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|---------------------------------------|----------|----------|----------|
| H | 0.18690 | 8.19440 | -0.68920 |
| 12-Acetoxy-marilzafurenyne_265 | | | |
| C | 1.66630 | 2.37790 | -1.47700 |
| O | 1.32140 | 1.00090 | -1.31710 |
| C | 0.40150 | 3.19440 | -1.81140 |
| C | 2.75940 | 2.42290 | -2.55510 |
| C | 2.34480 | 0.17210 | -1.85850 |
| C | -0.67780 | 3.13160 | -0.71380 |
| Br | -0.40730 | 2.50610 | -3.50080 |
| C | 2.79840 | 0.99590 | -3.06590 |
| C | 3.41880 | -0.08430 | -0.77970 |
| C | -0.28700 | 3.78880 | 0.63080 |
| Cl | 4.39990 | 0.53760 | -3.71000 |
| C | 2.85340 | -0.82820 | 0.41390 |
| C | -1.28300 | 3.54180 | 1.75750 |
| O | -0.14750 | 5.19530 | 0.45300 |
| C | 3.32830 | -1.99550 | 0.87970 |
| C | -2.47560 | 2.92380 | 1.66970 |
| C | 2.75430 | -2.64890 | 2.00770 |
| C | 2.23320 | -3.18590 | 2.97270 |
| C | -3.41080 | 2.71390 | 2.84150 |
| C | 1.06420 | 5.77470 | 0.41760 |
| C | 0.98310 | 7.28680 | 0.28350 |
| O | 2.14570 | 5.19120 | 0.46040 |
| H | 2.10340 | 2.72640 | -0.54170 |
| H | 0.67370 | 4.23320 | -1.99920 |
| H | 2.56320 | 3.14190 | -3.35080 |
| H | 3.71300 | 2.68930 | -2.09780 |
| H | 1.92170 | -0.78000 | -2.18160 |
| H | -1.58670 | 3.60530 | -1.08600 |
| H | -0.92590 | 2.08260 | -0.54860 |
| H | 2.07390 | 0.87560 | -3.87250 |
| H | 4.24080 | -0.66400 | -1.20040 |
| H | 3.84950 | 0.85250 | -0.42660 |
| H | 0.64630 | 3.34720 | 0.98110 |
| H | 2.01000 | -0.35610 | 0.89990 |
| H | -0.96730 | 3.91530 | 2.72100 |
| H | 4.17040 | -2.47970 | 0.40620 |
| H | -2.83040 | 2.53850 | 0.72490 |
| H | 1.77460 | -3.65330 | 3.81550 |
| H | -3.59230 | 1.64940 | 2.99210 |
| H | -2.99710 | 3.12390 | 3.76350 |
| H | -4.36780 | 3.20020 | 2.65070 |
| H | 1.98290 | 7.72020 | 0.26580 |
| H | 0.47000 | 7.55750 | -0.63880 |
| H | 0.43580 | 7.71060 | 1.12510 |

| 12-Acetoxy-marilzafurenyne_266 | | | |
|---------------------------------------|----------|----------|----------|
| C | 1.90560 | 2.91810 | -1.20790 |
| O | 1.60610 | 1.55510 | -1.51390 |
| C | 0.77570 | 3.82500 | -1.73610 |
| C | 3.29030 | 3.19760 | -1.81160 |
| C | 2.79210 | 0.85770 | -1.88010 |
| C | -0.61760 | 3.51190 | -1.14640 |
| Br | 0.64380 | 3.62100 | -3.71730 |
| C | 3.57590 | 1.94580 | -2.61760 |
| C | 3.45450 | 0.29330 | -0.60600 |
| C | -0.84020 | 3.83390 | 0.35100 |
| Cl | 5.32330 | 1.61400 | -2.77790 |
| C | 2.57290 | -0.73650 | 0.07110 |
| C | -0.51360 | 5.27620 | 0.69350 |
| O | -0.10410 | 2.96530 | 1.20140 |
| C | 2.97190 | -1.96890 | 0.42560 |
| C | -1.42300 | 6.19260 | 1.06340 |
| C | 2.09330 | -2.89170 | 1.06170 |
| C | 1.30850 | -3.66840 | 1.58230 |
| C | -1.09600 | 7.62950 | 1.40910 |
| C | -0.59460 | 1.75980 | 1.53190 |
| C | 0.32260 | 0.99500 | 2.47260 |
| O | -1.66380 | 1.28650 | 1.14990 |
| H | 1.99460 | 3.02080 | -0.12730 |
| H | 1.02790 | 4.86970 | -1.55460 |
| H | 3.33110 | 4.10050 | -2.42130 |
| H | 4.02350 | 3.30610 | -1.01160 |
| H | 2.55000 | 0.03700 | -2.55660 |
| H | -1.35040 | 4.09040 | -1.70940 |
| H | -0.86890 | 2.46860 | -1.34080 |
| H | 3.17010 | 2.05720 | -3.62400 |
| H | 4.41160 | -0.16800 | -0.85040 |
| H | 3.66540 | 1.08900 | 0.10800 |
| H | -1.90300 | 3.70180 | 0.56250 |
| H | 1.55700 | -0.42240 | 0.26770 |
| H | 0.52780 | 5.55690 | 0.63680 |
| H | 3.98270 | -2.30050 | 0.23700 |
| H | -2.46620 | 5.91520 | 1.12820 |
| H | 0.61970 | -4.34660 | 2.03420 |
| H | -1.40150 | 7.84880 | 2.43250 |
| H | -0.02760 | 7.82970 | 1.32140 |
| H | -1.62710 | 8.30800 | 0.74100 |
| H | 0.16300 | 1.32090 | 3.49990 |
| H | 0.12060 | -0.07430 | 2.41050 |
| H | 1.36630 | 1.16580 | 2.20930 |
| 12-Acetoxy-marilzafurenyne_267 | | | |
| C | 3.17280 | 2.65730 | -0.34710 |

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|----|----------|----------|----------|
| O | 2.81840 | 1.30000 | -0.09140 |
| C | 2.06140 | 3.59970 | 0.14850 |
| C | 3.52120 | 2.72770 | -1.83960 |
| C | 3.06160 | 0.50280 | -1.24870 |
| C | 0.67220 | 3.33230 | -0.46920 |
| Br | 2.60570 | 5.48390 | -0.20930 |
| C | 4.02530 | 1.32590 | -2.11350 |
| C | 3.52900 | -0.90940 | -0.86190 |
| C | -0.47290 | 4.13790 | 0.17980 |
| Cl | 5.72380 | 1.17730 | -1.56890 |
| C | 2.44540 | -1.67980 | -0.13470 |
| C | -0.63800 | 3.80600 | 1.65140 |
| O | -1.69470 | 3.85950 | -0.49250 |
| C | 1.95220 | -2.86380 | -0.53490 |
| C | -0.49990 | 4.69560 | 2.64810 |
| C | 0.93030 | -3.54100 | 0.19060 |
| C | 0.04580 | -4.08930 | 0.82930 |
| C | -0.66240 | 4.36700 | 4.11660 |
| C | -2.04330 | 4.55500 | -1.58740 |
| C | -3.39810 | 4.13720 | -2.13640 |
| O | -1.37200 | 5.43100 | -2.13010 |
| H | 4.08040 | 2.85770 | 0.22480 |
| H | 2.00300 | 3.49290 | 1.23240 |
| H | 2.63760 | 2.91720 | -2.44720 |
| H | 4.25330 | 3.50250 | -2.06920 |
| H | 2.11470 | 0.42770 | -1.78680 |
| H | 0.70330 | 3.55530 | -1.53470 |
| H | 0.43910 | 2.27000 | -0.38810 |
| H | 3.98550 | 1.05440 | -3.16890 |
| H | 3.83270 | -1.45810 | -1.75410 |
| H | 4.40130 | -0.85680 | -0.21010 |
| H | -0.25280 | 5.20450 | 0.10580 |
| H | 2.06780 | -1.21270 | 0.76520 |
| H | -0.88300 | 2.77860 | 1.88030 |
| H | 2.32020 | -3.34370 | -1.43030 |
| H | -0.25560 | 5.72320 | 2.41520 |
| H | -0.72520 | -4.56850 | 1.39080 |
| H | 0.26030 | 4.58380 | 4.65540 |
| H | -1.46140 | 4.96880 | 4.55050 |
| H | -0.90720 | 3.31480 | 4.26640 |
| H | -4.17040 | 4.27920 | -1.38110 |
| H | -3.65310 | 4.73500 | -3.01120 |
| H | -3.38040 | 3.08690 | -2.42560 |

| 12-Acetoxy-marilzafurenyne_268 | | | |
|---------------------------------------|----------|----------|----------|
| C | 1.70340 | 2.13500 | -2.17030 |
| O | 1.70920 | 1.64530 | -0.83180 |
| C | 1.63070 | 3.67480 | -2.17440 |
| C | 0.56580 | 1.39350 | -2.89060 |
| C | 1.03350 | 0.39330 | -0.76460 |
| C | 0.33260 | 4.31230 | -1.63340 |
| Br | 1.89030 | 4.29910 | -4.04850 |
| C | -0.09630 | 0.60530 | -1.77640 |
| C | 2.02310 | -0.74450 | -1.09470 |
| C | 0.04490 | 4.05950 | -0.14180 |
| Cl | -0.85600 | -0.90230 | -2.35750 |
| C | 3.16080 | -0.81140 | -0.09550 |
| C | -1.24450 | 4.74030 | 0.28130 |
| O | 1.13540 | 4.54620 | 0.62920 |
| C | 3.48260 | -1.90140 | 0.62110 |
| C | -2.29250 | 4.10270 | 0.82800 |
| C | 4.56500 | -1.90510 | 1.54700 |
| C | 5.49730 | -1.87120 | 2.33490 |
| C | -3.58050 | 4.77760 | 1.24820 |
| C | 1.48040 | 3.92940 | 1.77370 |
| C | 2.68130 | 4.57900 | 2.44250 |
| O | 0.91740 | 2.95540 | 2.27240 |
| H | 2.65070 | 1.83590 | -2.62190 |
| H | 2.47830 | 4.06130 | -1.60650 |
| H | -0.13250 | 2.04460 | -3.41560 |
| H | 0.99150 | 0.71590 | -3.63170 |
| H | 0.62930 | 0.24290 | 0.23760 |
| H | 0.39430 | 5.38940 | -1.79250 |
| H | -0.51830 | 3.97780 | -2.22570 |
| H | -0.88110 | 1.20730 | -1.31750 |
| H | 1.50240 | -1.70240 | -1.10160 |
| H | 2.44850 | -0.61690 | -2.08990 |
| H | -0.08090 | 2.98880 | 0.01560 |
| H | 3.73220 | 0.09980 | 0.02220 |
| H | -1.29250 | 5.80800 | 0.12190 |
| H | 2.92260 | -2.81940 | 0.51540 |
| H | -2.23890 | 3.03550 | 0.99440 |
| H | 6.31120 | -1.83810 | 3.02450 |
| H | -3.55450 | 5.84930 | 1.04810 |
| H | -4.42470 | 4.34860 | 0.70790 |
| H | -3.74870 | 4.63340 | 2.31580 |
| H | 3.55450 | 4.51210 | 1.79430 |
| H | 2.47630 | 5.62910 | 2.64840 |
| H | 2.90720 | 4.07730 | 3.38320 |

| 12-Acetoxy-marilzafurenyne_269 | | | |
|---------------------------------------|----------|----------|----------|
| C | 1.08750 | 2.25010 | -2.38290 |
| O | 1.89570 | 2.30020 | -1.21250 |
| C | 0.29640 | 3.55850 | -2.58370 |
| C | 0.28220 | 0.95190 | -2.26800 |
| C | 1.89440 | 1.03370 | -0.55570 |
| C | -0.83210 | 3.86490 | -1.57680 |
| Br | -0.50420 | 3.52710 | -4.40780 |
| C | 1.26780 | 0.04700 | -1.55560 |
| C | 3.29200 | 0.69530 | -0.01250 |
| C | -0.39210 | 3.96880 | -0.10570 |
| Cl | 2.45520 | -0.58880 | -2.73580 |
| C | 3.30170 | -0.58350 | 0.80200 |
| C | -1.57340 | 4.29360 | 0.79100 |
| O | 0.60800 | 4.97200 | 0.01240 |
| C | 4.01150 | -1.67890 | 0.48450 |
| C | -1.96920 | 3.53310 | 1.82480 |
| C | 3.98260 | -2.85730 | 1.28400 |
| C | 3.91990 | -3.86340 | 1.97300 |
| C | -3.14720 | 3.85170 | 2.72010 |
| C | 1.59530 | 4.83670 | 0.91650 |
| C | 2.58920 | 5.98610 | 0.86590 |
| O | 1.72260 | 3.91400 | 1.72130 |
| H | 1.78300 | 2.14930 | -3.21790 |
| H | 1.00630 | 4.38680 | -2.57820 |
| H | -0.59960 | 1.08460 | -1.64280 |
| H | -0.04290 | 0.56390 | -3.23380 |
| H | 1.21290 | 1.12940 | 0.29100 |
| H | -1.29810 | 4.80680 | -1.86790 |
| H | -1.61640 | 3.11370 | -1.66540 |
| H | 0.79490 | -0.80510 | -1.06620 |
| H | 4.01870 | 0.63670 | -0.82290 |
| H | 3.62720 | 1.50580 | 0.63570 |
| H | 0.00160 | 3.00200 | 0.20440 |
| H | 2.68530 | -0.58050 | 1.69070 |
| H | -2.10970 | 5.20270 | 0.55970 |
| H | 4.63130 | -1.69810 | -0.40090 |
| H | -1.42520 | 2.62800 | 2.05820 |
| H | 3.86910 | -4.74310 | 2.57540 |
| H | -3.63990 | 4.77680 | 2.41890 |
| H | -3.87970 | 3.04500 | 2.68080 |
| H | -2.81480 | 3.96210 | 3.75260 |
| H | 3.13510 | 5.96770 | -0.07680 |
| H | 2.06950 | 6.93980 | 0.95260 |
| H | 3.30450 | 5.90340 | 1.68390 |
| 12-Acetoxy-marilzafurenyne_270 | | | |
| C | 2.58610 | 2.13770 | 0.17390 |

| | | | |
|----|----------|----------|----------|
| O | 2.18870 | 1.16020 | -0.78910 |
| C | 1.72860 | 3.40580 | 0.01160 |
| C | 4.09330 | 2.35280 | -0.03070 |
| C | 3.32820 | 0.47080 | -1.29340 |
| C | 0.23330 | 3.12720 | 0.26050 |
| Br | 1.96100 | 4.14770 | -1.82750 |
| C | 4.38060 | 1.58200 | -1.30450 |
| C | 3.63700 | -0.73610 | -0.38190 |
| C | -0.65580 | 4.38790 | 0.26530 |
| Cl | 6.06630 | 0.99850 | -1.39040 |
| C | 2.50010 | -1.73870 | -0.36870 |
| C | -0.25600 | 5.35790 | 1.36200 |
| O | -2.01270 | 4.00990 | 0.45870 |
| C | 2.62630 | -3.03820 | -0.68560 |
| C | 0.18790 | 6.60640 | 1.14270 |
| C | 1.51970 | -3.93470 | -0.65540 |
| C | 0.54790 | -4.67360 | -0.63330 |
| C | 0.58780 | 7.57630 | 2.23380 |
| C | -2.79650 | 3.72240 | -0.59360 |
| C | -4.21520 | 3.36330 | -0.18150 |
| O | -2.45270 | 3.72730 | -1.77430 |
| H | 2.42780 | 1.72010 | 1.16960 |
| H | 2.08520 | 4.16450 | 0.70940 |
| H | 4.38180 | 3.40140 | -0.10810 |
| H | 4.64270 | 1.91930 | 0.80560 |
| H | 3.13260 | 0.11840 | -2.30700 |
| H | -0.12260 | 2.43350 | -0.50240 |
| H | 0.11620 | 2.61050 | 1.21360 |
| H | 4.21180 | 2.22540 | -2.16920 |
| H | 4.54540 | -1.23660 | -0.71830 |
| H | 3.82160 | -0.41440 | 0.64280 |
| H | -0.55200 | 4.90910 | -0.68810 |
| H | 1.53500 | -1.34520 | -0.07840 |
| H | -0.34750 | 4.99220 | 2.37470 |
| H | 3.58310 | -3.44720 | -0.97710 |
| H | 0.27610 | 6.96990 | 0.12770 |
| H | -0.30340 | -5.31730 | -0.61600 |
| H | -0.02950 | 8.47360 | 2.18360 |
| H | 0.46980 | 7.13550 | 3.22430 |
| H | 1.63030 | 7.87150 | 2.11210 |
| H | -4.82710 | 3.16740 | -1.06180 |
| H | -4.21150 | 2.47200 | 0.44520 |
| H | -4.66390 | 4.18330 | 0.37850 |