

Supplementary Materials

Marine Prostanoids with Cytotoxic Activity from Octocoral *Clavularia* spp.

Ming-Ya Cheng ^{1,†}, I-Chi Hsu ^{2,†}, Shi-Ying Huang ^{3,4}, Ya-Ting Chuang ⁵, Hsueh-Wei Chang ^{5,6,7}, Tian-Huei Chu ⁸, Ching-Yeu Chen ⁹ and Yuan-Bin Cheng ^{1,10,*}

Corresponding Author

Yuan-Bin Cheng – Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 80424, Taiwan; orcid.org/0000-0001-6581-1320; E-mail: jmb@mail.nsysu.edu.tw; Tel.: +886-7-5252-000-5212

Authors

Ming-Ya Cheng – Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 80424, Taiwan

I-Chi Hsu – Division of Pharmacy, Zuoying Branch of Kaohsiung Armed Forces General Hospital, Kaohsiung 813204, Taiwan

Shi-Ying Huang – College of Food and Biological Engineering, Jimei University, Xiamen 361021, China; Fujian Provincial Engineering Technology Research Center of Marine Functional Food, Xiamen 361021, China

Ya-Ting Chuang – Department of Biomedical Science and Environmental Biology, PhD program of Life Science, College of Life Science, Kaohsiung Medical University, Kaohsiung 80708, Taiwan

Hsueh-Wei Chang – Department of Biomedical Science and Environmental Biology, PhD program of Life Science, College of Life Science, Kaohsiung Medical University, Kaohsiung 80708, Taiwan; Center for Cancer Research, Kaohsiung Medical University, Kaohsiung 80708, Taiwan; Department of Medical Research, Kaohsiung Medical University Hospital, Kaohsiung 80708, Taiwan

Tian-Huei Chu – Medical Laboratory, Medical Education and Research Center, Kaohsiung Armed Forces General Hospital, Kaohsiung City, 802301

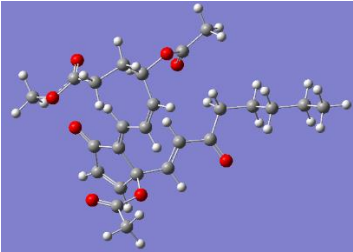
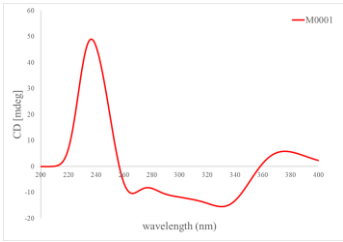
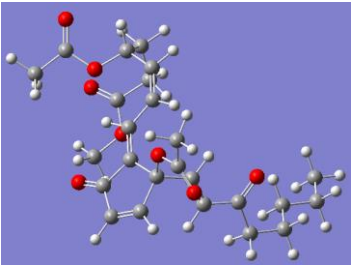
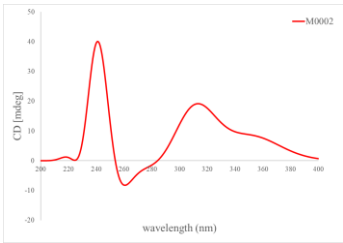
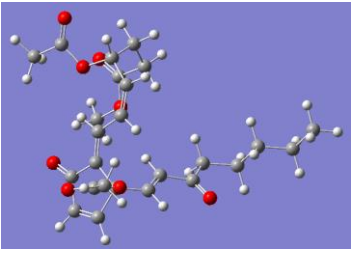
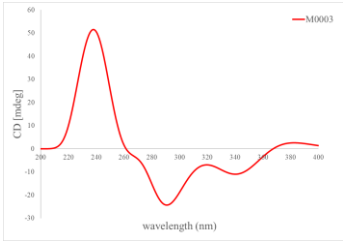
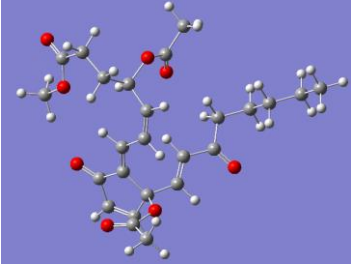
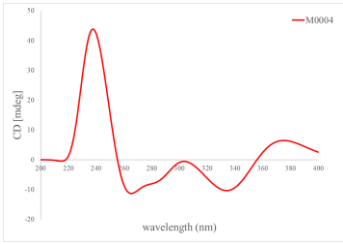
Ching-Yeu Chen – Department of Physical Therapy, Tzu-Hui Institute of Technology, Pingtung 926001, Taiwan

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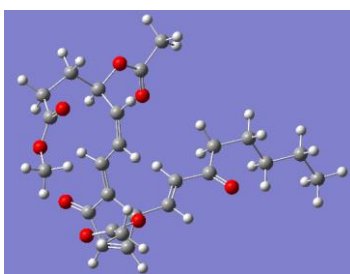
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Table S1. Energy analyses of 4*R*,12*S*-1/4*S*,12*R*-1 (fourteen conformers)

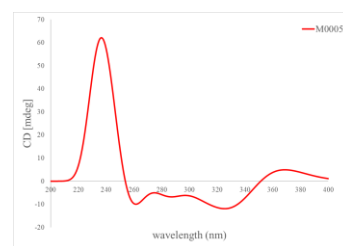
| NO. | 3D conformers B3LYP/6-31G(d,p) | G (Hartree) | Boltzmann distribution | Calculated ECD spectrum |
|-----|---|--------------|---------------------------|---|
| | | | | 4 <i>R</i> ,12 <i>S</i> -1 |
| 1 |  | -1573.243097 | 18.53 % |  |
| 2 |  | -1573.242279 | 7.79 % |  |
| 3 |  | -1573.240387 | 1.05 % |  |
| 4 |  | -1573.243648 | 33.21 % |  |

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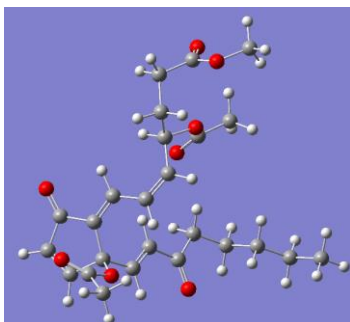


-1573.240860

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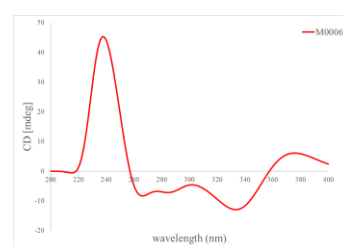


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-1573.241282

2.71 %

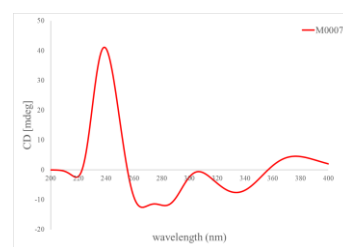


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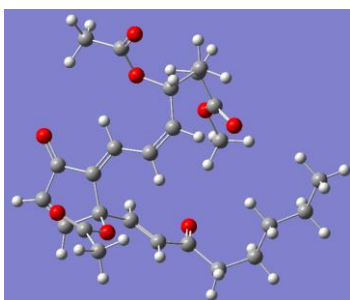


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11.63 %

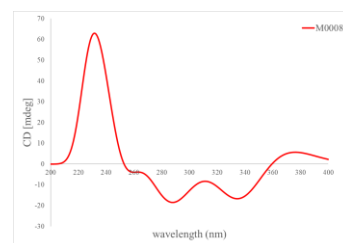


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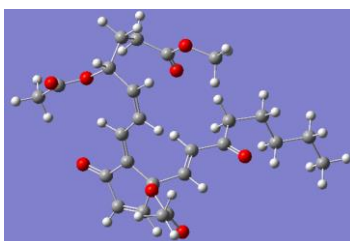


-1573.241846

4.93 %

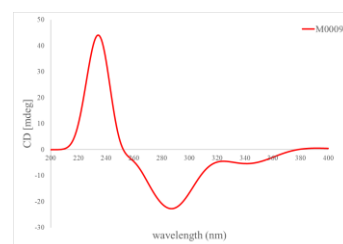


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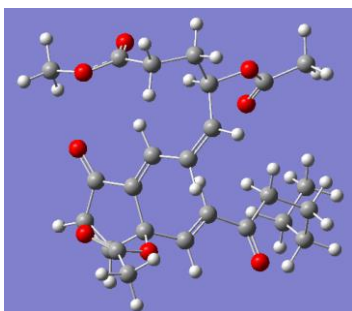


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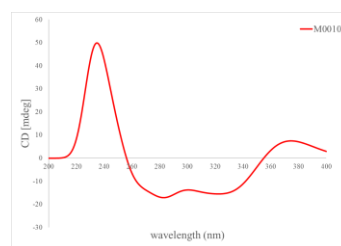


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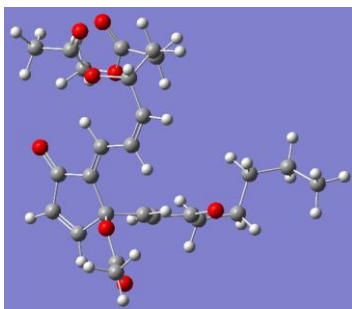


-1573.239958

0.67 %

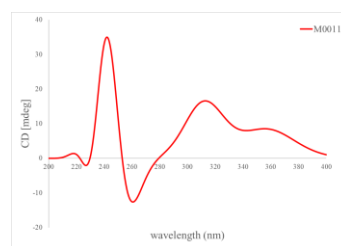


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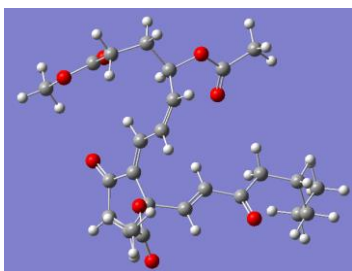


-1573.240849

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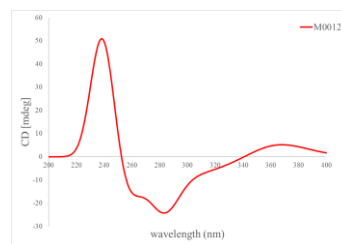


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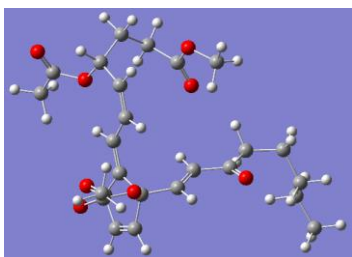


-1573.240968

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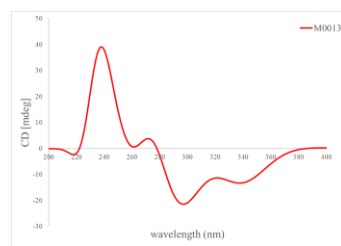


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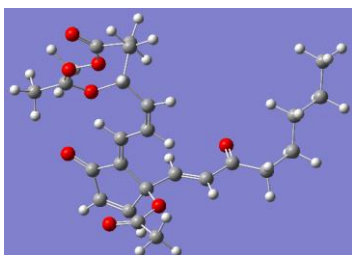


-1573.239961

0.67 %



14



-1573.242638

11.4 %

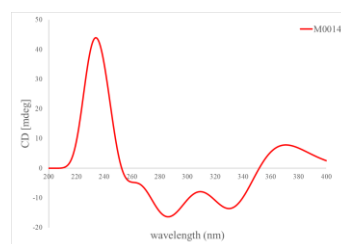


Table S2. Cartesian coordinates of the low-energy re-optimized conformers of 4*R*,12*S*-1/4*S*,12*R*-1 calculated at B3LYP/6-31G(d,p) level of theory.

| Conformer 1 | | | | | | | |
|-------------|---------------------------|---------|---------|-------------|---------------------------|---------|---------|
| Atomic Type | Standard Orientation (Å) | | | Atomic Type | Standard Orientation (Å) | | |
| | X | Y | Z | | X | Y | Z |
| C | -1.133 | -3.757 | -1.0164 | H | -0.7578 | -4.7693 | -0.9036 |
| C | -0.6894 | -2.6582 | -0.0532 | H | -2.3736 | -3.8718 | -2.7963 |
| C | -1.4742 | -1.4556 | -0.5425 | H | 1.36952 | -3.3393 | 0.3506 |
| C | -2.2508 | -1.8671 | -1.7517 | H | -2.0528 | 0.51974 | -0.6661 |
| C | -1.9483 | -3.3045 | -1.9767 | H | -0.4089 | -0.4845 | 1.78584 |
| O | -2.9916 | -1.1606 | -2.4181 | H | 1.01989 | -0.7159 | -1.2075 |
| C | 0.81798 | -2.5282 | -0.1232 | H | -0.0394 | 1.7951 | 2.35781 |
| C | -1.4702 | -0.1899 | -0.0822 | H | -1.1386 | 2.50708 | -0.4286 |
| C | -0.7785 | 0.27955 | 1.10641 | H | -1.7491 | 3.96149 | 2.19498 |
| C | 1.51177 | -1.5581 | -0.7293 | H | -2.1344 | 4.52437 | 0.56486 |
| C | -0.5547 | 1.56947 | 1.42423 | H | -3.3171 | 1.99533 | 1.87642 |
| C | -0.9025 | 2.77838 | 0.59942 | H | -4.125 | 3.54291 | 1.75532 |
| C | -2.0359 | 3.63076 | 1.18953 | H | 3.40045 | -0.5878 | -2.5698 |
| C | -3.3817 | 2.90174 | 1.26441 | H | 3.19127 | 0.49955 | -1.2262 |
| C | 3.008 | -1.5825 | -0.7479 | H | 5.61518 | -1.3766 | -1.5422 |
| C | 3.67375 | -0.4469 | -1.5112 | H | 5.59935 | 0.28627 | -2.1274 |
| O | 3.64369 | -2.471 | -0.1982 | H | 5.22337 | 1.1037 | 0.22041 |
| C | 5.19537 | -0.381 | -1.3541 | H | 5.25196 | -0.5612 | 0.7975 |
| C | 5.65328 | 0.10873 | 0.02668 | H | 7.6059 | -0.8117 | -0.0271 |
| C | 7.17899 | 0.18267 | 0.16496 | H | 7.58418 | 0.84375 | -0.6149 |
| C | 7.63705 | 0.6765 | 1.54107 | H | 8.73031 | 0.71533 | 1.61038 |
| O | -0.9218 | -3.0267 | 1.34698 | H | 7.25463 | 1.68384 | 1.7489 |
| O | -3.1768 | -3.1888 | 1.08333 | H | 7.27576 | 0.01549 | 2.33845 |
| C | -2.1923 | -3.2679 | 1.7781 | H | -3.192 | -3.8705 | 3.5667 |
| C | -2.1767 | -3.6377 | 3.24401 | H | -1.5219 | -4.4985 | 3.41245 |
| C | -3.9319 | 2.5175 | -0.1002 | H | -1.7814 | -2.8062 | 3.83709 |
| O | -3.4836 | 2.89885 | -1.1633 | H | -6.3949 | 0.59721 | -0.9394 |
| O | -4.9806 | 1.68674 | 0.01689 | H | -5.8282 | 2.02745 | -1.8668 |
| C | -5.5292 | 1.19442 | -1.2261 | H | -4.7895 | 0.57789 | -1.7431 |
| O | 0.25841 | 3.66397 | 0.56924 | H | 3.20139 | 4.03294 | -0.8441 |
| O | 1.28823 | 2.30794 | -0.9293 | H | 2.01627 | 5.3165 | -0.4592 |
| C | 1.2809 | 3.30862 | -0.2441 | H | 2.76921 | 4.40648 | 0.85129 |
| C | 2.39342 | 4.32898 | -0.1743 | | | | |

| Conformer 2 | | | | | | | |
|-------------|---------------------------|---------|---------|--------|---------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.8989 | -3.2806 | 1.6654 | H | -1.7084 | -3.9976 | 1.71769 |
| C | -0.6039 | -2.555 | 0.35793 | H | -0.1062 | -3.2457 | 3.68715 |
| C | 0.61684 | -1.7123 | 0.71626 | H | -1.783 | -1.5109 | -1.2043 |
| C | 0.88808 | -1.8883 | 2.17177 | H | 2.22836 | -0.4522 | 0.46223 |
| C | -0.0893 | -2.8964 | 2.66087 | H | 0.45818 | -1.2129 | -1.9796 |
| O | 1.74829 | -1.3228 | 2.83231 | H | -2.7279 | -1.282 | 1.7025 |
| C | -1.7556 | -1.7079 | -0.134 | H | 1.754 | 0.19024 | -3.2949 |
| C | 1.40898 | -0.9384 | -0.0547 | H | 3.99409 | 0.79208 | -2.7031 |
| C | 1.27187 | -0.6966 | -1.4769 | H | 3.85653 | 3.0069 | -1.7719 |
| C | -2.6933 | -1.1302 | 0.62598 | H | 2.53062 | 2.73927 | -2.9033 |
| C | 2.04025 | 0.10418 | -2.2466 | H | 1.63996 | 3.95559 | -1.0249 |
| C | 3.2381 | 0.95461 | -1.9265 | H | 0.97601 | 2.32746 | -0.9061 |
| C | 2.91519 | 2.4672 | -1.9128 | H | -5.3411 | -0.5864 | 1.35073 |
| C | 1.90229 | 2.90455 | -0.8452 | H | -4.2903 | 0.72369 | 1.83131 |
| C | -3.7344 | -0.2569 | 0.00897 | H | -6.1484 | 0.86312 | -0.613 |
| C | -4.7967 | 0.28676 | 0.95704 | H | -6.6292 | 1.41156 | 0.99192 |
| O | -3.7428 | -0.0146 | -1.1896 | H | -4.7507 | 3.08285 | 0.9798 |
| C | -5.7667 | 1.28788 | 0.32323 | H | -4.2837 | 2.53567 | -0.6293 |
| C | -5.1428 | 2.66152 | 0.04119 | H | -6.5209 | 3.2336 | -1.5199 |
| C | -6.1315 | 3.65458 | -0.5823 | H | -6.9994 | 3.77125 | 0.08295 |
| C | -5.5121 | 5.02834 | -0.8586 | H | -6.2408 | 5.71406 | -1.3061 |
| O | -0.1874 | -3.483 | -0.6975 | H | -5.1437 | 5.49084 | 0.0656 |
| O | -2.1915 | -4.5515 | -0.6709 | H | -4.6631 | 4.94747 | -1.5485 |
| C | -1.0774 | -4.4181 | -1.1251 | H | -1.1892 | -6.012 | -2.5417 |
| C | -0.4731 | -5.2509 | -2.2308 | H | -0.2141 | -4.6137 | -3.0828 |
| C | 2.45155 | 2.83408 | 0.57085 | H | 0.45144 | -5.7235 | -1.8842 |
| O | 3.56456 | 3.19124 | 0.90095 | H | 2.29665 | 1.2176 | 2.96878 |
| O | 1.52128 | 2.35742 | 1.42038 | H | 2.63981 | 2.97793 | 3.07472 |
| C | 1.89981 | 2.22279 | 2.80549 | H | 0.98162 | 2.35353 | 3.38046 |
| O | 3.82365 | 0.56907 | -0.6668 | H | 6.69456 | 0.34675 | 0.90493 |
| O | 5.88491 | 1.10394 | -1.4469 | H | 5.31252 | 1.31159 | 1.49657 |
| C | 5.17297 | 0.74473 | -0.5375 | H | 5.11722 | -0.4328 | 1.26946 |
| C | 5.61012 | 0.45995 | 0.87448 | | | | |

| Conformer 3 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.41482 | -3.7788 | 1.37924 | H | -0.1363 | -4.7127 | 1.42871 |
| C | 0.20243 | -2.816 | 0.21177 | H | 1.54832 | -3.7598 | 3.23236 |
| C | 1.2211 | -1.7286 | 0.49583 | H | -1.9572 | -3.1069 | -0.1449 |
| C | 1.82273 | -1.9986 | 1.83534 | H | 2.32147 | -0.0054 | 0.20152 |
| C | 1.26572 | -3.2973 | 2.29396 | H | 0.35531 | -1.0135 | -1.9888 |
| O | 2.60294 | -1.2781 | 2.44264 | H | -1.0528 | -0.4271 | 1.05237 |
| C | -1.2452 | -2.3693 | 0.22303 | H | 0.72026 | 0.95039 | -3.1742 |
| C | 1.57027 | -0.6521 | -0.2364 | H | 2.65123 | 2.34731 | -2.7802 |
| C | 1.02868 | -0.2908 | -1.5335 | H | 1.80753 | 4.15074 | -1.3902 |
| C | -1.7171 | -1.2027 | 0.67865 | H | 0.55845 | 3.52653 | -2.4651 |
| C | 1.24716 | 0.84834 | -2.2251 | H | -0.4582 | 3.97463 | -0.3209 |
| C | 2.0509 | 2.07714 | -1.9038 | H | -0.4369 | 2.22219 | -0.5226 |
| C | 1.15292 | 3.29369 | -1.5732 | H | -3.3405 | 0.37293 | 2.34849 |
| C | 0.20103 | 3.09867 | -0.3833 | H | -2.9577 | 1.20156 | 0.86305 |
| C | -3.1857 | -0.9238 | 0.68276 | H | -5.6865 | -0.1033 | 1.42279 |
| C | -3.6044 | 0.41454 | 1.27937 | H | -5.3369 | 1.58841 | 1.7746 |
| O | -3.9972 | -1.7312 | 0.254 | H | -4.8562 | 1.99074 | -0.6609 |
| C | -5.0862 | 0.75675 | 1.10257 | H | -5.219 | 0.30015 | -1.0044 |
| C | -5.4667 | 1.13404 | -0.3357 | H | -7.5594 | 0.62884 | -0.1695 |
| C | -6.9515 | 1.4853 | -0.4929 | H | -7.2041 | 2.31237 | 0.18633 |
| C | -7.3316 | 1.86802 | -1.9268 | H | -8.3975 | 2.10982 | -2.0078 |
| O | 0.33367 | -3.4674 | -1.0907 | H | -6.765 | 2.7437 | -2.2676 |
| O | 2.46005 | -4.1675 | -0.6835 | H | -7.1221 | 1.0473 | -2.6238 |
| C | 1.50347 | -4.0905 | -1.4154 | H | 2.31039 | -5.24 | -3.0238 |
| C | 1.41724 | -4.6496 | -2.8169 | H | 0.52042 | -5.266 | -2.931 |
| C | 0.91452 | 3.00198 | 0.95505 | H | 1.34552 | -3.8292 | -3.5394 |
| O | 1.82547 | 3.72141 | 1.3082 | H | 0.20796 | 1.35098 | 3.63235 |
| O | 0.37362 | 2.03384 | 1.7261 | H | 1.83933 | 1.17217 | 2.92518 |
| C | 0.97443 | 1.83305 | 3.02406 | H | 1.27259 | 2.78877 | 3.45779 |
| O | 2.96009 | 1.82833 | -0.8144 | H | 4.92038 | 1.25187 | 0.70687 |
| O | 4.40711 | 3.35738 | -1.6559 | H | 5.86609 | 2.74853 | 0.40555 |
| C | 4.09991 | 2.58169 | -0.7799 | H | 4.32824 | 2.80432 | 1.31434 |
| C | 4.86562 | 2.32252 | 0.48979 | | | | |

| Conformer 4 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.5509 | -4.0707 | -1.2026 | H | 0.02229 | -4.9914 | -1.248 |
| C | -0.2338 | -3.015 | -0.146 | H | -1.9123 | -4.2388 | -2.8876 |
| C | -1.291 | -1.9595 | -0.4098 | H | 1.95059 | -3.2919 | -0.0134 |
| C | -2.0737 | -2.3757 | -1.6128 | H | -2.2994 | -0.1715 | -0.19 |
| C | -1.5285 | -3.6913 | -2.0348 | H | -0.212 | -1.0294 | 1.95624 |
| O | -2.9756 | -1.7504 | -2.1509 | H | 0.9237 | -0.6308 | -1.15 |
| C | 1.20151 | -2.5639 | -0.3222 | H | -0.2273 | 1.25021 | 2.69552 |
| C | -1.5057 | -0.7909 | 0.2235 | H | -1.6046 | 1.89781 | 0.04309 |
| C | -0.7908 | -0.3032 | 1.39135 | H | -3.3982 | 1.61981 | 1.84241 |
| C | 1.62098 | -1.4029 | -0.8376 | H | -2.5933 | 2.89251 | 2.75882 |
| C | -0.7817 | 0.98025 | 1.79773 | H | -4.4252 | 3.93297 | 1.55746 |
| C | -1.4584 | 2.12864 | 1.09775 | H | -2.949 | 4.48294 | 0.80231 |
| C | -2.791 | 2.52465 | 1.74456 | H | 3.07102 | 0.18032 | -2.6502 |
| C | -3.5666 | 3.59315 | 0.96432 | H | 2.80724 | 1.01158 | -1.1427 |
| C | 3.08221 | -1.1095 | -0.9768 | H | 5.49671 | -0.2637 | -1.9368 |
| C | 3.42717 | 0.23135 | -1.6082 | H | 5.09495 | 1.42234 | -2.2596 |
| O | 3.9345 | -1.91 | -0.6189 | H | 4.82725 | 1.82634 | 0.20702 |
| C | 4.91535 | 0.58947 | -1.5665 | H | 5.2409 | 0.1423 | 0.52136 |
| C | 5.41803 | 0.97672 | -0.1689 | H | 7.49424 | 0.49644 | -0.5179 |
| C | 6.90633 | 1.34652 | -0.1443 | H | 7.08806 | 2.17397 | -0.8455 |
| C | 7.40755 | 1.73925 | 1.24923 | H | 8.47348 | 1.99442 | 1.23545 |
| O | -0.2365 | -3.5704 | 1.21013 | H | 6.86227 | 2.60914 | 1.63666 |
| O | -2.4215 | -4.1988 | 1.10461 | H | 7.27043 | 0.91872 | 1.96421 |
| C | -1.3771 | -4.1298 | 1.70633 | H | -2.037 | -5.1229 | 3.47799 |
| C | -1.1336 | -4.6356 | 3.10994 | H | -0.2953 | -5.3394 | 3.12102 |
| C | -4.1278 | 3.19617 | -0.3959 | H | -0.8684 | -3.802 | 3.76878 |
| O | -4.6424 | 3.98214 | -1.1601 | H | -4.2223 | 0.38132 | -2.0083 |
| O | -4.0074 | 1.8743 | -0.6502 | H | -5.6245 | 1.50945 | -1.9182 |
| C | -4.5348 | 1.42125 | -1.9175 | H | -4.1279 | 2.02656 | -2.7306 |
| O | -0.5979 | 3.30469 | 1.17367 | H | 2.10309 | 4.61446 | -0.1681 |
| O | 0.71597 | 2.46281 | -0.4707 | H | 0.61973 | 5.48242 | 0.32606 |
| C | 0.46021 | 3.3398 | 0.32669 | H | 1.60768 | 4.68354 | 1.54999 |
| C | 1.25426 | 4.61057 | 0.51627 | | | | |

| Conformer 5 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.00029 | -3.6393 | 1.02721 | H | -0.4751 | -4.5407 | 0.65351 |
| C | 0.18184 | -2.429 | 0.11428 | H | 0.38181 | -4.0944 | 3.11678 |
| C | 0.92711 | -1.4535 | 1.00443 | H | -1.6491 | -2.5962 | -1.1094 |
| C | 1.03562 | -2.0586 | 2.36815 | H | 1.83281 | 0.3059 | 1.57067 |
| C | 0.43153 | -3.4146 | 2.27418 | H | 1.11987 | -0.1995 | -1.4217 |
| O | 1.51681 | -1.5324 | 3.35772 | H | -1.4174 | -0.2073 | 0.80735 |
| C | -1.1775 | -1.9596 | -0.3621 | H | 1.55193 | 2.10061 | -1.8283 |
| C | 1.38331 | -0.2172 | 0.72928 | H | 1.60654 | 2.45319 | 1.23184 |
| C | 1.34787 | 0.43388 | -0.5679 | H | 3.4106 | 3.79288 | -0.8657 |
| C | -1.8436 | -0.8837 | 0.07184 | H | 3.18798 | 4.34425 | 0.7981 |
| C | 1.57198 | 1.74141 | -0.8007 | H | 5.23605 | 3.1113 | 0.77501 |
| C | 1.80995 | 2.81801 | 0.22236 | H | 4.09096 | 2.03979 | 1.57518 |
| C | 3.20373 | 3.45667 | 0.15594 | H | -3.9228 | 0.49564 | 1.24877 |
| C | 4.32693 | 2.51657 | 0.61899 | H | -3.1593 | 1.50601 | 0.05997 |
| C | -3.2014 | -0.5517 | -0.4613 | H | -5.4982 | 2.03861 | -0.1093 |
| C | -3.8647 | 0.66742 | 0.16192 | H | -5.1785 | 1.01467 | -1.5077 |
| O | -3.7245 | -1.2118 | -1.3479 | H | -6.104 | -0.9599 | -0.2749 |
| C | -5.2412 | 1.01438 | -0.4122 | H | -6.4188 | 0.05719 | 1.13002 |
| C | -6.3605 | 0.06169 | 0.03056 | H | -7.9829 | 1.46524 | -0.2508 |
| C | -7.7322 | 0.43542 | -0.5446 | H | -7.6738 | 0.43755 | -1.6422 |
| C | -8.8515 | -0.5097 | -0.0959 | H | -9.8177 | -0.2201 | -0.5252 |
| O | 0.85798 | -2.7916 | -1.1369 | H | -8.6449 | -1.5415 | -0.4054 |
| O | 2.79603 | -3.391 | -0.1058 | H | -8.9585 | -0.5078 | 0.99604 |
| C | 2.13401 | -3.2606 | -1.1095 | H | 3.57645 | -4.0535 | -2.4727 |
| C | 2.59837 | -3.5729 | -2.5143 | H | 1.87918 | -4.2238 | -3.0203 |
| C | 4.68116 | 1.45749 | -0.4121 | H | 2.66808 | -2.6483 | -3.098 |
| O | 4.821 | 1.67436 | -1.5976 | H | 4.93138 | -1.7471 | -0.1823 |
| O | 4.84287 | 0.25084 | 0.16467 | H | 4.66477 | -0.7529 | -1.6552 |
| C | 5.20486 | -0.8337 | -0.7096 | H | 6.28051 | -0.806 | -0.909 |
| O | 0.88013 | 3.913 | -0.0458 | H | -2.2418 | 4.83934 | 0.36672 |
| O | -0.8262 | 2.74554 | 0.889 | H | -0.7708 | 5.8604 | 0.30154 |
| C | -0.4098 | 3.73733 | 0.32877 | H | -1.3088 | 5.00813 | -1.1466 |
| C | -1.2412 | 4.93922 | -0.0552 | | | | |

| Conformer 6 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 4.5987 | -1.2215 | -0.9099 | H | 5.56908 | -0.7939 | -0.678 |
| C | 3.39818 | -0.9431 | -0.0075 | H | 4.94053 | -2.2655 | -2.7839 |
| C | 2.30344 | -1.7694 | -0.6547 | H | 3.86916 | 1.12347 | 0.60808 |
| C | 2.85428 | -2.372 | -1.9095 | H | 0.41347 | -2.5241 | -0.966 |
| C | 4.28223 | -1.9644 | -1.9775 | H | 1.08476 | -1.0306 | 1.68672 |
| O | 2.24033 | -3.0534 | -2.7133 | H | 1.42606 | 0.69464 | -1.2041 |
| C | 3.14964 | 0.55083 | 0.0243 | H | -1.2548 | -0.8638 | 2.09073 |
| C | 1.0188 | -1.927 | -0.2863 | H | -1.6342 | -1.807 | -0.8176 |
| C | 0.40608 | -1.3874 | 0.91593 | H | -2.2346 | -3.6727 | 0.71363 |
| C | 2.17921 | 1.21231 | -0.6167 | H | -3.2634 | -2.6006 | 1.66268 |
| C | -0.9166 | -1.2779 | 1.14166 | H | -3.7313 | -3.1755 | -1.33 |
| C | -2.0252 | -1.617 | 0.18426 | H | -4.4853 | -4.081 | -0.0092 |
| C | -2.8868 | -2.7937 | 0.65237 | H | 1.2587 | 3.17555 | -2.4178 |
| C | -4.0659 | -3.1074 | -0.2909 | H | 0.05469 | 2.75353 | -1.2337 |
| C | 2.08034 | 2.70245 | -0.5299 | H | 1.71904 | 5.34442 | -1.1323 |
| C | 0.9771 | 3.3378 | -1.3645 | H | 0.13597 | 5.24314 | -1.9015 |
| O | 2.85225 | 3.36081 | 0.15293 | H | -0.8861 | 4.58787 | 0.30083 |
| C | 0.75245 | 4.82775 | -1.093 | H | 0.69906 | 4.70234 | 1.06255 |
| C | 0.07956 | 5.11508 | 0.25631 | H | 0.81496 | 7.13433 | 0.46621 |
| C | -0.1501 | 6.61025 | 0.50958 | H | -0.7604 | 7.02832 | -0.3041 |
| C | -0.8259 | 6.8978 | 1.85413 | H | -0.9732 | 7.97309 | 2.00763 |
| O | 3.67453 | -1.2612 | 1.39584 | H | -1.8097 | 6.41539 | 1.91525 |
| O | 4.06039 | -3.4633 | 0.96979 | H | -0.2215 | 6.52162 | 2.68869 |
| C | 3.99576 | -2.5398 | 1.74466 | H | 4.55314 | -3.6335 | 3.49226 |
| C | 4.24652 | -2.6195 | 3.23343 | H | 5.02154 | -1.905 | 3.52811 |
| C | -5.1973 | -2.0957 | -0.2446 | H | 3.33562 | -2.3576 | 3.78219 |
| O | -5.6252 | -1.4689 | -1.1901 | H | -7.1136 | -1.1724 | 2.19979 |
| O | -5.7106 | -2.0057 | 1.00356 | H | -6.4499 | -0.0546 | 0.96432 |
| C | -6.7916 | -1.0743 | 1.16259 | H | -7.6108 | -1.3139 | 0.47988 |
| O | -2.9228 | -0.4723 | 0.0926 | H | -3.3829 | 2.3607 | -1.5079 |
| O | -1.5431 | 0.54525 | -1.3915 | H | -4.5947 | 1.0739 | -1.2082 |
| C | -2.582 | 0.52257 | -0.7672 | H | -3.8942 | 1.95153 | 0.15828 |
| C | -3.6812 | 1.55273 | -0.8391 | | | | |

| Conformer 7 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -4.1155 | -1.3668 | -1.1011 | H | -4.8782 | -2.1311 | -0.991 |
| C | -3.0264 | -1.2049 | -0.0427 | H | -4.5706 | -0.4683 | -3.0262 |
| C | -2.2469 | -0.0067 | -0.5545 | H | -2.7625 | -3.302 | 0.59106 |
| C | -2.8148 | 0.38317 | -1.8801 | H | -0.8066 | 1.47368 | -0.5675 |
| C | -3.9605 | -0.5277 | -2.1325 | H | -1.064 | -0.4442 | 1.88475 |
| O | -2.4106 | 1.27 | -2.6179 | H | -0.5023 | -2.0034 | -1.0258 |
| C | -2.2524 | -2.5025 | 0.05554 | H | 0.86816 | 0.65125 | 2.76324 |
| C | -1.2019 | 0.63604 | 0.00455 | H | 1.30279 | 1.88629 | 0.02632 |
| C | -0.5943 | 0.33131 | 1.28584 | H | -0.3033 | 3.45788 | 1.23786 |
| C | -1.056 | -2.7641 | -0.4823 | H | 0.8915 | 3.60154 | 2.52606 |
| C | 0.50233 | 0.9404 | 1.7793 | H | 1.14001 | 5.53324 | 1.07206 |
| C | 1.2916 | 2.0338 | 1.10736 | H | 2.55734 | 4.53281 | 0.84813 |
| C | 0.76947 | 3.43675 | 1.44868 | H | 1.11238 | -5.3882 | -1.0597 |
| C | 1.47586 | 4.56261 | 0.68369 | H | 0.90823 | -3.9009 | -2.0119 |
| C | -0.4397 | -4.1218 | -0.3514 | H | 1.8513 | -2.5486 | -0.0982 |
| C | 0.92423 | -4.3121 | -0.9922 | H | 2.05035 | -4.0291 | 0.83367 |
| O | -0.998 | -5.022 | 0.25871 | H | 3.63292 | -4.9102 | -0.9127 |
| C | 2.05004 | -3.6251 | -0.188 | H | 3.41922 | -3.4373 | -1.8504 |
| C | 3.43118 | -3.8324 | -0.8238 | H | 4.35277 | -2.086 | 0.0403 |
| C | 4.56461 | -3.1601 | -0.0385 | H | 4.57361 | -3.5529 | 0.98871 |
| C | 5.94153 | -3.3727 | -0.6765 | H | 6.73242 | -2.8854 | -0.0942 |
| O | -3.5778 | -1.053 | 1.30501 | H | 6.18958 | -4.4394 | -0.7449 |
| O | -4.7211 | 0.84429 | 0.78309 | H | 5.97524 | -2.9599 | -1.6923 |
| C | -4.3985 | -6E-05 | 1.58344 | H | -5.535 | 0.75484 | 3.22625 |
| C | -4.8268 | -0.0513 | 3.03216 | H | -5.2844 | -1.0187 | 3.26146 |
| C | 1.26008 | 4.6142 | -0.8235 | H | -3.9535 | 0.05977 | 3.68387 |
| O | 1.93219 | 5.28426 | -1.5759 | H | -0.8823 | 3.15713 | -2.7773 |
| O | 0.21689 | 3.85536 | -1.2251 | H | -0.407 | 4.88878 | -2.9276 |
| C | -0.0842 | 3.88534 | -2.638 | H | 0.80286 | 3.61628 | -3.2164 |
| O | 2.6698 | 1.99136 | 1.5743 | H | 5.50513 | 0.3852 | 1.13445 |
| O | 3.10272 | 0.24729 | 0.19464 | H | 5.28655 | 2.1408 | 1.39649 |
| C | 3.47472 | 1.04768 | 1.02549 | H | 4.84826 | 1.00918 | 2.67681 |
| C | 4.87174 | 1.14632 | 1.59069 | | | | |

| Conformer 8 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.91187 | 3.57864 | -1.3514 | H | 1.5588 | 4.60285 | -1.4165 |
| C | 1.23434 | 2.59467 | -0.3984 | H | 3.51395 | 3.49304 | -2.8141 |
| C | 2.05703 | 1.3266 | -0.5995 | H | -0.3184 | 1.90785 | -1.7963 |
| C | 3.0904 | 1.60115 | -1.6394 | H | 2.59602 | -0.6551 | -0.4132 |
| C | 2.89789 | 3.01684 | -2.0602 | H | 0.23289 | 0.49615 | 1.2488 |
| O | 3.9169 | 0.81251 | -2.0706 | H | -1.2214 | 3.15135 | 0.8569 |
| C | -0.1965 | 2.37877 | -0.823 | H | -0.1828 | -1.6149 | 2.08848 |
| C | 1.90004 | 0.0984 | -0.0635 | H | 1.73955 | -3.1824 | 2.1568 |
| C | 0.89452 | -0.2933 | 0.90226 | H | 0.92551 | -4.8979 | 0.74778 |
| C | -1.2956 | 2.67982 | -0.1176 | H | -0.4623 | -4.0369 | 1.41456 |
| C | 0.65661 | -1.5252 | 1.40143 | H | 0.59376 | -3.3834 | -1.3896 |
| C | 1.33015 | -2.8504 | 1.19453 | H | -0.4979 | -4.722 | -1.1237 |
| C | 0.36851 | -3.956 | 0.70547 | H | -3.5279 | 2.84867 | 1.27587 |
| C | -0.1803 | -3.7551 | -0.7109 | H | -4.1589 | 3.70899 | -0.1181 |
| C | -2.6475 | 2.3175 | -0.6266 | H | -5.915 | 2.19654 | 0.55584 |
| C | -3.8447 | 2.7135 | 0.23364 | H | -5.2187 | 1.53441 | -0.9227 |
| O | -2.8 | 1.7331 | -1.6929 | H | -3.8222 | -0.0551 | 0.48174 |
| C | -5.0157 | 1.72585 | 0.13731 | H | -4.5686 | 0.60328 | 1.93152 |
| C | -4.7457 | 0.40066 | 0.864 | H | -6.8214 | -0.168 | 1.10239 |
| C | -5.8884 | -0.6133 | 0.72727 | H | -6.0584 | -0.8192 | -0.3394 |
| C | -5.6085 | -1.928 | 1.46357 | H | -6.4268 | -2.6447 | 1.32711 |
| O | 1.18238 | 3.09482 | 0.96535 | H | -4.6836 | -2.3907 | 1.10052 |
| O | 3.44651 | 3.16713 | 1.18526 | H | -5.4927 | -1.7587 | 2.54159 |
| C | 2.34252 | 3.32978 | 1.64405 | H | 2.96269 | 4.05352 | 3.5544 |
| C | 2.03096 | 3.81111 | 3.04249 | H | 1.38116 | 4.69136 | 3.00877 |
| C | -1.3897 | -2.8386 | -0.7976 | H | 1.49869 | 3.03034 | 3.59629 |
| O | -2.0718 | -2.478 | 0.14172 | H | -2.9206 | -1.6956 | -3.4105 |
| O | -1.6354 | -2.5144 | -2.0787 | H | -3.6693 | -2.0954 | -1.8291 |
| C | -2.7882 | -1.6851 | -2.3282 | H | -2.6104 | -0.6641 | -1.9829 |
| O | 2.43634 | -2.7411 | 0.27096 | H | 5.55934 | -3.6453 | -0.187 |
| O | 3.68243 | -4.1708 | 1.51691 | H | 4.29701 | -3.7068 | -1.4442 |
| C | 3.56553 | -3.4513 | 0.55093 | H | 4.72217 | -2.1523 | -0.7291 |
| C | 4.60992 | -3.2195 | -0.5136 | | | | |

| Conformer 9 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.20674 | 3.58889 | 1.11238 | H | 0.94351 | 4.35221 | 0.90119 |
| C | -0.0775 | 2.48282 | 0.09387 | H | -0.4799 | 4.08757 | 3.11072 |
| C | -1.1603 | 1.67605 | 0.78644 | H | 1.88176 | 2.26975 | -0.9089 |
| C | -1.4163 | 2.27631 | 2.12798 | H | -2.5921 | 0.2269 | 1.06645 |
| C | -0.5156 | 3.45144 | 2.23356 | H | -1.1113 | 0.43604 | -1.6579 |
| O | -2.2229 | 1.88568 | 2.96056 | H | 0.94733 | -0.0125 | 0.92365 |
| C | 1.19794 | 1.74288 | -0.2477 | H | -2.3624 | -1.3693 | -2.4215 |
| C | -1.8832 | 0.62491 | 0.35082 | H | -4.5183 | -1.8184 | -1.3644 |
| C | -1.8164 | 0.00081 | -0.9547 | H | -4.0882 | -3.9063 | -0.2425 |
| C | 1.57464 | 0.55448 | 0.2409 | H | -3.017 | -3.7589 | -1.6335 |
| C | -2.5508 | -1.0416 | -1.3994 | H | -2.1396 | -3.1511 | 1.25586 |
| C | -3.6155 | -1.8824 | -0.7455 | H | -1.9739 | -4.7265 | 0.48617 |
| C | -3.2164 | -3.3677 | -0.6307 | H | 3.26155 | -0.9825 | 1.75078 |
| C | -2.0169 | -3.6464 | 0.29009 | H | 2.56193 | -2.0119 | 0.53425 |
| C | 2.90257 | -0.0321 | -0.1267 | H | 4.8347 | -2.7821 | 0.77184 |
| C | 3.33513 | -1.244 | 0.68336 | H | 4.81195 | -1.8852 | -0.7456 |
| O | 3.57921 | 0.43387 | -1.0329 | H | 5.77296 | 0.11306 | 0.4163 |
| C | 4.73012 | -1.776 | 0.34322 | H | 5.79081 | -0.7728 | 1.94001 |
| C | 5.87681 | -0.8897 | 0.84862 | H | 7.36423 | -2.4586 | 0.93089 |
| C | 7.26483 | -1.4474 | 0.51002 | H | 7.35075 | -1.5613 | -0.5799 |
| C | 8.40954 | -0.567 | 1.02182 | H | 9.38744 | -0.9886 | 0.76185 |
| O | -0.6785 | 3.0054 | -1.1482 | H | 8.35556 | 0.44054 | 0.59161 |
| O | 0.97516 | 4.52457 | -1.5234 | H | 8.37175 | -0.4621 | 2.11334 |
| C | -0.0657 | 3.99514 | -1.846 | H | -0.3908 | 5.16149 | -3.6055 |
| C | -0.8708 | 4.33605 | -3.0789 | H | -0.9349 | 3.46347 | -3.7374 |
| C | -0.6492 | -3.2587 | -0.2427 | H | -1.8928 | 4.61029 | -2.7994 |
| O | 0.24057 | -2.7759 | 0.42646 | H | 0.70159 | -3.6009 | -3.1706 |
| O | -0.509 | -3.5775 | -1.5485 | H | 0.97925 | -2.2087 | -2.0728 |
| C | 0.77187 | -3.2804 | -2.1309 | H | 1.56445 | -3.828 | -1.6147 |
| O | -3.9687 | -1.4262 | 0.57736 | H | -6.3394 | 0.06973 | 2.30061 |
| O | -5.9847 | -0.6687 | -0.1498 | H | -5.221 | -1.215 | 2.85147 |
| C | -5.1823 | -0.816 | 0.74223 | H | -4.5798 | 0.37265 | 2.43064 |
| C | -5.3481 | -0.366 | 2.17204 | | | | |

| Conformer 10 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.1504 | 3.69269 | 0.88031 | H | 0.34934 | 4.63124 | 0.66195 |
| C | -0.2233 | 2.59331 | -0.177 | H | -0.7553 | 3.91151 | 2.95551 |
| C | -1.0275 | 1.51498 | 0.5249 | H | 1.69828 | 2.91918 | -1.2121 |
| C | -1.316 | 1.98031 | 1.91575 | H | -1.8834 | -0.3397 | 0.81007 |
| C | -0.7063 | 3.32962 | 2.04262 | H | -0.9046 | 0.52095 | -2.0224 |
| O | -1.9352 | 1.3718 | 2.77506 | H | 1.38312 | 0.34589 | 0.43459 |
| C | 1.18471 | 2.20073 | -0.5746 | H | -1.1342 | -1.7488 | -2.6949 |
| C | -1.3875 | 0.29593 | 0.07942 | H | -1.4408 | -2.4388 | 0.2891 |
| C | -1.1807 | -0.2104 | -1.2669 | H | -3.0776 | -3.6014 | -2.0217 |
| C | 1.84651 | 1.10319 | -0.1914 | H | -3.0404 | -4.1916 | -0.3566 |
| C | -1.2948 | -1.4979 | -1.6464 | H | -4.0932 | -1.4227 | -1.2167 |
| C | -1.5848 | -2.6805 | -0.7631 | H | -5.0894 | -2.8166 | -0.8614 |
| C | -2.9788 | -3.2902 | -0.9748 | H | 3.84134 | -0.3493 | 1.01624 |
| C | -4.1294 | -2.3418 | -0.6216 | H | 3.24718 | -1.2422 | -0.3446 |
| C | 3.2548 | 0.85951 | -0.6362 | H | 5.60438 | -1.6872 | -0.3373 |
| C | 3.90383 | -0.3989 | -0.0815 | H | 5.36341 | -0.542 | -1.6482 |
| O | 3.8252 | 1.61857 | -1.407 | H | 7.35754 | 0.09831 | -0.4603 |
| C | 5.33994 | -0.6451 | -0.5569 | H | 6.13133 | 1.33046 | -0.2158 |
| C | 6.39978 | 0.29958 | 0.04102 | H | 7.32766 | 0.97525 | 1.85942 |
| C | 6.61631 | 0.1933 | 1.56096 | H | 5.68354 | 0.42629 | 2.09344 |
| C | 7.14554 | -1.1655 | 2.03544 | H | 7.34238 | -1.1581 | 3.11375 |
| O | -0.7963 | 3.07844 | -1.4364 | H | 6.43293 | -1.9749 | 1.83918 |
| O | -2.7996 | 3.60499 | -0.4927 | H | 8.08411 | -1.4217 | 1.52763 |
| C | -2.0727 | 3.55676 | -1.4557 | H | -3.4394 | 4.42466 | -2.8486 |
| C | -2.4332 | 4.00447 | -2.8541 | H | -1.7161 | 4.75022 | -3.2116 |
| C | -4.1591 | -1.9563 | 0.84904 | H | -2.3907 | 3.15458 | -3.5435 |
| O | -3.4792 | -2.4685 | 1.71632 | H | -5.8744 | 0.28477 | 2.4282 |
| O | -5.0327 | -0.9607 | 1.07097 | H | -5.306 | -1.2711 | 3.12322 |
| C | -5.0792 | -0.4609 | 2.42614 | H | -4.1217 | -0.0043 | 2.68925 |
| O | -0.6518 | -3.7507 | -1.105 | H | 2.46637 | -4.7026 | -0.6991 |
| O | 1.02389 | -2.6791 | -0.0143 | H | 1.00655 | -5.7369 | -0.7001 |
| C | 0.62088 | -3.6228 | -0.6608 | H | 1.47278 | -4.8883 | -2.1749 |
| C | 1.45156 | -4.8127 | -1.0826 | | | | |

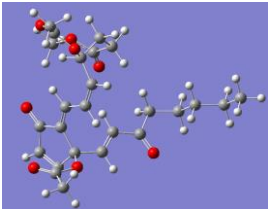
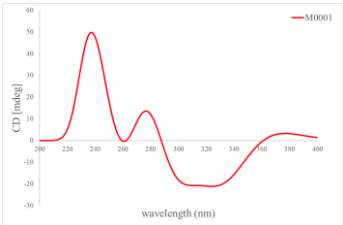
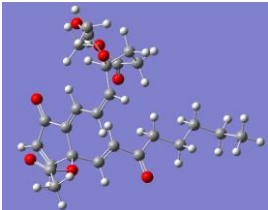
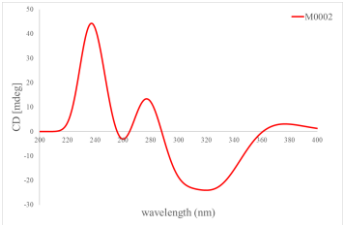
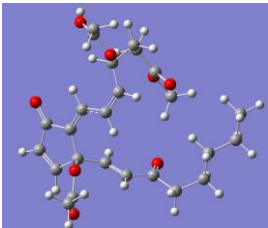
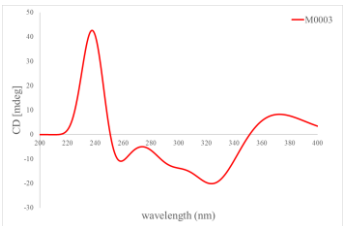
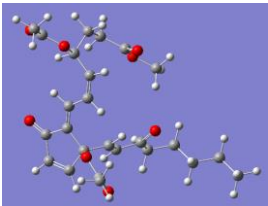
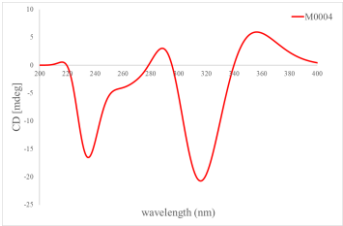
| Conformer 11 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.1504 | 3.69269 | 0.88031 | H | 0.34934 | 4.63124 | 0.66195 |
| C | -0.2233 | 2.59331 | -0.177 | H | -0.7553 | 3.91151 | 2.95551 |
| C | -1.0275 | 1.51498 | 0.5249 | H | 1.69828 | 2.91918 | -1.2121 |
| C | -1.316 | 1.98031 | 1.91575 | H | -1.8834 | -0.3397 | 0.81007 |
| C | -0.7063 | 3.32962 | 2.04262 | H | -0.9046 | 0.52095 | -2.0224 |
| O | -1.9352 | 1.3718 | 2.77506 | H | 1.38312 | 0.34589 | 0.43459 |
| C | 1.18471 | 2.20073 | -0.5746 | H | -1.1342 | -1.7488 | -2.6949 |
| C | -1.3875 | 0.29593 | 0.07942 | H | -1.4408 | -2.4388 | 0.2891 |
| C | -1.1807 | -0.2104 | -1.2669 | H | -3.0776 | -3.6014 | -2.0217 |
| C | 1.84651 | 1.10319 | -0.1914 | H | -3.0404 | -4.1916 | -0.3566 |
| C | -1.2948 | -1.4979 | -1.6464 | H | -4.0932 | -1.4227 | -1.2167 |
| C | -1.5848 | -2.6805 | -0.7631 | H | -5.0894 | -2.8166 | -0.8614 |
| C | -2.9788 | -3.2902 | -0.9748 | H | 3.84134 | -0.3493 | 1.01624 |
| C | -4.1294 | -2.3418 | -0.6216 | H | 3.24718 | -1.2422 | -0.3446 |
| C | 3.2548 | 0.85951 | -0.6362 | H | 5.60438 | -1.6872 | -0.3373 |
| C | 3.90383 | -0.3989 | -0.0815 | H | 5.36341 | -0.542 | -1.6482 |
| O | 3.8252 | 1.61857 | -1.407 | H | 7.35754 | 0.09831 | -0.4603 |
| C | 5.33994 | -0.6451 | -0.5569 | H | 6.13133 | 1.33046 | -0.2158 |
| C | 6.39978 | 0.29958 | 0.04102 | H | 7.32766 | 0.97525 | 1.85942 |
| C | 6.61631 | 0.1933 | 1.56096 | H | 5.68354 | 0.42629 | 2.09344 |
| C | 7.14554 | -1.1655 | 2.03544 | H | 7.34238 | -1.1581 | 3.11375 |
| O | -0.7963 | 3.07844 | -1.4364 | H | 6.43293 | -1.9749 | 1.83918 |
| O | -2.7996 | 3.60499 | -0.4927 | H | 8.08411 | -1.4217 | 1.52763 |
| C | -2.0727 | 3.55676 | -1.4557 | H | -3.4394 | 4.42466 | -2.8486 |
| C | -2.4332 | 4.00447 | -2.8541 | H | -1.7161 | 4.75022 | -3.2116 |
| C | -4.1591 | -1.9563 | 0.84904 | H | -2.3907 | 3.15458 | -3.5435 |
| O | -3.4792 | -2.4685 | 1.71632 | H | -5.8744 | 0.28477 | 2.4282 |
| O | -5.0327 | -0.9607 | 1.07097 | H | -5.306 | -1.2711 | 3.12322 |
| C | -5.0792 | -0.4609 | 2.42614 | H | -4.1217 | -0.0043 | 2.68925 |
| O | -0.6518 | -3.7507 | -1.105 | H | 2.46637 | -4.7026 | -0.6991 |
| O | 1.02389 | -2.6791 | -0.0143 | H | 1.00655 | -5.7369 | -0.7001 |
| C | 0.62088 | -3.6228 | -0.6608 | H | 1.47278 | -4.8883 | -2.1749 |
| C | 1.45156 | -4.8127 | -1.0826 | | | | |

| Conformer 12 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.09782 | 3.57189 | 1.25349 | H | 0.72602 | 4.44535 | 1.14154 |
| C | -0.0394 | 2.56369 | 0.11265 | H | -0.6463 | 3.74085 | 3.28646 |
| C | -0.9929 | 1.53703 | 0.69759 | H | 1.95014 | 2.74887 | -0.8369 |
| C | -1.3302 | 1.945 | 2.09314 | H | -2.1047 | -0.1947 | 0.79698 |
| C | -0.5978 | 3.2116 | 2.34155 | H | -0.9118 | 0.73363 | -1.9249 |
| O | -2.0756 | 1.36161 | 2.86702 | H | 1.23421 | 0.07969 | 0.5059 |
| C | 1.31946 | 2.04147 | -0.3036 | H | -1.3949 | -1.4369 | -2.7752 |
| C | -1.4925 | 0.41759 | 0.13752 | H | -1.8982 | -2.2978 | 0.13721 |
| C | -1.2982 | -0.0126 | -1.2365 | H | -3.5763 | -3.0602 | -2.3077 |
| C | 1.81122 | 0.82591 | -0.033 | H | -3.6773 | -3.7817 | -0.6979 |
| C | -1.5598 | -1.2443 | -1.7151 | H | -4.3378 | -0.8391 | -1.3449 |
| C | -2.0296 | -2.4413 | -0.9345 | H | -5.5167 | -2.1169 | -1.1483 |
| C | -3.4798 | -2.8491 | -1.2359 | H | 3.58265 | -0.9455 | 1.09506 |
| C | -4.5156 | -1.7931 | -0.8361 | H | 2.91048 | -1.6643 | -0.331 |
| C | 3.18626 | 0.43499 | -0.4782 | H | 5.19327 | -2.4016 | -0.3249 |
| C | 3.66125 | -0.9295 | -0.0027 | H | 5.12374 | -1.1508 | -1.5574 |
| O | 3.86264 | 1.16396 | -1.1895 | H | 7.15696 | -0.8455 | -0.3049 |
| C | 5.06507 | -1.3223 | -0.4761 | H | 6.08845 | 0.51144 | 0.00874 |
| C | 6.2216 | -0.5596 | 0.19764 | H | 7.18845 | -0.1272 | 2.06898 |
| C | 6.39231 | -0.793 | 1.70917 | H | 5.48478 | -0.4816 | 2.24513 |
| C | 6.74007 | -2.2357 | 2.0957 | H | 6.91414 | -2.3247 | 3.17429 |
| O | -0.7157 | 3.14293 | -1.0656 | H | 5.9373 | -2.9353 | 1.83563 |
| O | 0.71834 | 4.90198 | -1.2463 | H | 7.65015 | -2.5722 | 1.58291 |
| C | -0.2412 | 4.2773 | -1.6414 | H | -0.747 | 5.6001 | -3.2399 |
| C | -1.0808 | 4.64022 | -2.8446 | H | -0.9776 | 3.86944 | -3.616 |
| C | -4.5601 | -1.5345 | 0.66144 | H | -2.1389 | 4.6906 | -2.5704 |
| O | -3.9829 | -2.1977 | 1.4999 | H | -6.0762 | 0.74005 | 2.38972 |
| O | -5.3191 | -0.4626 | 0.94628 | H | -5.7085 | -0.9258 | 2.95058 |
| C | -5.3667 | -0.0863 | 2.34067 | H | -4.3765 | 0.23378 | 2.67494 |
| O | -1.2265 | -3.5943 | -1.3305 | H | 1.72719 | -4.9676 | -0.8997 |
| O | 0.52384 | -2.8303 | -0.1069 | H | 0.14991 | -5.8017 | -1.0328 |
| C | 0.03308 | -3.6645 | -0.8375 | H | 0.78361 | -4.9121 | -2.4183 |
| C | 0.72431 | -4.9167 | -1.3248 | | | | |

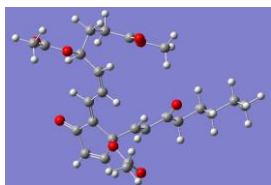
| Conformer 13 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.57209 | 3.68637 | 0.62326 | H | 1.26914 | 4.43822 | 0.26671 |
| C | 0.14454 | 2.53642 | -0.2882 | H | 0.21982 | 4.26258 | 2.68761 |
| C | -0.8608 | 1.79589 | 0.57226 | H | 1.985 | 2.23071 | -1.4619 |
| C | -0.8932 | 2.44569 | 1.91781 | H | -2.2613 | 0.38243 | 1.10415 |
| C | 0.04382 | 3.59764 | 1.85017 | H | -1.112 | 0.44409 | -1.7851 |
| O | -1.5622 | 2.09371 | 2.87748 | H | 1.25632 | 0.08476 | 0.61069 |
| C | 1.37962 | 1.75779 | -0.6898 | H | -2.4138 | -1.4064 | -2.3058 |
| C | -1.6383 | 0.73262 | 0.29057 | H | -4.4399 | -1.7849 | -0.9307 |
| C | -1.725 | 0.04234 | -0.9813 | H | -3.8861 | -3.8714 | 0.08154 |
| C | 1.81448 | 0.60846 | -0.1608 | H | -3.0171 | -3.7368 | -1.4437 |
| C | -2.4855 | -1.0315 | -1.2854 | H | -1.7387 | -3.1737 | 1.30282 |
| C | -3.4463 | -1.8533 | -0.4713 | H | -1.6967 | -4.7379 | 0.49237 |
| C | -3.065 | -3.3483 | -0.4211 | H | 3.56899 | -0.9508 | 1.23283 |
| C | -1.7543 | -3.6541 | 0.32196 | H | 2.79189 | -1.972 | 0.0636 |
| C | 3.1058 | 0.00336 | -0.6186 | H | 5.0631 | -2.7663 | 0.1528 |
| C | 3.57938 | -1.2104 | 0.16389 | H | 4.92789 | -1.8806 | -1.364 |
| O | 3.72108 | 0.45733 | -1.5738 | H | 7.04238 | -1.3068 | -0.39 |
| C | 4.94084 | -1.7614 | -0.2743 | H | 6.01883 | 0.11439 | -0.2872 |
| C | 6.15447 | -0.898 | 0.11328 | H | 5.57837 | -0.3988 | 2.14959 |
| C | 6.43981 | -0.8287 | 1.62018 | H | 6.55966 | -1.8486 | 2.01402 |
| C | 7.6888 | -0.0044 | 1.95081 | H | 7.87401 | 0.02955 | 3.03065 |
| O | -0.3741 | 3.00571 | -1.5757 | H | 8.58054 | -0.4281 | 1.47243 |
| O | -2.0593 | 4.20832 | -0.6298 | H | 7.58549 | 1.02884 | 1.59713 |
| C | -1.4678 | 3.81886 | -1.6075 | H | -2.6436 | 4.86419 | -3.0519 |
| C | -1.8253 | 4.14354 | -3.0402 | H | -0.9575 | 4.5482 | -3.57 |
| C | -0.4674 | -3.2653 | -0.3832 | H | -2.132 | 3.23106 | -3.5629 |
| O | 0.50242 | -2.7854 | 0.16591 | H | 0.49226 | -3.5933 | -3.4627 |
| O | -0.4989 | -3.5781 | -1.6978 | H | 0.90832 | -2.2054 | -2.4033 |
| C | 0.69581 | -3.2771 | -2.4393 | H | 1.5488 | -3.8258 | -2.0319 |
| O | -3.5597 | -1.3571 | 0.87907 | H | -5.741 | -0.4974 | 3.18022 |
| O | -5.8167 | -1.5966 | 0.83781 | H | -4.2593 | -1.4438 | 3.48003 |
| C | -4.8096 | -1.2631 | 1.41925 | H | -4.1184 | 0.19704 | 2.85114 |
| C | -4.7335 | -0.7083 | 2.82023 | | | | |

| Conformer 14 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.4847 | -3.5337 | 1.53607 | H | -1.2555 | -4.2943 | 1.60691 |
| C | -0.5688 | -2.4572 | 0.4549 | H | 0.82079 | -3.9631 | 3.21758 |
| C | 0.72644 | -1.6809 | 0.66712 | H | -1.7419 | -1.044 | 1.66854 |
| C | 1.39623 | -2.2255 | 1.88449 | H | 2.20092 | -0.2786 | 0.31799 |
| C | 0.56183 | -3.3636 | 2.35273 | H | -0.3249 | -0.3887 | -1.4953 |
| O | 2.42366 | -1.8113 | 2.40167 | H | -2.9642 | -2.0281 | -0.9658 |
| C | -1.7806 | -1.6014 | 0.73476 | H | 0.56759 | 1.33736 | -2.7698 |
| C | 1.24995 | -0.6572 | -0.0377 | H | 2.92984 | 1.73898 | -2.8821 |
| C | 0.65996 | -0.0304 | -1.2048 | H | 3.33783 | 3.61685 | -1.4335 |
| C | -2.8763 | -1.489 | -0.0273 | H | 1.68891 | 3.6748 | -2.0557 |
| C | 1.18706 | 0.96072 | -1.9556 | H | 1.6148 | 4.33954 | 0.2599 |
| C | 2.50072 | 1.6876 | -1.8748 | H | 0.86209 | 2.74705 | 0.18595 |
| C | 2.35477 | 3.14103 | -1.3666 | H | -4.8472 | -0.402 | -1.5659 |
| C | 1.80996 | 3.2772 | 0.06249 | H | -5.6212 | -1.6033 | -0.5623 |
| C | -4.0093 | -0.6131 | 0.39569 | H | -7.2085 | 0.19576 | -0.7203 |
| C | -5.211 | -0.5809 | -0.5424 | H | -6.5344 | 0.30074 | 0.90525 |
| O | -3.9807 | 0.01986 | 1.44103 | H | -4.9896 | 2.12208 | 0.15126 |
| C | -6.295 | 0.42962 | -0.1571 | H | -5.6499 | 2.01664 | -1.4801 |
| C | -5.9 | 1.89014 | -0.4152 | H | -7.9187 | 2.64758 | -0.592 |
| C | -7.0015 | 2.88745 | -0.0349 | H | -7.2489 | 2.76131 | 1.02842 |
| C | -6.6109 | 4.34533 | -0.2979 | H | -7.4153 | 5.03326 | -0.0135 |
| O | -0.7521 | -3.0045 | -0.8761 | H | -5.7167 | 4.62396 | 0.27298 |
| O | 1.17969 | -4.2041 | -0.8025 | H | -6.3904 | 4.51196 | -1.3598 |
| C | 0.19064 | -3.8458 | -1.3931 | H | 0.52192 | -4.9814 | -3.1701 |
| C | -0.1894 | -4.2421 | -2.8008 | H | -1.2043 | -4.6511 | -2.8248 |
| C | 2.79244 | 2.815 | 1.12727 | H | -0.1737 | -3.3611 | -3.4516 |
| O | 3.97902 | 3.07479 | 1.13155 | H | 2.31907 | 1.6152 | 4.05259 |
| O | 2.16026 | 2.11007 | 2.0846 | H | 3.23494 | 0.56047 | 2.94007 |
| C | 2.95943 | 1.59286 | 3.16916 | H | 3.8478 | 2.20889 | 3.315 |
| O | 3.43478 | 0.9717 | -1.043 | H | 5.20304 | -0.5398 | -0.0252 |
| O | 5.15314 | 1.68184 | -2.3413 | H | 6.63189 | 0.31833 | -0.6955 |
| C | 4.7587 | 1.09421 | -1.3603 | H | 5.6236 | 1.07286 | 0.57183 |
| C | 5.6155 | 0.4305 | -0.316 | | | | |

Table S3. Energy analyses of 4*S*,12*S*-1/4*R*,12*R*-1 (ten conformers)

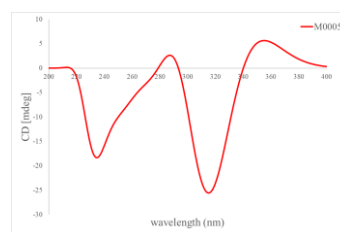
| NO. | 3D conformers B3LYP/6-31G(d,p) | G (Hartree) | Boltzmann distribution | Calculated ECD spectrum |
|-----|---|--------------|---------------------------|--|
| | | | | 4 <i>S</i> ,12 <i>S</i> -1 |
| 1 |  | -1573.242744 | 5.14 % |  |
| 2 |  | -1573.242248 | 3.04 % |  |
| 3 |  | -1573.241432 | 1.28 % |  |
| 4 |  | -1573.244033 | 20.12 % |  |

5

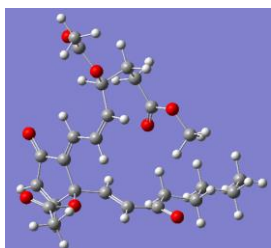


-1573.245111

63.01 %

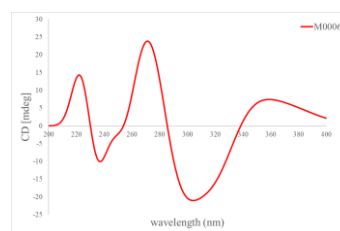


6



-1573.241519

1.4 %

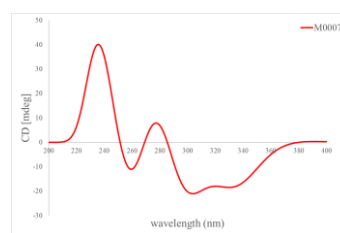


7

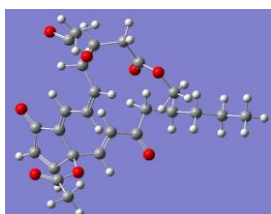


-1573.242182

2.83 %

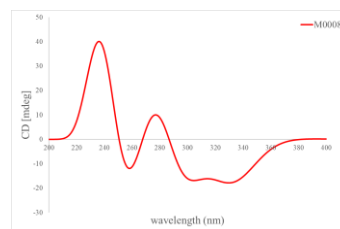


8

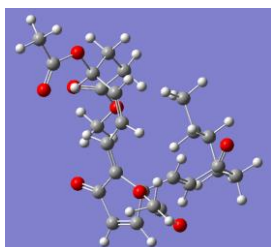


-1573.241161

0.96 %

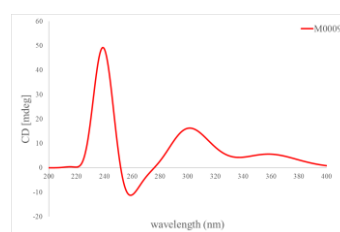


9

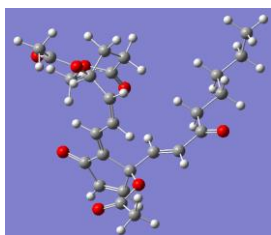


-1573.241458

1.32 %



10



-1573.240815

0.67 %

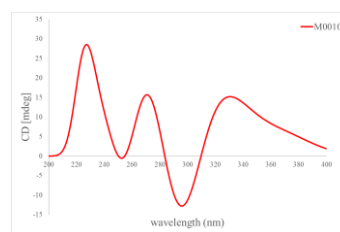


Table S4. Cartesian coordinates of the low-energy re-optimized conformers of 4*S*,12*S*-1/4*R*,12*R*-1 calculated at B3LYP/6-31G(d,p) level of theory.

| Conformer 1 | | | | | | | |
|-------------|---------------------------|---------|---------|--------|---------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.0539 | -4.0445 | 0.93033 | H | -0.6445 | -4.9314 | 0.72414 |
| C | -0.0324 | -2.8837 | -0.0623 | H | 0.75433 | -4.4235 | 2.91134 |
| C | 0.96889 | -1.9346 | 0.57075 | H | -2.0853 | -2.9052 | -0.876 |
| C | 1.32944 | -2.4739 | 1.91741 | H | 2.17669 | -0.2782 | 0.76761 |
| C | 0.65284 | -3.7891 | 2.03878 | H | 0.56759 | -0.7462 | -1.8654 |
| O | 2.02616 | -1.922 | 2.75694 | H | -1.3589 | -0.6885 | 1.12947 |
| C | -1.4399 | -2.3409 | -0.2044 | H | 1.27761 | 1.41429 | -2.5588 |
| C | 1.47409 | -0.7773 | 0.10282 | H | 2.8039 | 1.61434 | 0.12401 |
| C | 1.17436 | -0.1631 | -1.1771 | H | 2.14547 | 3.90915 | 0.309 |
| C | -1.9531 | -1.291 | 0.44718 | H | 1.262 | 3.8636 | -1.2219 |
| C | 1.56918 | 1.06597 | -1.5686 | H | -0.2981 | 3.8983 | 0.67738 |
| C | 2.34356 | 2.06258 | -0.7561 | H | -0.4998 | 2.42127 | -0.2457 |
| C | 1.50761 | 3.28441 | -0.3232 | H | -3.9054 | -0.1508 | 2.15243 |
| C | 0.19673 | 2.95542 | 0.40667 | H | -3.1123 | 1.02891 | 1.15307 |
| C | -3.3829 | -0.8965 | 0.24753 | H | -5.9534 | -0.0397 | 0.61692 |
| C | -3.881 | 0.24408 | 1.12354 | H | -5.6297 | 1.42189 | 1.54863 |
| O | -4.1035 | -1.473 | -0.5553 | H | -4.5229 | 2.45089 | -0.4616 |
| C | -5.2529 | 0.79672 | 0.728 | H | -4.8638 | 0.99038 | -1.3879 |
| C | -5.2357 | 1.6185 | -0.5683 | H | -7.3222 | 1.34727 | -1.0539 |
| C | -6.6123 | 2.17931 | -0.9462 | H | -6.9922 | 2.79898 | -0.121 |
| C | -6.5942 | 3.00424 | -2.2371 | H | -7.5911 | 3.38826 | -2.4823 |
| O | 0.29722 | -3.3109 | -1.4215 | H | -5.9188 | 3.86456 | -2.1489 |
| O | 2.30837 | -4.1839 | -0.8131 | H | -6.2512 | 2.40107 | -3.0868 |
| C | 1.4846 | -3.9381 | -1.6606 | H | 2.51478 | -4.8467 | -3.2955 |
| C | 1.60886 | -4.2622 | -3.1316 | H | 0.73205 | -4.8181 | -3.4776 |
| C | 0.29169 | 2.13929 | 1.68634 | H | 1.65967 | -3.3356 | -3.7137 |
| O | -0.6137 | 1.4497 | 2.11567 | H | 2.59376 | 1.9117 | 3.94936 |
| O | 1.47086 | 2.29303 | 2.30859 | H | 0.8228 | 1.78296 | 4.23002 |
| C | 1.64417 | 1.56236 | 3.54466 | H | 1.68464 | 0.48841 | 3.34642 |
| O | 3.41168 | 2.53611 | -1.6276 | H | 6.51092 | 3.62958 | -1.58 |
| O | 4.77547 | 2.85274 | 0.15896 | H | 5.79679 | 2.49297 | -2.7619 |
| C | 4.5819 | 2.88886 | -1.0355 | H | 5.18917 | 4.14691 | -2.6707 |
| C | 5.58988 | 3.32038 | -2.0751 | | | | |

| Conformer 2 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.15923 | -3.9419 | 1.14684 | H | -0.3261 | -4.8924 | 0.94888 |
| C | 0.27766 | -2.8915 | 0.04426 | H | 0.62935 | -4.0451 | 3.26577 |
| C | 1.08837 | -1.8013 | 0.72141 | H | -1.5958 | -3.1683 | -1.0923 |
| C | 1.24036 | -2.1663 | 2.163 | H | 2.13482 | -0.0392 | 0.92362 |
| C | 0.64145 | -3.5148 | 2.32092 | H | 1.04807 | -0.9104 | -1.8693 |
| O | 1.73985 | -1.4733 | 3.03778 | H | -1.3792 | -0.708 | 0.74181 |
| C | -1.1161 | -2.4866 | -0.3914 | H | 1.73159 | 1.21715 | -2.6815 |
| C | 1.59328 | -0.6611 | 0.21319 | H | 2.74107 | 1.82193 | 0.17908 |
| C | 1.48565 | -0.2105 | -1.1618 | H | 1.91817 | 4.06103 | -0.0211 |
| C | -1.8036 | -1.4244 | 0.0429 | H | 1.32963 | 3.7847 | -1.6653 |
| C | 1.86491 | 0.9994 | -1.6225 | H | -0.5461 | 3.88955 | -0.0797 |
| C | 2.41856 | 2.13591 | -0.8133 | H | -0.4867 | 2.31357 | -0.8463 |
| C | 1.44456 | 3.32406 | -0.6763 | H | -4.0168 | -0.2361 | 1.28742 |
| C | 0.04639 | 2.96698 | -0.15 | H | -3.2478 | 0.86762 | 0.19203 |
| C | -3.2012 | -1.1762 | -0.4329 | H | -5.1498 | 0.52077 | -1.468 |
| C | -3.9192 | -0.0032 | 0.21407 | H | -5.9141 | -0.5865 | -0.3515 |
| O | -3.7273 | -1.8795 | -1.2836 | H | -6.0713 | 1.26092 | 1.36945 |
| C | -5.2834 | 0.31037 | -0.4 | H | -5.3631 | 2.3843 | 0.22058 |
| C | -5.9892 | 1.48218 | 0.29546 | H | -8.0175 | 0.89413 | -0.175 |
| C | -7.3919 | 1.79493 | -0.2519 | H | -7.8612 | 2.54685 | 0.39694 |
| C | -7.4103 | 2.30596 | -1.6976 | H | -8.4291 | 2.56039 | -2.012 |
| O | 0.86724 | -3.4262 | -1.1824 | H | -6.7948 | 3.20842 | -1.8043 |
| O | 2.79313 | -4.0607 | -0.1503 | H | -7.0273 | 1.55817 | -2.4008 |
| C | 2.11619 | -3.9731 | -1.146 | H | 1.75349 | -5.0978 | -2.9473 |
| C | 2.51674 | -4.435 | -2.5283 | H | 2.60481 | -3.5726 | -3.1979 |
| C | -0.0411 | 2.29713 | 1.21258 | H | 3.47494 | -4.9523 | -2.4706 |
| O | -0.9642 | 1.58303 | 1.55507 | H | 1.82099 | 2.49683 | 3.85175 |
| O | 0.99389 | 2.61092 | 2.00746 | H | 0.04111 | 2.24517 | 3.83244 |
| C | 0.98667 | 2.02765 | 3.33083 | H | 1.1343 | 0.94662 | 3.26822 |
| O | 3.59377 | 2.60081 | -1.5395 | H | 6.55619 | 3.953 | -1.0947 |
| O | 4.59272 | 3.21715 | 0.40321 | H | 6.15002 | 2.62771 | -2.2243 |
| C | 4.61469 | 3.10944 | -0.8024 | H | 5.42541 | 4.21955 | -2.457 |
| C | 5.76469 | 3.50738 | -1.698 | | | | |

| Conformer 3 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.06977 | -3.6832 | -1.2463 | H | 3.11115 | -3.9582 | -1.1517 |
| C | 1.47851 | -2.5831 | -0.3587 | H | 1.34927 | -4.9632 | -2.8424 |
| C | 0.02718 | -2.5321 | -0.8356 | H | 2.14115 | -0.9149 | -1.6213 |
| C | -0.1495 | -3.5376 | -1.9239 | H | -1.931 | -1.9126 | -0.9483 |
| C | 1.17379 | -4.1892 | -2.1037 | H | 0.0073 | -0.6187 | 1.12681 |
| O | -1.1755 | -3.7629 | -2.545 | H | 2.82596 | -0.7644 | 1.36332 |
| C | 2.17157 | -1.2648 | -0.5905 | H | -1.7297 | 0.8771 | 1.69148 |
| C | -0.9883 | -1.7407 | -0.4299 | H | -3.5214 | -0.6355 | -0.3248 |
| C | -0.9322 | -0.7178 | 0.59293 | H | -4.6497 | 1.51353 | -0.6815 |
| C | 2.75732 | -0.4761 | 0.31901 | H | -3.3932 | 2.3729 | 0.2246 |
| C | -1.9238 | 0.13609 | 0.91918 | H | -2.6752 | 0.73688 | -2.2732 |
| C | -3.2989 | 0.21369 | 0.32474 | H | -3.3281 | 2.34499 | -2.4222 |
| C | -3.583 | 1.52149 | -0.437 | H | 3.62128 | 1.36086 | 2.00838 |
| C | -2.7832 | 1.68588 | -1.7341 | H | 5.05611 | 1.37616 | 0.99874 |
| C | 3.30721 | 0.85303 | -0.069 | H | 4.57991 | 3.69486 | 1.47524 |
| C | 3.9942 | 1.66794 | 1.02251 | H | 4.12433 | 3.42482 | -0.2066 |
| O | 3.22417 | 1.27228 | -1.2172 | H | 1.70445 | 3.15389 | 0.52879 |
| C | 3.85496 | 3.1838 | 0.82818 | H | 2.19672 | 3.48431 | 2.18415 |
| C | 2.44151 | 3.70009 | 1.13263 | H | 3.00802 | 5.76322 | 1.46971 |
| C | 2.27226 | 5.20249 | 0.87488 | H | 2.50903 | 5.41368 | -0.1779 |
| C | 0.85917 | 5.70414 | 1.19161 | H | 0.754 | 6.77226 | 0.96794 |
| O | 1.44629 | -2.9496 | 1.05427 | H | 0.10993 | 5.15638 | 0.60847 |
| O | 3.63933 | -3.5605 | 1.14813 | H | 0.61928 | 5.56238 | 2.25299 |
| C | 2.55661 | -3.4355 | 1.67278 | H | 3.14243 | -4.0996 | 3.61718 |
| C | 2.22859 | -3.8023 | 3.10188 | H | 1.75994 | -2.9588 | 3.61811 |
| C | -1.4044 | 2.30203 | -1.558 | H | 1.51161 | -4.6302 | 3.11457 |
| O | -0.9778 | 2.79952 | -0.5348 | H | 1.28922 | 2.26383 | -2.1597 |
| O | -0.729 | 2.26195 | -2.7195 | H | 0.8726 | 2.90005 | -3.7793 |
| C | 0.57977 | 2.86793 | -2.7293 | H | 0.53546 | 3.87668 | -2.3118 |
| O | -4.2039 | 0.1461 | 1.46805 | H | -7.2168 | -0.8448 | 2.33015 |
| O | -5.8046 | -0.8097 | 0.17518 | H | -5.7151 | -1.0258 | 3.2854 |
| C | -5.4268 | -0.4001 | 1.2508 | H | -6.3305 | 0.5893 | 2.93187 |
| C | -6.2308 | -0.4241 | 2.52976 | | | | |

| Conformer 4 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.8213 | 3.57712 | -1.1011 | H | -1.6908 | 4.15912 | -0.8227 |
| C | -0.3372 | 2.44726 | -0.2005 | H | -0.2333 | 4.41125 | -3.018 |
| C | 0.91852 | 1.96537 | -0.9206 | H | -1.1925 | 0.67964 | 0.82587 |
| C | 1.02462 | 2.70933 | -2.2115 | H | 2.65269 | 0.91842 | -1.2666 |
| C | -0.0843 | 3.70114 | -2.2124 | H | 1.15039 | 0.59342 | 1.44837 |
| O | 1.86456 | 2.54201 | -3.0803 | H | -2.5459 | 1.64855 | -1.7499 |
| C | -1.342 | 1.32991 | -0.0344 | H | 2.73355 | -1.0607 | 2.02826 |
| C | 1.85263 | 1.06803 | -0.5427 | H | 4.01535 | -0.5989 | -0.7533 |
| C | 1.90489 | 0.34042 | 0.70875 | H | 4.7248 | -2.9146 | -0.6563 |
| C | -2.3402 | 1.03489 | -0.8759 | H | 3.8736 | -3.1797 | 0.87552 |
| C | 2.81132 | -0.6003 | 1.04655 | H | 2.3275 | -2.3592 | -1.6475 |
| C | 3.92784 | -1.1312 | 0.1958 | H | 2.76814 | -4.0235 | -1.3597 |
| C | 3.83614 | -2.6434 | -0.0781 | H | -4.9118 | 0.66949 | -1.6726 |
| C | 2.58264 | -3.0682 | -0.8511 | H | -3.9659 | -0.4832 | -2.5819 |
| C | -3.2252 | -0.138 | -0.6283 | H | -6.0245 | -1.619 | -2.0779 |
| C | -4.3993 | -0.3005 | -1.5855 | H | -4.8181 | -2.3302 | -1.0081 |
| O | -3.0112 | -0.9305 | 0.28045 | H | -5.6197 | -0.8732 | 0.86773 |
| C | -5.3833 | -1.4123 | -1.2107 | H | -6.8221 | -0.1518 | -0.1992 |
| C | -6.2622 | -1.0779 | 0.00236 | H | -7.8854 | -2.4115 | -0.5144 |
| C | -7.2497 | -2.1967 | 0.35685 | H | -6.6895 | -3.1203 | 0.56014 |
| C | -8.1327 | -1.8602 | 1.56275 | H | -8.8244 | -2.6785 | 1.79361 |
| O | 0.08031 | 2.93815 | 1.11555 | H | -7.5259 | -1.6739 | 2.45723 |
| O | -2.0143 | 3.66514 | 1.60993 | H | -8.7318 | -0.9602 | 1.37694 |
| C | -0.8553 | 3.5094 | 1.92159 | H | 0.61699 | 4.57545 | 3.06908 |
| C | -0.2366 | 3.91184 | 3.23922 | H | -0.9865 | 4.41358 | 3.85144 |
| C | 1.36029 | -3.2774 | 0.02906 | H | 0.13772 | 3.02631 | 3.76365 |
| O | 1.37131 | -3.3597 | 1.24018 | H | -1.7069 | -3.9218 | -0.7627 |
| O | 0.2513 | -3.4049 | -0.7225 | H | -0.8452 | -4.4422 | 0.72548 |
| C | -0.977 | -3.6395 | -0.0035 | H | -1.3017 | -2.7276 | 0.50207 |
| O | 5.14636 | -0.879 | 0.95906 | H | 8.35722 | -0.2849 | 0.58692 |
| O | 6.348 | -0.7401 | -0.9605 | H | 7.25192 | 0.48311 | 1.76582 |
| C | 6.28681 | -0.6925 | 0.24856 | H | 7.57493 | -1.2476 | 1.87721 |
| C | 7.44842 | -0.4174 | 1.17477 | | | | |

| Conformer 5 | | | | | | | |
|----------------|---------------------------|---------|---------|----------------|---------------------------|---------|---------|
| Atomic Type | Standard Orientation (Å) | | | Atomic Type | Standard Orientation (Å) | | |
| | X | Y | Z | | X | Y | Z |
| C | 0.63291 | 3.59675 | 1.13915 | H | 1.39186 | 4.29211 | 0.80352 |
| C | 0.08804 | 2.54041 | 0.18565 | H | 0.3271 | 4.13163 | 3.2216 |
| C | -0.9812 | 1.85326 | 1.02959 | H | 0.87874 | 0.99392 | -1.1895 |
| C | -0.9164 | 2.42192 | 2.40926 | H | -2.5413 | 0.60458 | 1.50974 |
| C | 0.09489 | 3.51216 | 2.3626 | H | -1.5205 | 0.7634 | -1.434 |
| O | -1.5751 | 2.06831 | 3.37334 | H | 2.59823 | 1.79761 | 1.21925 |
| C | 1.13105 | 1.5555 | -0.2915 | H | -3.0453 | -0.9604 | -1.9655 |
| C | -1.8948 | 0.9196 | 0.69156 | H | -3.8452 | -0.9735 | 1.0268 |
| C | -2.1098 | 0.3473 | -0.6217 | H | -4.3773 | -3.3194 | 0.7299 |
| C | 2.2855 | 1.26881 | 0.32186 | H | -3.7947 | -3.3075 | -0.9439 |
| C | -2.9843 | -0.6327 | -0.9307 | H | -1.8922 | -2.6505 | 1.37503 |
| C | -3.8866 | -1.3739 | 0.01198 | H | -2.2463 | -4.303 | 0.93858 |
| C | -3.6298 | -2.8912 | 0.05506 | H | 5.0368 | 1.07352 | 0.45001 |
| C | -2.2293 | -3.2792 | 0.5425 | H | 4.35211 | -0.1026 | 1.54293 |
| C | 3.19986 | 0.22484 | -0.2219 | H | 4.93419 | -1.9555 | -0.0809 |
| C | 4.54552 | 0.08786 | 0.47513 | H | 5.61247 | -0.7779 | -1.1816 |
| O | 2.89042 | -0.4762 | -1.1765 | H | 7.31875 | -0.1243 | 0.56359 |
| C | 5.45387 | -0.9895 | -0.1168 | H | 6.63667 | -1.3066 | 1.6701 |
| C | 6.8038 | -1.0961 | 0.60285 | H | 7.20715 | -3.147 | 0.05421 |
| C | 7.7207 | -2.1759 | 0.0139 | H | 7.88804 | -1.9653 | -1.0518 |
| C | 9.06946 | -2.2806 | 0.73275 | H | 9.69989 | -3.0594 | 0.28879 |
| O | -0.5898 | 3.14117 | -0.9664 | H | 9.62202 | -1.3344 | 0.67927 |
| O | 1.32188 | 4.13141 | -1.6919 | H | 8.93578 | -2.5253 | 1.7938 |
| C | 0.14264 | 3.89623 | -1.8294 | H | -0.1384 | 5.03648 | -3.6127 |
| C | -0.7259 | 4.38648 | -2.9636 | H | -1.1066 | 3.53566 | -3.5385 |
| C | -1.1709 | -3.2553 | -0.5493 | H | -1.5917 | 4.9283 | -2.5703 |
| O | -1.3912 | -3.1866 | -1.7411 | H | 2.02776 | -3.6889 | -0.3768 |
| O | 0.06044 | -3.3651 | -0.0179 | H | 0.95671 | -4.0959 | -1.7607 |
| C | 1.15585 | -3.3843 | -0.9564 | H | 1.31742 | -2.3877 | -1.3725 |
| O | -5.2375 | -1.1544 | -0.496 | H | -8.3674 | -0.9377 | 0.48261 |
| O | -6.0856 | -1.3734 | 1.59705 | H | -7.553 | 0.07762 | -0.745 |
| C | -6.2443 | -1.1722 | 0.41295 | H | -7.754 | -1.6499 | -1.0406 |
| C | -7.5701 | | -0.9041 | | -0.2605 | | |

| Conformer 6 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.27991 | 3.83798 | 1.20683 | H | 0.96669 | 4.62023 | 0.89955 |
| C | -0.0648 | 2.70305 | 0.24449 | H | -0.1807 | 4.33777 | 3.26969 |
| C | -1.0953 | 1.90631 | 1.03721 | H | 1.55822 | 1.39828 | 0.8995 |
| C | -1.1955 | 2.50822 | 2.40295 | H | -2.4269 | 0.39276 | 1.46077 |
| C | -0.2966 | 3.69348 | 2.406 | H | -1.1814 | 0.66048 | -1.3894 |
| O | -1.8731 | 2.09327 | 3.32793 | H | 1.40617 | 2.15563 | -2.0835 |
| C | 1.1815 | 1.87837 | 0.00023 | H | -2.1851 | -1.4183 | -1.9326 |
| C | -1.7785 | 0.79961 | 0.68611 | H | -3.3042 | -1.4699 | 0.94841 |
| C | -1.7328 | 0.14515 | -0.6075 | H | -2.9323 | -3.8752 | 0.94199 |
| C | 1.79597 | 1.70267 | -1.1769 | H | -2.0885 | -3.8041 | -0.6103 |
| C | -2.2958 | -1.0404 | -0.9177 | H | -1.075 | -2.3819 | 1.93493 |
| C | -3.0345 | -1.9589 | 0.01002 | H | -0.6296 | -4.0206 | 1.4846 |
| C | -2.2719 | -3.2607 | 0.32178 | H | 3.95621 | 1.10356 | 0.5062 |
| C | -0.9494 | -3.0512 | 1.07864 | H | 3.054 | -0.3932 | 0.34329 |
| C | 2.98984 | 0.83812 | -1.3911 | H | 4.78512 | -1.2695 | -1.2634 |
| C | 3.74015 | 0.28028 | -0.1897 | H | 5.68775 | 0.22041 | -1.1214 |
| O | 3.32966 | 0.58199 | -2.5401 | H | 6.00794 | -0.2024 | 1.34838 |
| C | 5.02739 | -0.458 | -0.5658 | H | 5.09644 | -1.6972 | 1.20805 |
| C | 5.76549 | -1.0216 | 0.65444 | H | 6.8129 | -2.5905 | -0.4003 |
| C | 7.05411 | -1.7709 | 0.29148 | H | 7.7219 | -1.095 | -0.2613 |
| C | 7.79086 | -2.3322 | 1.5118 | H | 8.70523 | -2.8612 | 1.21959 |
| O | -0.506 | 3.17978 | -1.0508 | H | 8.07663 | -1.5317 | 2.2053 |
| O | -2.2883 | 4.29734 | -0.1857 | H | 7.16 | -3.0383 | 2.06587 |
| C | -1.6228 | 3.96125 | -1.1342 | H | -2.7428 | 5.00221 | -2.6234 |
| C | -1.8909 | 4.32324 | -2.5762 | H | -1.0093 | 4.79327 | -3.023 |
| C | 0.22712 | -2.5264 | 0.2729 | H | -2.1085 | 3.41886 | -3.1546 |
| O | 1.04738 | -1.7345 | 0.6893 | H | 1.32659 | -3.3103 | -2.6754 |
| O | 0.29627 | -3.1023 | -0.9457 | H | 1.38469 | -1.6538 | -1.9943 |
| C | 1.41775 | -2.7208 | -1.7629 | H | 2.35742 | -2.9478 | -1.2531 |
| O | -4.2685 | -2.3042 | -0.6842 | H | -7.3841 | -3.1961 | -0.1332 |
| O | -5.3132 | -2.6474 | 1.29981 | H | -6.8134 | -2.0202 | -1.3536 |
| C | -5.3396 | -2.6166 | 0.0893 | H | -6.3222 | -3.7102 | -1.48 |
| C | -6.5473 | -2.9078 | -0.7701 | | | | |

| Conformer 7 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.024 | 3.86668 | -0.6633 | H | -1.8251 | 4.456 | -0.2284 |
| C | -0.3943 | 2.72058 | 0.12646 | H | -0.8146 | 4.692 | -2.6612 |
| C | 0.69598 | 2.23642 | -0.8136 | H | -2.0209 | 1.90792 | 1.37912 |
| C | 0.5895 | 3.00937 | -2.0895 | H | 2.27562 | 1.07831 | -1.4684 |
| C | -0.5146 | 3.98654 | -1.8952 | H | 1.171 | 0.77449 | 1.43702 |
| O | 1.26781 | 2.84967 | -3.0905 | H | -1.2813 | 0.37912 | -1.1807 |
| C | -1.4618 | 1.70034 | 0.46821 | H | 2.5659 | -1.1307 | 1.66775 |
| C | 1.60799 | 1.26266 | -0.6273 | H | 3.79455 | -0.5153 | -1.0586 |
| C | 1.762 | 0.47057 | 0.5771 | H | 1.88926 | -1.8415 | -1.7933 |
| C | -1.7993 | 0.62951 | -0.2587 | H | 3.38408 | -2.7722 | -1.8637 |
| C | 2.55044 | -0.614 | 0.71036 | H | 1.82481 | -4.3127 | -0.9744 |
| C | 3.39014 | -1.2525 | -0.3606 | H | 2.6272 | -3.7495 | 0.49036 |
| C | 2.65306 | -2.3308 | -1.1792 | H | -3.5371 | -0.7484 | -1.8203 |
| C | 1.98787 | -3.4335 | -0.3378 | H | -2.5538 | -1.9546 | -1.0219 |
| C | -2.9201 | -0.2627 | 0.1708 | H | -4.775 | -2.8994 | -1.1368 |
| C | -3.3998 | -1.2703 | -0.861 | H | -4.5287 | -2.4416 | 0.54734 |
| O | -3.3957 | -0.1925 | 1.29669 | H | -5.8337 | -0.3386 | 0.17312 |
| C | -4.6635 | -2.0383 | -0.4641 | H | -6.0742 | -0.7794 | -1.5163 |
| C | -5.9447 | -1.1943 | -0.5048 | H | -7.3065 | -2.8503 | -0.7912 |
| C | -7.2013 | -1.9852 | -0.1204 | H | -7.0718 | -2.3976 | 0.89026 |
| C | -8.4812 | -1.1444 | -0.1676 | H | -9.3602 | -1.7354 | 0.11444 |
| O | 0.07756 | 3.14906 | 1.44495 | H | -8.419 | -0.291 | 0.51878 |
| O | 1.54533 | 4.66608 | 0.59354 | H | -8.6572 | -0.746 | -1.1746 |
| C | 1.03725 | 4.11369 | 1.5389 | H | 2.07196 | 5.20011 | 3.0583 |
| C | 1.36701 | 4.37085 | 2.9916 | H | 0.45826 | 4.60114 | 3.55621 |
| C | 0.61668 | -3.0357 | 0.18002 | H | 1.81112 | 3.47419 | 3.43726 |
| O | -0.2464 | -2.513 | -0.4968 | H | -0.785 | -3.3998 | 3.07766 |
| O | 0.45217 | -3.3669 | 1.47539 | H | -1.0618 | -2.0089 | 1.97792 |
| C | -0.8423 | -3.0773 | 2.03796 | H | -1.6211 | -3.6322 | 1.5084 |
| O | 4.51334 | -1.8565 | 0.34437 | H | 7.67385 | -2.6772 | -0.0389 |
| O | 5.82808 | -1.6121 | -1.4876 | H | 6.93132 | -1.9341 | 1.40841 |
| C | 5.68211 | -1.9643 | -0.3383 | H | 6.43033 | -3.5498 | 0.90751 |
| C | 6.75353 | -2.5719 | 0.53624 | | | | |

| Conformer 8 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.3053 | -4.3534 | -0.6215 | H | 0.27783 | -5.1761 | -0.2198 |
| C | -0.3485 | -3.0115 | 0.10852 | H | -1.0744 | -5.1435 | -2.493 |
| C | -1.3242 | -2.2134 | -0.7361 | H | 1.70756 | -2.9932 | 0.89791 |
| C | -1.6749 | -3.0315 | -1.9398 | H | -2.5213 | -0.636 | -1.3068 |
| C | -0.9872 | -4.3382 | -1.7732 | H | -0.9702 | -0.5435 | 1.40308 |
| O | -2.3807 | -2.68 | -2.8705 | H | 1.01874 | -0.9399 | -1.2779 |
| C | 1.06528 | -2.4752 | 0.18677 | H | -1.7303 | 1.7003 | 1.63078 |
| C | -1.8383 | -0.9849 | -0.5327 | H | -3.4906 | 1.30476 | -0.8284 |
| C | -1.5745 | -0.1241 | 0.603 | H | -1.412 | 1.96466 | -1.934 |
| C | 1.6039 | -1.4999 | -0.5537 | H | -2.6096 | 3.25852 | -1.946 |
| C | -2.0016 | 1.14768 | 0.7338 | H | -0.5626 | 4.35839 | -1.4617 |
| C | -2.7903 | 1.93594 | -0.2758 | H | -1.3149 | 4.23395 | 0.13043 |
| C | -1.9265 | 2.69636 | -1.3016 | H | 3.38242 | -0.5558 | -2.4208 |
| C | -0.8871 | 3.65058 | -0.6886 | H | 2.97614 | 0.75585 | -1.3455 |
| C | 3.0567 | -1.1604 | -0.4178 | H | 5.64308 | -0.7767 | -1.1856 |
| C | 3.59488 | -0.1507 | -1.4187 | H | 5.43323 | 0.65776 | -2.1875 |
| O | 3.75859 | -1.6863 | 0.43493 | H | 4.87074 | 2.00656 | -0.1567 |
| C | 5.08644 | 0.16502 | -1.2693 | H | 5.06148 | 0.57008 | 0.85152 |
| C | 5.41929 | 1.05601 | -0.0647 | H | 7.46451 | 0.40419 | 0.16542 |
| C | 6.91796 | 1.35289 | 0.07083 | H | 7.28151 | 1.82336 | -0.8542 |
| C | 7.24945 | 2.25307 | 1.26545 | H | 8.32645 | 2.44302 | 1.33844 |
| O | -0.7224 | -3.1505 | 1.51749 | H | 6.74593 | 3.22461 | 1.18243 |
| O | -2.7277 | -4.1156 | 1.0406 | H | 6.92787 | 1.79328 | 2.20814 |
| C | -1.9237 | -3.7087 | 1.84372 | H | -3.0093 | -4.2589 | 3.59835 |
| C | -2.0918 | -3.7264 | 3.34591 | H | -1.2319 | -4.2066 | 3.82284 |
| C | 0.36635 | 2.93378 | -0.2207 | H | -2.1468 | -2.7004 | 3.72594 |
| O | 0.99844 | 2.14427 | -0.8936 | H | 2.02139 | 3.0738 | 2.56076 |
| O | 0.71575 | 3.29765 | 1.03002 | H | 1.79728 | 1.59349 | 1.56962 |
| C | 1.90709 | 2.68086 | 1.55034 | H | 2.77386 | 2.94105 | 0.93777 |
| O | -3.5735 | 2.88433 | 0.50475 | H | -6.402 | 4.55997 | 0.46552 |
| O | -5.1814 | 2.91177 | -1.0947 | H | -5.6782 | 3.72278 | 1.87019 |
| C | -4.7614 | 3.28068 | -0.0207 | H | -4.8315 | 5.08875 | 1.14227 |
| C | -5.469 | 4.22667 | 0.92072 | | | | |

| Conformer 9 | | | | | | | |
|----------------|---------------------------|---------|---------|----------------|---------------------------|---------|---------|
| Atomic Type | Standard Orientation (Å) | | | Atomic Type | Standard Orientation (Å) | | |
| | X | Y | Z | | X | Y | Z |
| C | 1.73245 | 2.75292 | 1.81792 | H | 2.49752 | 3.51407 | 1.73158 |
| C | 0.8893 | 2.37411 | 0.60749 | H | 1.89637 | 2.08498 | 3.87841 |
| C | -0.0869 | 1.355 | 1.18935 | H | 1.20033 | 1.7778 | -1.5024 |
| C | 0.3246 | 1.07936 | 2.59674 | H | -1.6876 | 0.05657 | 1.26627 |
| C | 1.42825 | 2.02757 | 2.90215 | H | -1.2011 | 1.77912 | -1.2874 |
| O | -0.1456 | 0.23599 | 3.34581 | H | 3.4059 | 1.10365 | 0.51476 |
| C | 1.68342 | 1.76841 | -0.5267 | H | -2.8745 | 0.4866 | -2.3573 |
| C | -1.1566 | 0.75747 | 0.62341 | H | -3.3161 | -0.9826 | 0.30605 |
| C | -1.6489 | 0.96517 | -0.7242 | H | -3.5029 | -3.0777 | -0.9903 |
| C | 2.86659 | 1.15088 | -0.428 | H | -2.8944 | -2.2725 | -2.4407 |
| C | -2.6045 | 0.23318 | -1.3324 | H | -1.0638 | -3.5505 | -1.4517 |
| C | -3.3377 | -0.9584 | -0.7831 | H | -0.6822 | -1.8564 | -1.2477 |
| C | -2.825 | -2.2955 | -1.3467 | H | 5.19491 | -0.4469 | -2.4311 |
| C | -1.3882 | -2.6355 | -0.9396 | H | 5.5382 | 0.6124 | -1.0493 |
| C | 3.47881 | 0.50428 | -1.6268 | H | 5.85963 | -1.7359 | -0.4097 |
| C | 4.8426 | -0.1446 | -1.4399 | H | 4.55887 | -1.0311 | 0.5315 |
| O | 2.90808 | 0.49237 | -2.7085 | H | 2.85549 | -2.139 | -0.9112 |
| C | 4.83142 | -1.3565 | -0.4823 | H | 4.11624 | -2.7627 | -1.9633 |
| C | 3.89642 | -2.4916 | -0.9206 | H | 5.04371 | -4.1177 | -0.0761 |
| C | 4.01232 | -3.739 | -0.035 | H | 3.83535 | -3.4566 | 1.01331 |
| C | 3.03716 | -4.8517 | -0.4332 | H | 3.16315 | -5.738 | 0.19947 |
| O | 0.09836 | 3.50394 | 0.11624 | H | 1.99903 | -4.5135 | -0.3357 |
| O | 1.96 | 4.6992 | -0.3996 | H | 3.19433 | -5.1615 | -1.4738 |
| C | 0.75492 | 4.59134 | -0.3719 | H | 0.30731 | 6.50976 | -1.1954 |
| C | -0.2328 | 5.623 | -0.8626 | H | -0.8205 | 5.21473 | -1.6916 |
| C | -1.2318 | -2.8655 | 0.55392 | H | -0.934 | 5.88508 | -0.0641 |
| O | -2.1461 | -2.9445 | 1.34829 | H | 1.39811 | -3.2796 | 2.39348 |
| O | 0.06663 | -2.9734 | 0.89801 | H | 0.00297 | -2.2449 | 2.85259 |
| C | 0.32015 | -3.1388 | 2.31056 | H | -0.2132 | -4.0119 | 2.69384 |
| O | -4.7281 | -0.8796 | -1.2045 | H | -7.598 | 0.50341 | -0.3911 |
| O | -5.1886 | 0.51348 | 0.52671 | H | -6.9753 | 0.1648 | -2.0353 |
| C | -5.5509 | -0.1076 | -0.4458 | H | -7.3447 | -1.176 | -0.9497 |
| C | -6.9612 | -0.1509 | -0.9872 | | | | |

| Conformer 10 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.26533 | 3.68237 | 1.44494 | H | 0.97792 | 4.49444 | 1.34162 |
| C | 0.01246 | 2.73325 | 0.27645 | H | -0.3706 | 3.81538 | 3.51851 |
| C | -1.0963 | 1.83943 | 0.81867 | H | 1.49835 | 1.24724 | 0.86197 |
| C | -1.2927 | 2.17566 | 2.26096 | H | -2.4397 | 0.2778 | 0.85663 |
| C | -0.4134 | 3.33784 | 2.54668 | H | -1.0827 | 1.08205 | -1.8289 |
| O | -2.0126 | 1.58342 | 3.05187 | H | 1.78767 | 2.59134 | -1.8989 |
| C | 1.26428 | 1.91423 | 0.03644 | H | -1.7619 | -1.0279 | -2.6986 |
| C | -1.7354 | 0.81528 | 0.22304 | H | -2.8419 | -1.6623 | 0.13155 |
| C | -1.5691 | 0.3827 | -1.1538 | H | -1.9449 | -3.8742 | -0.0418 |
| C | 2.03045 | 1.94353 | -1.0619 | H | -1.3356 | -3.5872 | -1.6768 |
| C | -1.9367 | -0.8182 | -1.644 | H | 0.5118 | -3.6349 | -0.0586 |
| C | -2.4882 | -1.9674 | -0.8536 | H | 0.42412 | -2.0618 | -0.8321 |
| C | -1.4813 | -3.1266 | -0.692 | H | 3.98328 | 0.82955 | 0.70715 |
| C | -0.1022 | -2.7276 | -0.1431 | H | 2.89809 | -0.4374 | 0.19468 |
| C | 3.23672 | 1.0959 | -1.2775 | H | 4.65656 | -1.2823 | -1.4159 |
| C | 3.7294 | 0.19185 | -0.1537 | H | 5.74469 | -0.0167 | -0.8966 |
| O | 3.8079 | 1.14997 | -2.3587 | H | 5.66016 | -0.9112 | 1.46571 |
| C | 4.93194 | -0.6678 | -0.5508 | H | 4.61151 | -2.214 | 0.93193 |
| C | 5.42593 | -1.5512 | 0.60261 | H | 7.47765 | -1.7356 | -0.06 |
| C | 6.66472 | -2.399 | 0.2682 | H | 7.0188 | -2.8801 | 1.19003 |
| C | 6.4277 | -3.4783 | -0.795 | H | 7.32956 | -4.0814 | -0.9514 |
| O | -0.2825 | 3.42545 | -0.9602 | H | 5.62164 | -4.159 | -0.4922 |
| O | -2.1168 | 4.45514 | -0.0965 | H | 6.1507 | -3.0456 | -1.7627 |
| C | -1.366 | 4.25465 | -1.0197 | H | -2.3076 | 5.56672 | -2.4152 |
| C | -1.476 | 4.86171 | -2.3985 | H | -0.545 | 5.37103 | -2.6666 |
| C | -0.0617 | -2.0531 | 1.21917 | H | -1.6443 | 4.07556 | -3.1423 |
| O | 0.80025 | -1.2671 | 1.56375 | H | -1.8934 | -2.4284 | 3.8616 |
| O | -1.0661 | -2.4553 | 2.01449 | H | -0.1421 | -2.0243 | 3.83964 |
| C | -1.1044 | -1.8854 | 3.34169 | H | -1.3448 | -0.8207 | 3.28988 |
| O | -3.63 | -2.4658 | -1.6078 | H | -6.5671 | -3.8935 | -1.2341 |
| O | -4.6588 | -3.1095 | 0.31006 | H | -6.1513 | -2.5809 | -2.376 |
| C | -4.6533 | -3.005 | -0.896 | H | -5.3876 | -4.1614 | -2.5534 |
| C | -5.7659 | -3.442 | -1.82 | | | | |

Table S5. Experimental and calculated ^1H NMR data for compound **1**.

| No. | 1 , exptl. δ_{H} ^a | 4 <i>R</i> ,12 <i>S</i> - 1 , calcd. δ_{H} ^b | 4 <i>S</i> ,12 <i>S</i> - 1 , calcd. δ_{H} ^b |
|-------|--|--|--|
| 2 | 2.38 | 2.59 | 2.41 |
| | 1.29 | 2.44 | 2.28 |
| 3 | 2.05 | 2.45 | 2.29 |
| | 1.95 | 1.87 | 2.15 |
| 4 | 5.75 | 5.59 | 5.74 |
| 5 | 5.84 | 6.16 | 6.45 |
| 6 | 6.35 | 6.74 | 7.09 |
| 7 | 7.39 | 7.92 | 7.75 |
| 10 | 6.55 | 6.82 | 6.93 |
| 11 | 7.48 | 7.62 | 8.38 |
| 13 | 6.77 | 7.36 | 7.53 |
| 14 | 6.31 | 6.54 | 6.59 |
| 16 | 2.53 | 2.55 | 2.62 |
| 17 | 1.59 | 1.62 | 1.58 |
| 18 | 1.29 | 1.02 | 1.15 |
| 19 | 1.29 | 1.23 | 1.34 |
| 20 | 0.88 | 0.92 | 0.79 |
| 1-OMe | 3.7 | 3.87 | 3.70 |
| 2' | 2.04 | 2.20 | 2.14 |
| 2'' | 2.09 | 2.09 | 2.11 |

^a Recorded in CDCl_3 at 600 MHz.^b Calculated in CDCl_3

Table S6. Experimental and calculated ^{13}C NMR data for compound **1**.

| No. | 1 , exptl. δ_{C} ^a | 4 <i>R</i> ,12 <i>S</i> - 1 , calcd. δ_{C} ^b | 4 <i>S</i> ,12 <i>S</i> - 1 , calcd. δ_{C} ^b |
|-------|--|--|--|
| 1 | 172.9 | 178.2 | 179.6 |
| 2 | 29.7 | 28.2 | 27.1 |
| 3 | 29.7 | 26.8 | 25.5 |
| 4 | 69.3 | 68.1 | 66.1 |
| 5 | 140 | 144.1 | 144.9 |
| 6 | 124.4 | 126.2 | 126.5 |
| 7 | 126.6 | 129.2 | 127.7 |
| 8 | 135.7 | 132.4 | 131.6 |
| 9 | 192.7 | 192.9 | 191.4 |
| 10 | 136.4 | 139.8 | 140.3 |
| 11 | 155 | 156.2 | 157.3 |
| 12 | 83.5 | 80.7 | 79.5 |
| 13 | 141 | 144.7 | 143.5 |
| 14 | 129.2 | 131.0 | 130.5 |
| 15 | 199.6 | 204.8 | 202.6 |
| 16 | 41.2 | 39.7 | 42.3 |
| 17 | 23.5 | 26.4 | 23.4 |
| 18 | 31.3 | 30.3 | 30.3 |
| 19 | 22.4 | 21.9 | 22.2 |
| 20 | 13.9 | 11.0 | 10.9 |
| 1-OMe | 51.9 | 48.4 | 49.3 |
| 1' | 170 | 175.4 | 174.5 |
| 2' | 21.3 | 18.0 | 17.8 |
| 1'' | 168.8 | 172.5 | 174.4 |
| 2'' | 21.2 | 18.3 | 18.4 |

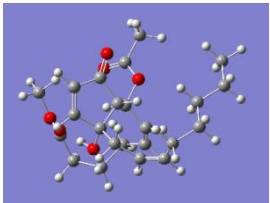
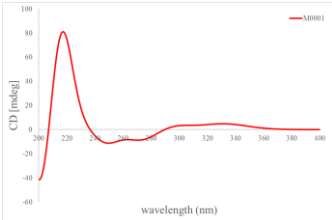
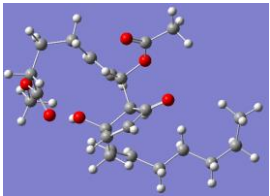
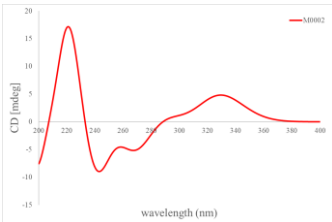
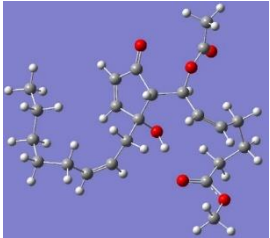
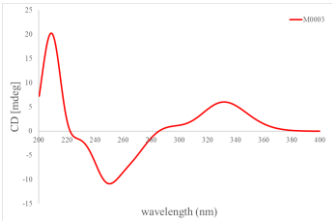

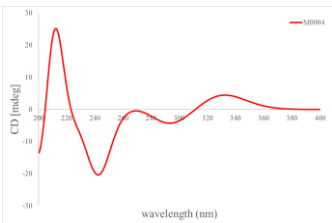
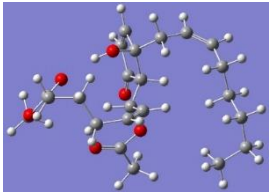
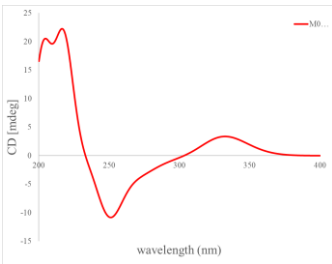
^a Recorded in CDCl₃ at 600 MHz.^b Calculated in CDCl₃

Table S7. DP4+ analyses of calculated and experimental NMR chemical shifts of **1** (unscaled). Isomer 1: 4*R*,12*S*-**1**; Isomer 2: 4*S*,12*S*-**1**

| Functional | Solvent? | Basis Set | Type of Data | | | |
|------------------|----------|--------------|-----------------|----------|----------|----------|
| mPW1PW91 | PCM | 6-311+G(d,p) | Unscaled Shifts | | | |
| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
| sDP4+ (H data) | 84.32% | 15.68% | - | - | - | - |
| sDP4+ (C data) | 99.51% | 0.49% | - | - | - | - |
| sDP4+ (all data) | 99.91% | 0.09% | - | - | - | - |
| uDP4+ (H data) | 96.66% | 3.34% | - | - | - | - |
| uDP4+ (C data) | 99.93% | 0.07% | - | - | - | - |
| uDP4+ (all data) | 100.00% | 0.00% | - | - | - | - |
| DP4+ (H data) | 99.36% | 0.64% | - | - | - | - |
| DP4+ (C data) | 100.00% | 0.00% | - | - | - | - |
| DP4+ (all data) | 100.00% | 0.00% | - | - | - | - |

| Functional | Solvent? | Basis Set | Type of Data | | | | |
|------------|----------|--------------|-----------------|------------|----------|----------|----------|
| mPW1PW91 | PCM | 6-311+G(d,p) | Unscaled Shifts | | | | |
| | DP4+ | 100.00% | 0.00% | - | - | - | - |
| Nuclei | sp2? | Experimenta | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 |
| C | x | 172.9 | 178.2 | 179.6 | | | |
| C | | 29.7 | 28.2 | 27.1 | | | |
| C | | 29.7 | 26.8 | 25.5 | | | |
| C | | 69.3 | 68.1 | 66.1 | | | |
| C | x | 140.0 | 144.1 | 144.9 | | | |
| C | x | 124.4 | 126.2 | 126.5 | | | |
| C | x | 126.6 | 129.2 | 127.7 | | | |
| C | x | 135.7 | 132.4 | 131.6 | | | |
| C | x | 192.7 | 192.9 | 191.4 | | | |
| C | x | 136.4 | 139.8 | 140.3 | | | |
| C | x | 155.0 | 156.2 | 157.3 | | | |
| C | | 83.5 | 80.65 | 79.53 | | | |
| C | x | 141.0 | 144.66 | 143.50 | | | |
| C | x | 129.2 | 130.97 | 130.53 | | | |
| C | x | 199.6 | 204.78 | 202.58 | | | |
| C | | 41.2 | 39.67 | 42.29 | | | |
| C | | 23.5 | 26.36 | 23.41 | | | |
| C | | 31.3 | 30.32 | 30.25 | | | |
| C | | 22.4 | 21.89 | 22.18 | | | |
| C | | 13.9 | 10.98 | 10.91 | | | |
| C | | 51.9 | 48.37 | 49.26 | | | |
| C | x | 170.0 | 175.41 | 174.47 | | | |
| C | | 21.3 | 18.04 | 17.76 | | | |
| C | x | 168.8 | 172.50 | 174.36 | | | |
| C | | 21.2 | 18.30 | 18.42 | | | |
| H | | 2.38 | 2.58518849 | 2.41448727 | | | |
| H | | 1.29 | 2.43990968 | 2.27709942 | | | |
| H | | 2.05 | 2.44954676 | 2.29200722 | | | |
| H | | 1.95 | 1.87121344 | 2.1475089 | | | |
| H | | 5.75 | 5.59041485 | 5.73881978 | | | |
| H | x | 5.84 | 6.16074762 | 6.4481194 | | | |
| H | x | 6.35 | 6.73651802 | 7.08593171 | | | |
| H | x | 7.39 | 7.91950138 | 7.75119996 | | | |
| H | x | 6.55 | 6.81510378 | 6.93090113 | | | |
| H | x | 7.48 | 7.61945923 | 8.37815606 | | | |
| H | x | 6.77 | 7.35598783 | 7.53311107 | | | |
| H | x | 6.31 | 6.54216996 | 6.58805942 | | | |
| H | | 2.53 | 2.55168596 | 2.61700834 | | | |
| H | | 1.59 | 1.61731089 | 1.57946925 | | | |
| H | | 1.29 | 1.01922143 | 1.14774555 | | | |
| H | | 1.29 | 1.22741903 | 1.3361358 | | | |
| H | | 0.88 | 0.91671997 | 0.79032632 | | | |
| H | | 3.70 | 3.87041314 | 3.70000147 | | | |
| H | | 2.04 | 2.19913453 | 2.14469985 | | | |
| H | | 2.09 | 2.08721569 | 2.10528836 | | | |

Table S8. Energy analyses of 7*S*,8*R*,12*R*-2/7*R*,8*S*,12*S*-2 (eleven conformers)

| NO. | 3D conformers B3LYP/6-31G(d,p) | G (Hartree) | Boltzmann distribution | Calculated ECD spectrum |
|-----|---|--------------|---------------------------|--|
| | | | | 7 <i>S</i> ,8 <i>R</i> ,12 <i>R</i> -2 |
| 1 |  | -1347.768036 | 3.55 % |  |
| 2 |  | -1347.766188 | 0.5 % |  |
| 3 |  | -1347.766520 | 0.71 % |  |
| 4 |  | -1347.770379 | 42.49 % |  |
| 5 |  | -1347.766810 | 0.97 % |  |

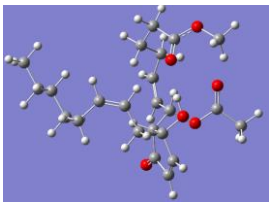
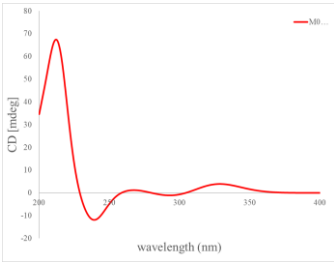
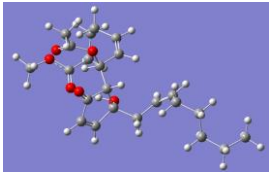
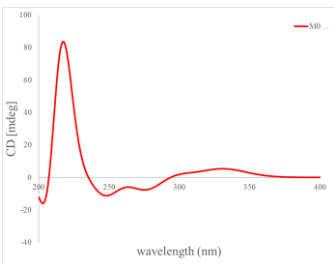
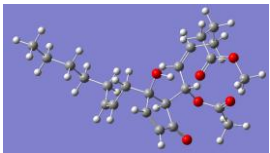
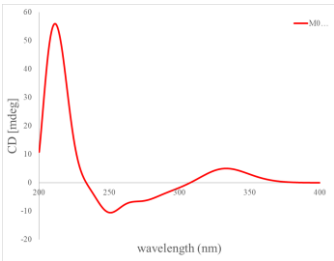
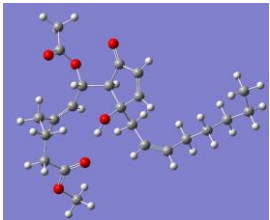
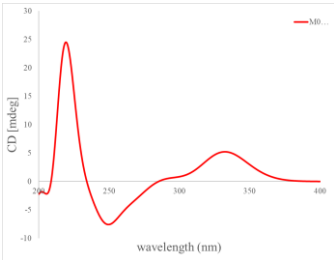

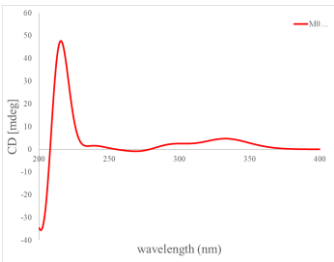
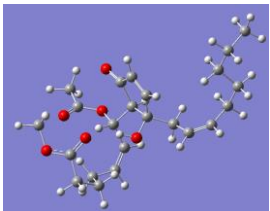
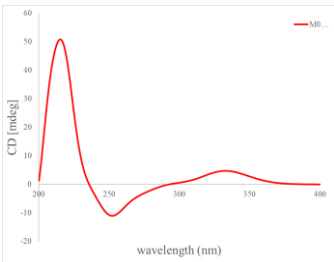
| | | | | |
|----|---|--------------|---------|--|
| 6 |  | -1347.768948 | 9.33 % |  |
| 7 |  | -1347.768453 | 5.53 % |  |
| 8 |  | -1347.770035 | 29.51 % |  |
| 9 |  | -1347.767498 | 2.01 % |  |
| 10 |  | -1347.767665 | 2.4 % |  |
| 11 |  | -1347.767761 | 2.66 % |  |

Table S9. Cartesian coordinates of the low-energy re-optimized conformers of 7*S*,8*R*,12*R*-2/7*R*,8*S*,12*S*-2 calculated at B3LYP/6-31G(d,p) level of theory.

| Conformer 1 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.288 | -0.0857 | 3.1934 | H | 1.17168 | -3.3259 | 1.67923 |
| C | -0.292 | -1.3387 | 2.72446 | H | 2.21528 | -1.9234 | 1.91488 |
| C | 0.194 | -1.4659 | 1.29198 | H | 1.26167 | -2.8627 | -0.8733 |
| C | 0.48856 | 0.02354 | 0.87213 | H | 3.50041 | -2.7117 | -1.5765 |
| C | 0.21157 | 0.84465 | 2.15904 | H | 4.23048 | -1.8664 | 1.31276 |
| O | 0.40106 | 2.03829 | 2.31081 | H | 5.11803 | -3.0666 | 0.38979 |
| C | 1.46113 | -2.3557 | 1.24909 | H | 6.32672 | -0.9914 | 0.23349 |
| C | 2.0085 | -2.5769 | -0.136 | H | 5.66647 | -1.3523 | -1.3544 |
| C | 3.2869 | -2.4894 | -0.5284 | H | 3.78623 | 0.27084 | -0.936 |
| C | 4.50677 | -2.156 | 0.29167 | H | 4.4479 | 0.62519 | 0.65312 |
| C | 5.38712 | -1.0537 | -0.333 | H | 6.55978 | 1.47502 | -0.4191 |
| C | 4.7266 | 0.32951 | -0.3699 | H | 5.89409 | 1.12395 | -2.006 |
| C | 5.6176 | 1.41739 | -0.983 | H | 5.60974 | 3.55067 | -1.4572 |
| C | 4.95197 | 2.79717 | -1.0088 | H | 4.02138 | 2.77727 | -1.5891 |
| O | -0.7858 | -2.1463 | 0.51651 | H | 4.69957 | 3.13415 | 0.00396 |
| C | -0.326 | 0.53267 | -0.341 | H | -1.6677 | -1.7438 | 0.65629 |
| C | 0.06107 | -0.0963 | -1.6547 | H | -1.3896 | 0.42627 | -0.1407 |
| C | -0.7889 | -0.4649 | -2.6204 | H | 1.13061 | -0.2168 | -1.8158 |
| C | -2.2939 | -0.3911 | -2.5582 | H | -0.3668 | -0.8952 | -3.5293 |
| O | -0.044 | 1.96006 | -0.4699 | H | -2.5956 | 0.38571 | -1.8473 |
| C | -2.9391 | -1.7441 | -2.1611 | H | -2.6885 | -0.0737 | -3.5326 |
| C | -4.328 | -1.5701 | -1.5244 | H | -2.2863 | -2.2604 | -1.4528 |
| C | -4.24 | -0.8062 | -0.2156 | H | -3.0278 | -2.394 | -3.0397 |
| C | -1.0501 | 2.8264 | -0.2331 | H | -4.7606 | -2.5545 | -1.3003 |
| O | -2.2065 | 2.50414 | -0.0371 | H | -5.0225 | -1.0526 | -2.1929 |
| C | -0.5342 | 4.2431 | -0.2269 | H | 0.05412 | 4.38382 | 0.68621 |
| O | -5.1907 | 0.12426 | -0.1028 | H | 0.12633 | 4.41977 | -1.0806 |
| O | -3.3997 | -1.0029 | 0.65147 | H | -1.3714 | 4.94223 | -0.2396 |
| C | -5.126 | 0.95995 | 1.07612 | H | -5.157 | 0.34567 | 1.9789 |
| H | -0.5832 | 0.25353 | 4.1803 | H | -4.2075 | 1.54995 | 1.05312 |
| H | -0.6123 | -2.2266 | 3.26354 | H | -6.0038 | 1.60318 | 1.01601 |
| H | 1.54996 | 0.15253 | 0.62824 | | | | |

| Conformer 2 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.91394 | 1.91254 | 3.04189 | H | -0.0374 | -1.8135 | 3.08879 |
| C | 0.08211 | 0.88212 | 3.22862 | H | 1.53209 | -1.2351 | 2.53574 |
| C | -0.1366 | 0.03064 | 1.99116 | H | -0.6077 | -2.5774 | 0.73739 |
| C | 0.61839 | 0.83093 | 0.86821 | H | 1.1578 | -3.5754 | -0.4141 |
| C | 1.37834 | 1.93916 | 1.6391 | H | 3.10667 | -2.0713 | 1.46645 |
| O | 2.23013 | 2.67769 | 1.17891 | H | 3.30965 | -3.7301 | 0.92645 |
| C | 0.49083 | -1.3759 | 2.22908 | H | 3.43349 | -2.9442 | -1.4601 |
| C | 0.40067 | -2.3211 | 1.05869 | H | 3.25929 | -1.283 | -0.9136 |
| C | 1.41766 | -2.8982 | 0.40231 | H | 5.38925 | -1.4856 | 0.40351 |
| C | 2.89828 | -2.7515 | 0.63252 | H | 5.52784 | -3.1723 | -0.0714 |
| C | 3.65178 | -2.2657 | -0.6218 | H | 7.03964 | -1.8877 | -1.4408 |
| C | 5.17038 | -2.19 | -0.4129 | H | 5.75426 | -2.4863 | -2.4756 |
| C | 5.96907 | -1.7792 | -1.6612 | H | 6.34234 | -0.0971 | -2.9983 |
| C | 5.70398 | -0.3478 | -2.1433 | H | 4.66408 | -0.2065 | -2.4579 |
| O | -1.5462 | -0.0453 | 1.82731 | H | 5.91 | 0.38066 | -1.3492 |
| C | -0.3211 | 1.41554 | -0.2122 | H | -1.812 | -0.8377 | 1.32024 |
| C | -0.8689 | 0.3771 | -1.1584 | H | -1.1117 | 1.99248 | 0.26247 |
| C | -2.0882 | 0.37444 | -1.7112 | H | -0.1618 | -0.3974 | -1.4526 |
| C | -3.2115 | 1.3489 | -1.4753 | H | -2.3092 | -0.4173 | -2.4308 |
| O | 0.47102 | 2.32152 | -1.0338 | H | -2.9425 | 2.07352 | -0.7006 |
| C | -4.5549 | 0.68031 | -1.1173 | H | -3.3683 | 1.93361 | -2.3945 |
| C | -4.5051 | -0.2172 | 0.13943 | H | -4.9249 | 0.09042 | -1.9641 |
| C | -3.9259 | -1.5968 | -0.0946 | H | -5.2939 | 1.47106 | -0.9435 |
| C | 0.20546 | 3.64679 | -0.941 | H | -5.5286 | -0.3708 | 0.5053 |
| O | -0.7114 | 4.11831 | -0.3021 | H | -3.9267 | 0.25494 | 0.93758 |
| C | 1.22414 | 4.43772 | -1.7234 | H | 2.17994 | 4.38295 | -1.1911 |
| O | -4.6039 | -2.2705 | -1.041 | H | 1.37091 | 4.00669 | -2.718 |
| O | -2.9837 | -2.0909 | 0.50405 | H | 0.90307 | 5.47732 | -1.8007 |
| C | -4.1422 | -3.6043 | -1.3204 | H | -4.8053 | -3.984 | -2.0978 |
| H | 1.2466 | 2.63655 | 3.77741 | H | -3.1075 | -3.585 | -1.6721 |
| H | -0.4199 | 0.61661 | 4.15483 | H | -4.2034 | -4.2258 | -0.4236 |
| H | 1.36307 | 0.20891 | 0.35869 | | | | |

| Conformer 3 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.7484 | 2.08618 | -1.1377 | H | -1.9614 | -0.3392 | 1.38627 |
| C | -1.6968 | 0.75066 | -1.1901 | H | -0.4665 | -1.2654 | 1.34144 |
| C | -0.6533 | 0.13703 | -0.2744 | H | -1.3936 | -2.5463 | -0.7111 |
| C | -0.0486 | 1.38182 | 0.47279 | H | -3.5423 | -3.3692 | -0.271 |
| C | -0.7605 | 2.6032 | -0.1681 | H | -4.2557 | -2.7215 | 2.14698 |
| O | -0.573 | 3.77597 | 0.09948 | H | -3.9075 | -1.0516 | 1.74685 |
| C | -1.285 | -0.8778 | 0.71455 | H | -5.9494 | -2.8722 | 0.35106 |
| C | -1.9842 | -2.0328 | 0.04564 | H | -6.3389 | -1.655 | 1.556 |
| C | -3.2135 | -2.4992 | 0.30186 | H | -5.1192 | -1.0652 | -1.1995 |
| C | -4.2197 | -2.0066 | 1.31008 | H | -6.8288 | -0.9589 | -0.8088 |
| C | -5.647 | -1.8872 | 0.73429 | H | -6.3037 | 0.81358 | 0.91745 |
| C | -5.8216 | -0.8456 | -0.3826 | H | -4.6158 | 0.76725 | 0.42874 |
| C | -5.6396 | 0.61159 | 0.06439 | H | -5.7895 | 2.64939 | -0.712 |
| C | -5.9277 | 1.6177 | -1.0548 | H | -5.2602 | 1.45905 | -1.911 |
| O | 0.28042 | -0.5065 | -1.139 | H | -6.9581 | 1.52188 | -1.4193 |
| C | 1.48888 | 1.47008 | 0.42717 | H | 0.65356 | -1.299 | -0.6998 |
| C | 2.17925 | 0.38258 | 1.21249 | H | 1.82724 | 1.49615 | -0.606 |
| C | 3.33832 | -0.2112 | 0.9006 | H | 1.70625 | 0.12631 | 2.16098 |
| C | 4.19611 | 0.01805 | -0.3155 | H | 3.73446 | -0.9387 | 1.61286 |
| O | 1.85689 | 2.72888 | 1.06103 | H | 3.72242 | 0.7277 | -1.0001 |
| C | 4.57328 | -1.2717 | -1.0724 | H | 5.13341 | 0.49538 | 0.00827 |
| C | 3.3661 | -2.0843 | -1.5918 | H | 5.19417 | -1.918 | -0.4409 |
| C | 2.68008 | -2.9323 | -0.5412 | H | 5.19117 | -0.9925 | -1.9336 |
| C | 2.51405 | 3.64166 | 0.30653 | H | 3.71322 | -2.7758 | -2.3701 |
| O | 2.93057 | 3.43355 | -0.8135 | H | 2.61348 | -1.4273 | -2.0358 |
| C | 2.62735 | 4.9475 | 1.05259 | H | 1.63013 | 5.39811 | 1.09975 |
| O | 3.52442 | -3.8163 | 0.0173 | H | 2.96729 | 4.78107 | 2.07897 |
| O | 1.50068 | -2.8758 | -0.2291 | H | 3.31147 | 5.61493 | 0.52694 |
| C | 2.96011 | -4.6829 | 1.01867 | H | 2.1596 | -5.2909 | 0.59 |
| H | -2.395 | 2.74499 | -1.7068 | H | 3.78396 | -5.3124 | 1.3549 |
| H | -2.2936 | 0.10802 | -1.8293 | H | 2.5579 | -4.0966 | 1.84861 |
| H | -0.3462 | 1.37449 | 1.53058 | | | | |

| Conformer 4 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.04008 | -3.4825 | -0.4917 | H | -0.493 | -1.1765 | 2.13009 |
| C | 2.07755 | -3.033 | 0.76917 | H | 0.44596 | -2.4537 | 2.89401 |
| C | 1.22764 | -1.8021 | 1.0052 | H | -0.5188 | -4.1549 | 1.26879 |
| C | 0.7731 | -1.3995 | -0.4395 | H | -2.7954 | -3.8886 | 0.81942 |
| C | 1.20493 | -2.5903 | -1.325 | H | -3.8499 | -1.9315 | 2.08229 |
| O | 0.89989 | -2.7584 | -2.4919 | H | -2.4925 | -0.9125 | 1.62726 |
| C | 0.01711 | -2.1251 | 1.9363 | H | -3.0803 | -1.225 | -0.8004 |
| C | -0.9447 | -3.1645 | 1.42909 | H | -4.4099 | -2.2777 | -0.3473 |
| C | -2.2507 | -3.01 | 1.17067 | H | -5.4834 | -0.3825 | 0.9182 |
| C | -3.0932 | -1.7684 | 1.29839 | H | -4.1581 | 0.67493 | 0.45805 |
| C | -3.8228 | -1.4106 | -0.0113 | H | -4.7444 | 0.35201 | -1.9682 |
| C | -4.7461 | -0.1935 | 0.12357 | H | -6.0697 | -0.7027 | -1.5069 |
| C | -5.4813 | 0.16421 | -1.1745 | H | -6.9114 | 1.60968 | -1.9754 |
| C | -6.4015 | 1.38102 | -1.0327 | H | -7.1717 | 1.20927 | -0.2706 |
| O | 2.05463 | -0.8463 | 1.65905 | H | -5.8368 | 2.27342 | -0.7349 |
| C | 1.35495 | -0.067 | -0.9484 | H | 1.49253 | -0.0897 | 1.91375 |
| C | 0.65562 | 0.41128 | -2.1964 | H | 1.29105 | 0.67624 | -0.1613 |
| C | 0.2908 | 1.67614 | -2.4477 | H | 0.41673 | -0.3654 | -2.9189 |
| C | 0.57712 | 2.91473 | -1.6338 | H | -0.2575 | 1.85514 | -3.3747 |
| O | 2.7775 | -0.2855 | -1.2078 | H | 1.39304 | 2.73728 | -0.9267 |
| C | -0.6414 | 3.50787 | -0.8905 | H | 0.94342 | 3.68531 | -2.3265 |
| C | -1.137 | 2.66032 | 0.29574 | H | -1.4786 | 3.63823 | -1.5883 |
| C | -0.0903 | 2.40704 | 1.36419 | H | -0.3751 | 4.50507 | -0.5245 |
| C | 3.65544 | 0.58033 | -0.6643 | H | -1.4923 | 1.68059 | -0.0352 |
| O | 3.35471 | 1.59926 | -0.0727 | H | -1.9842 | 3.16879 | 0.77611 |
| C | 5.07152 | 0.10193 | -0.8794 | H | 5.25966 | -0.7525 | -0.2196 |
| O | 0.60847 | 3.50561 | 1.66963 | H | 5.21398 | -0.2368 | -1.9094 |
| O | 0.10007 | 1.32318 | 1.89672 | H | 5.77071 | 0.90423 | -0.6402 |
| C | 1.70688 | 3.33003 | 2.59129 | H | 2.4701 | 2.69854 | 2.13058 |
| H | 2.52615 | -4.3655 | -0.8921 | H | 2.09388 | 4.33329 | 2.7687 |
| H | 2.62288 | -3.4828 | 1.59491 | H | 1.35504 | 2.88065 | 3.52265 |
| H | -0.3173 | -1.3172 | -0.4987 | | | | |

| Conformer 5 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.5913 | 2.46769 | -2.4332 | H | 1.48808 | 2.10501 | 1.45098 |
| C | -0.3889 | 3.12192 | -1.283 | H | 0.95532 | 3.73345 | 1.06818 |
| C | 0.05409 | 2.22433 | -0.1384 | H | 2.36535 | 3.74417 | -1.0383 |
| C | 0.32222 | 0.85302 | -0.8462 | H | 4.46599 | 2.74463 | -0.846 |
| C | -0.2719 | 1.0315 | -2.2665 | H | 5.07592 | 1.76636 | 1.36445 |
| O | -0.4369 | 0.1656 | -3.1067 | H | 3.41809 | 1.27019 | 1.6642 |
| C | 1.28151 | 2.78437 | 0.61936 | H | 3.53657 | -0.3251 | -0.2595 |
| C | 2.4979 | 3.01751 | -0.2357 | H | 5.17562 | 0.19029 | -0.6138 |
| C | 3.70483 | 2.446 | -0.1228 | H | 5.96724 | -0.6252 | 1.58979 |
| C | 4.16025 | 1.40875 | 0.86939 | H | 4.3349 | -1.0823 | 2.05104 |
| C | 4.45749 | 0.04761 | 0.20681 | H | 5.83436 | -2.2916 | -0.3374 |
| C | 5.0126 | -0.9939 | 1.18817 | H | 5.82089 | -2.9934 | 1.27131 |
| C | 5.22652 | -2.3881 | 0.57376 | H | 4.14285 | -4.1258 | -0.1776 |
| C | 3.92858 | -3.1398 | 0.25093 | H | 3.33047 | -3.295 | 1.15762 |
| O | -0.9849 | 2.202 | 0.83897 | H | 3.29989 | -2.5978 | -0.4644 |
| C | -0.1778 | -0.411 | -0.1236 | H | -1.8184 | 1.86411 | 0.45068 |
| C | 0.39068 | -0.6243 | 1.25453 | H | -1.2644 | -0.4238 | -0.1081 |
| C | -0.3086 | -0.9936 | 2.33502 | H | 1.4693 | -0.4992 | 1.34097 |
| C | -1.7997 | -1.2184 | 2.39476 | H | 0.23633 | -1.1199 | 3.27118 |
| O | 0.2645 | -1.5351 | -0.9501 | H | -2.1599 | -1.5314 | 1.40891 |
| C | -2.5774 | 0.03824 | 2.86663 | H | -2.0164 | -2.0558 | 3.07096 |
| C | -4.0311 | 0.05808 | 2.36187 | H | -2.0647 | 0.93381 | 2.50796 |
| C | -4.0883 | 0.13315 | 0.8465 | H | -2.5816 | 0.09205 | 3.9618 |
| C | -0.6833 | -2.3551 | -1.4505 | H | -4.5451 | 0.94627 | 2.75307 |
| O | -1.8594 | -2.3187 | -1.1451 | H | -4.5915 | -0.8202 | 2.69586 |
| C | -0.0824 | -3.306 | -2.4547 | H | 0.12893 | -2.7399 | -3.3685 |
| O | -4.9455 | -0.7484 | 0.32546 | H | 0.86191 | -3.7179 | -2.088 |
| O | -3.43 | 0.90207 | 0.15925 | H | -0.7895 | -4.107 | -2.6748 |
| C | -4.9952 | -0.8117 | -1.1185 | H | -5.7957 | -1.5162 | -1.3442 |
| H | -0.964 | 2.87054 | -3.3687 | H | -5.2165 | 0.17358 | -1.535 |
| H | -0.5742 | 4.17821 | -1.1048 | H | -4.0385 | -1.1756 | -1.4987 |
| H | 1.40576 | 0.74762 | -0.9928 | | | | |

| Conformer 6 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.06973 | -3.8961 | 0.1948 | H | -0.0623 | -1.9381 | 3.27401 |
| C | 1.3071 | -3.1948 | 1.31043 | H | -1.1567 | -2.5524 | 2.03481 |
| C | 0.73363 | -1.7902 | 1.28487 | H | -0.5888 | 0.45568 | 2.5299 |
| C | 0.26858 | -1.6291 | -0.2036 | H | -2.851 | 0.83241 | 2.14908 |
| C | 0.3653 | -3.053 | -0.7951 | H | -3.192 | -2.2263 | 1.82978 |
| O | -0.0687 | -3.4028 | -1.8776 | H | -4.3796 | -1.1203 | 2.49831 |
| C | -0.473 | -1.7317 | 2.27506 | H | -3.4289 | -1.136 | -0.418 |
| C | -1.2005 | -0.4136 | 2.29648 | H | -4.9148 | -1.8581 | 0.18301 |
| C | -2.506 | -0.1993 | 2.07312 | H | -5.7043 | 0.4251 | 0.9283 |
| C | -3.5795 | -1.2051 | 1.74654 | H | -4.251 | 1.13789 | 0.24103 |
| C | -4.2113 | -1.0295 | 0.34644 | H | -4.8882 | 0.25843 | -2.0248 |
| C | -4.9515 | 0.29783 | 0.13522 | H | -6.3461 | -0.4419 | -1.3416 |
| C | -5.639 | 0.39279 | -1.2334 | H | -6.8568 | 1.75417 | -2.4331 |
| C | -6.3769 | 1.71813 | -1.4484 | H | -7.1578 | 1.86493 | -0.6919 |
| O | 1.77452 | -0.9157 | 1.69632 | H | -5.6893 | 2.57048 | -1.382 |
| C | 1.09947 | -0.6215 | -1.0208 | H | 1.45493 | 0.00562 | 1.73085 |
| C | 0.44148 | -0.2424 | -2.3209 | H | 1.29076 | 0.26003 | -0.4158 |
| C | 0.21029 | 1.02077 | -2.7028 | H | 0.11714 | -1.0728 | -2.9436 |
| C | 0.61009 | 2.26056 | -1.9346 | H | -0.3143 | 1.17684 | -3.6456 |
| O | 2.39419 | -1.2531 | -1.2773 | H | 1.58926 | 2.09057 | -1.4732 |
| C | -0.4073 | 2.68047 | -0.8469 | H | 0.74524 | 3.09511 | -2.6345 |
| C | 0.19634 | 3.66768 | 0.17083 | H | -0.7571 | 1.79763 | -0.3012 |
| C | 1.28322 | 2.99354 | 0.98718 | H | -1.2915 | 3.13492 | -1.3097 |
| C | 3.50347 | -0.5125 | -1.0983 | H | -0.5819 | 3.99741 | 0.87073 |
| O | 3.51048 | 0.67372 | -0.8313 | H | 0.60544 | 4.55509 | -0.3206 |
| C | 4.74087 | -1.3631 | -1.2618 | H | 4.81624 | -2.0527 | -0.4137 |
| O | 2.44216 | 3.65601 | 0.9509 | H | 4.67549 | -1.9659 | -2.1722 |
| O | 1.12215 | 1.95124 | 1.60492 | H | 5.62427 | -0.7241 | -1.2916 |
| C | 3.55478 | 3.03233 | 1.63137 | H | 4.36832 | 3.75489 | 1.56718 |
| H | 1.32962 | -4.9307 | -0.0012 | H | 3.29739 | 2.83061 | 2.67372 |
| H | 1.82002 | -3.5542 | 2.19859 | H | 3.81756 | 2.10414 | 1.1202 |
| H | -0.7732 | -1.2961 | -0.257 | | | | |

| Conformer 7 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.06973 | -3.8961 | 0.1948 | H | -0.0623 | -1.9381 | 3.27401 |
| C | 1.3071 | -3.1948 | 1.31043 | H | -1.1567 | -2.5524 | 2.03481 |
| C | 0.73363 | -1.7902 | 1.28487 | H | -0.5888 | 0.45568 | 2.5299 |
| C | 0.26858 | -1.6291 | -0.2036 | H | -2.851 | 0.83241 | 2.14908 |
| C | 0.3653 | -3.053 | -0.7951 | H | -3.192 | -2.2263 | 1.82978 |
| O | -0.0687 | -3.4028 | -1.8776 | H | -4.3796 | -1.1203 | 2.49831 |
| C | -0.473 | -1.7317 | 2.27506 | H | -3.4289 | -1.136 | -0.418 |
| C | -1.2005 | -0.4136 | 2.29648 | H | -4.9148 | -1.8581 | 0.18301 |
| C | -2.506 | -0.1993 | 2.07312 | H | -5.7043 | 0.4251 | 0.9283 |
| C | -3.5795 | -1.2051 | 1.74654 | H | -4.251 | 1.13789 | 0.24103 |
| C | -4.2113 | -1.0295 | 0.34644 | H | -4.8882 | 0.25843 | -2.0248 |
| C | -4.9515 | 0.29783 | 0.13522 | H | -6.3461 | -0.4419 | -1.3416 |
| C | -5.639 | 0.39279 | -1.2334 | H | -6.8568 | 1.75417 | -2.4331 |
| C | -6.3769 | 1.71813 | -1.4484 | H | -7.1578 | 1.86493 | -0.6919 |
| O | 1.77452 | -0.9157 | 1.69632 | H | -5.6893 | 2.57048 | -1.382 |
| C | 1.09947 | -0.6215 | -1.0208 | H | 1.45493 | 0.00562 | 1.73085 |
| C | 0.44148 | -0.2424 | -2.3209 | H | 1.29076 | 0.26003 | -0.4158 |
| C | 0.21029 | 1.02077 | -2.7028 | H | 0.11714 | -1.0728 | -2.9436 |
| C | 0.61009 | 2.26056 | -1.9346 | H | -0.3143 | 1.17684 | -3.6456 |
| O | 2.39419 | -1.2531 | -1.2773 | H | 1.58926 | 2.09057 | -1.4732 |
| C | -0.4073 | 2.68047 | -0.8469 | H | 0.74524 | 3.09511 | -2.6345 |
| C | 0.19634 | 3.66768 | 0.17083 | H | -0.7571 | 1.79763 | -0.3012 |
| C | 1.28322 | 2.99354 | 0.98718 | H | -1.2915 | 3.13492 | -1.3097 |
| C | 3.50347 | -0.5125 | -1.0983 | H | -0.5819 | 3.99741 | 0.87073 |
| O | 3.51048 | 0.67372 | -0.8313 | H | 0.60544 | 4.55509 | -0.3206 |
| C | 4.74087 | -1.3631 | -1.2618 | H | 4.81624 | -2.0527 | -0.4137 |
| O | 2.44216 | 3.65601 | 0.9509 | H | 4.67549 | -1.9659 | -2.1722 |
| O | 1.12215 | 1.95124 | 1.60492 | H | 5.62427 | -0.7241 | -1.2916 |
| C | 3.55478 | 3.03233 | 1.63137 | H | 4.36832 | 3.75489 | 1.56718 |
| H | 1.32962 | -4.9307 | -0.0012 | H | 3.29739 | 2.83061 | 2.67372 |
| H | 1.82002 | -3.5542 | 2.19859 | H | 3.81756 | 2.10414 | 1.1202 |
| H | -0.7732 | -1.2961 | -0.257 | | | | |

| Conformer 8 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.47283 | -2.0409 | 2.6413 | H | -2.0581 | 0.68219 | 0.2691 |
| C | -0.2511 | -0.9201 | 2.74681 | H | -2.3085 | 0.73197 | 2.00395 |
| C | -0.4857 | -0.21 | 1.42424 | H | -2.8206 | -1.7881 | 1.99091 |
| C | 0.14771 | -1.1888 | 0.37223 | H | -4.2755 | -2.4162 | 0.27645 |
| C | 0.81928 | -2.2946 | 1.22519 | H | -3.3653 | 0.10363 | -1.2779 |
| O | 1.49339 | -3.2225 | 0.81555 | H | -3.6946 | -1.4672 | -1.9977 |
| C | -1.9869 | 0.07973 | 1.17898 | H | -5.6177 | -0.0676 | -2.3825 |
| C | -2.8708 | -1.1361 | 1.11786 | H | -6.083 | -1.3272 | -1.2489 |
| C | -3.7022 | -1.4981 | 0.13109 | H | -5.7993 | 0.30107 | 0.65878 |
| C | -3.981 | -0.7975 | -1.1729 | H | -5.3534 | 1.55558 | -0.4868 |
| C | -5.4678 | -0.4211 | -1.353 | H | -7.6067 | 1.34964 | -1.59 |
| C | -5.9639 | 0.64711 | -0.3711 | H | -8.0532 | 0.09797 | -0.442 |
| C | -7.4436 | 1.00553 | -0.5585 | H | -8.9928 | 2.31063 | 0.26268 |
| C | -7.9334 | 2.07767 | 0.42032 | H | -7.8157 | 1.74827 | 1.46005 |
| O | 0.11316 | 1.08164 | 1.48444 | H | -7.3665 | 3.00959 | 0.30365 |
| C | 1.09986 | -0.5549 | -0.6608 | H | 1.06491 | 1.00403 | 1.71276 |
| C | 0.45402 | 0.51605 | -1.5053 | H | 1.99593 | -0.1835 | -0.1694 |
| C | 1.0826 | 1.54616 | -2.0842 | H | -0.6163 | 0.40394 | -1.6717 |
| C | 2.5528 | 1.87684 | -2.0455 | H | 0.47271 | 2.23649 | -2.6701 |
| O | 1.51124 | -1.642 | -1.5468 | H | 3.13569 | 1.04442 | -1.6382 |
| C | 2.88702 | 3.17382 | -1.2759 | H | 2.89728 | 2.00783 | -3.0815 |
| C | 2.61511 | 3.08911 | 0.23749 | H | 2.29897 | 4.0078 | -1.6807 |
| C | 3.39214 | 1.99264 | 0.93923 | H | 3.94181 | 3.41882 | -1.4395 |
| C | 2.81805 | -1.9802 | -1.5652 | H | 1.55567 | 2.91124 | 0.43802 |
| O | 3.70565 | -1.3419 | -1.033 | H | 2.88996 | 4.0421 | 0.70935 |
| C | 3.01819 | -3.2671 | -2.3247 | H | 4.07668 | -3.4033 | -2.5506 |
| O | 4.68972 | 1.99243 | 0.6177 | H | 2.66846 | -4.0874 | -1.6885 |
| O | 2.90944 | 1.18316 | 1.72029 | H | 2.42417 | -3.2762 | -3.2427 |
| C | 5.47408 | 0.89941 | 1.14743 | H | 6.49279 | 1.09113 | 0.81057 |
| H | 0.80305 | -2.6947 | 3.44114 | H | 5.42228 | 0.88826 | 2.23839 |
| H | -0.6218 | -0.4801 | 3.66931 | H | 5.10165 | -0.0449 | 0.74447 |
| H | -0.6568 | -1.6843 | -0.1874 | | | | |

| Conformer 9 | | | | | | | |
|-------------|--------------------------|---------|---------|-------------|--------------------------|---------|---------|
| Atomic Type | Standard Orientation (Å) | | | Atomic Type | Standard Orientation (Å) | | |
| | X | Y | Z | | X | Y | Z |
| C | 1.38722 | 2.26044 | 1.36086 | H | 1.7097 | -0.124 | -1.2652 |
| C | 1.4393 | 0.92473 | 1.3241 | H | 0.23436 | -1.0843 | -1.23 |
| C | 0.40288 | 0.29521 | 0.40915 | H | 1.15781 | -2.4564 | 0.69872 |
| C | -0.248 | 1.53653 | -0.2995 | H | 3.40874 | -3.0573 | 0.44671 |
| C | 0.32175 | 2.76 | 0.46544 | H | 4.50687 | -2.2284 | -1.6721 |
| O | -0.0199 | 3.92183 | 0.34325 | H | 3.70831 | -0.6727 | -1.5085 |
| C | 1.04744 | -0.6898 | -0.602 | H | 4.93228 | -0.2689 | 0.64023 |
| C | 1.77316 | -1.8407 | 0.04531 | H | 5.71049 | -1.8388 | 0.50754 |
| C | 3.06019 | -2.1811 | -0.1039 | H | 6.75126 | -1.1329 | -1.678 |
| C | 4.12254 | -1.5085 | -0.9325 | H | 6.03408 | 0.46141 | -1.5005 |
| C | 5.30681 | -1.0036 | -0.084 | H | 8.06092 | -0.7894 | 0.43658 |
| C | 6.43134 | -0.3923 | -0.9309 | H | 8.45066 | 0.35492 | -0.8362 |
| C | 7.66168 | 0.06459 | -0.1294 | H | 8.32251 | 1.54738 | 1.32768 |
| C | 7.39899 | 1.23337 | 0.82796 | H | 7.00084 | 2.10244 | 0.28912 |
| O | -0.501 | -0.3825 | 1.28077 | H | 6.6775 | 0.96899 | 1.60911 |
| C | -1.7839 | 1.52349 | -0.3862 | H | -0.895 | -1.1523 | 0.82466 |
| C | -2.3313 | 0.37384 | -1.19 | H | -2.2173 | 1.55383 | 0.61119 |
| C | -3.3771 | -0.3959 | -0.8648 | H | -1.8329 | 0.20251 | -2.1447 |
| C | -4.2367 | -0.2993 | 0.37296 | H | -3.6537 | -1.1776 | -1.5747 |
| O | -2.1521 | 2.74881 | -1.0851 | H | -4.2168 | 0.72248 | 0.76487 |
| C | -3.8593 | -1.2678 | 1.51716 | H | -5.2779 | -0.4978 | 0.08031 |
| C | -3.9238 | -2.7599 | 1.15853 | H | -4.5575 | -1.0948 | 2.34487 |
| C | -2.7645 | -3.2743 | 0.32892 | H | -2.8621 | -1.0211 | 1.89329 |
| C | -3.0622 | 3.55638 | -0.4946 | H | -4.8593 | -3.0147 | 0.64848 |
| O | -3.6981 | 3.26606 | 0.49718 | H | -3.91 | -3.3582 | 2.08124 |
| C | -3.1476 | 4.87039 | -1.2304 | H | -2.2205 | 5.42404 | -1.0461 |
| O | -3.1236 | -4.3378 | -0.4104 | H | -3.2292 | 4.70717 | -2.3091 |
| O | -1.6244 | -2.8416 | 0.33846 | H | -4.0008 | 5.44352 | -0.8656 |
| C | -2.0744 | -4.9545 | -1.1801 | H | -2.5481 | -5.7865 | -1.7008 |
| H | 1.99415 | 2.92868 | 1.96204 | H | -1.6546 | -4.2412 | -1.8937 |
| H | 2.1022 | 0.28936 | 1.90256 | H | -1.278 | -5.3129 | -0.5231 |
| H | 0.13594 | 1.6177 | -1.3267 | | | | |

| Conformer 10 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 0.66841 | 4.3221 | 0.04909 | H | -1.205 | 1.98758 | -2.5488 |
| C | 0.30068 | 3.73422 | -1.0952 | H | -1.8826 | 2.12444 | -0.9238 |
| C | 0.28502 | 2.21638 | -1.0313 | H | -0.3927 | -0.3861 | -1.9844 |
| C | 0.57356 | 1.92993 | 0.48276 | H | -1.9725 | -1.6722 | -0.8822 |
| C | 0.95726 | 3.30139 | 1.08096 | H | -3.2269 | -0.5377 | 0.99175 |
| O | 1.38629 | 3.50251 | 2.20117 | H | -3.3119 | 0.95823 | 0.07198 |
| C | -1.0822 | 1.65593 | -1.5075 | H | -4.7013 | -0.1957 | -1.6726 |
| C | -1.1707 | 0.15403 | -1.4445 | H | -4.5898 | -1.7017 | -0.7755 |
| C | -2.089 | -0.5901 | -0.8121 | H | -5.7595 | -0.6296 | 1.17917 |
| C | -3.2917 | -0.1334 | -0.0304 | H | -5.8757 | 0.87838 | 0.28452 |
| C | -4.6177 | -0.6087 | -0.6579 | H | -7.265 | -0.2698 | -1.4701 |
| C | -5.8512 | -0.2151 | 0.16393 | H | -7.15 | -1.7765 | -0.5755 |
| C | -7.1739 | -0.684 | -0.456 | H | -9.3294 | -0.6364 | -0.0988 |
| C | -8.4021 | -0.2875 | 0.36974 | H | -8.357 | -0.7161 | 1.37858 |
| O | 1.32018 | 1.80661 | -1.925 | H | -8.4728 | 0.80201 | 0.47722 |
| C | 1.55271 | 0.78953 | 0.8152 | H | 1.48437 | 0.85096 | -1.832 |
| C | 1.57557 | 0.41143 | 2.27501 | H | 1.31748 | -0.0775 | 0.1976 |
| C | 0.9994 | -0.6683 | 2.81749 | H | 2.10601 | 1.11571 | 2.90936 |
| C | 0.16855 | -1.726 | 2.13811 | H | 1.12475 | -0.8037 | 3.8935 |
| O | 2.91409 | 1.21724 | 0.48935 | H | -0.7867 | -1.8031 | 2.6781 |
| C | 0.82228 | -3.1258 | 2.14037 | H | -0.0815 | -1.4505 | 1.11156 |
| C | 2.08963 | -3.2385 | 1.28527 | H | 0.08457 | -3.8565 | 1.78865 |
| C | 1.83734 | -3.1887 | -0.2112 | H | 1.07765 | -3.4051 | 3.17117 |
| C | 3.56803 | 0.59425 | -0.5028 | H | 2.62767 | -4.169 | 1.50115 |
| O | 3.09275 | -0.2962 | -1.1884 | H | 2.79124 | -2.4278 | 1.52439 |
| C | 4.95013 | 1.1669 | -0.6887 | H | 4.86396 | 2.10112 | -1.2558 |
| O | 2.94863 | -3.5348 | -0.8889 | H | 5.41301 | 1.39979 | 0.27324 |
| O | 0.79002 | -2.8843 | -0.7485 | H | 5.5639 | 0.46483 | -1.2548 |
| C | 2.86855 | -3.4283 | -2.3213 | H | 2.00998 | -3.9873 | -2.7015 |
| H | 0.77818 | 5.38452 | 0.23742 | H | 2.78528 | -2.378 | -2.6071 |
| H | 0.05779 | 4.24102 | -2.0253 | H | 3.8003 | -3.8539 | -2.6961 |
| H | -0.3735 | 1.64789 | 0.9615 | | | | |

| Conformer 11 | | | | | | | |
|--------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.00313 | 1.44384 | 1.42443 | H | 2.31412 | 0.17301 | -1.6542 |
| C | 1.41723 | 0.23939 | 1.01189 | H | 1.11992 | -1.0041 | -2.2048 |
| C | 0.72446 | -0.2463 | -0.2498 | H | 2.06953 | -2.6942 | -0.5156 |
| C | -0.1211 | 0.99926 | -0.6982 | H | 4.4095 | -2.8463 | -0.677 |
| C | -0.0034 | 1.99141 | 0.48978 | H | 5.32136 | -1.275 | -2.5048 |
| O | -0.6023 | 3.0429 | 0.62663 | H | 4.40498 | 0.04255 | -1.7935 |
| C | 1.72434 | -0.6942 | -1.3401 | H | 6.6127 | -1.561 | -0.3814 |
| C | 2.60796 | -1.8395 | -0.9202 | H | 6.82159 | 0.01281 | -1.1351 |
| C | 3.94198 | -1.9183 | -1.0142 | H | 5.18549 | 1.01246 | 0.49045 |
| C | 4.91273 | -0.8995 | -1.5538 | H | 4.92917 | -0.5709 | 1.20644 |
| C | 6.0954 | -0.6155 | -0.604 | H | 6.42373 | 0.65536 | 2.64688 |
| C | 5.68359 | 0.05631 | 0.71277 | H | 7.33934 | -0.6503 | 1.91379 |
| C | 6.84172 | 0.30517 | 1.69334 | H | 8.64917 | 1.49543 | 1.9701 |
| C | 7.88216 | 1.32138 | 1.20669 | H | 8.3944 | 0.98161 | 0.29955 |
| O | -0.0445 | -1.4052 | 0.06345 | H | 7.41333 | 2.28748 | 0.98059 |
| C | -1.5725 | 0.71396 | -1.1286 | H | -0.6805 | -1.2225 | 0.78552 |
| C | -1.7029 | -0.1841 | -2.3309 | H | -2.1402 | 0.3317 | -0.2843 |
| C | -2.5758 | -1.1914 | -2.4559 | H | -1.0461 | 0.05528 | -3.1671 |
| C | -3.5586 | -1.6496 | -1.4063 | H | -2.5665 | -1.7566 | -3.3885 |
| O | -2.1443 | 2.00737 | -1.4972 | H | -3.8212 | -0.8053 | -0.7598 |
| C | -3.0164 | -2.8215 | -0.5474 | H | -4.4947 | -1.9566 | -1.8911 |
| C | -3.6852 | -2.8997 | 0.83641 | H | -1.9387 | -2.7008 | -0.4152 |
| C | -3.3841 | -1.6665 | 1.66958 | H | -3.168 | -3.7742 | -1.0685 |
| C | -3.2075 | 2.4474 | -0.7931 | H | -3.2954 | -3.7673 | 1.38546 |
| O | -3.8142 | 1.78615 | 0.02733 | H | -4.7699 | -3.0202 | 0.75928 |
| C | -3.5222 | 3.87741 | -1.1525 | H | -2.7573 | 4.51428 | -0.695 |
| O | -4.4775 | -1.1679 | 2.25233 | H | -3.4798 | 4.02659 | -2.235 |
| O | -2.2757 | -1.1669 | 1.80567 | H | -4.5058 | 4.14867 | -0.7666 |
| C | -4.2993 | 0.05991 | 2.99538 | H | -5.2695 | 0.25937 | 3.45038 |
| H | 1.31213 | 1.98024 | 2.31507 | H | -3.5307 | -0.0673 | 3.761 |
| H | 2.13798 | -0.3993 | 1.51302 | H | -4.019 | 0.86152 | 2.30909 |
| H | 0.37952 | 1.48666 | -1.5468 | | | | |

Table S10. Energy analyses of 7*S*,8*R*,12*S*-2/7*R*,8*S*,12*R*-2 (five conformers)

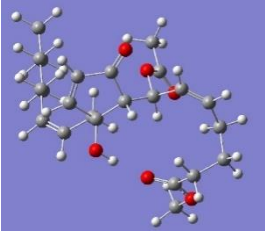
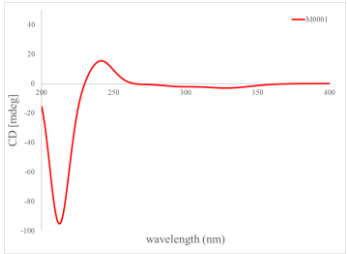
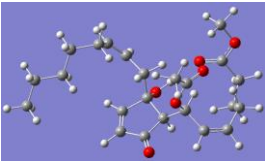
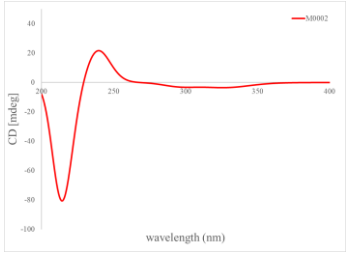

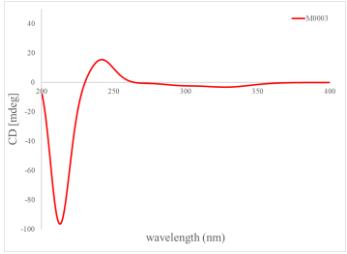
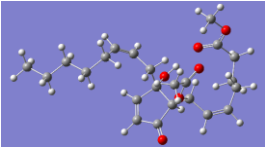
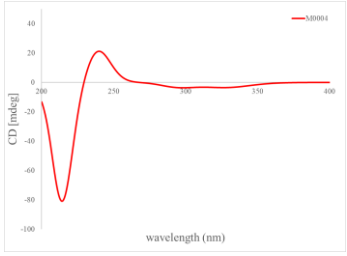
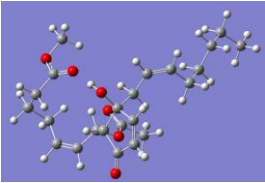
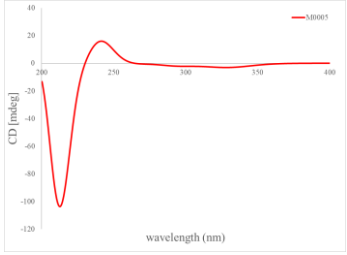
| NO. | 3D conformers B3LYP/6-31G(d,p) | G (Hartree) | Boltzmann distribution | Calculated ECD spectrum 7 <i>S</i> ,8 <i>R</i> ,12 <i>S</i> -2 |
|-----|---|--------------|---------------------------|--|
| | | | | |
| 1 |  | -1347.771487 | 80.14 % |  |
| 2 |  | -1347.768911 | 5.24 % |  |
| 3 |  | -1347.769451 | 9.28 % |  |
| 4 |  | -1347.768154 | 2.35 % |  |
| 5 |  | -1347.768328 | 2.82 % |  |

Table S11. Cartesian coordinates of the low-energy re-optimized conformers of 7*S*,8*R*,12*S*-2/7*R*,8*S*,12*R*-2 calculated at B3LYP/6-31G(d,p) level of theory.

| Conformer 1 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.1847 | 3.67554 | 1.19432 | H | -1.3064 | 0.7008 | 0.32669 |
| C | -0.3307 | 2.64492 | 2.03732 | H | -0.1865 | -0.5734 | 0.80352 |
| C | 0.34759 | 1.37156 | 1.57032 | H | -1.0607 | -0.3857 | 3.21422 |
| C | 1.23631 | 1.88519 | 0.38482 | H | -3.4085 | -0.4401 | 3.28872 |
| C | 0.6948 | 3.29695 | 0.06811 | H | -4.592 | 1.03998 | 1.63154 |
| O | 0.97972 | 3.98061 | -0.8985 | H | -3.4008 | 0.66479 | 0.39572 |
| C | -0.7228 | 0.31588 | 1.16648 | H | -4.1135 | -1.7435 | 0.44264 |
| C | -1.6045 | -0.0846 | 2.32057 | H | -5.2809 | -1.3809 | 1.70387 |
| C | -2.943 | -0.1047 | 2.35973 | H | -6.4772 | 0.19783 | 0.14981 |
| C | -3.9183 | 0.24843 | 1.26805 | H | -5.3145 | -0.1656 | -1.1162 |
| C | -4.7754 | -0.9543 | 0.82523 | H | -6.0199 | -2.5798 | -1.0713 |
| C | -5.8204 | -0.5952 | -0.2383 | H | -7.1826 | -2.2166 | 0.19356 |
| C | -6.6764 | -1.7881 | -0.6832 | H | -8.3122 | -2.2942 | -2.0414 |
| C | -7.7181 | -1.422 | -1.7455 | H | -8.4113 | -0.6572 | -1.374 |
| O | 1.13662 | 0.8877 | 2.65085 | H | -7.2401 | -1.0228 | -2.6486 |
| C | 1.47626 | 0.98377 | -0.8331 | H | 1.58475 | 0.07246 | 2.34919 |
| C | 2.68184 | 1.42697 | -1.6242 | H | 1.58447 | -0.0512 | -0.5104 |
| C | 3.69691 | 0.65121 | -2.0261 | H | 2.69521 | 2.48857 | -1.8577 |
| C | 3.8768 | -0.8376 | -1.8649 | H | 4.51142 | 1.1488 | -2.5564 |
| O | 0.28549 | 1.0569 | -1.6819 | H | 2.92531 | -1.3251 | -1.6291 |
| C | 4.95973 | -1.2301 | -0.8348 | H | 4.18371 | -1.2414 | -2.8395 |
| C | 4.53499 | -1.0182 | 0.63087 | H | 5.87045 | -0.645 | -1.0154 |
| C | 3.37492 | -1.8936 | 1.05882 | H | 5.22654 | -2.2828 | -0.9747 |
| C | -0.0595 | -0.0567 | -2.3642 | H | 4.24858 | 0.02048 | 0.81582 |
| O | 0.50692 | -1.1263 | -2.2685 | H | 5.38086 | -1.2511 | 1.29119 |
| C | -1.2514 | 0.21413 | -3.253 | H | -2.0919 | 0.58782 | -2.6591 |
| O | 3.58656 | -3.1866 | 0.77485 | H | -1.0004 | 0.99023 | -3.9834 |
| O | 2.3546 | -1.5061 | 1.60704 | H | -1.5375 | -0.7034 | -3.7683 |
| C | 2.52392 | -4.0954 | 1.12527 | H | 2.87674 | -5.0813 | 0.82328 |
| H | -0.6136 | 4.66744 | 1.28704 | H | 2.33524 | -4.064 | 2.20099 |
| H | -0.8946 | 2.64901 | 2.96464 | H | 1.60927 | -3.831 | 0.58941 |
| H | 2.21918 | 2.05437 | 0.84533 | | | | |

| Conformer 2 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.9169 | -2.2156 | -1.2298 | H | -1.2249 | 0.31534 | 0.66134 |
| C | -1.7238 | -0.986 | -1.7281 | H | 0.20267 | 1.19552 | 0.11713 |
| C | -0.4359 | -0.3371 | -1.2579 | H | -1.2486 | 2.2745 | -1.7331 |
| C | 0.34126 | -1.5658 | -0.6743 | H | -3.1798 | 3.2364 | -0.8023 |
| C | -0.7398 | -2.6367 | -0.4364 | H | -2.9192 | 1.20959 | 1.5245 |
| O | -0.6251 | -3.6478 | 0.23201 | H | -3.2719 | 2.91605 | 1.74694 |
| C | -0.7568 | 0.77229 | -0.2142 | H | -5.3529 | 1.69844 | 1.88104 |
| C | -1.6054 | 1.87974 | -0.7833 | H | -5.3804 | 2.68319 | 0.42592 |
| C | -2.7066 | 2.42268 | -0.2481 | H | -4.7849 | 0.66632 | -0.9519 |
| C | -3.3943 | 2.075 | 1.04688 | H | -4.7424 | -0.3187 | 0.50035 |
| C | -4.9042 | 1.80313 | 0.88329 | H | -7.174 | 0.18258 | 0.91324 |
| C | -5.2284 | 0.55881 | 0.04784 | H | -7.2173 | 1.16974 | -0.5385 |
| C | -6.7327 | 0.29161 | -0.0879 | H | -8.1334 | -1.1158 | -1.0022 |
| C | -7.0525 | -0.952 | -0.9239 | H | -6.6556 | -0.8575 | -1.9423 |
| O | 0.22315 | 0.22133 | -2.3878 | H | -6.6106 | -1.8524 | -0.4795 |
| C | 1.35668 | -1.3489 | 0.45098 | H | 0.99511 | 0.73107 | -2.0705 |
| C | 2.34403 | -2.4831 | 0.55777 | H | 1.87695 | -0.4075 | 0.28068 |
| C | 3.66137 | -2.3564 | 0.35331 | H | 1.90626 | -3.4536 | 0.77715 |
| C | 4.37651 | -1.0635 | 0.02966 | H | 4.27358 | -3.2561 | 0.40985 |
| O | 0.63448 | -1.2178 | 1.7165 | H | 3.95481 | -0.2631 | 0.64959 |
| C | 4.29255 | -0.6638 | -1.4629 | H | 5.43188 | -1.1433 | 0.31851 |
| C | 4.66352 | 0.81273 | -1.7072 | H | 3.27527 | -0.8242 | -1.8356 |
| C | 3.66138 | 1.72174 | -1.0242 | H | 4.949 | -1.3042 | -2.0636 |
| C | 1.11288 | -0.3276 | 2.6101 | H | 4.62934 | 1.02671 | -2.7823 |
| O | 2.05802 | 0.41117 | 2.4109 | H | 5.66993 | 1.04013 | -1.3448 |
| C | 0.30642 | -0.3692 | 3.88695 | H | -0.7478 | -0.1626 | 3.67551 |
| O | 4.22895 | 2.52489 | -0.1192 | H | 0.35871 | -1.3704 | 4.32681 |
| O | 2.45799 | 1.70991 | -1.241 | H | 0.69666 | 0.36769 | 4.58975 |
| C | 3.32976 | 3.33819 | 0.66759 | H | 3.97592 | 3.98512 | 1.26068 |
| H | -2.7849 | -2.8513 | -1.367 | H | 2.68073 | 3.92794 | 0.01676 |
| H | -2.4063 | -0.4398 | -2.3714 | H | 2.7284 | 2.69466 | 1.31401 |
| H | 0.91551 | -1.9365 | -1.5343 | | | | |

| Conformer 3 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.1017 | 3.84985 | -1.183 | H | 1.34847 | 1.1338 | -0.0234 |
| C | 0.32611 | 2.83743 | -1.9486 | H | 0.53394 | -0.3244 | -0.5851 |
| C | -0.1955 | 1.48082 | -1.516 | H | 1.70738 | -0.0716 | -2.8516 |
| C | -1.3167 | 1.86919 | -0.491 | H | 4.01365 | 0.30141 | -2.6111 |
| C | -1.0578 | 3.35762 | -0.1685 | H | 4.62628 | 2.07686 | -0.9255 |
| O | -1.5805 | 4.00713 | 0.71902 | H | 3.41259 | 1.47259 | 0.19241 |
| C | 0.96368 | 0.63296 | -0.9149 | H | 5.8539 | -0.1005 | -0.7979 |
| C | 2.05707 | 0.3562 | -1.9136 | H | 5.76315 | 0.75284 | 0.736 |
| C | 3.37019 | 0.58051 | -1.7737 | H | 3.84285 | -0.7056 | 1.43986 |
| C | 4.1085 | 1.16323 | -0.5965 | H | 3.95885 | -1.5945 | -0.0694 |
| C | 5.16095 | 0.20246 | -0.001 | H | 6.17566 | -1.421 | 2.05055 |
| C | 4.55306 | -1.0375 | 0.66813 | H | 5.03704 | -2.7471 | 1.88817 |
| C | 5.57906 | -1.9818 | 1.31635 | H | 7.18705 | -3.3773 | 0.83834 |
| C | 6.51751 | -2.6787 | 0.32341 | H | 5.94866 | -3.2503 | -0.4208 |
| O | -0.7307 | 0.84149 | -2.6686 | H | 7.14548 | -1.9629 | -0.219 |
| C | -1.5865 | 0.9683 | 0.72101 | H | -1.0777 | -0.0298 | -2.3911 |
| C | -2.9484 | 1.22977 | 1.3148 | H | -1.4843 | -0.0775 | 0.43295 |
| C | -3.8775 | 0.31024 | 1.60645 | H | -3.1616 | 2.28055 | 1.49401 |
| C | -3.7965 | -1.1916 | 1.49309 | H | -4.8283 | 0.68262 | 1.99317 |
| O | -0.5572 | 1.24981 | 1.72342 | H | -2.7559 | -1.5244 | 1.4229 |
| C | -4.6351 | -1.7803 | 0.33635 | H | -4.1811 | -1.6154 | 2.43098 |
| C | -4.0289 | -1.5426 | -1.0597 | H | -5.6423 | -1.3447 | 0.35119 |
| C | -2.6937 | -2.2281 | -1.2668 | H | -4.7537 | -2.858 | 0.48887 |
| C | -0.1422 | 0.2199 | 2.49268 | H | -3.8844 | -0.4766 | -1.2548 |
| O | -0.5152 | -0.9286 | 2.36598 | H | -4.7159 | -1.9283 | -1.8245 |
| C | 0.85964 | 0.69514 | 3.51953 | H | 1.73201 | 1.13201 | 3.02188 |
| O | -2.7362 | -3.527 | -0.9384 | H | 0.41477 | 1.47861 | 4.14128 |
| O | -1.6783 | -1.6963 | -1.689 | H | 1.17064 | -0.1453 | 4.14103 |
| C | -1.5015 | -4.2577 | -1.0785 | H | -1.7333 | -5.2768 | -0.7698 |
| H | 0.17004 | 4.89675 | -1.264 | H | -1.1614 | -4.2351 | -2.1166 |
| H | 1.00668 | 2.91238 | -2.7907 | H | -0.7319 | -3.8243 | -0.4356 |
| H | -2.2362 | 1.86502 | -1.0921 | | | | |

| Conformer 4 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.5075 | -2.4158 | -1.5313 | H | -1.1219 | -0.1171 | 0.7086 |
| C | -1.4961 | -1.1123 | -1.8449 | H | 0.15385 | 1.0295 | 0.29237 |
| C | -0.2987 | -0.3659 | -1.2877 | H | -1.4548 | 2.18299 | -1.337 |
| C | 0.6526 | -1.5462 | -0.8924 | H | -3.544 | 2.61325 | -0.3604 |
| C | -0.2658 | -2.7798 | -0.811 | H | -2.8492 | 0.47463 | 1.75774 |
| O | 0.00164 | -3.8513 | -0.299 | H | -3.9414 | 1.83469 | 1.95888 |
| C | -0.7449 | 0.52529 | -0.0909 | H | -4.428 | -0.5828 | 0.13832 |
| C | -1.7567 | 1.56736 | -0.4913 | H | -5.1258 | -0.3432 | 1.73604 |
| C | -2.9498 | 1.80617 | 0.06932 | H | -6.2952 | 1.73391 | 0.898 |
| C | -3.5888 | 1.08812 | 1.23109 | H | -5.6533 | 1.43254 | -0.711 |
| C | -4.7822 | 0.188 | 0.83674 | H | -6.8373 | -0.7836 | -0.77 |
| C | -5.9703 | 0.93372 | 0.21533 | H | -7.4869 | -0.4782 | 0.83249 |
| C | -7.1631 | 0.01902 | -0.093 | H | -9.1836 | 0.08185 | -0.9238 |
| C | -8.3495 | 0.7618 | -0.7159 | H | -8.72 | 1.54863 | -0.0472 |
| O | 0.25166 | 0.43647 | -2.3248 | H | -8.0657 | 1.23962 | -1.6618 |
| C | 1.65432 | -1.3547 | 0.24969 | H | 0.95208 | 0.99861 | -1.9378 |
| C | 2.79191 | -2.3417 | 0.1849 | H | 2.03463 | -0.3347 | 0.21852 |
| C | 4.0735 | -2.0021 | -0.0033 | H | 2.49866 | -3.3857 | 0.26038 |
| C | 4.59403 | -0.588 | -0.135 | H | 4.80598 | -2.8051 | -0.0822 |
| O | 0.951 | -1.512 | 1.52269 | H | 4.08082 | 0.04569 | 0.59839 |
| C | 4.41883 | 0.00938 | -1.5516 | H | 5.65708 | -0.5597 | 0.13471 |
| C | 4.57675 | 1.54305 | -1.5764 | H | 3.42445 | -0.2355 | -1.9399 |
| C | 3.47543 | 2.19331 | -0.7632 | H | 5.14219 | -0.4384 | -2.243 |
| C | 1.32108 | -0.7016 | 2.53578 | H | 4.48765 | 1.90449 | -2.608 |
| O | 2.14986 | 0.18356 | 2.44458 | H | 5.55056 | 1.8537 | -1.1877 |
| C | 0.556 | -1.039 | 3.79405 | H | 0.74496 | -2.0796 | 4.07673 |
| O | 3.94812 | 2.92644 | 0.24931 | H | 0.86424 | -0.3712 | 4.5992 |
| O | 2.28033 | 2.04543 | -0.9759 | H | -0.5205 | -0.941 | 3.6193 |
| C | 2.96437 | 3.48186 | 1.15084 | H | 3.52917 | 4.11842 | 1.83173 |
| H | -2.2823 | -3.14 | -1.7588 | H | 2.22531 | 4.06451 | 0.59682 |
| H | -2.2609 | -0.5781 | -2.3996 | H | 2.47263 | 2.67283 | 1.69606 |
| H | 1.25228 | -1.7052 | -1.799 | | | | |

| Conformer 5 | | | | | | | |
|-------------|--------------------------|---------|---------|--------|--------------------------|---------|---------|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -0.0578 | 3.69214 | -1.3962 | H | 1.25863 | 0.98878 | -0.0556 |
| C | 0.3247 | 2.61364 | -2.0925 | H | 0.37855 | -0.4612 | -0.5301 |
| C | -0.2623 | 1.31356 | -1.5778 | H | 1.56784 | -0.3885 | -2.8097 |
| C | -1.3675 | 1.81919 | -0.587 | H | 3.88777 | -0.1421 | -2.5622 |
| C | -1.0406 | 3.31171 | -0.3595 | H | 4.73974 | 1.52688 | -0.9458 |
| O | -1.5364 | 4.04094 | 0.48027 | H | 3.31731 | 1.36587 | 0.07091 |
| C | 0.85359 | 0.45236 | -0.9172 | H | 5.16969 | 0.2795 | 1.16347 |
| C | 1.93595 | 0.06301 | -1.89 | H | 4.01116 | -0.9604 | 0.69298 |
| C | 3.25945 | 0.21318 | -1.7449 | H | 5.41556 | -1.5289 | -1.3029 |
| C | 4.00207 | 0.80091 | -0.5717 | H | 6.57662 | -0.2878 | -0.852 |
| C | 4.74336 | -0.2427 | 0.29669 | H | 5.87284 | -2.7486 | 0.84408 |
| C | 5.85159 | -1.0072 | -0.441 | H | 7.25841 | -2.6264 | -0.2263 |
| C | 6.59836 | -2.0369 | 0.42443 | H | 7.98331 | -2.2114 | 2.1008 |
| C | 7.43491 | -1.4324 | 1.55867 | H | 8.17127 | -0.7187 | 1.16779 |
| O | -0.8235 | 0.6278 | -2.6907 | H | 6.81435 | -0.9011 | 2.28888 |
| C | -1.6824 | 1.01222 | 0.67914 | H | -1.2098 | -0.2079 | -2.3606 |
| C | -3.0336 | 1.37204 | 1.24543 | H | -1.6259 | -0.0537 | 0.46054 |
| C | -4.0034 | 0.51543 | 1.59104 | H | -3.2006 | 2.44069 | 1.35394 |
| C | -3.9884 | -0.9928 | 1.57697 | H | -4.9382 | 0.95382 | 1.94633 |
| O | -0.6462 | 1.31262 | 1.66887 | H | -2.9633 | -1.3748 | 1.53569 |
| C | -4.8478 | -1.6189 | 0.45557 | H | -4.3951 | -1.3366 | 2.53796 |
| C | -4.226 | -1.5007 | -0.9488 | H | -5.8346 | -1.1394 | 0.43477 |
| C | -2.921 | -2.2554 | -1.1012 | H | -5.0147 | -2.678 | 0.67779 |
| C | -0.2776 | 0.3164 | 2.5034 | H | -4.0344 | -0.4573 | -1.2131 |
| O | -0.6938 | -0.8227 | 2.44265 | H | -4.9261 | -1.9062 | -1.6913 |
| C | 0.728 | 0.81663 | 3.51447 | H | 1.59164 | 1.25815 | 3.00688 |
| O | -3.0203 | -3.5258 | -0.6852 | H | 0.27574 | 1.60283 | 4.12804 |
| O | -1.8827 | -1.7974 | -1.5528 | H | 1.04971 | -0.0104 | 4.14836 |
| C | -1.8177 | -4.3164 | -0.7681 | H | -2.0944 | -5.3016 | -0.3932 |
| H | 0.26361 | 4.71771 | -1.5422 | H | -1.4731 | -4.3782 | -1.803 |
| H | 1.01172 | 2.60234 | -2.9326 | H | -1.0326 | -3.8741 | -0.1504 |
| H | -2.2844 | 1.81855 | -1.1922 | | | | |

Table S12. Experimental and calculated ^1H NMR data for compound **2**.

| No. | 2 , exptl. δ_{H} ^a | 7 <i>S</i> ,8 <i>R</i> ,12 <i>R</i> - 2 , calcd. δ_{H} ^b | 7 <i>S</i> ,8 <i>R</i> ,12 <i>S</i> - 2 , calcd. δ_{H} ^b |
|-------|--|--|--|
| 2 | 2.34 | 2.48 | 2.38 |
| 3 | 1.72 | 1.88 | 1.89 |
| 4 | 2.22 | 2.40 | 2.46 |
| 5 | 5.57 | 6.10 | 6.02 |
| 6 | 5.85 | 6.55 | 7.01 |
| 7 | 5.94 | 5.81 | 5.90 |
| 8 | 2.55 | 2.41 | 2.71 |
| 10 | 6.17 | 6.40 | 6.36 |
| 11 | 7.43 | 7.94 | 8.09 |
| 13 | 2.56 | 3.11 | 2.58 |
| | 2.34 | 2.40 | 2.48 |
| 14 | 5.36 | 5.70 | 6.42 |
| 15 | 5.65 | 6.01 | 6.07 |
| 16 | 2 | 2.25 | 2.05 |
| 17 | 1.35 | 1.41 | 1.31 |
| 18 | 1.27 | 1.29 | 1.28 |
| 19 | 1.3 | 1.38 | 1.40 |
| 20 | 0.89 | 1.02 | 1.02 |
| 1-OMe | 3.68 | 4.04 | 3.94 |
| 2' | 1.99 | 2.06 | 2.02 |



















^a Recorded in CDCl_3 at 600 MHz.^b Calculated in CDCl_3

Table S13. Experimental and calculated ^{13}C NMR data for compound **2**.

| No. | 2 , exptl. δ_{C} ^a | 7 <i>S</i> ,8 <i>R</i> ,12 <i>R</i> - 2 , calcd. δ_{C} ^b | 7 <i>S</i> ,8 <i>R</i> ,12 <i>S</i> - 2 , calcd. δ_{C} ^b |
|-------|--|--|--|
| 1 | 174 | 178.7 | 180.1 |
| 2 | 33.4 | 30.5 | 31.3 |
| 3 | 24.5 | 23.1 | 23.1 |
| 4 | 27 | 24.4 | 23.9 |
| 5 | 133.3 | 136.5 | 134.6 |
| 6 | 129.6 | 130.8 | 131.3 |
| 7 | 68.3 | 65.0 | 63.7 |
| 8 | 57.2 | 52.5 | 61.9 |
| 9 | 204.8 | 206.9 | 204.0 |
| 10 | 133.7 | 134.1 | 132.6 |
| 11 | 165.4 | 171.6 | 172.8 |
| 12 | 79.5 | 79.0 | 79.9 |
| 13 | 39.3 | 36.5 | 33.4 |
| 14 | 121.8 | 125.3 | 126.8 |
| 15 | 135.7 | 136.7 | 133.7 |
| 16 | 27.4 | 26.3 | 27.1 |
| 17 | 29.1 | 28.0 | 28.6 |
| 18 | 31.5 | 29.6 | 30.4 |
| 19 | 22.5 | 21.8 | 21.9 |
| 20 | 14 | 10.4 | 10.4 |
| 1-OMe | 51.6 | 48.9 | 49.8 |
| 1' | 170.3 | 170.2 | 171.9 |
| 2' | 21.2 | 17.0 | 18.0 |

^a Recorded in CDCl_3 at 600 MHz.^b Calculated in CDCl_3

Table S14. DP4+ analyses of calculated and experimental NMR chemical shifts of **2** (unscaled). Isomer 1: 7*S*,8*R*,12*R*-**2**; Isomer 2: 7*S*,8*R*,12*S*-**2**

| Functional | Solvent? | | Basis Set | | Type of Data | |
|------------------|---|--|--------------|----------|-----------------|----------|
| mPW1PW91 | PCM | | 6-311+G(d,p) | | Unscaled Shifts | |
| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
| sDP4+ (H data) |  83.83% |  16.17% | - | - | - | - |
| sDP4+ (C data) |  100.00% |  0.00% | - | - | - | - |
| sDP4+ (all data) |  100.00% |  0.00% | - | - | - | - |
| uDP4+ (H data) |  99.02% |  0.98% | - | - | - | - |
| uDP4+ (C data) |  3.91% |  96.09% | - | - | - | - |
| uDP4+ (all data) |  80.49% |  19.51% | - | - | - | - |
| DP4+ (H data) |  99.81% |  0.19% | - | - | - | - |
| DP4+ (C data) |  100.00% |  0.00% | - | - | - | - |
| DP4+ (all data) |  100.00% |  0.00% | - | - | - | - |

| Functional mPW1PW91 | | Solvent? PCM | | Basis Set 6-311+G(d,p) | | Type of Data Unscaled Shifts | |
|------------------------|------|-----------------|------------|---------------------------|----------|---------------------------------|----------|
| | | DP4+ | 100.00% | 0.00% | - | - | - |
| Nuclei | sp2? | Experimenta | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 |
| C | x | 174.0 | 178.7 | 180.1 | | | |
| C | | 33.4 | 30.5 | 31.3 | | | |
| C | | 24.5 | 23.1 | 23.1 | | | |
| C | | 27.0 | 24.4 | 23.9 | | | |
| C | x | 133.3 | 136.5 | 134.6 | | | |
| C | x | 129.6 | 130.8 | 131.3 | | | |
| C | | 68.3 | 65.0 | 63.7 | | | |
| C | | 57.2 | 52.5 | 61.9 | | | |
| C | x | 204.8 | 206.9 | 204.0 | | | |
| C | x | 133.7 | 134.1 | 132.6 | | | |
| C | x | 165.4 | 171.6 | 172.8 | | | |
| C | | 79.5 | 78.98 | 79.91 | | | |
| C | | 39.3 | 36.45 | 33.45 | | | |
| C | x | 121.8 | 125.30 | 126.77 | | | |
| C | x | 135.7 | 136.73 | 133.75 | | | |
| C | | 27.4 | 26.28 | 27.10 | | | |
| C | | 29.1 | 27.98 | 28.59 | | | |
| C | | 31.5 | 29.58 | 30.36 | | | |
| C | | 22.5 | 21.79 | 21.89 | | | |
| C | | 14.0 | 10.40 | 10.36 | | | |
| C | | 51.6 | 48.87 | 49.75 | | | |
| C | x | 170.3 | 170.22 | 171.86 | | | |
| C | | 21.2 | 17.03 | 17.99 | | | |
| H | | 2.3 | 2.48 | 2.38 | | | |
| H | | 1.7 | 1.88 | 1.89 | | | |
| H | | 2.22 | 2.3999751 | 2.45825543 | | | |
| H | x | 5.57 | 6.10101227 | 6.02000694 | | | |
| H | x | 5.85 | 6.55245404 | 7.01225953 | | | |
| H | | 5.94 | 5.81206222 | 5.89869416 | | | |
| H | | 2.55 | 2.4114666 | 2.71207999 | | | |
| H | x | 6.17 | 6.40119312 | 6.35704911 | | | |
| H | x | 7.43 | 7.94088827 | 8.0875924 | | | |
| H | | 2.56 | 3.11240124 | 2.58422038 | | | |
| H | | 2.34 | 2.40440269 | 2.48382623 | | | |
| H | x | 5.36 | 5.70232067 | 6.42483296 | | | |
| H | x | 5.65 | 6.00938708 | 6.07013901 | | | |
| H | | 2.00 | 2.2537362 | 2.05059299 | | | |
| H | | 1.35 | 1.41051741 | 1.31460266 | | | |
| H | | 1.27 | 1.29085926 | 1.27875256 | | | |
| H | | 1.30 | 1.37931264 | 1.39857795 | | | |
| H | | 0.89 | 1.01984823 | 1.02190545 | | | |
| H | | 3.68 | 4.04144572 | 3.94368397 | | | |
| H | | 1.99 | 2.05722616 | 2.02193488 | | | |

Table S15. *In silico* prediction of cytotoxicity of the compounds for human tumor cell lines.

| | Cell-line | Description | Tissue/Organ | <i>Pa</i> | <i>Pi</i> | IAP |
|----|-----------|---------------------------------------|--------------|-----------|-----------|-------|
| 1 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.814 | 0.026 | 0.838 |
| 1 | PC-3 | Prostate carcinoma | Prostate | 0.798 | 0.005 | 0.883 |
| 2 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.928 | 0.004 | 0.838 |
| 3 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.896 | 0.006 | 0.838 |
| 3 | PC-3 | Prostate carcinoma | Prostate | 0.767 | 0.007 | 0.883 |
| 4 | PC-3 | Prostate carcinoma | Prostate | 0.911 | 0.004 | 0.883 |
| 4 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.904 | 0.005 | 0.838 |
| 5 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.869 | 0.011 | 0.838 |
| 5 | PC-3 | Prostate carcinoma | Prostate | 0.858 | 0.005 | 0.883 |
| 6 | PC-3 | Prostate carcinoma | Prostate | 0.828 | 0.005 | 0.883 |
| 6 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.790 | 0.035 | 0.838 |
| 7 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.869 | 0.011 | 0.838 |
| 7 | PC-3 | Prostate carcinoma | Prostate | 0.858 | 0.005 | 0.883 |
| 8 | PC-3 | Prostate carcinoma | Prostate | 0.982 | 0.003 | 0.883 |
| 8 | HT-29 | Colon adenocarcinoma | Colon | 0.935 | 0.004 | 0.888 |
| 8 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.846 | 0.017 | 0.838 |
| 9 | PC-3 | Prostate carcinoma | Prostate | 0.854 | 0.005 | 0.883 |
| 9 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.747 | 0.051 | 0.838 |
| 10 | PC-3 | Prostate carcinoma | Prostate | 0.920 | 0.004 | 0.883 |
| 10 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.904 | 0.005 | 0.838 |
| 11 | PC-3 | Prostate carcinoma | Prostate | 0.911 | 0.004 | 0.883 |
| 11 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.904 | 0.005 | 0.838 |
| 12 | PC-3 | Prostate carcinoma | Prostate | 0.879 | 0.005 | 0.883 |
| 12 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.859 | 0.013 | 0.838 |
| 13 | PC-3 | Prostate carcinoma | Prostate | 0.879 | 0.005 | 0.883 |
| 13 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovary | 0.859 | 0.013 | 0.838 |

Pa: the probability of “to be active”.

Pi: the probability of “to be inactive”.

IAP: Invariant accuracy of prediction.

Table S16. *In silico* prediction of the nitric oxide (NO) production inhibition activity of the compounds.

| | Predictions |
|-----------------------|--------------------|
| 1 | 0.319 |
| 2 | 0.329 |
| 3 | 0.344 |
| 4 | 0.325 |
| 5 | 0.365 |
| 6 | 0.430 |
| 7 | 0.339 |
| 8 | 0.326 |
| 9 | 0.310 |
| 10 | 0.383 |
| 11 | 0.345 |
| 12 | 0.344 |
| 13 | 0.372 |
| Aminoguanidine | 0.657 |
| Apigenin | 0.621 |

Predictions: the predicted probabilities of test compounds with the IC₅₀ (inhibition for NO production) < 50 µM in macrophages.

Table S17. The *in silico* predicted water solubility of the compounds.

| | ESOL model | | Ali model | | SILICOS-IT model | |
|----|--------------|--------------------|--------------|--------------------|------------------|--------------------|
| | Log <i>S</i> | Class | Log <i>S</i> | Class | Log <i>S</i> | Class |
| 1 | -3.48 | Soluble | -4.96 | Moderately soluble | -3.79 | Soluble |
| 2 | -3.61 | Soluble | -5.13 | Moderately soluble | -3.79 | Soluble |
| 3 | -4.81 | Moderately soluble | -5.82 | Moderately soluble | -4.83 | Moderately soluble |
| 4 | -3.99 | Soluble | -5.43 | Moderately soluble | -4.20 | Moderately soluble |
| 5 | -3.39 | Soluble | -4.71 | Moderately soluble | -3.26 | Soluble |
| 6 | -- | -- | -- | -- | -- | -- |
| 7 | -3.39 | Soluble | -4.71 | Moderately soluble | -3.26 | Soluble |
| 8 | -4.70 | Moderately soluble | -5.40 | Moderately soluble | -4.64 | Moderately soluble |
| 9 | -- | -- | -- | -- | -- | -- |
| 10 | -3.50 | Soluble | -4.72 | Moderately soluble | -3.58 | Soluble |
| 11 | -4.35 | Moderately soluble | -6.00 | Moderately soluble | -4.60 | Moderately soluble |
| 12 | -- | -- | -- | -- | -- | -- |
| 13 | -- | -- | -- | -- | -- | -- |

Class: solubility class, Log *S* scale, Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 < Very < 0 < Highly.

--: the compounds were not suitable for the *in silico* tool.

Table S18. The *in silico* predicted pharmacokinetics of the compounds.

| | GI absorption | BBB permeant | P-gp substrate | Inhibitors for CYP | | | | | Log <i>K_p</i> (cm/s) |
|----|---------------|--------------|----------------|--------------------|------|-----|-----|-----|---------------------------------|
| | | | | 1A2 | 2C19 | 2C9 | 2D6 | 3A4 | |
| 1 | High | No | Yes | No | Yes | Yes | Yes | No | -7.04 |
| 2 | High | No | Yes | No | Yes | Yes | Yes | No | -6.25 |
| 3 | High | No | Yes | Yes | Yes | No | Yes | Yes | -6.55 |
| 4 | High | Yes | Yes | Yes | Yes | Yes | Yes | No | -5.56 |
| 5 | High | No | Yes | Yes | Yes | Yes | Yes | No | -6.45 |
| 6 | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| 7 | High | No | Yes | Yes | Yes | Yes | Yes | No | -6.45 |
| 8 | High | Yes | Yes | Yes | Yes | Yes | Yes | No | -6.01 |
| 9 | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| 10 | High | Yes | Yes | Yes | Yes | Yes | Yes | No | -5.71 |
| 11 | High | Yes | Yes | Yes | Yes | Yes | Yes | Yes | -5.26 |
| 12 | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| 13 | -- | -- | -- | -- | -- | -- | -- | -- | -- |

GI absorption: Gastrointestinal absorption; **BBB permeation:** blood-brain barrier permeation; **P-gp substrate:** P-glycoprotein substrate; **CYP:** Cytochrome P450; **Log *K_p*:** for skin permeation.

--: the compounds were not suitable for the *in silico* tool.

Table S19. The *in silico* evaluation of the compounds for druglikeness.

| | Lipinsk | Ghose | Veber | Egan | Muegge | Bioavailability score |
|-----------|---|---|--|-------------|--|------------------------------|
| 1 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | No ; 1 violation: Rotors > 15 | 0.55 |
| 2 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 3 | No ; 1 violation: MW > 500 | No ; 1 violation: MW > 480 | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 4 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 5 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 6 | -- | -- | -- | -- | -- | -- |
| 7 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 8 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 9 | -- | -- | -- | -- | -- | -- |
| 10 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 11 | Yes | Yes | No ; 1 violation: Rotors > 10 | Yes | Yes | 0.55 |
| 12 | -- | -- | -- | -- | -- | -- |
| 13 | -- | -- | -- | -- | -- | -- |

--: the compounds were not suitable for the *in silico* tool.

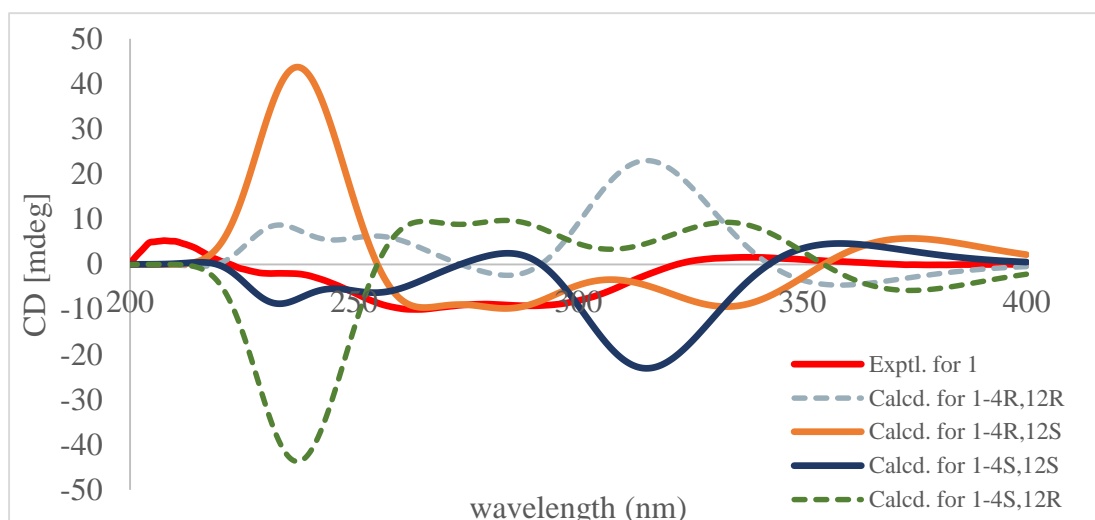
Table S20. The *in silico* evaluation of the compounds for medicinal chemistry.

| | PAINS | Brenk | Leadlikeness | Synthetic accessibility |
|-----------|--------------------------------|---|---|--------------------------------|
| 1 | 0 alert | 2 alerts: michael acceptor 1, more than 2 esters | No ; 2 violations: MW > 350, Rotors > 7 | 5.39 |
| 2 | 0 alert | 2 alerts: isolated alkene, more than 2 esters | No ; 3 violations: MW > 350, Rotors > 7, XLOGP3 > 3.5 | 5.22 |
| 3 | 1 alert: ene one hal | 3 alerts: iodine, isolated alkene, more than 2 esters | No ; 3 violations: MW > 350, Rotors > 7, XLOGP3 > 3.5 | 5.41 |
| 4 | 0 alert | 3 alerts: isolated alkene, michael acceptor 1, more than 2 esters | No ; 3 violations: MW > 350, Rotors > 7, XLOGP3 > 3.5 | 4.83 |
| 5 | 0 alert | 3 alerts: isolated alkene, michael acceptor 1, more than 2 esters | No ; 2 violations: MW > 350, Rotors > 7 | 5.20 |
| 6 | -- | -- | -- | -- |
| 7 | 0 alert | 3 alerts: isolated alkene, michael acceptor 1, more than 2 esters | No ; 2 violations: MW > 350, Rotors > 7 | 5.20 |
| 8 | 1 alert: ene one hal | 3 alerts: iodine, isolated alkene, michael acceptor 1 | No ; 3 violations: MW > 350, Rotors > 7, XLOGP3 > 3.5 | 4.78 |
| 9 | -- | -- | -- | -- |
| 10 | 0 alert | 2 alerts: isolated alkene, michael acceptor 1 | No ; 2 violations: Rotors > 7, XLOGP3 > 3.5 | 4.58 |
| 11 | 0 alert | 3 alerts: isolated alkene, michael acceptor 1, more than 2 esters | No ; 3 violations: MW > 350, Rotors > 7, XLOGP3 > 3.5 | 4.95 |
| 12 | -- | -- | -- | -- |
| 13 | -- | -- | -- | -- |

PAINS: Pan Assay Interference Structures.

Synthetic score: the synthetic accessibility score; from 1 (very easy) to 10 (very difficult).

--: the compounds were not suitable for the *in silico* tool.



Note: The ECD curves of *4R,12S* and *4S,12S* were generated by software calculation. The curves of *4R,12R* and *4S,12R* are directly transformed from their enantiomers *4R,12S* and *4S,12S*.

Figure S1. Experimental and Calculated ECD of **1**

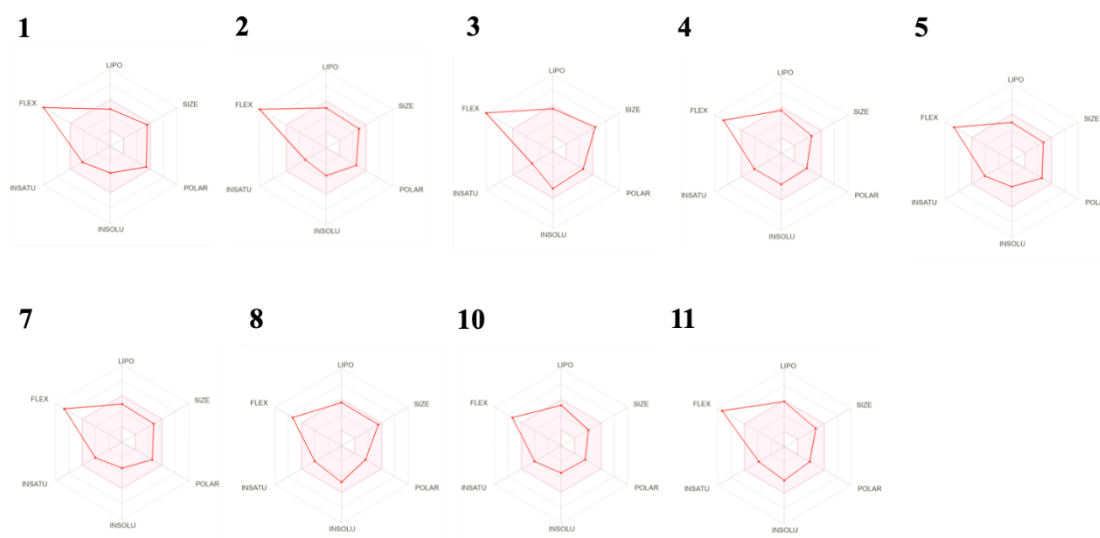


Figure S2. The predicted oral bioavailability of nine compounds.

The colored zone could be the suitable physicochemical space of the ideal compound predicted by the in silico tool SwissADME, and six red spots were the predicted values of the test compound. Lipophilicity (LIPO): $-0.7 < \text{XLOGP3} < +5.0$; size (SIZE): $150\text{g/mol} < \text{MW} < 500\text{ g/mol}$; polarity (POLAR): $20 \text{ \AA}^2 < \text{TPSA} < 130 \text{ \AA}^2$; insolubility (INSOLU): $-6 < \text{Log S (ESOL)} < 0$; insaturation (INSATU): $0.25 < \text{Fraction Csp3} < 1$; flexibility (FLEX): $0 < \text{Num. rotatable bonds} < 9$. Almost all of the five values of nine compounds were located in the colored zone, but only one value (size) of compound **3** was not located in the colored zone. Only one value (flexibility) of nine compounds was not located in the colored zone.

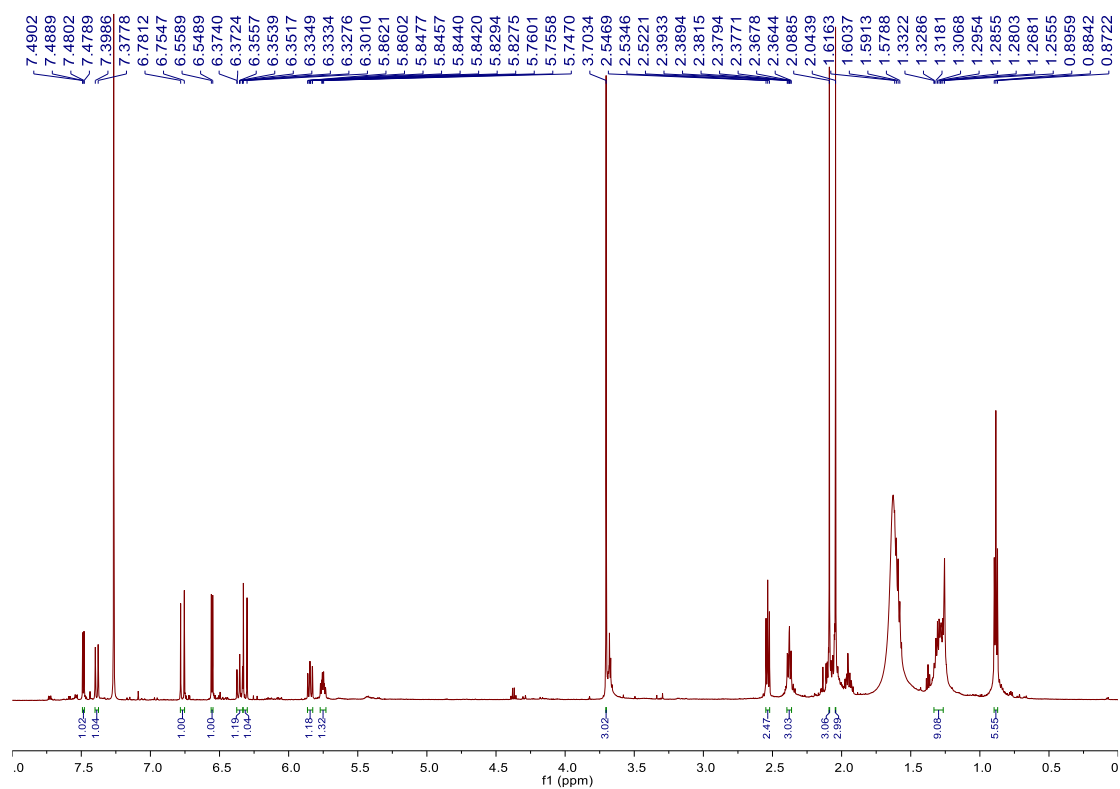


Figure S3. ¹H NMR spectrum of **1** (600 MHz, CDCl₃)

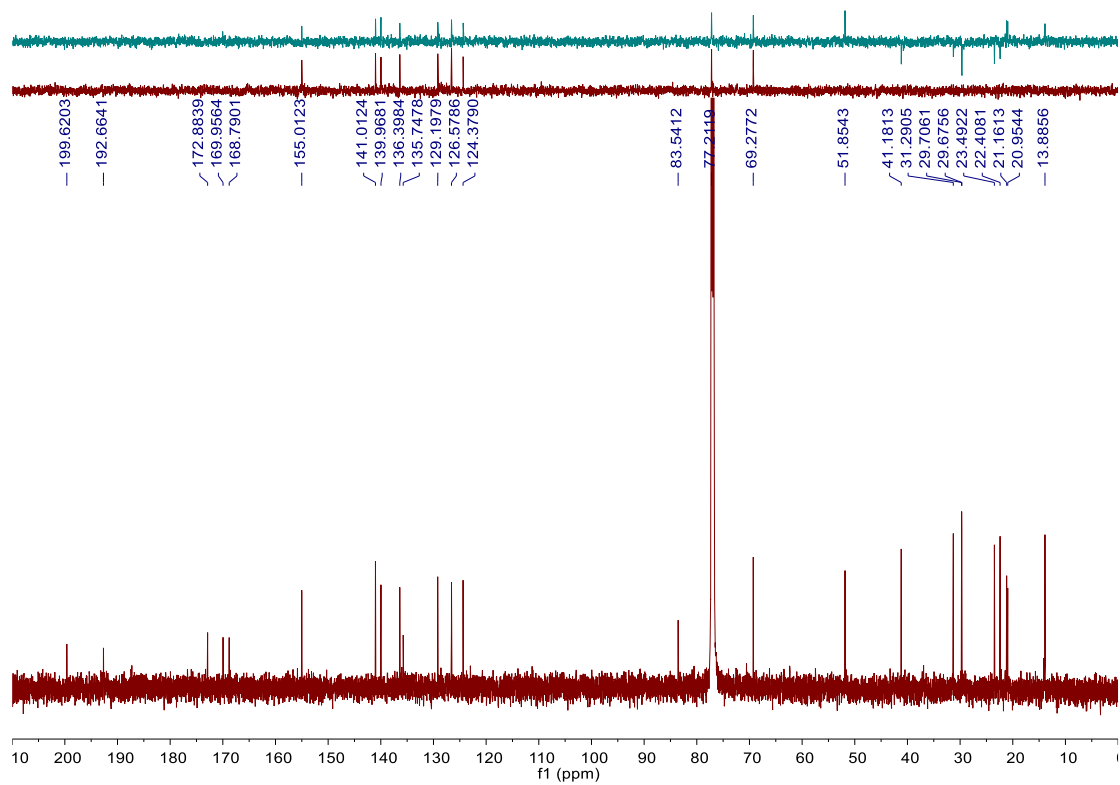


Figure S4. ¹³C NMR spectrum of **1** (125 MHz, CDCl₃)

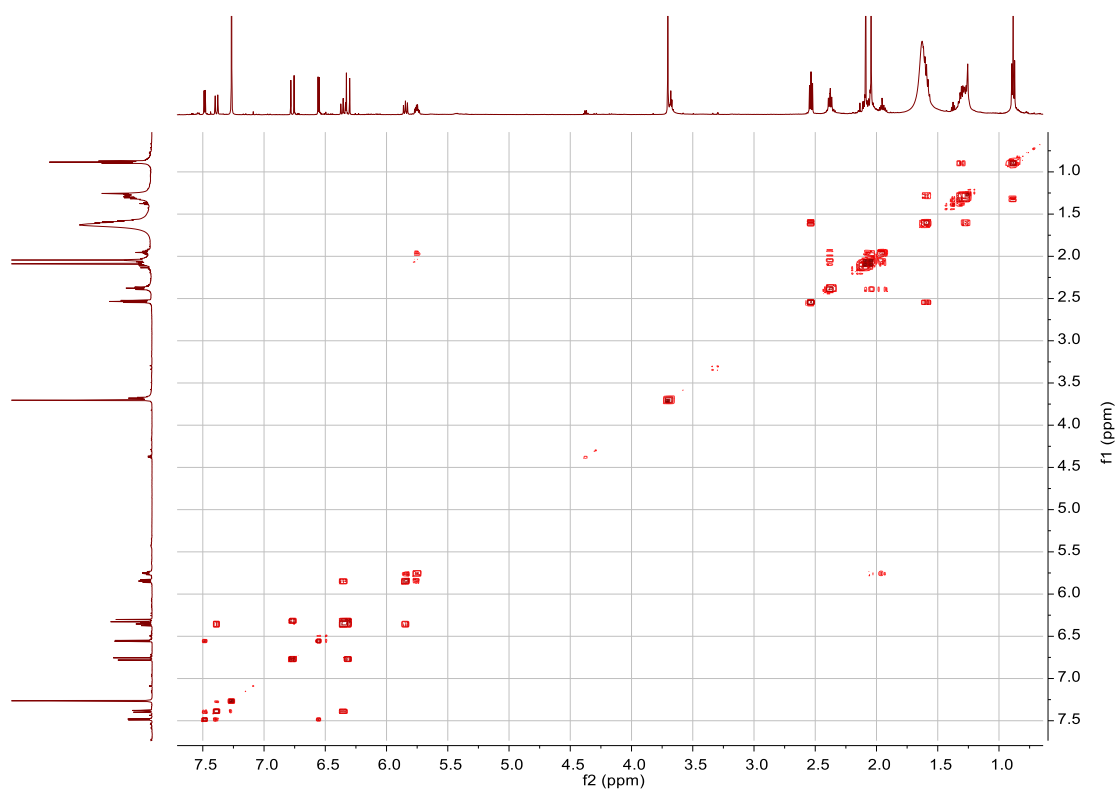


Figure S5. COSY spectrum of **1**

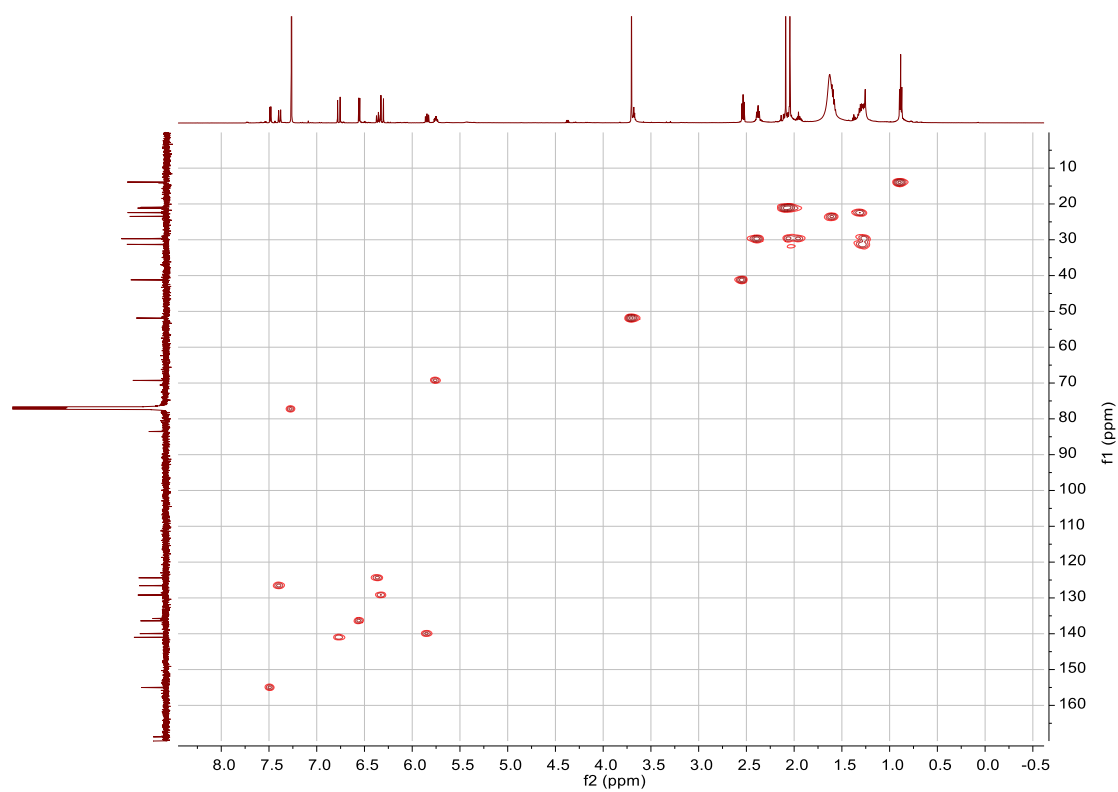


Figure S6. HSQC spectrum of **1**

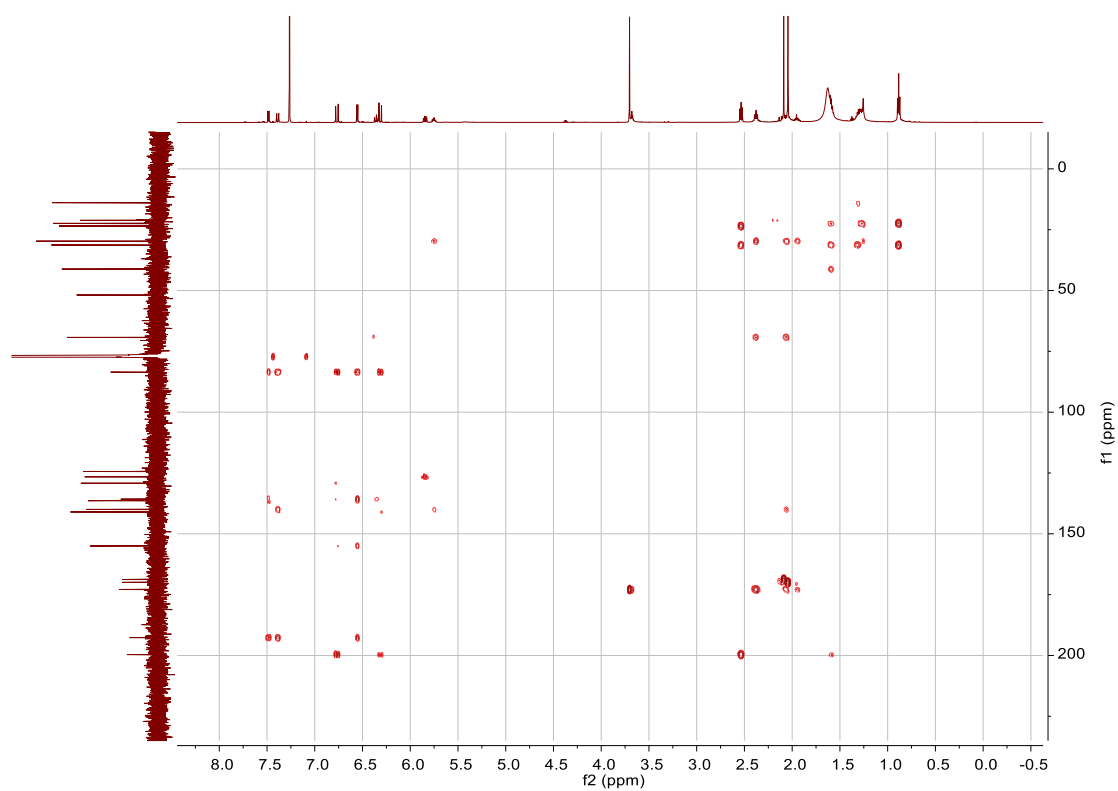


Figure S7. HMBC spectrum of **1**

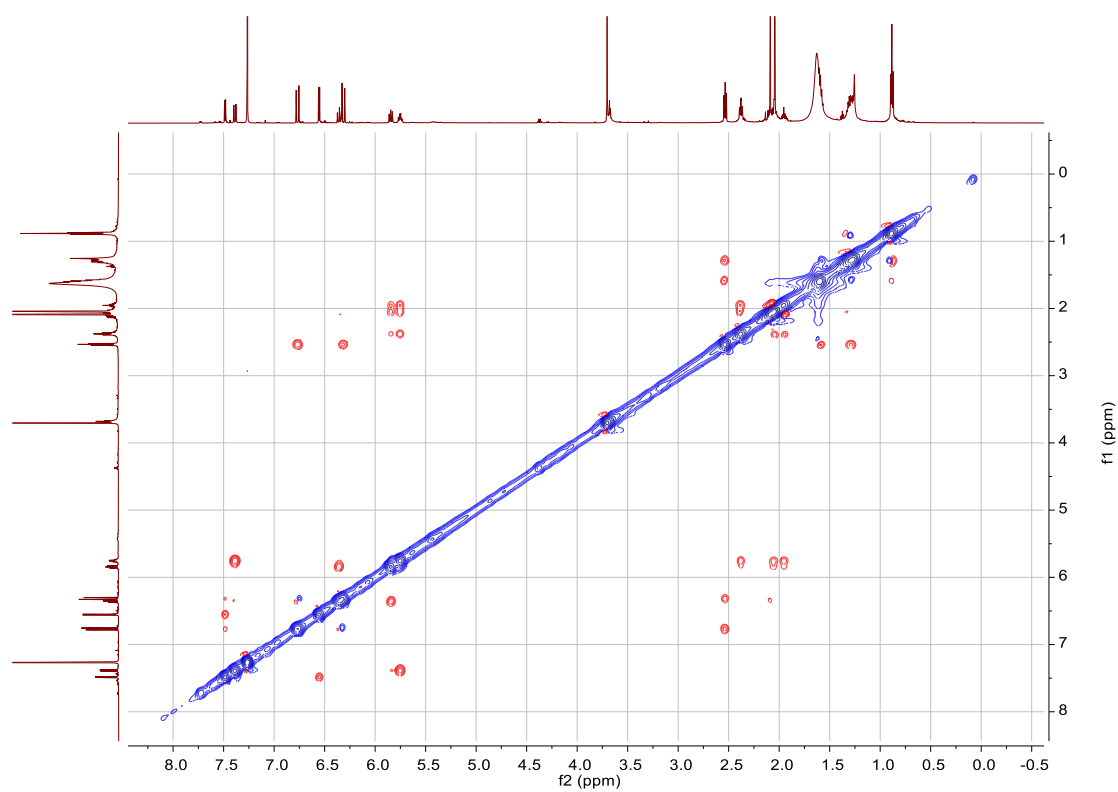


Figure S8. NOESY spectrum of **1**

CI-AU_20230609013709 #17 RT: 0.12 AV: 1 NL: 2.74E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

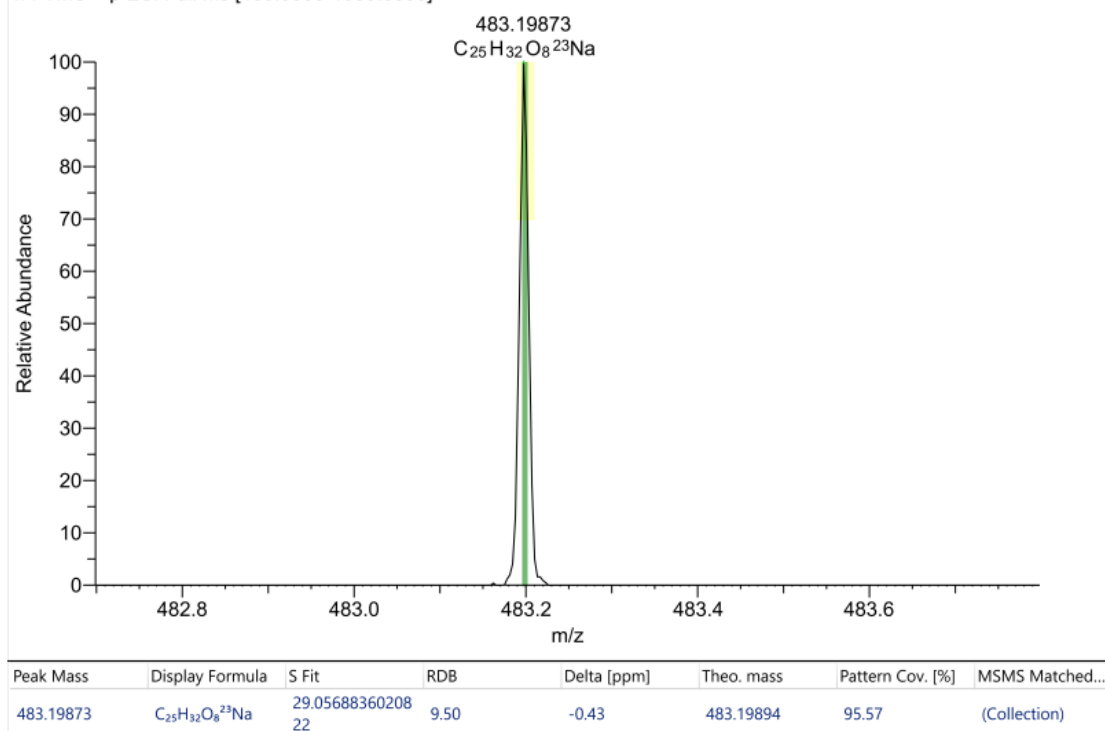


Figure S9. HRESIMS spectrum of **1**

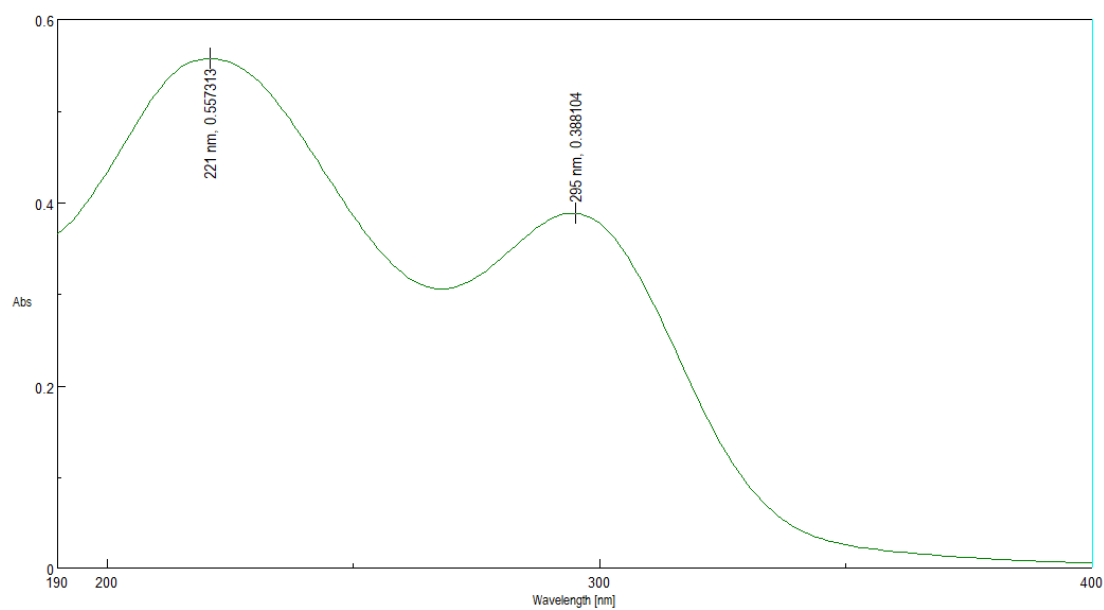


Figure S10. UV spectrum of **1**

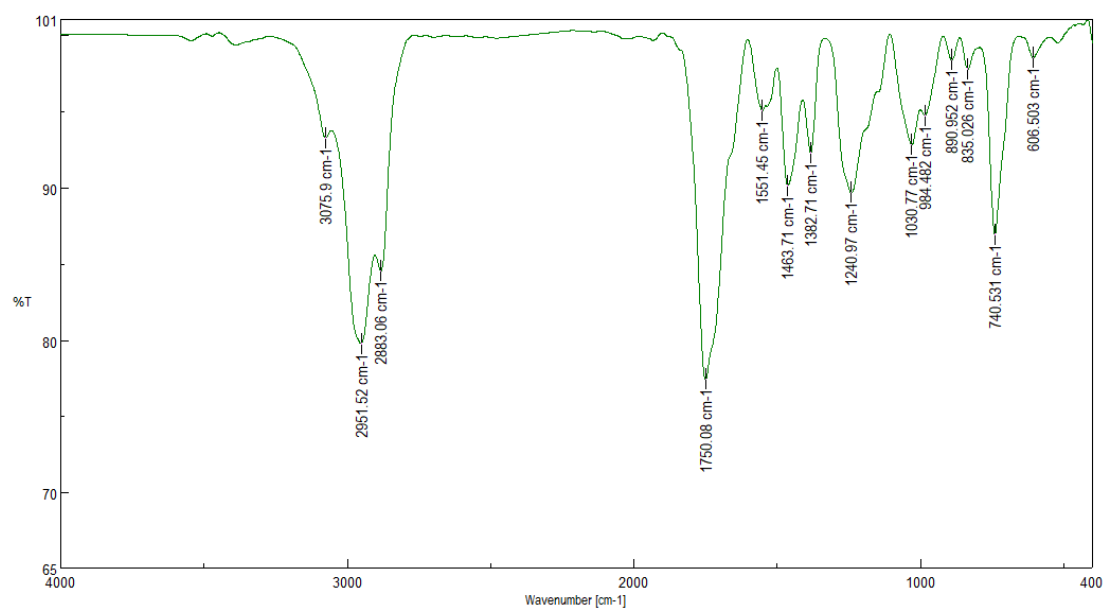


Figure S11. IR spectrum of **1**

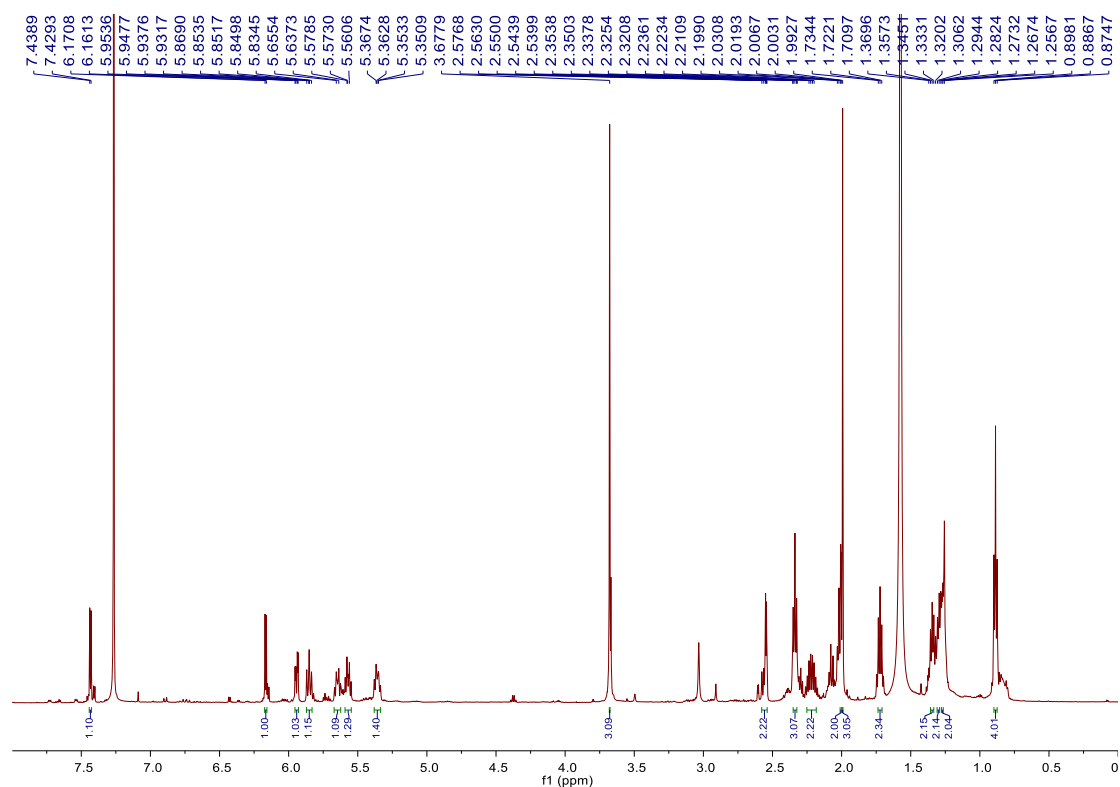


Figure S12. ¹H NMR spectrum of **2** (600 MHz, CDCl₃)

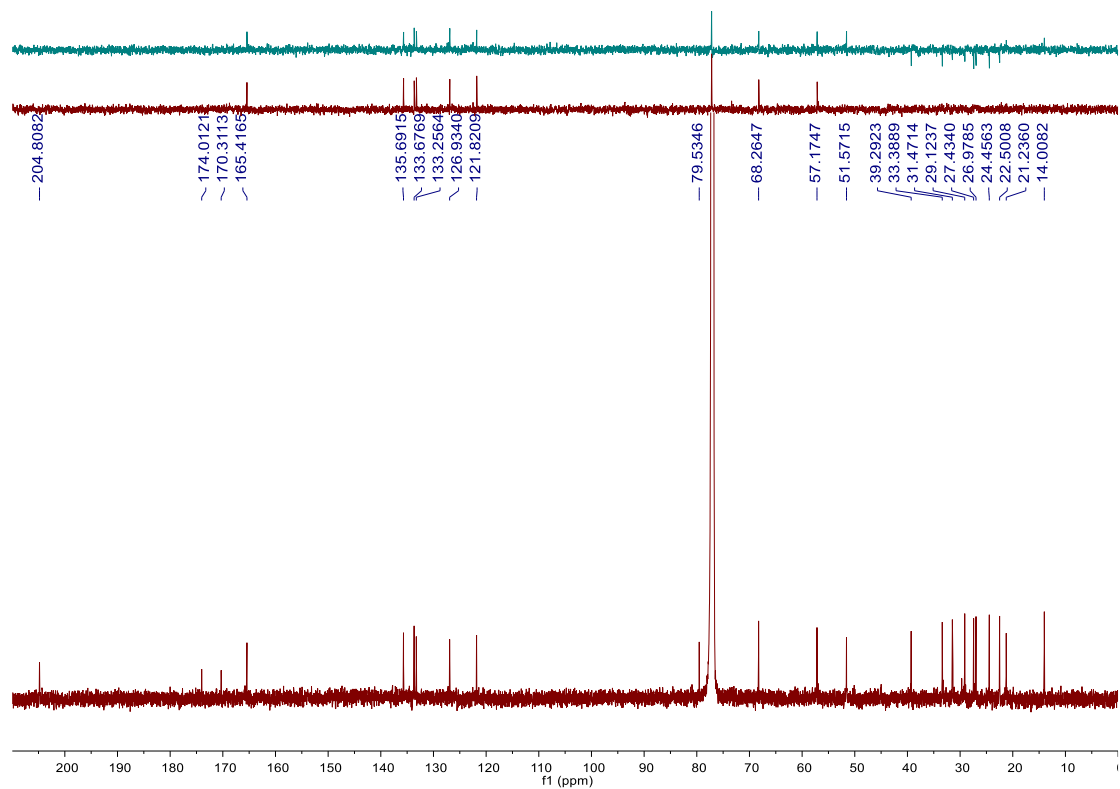


Figure S13. ¹³C NMR spectrum of **2** (125 MHz, CDCl₃)

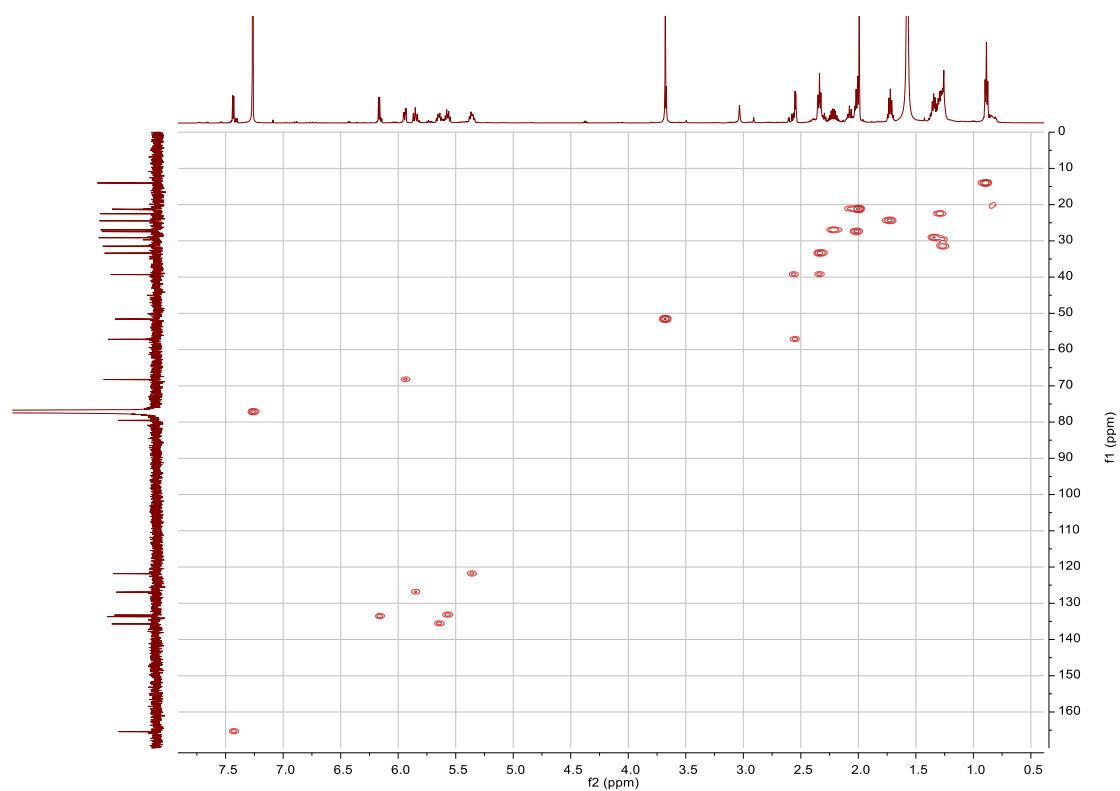


Figure S14. COSY spectrum of **2**

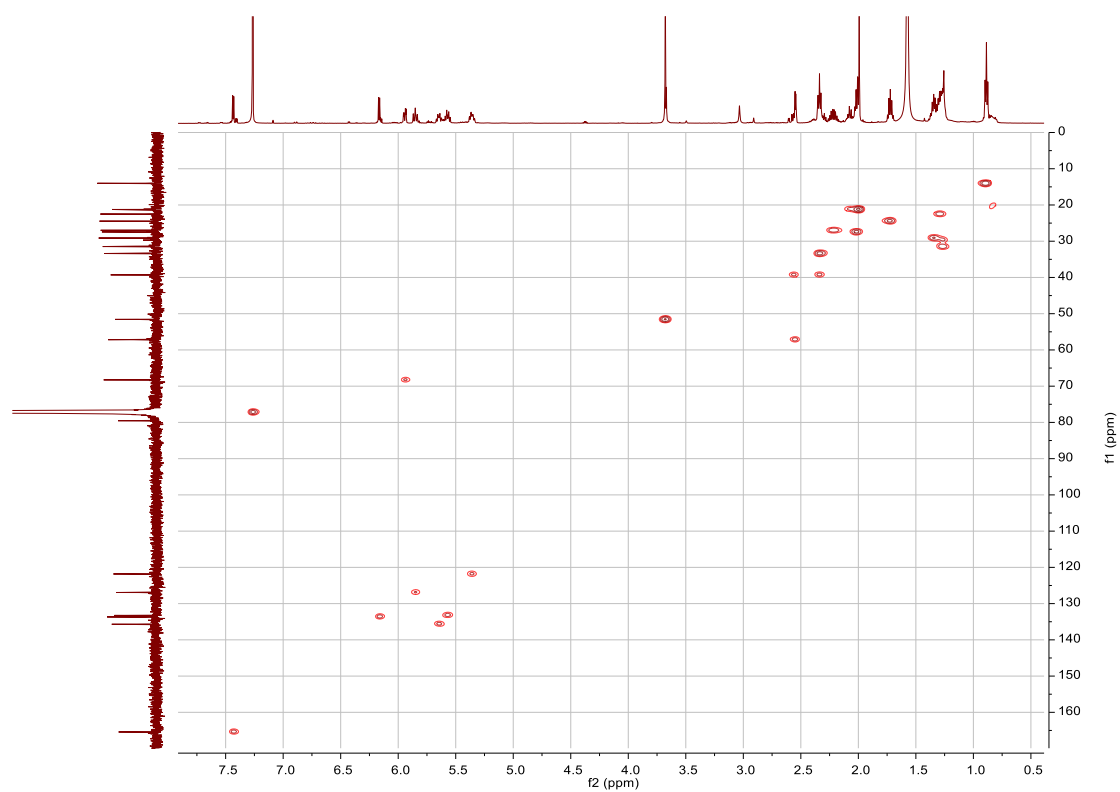


Figure S15. HSQC spectrum of **2**

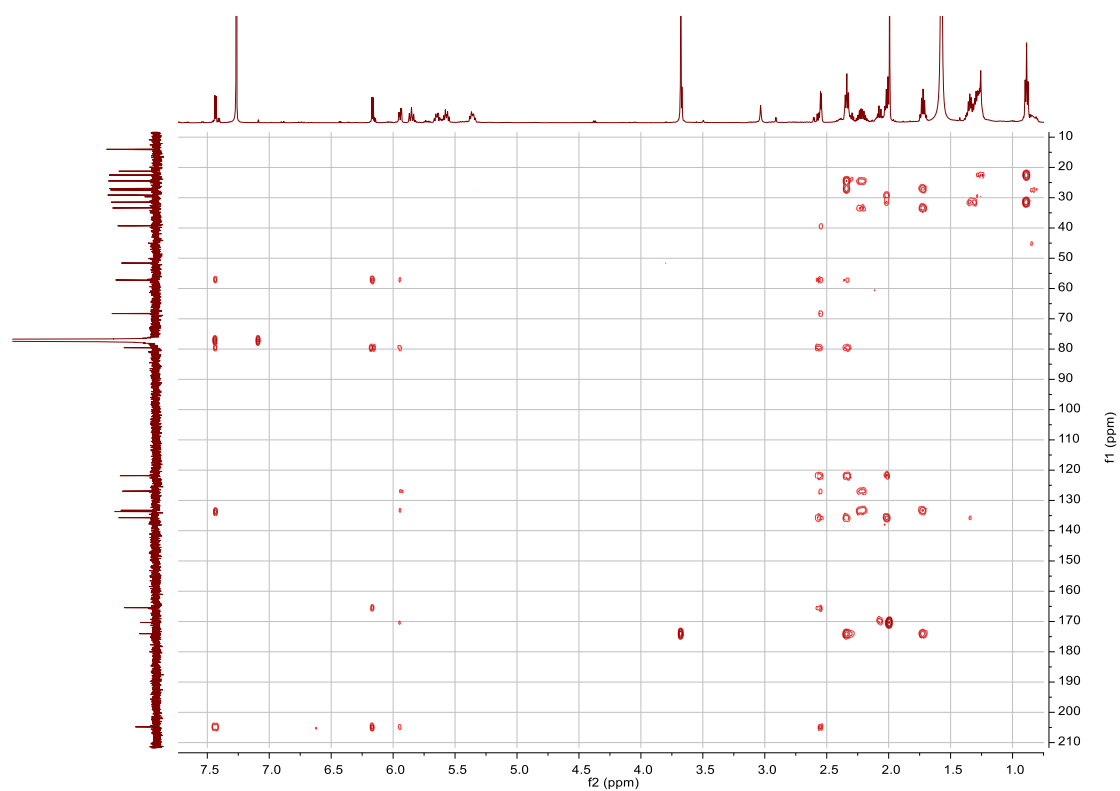


Figure S16. HMBC spectrum of **2**

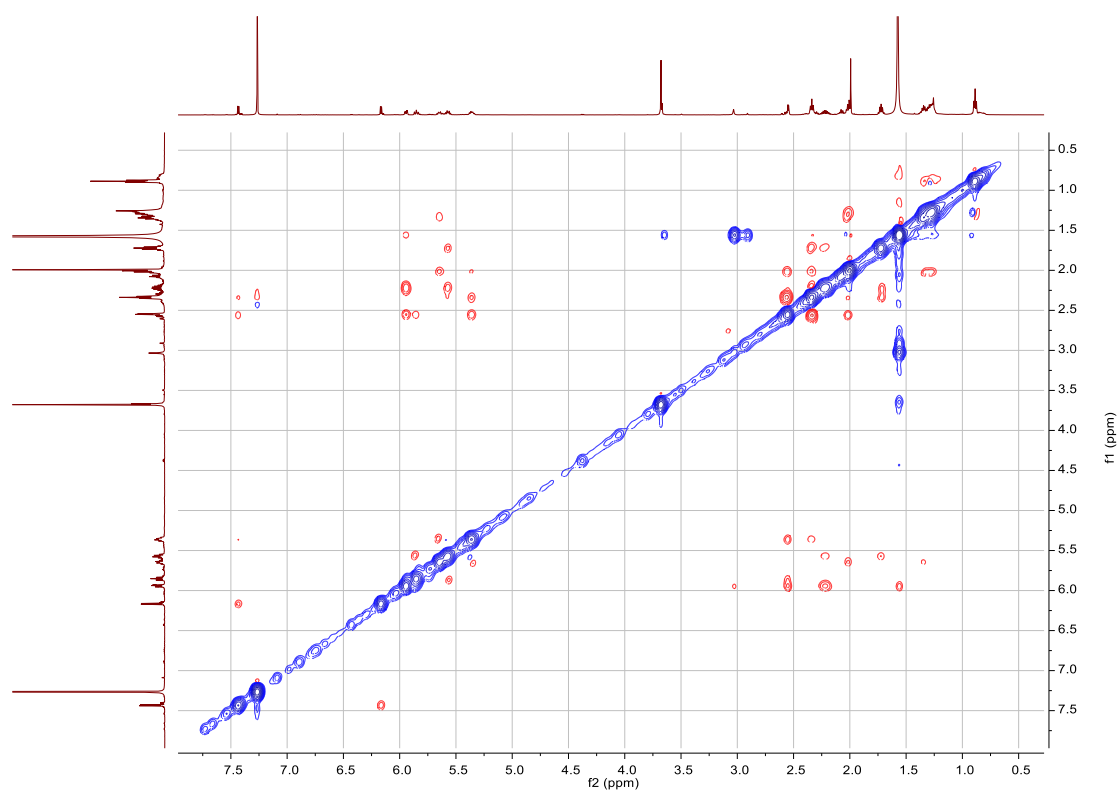


Figure S17. NOESY spectrum of **2**

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\1107\CIACR.d
Method tune_wide_pos_20220422.m
Sample Name CI-AC
Comment ESI Positive

11/8/2022 2:45:15 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER micrOTOF-Q

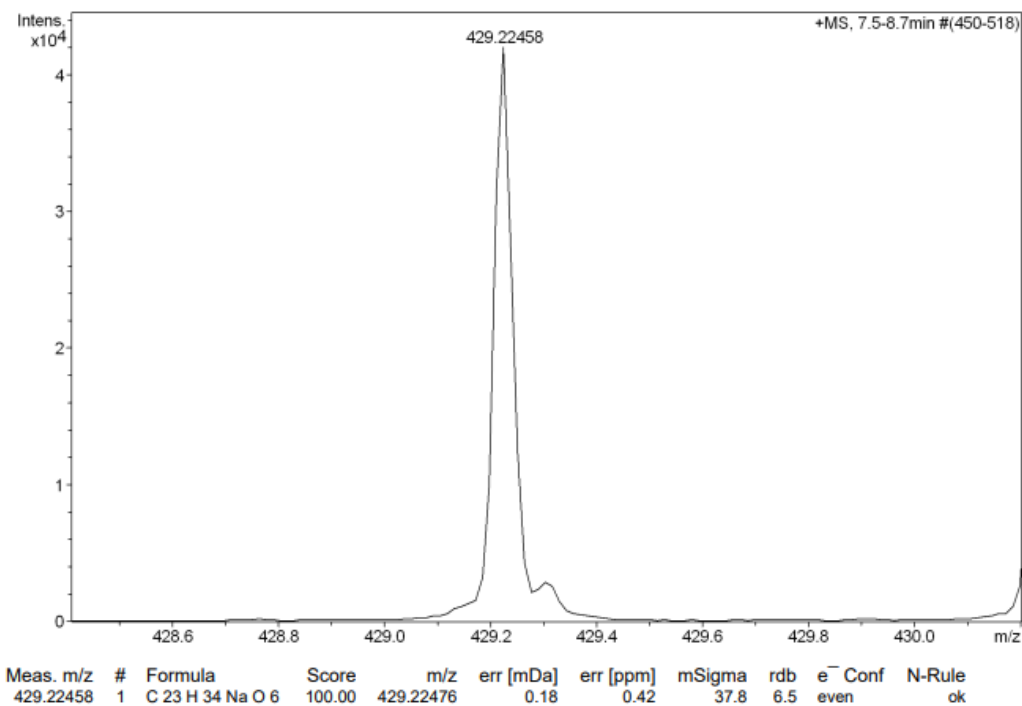


Figure S18. HRESIMS spectrum of **2**

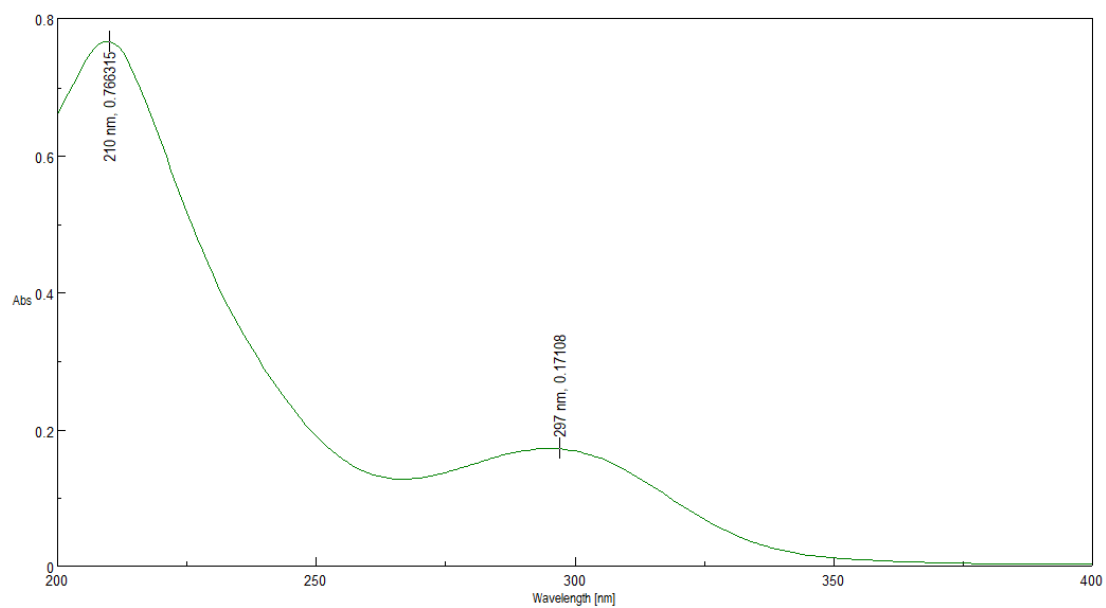


Figure S19. UV spectrum of **2**

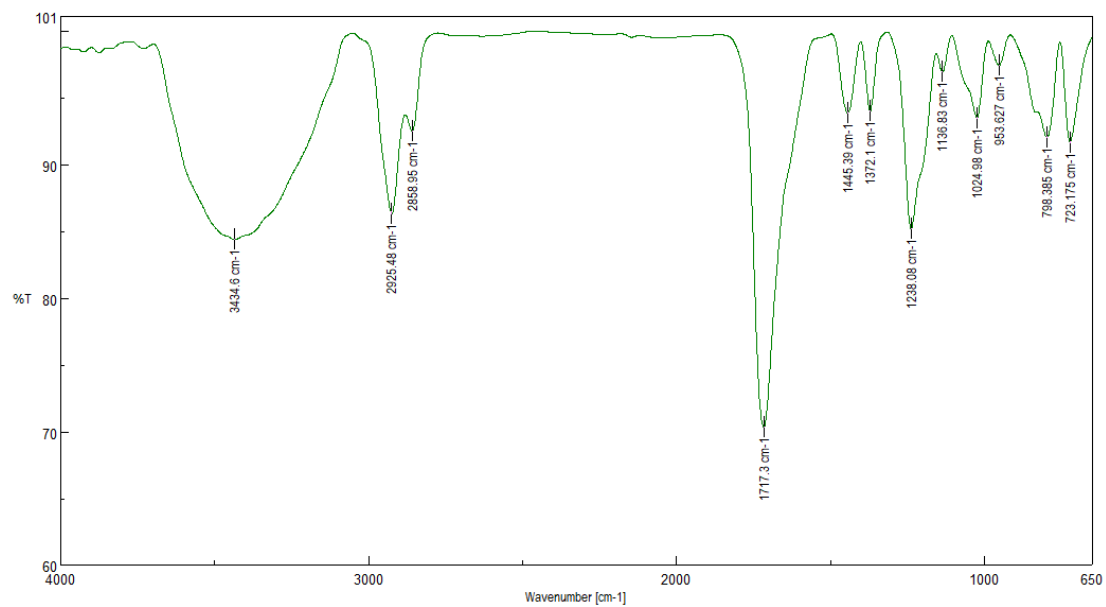


Figure S20. IR spectrum of **2**