***Supporting Information***

Four new diterpenoids from the South China Sea soft coral *Sinularia nanolobata* and DFT-based structure elucidation

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**Content**

1. **Original spectra of 13**

**Figure S1a.** 1H NMR spectrum (600 MHz) of **1** in CDCl3**3**

**Figure S1b.** DEPT135/13C NMR spectrum (150 MHz) of **1** in CDCl3**3**

**Figure S1c.** HSQC spectrum (600 MHz) of **1** in CDCl3**4**

**Figure S1d.** 1H-1H COSY spectrum of (600 MHz) **1** in CDCl3**4**

**Figure S1e.** HMBC spectrum (600 MHz) of **1** in CDCl3**5**

**Figure S1f.** NOESY spectrum (600 MHz) of **1** in CDCl3**5**

**Figure S1g.** HR-EIMS of **16**

**Figure S1h.** IR spectrum of **16**

**Figure S1i.** ECD and UV spectra of **17**

1. **Original spectra of 28**

**Figure S2a.** 1H NMR spectrum (600 MHz) of **2** in CDCl3**8**

**Figure S2b.** DEPT135/13C NMR spectrum (150 MHz) of **2** in CDCl3**8**

**Figure S2c.** HSQC spectrum (600 MHz) of **2** in CDCl3**9**

**Figure S2d.** 1H-1H COSY spectrum (600 MHz) of **2** in CDCl3**9**

**Figure S2e.** HMBC spectrum (600 MHz) of **2** in CDCl3**10**

**Figure S2f.** NOESY spectrum (600 MHz) of **2** in CDCl3**10**

**Figure S2g.** HR-EIMS of **211**

**Figure S2h.** IR spectrum of **211**

**Figure S2i.** ECD and UV spectra of **212**

1. **Original spectra of 313**

**Figure S3a.** 1H NMR spectrum (600 MHz) of **3** in CDCl3**13**

**Figure S3b.** DEPT135/13C NMR spectrum (150 MHz) of **3** in CDCl3**13**

**Figure S3c.** HSQC spectrum (600 MHz) of **3** in CDCl3**14**

**Figure S3d.** 1H-1H COSY spectrum (600 MHz) of **3** in CDCl3**14**

**Figure S3e.** HMBC spectrum (600 MHz) of **3** in CDCl3**15**

**Figure S3f.** NOESY spectrum (600 MHz) of **3** in CDCl3**15**

**Figure S3g.** HR-EIMS of **316**

**Figure S3h.** IR spectrum of **316**

**Figure S3i.** ECD and UV spectra of **317**

1. **Original spectra of 418**

**Figure S4a.** 1H NMR spectrum (600 MHz) of **4** in CDCl3**18**

**Figure S4b.** DEPT135/13C NMR spectrum (150 MHz) of **4** in CDCl3**18**

**Figure S4c.** HSQC spectrum (600 MHz) of **4** in CDCl3**19**

**Figure S4d.** 1H-1H COSY spectrum (600 MHz) of **4** in CDCl3**19**

**Figure S4e.** HMBC spectrum (600 MHz) of **4** in CDCl3**20**

**Figure S4f.** NOESY spectrum (600 MHz) of **4** in CDCl3**20**

**Figure S4g.** HR-EIMS of **421**

**Figure S4h.** IR spectrum of **421**

**Figure S4i.** ECD and UV spectra of **421**

1. **QM-NMR calculation and DP4+ analysis of compound 322**

**Figure S5a.** Structures of studied isomers for compound **3** **22**

**Figure S5b.** DP4+ results obtained using experimental data of **3** *versus* isomers 1 (**3a**) and 2 (**3b**)**22**

1. **TDDFT-ECD calculations of compounds 1-423**

**Figure S6a.** Experimental ECD curve of **1**, and calculated ECD spectrum of (12*S*)-**123**

**Figure S6b.** Experimental ECD curve of **2**, and calculated ECD spectrum of (11*R*,12*R*)-**223**

**Figure S6c.** Experimental ECD curve of **3**, and calculated ECD spectrum of (4*S*,10*R*,12*R*)-**324**

**Figure S6d.** Experimental ECD curve of **4**, and calculated ECD spectrum of (1*S*, 2*R*)-**424**

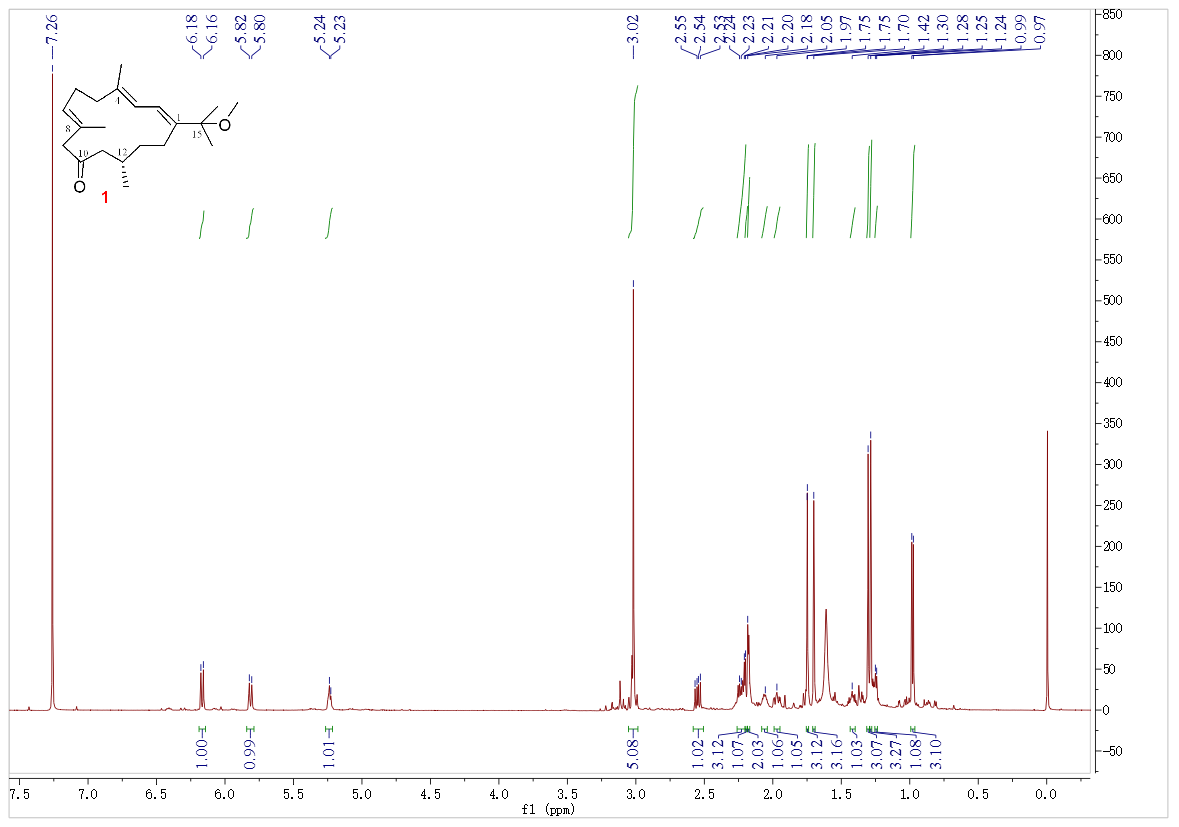
**Figure S6e.** Re-optimized conformers of (12*S*)-**1** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. **27**

**Figure S6f.** Re-optimized conformers of (11*R*, 12*R*)-**2** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. **30**

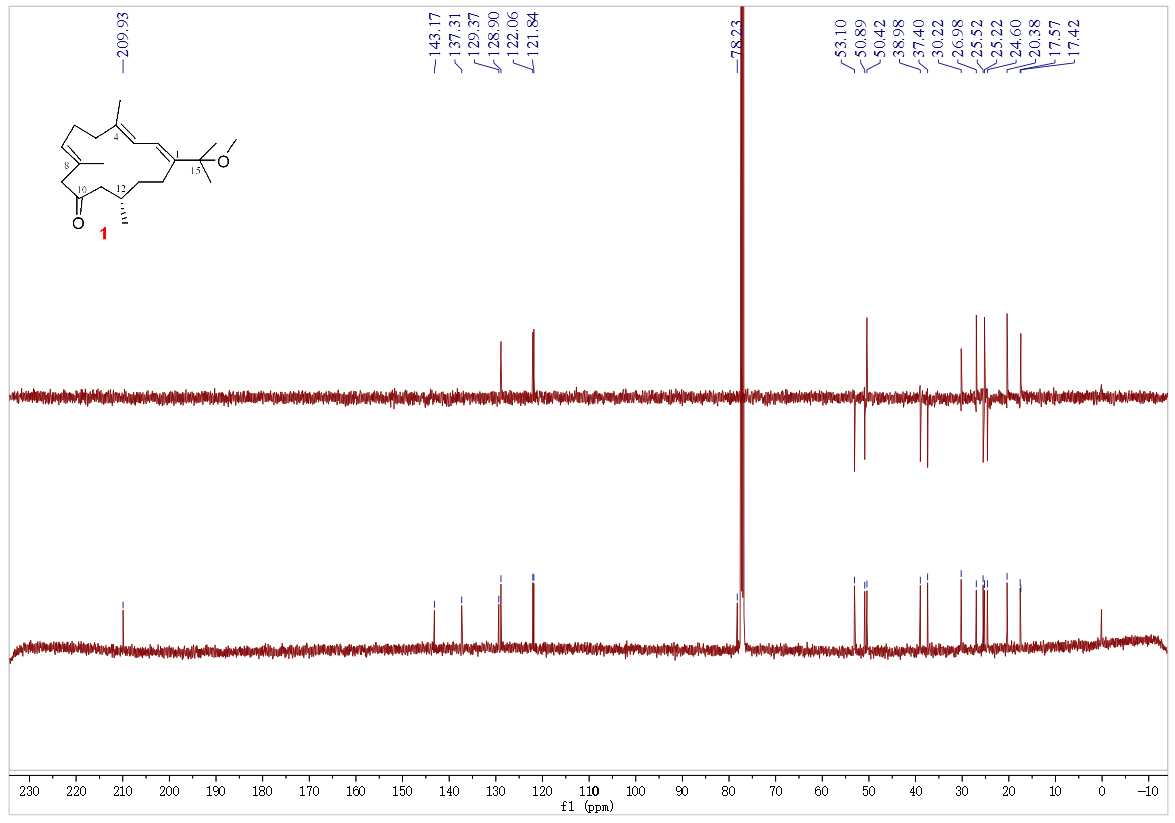
**Figure S6g.** Re-optimized conformers of (4*S*, 11*R*, 12*R*)-**3** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. **33**

**Figure S6h.** Re-optimized conformers of (1*S*, 2*R*)-**4** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. **35**

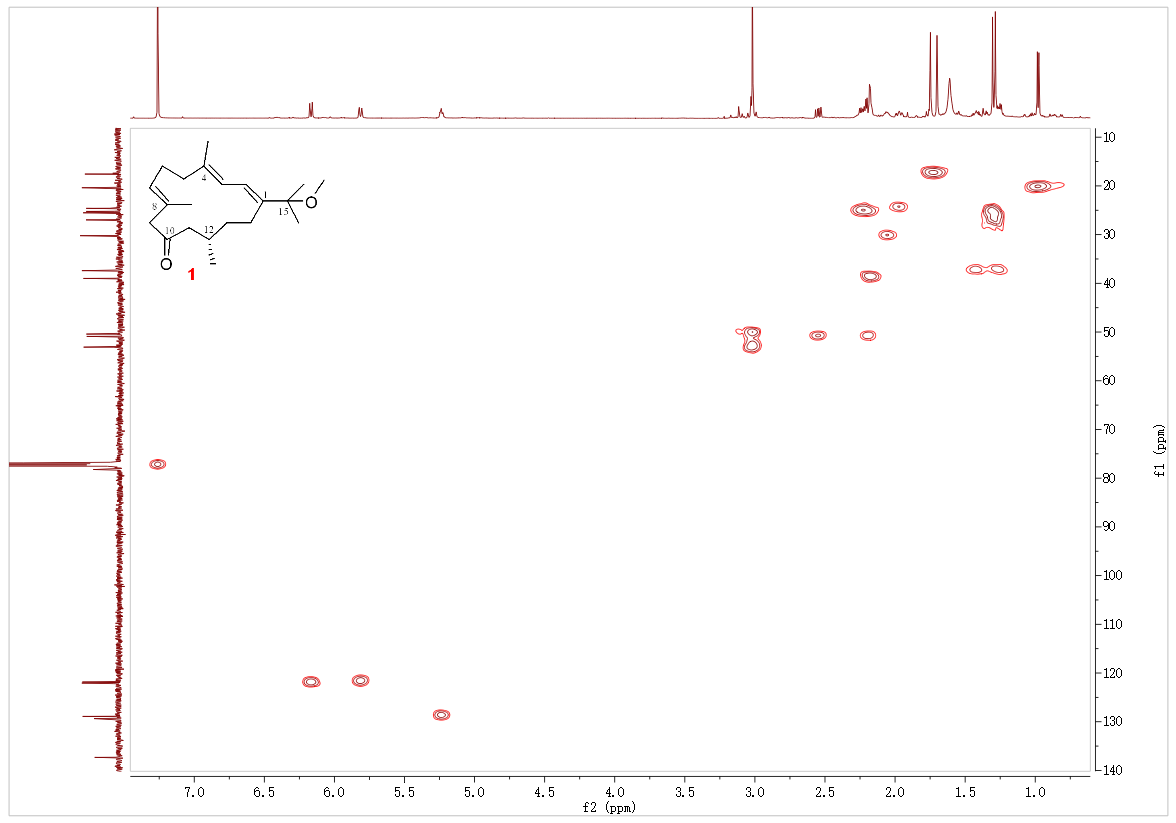
1. **Original spectra of 1**



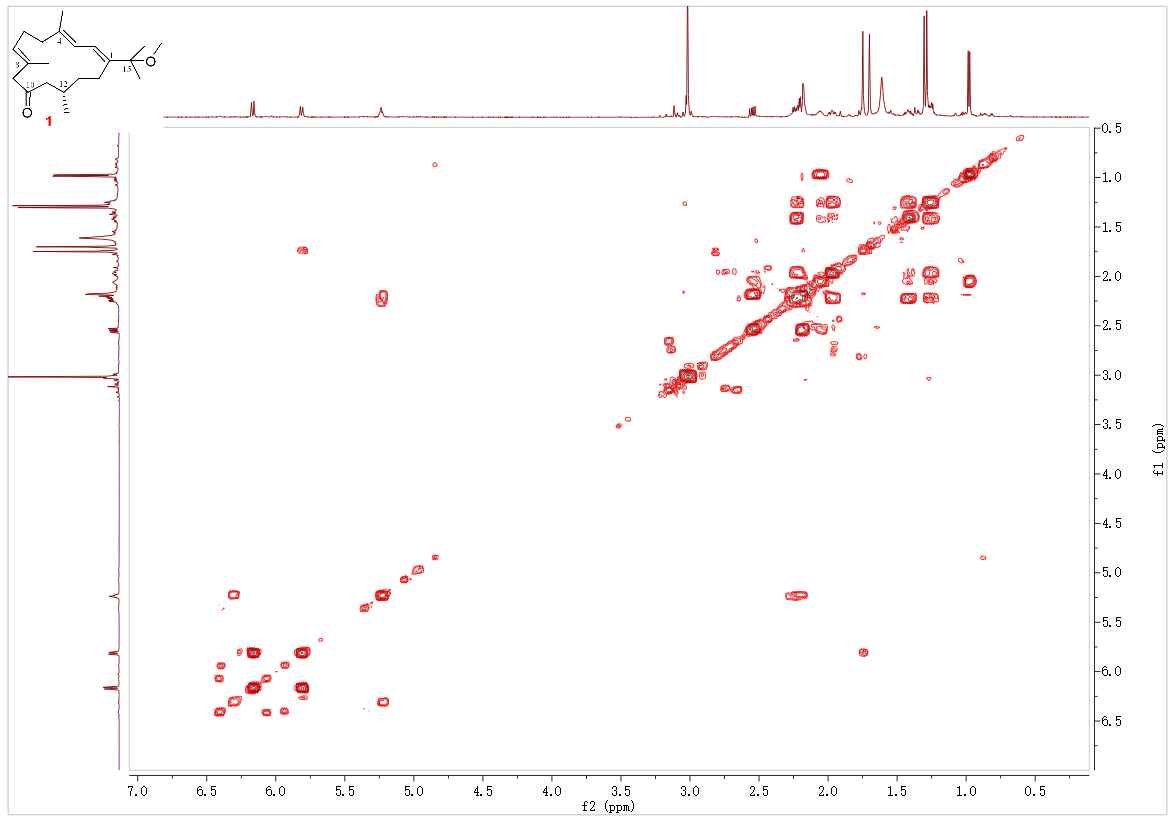
**Figure S1a.** 1H NMR spectrum (600 MHz) of **1** in CDCl3



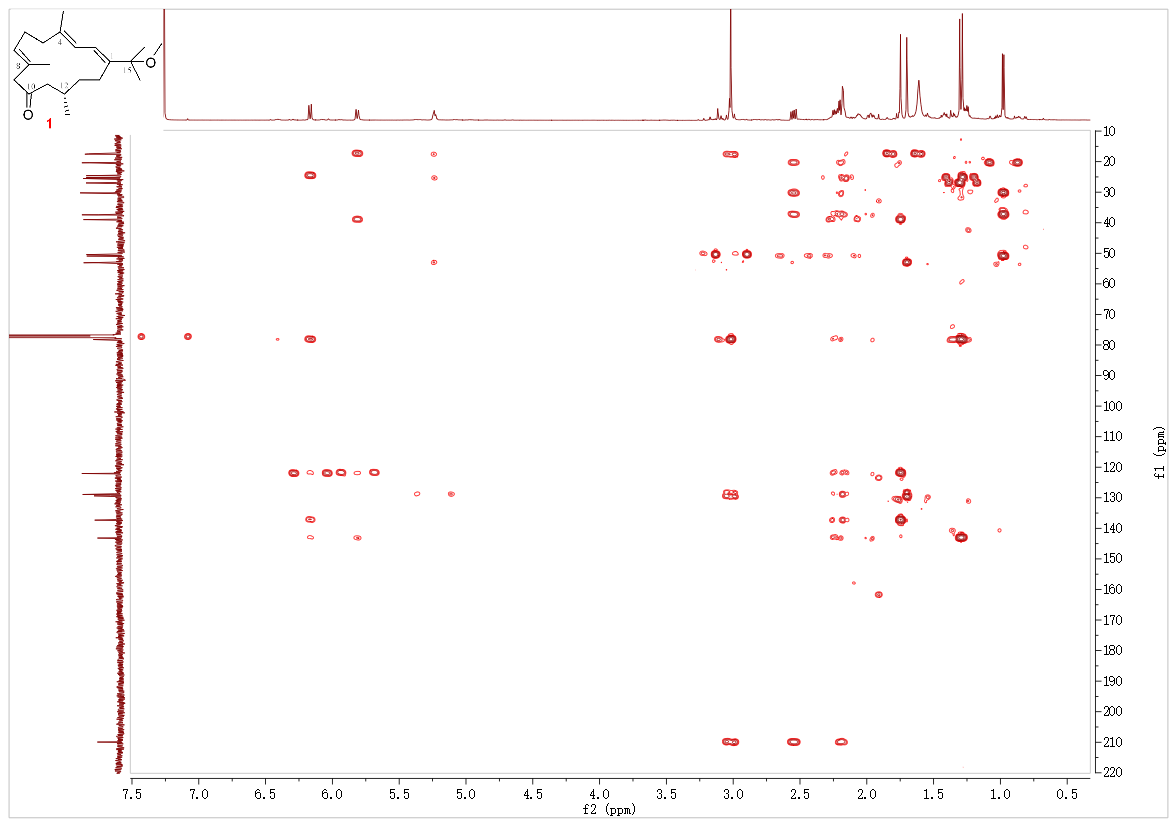
**Figure S1b.** DEPT135/13C NMR spectrum (150 MHz) of **1** in CDCl3

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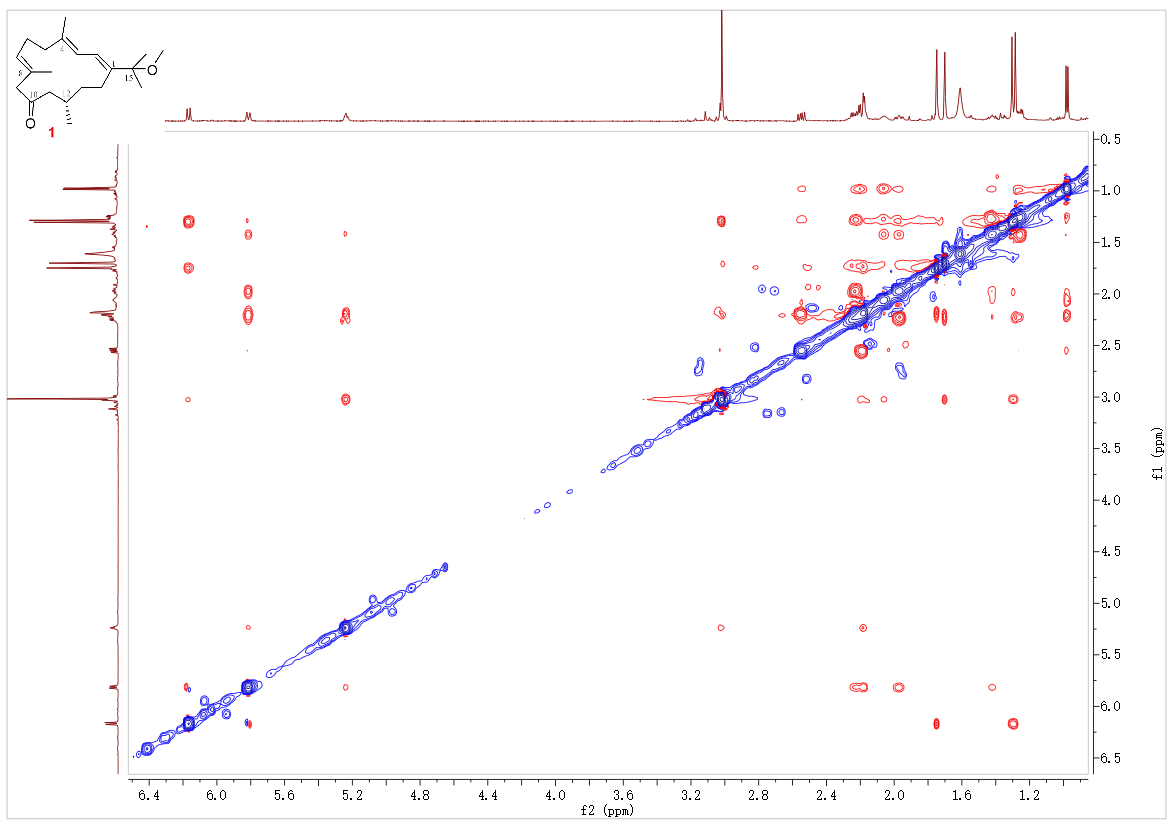
**Figure S1c.** HSQC spectrum (600 MHz) of **1** in CDCl3



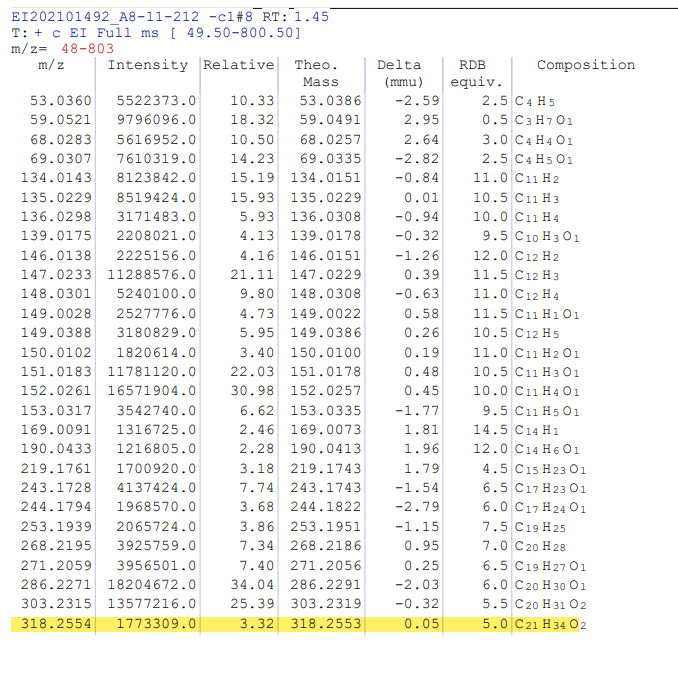
**Figure S1d.** 1H-1H COSY spectrum of (600 MHz) **1** in CDCl3



**Figure S1e.** HMBC spectrum (600 MHz) of **1** in CDCl3



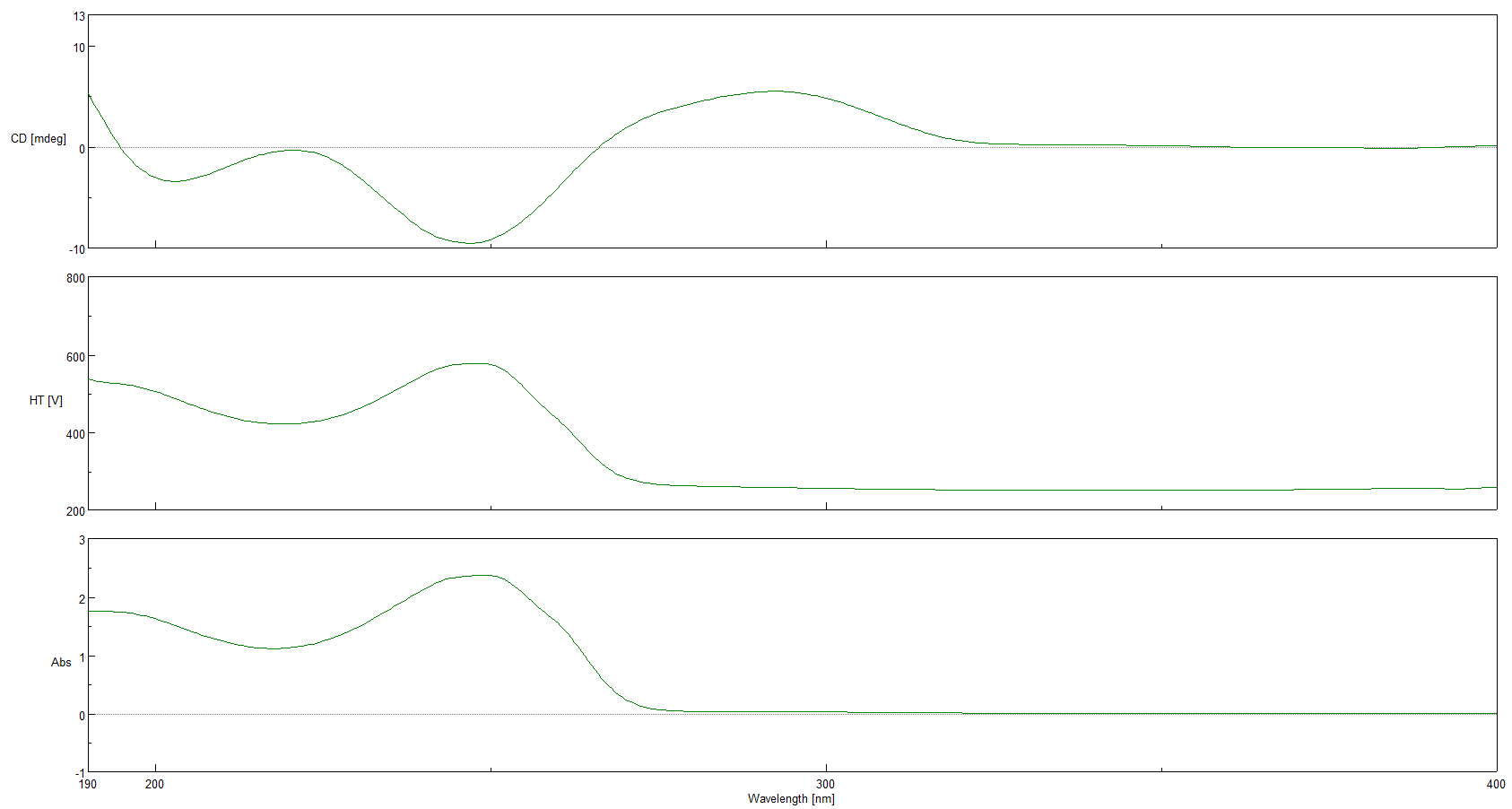
**Figure S1f.** NOESY spectrum (600 MHz) of **1** in CDCl3



**Figure S1g.** HR-EIMS of **1**

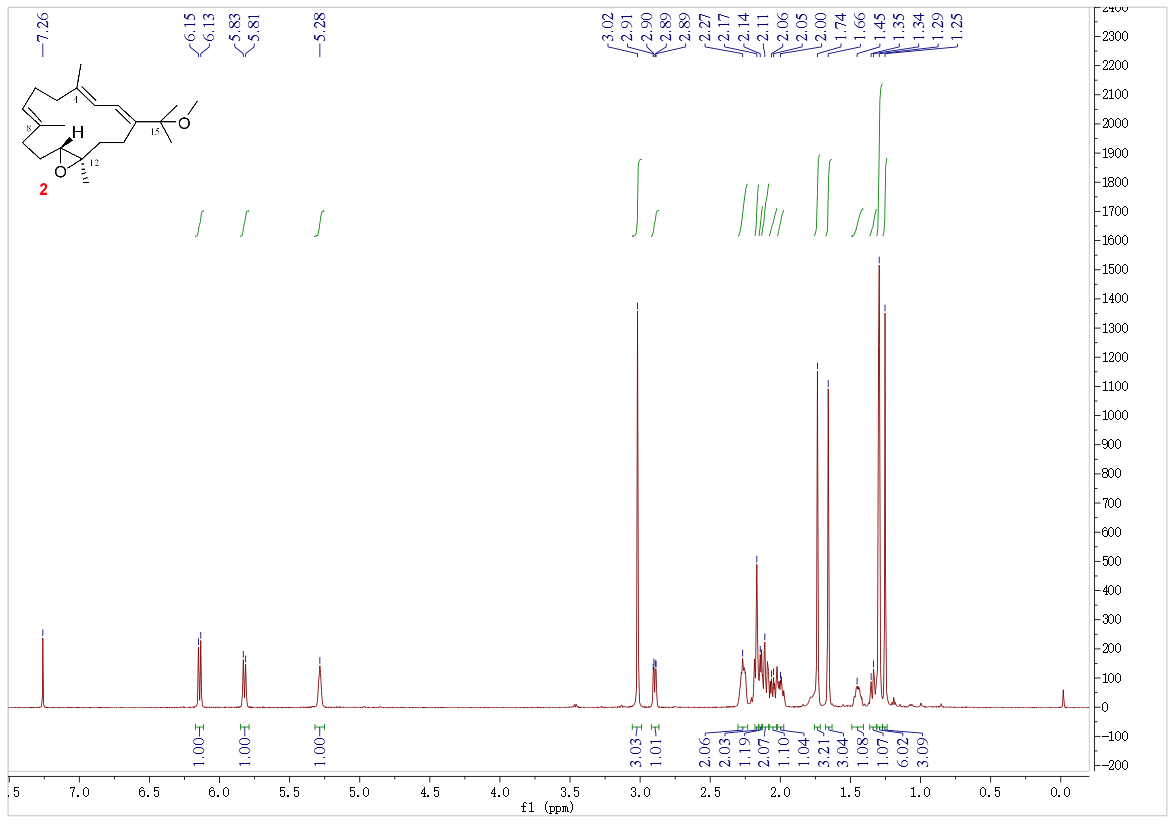


**Figure S1h.** IR spectrum of **1**

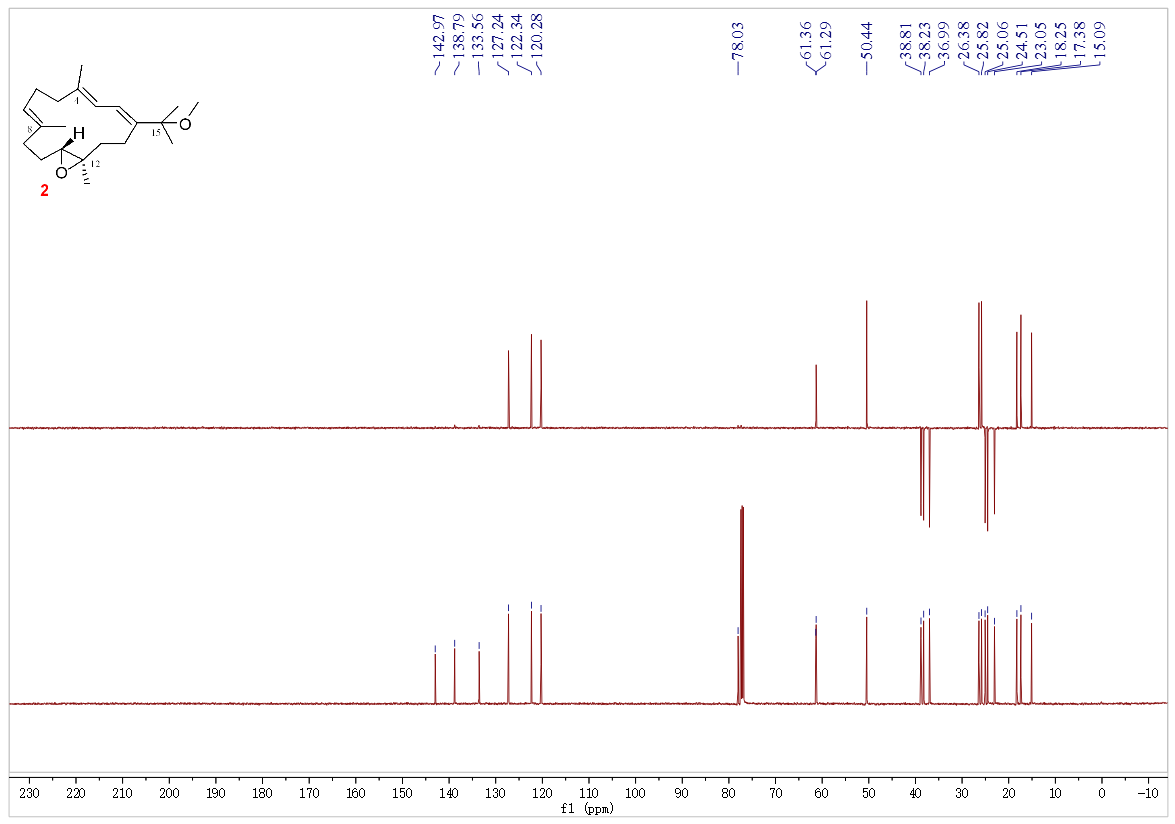


**Figure S2i.** ECD and UV spectra of **1**

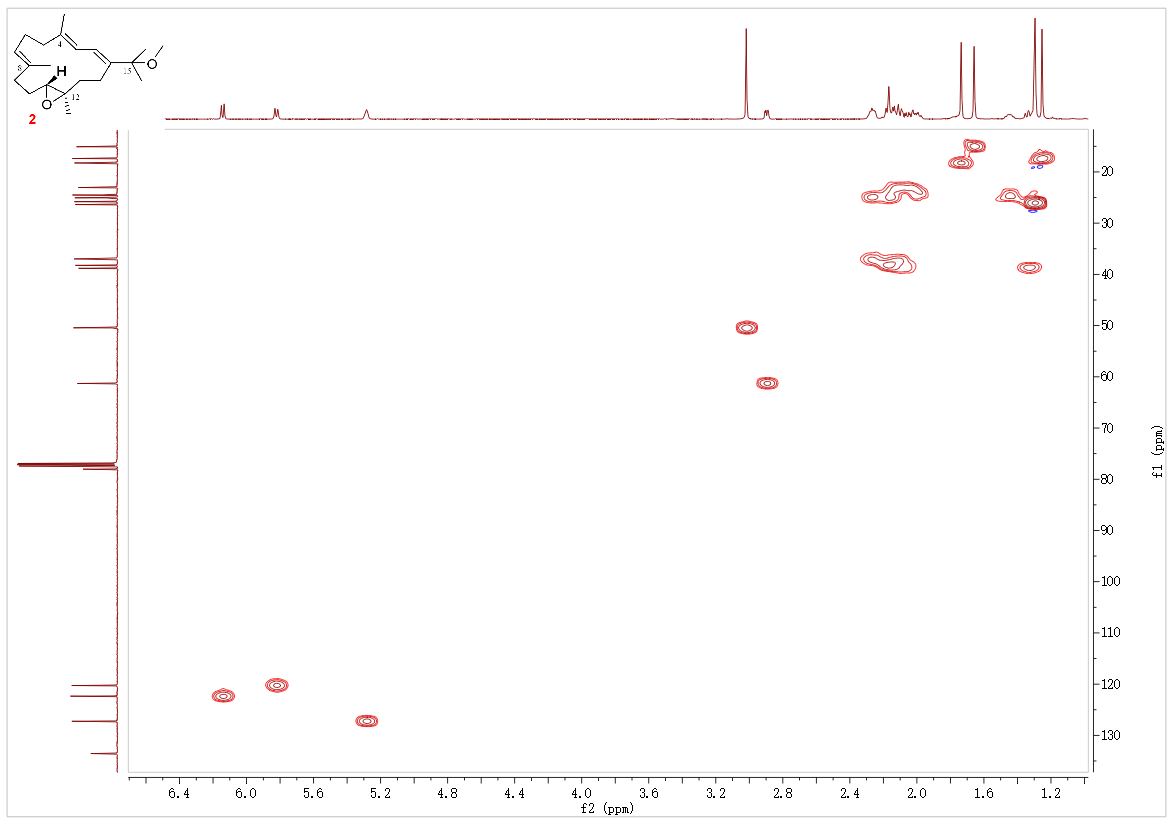
1. **Original spectra of 2**



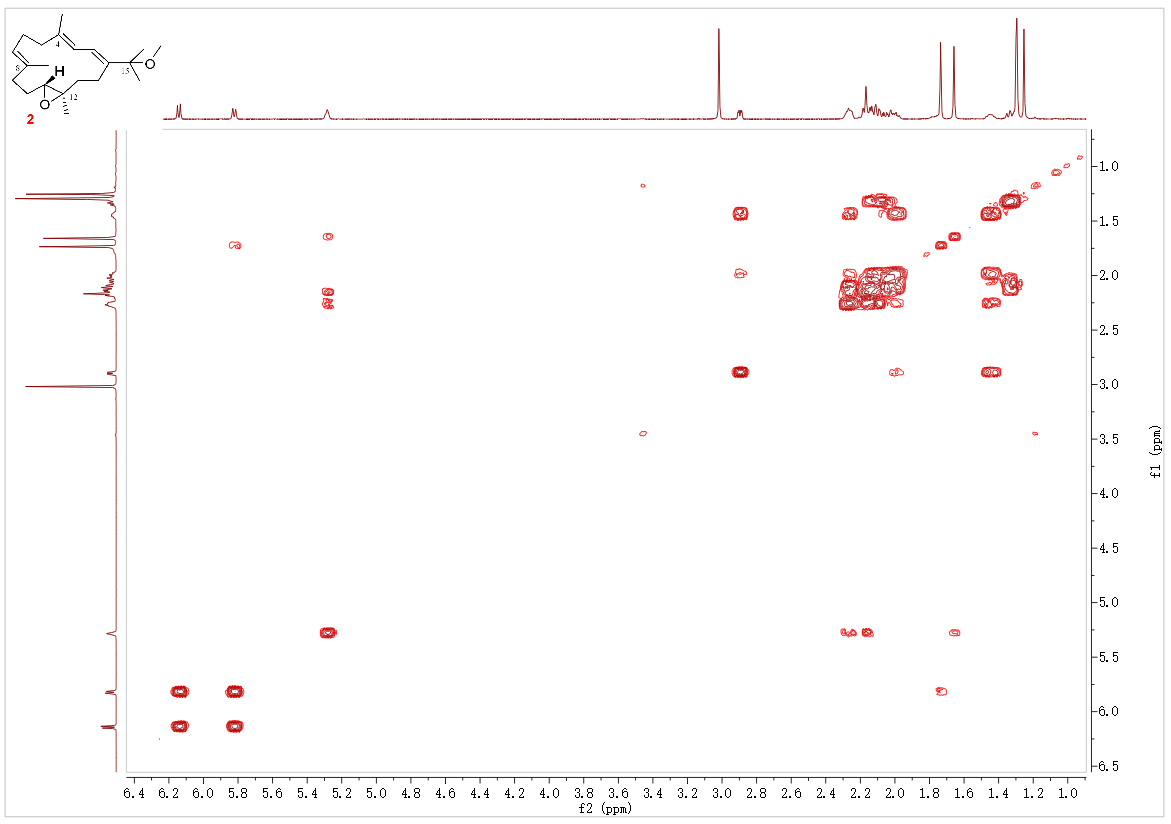
**Figure S2a.** 1H NMR spectrum (600 MHz) of **2** in CDCl3



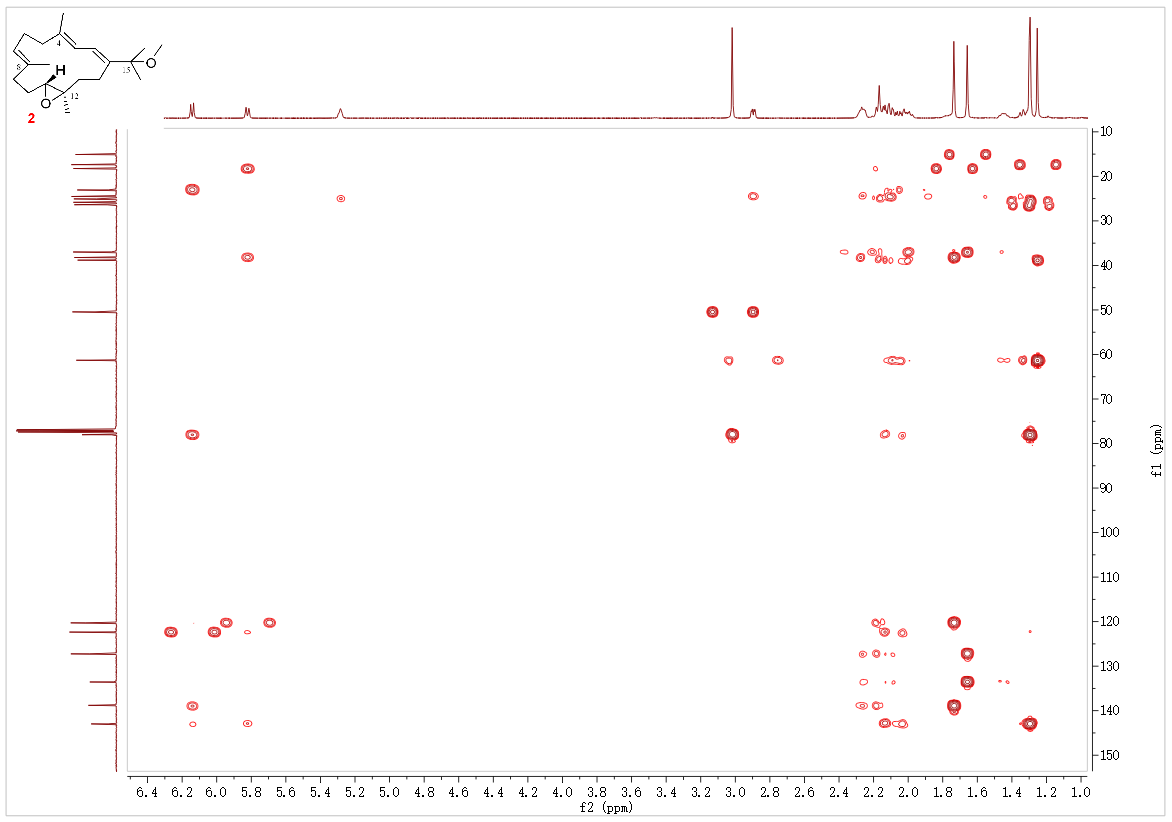
**Figure S2b.** DEPT135/13C NMR spectrum (150 MHz) of **2** in CDCl3

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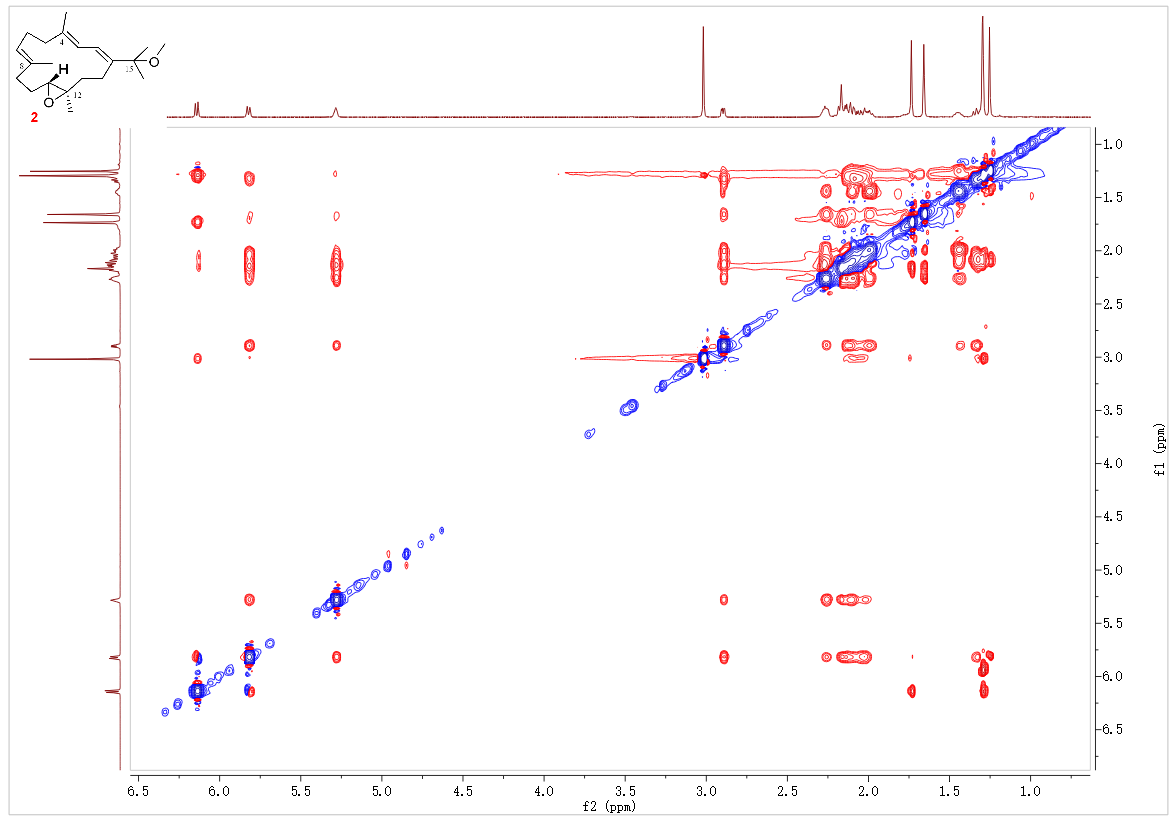
**Figure S2c.** HSQC spectrum (600 MHz) of **2** in CDCl3



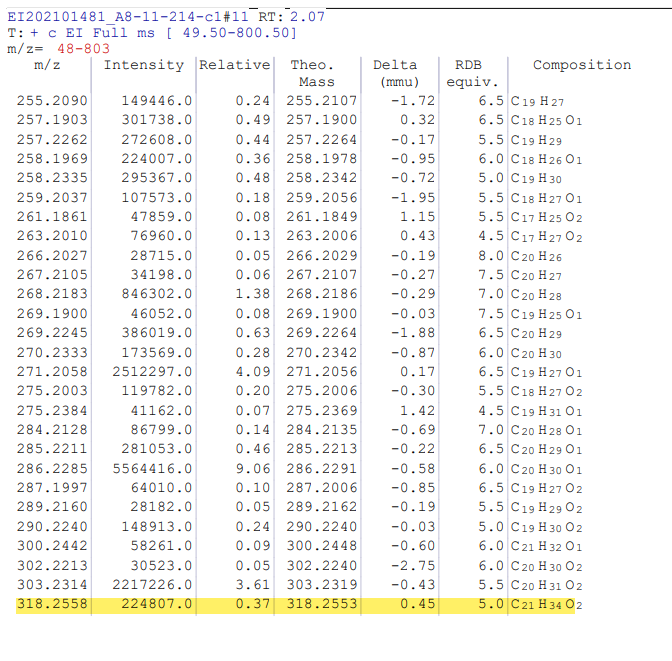
**Figure S2d.** 1H-1H COSY spectrum (600 MHz) of **2** in CDCl3

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**Figure S2e.** HMBC spectrum (600 MHz) of **2** in CDCl3



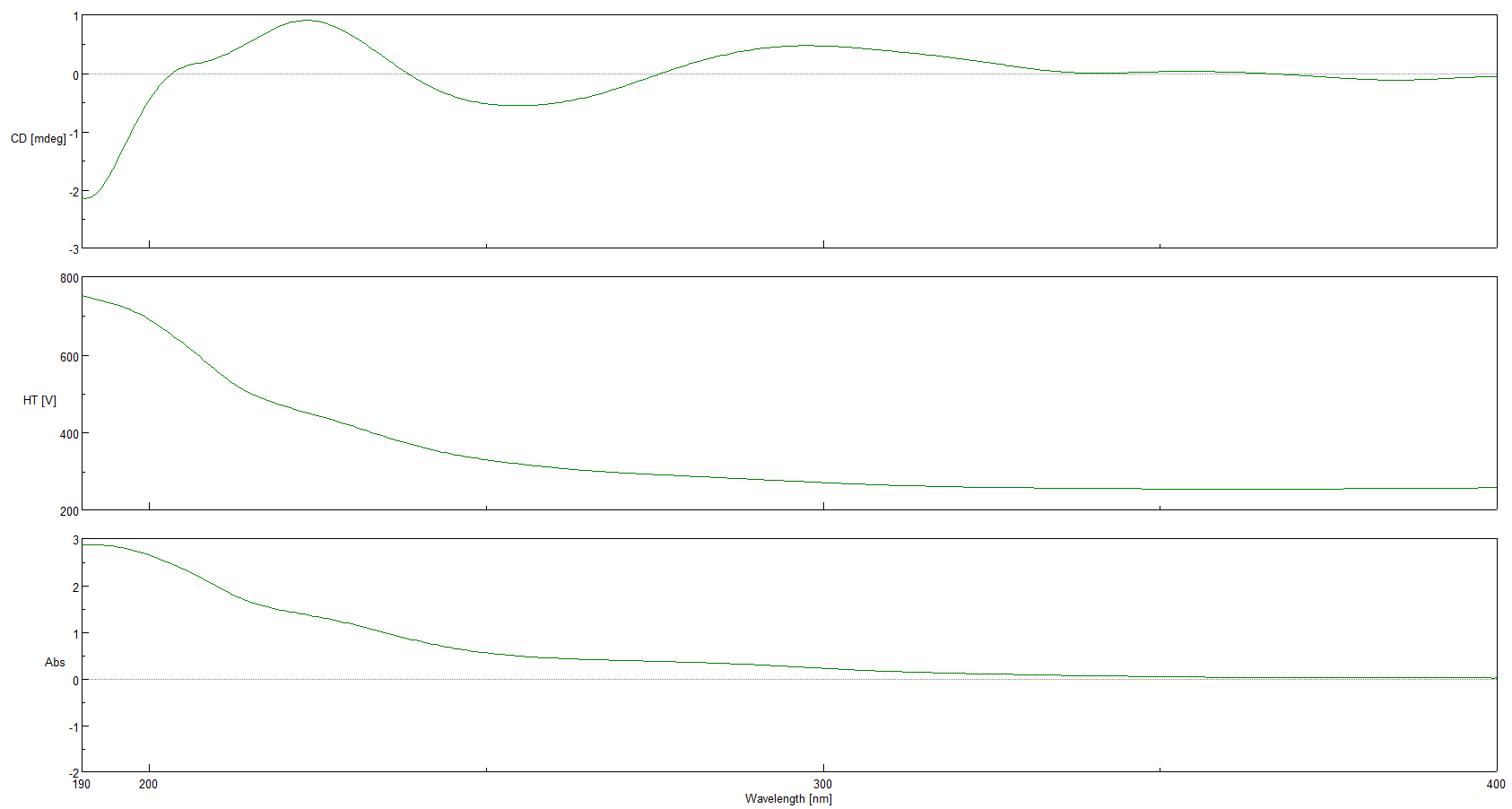
**Figure S2f.** NOESY spectrum (600 MHz) of **2** in CDCl3

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**Figure S2g.** HR-EIMS of **2**

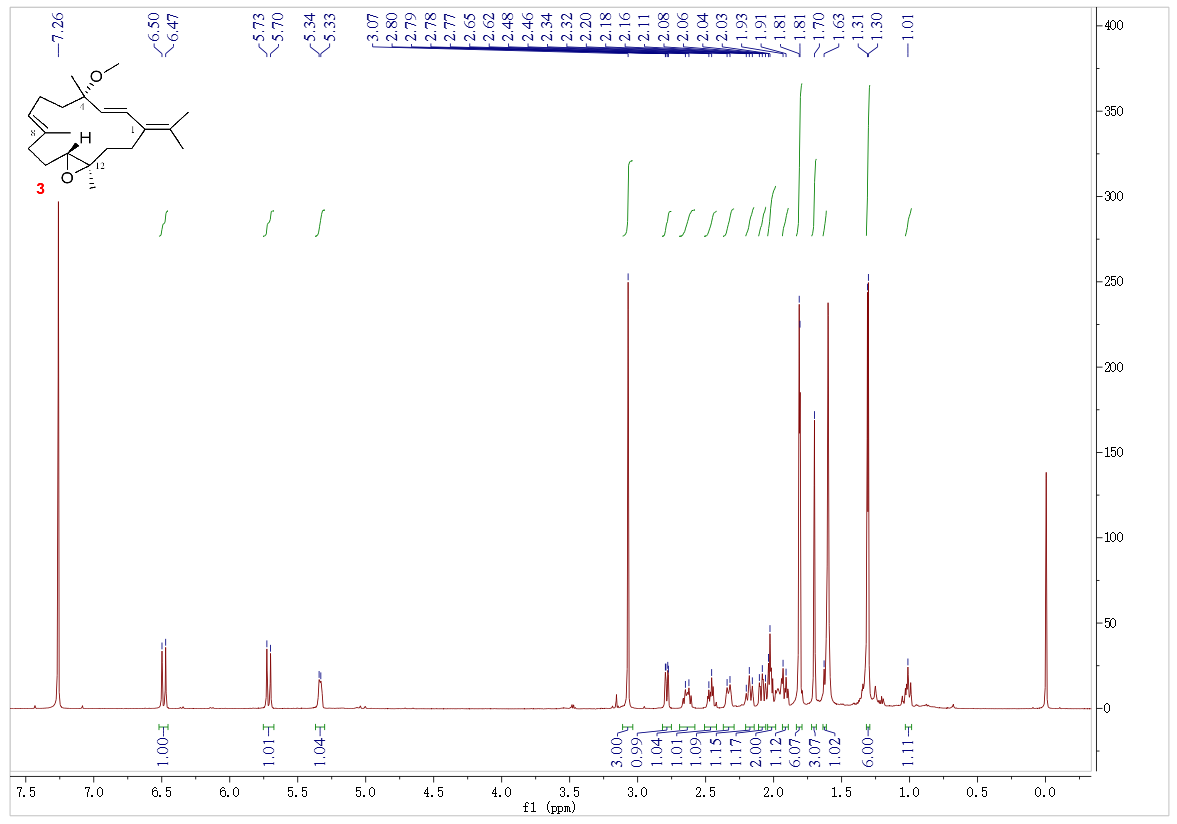


**Figure S2h.** IR spectrum of **2**

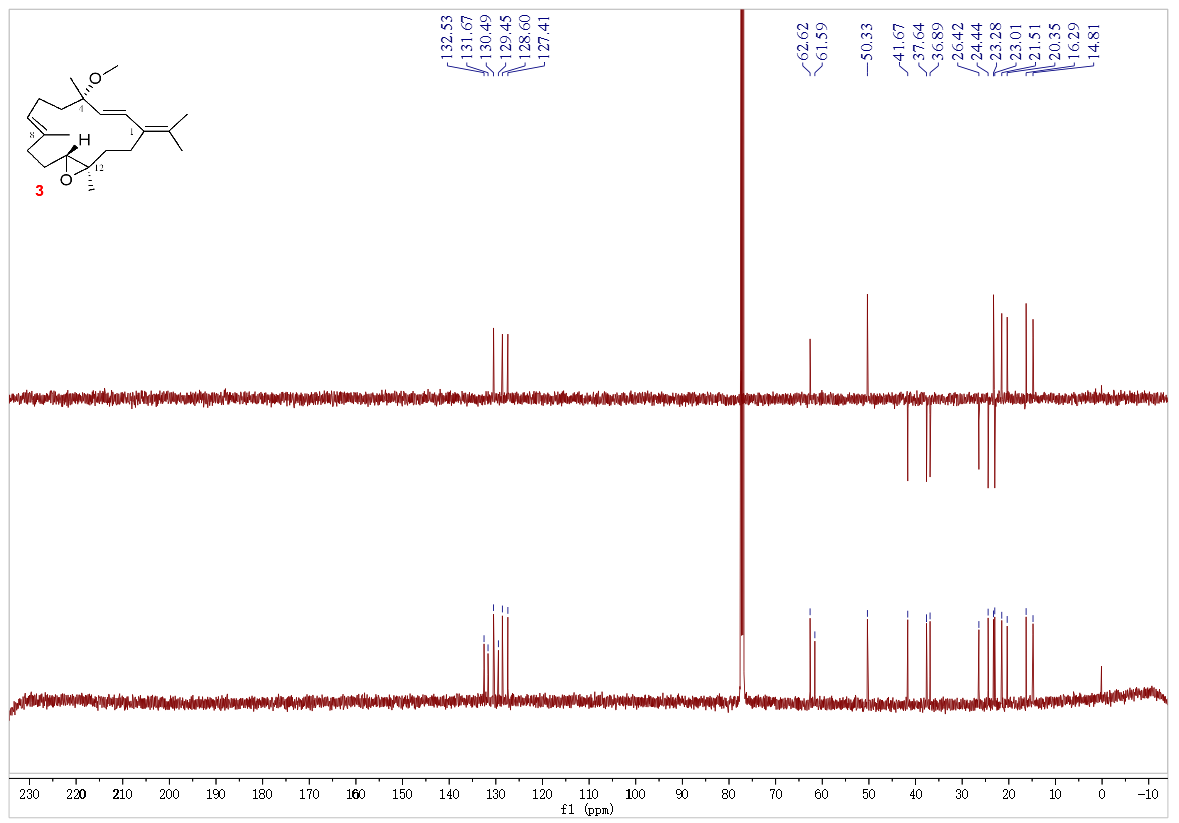


**Figure S2i.** ECD and UV spectra of **2**

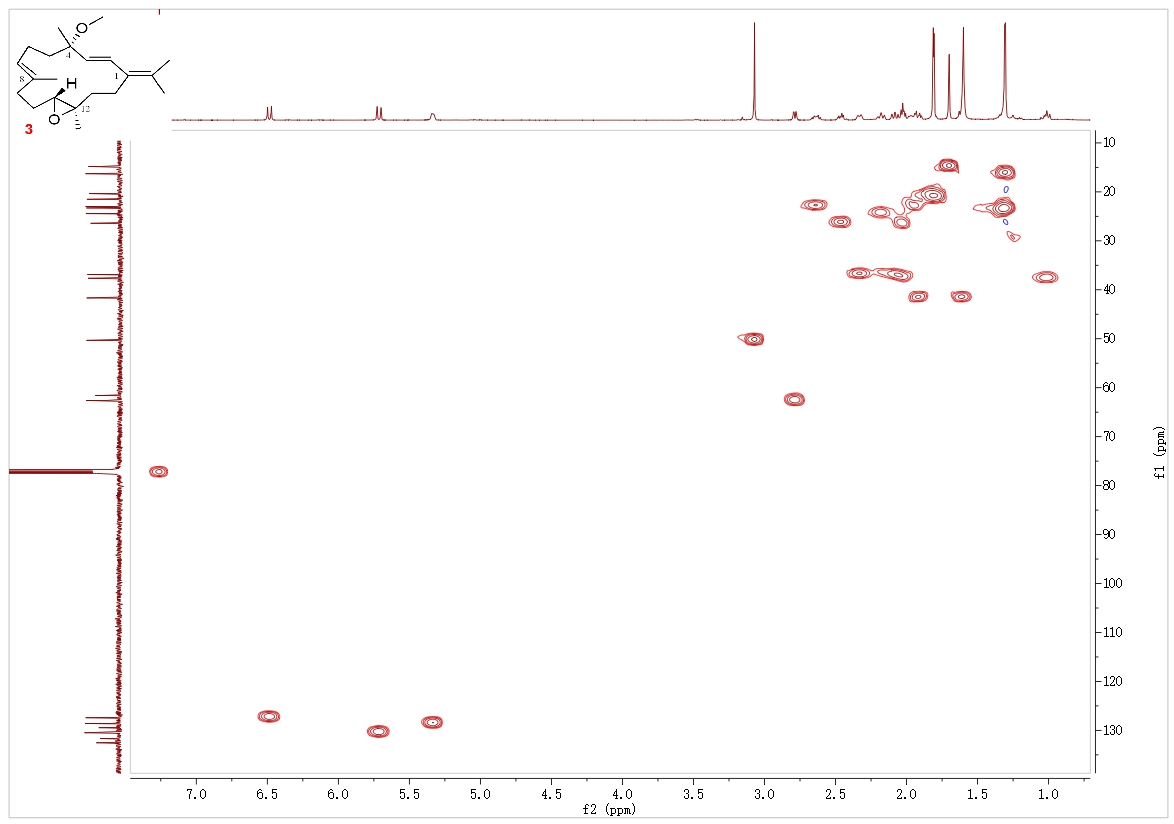
1. **Original spectra of 3**

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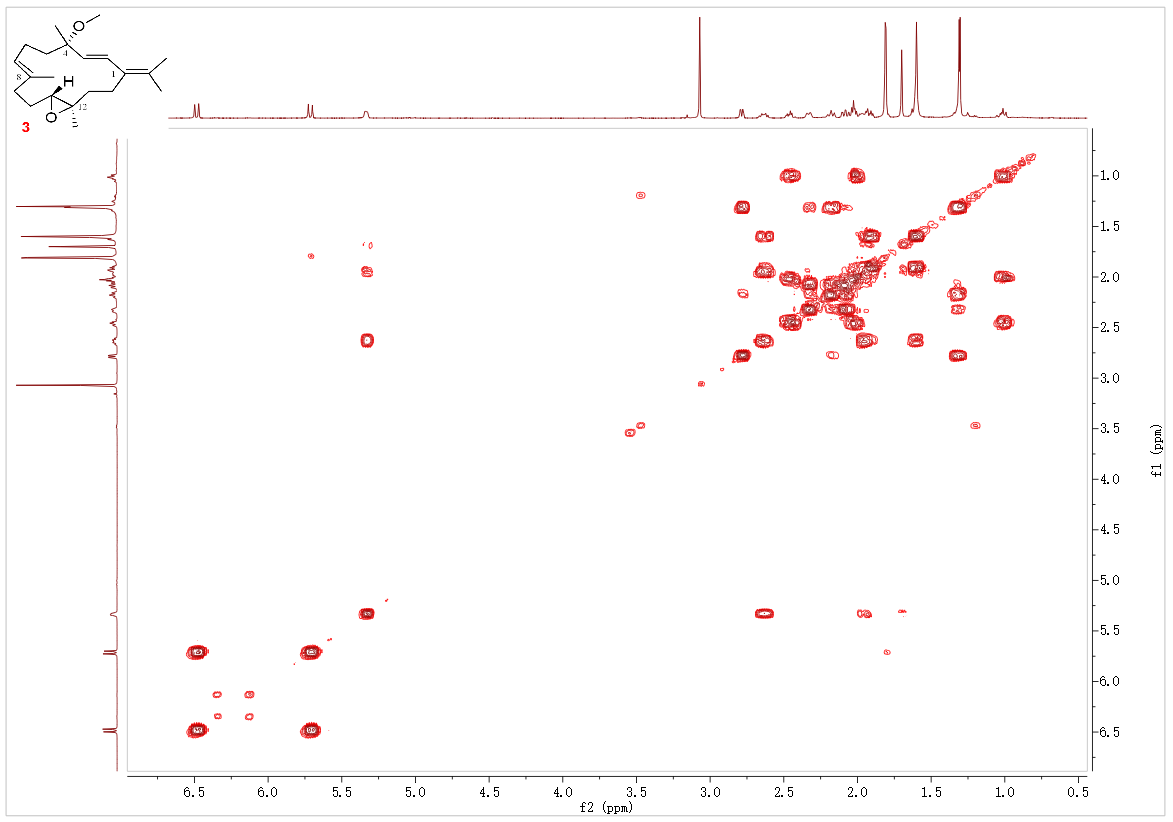
**Figure S3a.** 1H NMR spectrum (600 MHz) of **3** in CDCl3



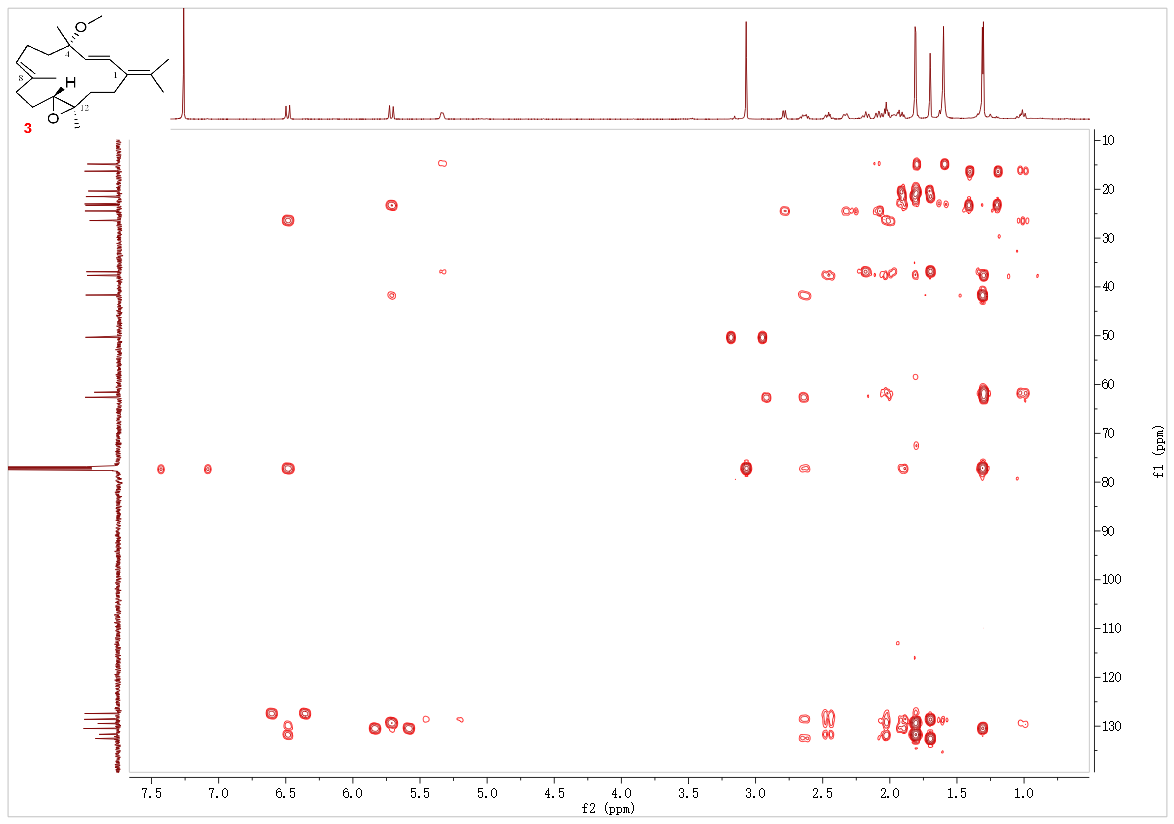
**Figure S3b.** DEPT135/13C NMR spectrum (150 MHz) of **3** in CDCl3

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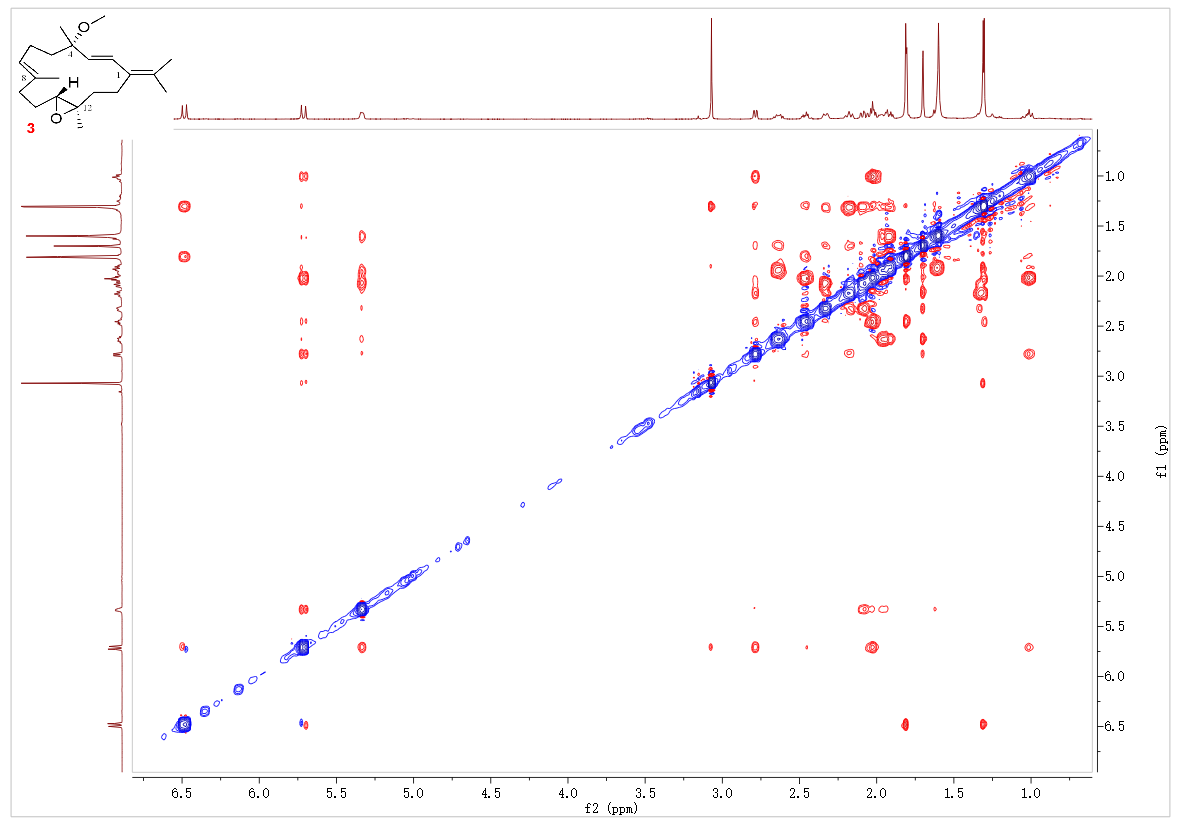
**Figure S3c.** HSQC spectrum (600 MHz) of **3** in CDCl3



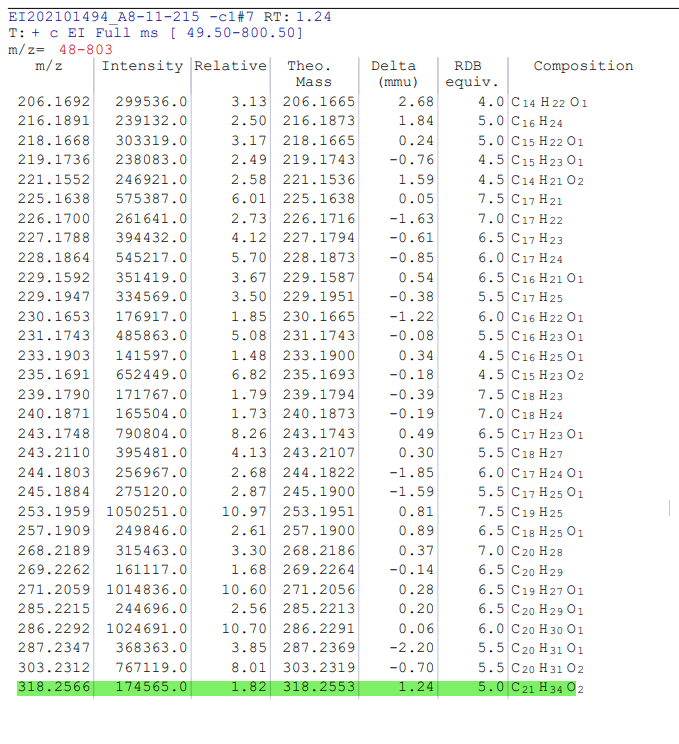
**Figure S3d.** 1H-1H COSY spectrum (600 MHz) of **3** in CDCl3

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**Figure S3e.** HMBC spectrum (600 MHz) of **3** in CDCl3



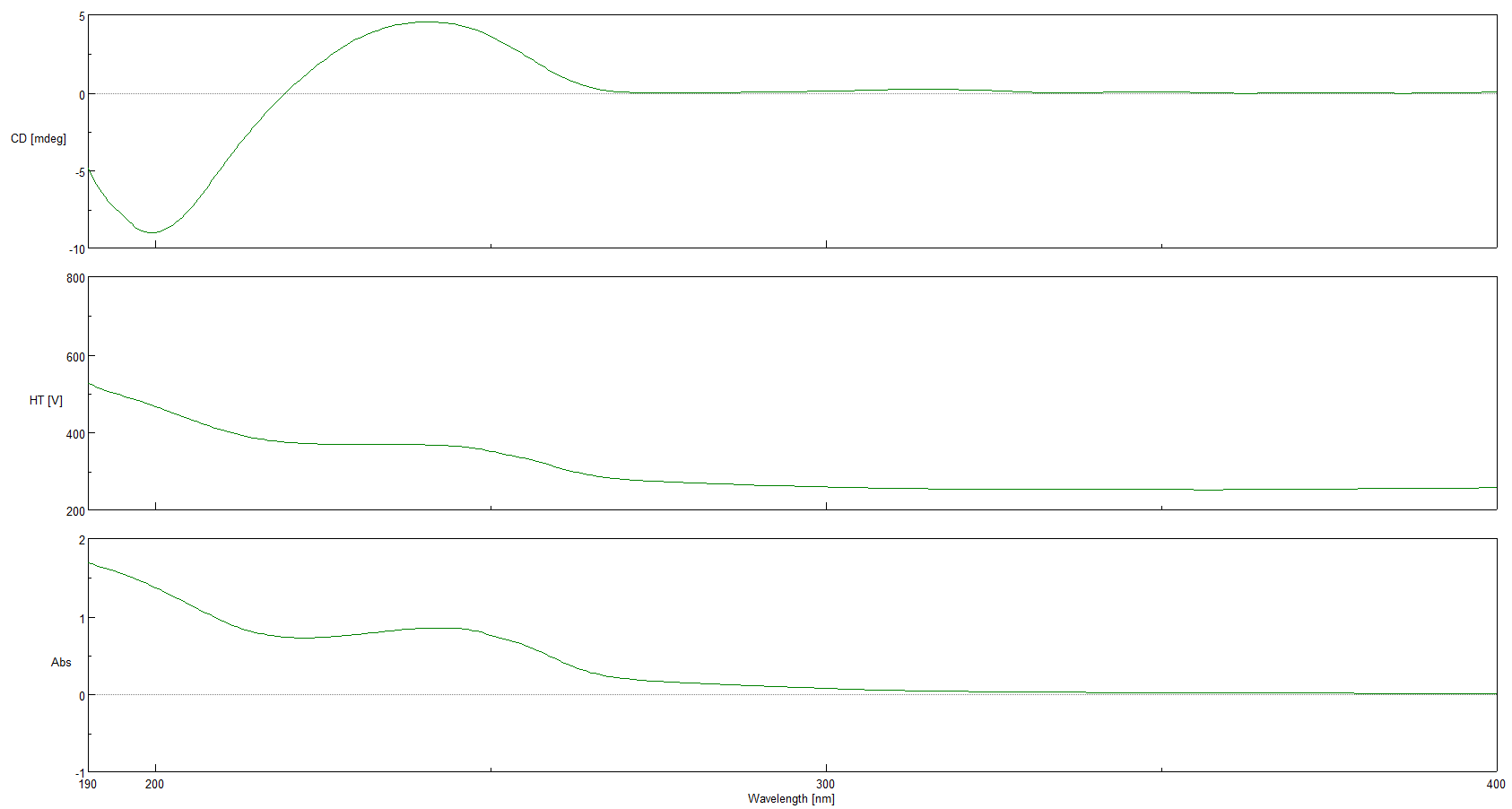
**Figure S3f.** NOESY spectrum (600 MHz) of **3** in CDCl3

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**Figure S3g.** HR-EIMS of **3**

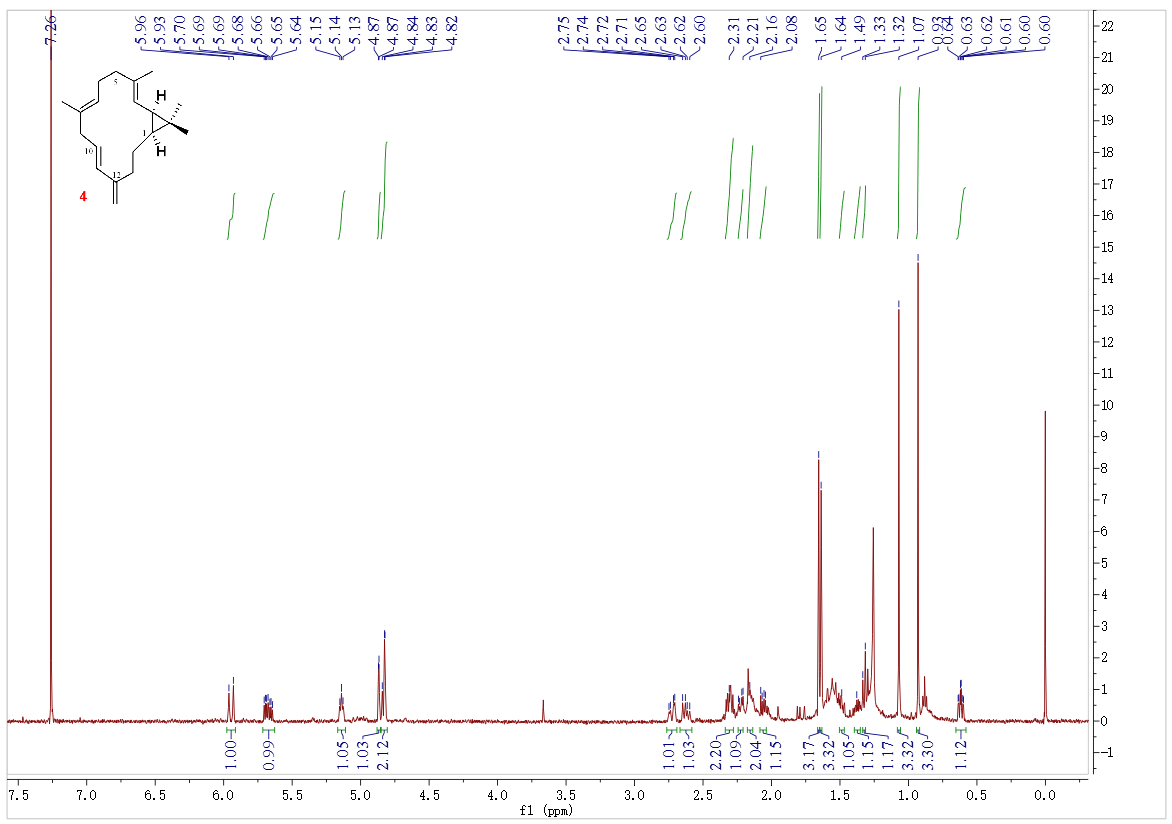


**Figure S3h.** IR spectrum of **3**

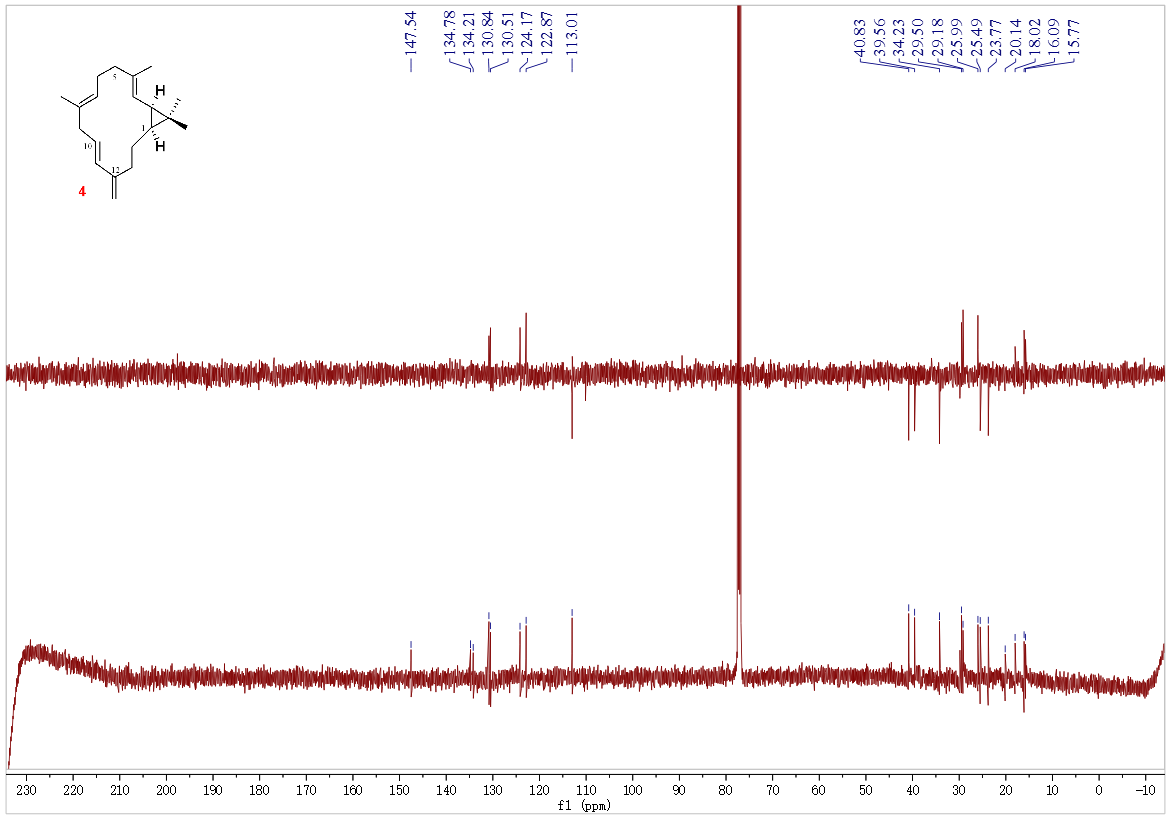


**Figure S3i.** ECD and UV spectra of **3**

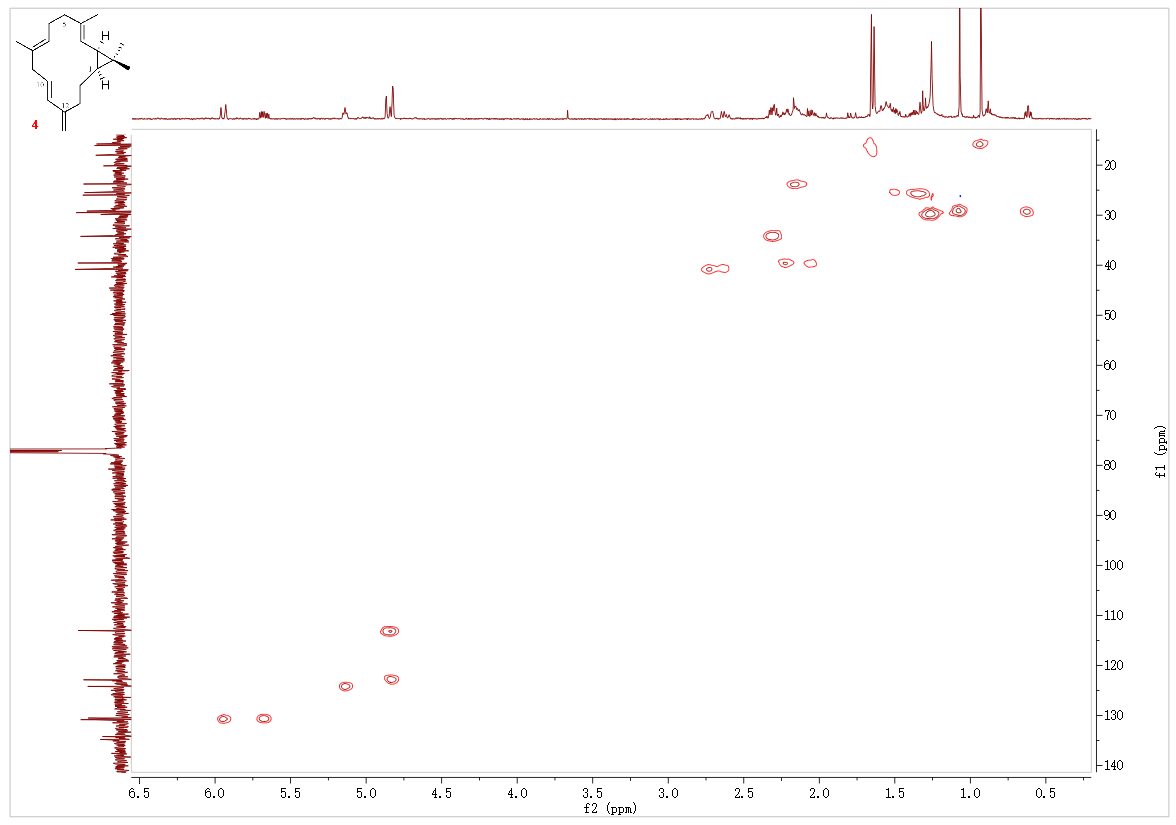
1. **Original spectra of 4**

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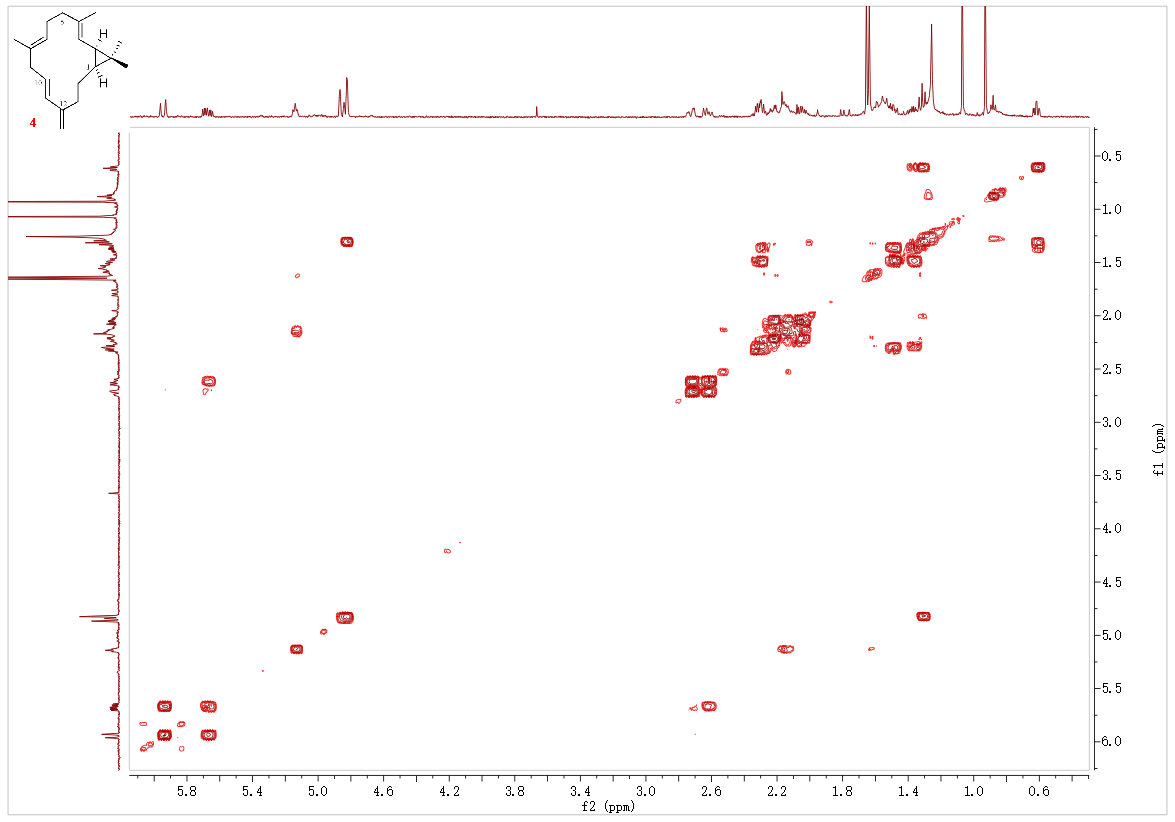
**Figure S4a.** 1H NMR spectrum (600 MHz) of **4** in CDCl3

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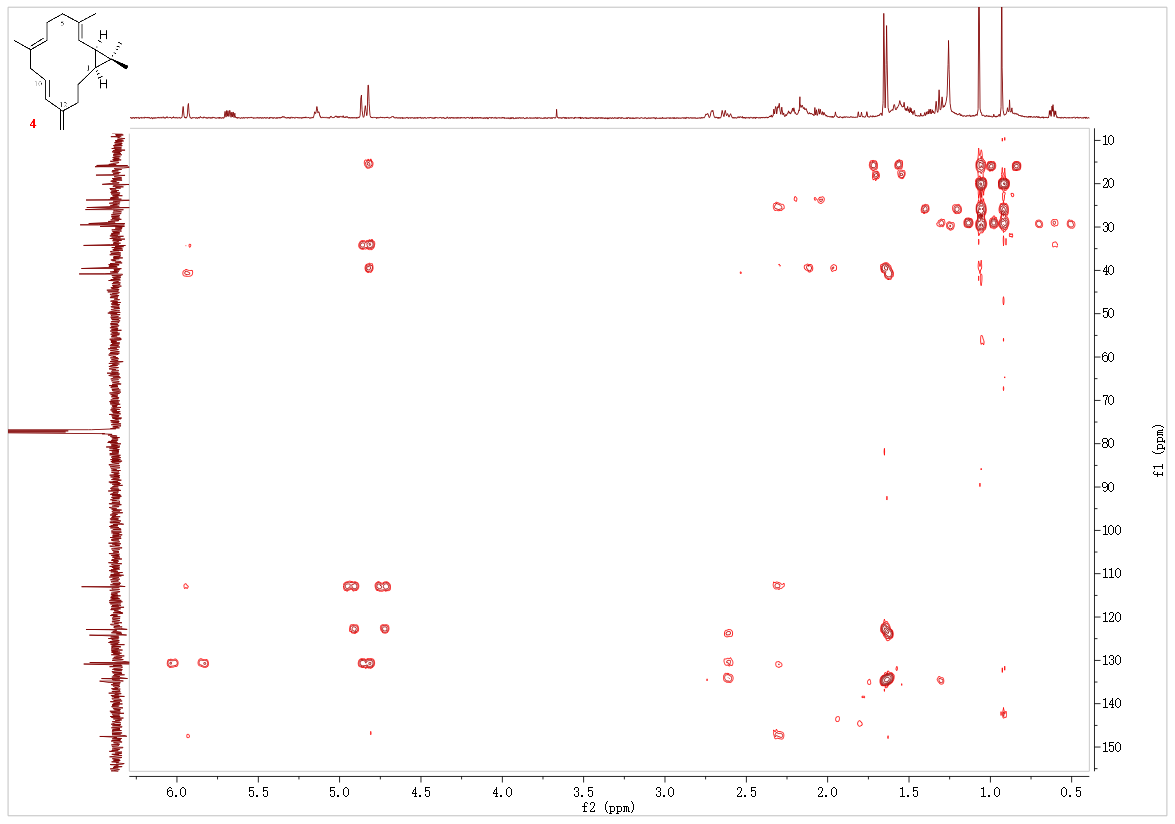
**Figure S4b.** DEPT135/13C NMR spectrum (150 MHz) of **4** in CDCl3

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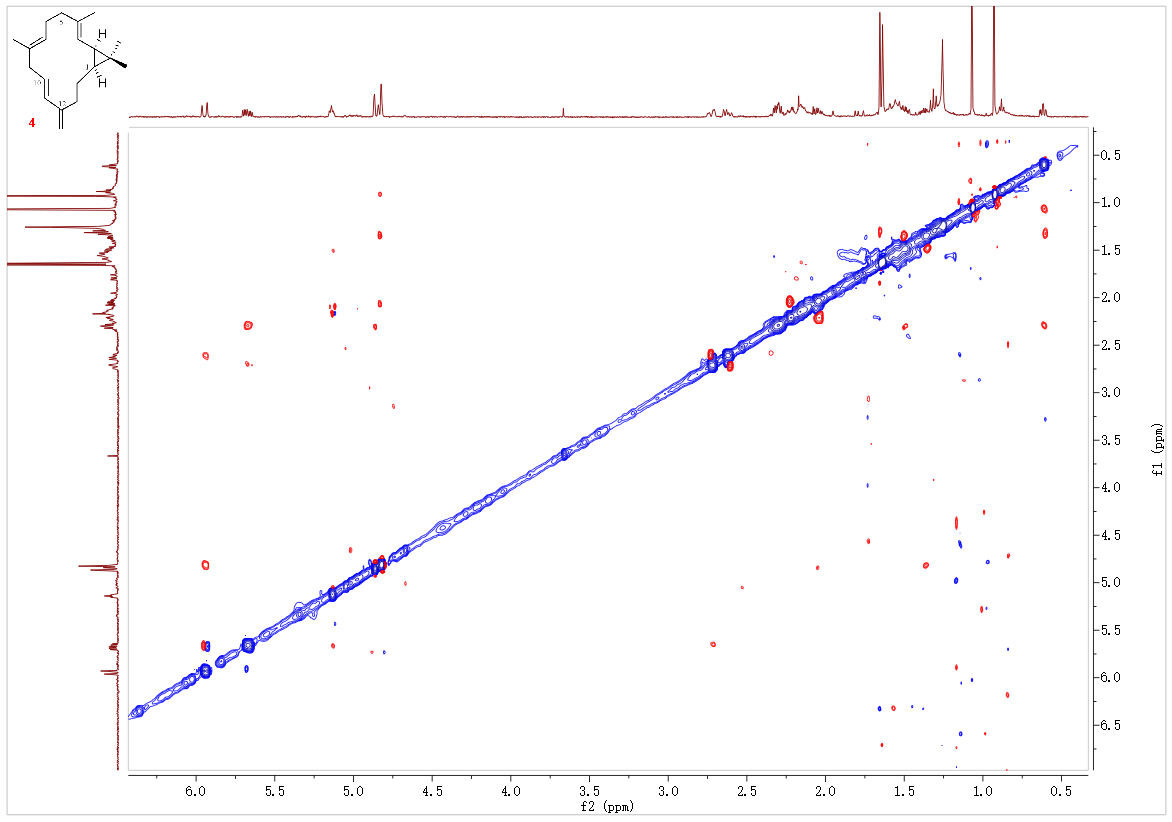
**Figure S4c.** HSQC spectrum (600 MHz) of **4** in CDCl3

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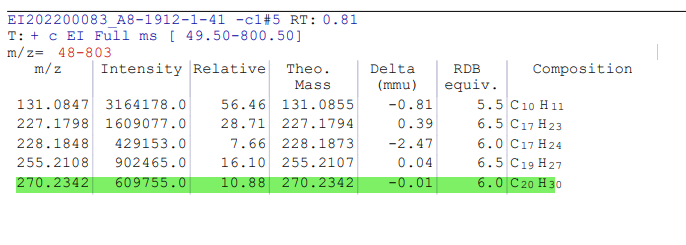
**Figure S4d.** 1H-1H COSY spectrum (600 MHz) of **4** in CDCl3

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**Figure S4e.** HMBC spectrum (600 MHz) of **4** in CDCl3

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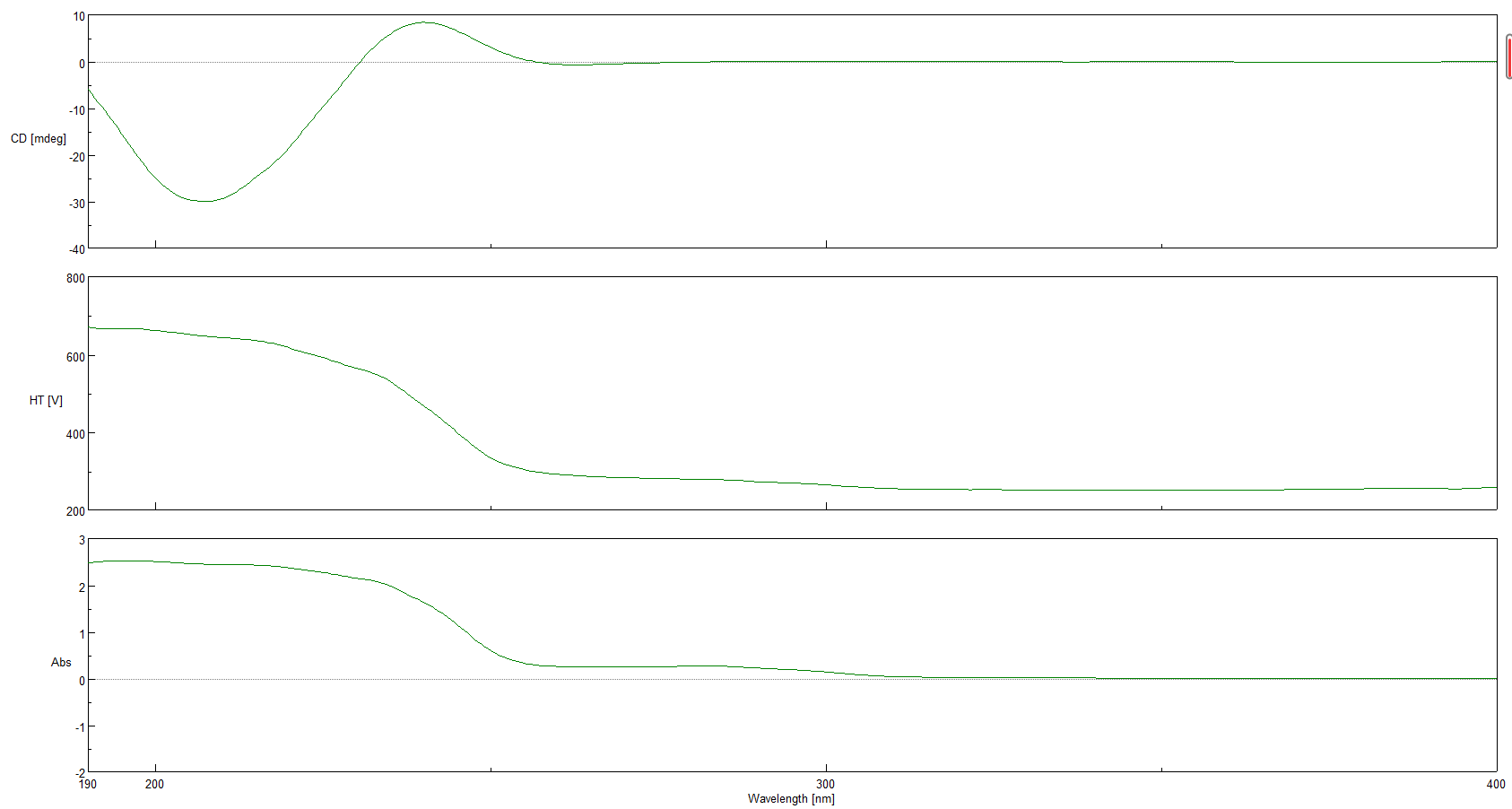
**Figure S4f.** NOESY spectrum (600 MHz) of **4** in CDCl3

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**Figure S4g.** HR-EIMS of **4**



**Figure S4h.** IR spectrum of **4**



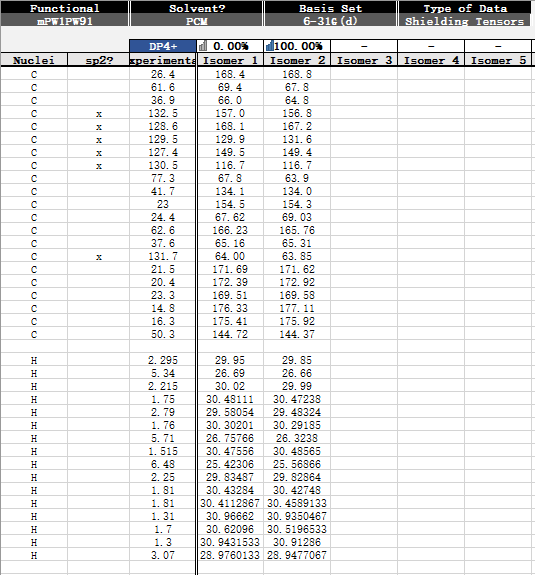
**Figure S4i.** ECD and UV spectra of **4**

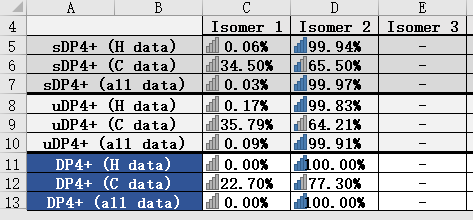
1. **QM-NMR calculation and DP4+ analysis of compound 3**

**Figure S5a.** Structures of studied isomers for compound **3**



**Figure S5b.** DP4+ results obtained using experimental data of **3** *versus* isomers 1 (**3a**) and 2 (**3b**).





1. **TDDFT-EDC calculations of compounds 1-4**

Torsional sampling (MCMM) conformational searches using MMFFs force field were carried out by means of the conformational search module in the Macromodel1 applying an energy window of 21 kJ/mol, which afforded 145, 171, 125, 126 conformers for (12*S*)-**1**, (11*R*, 12*R*)-**2**, (4*S*, 11*R*, 12*R*)-**3**, (1*S*, 2*R*)-**4**, respectively. The Boltzmann populations of the conformers were obtained based on the potential energy provided by the MMFFs force field, which afforded 5, 5, 5, 4 conformers for re-optimization. The re-optimization and the following TDDFT calculations of the re-optimized geometries were all performed with Gaussian 09 at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. Frequency analysis was performed as well to confirm that the re-optimized geometries were at the energy minima. Finally, the SpecDis 1.62 software was used to obtain the Boltzmann-averaged ECD spectra and visualize the results.



**Figure S6a.** Experimental ECD curve of **1**, and calculated ECD spectrum of (12*S*)-**1**



**Figure S6b.** Experimental ECD curve of **2**, and calculated ECD spectrum of (11*R*, 12*R*)-**2**



**Figure S6c.** Experimental ECD curve of **3**, and calculated ECD spectrum of (4*S*, 11*R*, 12*R*)-**3**



**Figure S6d.** Experimental ECD curve of **4**, and calculated ECD spectrum of (1*S*, 2*R*)-**4**

|  |  |  |
| --- | --- | --- |
|  |  |  |
| Conf. 1  3.16%  -971.22082194 a. u. | Conf. 2  9.43%  -971.22210426 a. u. | Conf. 3  16.36%  -971.22196749 a. u. |
|  |  |  |
| Conf. 4  5.73%  -971.22087028 a. u. | Conf. 5  65.32%  -971.22319110 a. u. |  |

|  |  |  |  |
| --- | --- | --- | --- |
| Conf. 1 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.93858 | -2.73139 | -0.37242 |
| C | 3.25353 | -1.26776 | -0.22732 |
| C | 3.14115 | -0.4776 | 0.84943 |
| C | 3.57909 | 0.9813 | 0.76691 |
| C | 2.38076 | 1.93369 | 0.76491 |
| C | 1.9124 | 2.41783 | -0.59845 |
| C | 1.8815 | -3.02857 | -1.47663 |
| C | 0.44522 | -2.83282 | -1.02916 |
| C | -0.08728 | -1.59638 | -0.9677 |
| C | 0.53746 | 3.11018 | -0.66008 |
| C | -0.6164 | 2.11737 | -0.91461 |
| C | -1.44456 | -1.23358 | -0.56766 |
| C | -0.80447 | 1.05656 | 0.188 |
| C | -1.82645 | -0.02793 | -0.0984 |
| C | -3.32664 | 0.24448 | 0.14523 |
| C | -3.58568 | 1.30422 | 1.22865 |
| C | -3.99279 | 0.68716 | -1.16861 |
| O | -4.02832 | -0.9794 | 0.46707 |
| C | -0.28146 | -4.08826 | -0.62352 |
| C | 2.63491 | -0.91462 | 2.20027 |
| C | 0.53523 | 4.20279 | -1.74009 |
| O | 1.86503 | 2.29552 | 1.80501 |
| C | -3.76931 | -1.55618 | 1.74101 |
| H | 3.86512 | -3.24526 | -0.65875 |
| H | 2.61891 | -3.17631 | 0.5725 |
| H | 3.65134 | -0.81449 | -1.13526 |
| H | 4.17466 | 1.13923 | -0.13417 |
| H | 4.18944 | 1.23212 | 1.64034 |
| H | 2.69785 | 3.11945 | -0.91531 |
| H | 1.9787 | 1.58959 | -1.31344 |
| H | 2.0145 | -4.06267 | -1.8082 |
| H | 2.09824 | -2.39411 | -2.34217 |
| H | 0.5649 | -0.77814 | -1.25737 |
| H | 0.37077 | 3.58748 | 0.31183 |
| H | -1.54122 | 2.69217 | -1.03118 |
| H | -0.44509 | 1.61519 | -1.87539 |
| H | -2.21447 | -1.99155 | -0.67038 |
| H | 0.15154 | 0.56662 | 0.37319 |
| H | -1.05408 | 1.56689 | 1.12175 |
| H | -4.66074 | 1.36757 | 1.41372 |
| H | -3.08638 | 1.0717 | 2.17129 |
| H | -3.24208 | 2.28757 | 0.9024 |
| H | -5.05367 | 0.89056 | -0.99778 |
| H | -3.52393 | 1.58907 | -1.56597 |
| H | -3.90268 | -0.10587 | -1.91342 |
| H | 0.28083 | -4.61961 | 0.15379 |
| H | -1.2829 | -3.89821 | -0.23846 |
| H | -0.36192 | -4.77913 | -1.47108 |
| H | 1.87562 | -0.22095 | 2.5722 |
| H | 2.20696 | -1.91638 | 2.18631 |
| H | 3.45079 | -0.90264 | 2.9329 |
| H | -0.43122 | 4.71317 | -1.77921 |
| H | 1.30471 | 4.95517 | -1.54432 |
| H | 0.72766 | 3.77765 | -2.73114 |
| H | -4.25307 | -2.5342 | 1.73892 |
| H | -2.69728 | -1.69317 | 1.9203 |
| H | -4.19416 | -0.96043 | 2.55637 |

|  |  |  |  |
| --- | --- | --- | --- |
| Conf. 2 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.9733 | -2.70612 | -0.36256 |
| C | 3.29655 | -1.2395 | -0.28175 |
| C | 3.22462 | -0.4093 | 0.76798 |
| C | 3.65123 | 1.04698 | 0.61315 |
| C | 2.4441 | 1.98755 | 0.58686 |
| C | 1.90068 | 2.3344 | -0.79 |
| C | 1.84028 | -3.03053 | -1.38192 |
| C | 0.43967 | -2.85282 | -0.82787 |
| C | -0.11571 | -1.62662 | -0.75513 |
| C | 0.50347 | 2.9805 | -0.85838 |
| C | -0.62972 | 1.93583 | -0.94584 |
| C | -1.43686 | -1.28379 | -0.23902 |
| C | -0.80939 | 1.07204 | 0.31944 |
| C | -1.80945 | -0.0659 | 0.20281 |
| C | -3.23181 | 0.15494 | 0.74878 |
| C | -3.21286 | 0.0131 | 2.28075 |
| C | -3.8075 | 1.53181 | 0.36974 |
| O | -4.12526 | -0.89792 | 0.327 |
| C | -0.21926 | -4.11376 | -0.33234 |
| C | 2.77051 | -0.79453 | 2.15276 |
| C | 0.42187 | 3.94207 | -2.05422 |
| O | 1.97973 | 2.4442 | 1.61372 |
| C | -4.57754 | -0.87058 | -1.02238 |
| H | 3.87795 | -3.22881 | -0.6979 |
| H | 2.72069 | -3.12313 | 0.61485 |
| H | 3.65752 | -0.82088 | -1.22118 |
| H | 4.22735 | 1.16816 | -0.30633 |
| H | 4.27519 | 1.34252 | 1.46214 |
| H | 2.64986 | 3.02708 | -1.20087 |
| H | 1.9626 | 1.44861 | -1.43204 |
| H | 1.9636 | -4.06596 | -1.71326 |
| H | 1.98054 | -2.40157 | -2.26693 |
| H | 0.49093 | -0.80275 | -1.11737 |
| H | 0.36603 | 3.56221 | 0.05989 |
| H | -1.56627 | 2.45997 | -1.15779 |
| H | -0.44302 | 1.28629 | -1.80979 |
| H | -2.18197 | -2.07107 | -0.20666 |
| H | 0.15422 | 0.64236 | 0.59753 |
| H | -1.08567 | 1.72889 | 1.14945 |
| H | -4.20806 | 0.21359 | 2.68652 |
| H | -2.92059 | -1.0031 | 2.55228 |
| H | -2.5062 | 0.71102 | 2.73446 |
| H | -4.83651 | 1.60293 | 0.73163 |
| H | -3.23301 | 2.3352 | 0.83316 |
| H | -3.80812 | 1.69881 | -0.70839 |
| H | 0.41954 | -4.61183 | 0.40699 |
| H | -1.18977 | -3.93921 | 0.13121 |
| H | -0.35278 | -4.82774 | -1.15371 |
| H | 2.0174 | -0.09311 | 2.52358 |
| H | 2.35131 | -1.7992 | 2.19485 |
| H | 3.61126 | -0.74572 | 2.85501 |
| H | -0.55499 | 4.43163 | -2.09783 |
| H | 1.18614 | 4.72175 | -1.98804 |
| H | 0.56965 | 3.40862 | -2.99953 |
| H | -5.08602 | -1.82085 | -1.19264 |
| H | -5.29086 | -0.05851 | -1.19941 |
| H | -3.75082 | -0.78109 | -1.73493 |

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| Conf. 3 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 3.16654 | -2.43402 | -0.2557 |
| C | 3.34404 | -0.95519 | -0.04902 |
| C | 3.05602 | -0.20425 | 1.02276 |
| C | 3.35611 | 1.29114 | 1.00201 |
| C | 2.07962 | 2.11247 | 0.80254 |
| C | 1.72752 | 2.45336 | -0.63633 |
| C | 2.22153 | -2.77759 | -1.44618 |
| C | 0.74857 | -2.76599 | -1.08611 |
| C | 0.06811 | -1.60322 | -1.02918 |
| C | 0.30441 | 2.97341 | -0.9159 |
| C | -0.70134 | 1.83657 | -1.19686 |
| C | -1.33784 | -1.42168 | -0.67965 |
| C | -1.03617 | 0.95897 | 0.02831 |
| C | -1.88915 | -0.27067 | -0.24156 |
| C | -3.38149 | -0.15829 | 0.10455 |
| C | -4.05213 | 0.95376 | -0.71656 |
| C | -4.17702 | -1.45761 | -0.08374 |
| O | -3.52424 | 0.31299 | 1.47369 |
| C | 0.16146 | -4.1138 | -0.75732 |
| C | 2.45358 | -0.71245 | 2.30759 |
| C | 0.32502 | 3.95873 | -2.09525 |
| O | 1.41677 | 2.48506 | 1.75128 |
| C | -3.03095 | -0.53928 | 2.49875 |
| H | 4.15153 | -2.86059 | -0.48293 |
| H | 2.81453 | -2.93457 | 0.64891 |
| H | 3.78987 | -0.44678 | -0.90386 |
| H | 4.06285 | 1.51628 | 0.20065 |
| H | 3.79506 | 1.59671 | 1.95626 |
| H | 2.46415 | 3.22269 | -0.91103 |
| H | 1.97122 | 1.59749 | -1.27547 |
| H | 2.48838 | -3.77031 | -1.8207 |
| H | 2.41863 | -2.07346 | -2.2607 |
| H | 0.63188 | -0.70432 | -1.25454 |
| H | -0.02796 | 3.51427 | -0.0229 |
| H | -1.62408 | 2.28181 | -1.5798 |
| H | -0.30912 | 1.21276 | -2.00908 |
| H | -1.97325 | -2.29309 | -0.78542 |
| H | -0.1062 | 0.62627 | 0.49248 |
| H | -1.53816 | 1.57846 | 0.77529 |
| H | -5.1061 | 1.02758 | -0.437 |
| H | -3.58362 | 1.91923 | -0.52275 |
| H | -3.98643 | 0.73879 | -1.78521 |
| H | -5.20001 | -1.29532 | 0.26342 |
| H | -4.21674 | -1.74155 | -1.13742 |
| H | -3.75681 | -2.29485 | 0.47521 |
| H | 0.7559 | -4.60694 | 0.02096 |
| H | -0.8689 | -4.06473 | -0.40649 |
| H | 0.19592 | -4.77256 | -1.63315 |
| H | 1.58814 | -0.10826 | 2.59587 |
| H | 2.13758 | -1.75311 | 2.24349 |
| H | 3.17805 | -0.62592 | 3.12607 |
| H | -0.67298 | 4.36328 | -2.28554 |
| H | 0.99653 | 4.79944 | -1.89796 |
| H | 0.66586 | 3.4676 | -3.01332 |
| H | -3.62385 | -1.45583 | 2.59746 |
| H | -1.98265 | -0.81539 | 2.33693 |
| H | -3.10785 | 0.02436 | 3.42963 |

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| Conf. 4 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 3.47477 | -2.11049 | -0.46038 |
| C | 3.49018 | -0.61412 | -0.31235 |
| C | 3.26941 | 0.13486 | 0.77671 |
| C | 3.36873 | 1.65422 | 0.68399 |
| C | 1.98235 | 2.30398 | 0.67569 |
| C | 1.38012 | 2.56673 | -0.69507 |
| C | 2.42439 | -2.61109 | -1.49643 |
| C | 1.02389 | -2.75527 | -0.93364 |
| C | 0.21751 | -1.68099 | -0.82063 |
| C | -0.11874 | 2.91784 | -0.75531 |
| C | -1.02284 | 1.67284 | -0.87844 |
| C | -1.14637 | -1.65426 | -0.29753 |
| C | -1.0272 | 0.75375 | 0.35925 |
| C | -1.7667 | -0.56763 | 0.20775 |
| C | -3.2007 | -0.63171 | 0.75498 |
| C | -3.93984 | -1.9392 | 0.43362 |
| C | -3.20716 | -0.43442 | 2.2806 |
| O | -3.95172 | 0.50955 | 0.25928 |
| C | 0.65761 | -4.1443 | -0.47979 |
| C | 2.93401 | -0.39619 | 2.14677 |
| C | -0.39116 | 3.87626 | -1.92532 |
| O | 1.4257 | 2.61002 | 1.71248 |
| C | -4.35431 | 0.45809 | -1.10373 |
| H | 4.46448 | -2.42263 | -0.81667 |
| H | 3.31753 | -2.61418 | 0.49593 |
| H | 3.73485 | -0.08725 | -1.23462 |
| H | 3.90943 | 1.93623 | -0.22187 |
| H | 3.90694 | 2.04611 | 1.55214 |
| H | 1.97371 | 3.40571 | -1.08695 |
| H | 1.62135 | 1.72676 | -1.3562 |
| H | 2.75525 | -3.58097 | -1.87988 |
| H | 2.4219 | -1.92325 | -2.34796 |
| H | 0.62803 | -0.73243 | -1.15069 |
| H | -0.37051 | 3.43609 | 0.17678 |
| H | -2.04571 | 2.00959 | -1.06351 |
| H | -0.71876 | 1.10487 | -1.76656 |
| H | -1.68562 | -2.59401 | -0.32421 |
| H | 0.00259 | 0.52933 | 0.64234 |
| H | -1.45036 | 1.32104 | 1.19049 |
| H | -4.98062 | -1.84457 | 0.75229 |
| H | -3.92514 | -2.18027 | -0.63029 |
| H | -3.49861 | -2.77708 | 0.97647 |
| H | -4.23542 | -0.47362 | 2.64838 |
| H | -2.62792 | -1.21985 | 2.77079 |
| H | -2.78659 | 0.53265 | 2.55785 |
| H | 1.40578 | -4.52148 | 0.22752 |
| H | -0.31566 | -4.19799 | 0.00716 |
| H | 0.65826 | -4.83965 | -1.3275 |
| H | 2.05682 | 0.11424 | 2.55496 |
| H | 2.73829 | -1.46785 | 2.14793 |
| H | 3.7588 | -0.19929 | 2.84195 |
| H | -1.44755 | 4.15615 | -1.96428 |
| H | 0.19662 | 4.79409 | -1.83172 |
| H | -0.13444 | 3.4114 | -2.88354 |
| H | -4.70644 | 1.45836 | -1.36062 |
| H | -3.52614 | 0.19422 | -1.77119 |
| H | -5.17466 | -0.25051 | -1.26326 |

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| Conf. 5 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 3.17426 | -2.59145 | -0.55996 |
| C | 3.37979 | -1.10309 | -0.60385 |
| C | 3.51721 | -0.24099 | 0.41252 |
| C | 3.75128 | 1.23755 | 0.12176 |
| C | 2.50247 | 2.06716 | 0.42721 |
| C | 1.63578 | 2.45057 | -0.76088 |
| C | 1.88641 | -3.05027 | -1.30183 |
| C | 0.60409 | -2.80354 | -0.53682 |
| C | -0.11565 | -1.68351 | -0.75706 |
| C | 0.29276 | 3.10836 | -0.40998 |
| C | -0.7214 | 2.10725 | 0.19008 |
| C | -1.37411 | -1.31105 | -0.1279 |
| C | -1.34764 | 1.10683 | -0.81473 |
| C | -1.98149 | -0.10555 | -0.16211 |
| C | -3.33779 | 0.05266 | 0.56438 |
| C | -3.11301 | 0.33616 | 2.05924 |
| C | -4.21702 | 1.15955 | -0.04123 |
| O | -4.06193 | -1.20073 | 0.58185 |
| C | 0.24228 | -3.86746 | 0.4673 |
| C | 3.48177 | -0.60469 | 1.87464 |
| C | -0.27523 | 3.88038 | -1.60958 |
| O | 2.236 | 2.40058 | 1.56643 |
| C | -4.59188 | -1.66045 | -0.65558 |
| H | 4.02689 | -3.06946 | -1.05919 |
| H | 3.1674 | -2.97013 | 0.46417 |
| H | 3.44099 | -0.6956 | -1.6128 |
| H | 4.03952 | 1.37158 | -0.92239 |
| H | 4.55628 | 1.61742 | 0.7593 |
| H | 2.24881 | 3.13881 | -1.36021 |
| H | 1.51351 | 1.56697 | -1.39735 |
| H | 1.97831 | -4.12247 | -1.50803 |
| H | 1.84794 | -2.54492 | -2.27202 |
| H | 0.28437 | -0.99738 | -1.49778 |
| H | 0.50459 | 3.83358 | 0.38272 |
| H | -0.22503 | 1.55076 | 0.98921 |
| H | -1.51868 | 2.68427 | 0.66999 |
| H | -1.89878 | -2.09494 | 0.40839 |
| H | -2.08367 | 1.6306 | -1.43012 |
| H | -0.57279 | 0.7691 | -1.50466 |
| H | -4.07708 | 0.44231 | 2.56432 |
| H | -2.56815 | -0.49303 | 2.51464 |
| H | -2.53776 | 1.25054 | 2.20838 |
| H | -5.19782 | 1.13694 | 0.43999 |
| H | -3.78025 | 2.14437 | 0.13168 |
| H | -4.35782 | 1.04046 | -1.1172 |
| H | 1.07748 | -4.05223 | 1.15257 |
| H | -0.62875 | -3.61351 | 1.07022 |
| H | 0.04343 | -4.82012 | -0.03828 |
| H | 4.468 | -0.44714 | 2.32761 |
| H | 2.78616 | 0.0425 | 2.41564 |
| H | 3.19307 | -1.64102 | 2.04652 |
| H | -1.2321 | 4.34665 | -1.35627 |
| H | 0.41068 | 4.67331 | -1.9215 |
| H | -0.44032 | 3.22884 | -2.47279 |
| H | -4.96367 | -2.66983 | -0.47304 |
| H | -5.42611 | -1.04058 | -1.00188 |
| H | -3.82835 | -1.70216 | -1.43996 |

**Figure S6e**. Re-optimized conformers of (12*S*)-**1** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile.

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| Conf. 1  20.79%  -971.16409466 a. u. | Conf. 2  4.59%  -971.16296862 a. u. | Conf. 3  1.77%  -971.15570297 a. u. |
|  |  |  |
| Conf. 4  70.48%  -971.16454601 a. u. | Conf. 5  2.38%  -971.15664626 a. u. |  |

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| Conf. 1 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.66625 | 2.8229 | 0.48781 |
| C | 2.75898 | 1.37958 | 0.91351 |
| C | 3.6683 | 0.46786 | 0.53723 |
| C | 3.58609 | -0.95919 | 1.05036 |
| C | 3.33129 | -2.03874 | -0.03037 |
| C | 1.99554 | -1.86952 | -0.71332 |
| C | 1.6832 | 3.0661 | -0.6958 |
| C | 0.21718 | 2.86385 | -0.35861 |
| C | -0.31485 | 1.62531 | -0.37695 |
| C | 0.75107 | -2.60014 | -0.39352 |
| C | -0.56942 | -1.90152 | -0.68544 |
| C | -1.69395 | 1.23563 | -0.10426 |
| C | -1.07988 | -1.10023 | 0.5387 |
| C | -2.09184 | -0.00491 | 0.24365 |
| C | -3.58057 | -0.30575 | 0.48778 |
| C | -3.99074 | -1.697 | -0.03027 |
| C | -3.88335 | -0.20656 | 1.99256 |
| O | -4.42033 | 0.71554 | -0.09108 |
| C | -0.54261 | 4.10767 | 0.01976 |
| C | 4.82469 | 0.7545 | -0.38989 |
| C | 0.70001 | -3.69314 | 0.65091 |
| O | 1.52523 | -2.93211 | -1.5752 |
| C | -4.58758 | 0.69933 | -1.50497 |
| H | 3.64636 | 3.20202 | 0.18754 |
| H | 2.34791 | 3.43169 | 1.34166 |
| H | 1.96953 | 1.04265 | 1.58143 |
| H | 4.5312 | -1.2109 | 1.54774 |
| H | 2.8023 | -1.02726 | 1.81069 |
| H | 3.40291 | -3.02598 | 0.43023 |
| H | 4.1161 | -1.99798 | -0.79359 |
| H | 1.86078 | -0.88681 | -1.16359 |
| H | 1.97244 | 2.40272 | -1.5162 |
| H | 1.83016 | 4.09148 | -1.05143 |
| H | 0.36625 | 0.82032 | -0.63211 |
| H | -0.42002 | -1.23168 | -1.53556 |
| H | -1.31324 | -2.64355 | -0.99372 |
| H | -2.46224 | 1.99458 | -0.20508 |
| H | -0.21529 | -0.64032 | 1.02577 |
| H | -1.49242 | -1.79736 | 1.27212 |
| H | -5.06983 | -1.82114 | 0.09144 |
| H | -3.74259 | -1.83621 | -1.08373 |
| H | -3.49783 | -2.48708 | 0.53799 |
| H | -4.92825 | -0.46698 | 2.18087 |
| H | -3.24823 | -0.88093 | 2.57054 |
| H | -3.70827 | 0.81492 | 2.33585 |
| H | -0.57058 | 4.81355 | -0.81884 |
| H | -1.56679 | 3.90503 | 0.33239 |
| H | -0.038 | 4.62775 | 0.84272 |
| H | 5.76667 | 0.41489 | 0.0556 |
| H | 4.71689 | 0.21455 | -1.33699 |
| H | 4.92478 | 1.81303 | -0.62829 |
| H | -0.04222 | -4.44325 | 0.36064 |
| H | 1.66142 | -4.19439 | 0.75609 |
| H | 0.40906 | -3.2946 | 1.6263 |
| H | -5.22103 | -0.13186 | -1.83289 |
| H | -5.08359 | 1.63593 | -1.76417 |
| H | -3.6304 | 0.64947 | -2.03444 |

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| Conf. 2 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.52434 | 2.92305 | 0.44295 |
| C | 2.63295 | 1.50382 | 0.9411 |
| C | 3.58407 | 0.60271 | 0.65242 |
| C | 3.52069 | -0.7983 | 1.23504 |
| C | 3.3864 | -1.94384 | 0.20205 |
| C | 2.10019 | -1.8708 | -0.58556 |
| C | 1.62128 | 3.08146 | -0.81635 |
| C | 0.14402 | 2.8296 | -0.57734 |
| C | -0.33625 | 1.57043 | -0.59943 |
| C | 0.86605 | -2.63782 | -0.31583 |
| C | -0.45437 | -2.01082 | -0.73972 |
| C | -1.7175 | 1.13055 | -0.42628 |
| C | -1.05354 | -1.13008 | 0.38552 |
| C | -2.09218 | -0.10819 | -0.04492 |
| C | -3.58608 | -0.49323 | -0.06211 |
| C | -3.9578 | -1.03797 | -1.45157 |
| C | -3.96242 | -1.53223 | 1.00815 |
| O | -4.42123 | 0.68 | 0.06606 |
| C | -0.6897 | 4.04927 | -0.28752 |
| C | 4.77582 | 0.88114 | -0.23147 |
| C | 0.78185 | -3.6712 | 0.78537 |
| O | 1.74009 | -2.99896 | -1.41676 |
| C | -4.47148 | 1.29943 | 1.34578 |
| H | 3.51089 | 3.32245 | 0.19388 |
| H | 2.12815 | 3.55743 | 1.24387 |
| H | 1.82147 | 1.17555 | 1.58663 |
| H | 4.43859 | -0.98299 | 1.80735 |
| H | 2.69006 | -0.85883 | 1.9447 |
| H | 3.46119 | -2.90078 | 0.72232 |
| H | 4.22375 | -1.9115 | -0.50365 |
| H | 1.9595 | -0.92078 | -1.09995 |
| H | 1.99466 | 2.40071 | -1.58682 |
| H | 1.75373 | 4.09844 | -1.20077 |
| H | 0.39283 | 0.78793 | -0.7836 |
| H | -0.27412 | -1.40548 | -1.63156 |
| H | -1.15687 | -2.80073 | -1.0278 |
| H | -2.50466 | 1.84307 | -0.64958 |
| H | -0.22989 | -0.59027 | 0.86007 |
| H | -1.46502 | -1.77731 | 1.16138 |
| H | -5.01004 | -1.3353 | -1.46653 |
| H | -3.79963 | -0.26443 | -2.20542 |
| H | -3.34701 | -1.90465 | -1.71174 |
| H | -5.04874 | -1.64934 | 1.02171 |
| H | -3.52477 | -2.50512 | 0.77809 |
| H | -3.63268 | -1.24342 | 2.00812 |
| H | -0.68422 | 4.73425 | -1.14369 |
| H | -1.72501 | 3.81061 | -0.04452 |
| H | -0.26732 | 4.60794 | 0.5561 |
| H | 5.70296 | 0.57746 | 0.26772 |
| H | 4.72233 | 0.30671 | -1.1629 |
| H | 4.86559 | 1.93277 | -0.50258 |
| H | 0.0808 | -4.46027 | 0.49631 |
| H | 1.74945 | -4.13377 | 0.97599 |
| H | 0.42101 | -3.22766 | 1.71703 |
| H | -3.47189 | 1.51527 | 1.73842 |
| H | -5.00666 | 2.24049 | 1.21006 |
| H | -5.01744 | 0.69135 | 2.07533 |

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| Conf. 3 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | -2.32811 | 2.91043 | 0.33956 |
| C | -2.66468 | 1.68257 | -0.48236 |
| C | -3.60816 | 0.77504 | -0.19737 |
| C | -3.78586 | -0.46169 | -1.05609 |
| C | -3.60103 | -1.79637 | -0.2927 |
| C | -2.27775 | -1.88004 | 0.43015 |
| C | -1.1136 | 3.71846 | -0.14388 |
| C | 0.27165 | 3.10883 | -0.02445 |
| C | 0.47974 | 1.79188 | 0.17428 |
| C | -1.06849 | -2.6031 | -0.01355 |
| C | 0.27346 | -2.08493 | 0.48321 |
| C | 1.76983 | 1.11302 | 0.29006 |
| C | 0.92159 | -1.09784 | -0.5174 |
| C | 2.00353 | -0.1919 | 0.03966 |
| C | 3.40392 | -0.77688 | 0.32713 |
| C | 3.48456 | -1.22972 | 1.79479 |
| C | 3.76787 | -1.95498 | -0.59185 |
| O | 4.4193 | 0.24981 | 0.24669 |
| C | 1.38256 | 4.1132 | -0.20282 |
| C | -4.53472 | 0.89971 | 0.9885 |
| C | -1.03717 | -3.42766 | -1.28078 |
| O | -1.91308 | -3.14179 | 1.03648 |
| C | 4.74132 | 0.73925 | -1.04968 |
| H | -2.16891 | 2.62654 | 1.3867 |
| H | -3.18682 | 3.59327 | 0.34857 |
| H | -2.06116 | 1.52236 | -1.37344 |
| H | -4.79473 | -0.4682 | -1.48795 |
| H | -3.08213 | -0.42389 | -1.89296 |
| H | -3.71555 | -2.62802 | -0.99069 |
| H | -4.39699 | -1.90831 | 0.45228 |
| H | -2.09343 | -1.0363 | 1.09413 |
| H | -1.10372 | 4.66885 | 0.40432 |
| H | -1.26703 | 4.00671 | -1.19486 |
| H | -0.39723 | 1.1608 | 0.2546 |
| H | 0.11019 | -1.58705 | 1.44277 |
| H | 0.93613 | -2.93624 | 0.67429 |
| H | 2.61898 | 1.70629 | 0.61265 |
| H | 0.13025 | -0.47184 | -0.93415 |
| H | 1.32394 | -1.66253 | -1.36305 |
| H | 4.4722 | -1.65215 | 1.99954 |
| H | 3.32485 | -0.374 | 2.45351 |
| H | 2.72901 | -1.98434 | 2.01943 |
| H | 4.80393 | -2.24622 | -0.40286 |
| H | 3.13431 | -2.8198 | -0.38765 |
| H | 3.66654 | -1.70808 | -1.65046 |
| H | 1.34741 | 4.87184 | 0.58779 |
| H | 2.37379 | 3.66187 | -0.20076 |
| H | 1.26093 | 4.64985 | -1.15111 |
| H | -4.2847 | 0.18116 | 1.77782 |
| H | -4.50888 | 1.89533 | 1.4318 |
| H | -5.56743 | 0.68727 | 0.69073 |
| H | -0.34486 | -4.26647 | -1.15838 |
| H | -2.02034 | -3.83368 | -1.5164 |
| H | -0.69578 | -2.83252 | -2.13164 |
| H | 5.28717 | -0.00115 | -1.64444 |
| H | 3.85051 | 1.05504 | -1.60337 |
| H | 5.38687 | 1.60579 | -0.89863 |

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| Conf. 4 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.71426 | 2.74152 | 0.50437 |
| C | 2.68641 | 1.31639 | 0.99462 |
| C | 3.57826 | 0.34549 | 0.7466 |
| C | 3.36337 | -1.05446 | 1.29458 |
| C | 3.17382 | -2.1575 | 0.22466 |
| C | 1.95419 | -1.9228 | -0.63418 |
| C | 1.8808 | 2.97252 | -0.79195 |
| C | 0.37907 | 2.85996 | -0.60925 |
| C | -0.21875 | 1.65283 | -0.66844 |
| C | 0.63643 | -2.57518 | -0.48475 |
| C | -0.5888 | -1.80733 | -0.95941 |
| C | -1.64073 | 1.35406 | -0.53095 |
| C | -1.24631 | -1.00804 | 0.19443 |
| C | -2.15078 | 0.14849 | -0.20378 |
| C | -3.66196 | -0.1126 | -0.13094 |
| C | -4.53165 | 1.12725 | -0.37995 |
| C | -4.06448 | -1.21203 | -1.12621 |
| O | -3.99354 | -0.69555 | 1.1594 |
| C | -0.3388 | 4.15334 | -0.32821 |
| C | 4.83735 | 0.53673 | -0.06363 |
| C | 0.38211 | -3.64934 | 0.54967 |
| O | 1.54433 | -2.96665 | -1.54761 |
| C | -3.76399 | 0.11613 | 2.3038 |
| H | 3.73897 | 3.06216 | 0.3004 |
| H | 2.33501 | 3.4033 | 1.29118 |
| H | 1.81562 | 1.04712 | 1.58812 |
| H | 4.23113 | -1.33514 | 1.90463 |
| H | 2.49586 | -1.05348 | 1.96132 |
| H | 3.11494 | -3.12838 | 0.72058 |
| H | 4.05156 | -2.19876 | -0.4297 |
| H | 1.93976 | -0.9393 | -1.10181 |
| H | 2.21889 | 2.25435 | -1.54439 |
| H | 2.12057 | 3.97043 | -1.17432 |
| H | 0.43626 | 0.80513 | -0.83718 |
| H | -0.28064 | -1.13508 | -1.76362 |
| H | -1.30682 | -2.50998 | -1.39483 |
| H | -2.32474 | 2.17231 | -0.72465 |
| H | -0.44662 | -0.60915 | 0.82624 |
| H | -1.81867 | -1.69076 | 0.82473 |
| H | -5.57833 | 0.85874 | -0.21981 |
| H | -4.28472 | 1.95413 | 0.28753 |
| H | -4.42508 | 1.47972 | -1.40784 |
| H | -5.13673 | -1.40658 | -1.043 |
| H | -3.84115 | -0.90547 | -2.1502 |
| H | -3.53531 | -2.14224 | -0.9155 |
| H | -0.24271 | 4.84001 | -1.17749 |
| H | -1.39876 | 4.02067 | -0.11244 |
| H | 0.11586 | 4.66107 | 0.53061 |
| H | 4.80001 | -0.03598 | -0.99685 |
| H | 5.01606 | 1.57848 | -0.32838 |
| H | 5.70935 | 0.17101 | 0.49048 |
| H | -0.37232 | -4.34889 | 0.17632 |
| H | 1.28684 | -4.21492 | 0.76915 |
| H | 0.00726 | -3.21972 | 1.48216 |
| H | -3.9501 | -0.51777 | 3.17189 |
| H | -2.73222 | 0.48402 | 2.34796 |
| H | -4.4444 | 0.97406 | 2.34777 |

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| Conf. 5 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | -2.74365 | 2.89377 | -0.24394 |
| C | -2.9617 | 1.47411 | -0.70675 |
| C | -3.65815 | 0.49382 | -0.11673 |
| C | -3.79944 | -0.85324 | -0.80413 |
| C | -3.37848 | -2.0826 | 0.03078 |
| C | -1.96733 | -2.00523 | 0.56033 |
| C | -1.40857 | 3.49487 | -0.75368 |
| C | -0.16368 | 2.96332 | -0.06947 |
| C | 0.4542 | 1.85996 | -0.53543 |
| C | -0.76171 | -2.64011 | -0.01546 |
| C | 0.58461 | -2.02798 | 0.33954 |
| C | 1.69175 | 1.26175 | -0.03973 |
| C | 1.16222 | -1.08015 | -0.74601 |
| C | 2.08777 | -0.01955 | -0.18419 |
| C | 3.48928 | -0.42841 | 0.32405 |
| C | 3.44845 | -0.7637 | 1.82439 |
| C | 4.07555 | -1.61926 | -0.45346 |
| O | 4.39928 | 0.69547 | 0.27288 |
| C | 0.28243 | 3.72818 | 1.14927 |
| C | -4.38929 | 0.64949 | 1.19422 |
| C | -0.80357 | -3.49263 | -1.26266 |
| O | -1.4236 | -3.21204 | 1.14307 |
| C | 4.81602 | 1.136 | -1.01413 |
| H | -2.79282 | 2.97221 | 0.84574 |
| H | -3.55519 | 3.52596 | -0.63007 |
| H | -2.51568 | 1.2447 | -1.67381 |
| H | -4.851 | -0.99888 | -1.08466 |
| H | -3.22671 | -0.83942 | -1.73621 |
| H | -3.50988 | -2.98352 | -0.57197 |
| H | -4.04698 | -2.19293 | 0.89232 |
| H | -1.77713 | -1.12272 | 1.17093 |
| H | -1.44894 | 4.58104 | -0.62035 |
| H | -1.34371 | 3.31583 | -1.83192 |
| H | 0. | 1.38053 | -1.39836 |
| H | 0.45596 | -1.47578 | 1.27331 |
| H | 1.28695 | -2.84227 | 0.54903 |
| H | 2.38997 | 1.93029 | 0.45486 |
| H | 0.32406 | -0.5869 | -1.24049 |
| H | 1.66604 | -1.67226 | -1.51481 |
| H | 4.45152 | -1.0303 | 2.16833 |
| H | 3.10447 | 0.10521 | 2.3888 |
| H | 2.77743 | -1.59829 | 2.02998 |
| H | 5.10691 | -1.78187 | -0.1312 |
| H | 3.51325 | -2.53252 | -0.25247 |
| H | 4.07266 | -1.45499 | -1.53268 |
| H | -0.53943 | 3.80927 | 1.87046 |
| H | 1.12629 | 3.26458 | 1.65987 |
| H | 0.56044 | 4.75482 | 0.88258 |
| H | -4.00877 | -0.0414 | 1.95423 |
| H | -4.31837 | 1.6595 | 1.59693 |
| H | -5.45249 | 0.41384 | 1.06654 |
| H | -0.05945 | -4.29186 | -1.18908 |
| H | -1.78105 | -3.95286 | -1.40378 |
| H | -0.57011 | -2.89858 | -2.15026 |
| H | 5.36799 | 2.06365 | -0.85567 |
| H | 5.48169 | 0.41443 | -1.50008 |
| H | 3.96633 | 1.33955 | -1.6746 |

**Figure S6f**. Re-optimized conformers of (11*R*, 12*R*)-**2** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile.

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| --- | --- | --- |
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| Conf. 1  0.02%  -971.15464835 a. u. | Conf. 2  74.32%  -971.15296407 a. u. | Conf. 3  0.00%  -971.14545343 a. u. |
|  |  |  |
| Conf. 4  25.66%  -971.15480698 a. u. | Conf. 5  0.01%  -971.15368466 a. u. |  |

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| Conf. 1 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | -2.26388 | 2.17362 | -0.8949 |
| C | -0.82079 | 2.05678 | -1.32887 |
| C | 0.2131 | 2.82783 | -0.95775 |
| C | 1.56693 | 2.67386 | -1.62539 |
| C | 2.76526 | 2.36661 | -0.70213 |
| C | 2.91193 | 0.91849 | -0.27961 |
| C | -3.09656 | 0.89481 | -1.08702 |
| C | -2.98224 | -0.17854 | 0.02399 |
| C | -1.54976 | -0.63551 | 0.25064 |
| C | 2.5759 | 0.32229 | 1.03506 |
| C | 2.46611 | -1.19503 | 1.16704 |
| C | -0.97823 | -1.73547 | -0.26985 |
| C | 1.06434 | -1.8439 | 1.29483 |
| C | 0.36293 | -2.27754 | 0.00686 |
| C | 0.88969 | -3.24783 | -0.78752 |
| C | 2.1513 | -4.01043 | -0.45278 |
| C | 0.28153 | -3.69845 | -2.09766 |
| C | -3.93687 | -1.33503 | -0.32156 |
| C | 0.09277 | 3.96307 | 0.03242 |
| C | 1.94927 | 1.13654 | 2.14858 |
| O | 3.93843 | 0.68426 | 0.70072 |
| O | -3.43852 | 0.51303 | 1.20874 |
| C | -3.53823 | -0.25286 | 2.39481 |
| H | -2.74152 | 2.96365 | -1.4955 |
| H | -2.35388 | 2.49543 | 0.14747 |
| H | -0.62889 | 1.29273 | -2.08402 |
| H | 1.50529 | 1.90434 | -2.4062 |
| H | 1.79483 | 3.61653 | -2.14674 |
| H | 2.75663 | 3.01536 | 0.1788 |
| H | 3.68968 | 2.61579 | -1.24184 |
| H | 2.94598 | 0.21981 | -1.12247 |
| H | -2.84226 | 0.42538 | -2.04625 |
| H | -4.15697 | 1.17123 | -1.13682 |
| H | -0.98096 | 0.03102 | 0.8952 |
| H | 3.01702 | -1.63806 | 0.33346 |
| H | 3.03831 | -1.44614 | 2.07189 |
| H | -1.58957 | -2.34067 | -0.9335 |
| H | 0.40578 | -1.1855 | 1.86662 |
| H | 1.17717 | -2.73608 | 1.92515 |
| H | 2.00687 | -5.07794 | -0.66883 |
| H | 2.99866 | -3.68584 | -1.07424 |
| H | 2.45563 | -3.9216 | 0.59233 |
| H | -0.15908 | -4.7024 | -2.00611 |
| H | -0.48256 | -3.02479 | -2.48869 |
| H | 1.0652 | -3.77798 | -2.86332 |
| H | -3.86082 | -2.15699 | 0.3963 |
| H | -4.96821 | -0.96719 | -0.32631 |
| H | -3.71937 | -1.73998 | -1.31514 |
| H | -0.91791 | 4.06422 | 0.43393 |
| H | 0.77552 | 3.8394 | 0.88252 |
| H | 0.35953 | 4.91822 | -0.44253 |
| H | 2.22954 | 0.72293 | 3.12515 |
| H | 2.28874 | 2.17381 | 2.11775 |
| H | 0.8557 | 1.13181 | 2.07958 |
| H | -2.61153 | -0.80135 | 2.61736 |
| H | -3.73137 | 0.4568 | 3.20446 |
| H | -4.36738 | -0.97416 | 2.35946 |

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| Conf. 2 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | -1.59768 | 3.09968 | -0.51245 |
| C | -2.1291 | 1.75253 | -0.93882 |
| C | -3.15764 | 1.05795 | -0.42315 |
| C | -3.57027 | -0.27027 | -1.03604 |
| C | -3.58005 | -1.47059 | -0.06025 |
| C | -2.24029 | -1.69934 | 0.60205 |
| C | -0.06665 | 3.28432 | -0.62148 |
| C | 0.85647 | 2.51831 | 0.37018 |
| C | 0.97175 | 1.04282 | 0.01942 |
| C | -1.23242 | -2.72017 | 0.23255 |
| C | 0.22225 | -2.42095 | 0.56728 |
| C | 2.107 | 0.32603 | 0.10759 |
| C | 1.0296 | -1.85771 | -0.62668 |
| C | 2.27985 | -1.10172 | -0.20016 |
| C | 3.48676 | -1.71815 | -0.08253 |
| C | 3.69951 | -3.19461 | -0.32909 |
| C | 4.77426 | -1.03249 | 0.31718 |
| C | 0.35629 | 2.66556 | 1.8171 |
| C | -4.0036 | 1.52994 | 0.7369 |
| C | -1.46581 | -3.73414 | -0.869 |
| O | -2.07543 | -2.88778 | 1.39556 |
| O | 2.1533 | 3.14985 | 0.40508 |
| C | 2.80884 | 3.37423 | -0.83244 |
| H | -1.92818 | 3.35423 | 0.49907 |
| H | -2.03998 | 3.86635 | -1.16878 |
| H | -1.62382 | 1.32388 | -1.80694 |
| H | -4.58549 | -0.1735 | -1.45029 |
| H | -2.90989 | -0.50012 | -1.88149 |
| H | -3.9043 | -2.36817 | -0.59616 |
| H | -4.32486 | -1.30532 | 0.7297 |
| H | -1.84296 | -0.80601 | 1.0913 |
| H | 0.14445 | 4.34971 | -0.46358 |
| H | 0.2393 | 3.05323 | -1.65035 |
| H | 0.03716 | 0.57842 | -0.2804 |
| H | 0.24213 | -1.7049 | 1.39561 |
| H | 0.70314 | -3.33661 | 0.93833 |
| H | 2.98187 | 0.86682 | 0.45313 |
| H | 0.3886 | -1.18027 | -1.20243 |
| H | 1.28313 | -2.66689 | -1.31709 |
| H | 4.3683 | -3.35378 | -1.18779 |
| H | 4.20113 | -3.65221 | 0.53515 |
| H | 2.78245 | -3.75699 | -0.50883 |
| H | 5.11364 | -1.38799 | 1.30083 |
| H | 5.57161 | -1.29199 | -0.39312 |
| H | 4.71568 | 0.05522 | 0.35969 |
| H | 0.18861 | 3.72112 | 2.06138 |
| H | -0.57405 | 2.11186 | 1.97531 |
| H | 1.11345 | 2.26649 | 2.49778 |
| H | -5.06537 | 1.54276 | 0.45396 |
| H | -3.92188 | 0.85733 | 1.6008 |
| H | -3.7405 | 2.53463 | 1.07417 |
| H | -0.95246 | -4.67231 | -0.62404 |
| H | -2.52757 | -3.96 | -0.98958 |
| H | -1.0729 | -3.37902 | -1.82874 |
| H | 2.84277 | 2.47318 | -1.45893 |
| H | 2.34684 | 4.18804 | -1.40852 |
| H | 3.83264 | 3.66881 | -0.58318 |

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| Conf. 3 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | -2.3879 | 2.03634 | 1.144 |
| C | -0.90013 | 1.92135 | 1.36974 |
| C | 0.06853 | 2.79233 | 1.04321 |
| C | 1.51699 | 2.47233 | 1.37214 |
| C | 2.46439 | 2.411 | 0.15085 |
| C | 2.00669 | 1.43685 | -0.91348 |
| C | -3.10493 | 0.69501 | 0.8945 |
| C | -2.79688 | -0.08391 | -0.41364 |
| C | -1.33511 | -0.51478 | -0.48226 |
| C | 2.57096 | 0.09513 | -1.19659 |
| C | 1.70786 | -0.92906 | -1.92954 |
| C | -0.85454 | -1.60886 | 0.12617 |
| C | 1.28494 | -2.2169 | -1.17797 |
| C | 0.54188 | -2.12231 | 0.15169 |
| C | 1.03424 | -2.63505 | 1.30909 |
| C | 2.36396 | -3.33619 | 1.47604 |
| C | 0.27489 | -2.57873 | 2.61841 |
| C | -3.16305 | 0.75469 | -1.64974 |
| C | -0.17516 | 4.12308 | 0.37 |
| C | 3.7619 | -0.44763 | -0.435 |
| O | 2.87421 | 1.23411 | -2.04053 |
| O | -3.6688 | -1.22503 | -0.27904 |
| C | -3.77474 | -2.09638 | -1.39121 |
| H | -2.61502 | 2.74197 | 0.33697 |
| H | -2.8521 | 2.46697 | 2.04567 |
| H | -0.59412 | 1.01019 | 1.88354 |
| H | 1.91365 | 3.23609 | 2.05849 |
| H | 1.56169 | 1.51631 | 1.90759 |
| H | 3.47549 | 2.16596 | 0.49114 |
| H | 2.536 | 3.40204 | -0.31745 |
| H | 0.96456 | 1.5848 | -1.20582 |
| H | -4.18815 | 0.86879 | 0.90397 |
| H | -2.89355 | 0.01101 | 1.72582 |
| H | -0.67582 | 0.15937 | -1.01844 |
| H | 0.83139 | -0.41708 | -2.3372 |
| H | 2.28838 | -1.25697 | -2.8041 |
| H | -1.58689 | -2.20601 | 0.66909 |
| H | 2.17665 | -2.83435 | -1.05113 |
| H | 0.64191 | -2.77201 | -1.87602 |
| H | 3.00655 | -2.79167 | 2.1823 |
| H | 2.20489 | -4.33061 | 1.91744 |
| H | 2.92974 | -3.47448 | 0.55417 |
| H | 0.91639 | -2.16618 | 3.40949 |
| H | -0.6272 | -1.96701 | 2.5777 |
| H | -0.00901 | -3.58812 | 2.95084 |
| H | -4.22275 | 1.03127 | -1.62241 |
| H | -2.56664 | 1.67219 | -1.68314 |
| H | -2.97026 | 0.21062 | -2.58005 |
| H | 0.24228 | 4.94029 | 0.97501 |
| H | 0.31754 | 4.18237 | -0.60975 |
| H | -1.23662 | 4.3342 | 0.22074 |
| H | 4.33382 | -1.13573 | -1.07015 |
| H | 4.43458 | 0.35805 | -0.13314 |
| H | 3.44484 | -0.99524 | 0.45742 |
| H | -4.33367 | -1.64494 | -2.22298 |
| H | -2.79266 | -2.42265 | -1.75825 |
| H | -4.32797 | -2.97194 | -1.03934 |

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| Conf. 4 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 1.46486 | -2.93532 | -1.18977 |
| C | 1.99022 | -1.52422 | -1.29073 |
| C | 3.05749 | -0.98121 | -0.67741 |
| C | 3.48121 | 0.44645 | -0.98677 |
| C | 3.51907 | 1.41569 | 0.22027 |
| C | 2.16082 | 1.5887 | 0.86049 |
| C | -0.06645 | -3.10074 | -1.06747 |
| C | -0.77933 | -2.53115 | 0.19484 |
| C | -0.92613 | -1.0231 | 0.08453 |
| C | 1.19685 | 2.67618 | 0.57865 |
| C | -0.28314 | 2.35704 | 0.741 |
| C | -2.05938 | -0.37544 | -0.2376 |
| C | -0.91732 | 1.8659 | -0.58435 |
| C | -2.21005 | 1.07886 | -0.41934 |
| C | -3.43067 | 1.67645 | -0.45299 |
| C | -3.63236 | 3.16402 | -0.63004 |
| C | -4.74787 | 0.95242 | -0.28828 |
| C | -0.0069 | -2.90176 | 1.47399 |
| C | 3.95209 | -1.7176 | 0.29392 |
| C | 1.52339 | 3.82931 | -0.34978 |
| O | 1.96576 | 2.65761 | 1.80356 |
| O | -2.06351 | -3.18308 | 0.14402 |
| C | -2.86539 | -3.14389 | 1.31195 |
| H | 1.95497 | -3.4794 | -0.37667 |
| H | 1.74978 | -3.46858 | -2.11075 |
| H | 1.44543 | -0.89172 | -1.99452 |
| H | 4.49175 | 0.42558 | -1.42262 |
| H | 2.81999 | 0.86309 | -1.75666 |
| H | 3.91182 | 2.3829 | -0.10851 |
| H | 4.21991 | 1.04659 | 0.98064 |
| H | 1.72398 | 0.64627 | 1.20113 |
| H | -0.28601 | -4.17534 | -1.07711 |
| H | -0.5617 | -2.67372 | -1.94766 |
| H | -0.00441 | -0.47519 | 0.25656 |
| H | -0.38819 | 1.59093 | 1.51614 |
| H | -0.81884 | 3.24404 | 1.10582 |
| H | -2.93906 | -0.99062 | -0.39502 |
| H | -0.193 | 1.22355 | -1.09862 |
| H | -1.07184 | 2.72046 | -1.24902 |
| H | -4.25698 | 3.36704 | -1.51213 |
| H | -4.17729 | 3.5787 | 0.22998 |
| H | -2.70736 | 3.73261 | -0.73473 |
| H | -5.27785 | 1.3262 | 0.59953 |
| H | -5.40536 | 1.15656 | -1.14517 |
| H | -4.66026 | -0.1291 | -0.18437 |
| H | 0.11872 | -3.98839 | 1.54753 |
| H | 0.98408 | -2.43888 | 1.46777 |
| H | -0.52344 | -2.54946 | 2.37168 |
| H | 4.9954 | -1.68981 | -0.05034 |
| H | 3.94304 | -1.24995 | 1.28735 |
| H | 3.67543 | -2.76619 | 0.42127 |
| H | 1.00551 | 4.73467 | -0.00964 |
| H | 2.59374 | 4.04557 | -0.36203 |
| H | 1.19717 | 3.62397 | -1.37586 |
| H | -2.48622 | -3.81165 | 2.09832 |
| H | -2.96016 | -2.13105 | 1.72548 |
| H | -3.8569 | -3.49539 | 1.01084 |

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| Conf. 5 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.48295 | 1.94953 | -0.15239 |
| C | 1.00229 | 2.21438 | 0.0199 |
| C | 0.41274 | 2.76993 | 1.08915 |
| C | -1.07178 | 3.07335 | 1.17035 |
| C | -1.95805 | 2.83417 | -0.06362 |
| C | -2.49469 | 1.42259 | -0.23623 |
| C | 3.04167 | 0.69635 | 0.559 |
| C | 2.79376 | -0.67043 | -0.12614 |
| C | 1.3146 | -0.96387 | -0.31934 |
| C | -2.36655 | 0.53016 | -1.41673 |
| C | -2.66268 | -0.95924 | -1.26242 |
| C | 0.53035 | -1.66665 | 0.51592 |
| C | -1.48272 | -1.93948 | -1.06551 |
| C | -0.88286 | -2.03473 | 0.33693 |
| C | -1.59785 | -2.55317 | 1.37207 |
| C | -2.98888 | -3.12631 | 1.22515 |
| C | -1.10006 | -2.63302 | 2.79919 |
| C | 3.51843 | -1.75557 | 0.69132 |
| C | 1.16561 | 3.18623 | 2.33248 |
| C | -1.59397 | 0.92719 | -2.65778 |
| O | -3.56377 | 1.31008 | -1.19227 |
| O | 3.41055 | -0.52225 | -1.42392 |
| C | 3.433 | -1.66929 | -2.25251 |
| H | 3.05144 | 2.81135 | 0.21949 |
| H | 2.72002 | 1.87108 | -1.21829 |
| H | 0.37273 | 1.93603 | -0.8208 |
| H | -1.5 | 2.53019 | 2.02932 |
| H | -1.16699 | 4.13469 | 1.44686 |
| H | -1.45707 | 3.18643 | -0.97089 |
| H | -2.85079 | 3.46412 | 0.04601 |
| H | -2.71082 | 0.92081 | 0.7128 |
| H | 2.64362 | 0.64148 | 1.57868 |
| H | 4.13139 | 0.80552 | 0.63836 |
| H | 0.90576 | -0.52755 | -1.22773 |
| H | -3.3789 | -1.0643 | -0.44255 |
| H | -3.20142 | -1.25796 | -2.17378 |
| H | 0.99694 | -2.05445 | 1.41684 |
| H | -0.6946 | -1.71657 | -1.7898 |
| H | -1.84536 | -2.93615 | -1.34912 |
| H | -3.067 | -4.06192 | 1.79566 |
| H | -3.74901 | -2.45023 | 1.64319 |
| H | -3.27173 | -3.34265 | 0.19283 |
| H | -1.8937 | -2.31349 | 3.48794 |
| H | -0.85412 | -3.66908 | 3.07573 |
| H | -0.22798 | -2.00994 | 3.00289 |
| H | 4.59703 | -1.56805 | 0.67052 |
| H | 3.19423 | -1.74127 | 1.73681 |
| H | 3.32842 | -2.75866 | 0.29827 |
| H | 0.98306 | 4.24484 | 2.56528 |
| H | 0.82132 | 2.61505 | 3.20656 |
| H | 2.24529 | 3.04241 | 2.24951 |
| H | -2.11337 | 0.5535 | -3.54883 |
| H | -1.51314 | 2.01231 | -2.75201 |
| H | -0.58328 | 0.50425 | -2.66052 |
| H | 4.13323 | -2.43542 | -1.88956 |
| H | 2.43957 | -2.12979 | -2.35581 |
| H | 3.76922 | -1.33191 | -3.2372 |

**Figure S6g**. Re-optimized conformers of (4*S*, 11*R*, 12*R*)-**3** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile.

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|  |  |
| Conf. 1  4.29%  -780.12918558 a. u. | Conf. 2  2.00%  -780.13733449 a. u. |
|  |  |
| Conf. 3  14.36%  -780.13310085 a. u. | Conf. 4  79.34%  -780.13557317 a. u. |

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| Conf. 1 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | -2.89044 | -0.76114 | -1.61945 |
| C | -2.72948 | -2.05723 | -0.77478 |
| C | -2.46782 | 0.51826 | -0.92405 |
| C | -1.35037 | 1.15542 | -1.30125 |
| C | 0.82019 | -3.09002 | 0.60562 |
| C | 1.67845 | -1.84995 | 0.59005 |
| C | 2.74323 | -1.6453 | -0.19686 |
| C | 3.4903 | -0.38038 | -0.3276 |
| C | 2.81247 | 0.91378 | 0.08984 |
| C | 1.59188 | 1.20534 | -0.8127 |
| C | -0.74181 | 2.40198 | -0.73756 |
| C | 0.76948 | 2.4381 | -0.48706 |
| C | -0.19355 | 2.53781 | 0.68089 |
| C | 4.7059 | -0.3745 | -0.89749 |
| C | -0.32819 | 3.9098 | 1.32242 |
| C | -0.32833 | 1.40512 | 1.6811 |
| H | -1.15837 | 3.32375 | -1.14123 |
| H | 1.2597 | 3.37461 | -0.74353 |
| C | -3.38428 | 1.01018 | 0.167 |
| C | -1.2978 | -2.46829 | -0.55169 |
| C | -0.66397 | -2.71614 | 0.60193 |
| C | -1.28489 | -2.61456 | 1.97185 |
| H | -3.947 | -0.68365 | -1.90489 |
| H | -2.32084 | -0.87786 | -2.54695 |
| H | -3.23862 | -2.85935 | -1.32524 |
| H | -3.26707 | -1.95347 | 0.16998 |
| H | -0.80759 | 0.72074 | -2.13964 |
| H | 1.03094 | -3.68442 | 1.50419 |
| H | 1.06555 | -3.71772 | -0.25533 |
| H | 1.34667 | -1.05202 | 1.24816 |
| H | 3.08918 | -2.46278 | -0.82808 |
| H | 2.48994 | 0.85494 | 1.13433 |
| H | 3.5332 | 1.73433 | 0.03038 |
| H | 1.94902 | 1.29536 | -1.84628 |
| H | 0.94831 | 0.3267 | -0.80219 |
| H | 5.17372 | -1.29081 | -1.24344 |
| H | 5.26719 | 0.54408 | -1.02965 |
| H | -1.30493 | 4.0225 | 1.8062 |
| H | 0.44104 | 4.05914 | 2.08838 |
| H | -0.2255 | 4.70997 | 0.58471 |
| H | -1.26556 | 1.49806 | 2.23805 |
| H | -0.32683 | 0.42625 | 1.20427 |
| H | 0.48744 | 1.43807 | 2.41095 |
| H | -3.0459 | 1.95477 | 0.59172 |
| H | -4.39543 | 1.15683 | -0.23113 |
| H | -3.47404 | 0.28307 | 0.9809 |
| H | -0.71762 | -2.57997 | -1.46854 |
| H | -2.30626 | -2.23574 | 1.9563 |
| H | -1.29472 | -3.59734 | 2.45792 |
| H | -0.69163 | -1.95771 | 2.61836 |

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| Conf. 2 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 2.79185 | 1.6769 | -1.17822 |
| C | 2.13313 | 2.57388 | -0.11303 |
| C | 2.56493 | 0.17615 | -1.12241 |
| C | 1.89171 | -0.42553 | -0.13087 |
| C | -1.76193 | 2.79115 | 0.48725 |
| C | -2.23552 | 1.36574 | 0.36184 |
| C | -2.96916 | 0.86465 | -0.64052 |
| C | -3.25069 | -0.56579 | -0.86549 |
| C | -2.32651 | -1.59511 | -0.23478 |
| C | -0.88604 | -1.44628 | -0.77665 |
| C | 1.59395 | -1.87953 | 0.00385 |
| C | 0.16345 | -2.40682 | -0.24864 |
| C | 0.74366 | -2.41142 | 1.15004 |
| C | -4.23898 | -0.93602 | -1.69513 |
| C | 1.14389 | -3.76819 | 1.70889 |
| C | 0.22595 | -1.46989 | 2.22303 |
| H | 2.38376 | -2.54755 | -0.32553 |
| H | 0.1277 | -3.39122 | -0.70979 |
| C | 3.16003 | -0.56522 | -2.29467 |
| C | 0.62745 | 2.65539 | -0.2108 |
| C | -0.25929 | 2.80551 | 0.78132 |
| C | 0.09723 | 2.92458 | 2.24099 |
| H | 3.87542 | 1.85703 | -1.156 |
| H | 2.47378 | 2.02679 | -2.17083 |
| H | 2.55265 | 3.57974 | -0.24961 |
| H | 2.44684 | 2.25769 | 0.88557 |
| H | 1.49115 | 0.21273 | 0.64788 |
| H | -2.28951 | 3.3026 | 1.30205 |
| H | -1.9866 | 3.33762 | -0.43281 |
| H | -1.86895 | 0.69298 | 1.1327 |
| H | -3.36524 | 1.54774 | -1.39062 |
| H | -2.32048 | -1.48435 | 0.85467 |
| H | -2.7095 | -2.59786 | -0.44474 |
| H | -0.92134 | -1.56201 | -1.86694 |
| H | -0.55794 | -0.42215 | -0.60828 |
| H | -4.87053 | -0.20266 | -2.1866 |
| H | -4.44505 | -1.98038 | -1.90271 |
| H | 1.92298 | -3.66206 | 2.47199 |
| H | 0.28734 | -4.26852 | 2.17421 |
| H | 1.53075 | -4.4253 | 0.92566 |
| H | -0.12285 | -0.51794 | 1.82485 |
| H | -0.60936 | -1.93038 | 2.7601 |
| H | 1.01038 | -1.25468 | 2.95697 |
| H | 3.02196 | -1.64413 | -2.2268 |
| H | 2.70539 | -0.22724 | -3.2335 |
| H | 4.23421 | -0.36257 | -2.38028 |
| H | 0.23417 | 2.58861 | -1.22554 |
| H | 1.16326 | 2.80665 | 2.43416 |
| H | -0.20665 | 3.90559 | 2.62537 |
| H | -0.44224 | 2.18036 | 2.83844 |

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| Conf. 3 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 0.49333 | -3.06251 | -0.64017 |
| C | 1.50303 | -2.77987 | 0.51375 |
| C | -0.8605 | -2.38844 | -0.48416 |
| C | -1.0733 | -1.1538 | -0.96411 |
| C | 3.55114 | 0.5484 | 0.00252 |
| C | 2.34564 | 1.38296 | -0.31972 |
| C | 2.01921 | 2.55076 | 0.24812 |
| C | 0.82749 | 3.35812 | -0.06179 |
| C | -0.33969 | 2.7149 | -0.78791 |
| C | -1.14887 | 1.79171 | 0.15127 |
| C | -2.32893 | -0.34114 | -0.95769 |
| C | -2.34307 | 1.11747 | -0.50037 |
| C | -3.15372 | 0.08037 | 0.25469 |
| C | 0.75498 | 4.62908 | 0.36582 |
| C | -4.66258 | 0.1209 | 0.07436 |
| C | -2.73644 | -0.28604 | 1.66979 |
| H | -2.93751 | -0.51196 | -1.8457 |
| H | -2.93089 | 1.78786 | -1.12426 |
| C | -1.90853 | -3.21365 | 0.21786 |
| C | 2.02041 | -1.37068 | 0.45241 |
| C | 3.26298 | -0.93738 | 0.20214 |
| C | 4.47752 | -1.82041 | 0.06339 |
| H | 0.34403 | -4.14567 | -0.70352 |
| H | 0.95964 | -2.75168 | -1.57973 |
| H | 2.31478 | -3.50705 | 0.44365 |
| H | 1.00278 | -2.95898 | 1.47382 |
| H | -0.24457 | -0.68885 | -1.49706 |
| H | 4.07906 | 0.95451 | 0.87466 |
| H | 4.26533 | 0.627 | -0.83125 |
| H | 1.70537 | 0.97485 | -1.09699 |
| H | 2.68107 | 2.96564 | 1.00717 |
| H | -0.99652 | 3.49965 | -1.17433 |
| H | 0.00882 | 2.14571 | -1.65586 |
| H | -0.47785 | 1.04255 | 0.57561 |
| H | -1.49907 | 2.40071 | 0.99359 |
| H | 1.56238 | 5.08337 | 0.93117 |
| H | -0.11054 | 5.24938 | 0.16004 |
| H | -5.11032 | -0.8597 | 0.27175 |
| H | -5.1176 | 0.83807 | 0.76696 |
| H | -4.93727 | 0.4175 | -0.94141 |
| H | -3.27518 | -1.17368 | 2.01311 |
| H | -1.66974 | -0.49322 | 1.75499 |
| H | -2.97978 | 0.52925 | 2.36007 |
| H | -2.86614 | -2.70068 | 0.28613 |
| H | -2.0623 | -4.15628 | -0.32038 |
| H | -1.58822 | -3.48445 | 1.23069 |
| H | 1.24622 | -0.61612 | 0.55263 |
| H | 4.27588 | -2.86528 | 0.29779 |
| H | 4.88103 | -1.77128 | -0.95485 |
| H | 5.2764 | -1.47565 | 0.73023 |

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| Conf. 4 | Coordinates (Angstroms) | | |
| atom | X | Y | Z |
| C | 1.3532 | -2.96762 | -0.27965 |
| C | 2.55963 | -2.0787 | -0.7012 |
| C | -0.00588 | -2.47155 | -0.73342 |
| C | -0.91153 | -2.0594 | 0.16625 |
| C | 2.8657 | 1.50737 | 0.94147 |
| C | 1.45597 | 1.92076 | 0.63694 |
| C | 1.08512 | 2.83225 | -0.27242 |
| C | -0.2942 | 3.17429 | -0.65903 |
| C | -1.44838 | 2.30137 | -0.19611 |
| C | -1.35847 | 0.86434 | -0.75854 |
| C | -2.285 | -1.52917 | -0.09851 |
| C | -2.53168 | -0.05557 | -0.47342 |
| C | -2.94292 | -0.57818 | 0.88911 |
| C | -0.50938 | 4.22281 | -1.47089 |
| C | -4.43356 | -0.75755 | 1.12857 |
| C | -2.18892 | -0.16983 | 2.14275 |
| H | -2.96138 | -2.23292 | -0.57872 |
| H | -3.37097 | 0.09104 | -1.14933 |
| C | -0.2597 | -2.46862 | -2.21934 |
| C | 2.43044 | -0.64896 | -0.25253 |
| C | 3.18846 | 0.04854 | 0.60393 |
| C | 4.41504 | -0.48007 | 1.30357 |
| H | 1.35524 | -3.05838 | 0.81058 |
| H | 1.52741 | -3.97293 | -0.68518 |
| H | 2.6451 | -2.09924 | -1.79483 |
| H | 3.46957 | -2.54426 | -0.31638 |
| H | -0.61727 | -2.1139 | 1.21261 |
| H | 3.05732 | 1.64718 | 2.01461 |
| H | 3.57786 | 2.16373 | 0.42497 |
| H | 0.69318 | 1.38518 | 1.19523 |
| H | 1.86377 | 3.37089 | -0.81131 |
| H | -1.47153 | 2.26238 | 0.89782 |
| H | -2.38729 | 2.76533 | -0.51168 |
| H | -1.24443 | 0.9306 | -1.84707 |
| H | -0.44453 | 0.39775 | -0.3988 |
| H | 0.30971 | 4.83538 | -1.83403 |
| H | -1.50804 | 4.49764 | -1.79205 |
| H | -4.61748 | -1.51842 | 1.89539 |
| H | -4.89243 | 0.17702 | 1.47001 |
| H | -4.94924 | -1.0707 | 0.21698 |
| H | -2.26967 | -0.94828 | 2.90984 |
| H | -1.12752 | 0.00277 | 1.96286 |
| H | -2.61154 | 0.74844 | 2.56235 |
| H | -1.26323 | -2.1187 | -2.46226 |
| H | 0.45663 | -1.82802 | -2.7456 |
| H | -0.13651 | -3.47651 | -2.63306 |
| H | 1.58648 | -0.12679 | -0.69235 |
| H | 4.6788 | -1.49251 | 0.99844 |
| H | 5.27758 | 0.16711 | 1.10559 |
| H | 4.27073 | -0.47992 | 2.39018 |

**Figure S6h**. Re-optimized conformers of (1*S*, 2*R*)-**4** calculated at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile.