# Extending the structural diversity of labdane diterpenoids from marine derived fungus *Talaromyces* sp. HDN151403 using heterologous expression

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**Table S1.** Fungal strains and plasmids used in this study.

| Strain/plasmid | Primer name | Descrption | Reference |
|---|---|---|---|
| *Talaromyces* sp. HDN151403 | | Antarctica sponge-derived fungus, GenBank: MW888514 | [34] |
| *E. coli* XL1-blue | | *recA1 endA1 gyrA96 thi-1 hsdR17supE44 relA1 lac* [*F' pro AB lac IqZΔM15 Tn10* (*Tetr*)] | This study |
| *Saccharomyces cerevisiae* BJ5464-NpgA | | (*MATα ura3-52 his3-Δ200 leu2-Δ1 trp1 pep4::HIS3 prb1 Δ1.6R can1 GAL*) | This study |
| *Aspergillus nidulans* A1145 | | *pyrG89*; *pyroA4*; *nkuA::argB*; *riboB2* | This study |
| AN-empty vectors | | Harboring three empty pANU, pANR, and pANP vectors | This study |
| AN-*labdA* | | Harboring the plasmid pANU-*labdA* | This study |
| AN-*labdAB* | | Harboring the plasmids pANU-*labdA* and pANP-*labdB* | This study |
| AN-*labdABE* | | Harboring the plasmids pANU-*labdA*-*labdE* and pANP-*labdB* | This study |
| AN-*labdABF* | | Harboring the plasmids pANU-*labdA*-*labdF* and pANP-*labdB* | This study |
| AN-*labdABEF* | | Harboring the plasmids pANU-*labdA-labdE-labdF* and pANP-*labdB* | This study |
| AN-*labdABEFG* | | Harboring the plasmids pANU-*labdA-labdE-labdF*, pANP-*labdB* and pANR-*labdG* | This study |
| AN-*labdABDEFG* | | Harboring the plasmids pANU-*labdA-labdE-labdF*, pANP-*labdB* and pANR-*labdD-labdG* | This study |
| AN-*labdABCDEG* | | Harboring the plasmids pANU-*labdA-labdE*, pANP-*labdB* and pANR-*labdC-labdD-labdG* | This study |
| AN-*labdABCDEFG* | | Harboring the plasmids pANU-*labdA-labdE-labdF*, pANP-*labdB* and pANR-*labdC-labdD-labdG* | This study |
| AN-*labdCDEFG* | | Harboring the plasmids pANU-*labdE-labdF* and pANR-*labdC-labdD-labdG* | This study |
| AN-*labdE* | | Harboring the plasmids pANU-*labdE* | This study |
| AN-*labdG* | | Harboring the plasmids pANR-*labdG* | This study |
| pANR | | *E. coli*-yeast-fungal shuttle vectors, ampicillin resistance, selection is by *riboB*. | [35] |
| pANP | | *E. coli*-yeast-fungal shuttle vectors, ampicillin resistance, selection is by *pyroA*. | [35] |
| pANU | | *E. coli*-yeast-fungal shuttle vectors, ampicillin resistance, selection is by *pyrG*. | [35] |
| pANU-*labdA* | U-*labdA*-F1/U-*labdA*-R1 | *labdA* gDNA with downstream 400 bp used the promoter *glaA* in *Pac*I-linearized pANU | This study |
| pANU-*labdA-labdE-labdF* | U-*labdA*-F2/U-*labdA*-R2<br>U-*labdE*-F1/U-*labdE*-R1 | *labdA* gDNA with downstream 400 bp, *labdE* gDNA with downstream 500 bp and *labdF* gDNA with | This study |

| | | | |
|---|---|---|---|
| | U-*labdF*-F1/U-*labdF*-R1 | downstream 400 bp in *Pac*I-linearized pANU | |
| pANU-*labdA*-*labdE* | U-*labdA*-F2/U-*labdA*-R2<br>U-*labdE*-F1/U-*labdE*-R2 | *labdA* gDNA with downstream 400 bp and *labdE* gDNA with downstream 500 bp in *Pac*I-linearized pANU | This study |
| pANU-*labdA*-*labdF* | U-*labdA*-F2/U-*labdA*-R2<br>U-*labdF*-F2/U-*labdF*-R1 | *labdA* gDNA with downstream 400 bp and *labdF* gDNA with downstream 400 bp in *Pac*I-linearized pANU | This study |
| pANU-*labdE*-*labdF* | U-*labdE*-F2/U-*labdE*-R1<br>U-*labdF*-F1/U-*labdF*-R1 | *labdE* gDNA with downstream 500 bp and *labdF* gDNA with downstream 400 bp in *Pac*I-linearized pANU | This study |
| pANU-*labdE* | U-*labdE*-F2/U-*labdE*-R2 | *labdE* gDNA with downstream 500 bp in *Pac*I-linearized pANU | This study |
| pANR-*labdC*-*labdD*-*labdG* | R-*labdC*-F1/R-*labdC*-R1<br>R-*labdD*-F1/R-*labdD*-R1<br>R-*labdG*-F1/R-*labdG*-R1 | *labdC* gDNA with downstream 500 bp, *labdD* gDNA with downstream 500 bp and *labdG* gDNA with downstream 500 bp in *Pac*I-linearized pANR | This study |
| pANR-*labdD*-*labdG* | R-*labdD*-F2/R-*labdD*-R1<br>R-*labdG*-F1/R-*labdG*-R1 | *labdD* gDNA with downstream 500 bp and *labdG* gDNA with downstream 500 bp in *Pac*I-linearized pANR | This study |
| pANR-*labdG* | R-*labdG*-F1/R-*labdG*-R2 | *labdG* gDNA with downstream 500 bp in *Pac*I-linearized pANR | This study |
| pANP-*labdB* | P-*labdB*-F1/P-*labdB*-R1 | *labdB* gDNA with downstream 500 bp used the promoter *amyB* in *Pac*I-linearized pANP | This study |

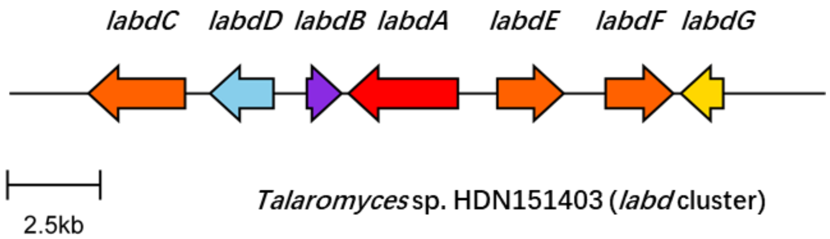
**Table S2.** PCR primer sets utilized in this study.

| Primer name | Oligonucleotide sequence (5′→3′)[a] |
|---|---|
| *amyB*-F | GATTAAAGGTGCCGAACGAGC |
| *amyB*-R | AAATGCCTTCTGTGGGGTTTATTG |
| *glaA*-F | CCTGATCTTCCGAACTGGTCG |
| *glaA*-R | TGCTGAGGTGTAATGATGCTGG |
| *gpdA*-F | ACTCCGGTGAATTGATTTGGGTG |
| *gpaA*-R | TGTTTAGATGTGTCTATGTGGCGG |
| *labdA*-F | ATGGGCCCAATGGATTTGC |
| *labdA*-R | TCATAACTCAAGGGACATGCGG |
| *labdB*-F | ATGTCTAATGACACCACTACCACGG |
| *labdB*-R | TCAATTCGTAATGGCCAGTGTATGAC |
| *labdC*-F | ATGATCACAGATCATGTCTCCCAGC |
| *labdC*-R | CCAAGCGGCGTAGTATGCC |
| *labdD*-F | GTCCAGTATGACAATGCTGCAG |
| *labdD*-R | GCGTGCCTAGAACAGCGATAG |
| *labdE*-F | ATGGCTCCCAGGATCAGTC |
| *labdE*-R | TCAAGCTTTTGTAGCTCTGGTGG |
| *labdF*-F | ATGTCCACCGCAAAGCGTG |
| *labdF*-R | TCACACAAGTATCGGTCGTAGTCG |
| *labdG*-F | ATGGCATCTAAACTGCCCCGC |
| *labdG*-R | TCAATCCAAGGGTTTGTGAGG |
| ITS-1 | TCCGTAGGTGAACCTGCGG |
| ITS-4 | TCCTCCGCTTATTGATATGC |
| Tubulin-F | ATTTGCCATCTTCACATCGGTCAGGCTG |
| Tubulin-R | TTAGTACTCGGCATCACCCTCGACATCC |
| U-*labdA*-F1 | ATCCCCAGCATCATTACACCTCAGCATTAATTAAGGCATGGGCCCAATGGATTTGCAAG |
| U-*labdA*-R1 | CTGCAGCCCGGGGGATCCACTAGTTCTAGAGCGGCCGGTACCAGACGACACGATAGTTG |
| U-*labdA*-F2 | CTGAGCTTCATCCCCAGCATCATTACACCTCAGCATTAATATGGGCCCAATGGATTTGC |
| U-*labdA*-R2 | CTTGGGTCTCTCCCGTCACCCAAATCAATTCACCGGAGTGGTACCAGACGACACGATAG |
| P-*labdB*-F1 | TTCTCTGAACAATAAACCCCACAGAAGGCATTTTTAATATGTCTAATGACACCACTACC |
| P-*labdB*-R1 | CGATAAGCTTGATATCGAATTCCTGCAGCCCGGGGGATCTTGAATCTGAAGTCCACGGC |
| U-*labdE*-F1 | TTGACTAACCATTACCCCGCCACATAGACACATCTAAACAATGGCTCCCAGGATCAGTC |
| U-*labdE*-F2 | CTGAGCTTCATCCCCAGCATCATTACACCTCAGCATTAATATGGCTCCCAGGATCAGTC |
| U-*labdE*-R1 | ATTGTTATATCATTTATAGCTCGTTCGGCACCTTTAATCTAGGTTGGATGACGTGCCAG |
| U-*labdE*-R2 | TCCTGCAGCCCGGGGGATCCACTAGTTCTAGAGCGGCCTAGGTTGGATGACGTGCCAGG |
| U-*labdF*-F1 | AGCTCTCCCTTCTCTGAACAATAAACCCCACAGAAGGCATTTATGTCCACCGCAAAGCG |
| U-*labdF*-F2 | CTCTCCCTTCTCTGAACAATAAACCCCACAGAAGGCATTTATGTCCACCGCAAAGCGTG |
| U-*labdF*-R1 | CCTGCAGCCCGGGGGATCCACTAGTTCTAGAGCGGCCGCGTATCATGTGTAGCACCATC |
| R-*labdC*-F1 | GCCTGAGCTTCATCCCCAGCATCATTACACCTCAGCAATGATCACAGATCATGTCTCCC |
| R-*labdC*-R1 | TGTTATATCATTTATAGCTCGTTCGGCACCTTTAATCCCTGACGGCGATACATACCTAG |
| R-*labdD*-F1 | CTCCCTTCTCTGAACAATAAACCCCACAGAAGGCATTTATGTCTACTGCGAAAGTCCAG |
| R-*labdD*-F2 | TGAGCTTCATCCCCAGCATCATTACACCTCAGCAATGTCTACTGCGAAAGTCCAGTATG |
| R-*labdD*-R1 | GATAAGCTTGATATCGAATTCCTGCAGCCCGGGGGATCCGAGCGTTACCTCACTTACAG |

| | |
|---|---|
| R-*labdG*-F1 | CCATTACCCCGCCACATAGACACATCTAAACATTAATGACACAATTGCCTTCAAGATGC |
| R-*labdG*-R1 | GTCATAGGTCGCCAGGTACGACCAGTTCGGAAGATCAGGCCTGAACGATGGATGAAGCC |
| R-*labdG*-R2 | CGATAAGCTTGATATCGAATTCCTGCAGCCCGGGGGATCCCTGAACGATGGATGAAGCC |

[a] The underlined sequence is a homologous recombination binding region.

**Table S3.** Annotation of each gene in the *labd* cluster from *Talaromyces* sp. HDN151403.




| Genes | Size | Translate | Putative Function | Closest Homolog (Origin, Accession No.) | Identity (%) |
|---|---|---|---|---|---|
| *labdC* | 780 | – | Bifunctional P450/methyltransferase. | *Talaromyces verruculosus*, KUL89355.1 | 758/780(97%) |
| *labdD* | 509 | – | Aldehyde dehydrogenase | *Talaromyces pinophilus*, GAM41999.1 | 484/509(95%) |
| *labdB* | 311 | + | Tyrosine phosphatase | *Talaromyces verruculosus*, KUL89334.1 | 300/311(96%) |
| *labdA* | 960 | – | Type II terpene cyclase | *Talaromyces verruculosus*, A0A348FUE1.1 | 860/963(89%) |
| *labdE* | 501 | + | P450 | *Talaromyces pinophilus*, KAF3385867.1 | 500/501(99%) |
| *labdF* | 542 | + | P450 | *Talaromyces verruculosus*, KUL89225.1 | 527/542(97%) |
| *labdG* | 314 | – | SDR | *Talaromyces verruculosus*, KUL89357.1 | 308/314(98%) |

**Table S4.** $^1$H and $^{13}$C NMR Spectroscopic Data for Compounds **1** and **2** in $CD_3OD$ (125 and 500 MHz).

| no. | **1** | | **2** | |
|---|---|---|---|---|
| | **$\delta_C$, mult** | **$\delta_H$ ($J$ in Hz)** | **$\delta_C$, mult** | **$\delta_H$ ($J$ in Hz)** |
| 1a | 38.3, $CH_2$ | 1.81, m | 38.3, $CH_2$ | 1.81, m |
| 1b | | 1.19, m | | 1.19, m |
| 2 | 28.6, $CH_2$ | 1.65 m | 28.6, $CH_2$ | 1.65, m |
| 3 | 79.4, CH | 3.20, m | 79.4, CH | 3.20, m |
| 4 | 40.2, C | – | 40.2, C | – |
| 5 | 56.0, CH | 1.12, dd (12.5, 2.8) | 56.0, CH | 1.12, dd (12.5, 3.3) |
| 6a | 25.3, $CH_2$ | 1.76, m | 25.2, $CH_2$ | 1.76, m |
| 6b | | 1.41, m | | 1.40, m |
| 7a | 39.3, $CH_2$ | 2.40, m | 39.4, $CH_2$ | 2.40, m |
| 7b | | 1.98, m | | 1.98, m |
| 8 | 149.3, C | – | 149.5, C | – |
| 9 | 57.1, CH | 1.61, m | 58.3, CH | 1.56, m |
| 10 | 40.4, C | – | 40.5, C | – |
| 11a | 22.8, $CH_2$ | 1.68, m | 22.2, $CH_2$ | 1.54, m |
| 11b | | 1.56, m | | 1.33, m |
| 12a | 40.7, $CH_2$ | 2.31, m | 37.0, $CH_2$ | 1.51, m |
| 12b | | 2.01, m | | 1.02, m |
| 13 | 161.9, C | – | 32.2, CH | 1.89, m |
| 14a | 116.8, CH | 5.61, s | 42.5, $CH_2$ | 2.28, dd (14.7, 6.6) |
| 14b | | | | 2.06, dd (14.7, 8.0) |
| 15 | 170.3, C | – | 177.2, C | – |
| 16 | 18.9, $CH_3$ | 2.13, d (1.2) | 20.4, $CH_3$ | 0.96, d (6.6) |
| 17a | 107.2, $CH_2$ | 4.89, s | 107.2, $CH_2$ | 4.83, s |
| 17b | | 4.55, s | | 4.52, s |
| 18 | 16.1, $CH_3$ | 0.77, s | 16.1, $CH_2$ | 0.77, s |
| 19 | 28.9, $CH_3$ | 0.98, s | 28.9, $CH_3$ | 0.98, s |
| 20 | 15.0, $CH_3$ | 0.73, s | 15.0, $CH_3$ | 0.72, s |

**Table S5.** $^{1}H$ and $^{13}C$ NMR Spectroscopic Data for Compounds **8–10** in $CD_3OD$ (125 and 500 MHz).

| no. | **8** | | **9** | | **10** | |
|---|---|---|---|---|---|---|
| | $\delta_C$, **mult** | $\delta_H$ **(*J* in Hz)** | $\delta_C$, **mult** | $\delta_H$ **(*J* in Hz)** | $\delta_C$, **mult** | $\delta_H$ **(*J* in Hz)** |
| 1a | 40.8, $CH_2$ | 1.85–1.94, m | 47.5, $CH_2$ | 2.37–2.44, m | 41.8, $CH_2$ | 1.70–1.79, m |
| 1b | | 1.05–1.15, m | | 0.98–1.04, m | | 1.47, t (12.2) |
| 2a | 21.2, $CH_2$ | 1.85–1.94, m | 65.5, CH | 4.11, m | 67.7, CH | 4.16, m |
| 2b | | 1.49–1.57 m | | | | |
| 3a | 39.9, $CH_2$ | 2.11–2.15, m | 48.9, $CH_2$ | 1.99–2.06, m | 75.1, CH | 3.96, d (2.6) |
| 3b | | 1.05–1.15, m | | 0.98–1.04, m | | |
| 4 | 45.1, C | – | 46.0, C | – | 49.8, C | – |
| 5 | 57.4, CH | 1.36, m | 56.7, CH | 1.34, dd (12.5, 2.9) | 48.9, CH | 1.70–1.79, m |
| 6a | 27.6, $CH_2$ | 1.99–2.04, m | 27.1, $CH_2$ | 1.99–2.06, m | 26.7, $CH_2$ | 1.86–1.95, m |
| 6b | | 1.85–1.94, m | | 1.83, m | | |
| 7a | 40.4, $CH_2$ | 2.42, m | 39.6, $CH_2$ | 2.37–2.44, m | 39.7, $CH_2$ | 2.42, m |
| 7b | | 1.85–1.94, m | | 1.94, m | | 1.86–1.95, m |
| 8 | 149.4, C | – | 148.8, C | – | 149.0, C | – |
| 9 | 56.6, CH | 1.64, dd (11.0, 1.7) | 56.5, CH | 1.69, m | 56.4, CH | 1.70–1.79, m |
| 10 | 41.5, C | – | 42.4, C | – | 41.7, C | – |
| 11a | 22.9, $CH_2$ | 1.73, m | 23.0, $CH_2$ | 1.76, m | 23.0, $CH_2$ | 1.70–1.79, m |
| 11b | | 1.49–1.57 m | | 1.57, m | | 1.57, m |
| 12a | 39.3, $CH_2$ | 2.30, m | 40.7, $CH_2$ | 2.31, m | 40.7, $CH_2$ | 2.31, m |
| 12b | | 1.99–2.04, m | | 2.11, m | | 2.04, m |
| 13 | 162.0, C | – | 161.9, C | – | 161.9, C | – |
| 14 | 116.7, CH | 5.61, d (1.2) | 116.8, CH | 5.62, d (1.2) | 116.9, CH | 5.62, s |
| 15 | 170.2, C | – | 170.2, C | – | 170.3, C | – |
| 16 | 18.9, $CH_3$ | 2.13, d (1.2) | 18.9, $CH_3$ | 2.14, d (1.2) | 18.9, $CH_3$ | 2.14, d (1.2) |
| 17a | 106.9, $CH_2$ | 4.89, s | 107.6, $CH_2$ | 4.93, s | 107.4, $CH_2$ | 4.92, s |
| 17b | | 4.54, s | | 4.57, s | | 4.56, s |
| 18 | 181.2, C | – | 180.5, C | – | 180.3, C | – |
| 19 | 29.6, $CH_3$ | 1.20, s | 29.5, $CH_3$ | 1.26, s | 25.0, $CH_3$ | 1.30, s |
| 20 | 13.4, $CH_3$ | 0.65, s | 14.2, $CH_3$ | 0.66, s | 14.2, $CH_3$ | 0.67, s |

**Table S6.** $^{1}H$ and $^{13}C$ NMR Spectroscopic Data for Compounds **11–13** in $CD_3OD$ (125 and 500 MHz).

| no. | **11** | | **12** | | **13** | |
|---|---|---|---|---|---|---|
| | $\delta_C$, **mult** | $\delta_H$ (***J*** **in Hz**) | $\delta_C$, **mult** | $\delta_H$ (***J*** **in Hz**) | $\delta_C$, **mult** | $\delta_H$ (***J*** **in Hz**) |
| 1a | 54.8, $CH_2$ | 2.49, m | 51.5, $CH_2$ | 2.62, m | 38.5, $CH_2$ | 3.09, d (15.0) |
| 1b | | 2.27–2.34, m | | 2.36, m | | 2.71, d (15.0) |
| 2 | 212.0, C | – | 194.5, C | – | 173.9, C | – |
| 3a | 52.2, $CH_2$ | 2.75, dd (14.0, 2.1) | 146.4, C | – | – | – |
| 3b | | 2.27–2.34, m | | | | |
| 4 | 48.9, C | – | 134.7, C | – | 39.3, CH | 2.89, p (7.5) |
| 5 | 56.1, CH | 1.92, m | 55.0, CH | 2.58, d (11.0) | 52.9, CH | 2.66, dd (11.4, 7.5) |
| 6a | 26.9, $CH_2$ | 2.15, m | 70.2, CH | 3.85, td (11.0, 5.1) | 78.7, CH | 4.99, td (11.4, 4.8) |
| 6b | | 1.84, m | | | | |
| 7a | 39.0, $CH_2$ | 2.45, m | 48.8, $CH_2$ | 2.77, m | 43.0, $CH_2$ | 3.03, dd (11.4, 4.8) |
| 7b | | 2.06, m | | 2.15, m | | 2.25, t (11.4) |
| 8 | 148.2, C | – | 145.0, C | – | 142.8, C | – |
| 9 | 55.4, CH | 2.00, m | 53.0, CH | 2.02, m | 49.5, CH | 2.48, d (10.6) |
| 10 | 45.0, C | – | 45.0, C | – | 51.9, C | – |
| 11a | 22.9, $CH_2$ | 1.59, m | 23.0, $CH_2$ | 1.62, m | 24.7, $CH_2$ | 1.86, m |
| 11b | | | | | | 1.46, m |
| 12a | 40.4, $CH_2$ | 2.27–2.34, m | 40.3, $CH_2$ | 2.36, m | 40.5, $CH_2$ | 2.34, m |
| 12b | | 2.06, m | | 2.11, m | | 2.10, m |
| 13 | 161.5, C | – | 161.3, C | – | 160.8, C | – |
| 14 | 117.0, CH | 5.62, d (1.2) | 117.0, CH | 5.65, s | 117.1, CH | 5.62, s |
| 15 | 170.1, C | – | 170.1, C | – | 170.1, C | – |
| 16 | 18.9, $CH_3$ | 2.13, d (1.2) | 18.8, $CH_3$ | 2.16, d (1.2) | 18.9, $CH_3$ | 2.15, d (1.2) |
| 17a | 108.1, $CH_2$ | 4.98, s | 110.0, $CH_2$ | 5.08, s | 114.3, $CH_2$ | 5.20, s |
| 17b | | 4.62, s | | 4.72, s | | 4.88, s |
| 18 | 179.5, C | – | – | – | 180.9, C | – |
| 19 | 28.3, $CH_3$ | 1.35, s | 15.3, $CH_3$ | 2.10, d (2.0) | 10.4, $CH_3$ | 1.07, d (7.5) |
| 20 | 14.2, $CH_3$ | 0.66, s | 14.0, $CH_3$ | 0.71, s | 173.3, C | – |
| -COOC$H_3$ | – | – | – | – | 52.2, $CH_3$ | 3.65, s |

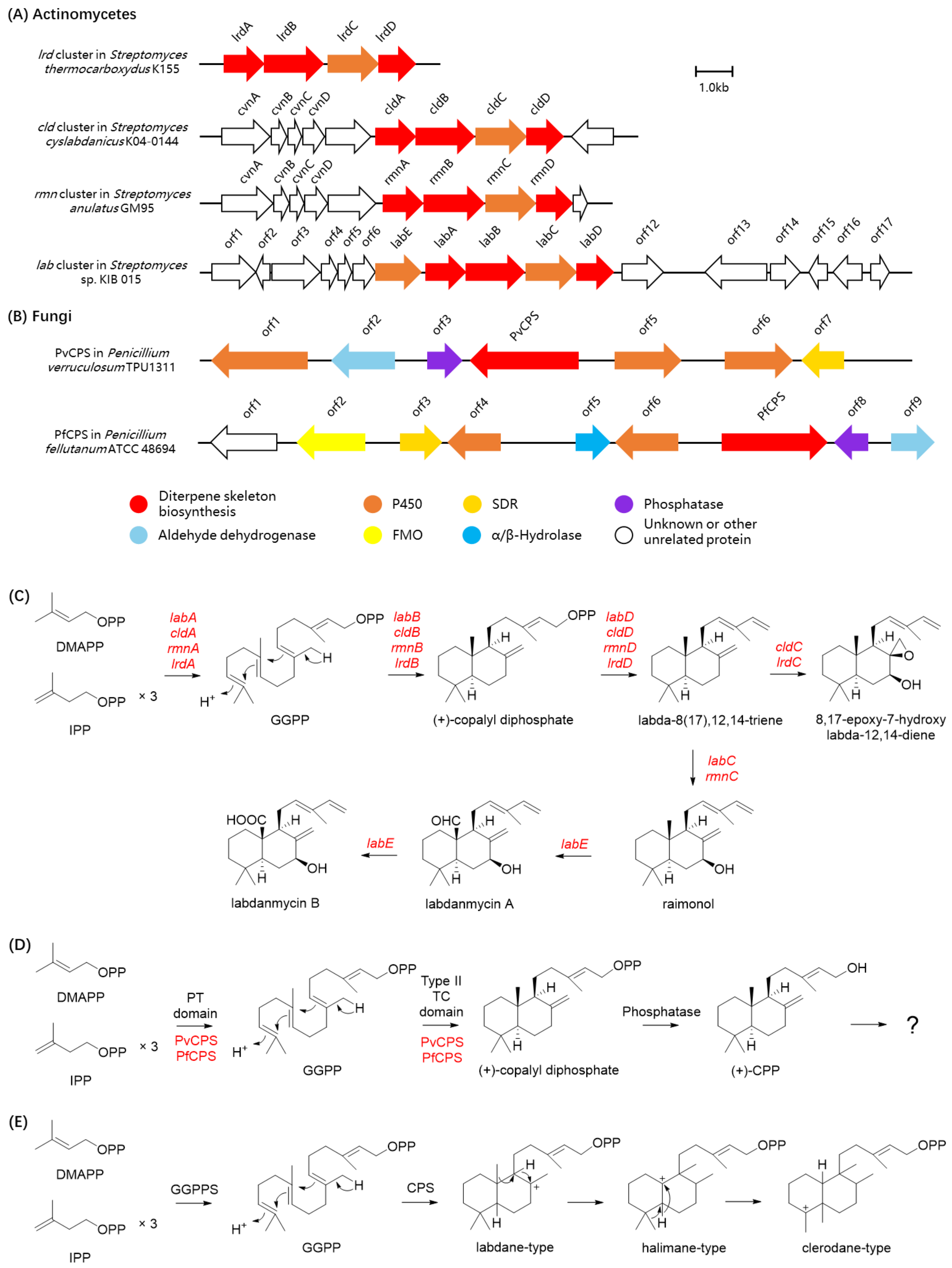



**Figure S1.** Representative labdane diterpenoid biosynthetic gene clusters and their biosynthetic pathways in Actinomycetes, fungi and plants. (A) The *lrd*, *cld*, *rmn* and *lab* BGCs clusters in *Streptomyces*. [16, 20,33]. (B) The BGCs containing the bifunctional terpene synthase PvCPS and PfCPS in *Penicillium*. [15]. (C) Proposed biosynthetic pathway of labdane-type bicyclic diterpenes catalyzed by *lrd*, *cld*, *rmn* and *lab* BGCs. [16,20,33]. (D) The reactions catalyzed by PvCPS and PfCPS. (E) Biosynthetic pathway of halimane and clerodane diterpenes in plants. [7,18].

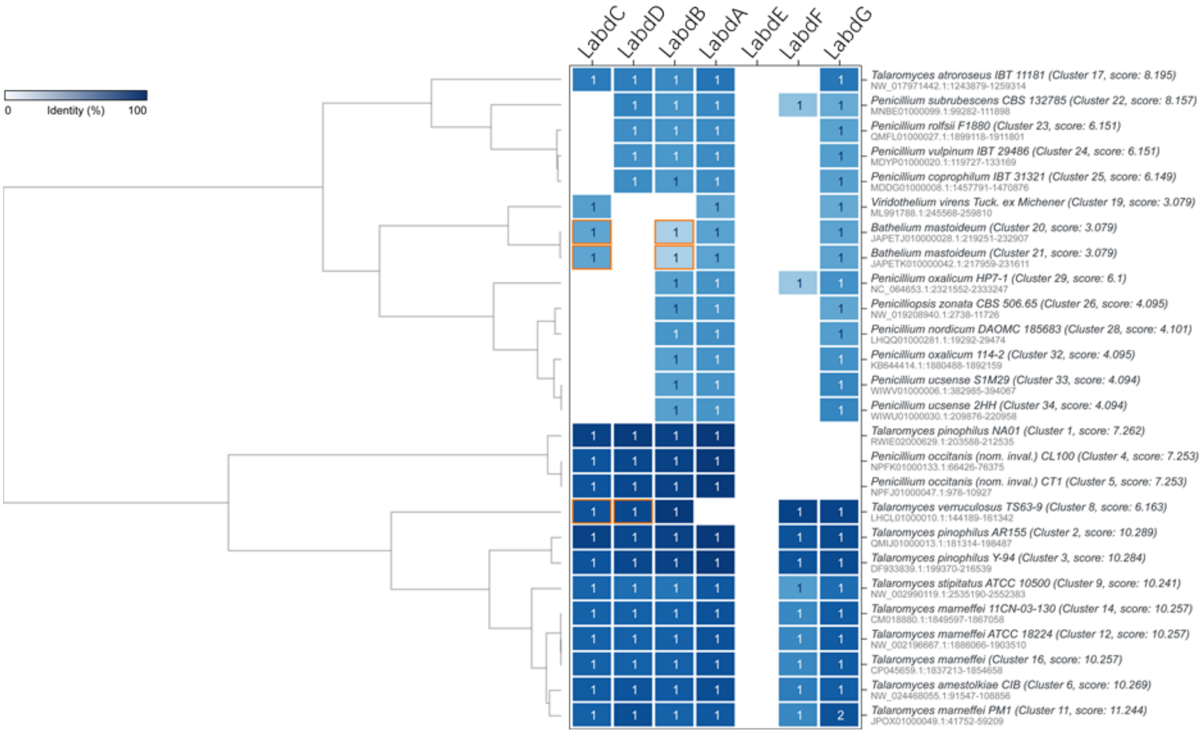



**Figure S2.** Cluster heatmap visualization of cblaster[9] search results using the *labd* cluster to query the fungal genomes from online database.

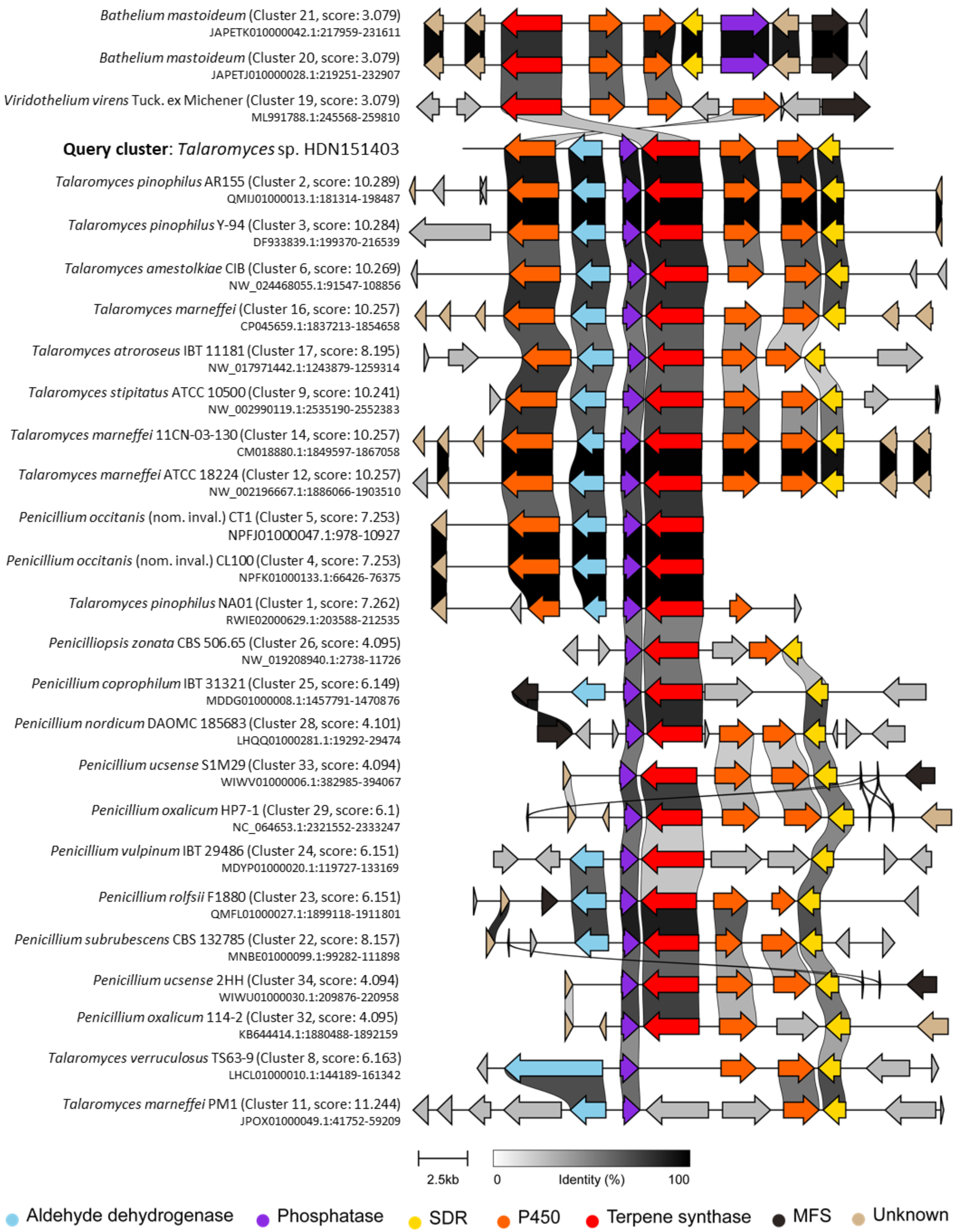



**Figure S3.** Visualization of gene clusters homologous to *labd* cluster searched by cblaster using clinker tool. [23].

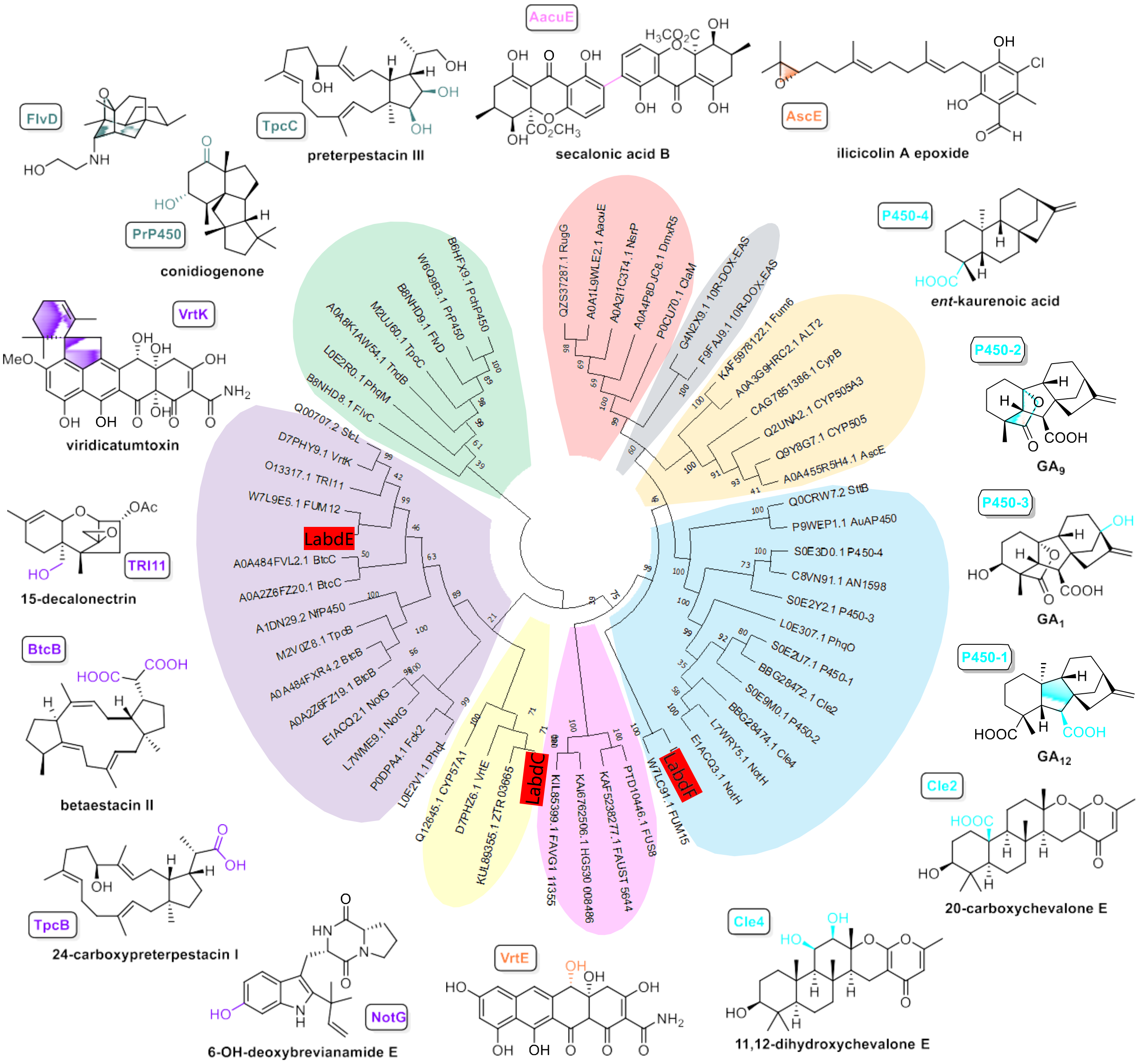


**Figure S4.** Neighbor joining method based phylogenetic analysis of P450s from Ascomycetes fungi using MEGA X software. The bootstrap consensus tree inferred from 1000 replicates is taken to represent the evolutionary history of the taxa analyzed. Protein names and accession numbers are shown at the leaves of the tree. The representative structures are listed in the figure, and the key catalytic sites of the relevant P450 enzymes are highlighted in different colors.

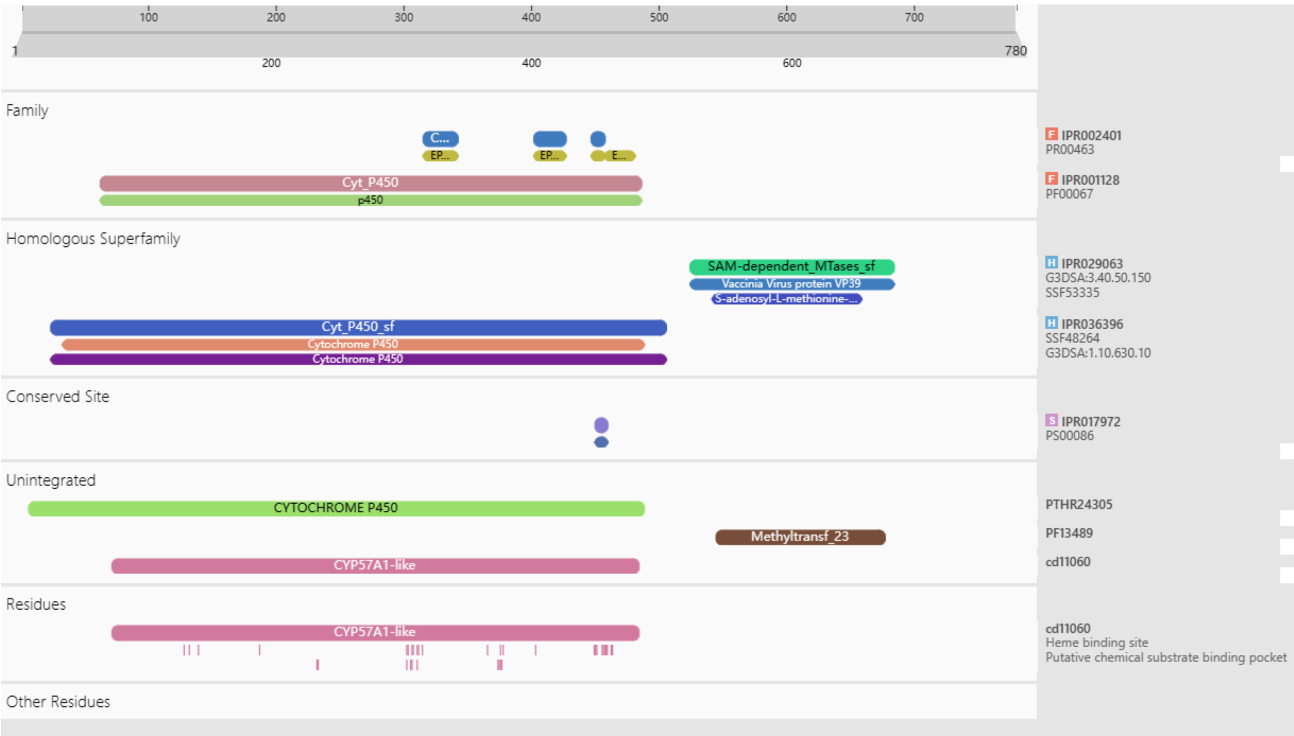



**Figure S5.** Results of protein family classification analysis of LabdC using InterPro database. The results showed that LabdC is a bifunctional P450 enzyme, including two functional domains of cytochrome P450 and methyltransferase.

| Description | Scientific Name | Max Score | Total Score | Query Cover | E value | Per. Ident | Acc. Len | Accession |
|---|---|---|---|---|---|---|---|---|
| hypothetical protein ZTR_03665 [Talaromyces verruculosus] | Talaromyces verruculosus | 1578 | 1578 | 100% | 0.0 | 97.18% | 1333 | KUL89355.1 |
| hypothetical protein TCE0_043r15581 [Talaromyces pinophilus] | Talaromyces pinophilus | 1562 | 1562 | 100% | 0.0 | 96.04% | 782 | GAM41998.1 |
| Cytochrome P450 [Penicillium occitanis (nom. inval.)] | Penicillium occitanis (nom. inval.) | 1561 | 1561 | 100% | 0.0 | 95.78% | 782 | PCG99752.1 |
| Cytochrome P450 monooxygenase vrtE [Talaromyces pinophilus] | Talaromyces pinophilus | 1538 | 1538 | 100% | 0.0 | 92.45% | 808 | KAF3385863.1 |
| uncharacterized protein BHQ10_008362 [Talaromyces amestolkiae] | Talaromyces amestolkiae | 1521 | 1521 | 100% | 0.0 | 93.09% | 782 | XP_040736864.1 |
| uncharacterized protein EYB26_009327 [Talaromyces marneffei] | Talaromyces marneffei | 1447 | 1447 | 99% | 0.0 | 89.74% | 782 | XP_054124552.1 |
| benzoate 4-monooxygenase cytochrome P450, putative [Talaromyces stipitatus ATCC ... | Talaromyces stipitatus ATCC 10500 | 1444 | 1444 | 100% | 0.0 | 87.47% | 782 | XP_002486679.1 |
| hypothetical protein EIK77_007927 [Talaromyces pinophilus] | Talaromyces pinophilus | 960 | 960 | 61% | 0.0 | 91.49% | 517 | KAI7970747.1 |
| hypothetical protein UA08_07234 [Talaromyces atroroseus] | Talaromyces atroroseus | 776 | 1115 | 84% | 0.0 | 80.17% | 692 | XP_020117855.1 |
| cytochrome P450 [Viridothelium virens] | Viridothelium virens | 650 | 650 | 62% | 0.0 | 61.81% | 720 | KAF2235944.1 |
| hypothetical protein M1822_007084 [Bathelium mastoideum] | Bathelium mastoideum | 643 | 643 | 63% | 0.0 | 60.45% | 810 | KAI9681732.1 |
| hypothetical protein M1821_005805 [Bathelium mastoideum] | Bathelium mastoideum | 642 | 642 | 63% | 0.0 | 60.45% | 810 | KAI9654811.1 |
| uncharacterized protein PgNI_02220 [Pyricularia grisea] | Pyricularia grisea | 545 | 545 | 62% | 0.0 | 49.80% | 501 | XP_030986481.1 |
| hypothetical protein FGRMN_6520 [Fusarium graminum] | Fusarium graminum | 545 | 545 | 60% | 0.0 | 50.42% | 523 | KAF4993391.1 |
| uncharacterized protein FTOL_07655 [Fusarium torulosum] | Fusarium torulosum | 541 | 541 | 59% | 0.0 | 49.89% | 480 | SPJ79264.1 |
| uncharacterized protein PpBr36_10745 [Pyricularia pennisetigena] | Pyricularia pennisetigena | 532 | 532 | 60% | 9e-179 | 51.58% | 501 | XP_029743706.1 |
| benzoate 4-monooxygenase cytochrome P450 [Pyricularia oryzae] | Pyricularia oryzae | 527 | 527 | 59% | 9e-177 | 50.53% | 501 | KAI7909201.1 |
| benzoate 4-monooxygenase cytochrome P450 [Pyricularia oryzae 70-15] | Pyricularia oryzae 70-15 | 527 | 527 | 59% | 1e-176 | 50.53% | 508 | XP_003720475.1 |
| hypothetical protein MCOR01_010310 [Pyricularia oryzae] | Pyricularia oryzae | 525 | 525 | 59% | 6e-176 | 50.32% | 501 | KAH8838880.1 |
| hypothetical protein PspLS_10363 [Pyricularia sp. CBS 133598] | Pyricularia sp. CBS 133598 | 468 | 468 | 59% | 2e-154 | 47.77% | 467 | TLD18038.1 |
| hypothetical protein F66182_12136 [Fusarium sp. NRRL 66182] | Fusarium sp. NRRL 66182 | 444 | 444 | 28% | 9e-149 | 95.43% | 219 | KAF5016246.1 |
| hypothetical protein M1820_009678 [Bogoriella megaspora] | Bogoriella megaspora | 456 | 456 | 47% | 8e-147 | 55.65% | 646 | KAI9691406.1 |
| benzoate 4-monooxygenase cytochrome P450 [Hyaloscypha variabilis F] | Hyaloscypha variabilis F | 384 | 384 | 59% | 3e-121 | 40.94% | 489 | PMD45842.1 |
| cytochrome P450 [Hyaloscypha hepaticicola] | Hyaloscypha hepaticicola | 378 | 378 | 60% | 9e-119 | 39.62% | 495 | PMD22400.1 |
| hypothetical protein B0A52_00440 [Exophiala mesophila] | Exophiala mesophila | 364 | 364 | 62% | 3e-113 | 38.49% | 506 | RVX76083.1 |
| hypothetical protein AYO20_04127 [Fonsecaea nubica] | Fonsecaea nubica | 362 | 362 | 61% | 2e-112 | 37.92% | 519 | XP_022501523.1 |
| hypothetical protein B0A52_07104 [Exophiala mesophila] | Exophiala mesophila | 353 | 353 | 61% | 3e-109 | 36.76% | 497 | RVX68677.1 |
| hypothetical protein FE257_012986 [Aspergillus nanangensis] | Aspergillus nanangensis | 353 | 353 | 61% | 6e-109 | 35.88% | 513 | KAF9885369.1 |
| hypothetical protein A1O9_04703 [Exophiala aquamarina CBS 119918] | Exophiala aquamarina CBS 119918 | 351 | 351 | 62% | 2e-108 | 36.73% | 499 | XP_013262445.1 |

**Figure S6.** Protein sequence alignment of LabdC with other homologs using Blastp (protein-protein BLAST).

| Description | Scientific Name | Max Score | Total Score | Query Cover | E value | Per. Ident | Acc. Len | Accession |
|---|---|---|---|---|---|---|---|---|
| Isotrichodermin C-15 hydroxylase [Talaromyces pinophilus] | Talaromyces pinophilus | 1040 | 1040 | 100% | 0.0 | 99.80% | 501 | KAF3385867.1 |
| hypothetical protein PENOC_085340 [Penicillium occitanis (nom. inval.)] | Penicillium occitanis (nom. inval.) | 1038 | 1038 | 100% | 0.0 | 99.40% | 501 | PCG93888.1 |
| hypothetical protein ZTR_03649 [Talaromyces verruculosus] | Talaromyces verruculosus | 1037 | 1037 | 100% | 0.0 | 99.60% | 501 | KUL89333.1 |
| uncharacterized protein BHQ10_008366 [Talaromyces amestolkiae] | Talaromyces amestolkiae | 1031 | 1031 | 100% | 0.0 | 98.60% | 503 | XP_040736868.1 |
| uncharacterized protein EYB26_009323 [Talaromyces marneffei] | Talaromyces marneffei | 996 | 996 | 100% | 0.0 | 94.21% | 501 | XP_054124548.1 |
| cytochrome P450, putative [Talaromyces stipitatus ATCC 10500] | Talaromyces stipitatus ATCC 10500 | 985 | 985 | 99% | 0.0 | 94.79% | 500 | XP_002486675.1 |
| hypothetical protein UA08_07230 [Talaromyces atroroseus] | Talaromyces atroroseus | 942 | 942 | 100% | 0.0 | 92.02% | 501 | XP_020117851.1 |
| Isotrichodermin C-15 hydroxylase [Penicillium rolfsii] | Penicillium rolfsii | 906 | 906 | 97% | 0.0 | 87.12% | 497 | KAF3385030.1 |
| Averantin hydroxylase [Penicillium vulpinum] | Penicillium vulpinum | 902 | 902 | 98% | 0.0 | 86.38% | 497 | XP_057110490.1 |
| Averantin hydroxylase [Penicillium subrubescens] | Penicillium subrubescens | 899 | 899 | 97% | 0.0 | 86.91% | 497 | XP_057003734.1 |
| Averantin hydroxylase [Penicillium oxalicum] | Penicillium oxalicum | 899 | 899 | 98% | 0.0 | 86.76% | 497 | XP_049969383.1 |
| Averantin hydroxylase [Penicillium cataractarum] | Penicillium cataractarum | 898 | 898 | 97% | 0.0 | 86.71% | 497 | XP_056554907.1 |
| hypothetical protein PDE_07206 [Penicillium oxalicum 114-2] | Penicillium oxalicum 114-2 | 898 | 898 | 98% | 0.0 | 86.56% | 497 | EPS32246.1 |
| Averantin hydroxylase [Penicillium tannophilum] | Penicillium tannophilum | 897 | 897 | 97% | 0.0 | 86.71% | 497 | KAJ5904104.1 |
| Cytochrome P450 monooxygenase [Penicillium ucsense] | Penicillium ucsense | 893 | 893 | 98% | 0.0 | 85.98% | 497 | KAF7719414.1 |
| Averantin hydroxylase [Penicillium odoratum] | Penicillium odoratum | 893 | 893 | 98% | 0.0 | 84.99% | 504 | XP_056993152.1 |
| Averantin hydroxylase [Penicillium robsamsonii] | Penicillium robsamsonii | 892 | 892 | 98% | 0.0 | 85.57% | 497 | XP_057088019.1 |
| Averantin hydroxylase [Penicillium glabrum] | Penicillium glabrum | 892 | 892 | 97% | 0.0 | 86.09% | 497 | KAJ5553235.1 |
| Averantin hydroxylase [Penicillium diatomitis] | Penicillium diatomitis | 891 | 891 | 98% | 0.0 | 85.77% | 497 | XP_056791296.1 |
| Averantin hydroxylase [Penicillium longicatenatum] | Penicillium longicatenatum | 890 | 890 | 97% | 0.0 | 87.09% | 497 | KAJ5664045.1 |
| Averantin hydroxylase [Penicillium longicatenatum] | Penicillium longicatenatum | 890 | 890 | 97% | 0.0 | 87.09% | 497 | XP_056977175.1 |
| Averantin hydroxylase [Penicillium concentricum] | Penicillium concentricum | 889 | 889 | 98% | 0.0 | 85.37% | 497 | XP_056582103.1 |
| Averantin hydroxylase [Penicillium lividum] | Penicillium lividum | 889 | 889 | 98% | 0.0 | 84.58% | 504 | KAJ5627861.1 |
| Averantin hydroxylase [Penicillium samsonianum] | Penicillium samsonianum | 885 | 885 | 97% | 0.0 | 85.10% | 497 | XP_057135627.1 |
| hypothetical protein ASPZODRAFT_1503734 [Penicilliopsis zonata CBS 506.65] | Penicilliopsis zonata CBS 506.65 | 885 | 885 | 94% | 0.0 | 87.26% | 471 | XP_022576702.1 |
| Averantin hydroxylase [Penicillium verhagenii] | Penicillium verhagenii | 884 | 884 | 96% | 0.0 | 86.16% | 497 | XP_057016147.1 |
| Averantin hydroxylase [Penicillium glabrum] | Penicillium glabrum | 882 | 882 | 97% | 0.0 | 84.88% | 504 | KAJ5554181.1 |
| Averantin hydroxylase [Penicillium sp. IBT 16267x] | Penicillium sp. IBT 16267x | 881 | 881 | 94% | 0.0 | 87.74% | 497 | KAJ6109479.1 |
| Averantin hydroxylase [Penicillium sp. IBT 35674x] | Penicillium sp. IBT 35674x | 879 | 879 | 94% | 0.0 | 87.13% | 497 | KAJ5987131.1 |
| Averantin hydroxylase [Penicillium sp. IBT 35674x] | Penicillium sp. IBT 35674x | 879 | 879 | 94% | 0.0 | 87.13% | 497 | KAJ5987131.1 |
| hypothetical protein ACN38_g11222 [Penicillium nordicum] | Penicillium nordicum | 879 | 879 | 97% | 0.0 | 84.29% | 497 | KOS37964.1 |
| Averantin hydroxylase [Penicillium verrucosum] | Penicillium verrucosum | 878 | 878 | 97% | 0.0 | 84.29% | 497 | XP_057076769.1 |
| Averantin hydroxylase [Penicillium verhagenii] | Penicillium verhagenii | 877 | 877 | 96% | 0.0 | 86.36% | 497 | KAJ5937840.1 |
| Averantin hydroxylase [Penicillium angulare] | Penicillium angulare | 874 | 874 | 96% | 0.0 | 85.30% | 498 | KAJ5114237.1 |
| hypothetical protein VN97_g8291 [Penicillium thymicola] | Penicillium thymicola | 874 | 874 | 97% | 0.0 | 84.29% | 497 | KAJ9485073.1 |
| Averantin hydroxylase [Penicillium pulvis] | Penicillium pulvis | 801 | 801 | 87% | 0.0 | 86.10% | 468 | XP_056924516.1 |
| hypothetical protein PENCOP_c008G02740 [Penicillium coprophilum] | Penicillium coprophilum | 786 | 786 | 84% | 0.0 | 87.91% | 446 | OQE38664.1 |
| putative cytochrome P450 [Viridothelium virens] | Viridothelium virens | 755 | 755 | 92% | 0.0 | 76.61% | 505 | KAF2235947.1 |
| hypothetical protein M1820_009681 [Bogoriella megaspora] | Bogoriella megaspora | 753 | 753 | 98% | 0.0 | 72.76% | 505 | KAI9691409.1 |
| hypothetical protein M1821_005808 [Bathelium mastoideum] | Bathelium mastoideum | 746 | 746 | 93% | 0.0 | 75.11% | 498 | KAI9654814.1 |
| hypothetical protein M1822_007087 [Bathelium mastoideum] | Bathelium mastoideum | 745 | 745 | 93% | 0.0 | 75.11% | 498 | KAI9681735.1 |
| Isotrichodermin C-15 hydroxylase [Penicillium subrubescens] | Penicillium subrubescens | 695 | 695 | 76% | 0.0 | 86.20% | 402 | OKP14338.1 |
| hypothetical protein EIK77_007931 [Talaromyces pinophilus] | Talaromyces pinophilus | 686 | 686 | 66% | 0.0 | 97.94% | 359 | KAI7970751.1 |
| uncharacterized protein N7510_007632 [Penicillium lagena] | Penicillium lagena | 530 | 530 | 98% | 0.0 | 53.55% | 498 | XP_056832600.1 |
| Cytochrome p450 protein [Lasiodiplodia theobromae] | Lasiodiplodia theobromae | 525 | 525 | 96% | 3e-180 | 52.47% | 491 | XP_035367558.1 |
| Cytochrome P450 monooxygenase hmp1 [Lasiodiplodia hormozganensis] | Lasiodiplodia hormozganensis | 524 | 524 | 96% | 1e-179 | 52.36% | 491 | KAK0647576.1 |
| Cytochrome p450 protein [Neofusicoccum parvum] | Neofusicoccum parvum | 516 | 516 | 94% | 3e-176 | 51.26% | 529 | GME59351.1 |
| putative cytochrome p450 protein [Neofusicoccum parvum UCRNP2] | Neofusicoccum parvum UCRNP2 | 515 | 515 | 94% | 1e-175 | 51.26% | 529 | EOD48095.1 |
| Cytochrome p450 protein [Neofusicoccum parvum] | Neofusicoccum parvum | 513 | 513 | 94% | 5e-175 | 51.05% | 529 | GME34285.1 |
| putative cytochrome P450 [Pestalotiopsis sp. NC0098] | Pestalotiopsis sp. NC0098 | 508 | 508 | 92% | 1e-173 | 51.84% | 488 | KAI0146810.1 |
| putative cytochrome P450 [Corynespora cassiicola Philippines] | Corynespora cassiicola Philippines | 505 | 505 | 97% | 2e-172 | 51.53% | 490 | PSN63043.1 |
| hypothetical protein PFICI_06539 [Pestalotiopsis fici W106-1] | Pestalotiopsis fici W106-1 | 503 | 503 | 93% | 2e-171 | 51.17% | 490 | XP_007833311.1 |
| Cytochrome p450 protein [Lasiodiplodia theobromae] | Lasiodiplodia theobromae | 502 | 502 | 96% | 2e-171 | 49.38% | 476 | XP_035368502.1 |
| Heterokaryon incompatibility [Botryosphaeria dothidea] | Botryosphaeria dothidea | 493 | 493 | 93% | 2e-167 | 51.06% | 499 | KAF4300746.1 |
| hypothetical protein PFICI_06539 [Neofusicoccum parvum] | Neofusicoccum parvum | 492 | 492 | 93% | 3e-167 | 49.89% | 494 | GME59698.1 |
| hypothetical protein S40288_03084 [Stachybotrys chartarum IBT 40288] | Stachybotrys chartarum IBT 40288 | 493 | 493 | 92% | 3e-167 | 50.64% | 500 | KFA77429.1 |
| hypothetical protein S7711_03465 [Stachybotrys chartarum IBT 7711] | Stachybotrys chartarum IBT 7711 | 491 | 491 | 92% | 8e-167 | 50.43% | 500 | KEY64172.1 |
| Isotrichodermin C-15 hydroxylase [Diplodia seriata] | Diplodia seriata | 488 | 488 | 96% | 9e-166 | 49.48% | 491 | OMP83594.1 |

**Figure S7.** Protein sequence alignment of LabdE with other homologs using Blastp (protein-protein BLAST).

| Description | Scientific Name | Max Score | Total Score | Query Cover | E value | Per. Ident | Acc. Len | Accession |
|---|---|---|---|---|---|---|---|---|
| hypothetical protein ZTR_03650 [Talaromyces verruculosus] | Talaromyces verruculosus | 1086 | 1086 | 100% | 0.0 | 97.23% | 542 | KUL89225.1 |
| hypothetical protein PENOC_085350 [Penicillium occitanis (nom. inval.)] | Penicillium occitanis (nom. inval.) | 1068 | 1068 | 100% | 0.0 | 95.39% | 542 | PCG93889.1 |
| hypothetical protein TCE0_043f15589 [Talaromyces pinophilus] | Talaromyces pinophilus | 1060 | 1060 | 100% | 0.0 | 95.20% | 540 | GAM42003.1 |
| uncharacterized protein BHQ10_008367 [Talaromyces amestolkiae] | Talaromyces amestolkiae | 1021 | 1021 | 100% | 0.0 | 90.28% | 545 | XP_040736869.1 |
| uncharacterized protein EYB26_009322 [Talaromyces marneffei] | Talaromyces marneffei | 1005 | 1005 | 100% | 0.0 | 88.56% | 542 | XP_054124547.1 |
| cytochrome P450, putative [Talaromyces stipitatus ATCC 10500] | Talaromyces stipitatus ATCC 10500 | 929 | 929 | 100% | 0.0 | 82.87% | 543 | XP_002486674.1 |
| hypothetical protein UA08_07229 [Talaromyces atroroseus] | Talaromyces atroroseus | 831 | 831 | 94% | 0.0 | 77.93% | 518 | XP_020117852.1 |
| Cytochrome P450 3A12 [Talaromyces pinophilus] | Talaromyces pinophilus | 802 | 802 | 77% | 0.0 | 93.57% | 422 | KAF3385868.1 |
| hypothetical protein N7451_011497 [Penicillium sp. IBT 35674x] | Penicillium sp. IBT 35674x | 751 | 751 | 99% | 0.0 | 67.96% | 534 | KAJ5987132.1 |
| hypothetical protein N7486_001713 [Penicillium sp. IBT 16267x] | Penicillium sp. IBT 16267x | 751 | 751 | 99% | 0.0 | 67.47% | 534 | KAJ6109478.1 |
| hypothetical protein N7494_002614 [Penicillium glabrum] | Penicillium glabrum | 749 | 749 | 99% | 0.0 | 67.28% | 534 | KAJ5553236.1 |
| hypothetical protein N7504_006488 [Penicillium tannophilum] | Penicillium tannophilum | 749 | 749 | 99% | 0.0 | 67.65% | 544 | KAJ5904105.1 |
| uncharacterized protein N7503_004055 [Penicillium pulvis] | Penicillium pulvis | 748 | 748 | 99% | 0.0 | 67.46% | 534 | XP_056924517.1 |
| uncharacterized protein N7520_009929 [Penicillium odoratum] | Penicillium odoratum | 748 | 748 | 99% | 0.0 | 67.83% | 537 | XP_056993151.1 |
| hypothetical protein N7513_004139 [Penicillium glabrum] | Penicillium glabrum | 748 | 748 | 99% | 0.0 | 67.10% | 534 | KAJ5554180.1 |
| hypothetical protein N7454_004183 [Penicillium verhagenii] | Penicillium verhagenii | 748 | 748 | 99% | 0.0 | 67.78% | 536 | KAJ5937841.1 |
| uncharacterized protein N7496_006566 [Penicillium cataractarum] | Penicillium cataractarum | 743 | 743 | 99% | 0.0 | 67.03% | 535 | XP_056554908.1 |
| hypothetical protein N7490_010090 [Penicillium lividum] | Penicillium lividum | 739 | 739 | 99% | 0.0 | 68.26% | 537 | KAJ5627862.1 |
| uncharacterized protein N7473_011946 [Penicillium subrubescens] | Penicillium subrubescens | 739 | 739 | 99% | 0.0 | 66.98% | 535 | XP_057003735.1 |
| uncharacterized protein N7471_008649 [Penicillium samsonianum] | Penicillium samsonianum | 738 | 738 | 99% | 0.0 | 67.53% | 540 | XP_057135628.1 |
| uncharacterized protein N7479_003469 [Penicillium vulpinum] | Penicillium vulpinum | 738 | 738 | 99% | 0.0 | 67.89% | 540 | XP_057110491.1 |
| uncharacterized protein N7517_000237 [Penicillium concentricum] | Penicillium concentricum | 732 | 732 | 99% | 0.0 | 67.71% | 540 | XP_056582102.1 |
| Cytochrome P450 monooxygenase [Penicillium ucsense] | Penicillium ucsense | 731 | 731 | 99% | 0.0 | 66.61% | 539 | KAF7719415.1 |
| Cytochrome P450 3A13 [Penicillium subrubescens] | Penicillium subrubescens | 728 | 728 | 99% | 0.0 | 64.58% | 553 | OKP14337.1 |
| hypothetical protein POX_d05589 [Penicillium oxalicum] | Penicillium oxalicum | 727 | 727 | 98% | 0.0 | 66.85% | 535 | XP_049969382.1 |
| uncharacterized protein N7516_002167 [Penicillium verrucosum] | Penicillium verrucosum | 726 | 726 | 99% | 0.0 | 66.91% | 540 | XP_057076770.1 |
| uncharacterized protein ASPVEDRAFT_138421 [Aspergillus versicolor CBS 583.65] | Aspergillus versicolor CBS 583.65 | 725 | 725 | 99% | 0.0 | 65.99% | 541 | XP_040671551.1 |
| hypothetical protein N7507_004777 [Penicillium longicatenatum] | Penicillium longicatenatum | 724 | 724 | 90% | 0.0 | 70.06% | 508 | KAJ5664046.1 |
| uncharacterized protein N7447_004402 [Penicillium robsamsonii] | Penicillium robsamsonii | 720 | 720 | 99% | 0.0 | 67.53% | 540 | XP_057088018.1 |
| uncharacterized protein N7447_004402 [Penicillium robsamsonii] | Penicillium robsamsonii | 720 | 720 | 99% | 0.0 | 67.53% | 540 | XP_057088018.1 |
| hypothetical protein PDE_07207 [Penicillium oxalicum 114-2] | Penicillium oxalicum 114-2 | 716 | 716 | 92% | 0.0 | 69.50% | 506 | EPS32247.1 |
| hypothetical protein N7456_002772 [Penicillium angulare] | Penicillium angulare | 700 | 700 | 98% | 0.0 | 67.22% | 537 | KAJ5114238.1 |
| uncharacterized protein N7539_004152 [Penicillium diatomitis] | Penicillium diatomitis | 691 | 691 | 88% | 0.0 | 70.15% | 494 | XP_056791295.1 |
| uncharacterized protein N7466_011027 [Penicillium verhagenii] | Penicillium verhagenii | 668 | 668 | 89% | 0.0 | 66.74% | 494 | XP_057016148.1 |
| hypothetical protein ACN38_g11223 [Penicillium nordicum] | Penicillium nordicum | 646 | 646 | 89% | 0.0 | 65.92% | 489 | KOS37976.1 |
| hypothetical protein VN97_g8292 [Penicillium thymicola] | Penicillium thymicola | 642 | 642 | 89% | 0.0 | 65.78% | 489 | KAJ9485072.1 |
| hypothetical protein EIK77_007932 [Talaromyces pinophilus] | Talaromyces pinophilus | 638 | 638 | 59% | 0.0 | 95.65% | 336 | KAI7970752.1 |
| hypothetical protein ASPZODRAFT_77483 [Penicilliopsis zonata CBS 506.65] | Penicilliopsis zonata CBS 506.65 | 634 | 634 | 92% | 0.0 | 61.90% | 514 | XP_022576701.1 |
| putative cytochrome P450 [Viridothelium virens] | Viridothelium virens | 580 | 580 | 91% | 0.0 | 58.37% | 496 | KAF2235946.1 |
| cytochrome p450 [Lasallia pustulata] | Lasallia pustulata | 568 | 568 | 96% | 0.0 | 51.87% | 543 | SLM39940.1 |
| cytochrome P450 [Lasallia pustulata] | Lasallia pustulata | 565 | 565 | 96% | 0.0 | 51.50% | 543 | KAA6413515.1 |
| hypothetical protein [Hypocenomyce scalaris] | Hypocenomyce scalaris | 555 | 555 | 97% | 0.0 | 52.04% | 545 | MCJ1304961.1 |
| hypothetical protein LQ347_000766 [Umbilicaria vellea] | Umbilicaria vellea | 555 | 555 | 93% | 0.0 | 52.05% | 545 | KAI4135313.1 |
| hypothetical protein M1821_005807 [Bathelium mastoideum] | Bathelium mastoideum | 552 | 552 | 86% | 0.0 | 57.69% | 463 | KAI9654813.1 |
| hypothetical protein M1820_009680 [Bogoriella megaspora] | Bogoriella megaspora | 550 | 550 | 86% | 0.0 | 56.84% | 466 | KAI9691408.1 |
| hypothetical protein [Lignoscripta atroalba] | Lignoscripta atroalba | 545 | 545 | 96% | 0.0 | 50.18% | 548 | MCJ1254213.1 |
| hypothetical protein [Acarospora aff. strigata] | Acarospora aff. strigata | 541 | 541 | 99% | 0.0 | 49.18% | 547 | MCJ1362699.1 |
| cytochrome P450 [Saccharata proteae CBS 121410] | Saccharata proteae CBS 121410 | 538 | 538 | 93% | 0.0 | 51.76% | 542 | KAF2092013.1 |
| hypothetical protein B0A49_00372 [Cryomyces minteri] | Cryomyces minteri | 537 | 537 | 99% | 0.0 | 51.38% | 541 | TKA81886.1 |
| uncharacterized protein HO173_001655 [Letharia columbiana] | Letharia columbiana | 536 | 536 | 97% | 0.0 | 49.81% | 546 | XP_037169314.1 |
| hypothetical protein [Lobaria immixta] | Lobaria immixta | 535 | 535 | 98% | 0.0 | 47.91% | 547 | MCJ1266096.1 |
| hypothetical protein [Xylographa bjoerkii] | Xylographa bjoerkii | 535 | 535 | 91% | 0.0 | 50.79% | 548 | MCJ1387575.1 |
| hypothetical protein [Ptychographa xylographoides] | Ptychographa xylographoides | 533 | 533 | 98% | 0.0 | 49.36% | 548 | MCJ1406239.1 |
| hypothetical protein [Xylographa carneopallida] | Xylographa carneopallida | 533 | 533 | 96% | 0.0 | 48.89% | 548 | MCJ1295844.1 |
| hypothetical protein L6R40_003711 [Xanthomendoza cf. fulva] | Xanthomendoza cf. fulva | 532 | 532 | 95% | 0.0 | 50.19% | 547 | KAI4243020.1 |
| Cytochrome P450 3A13 [Penicillium rolfsii] | Penicillium rolfsii | 528 | 528 | 69% | 0.0 | 67.09% | 392 | KAF3385029.1 |
| hypothetical protein [Xylographa vitiligo] | Xylographa vitiligo | 530 | 530 | 95% | 1e-180 | 48.69% | 548 | MCJ1316429.1 |
| hypothetical protein M1833_006363 [Piccolia ochrophora] | Piccolia ochrophora | 529 | 529 | 91% | 3e-180 | 51.29% | 544 | KAI9796358.1 |
| uncharacterized protein HO133_007892 [Letharia lupina] | Letharia lupina | 528 | 528 | 97% | 4e-180 | 49.26% | 546 | XP_037156096.1 |

**Figure S8.** Protein sequence alignment of LabdF with other homologs using Blastp (protein-protein BLAST).

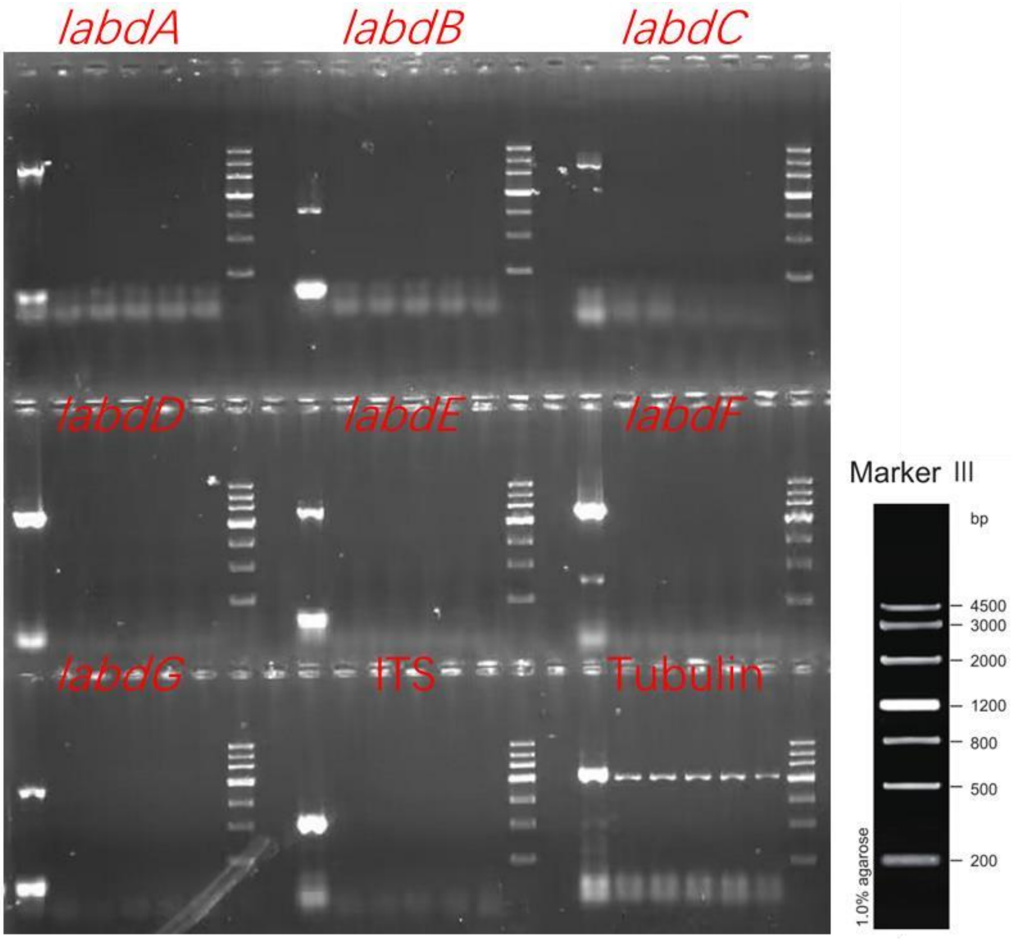
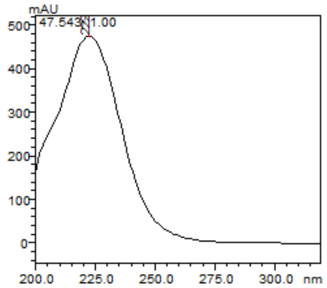
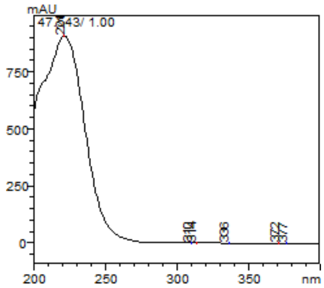


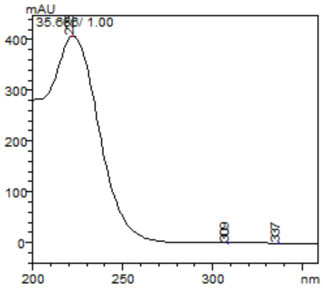

**Figure S9.** RT-PCR results of *labd* cluster of *Talaromyces* sp. HDN 151403 under different laboratory culture conditions. The PCR templates from left to right are: gDNA of *Talaromyces* sp. HDN 151403, cDNA of *Talaromyces* sp. HDN 151403 from five different media: PDB, fungal modified No. 2 medium, rice medium, glycerol medium, and trypticase (tryptic) soy broth.




**1**




**2**

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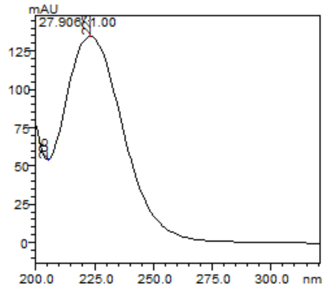


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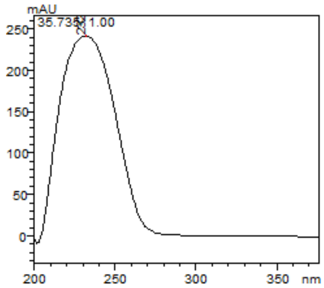


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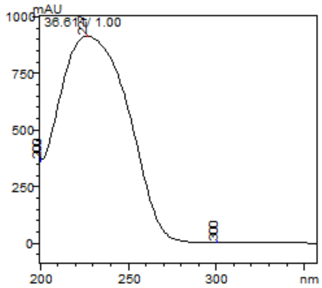


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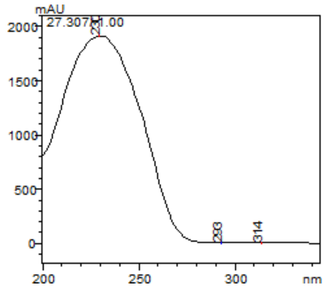


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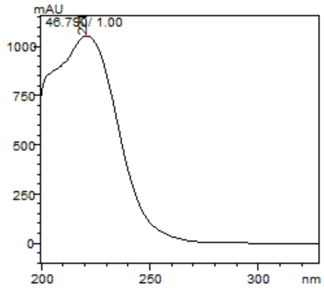


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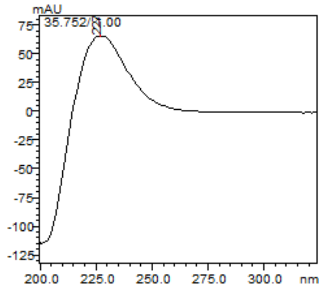


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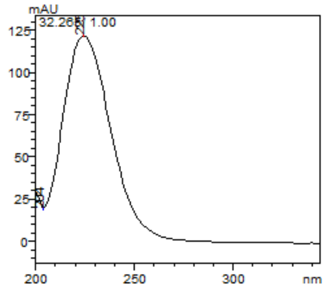


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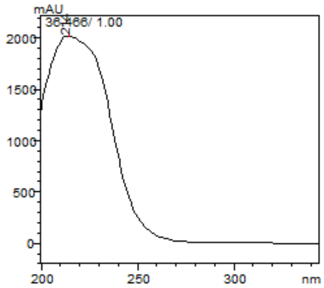
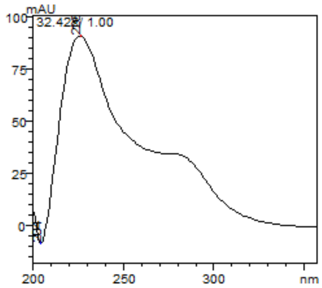
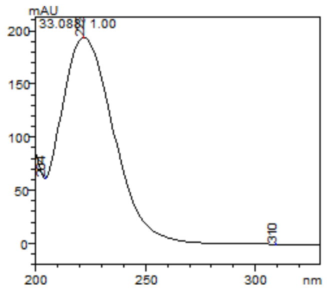



**11**




**12**




**13**

**Figure S10.** UV-vis spectra of purified compounds. All spectra were measured with a Shimadzu UFLC system equipped with a variable wavelength detector.

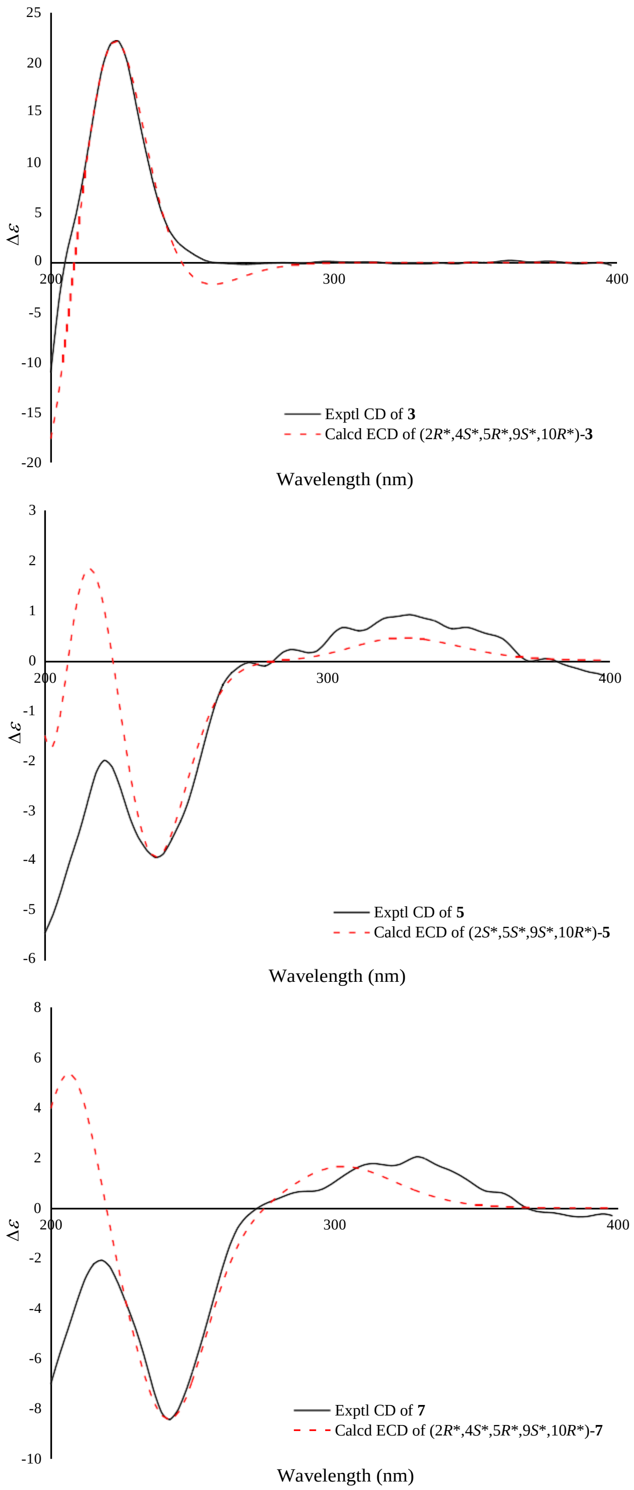



**Figure S11.** Comparison of calculated and experimental ECD spectra of **3–7** in methanol.

**Figure S12.** $^1$H NMR of **3** in $CD_3OD$.

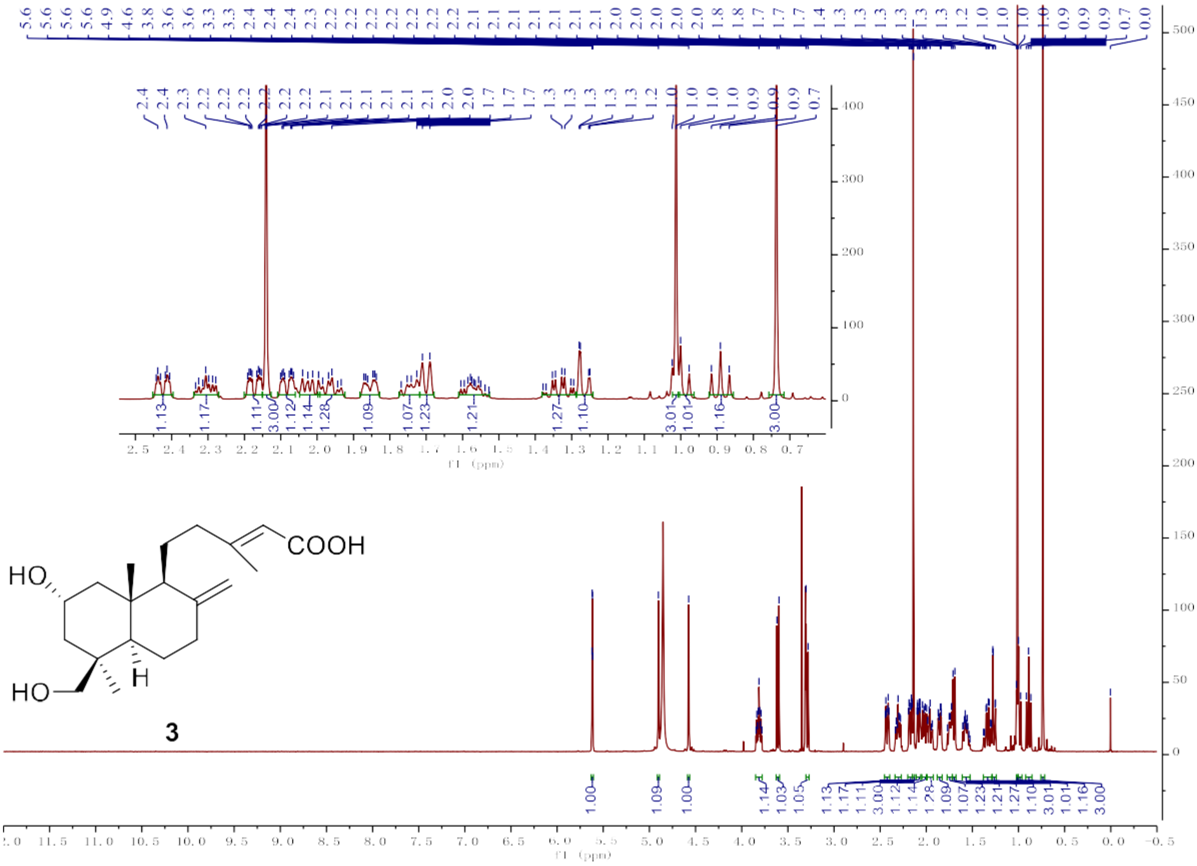


**Figure S13.** $^{13}$C NMR of **3** in $CD_3OD$.

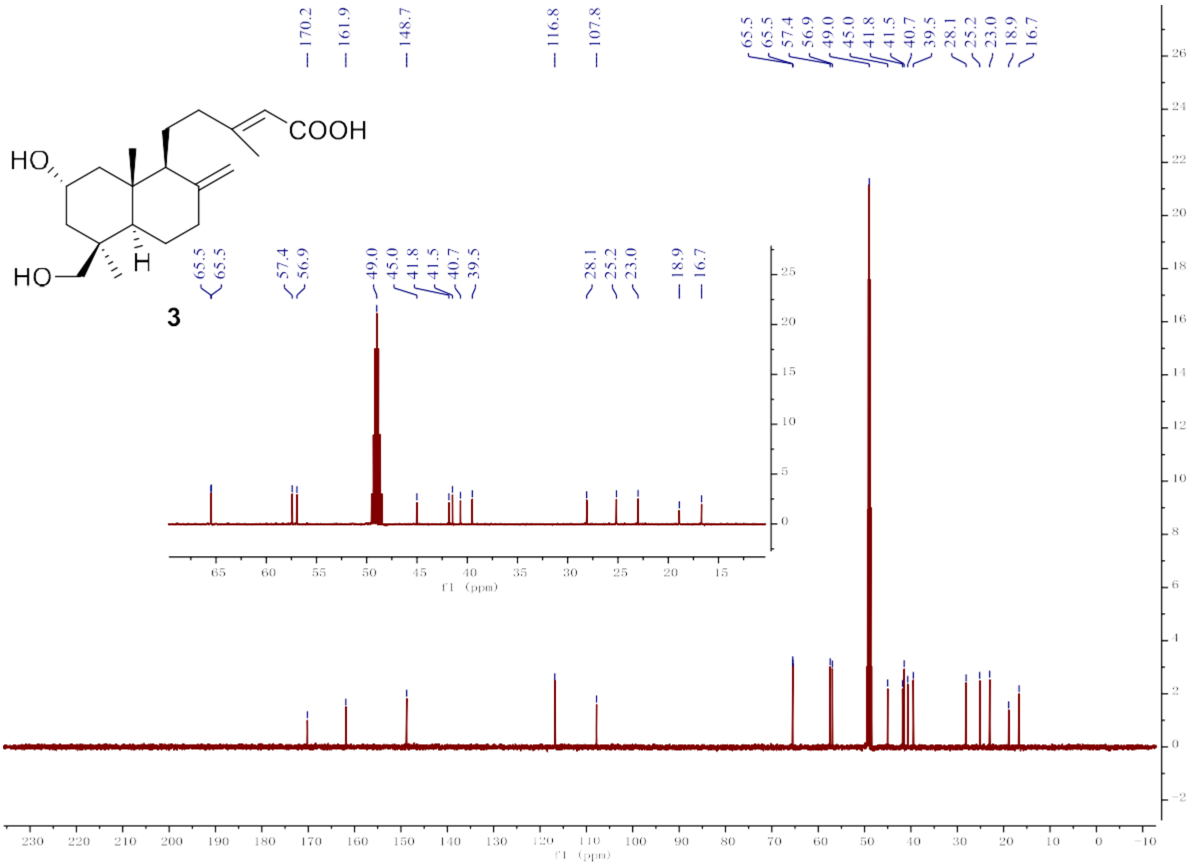


**Figure S14.** HSQC of **3** in $CD_3OD$.

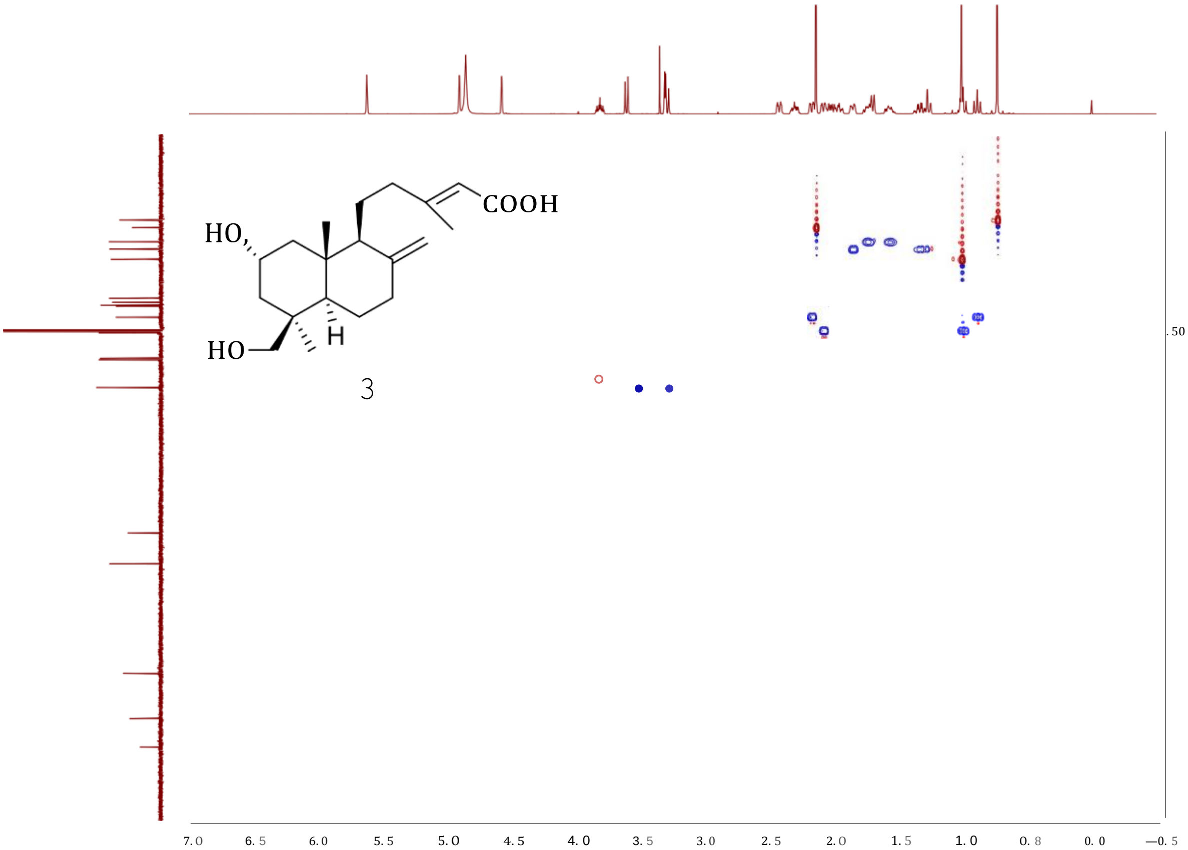



**Figure S15.** HMBC of **3** in $CD_3OD$.

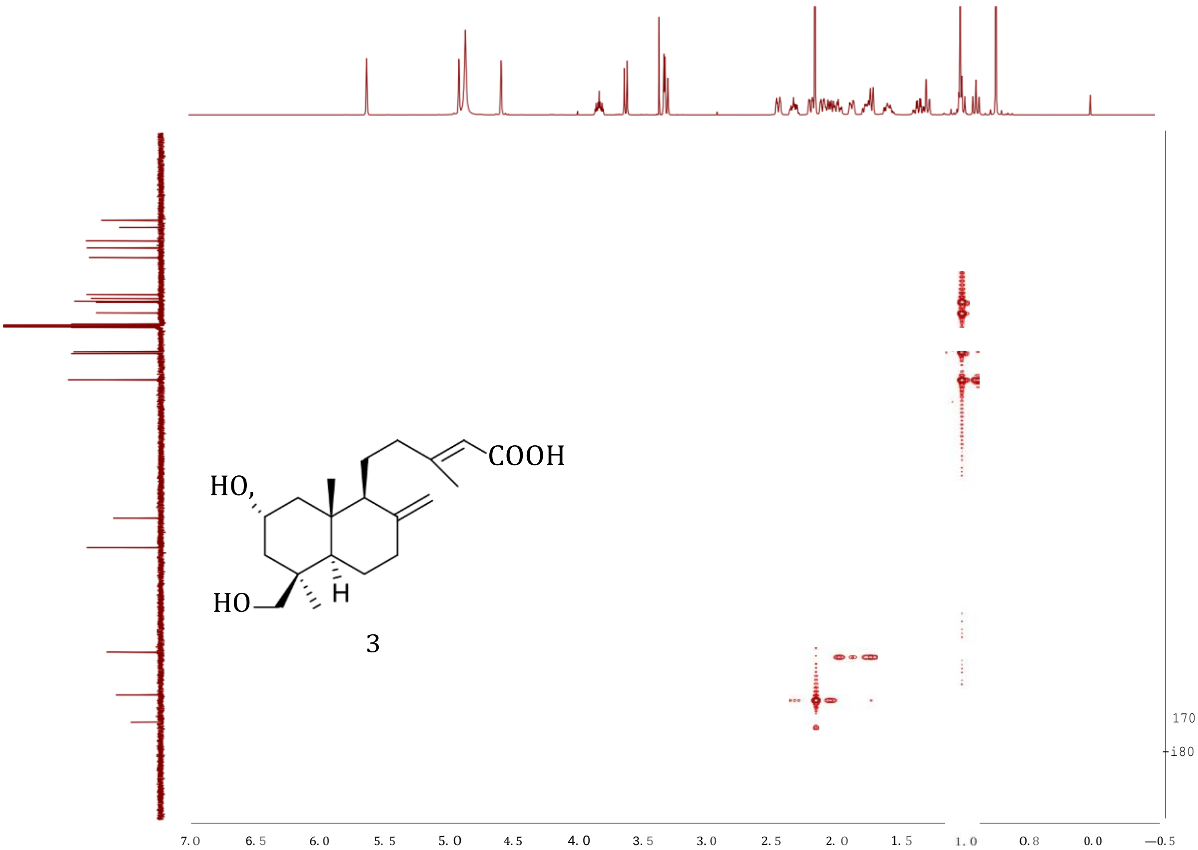


**Figure S16.** $^1$H-$^1$H COSY of **3** in $CD_3OD$.

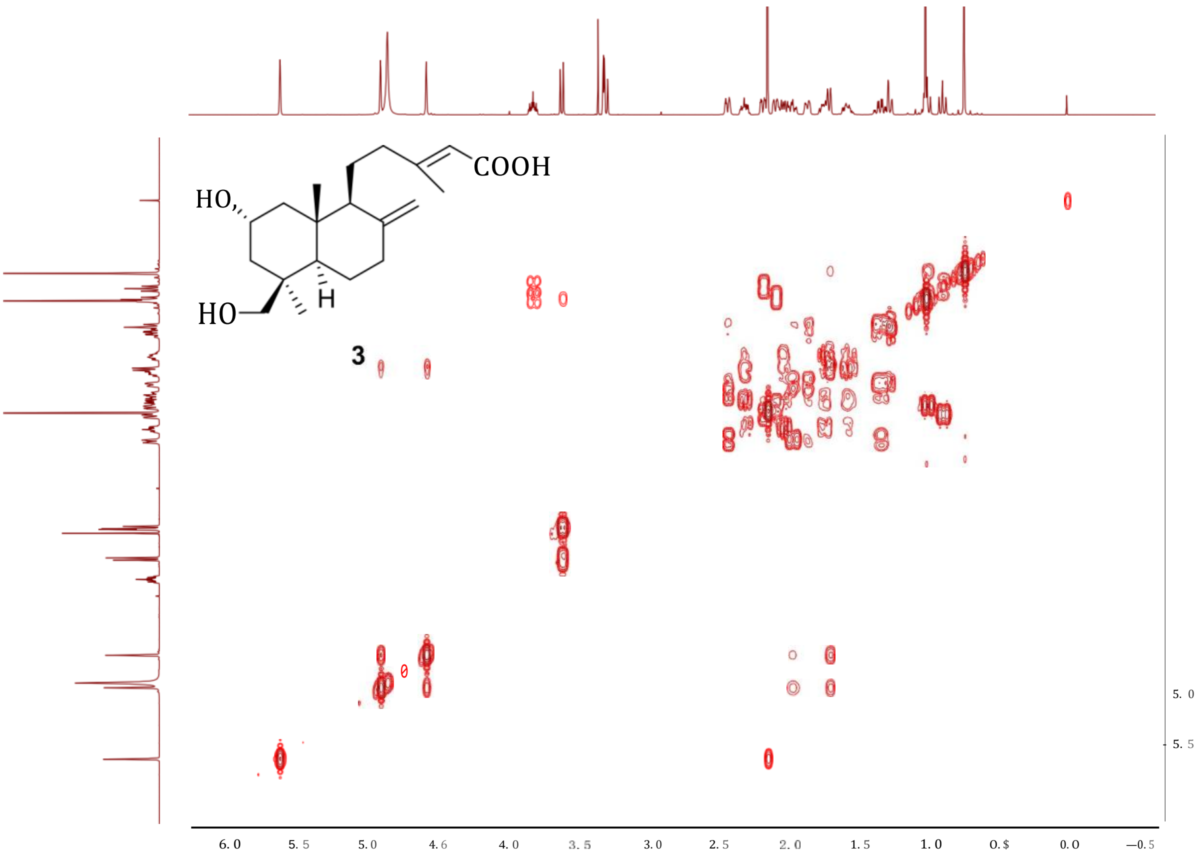



**Figure S17.** ROESY of **3** in $CD_3OD$.

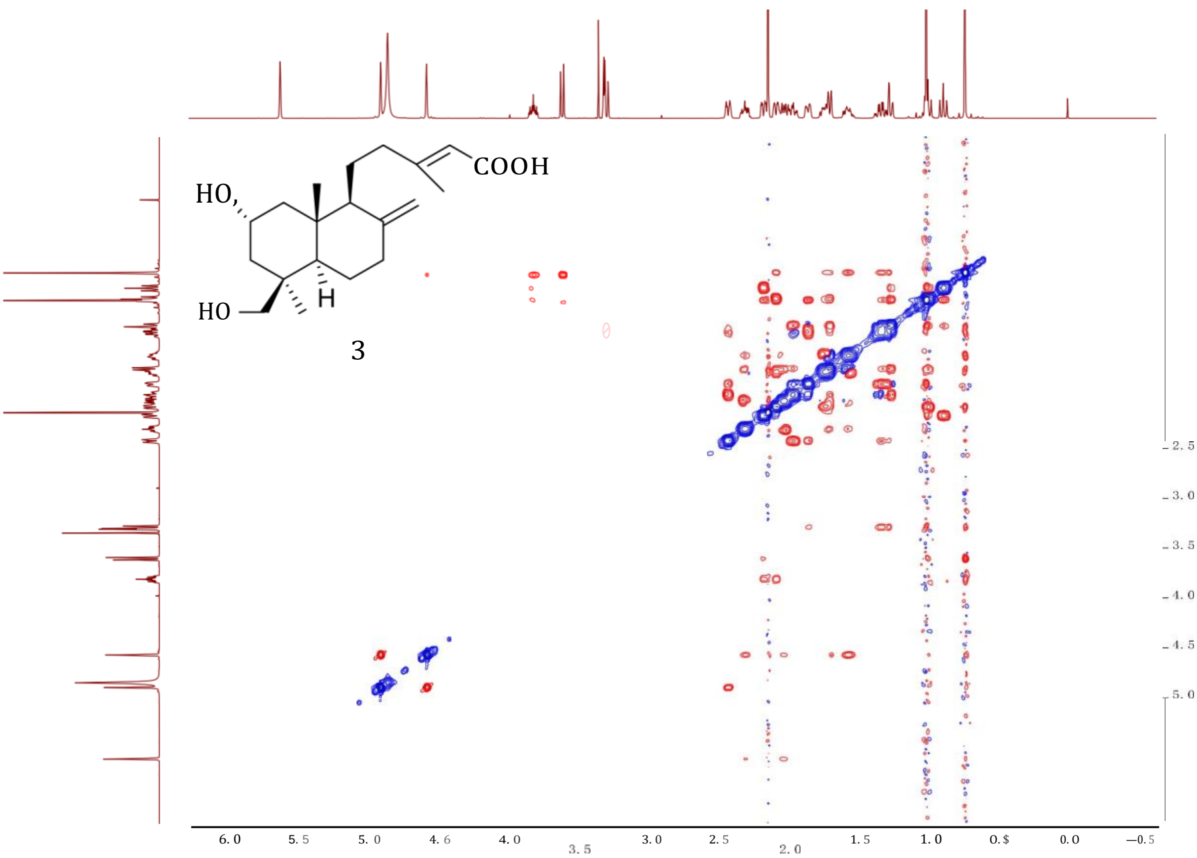


**Figure S18.** HRESIMS of **3**.

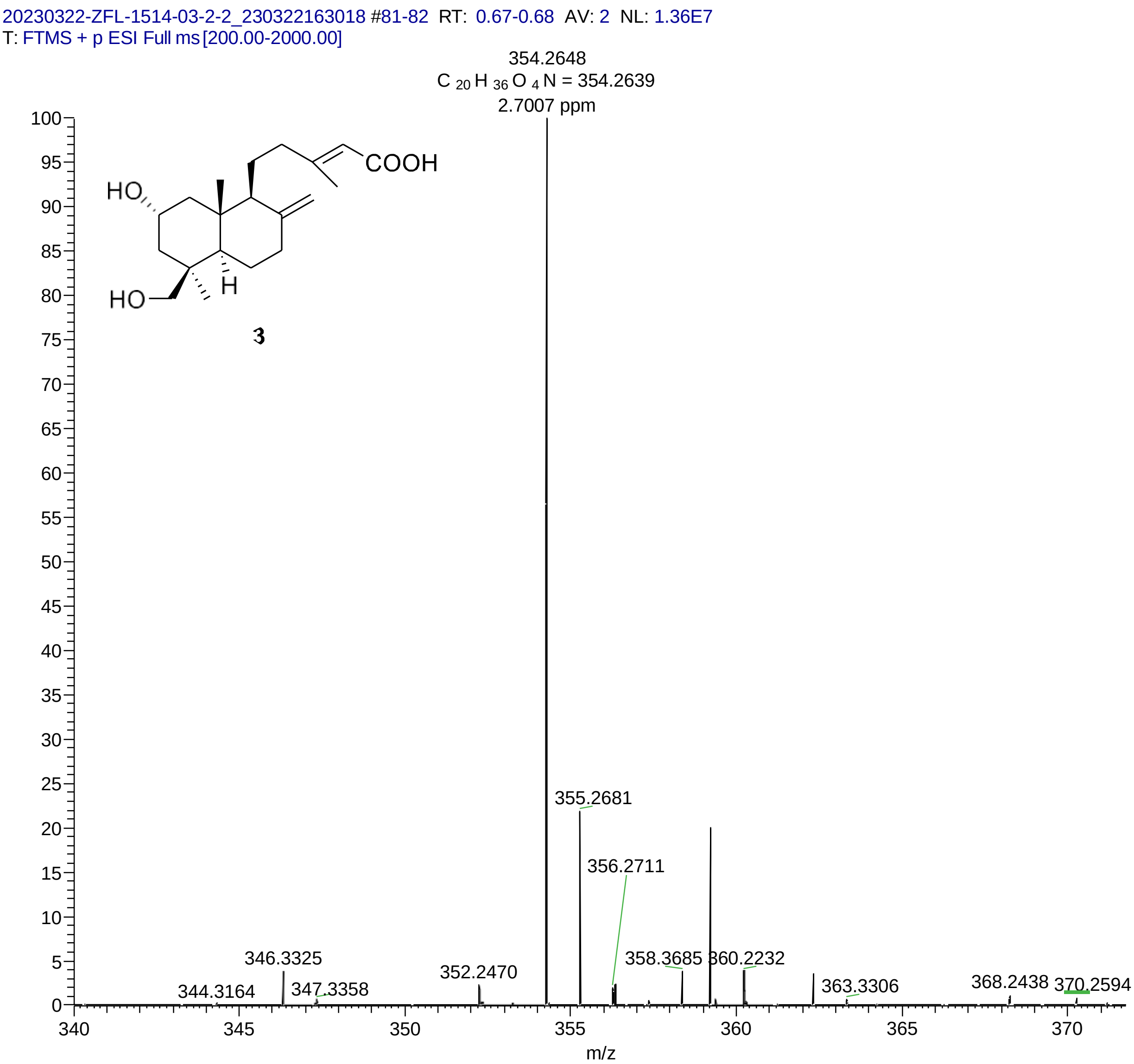



**Figure S19.** UV spectrum of **3**.

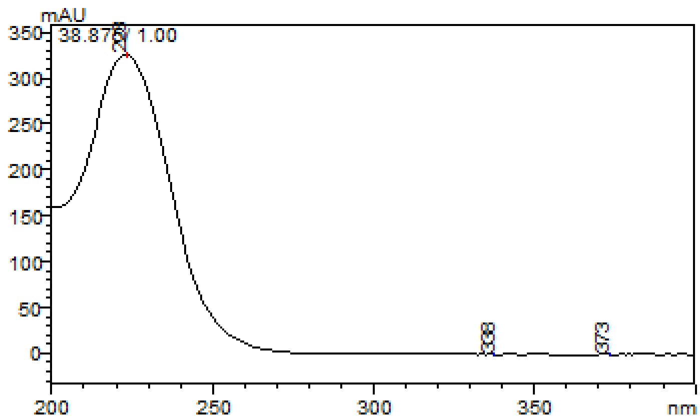


**Figure S20.** $^{1}$H NMR of **4** in $CD_3OD$.

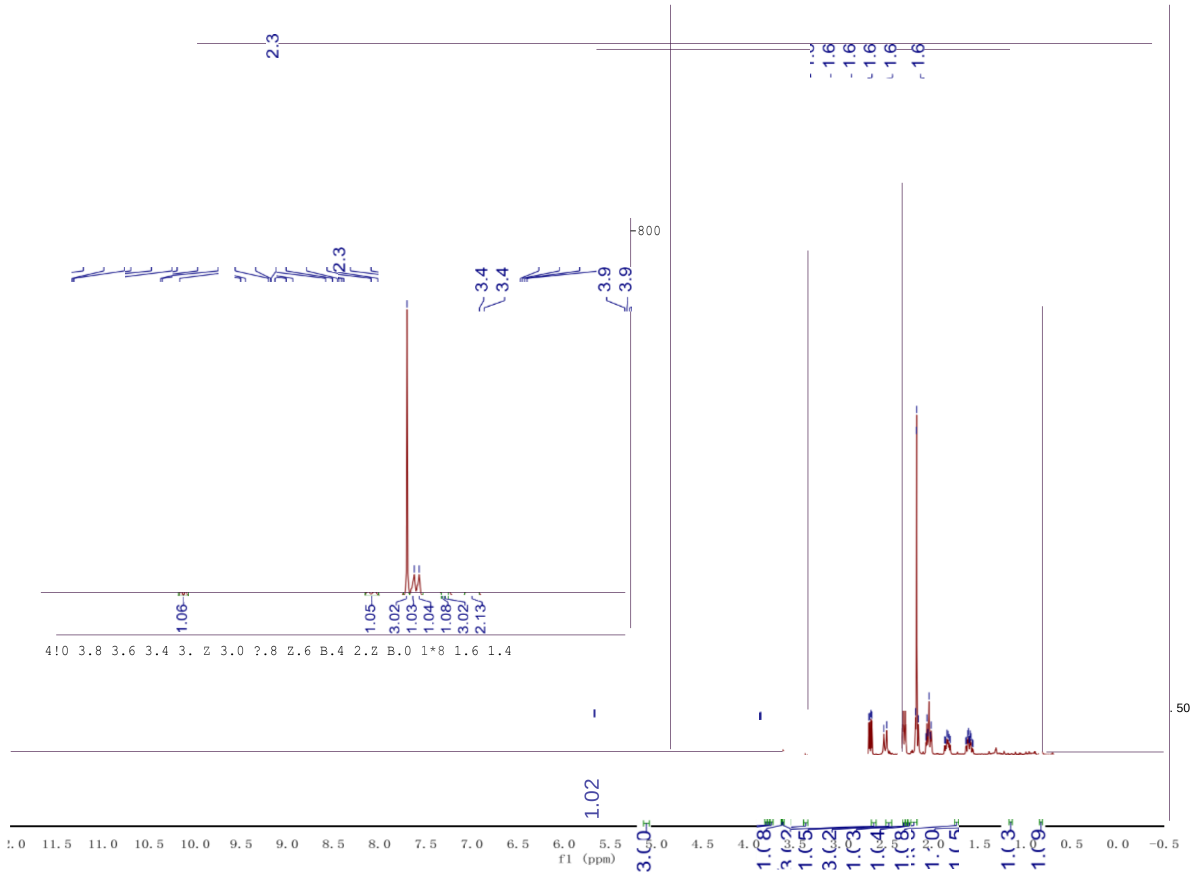


**Figure S21.** $^{13}$C NMR and DEPT of **4** in $CD_3OD$.

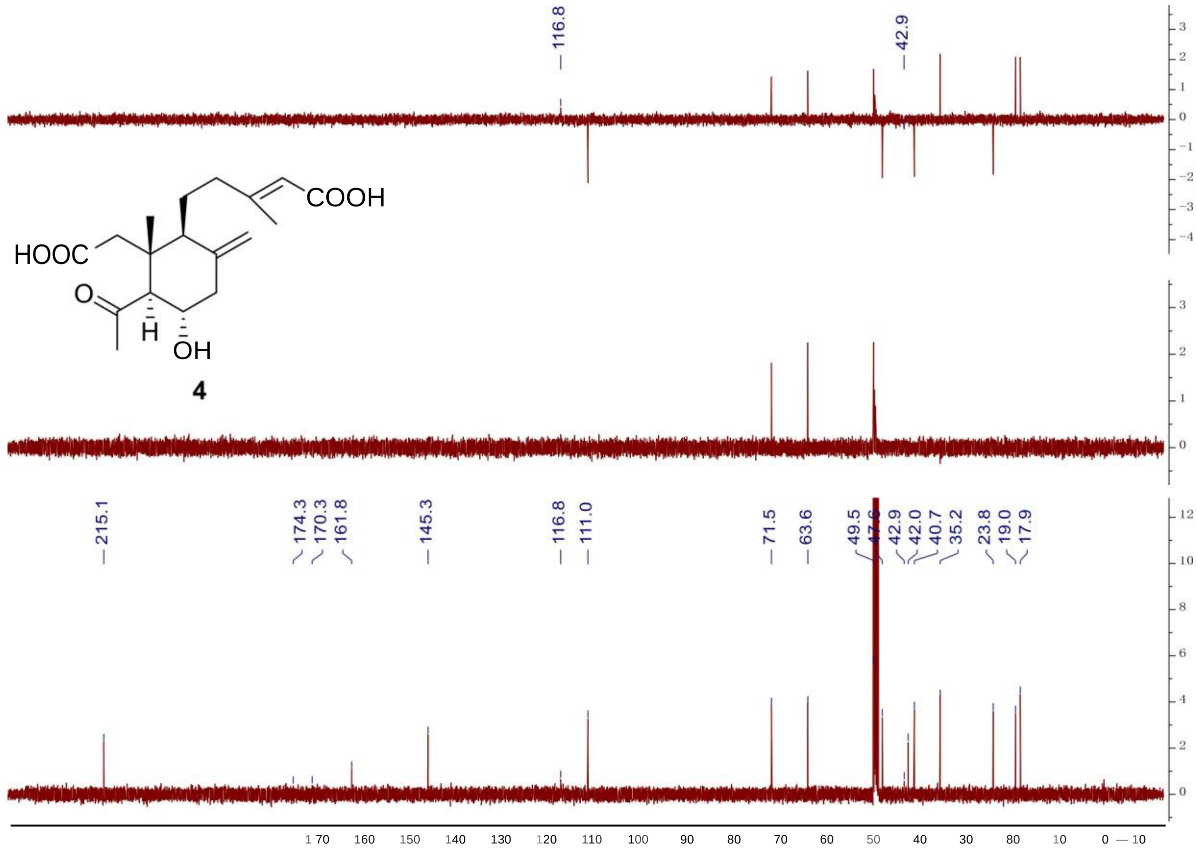


**Figure S22.** HSQC of **4** in $CD_3OD$.

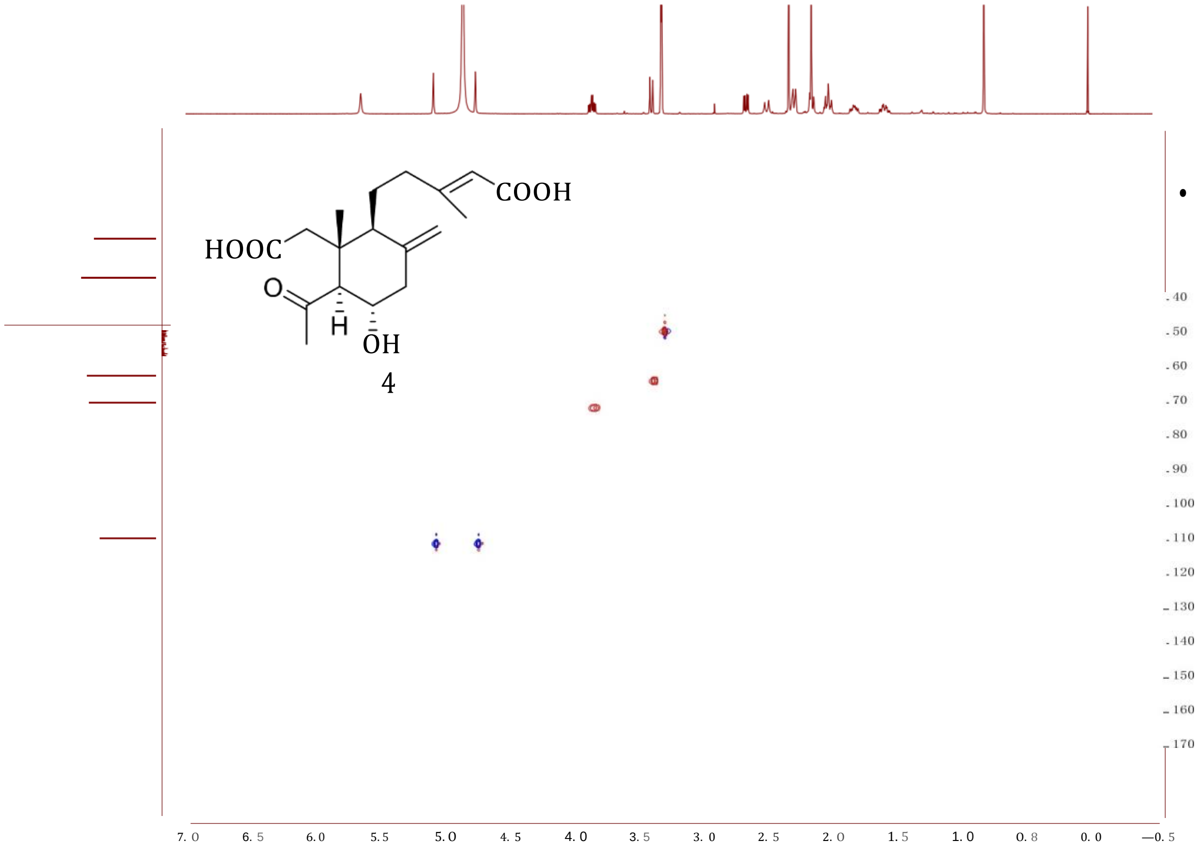



**Figure S23.** HMBC of **4** in $CD_3OD$.

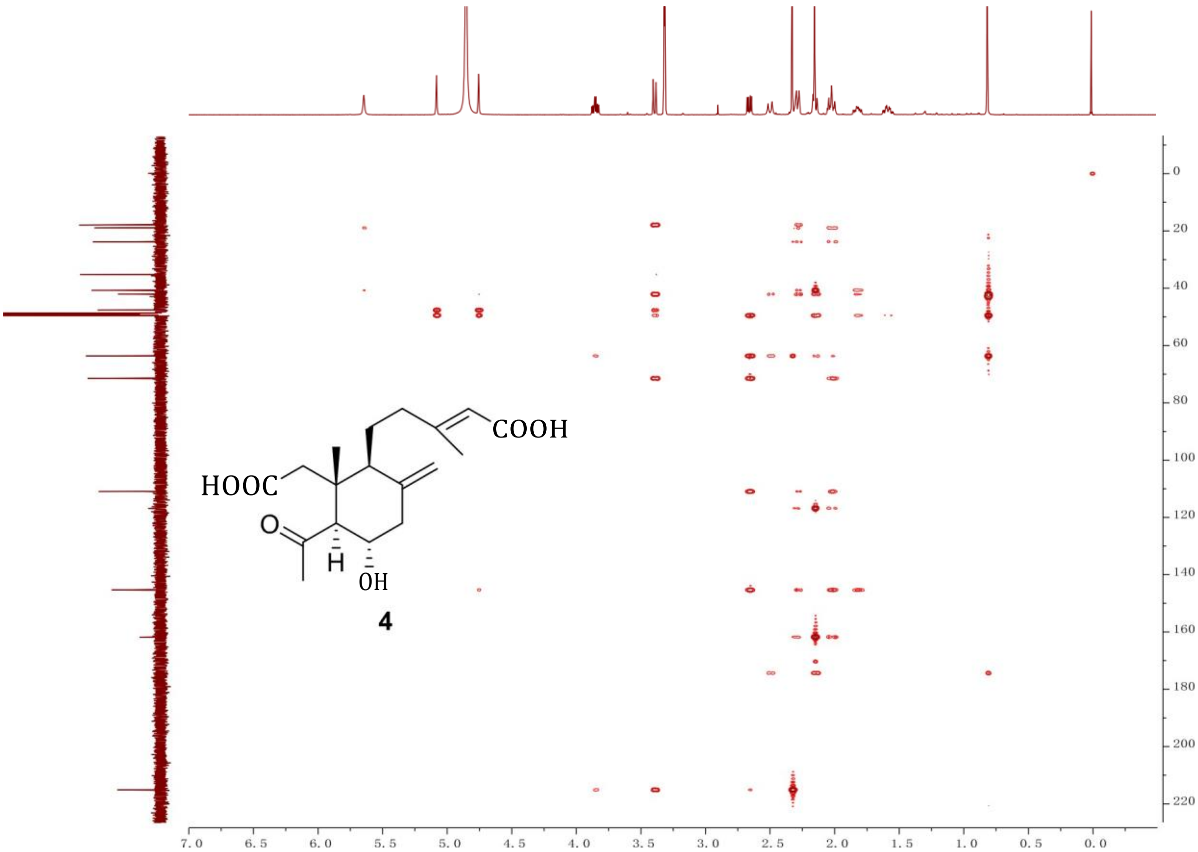


**Figure S24.** $^1$H-$^1$H COSY of **4** in $CD_3OD$.

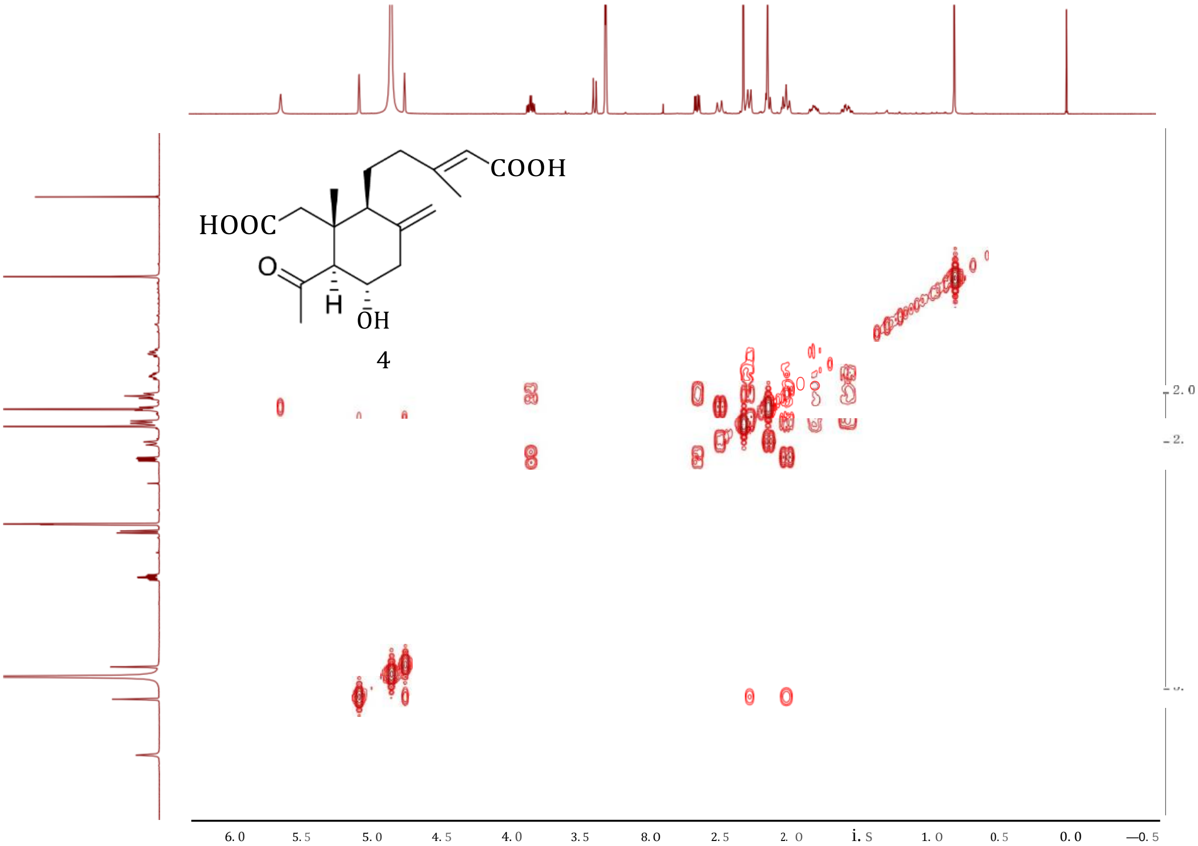



**Figure S25.** ROESY of **4** in $CD_3OD$.

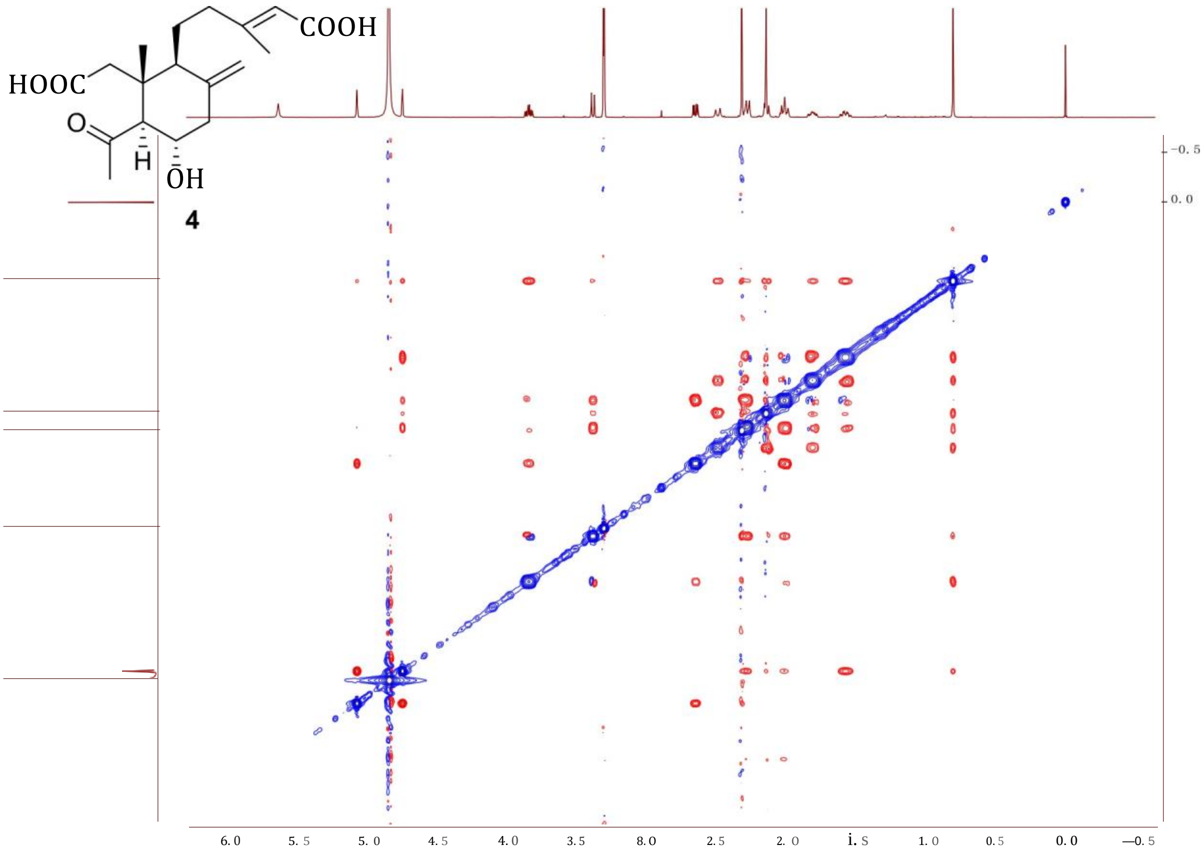


**Figure S26.** HRESIMS of **4**.

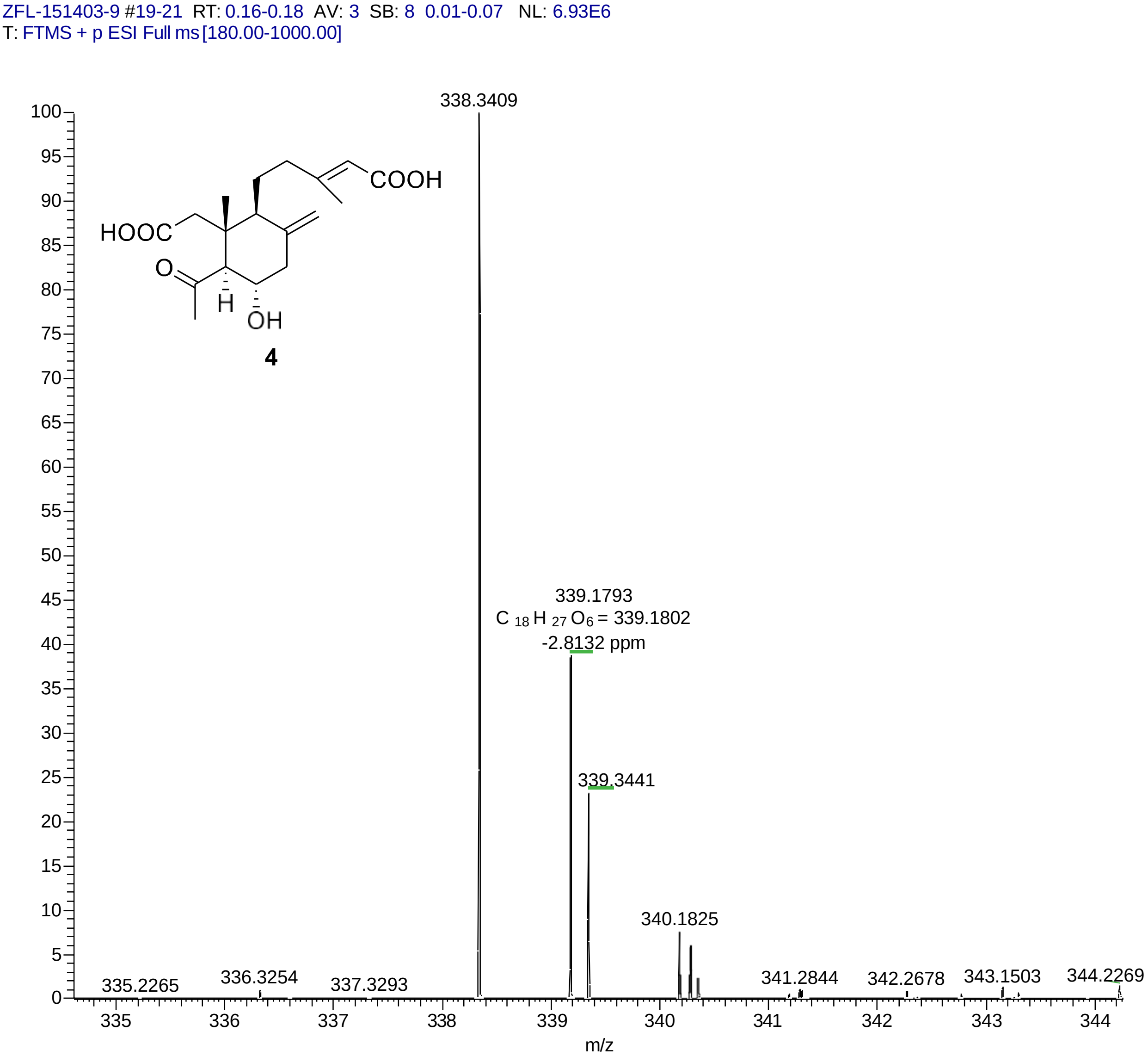



**Figure S27.** UV spectrum of **4**.

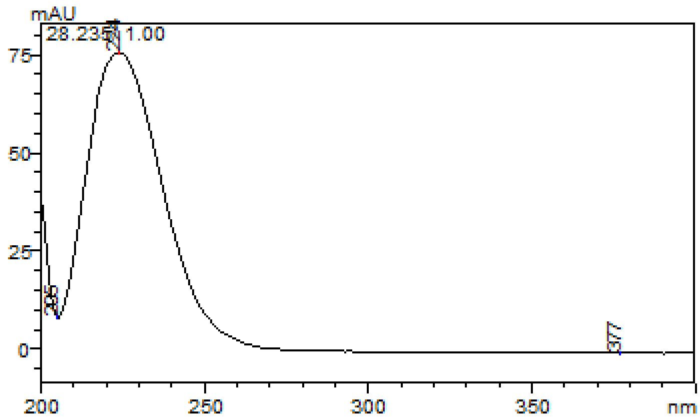


**Figure S28.** $^{1}H$ NMR of **5** in $CD_3OD$.

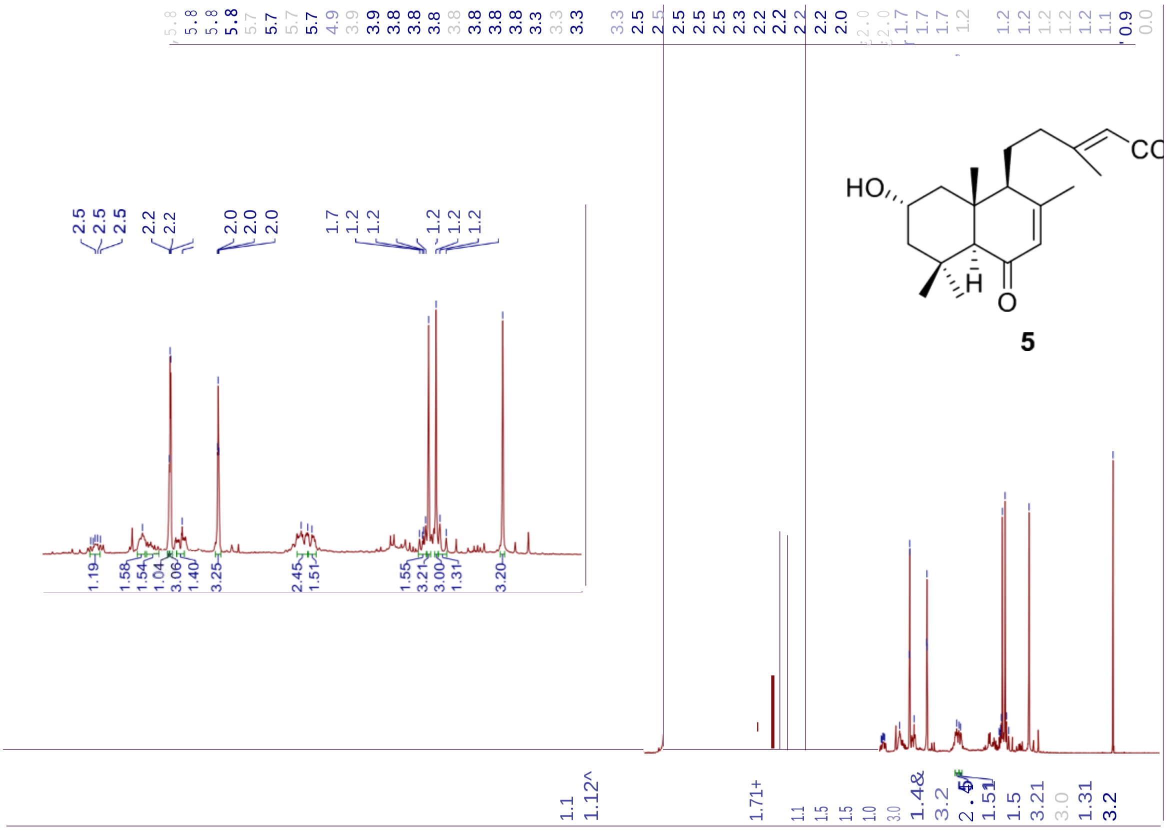


**Figure S29.** $^{13}C$ NMR of **5** in $CD_3OD$.

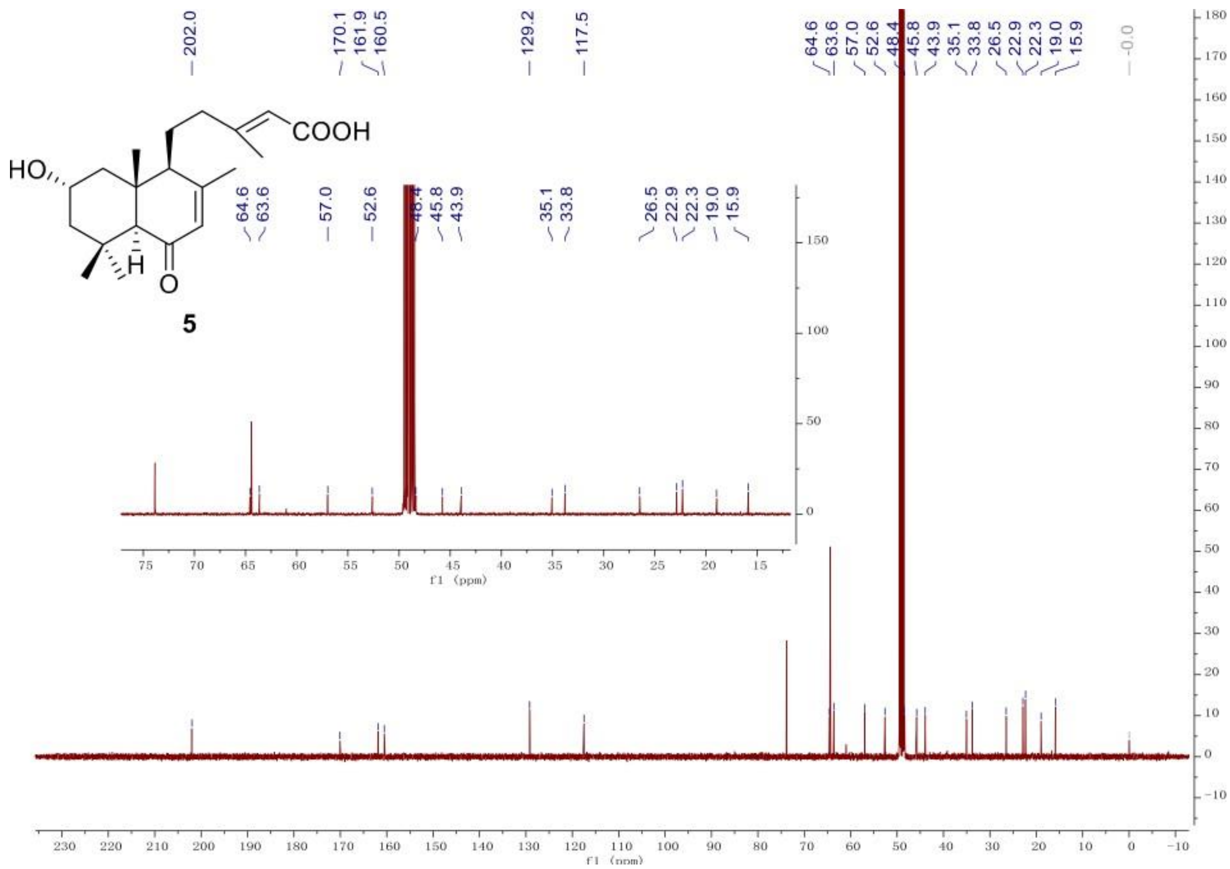


**Figure S30.** HSQC of **5** in $CD_3OD$.

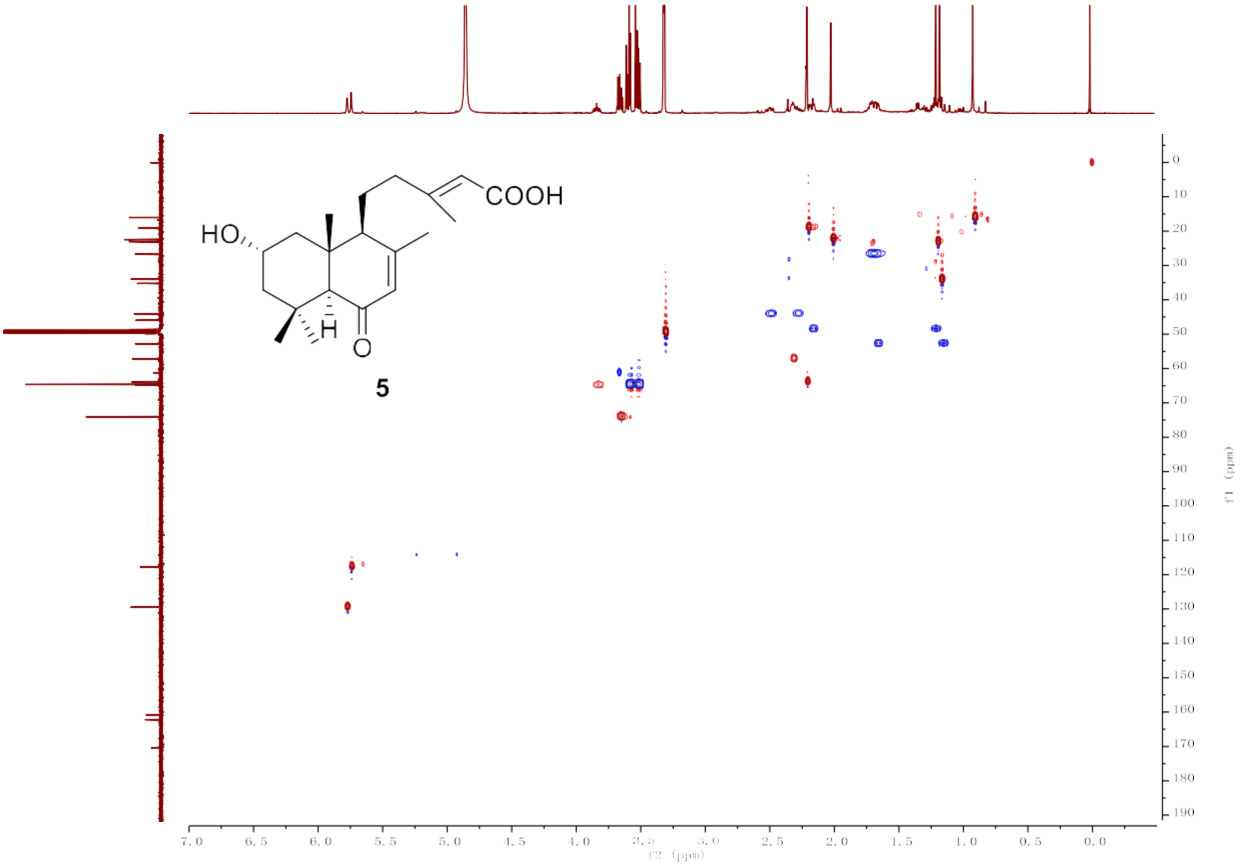


**Figure S31.** HMBC of **5** in $CD_3OD$.

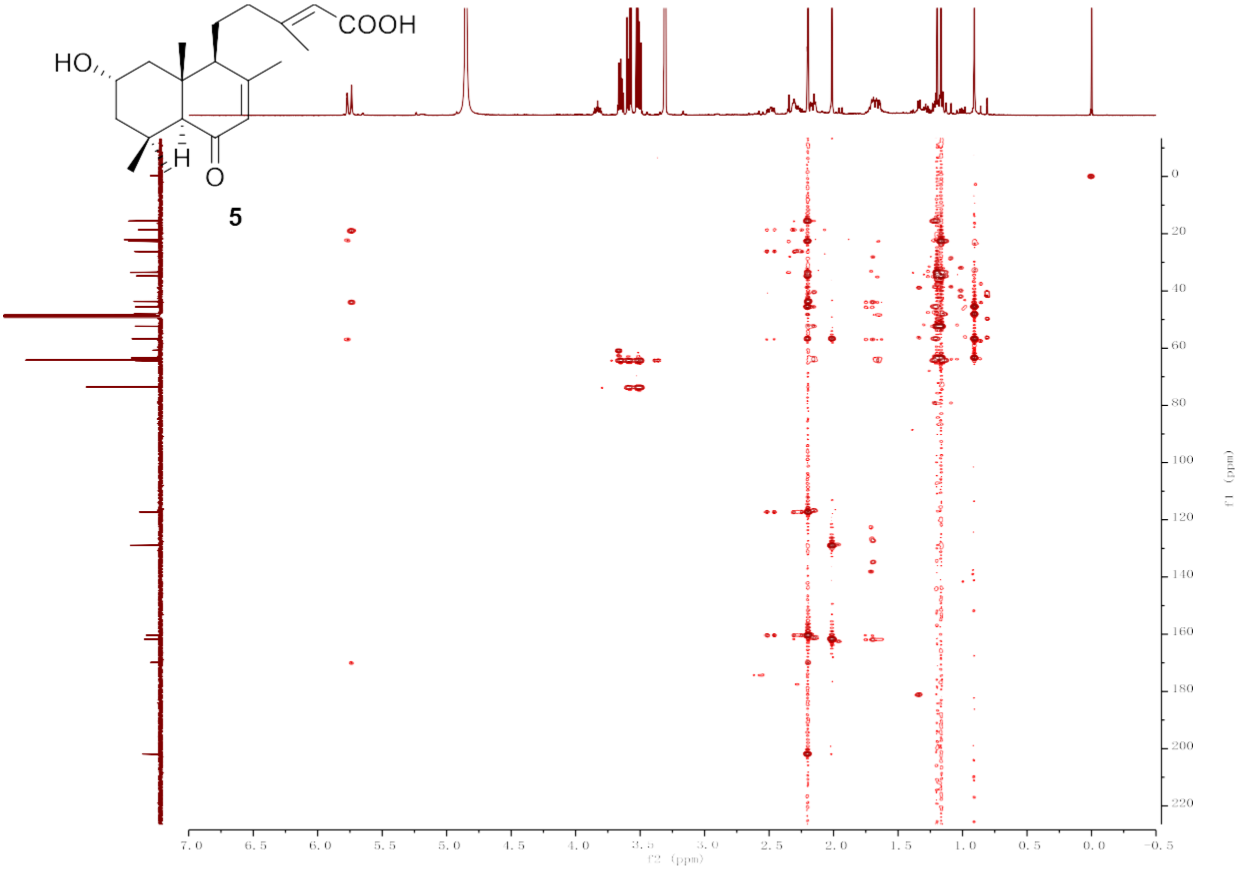


**Figure S32.** $^{1}$H-$^{1}$H COSY of **5** in $CD_3OD$.

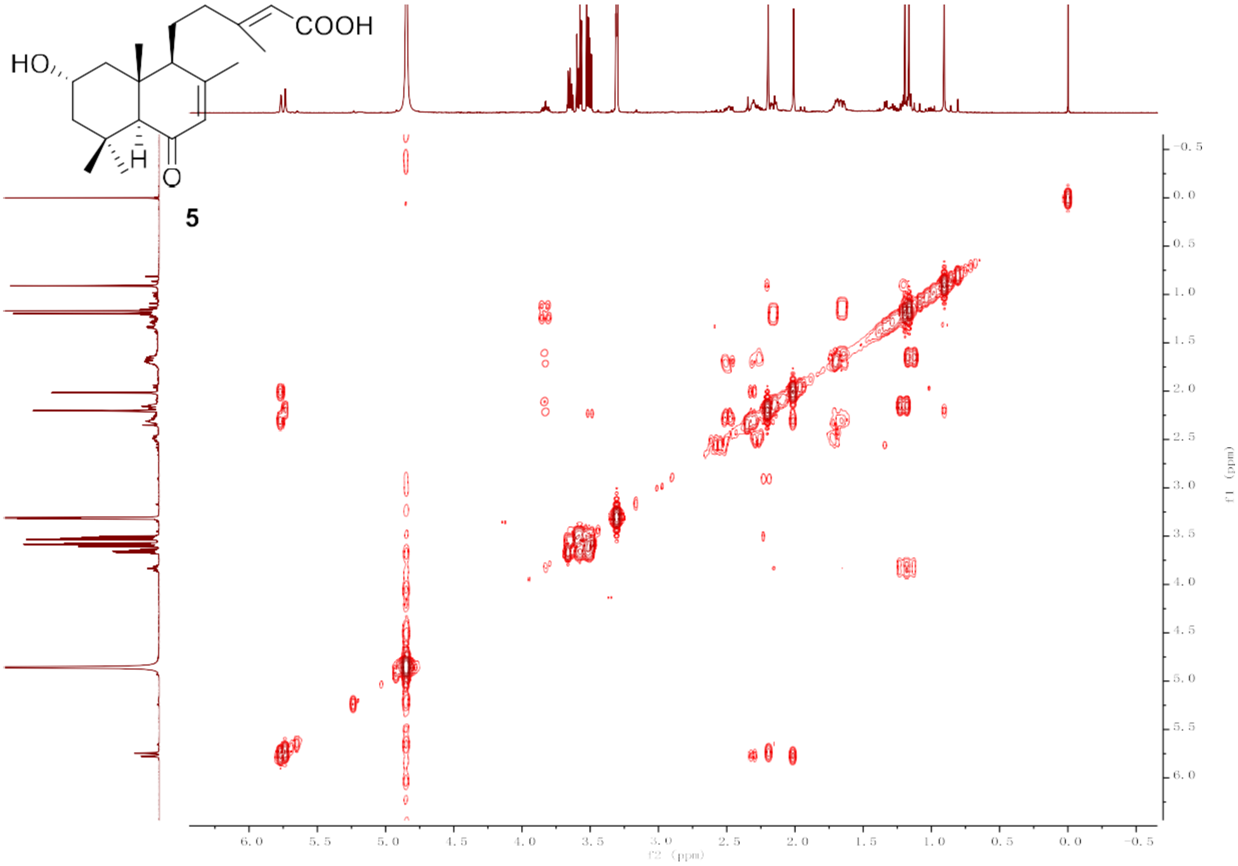



**Figure S33.** ROESY of **5** in $CD_3OD$.

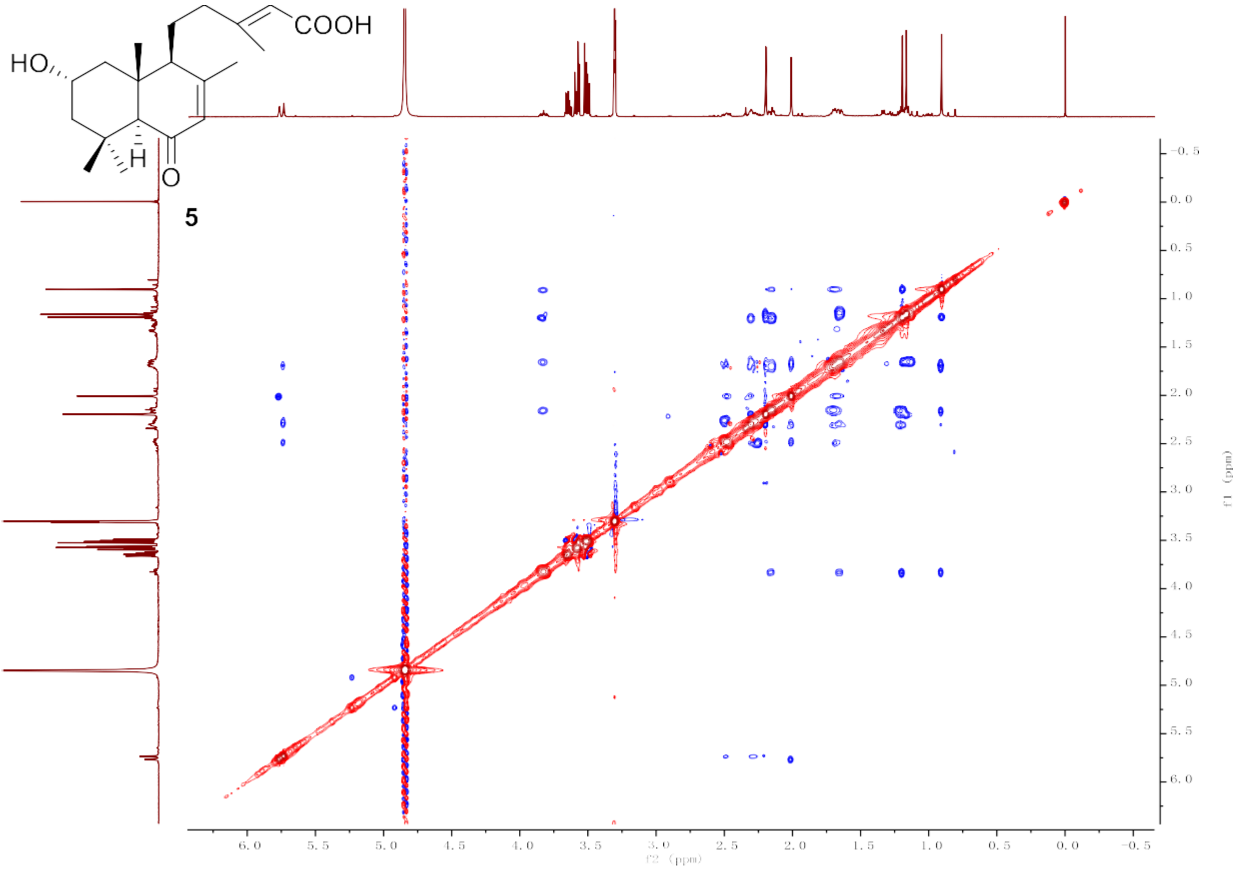


**Figure S34.** HRESIMS of **5**.

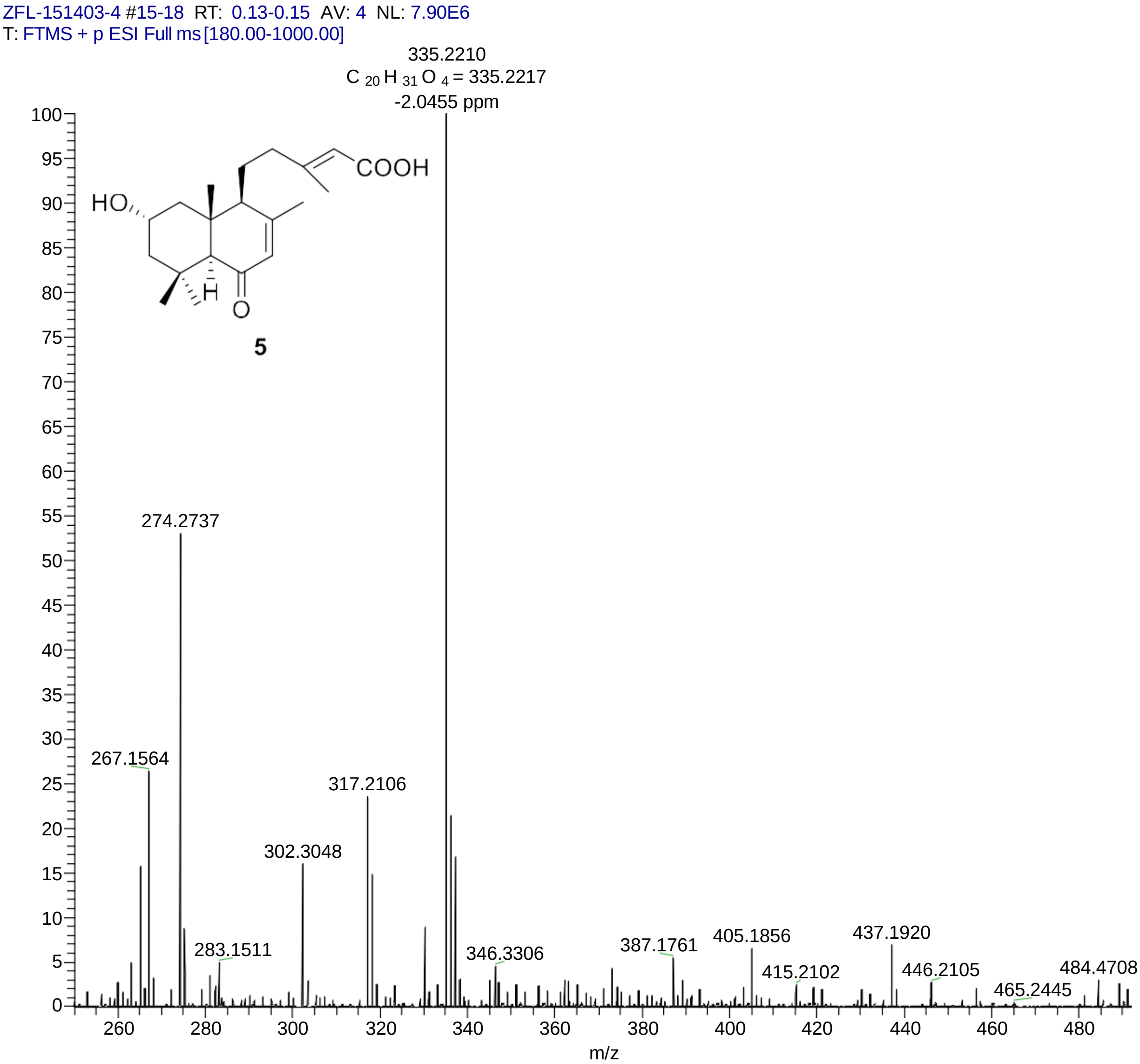



**Figure S35.** UV spectrum of **5**.

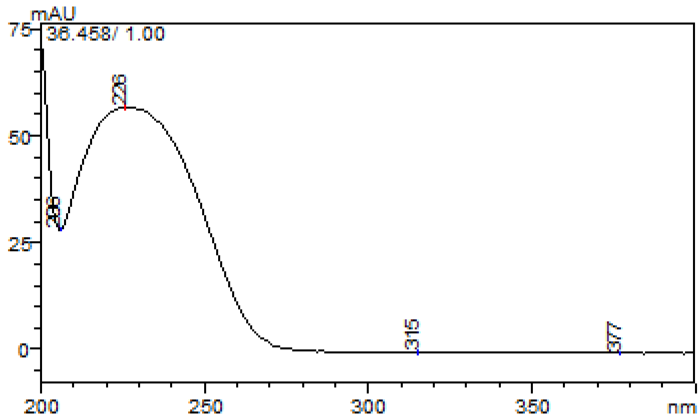


**Figure S36.** $^{1}H$ NMR of **6** in $CD_3OD$.

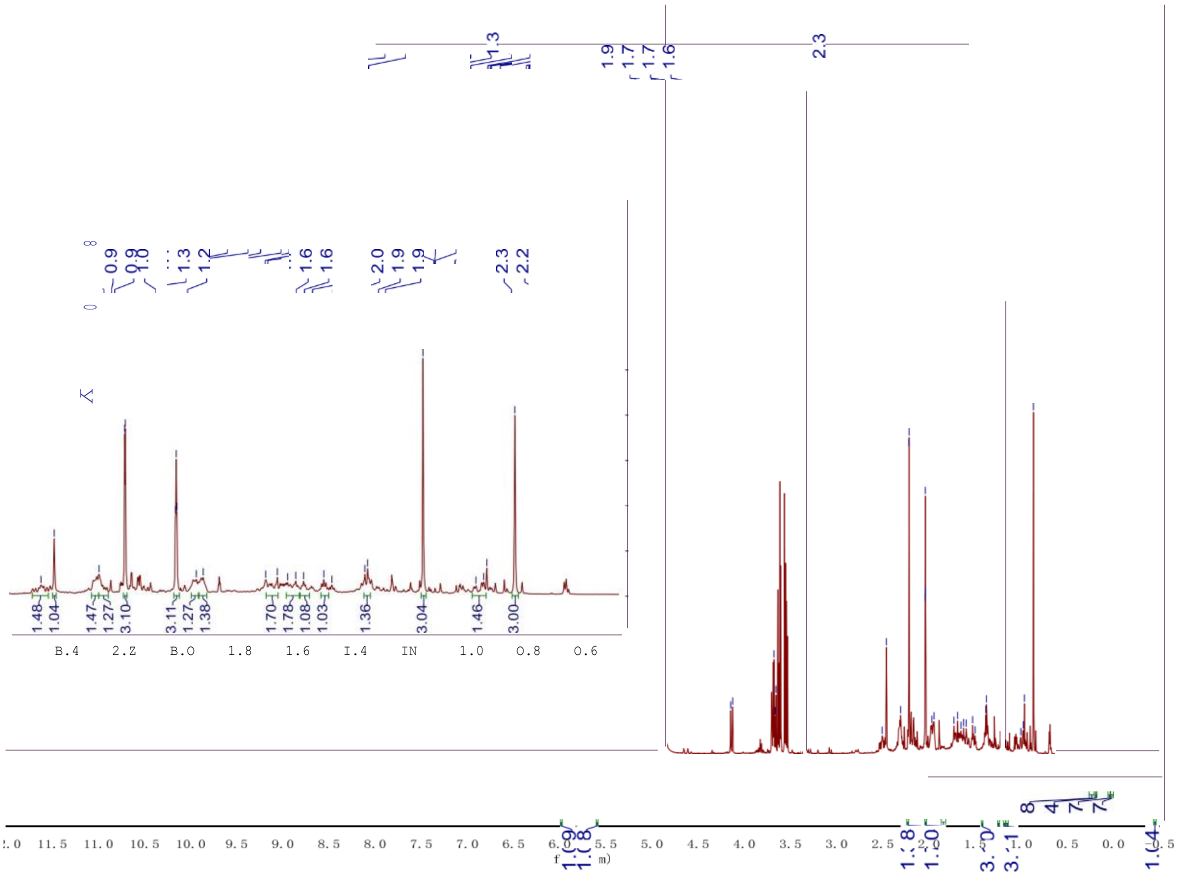


**Figure S37.** $^{13}C$ NMR of **6** in $CD_3OD$.

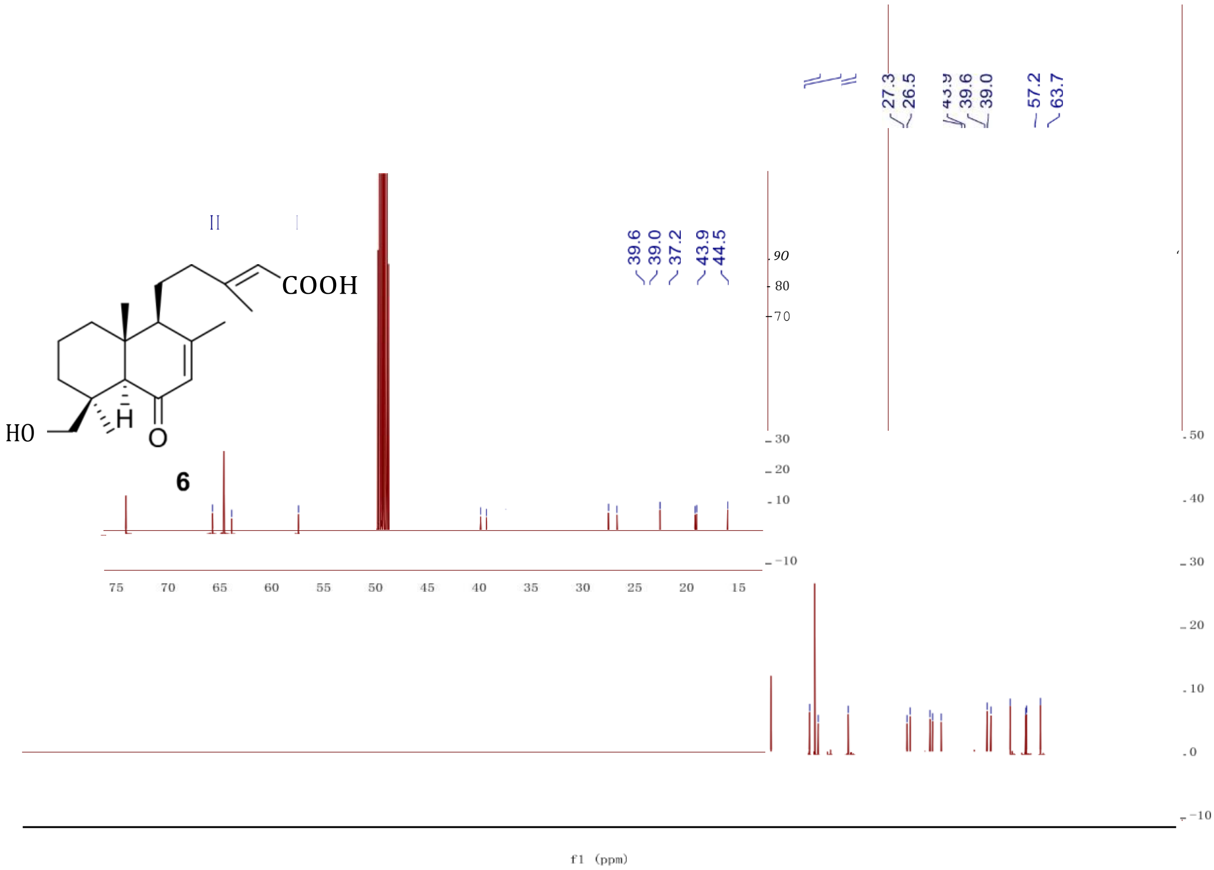


**Figure S38.** HSQC of **6** in $CD_3OD$.

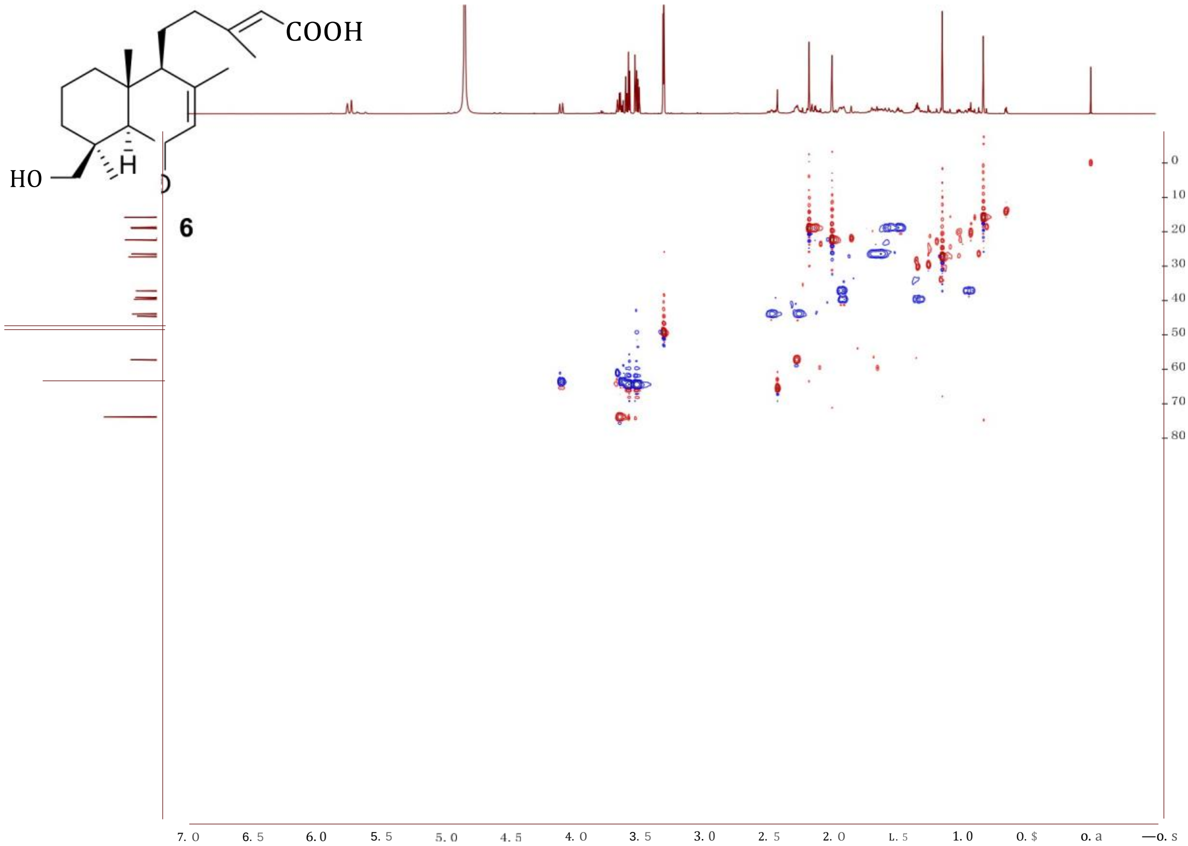



**Figure S39.** HMBC of **6** in $CD_3OD$.

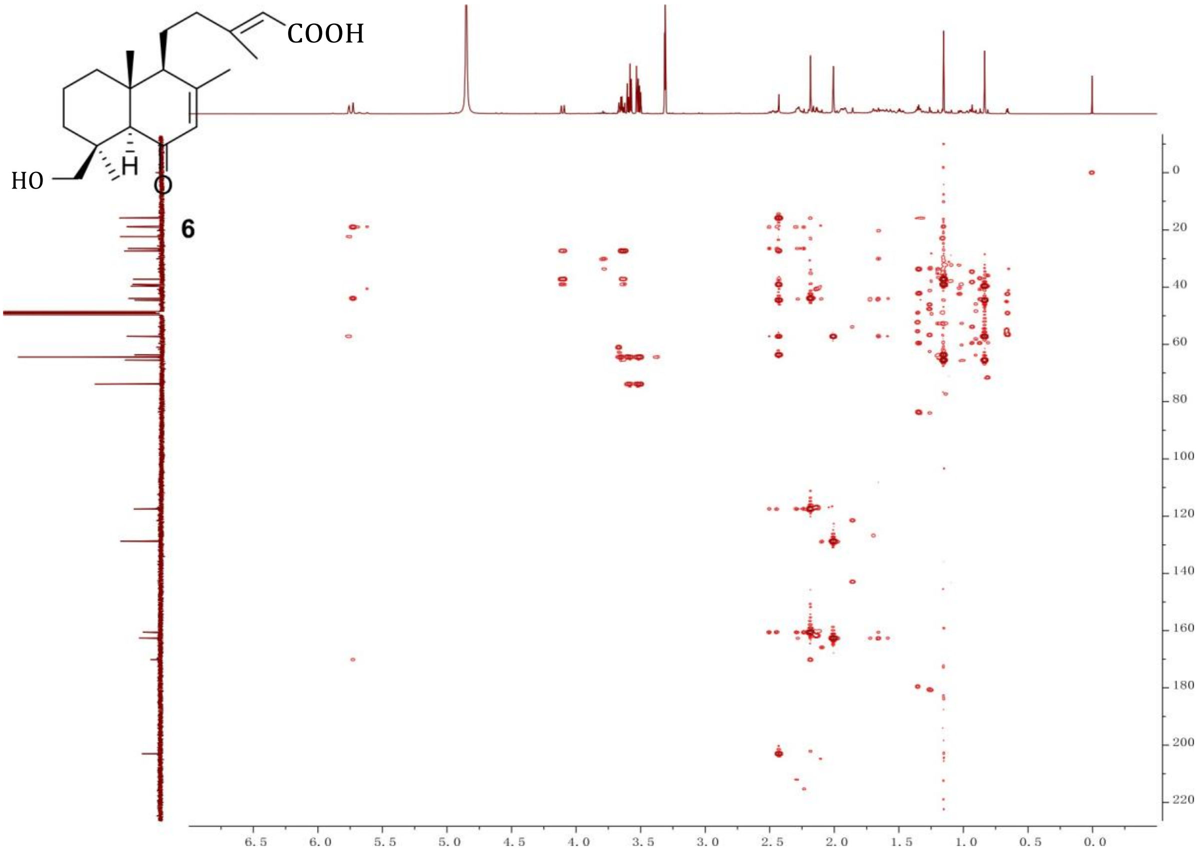


**Figure S40.** $^{1}H$-$^{1}H$ COSY of **6** in $CD_3OD$.

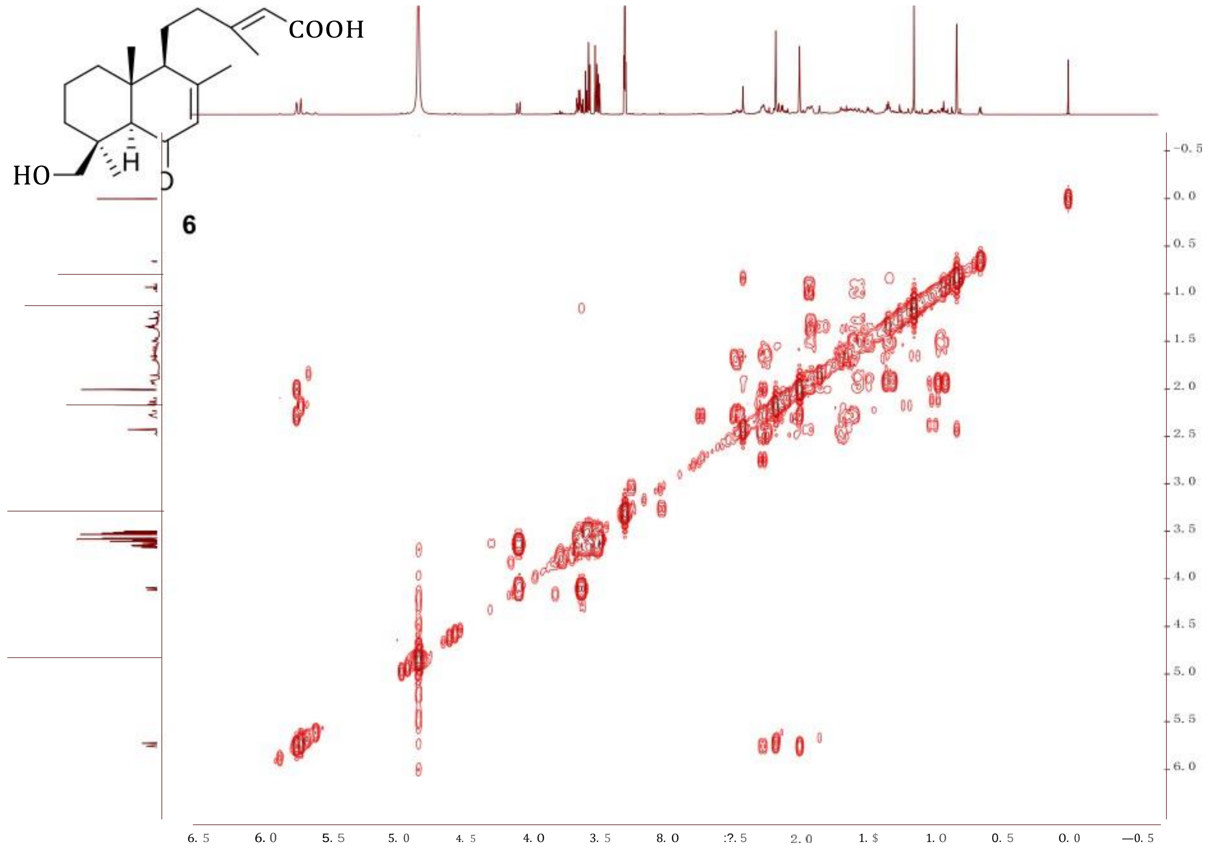



**Figure S41.** ROESY of **6** in $CD_3OD$.

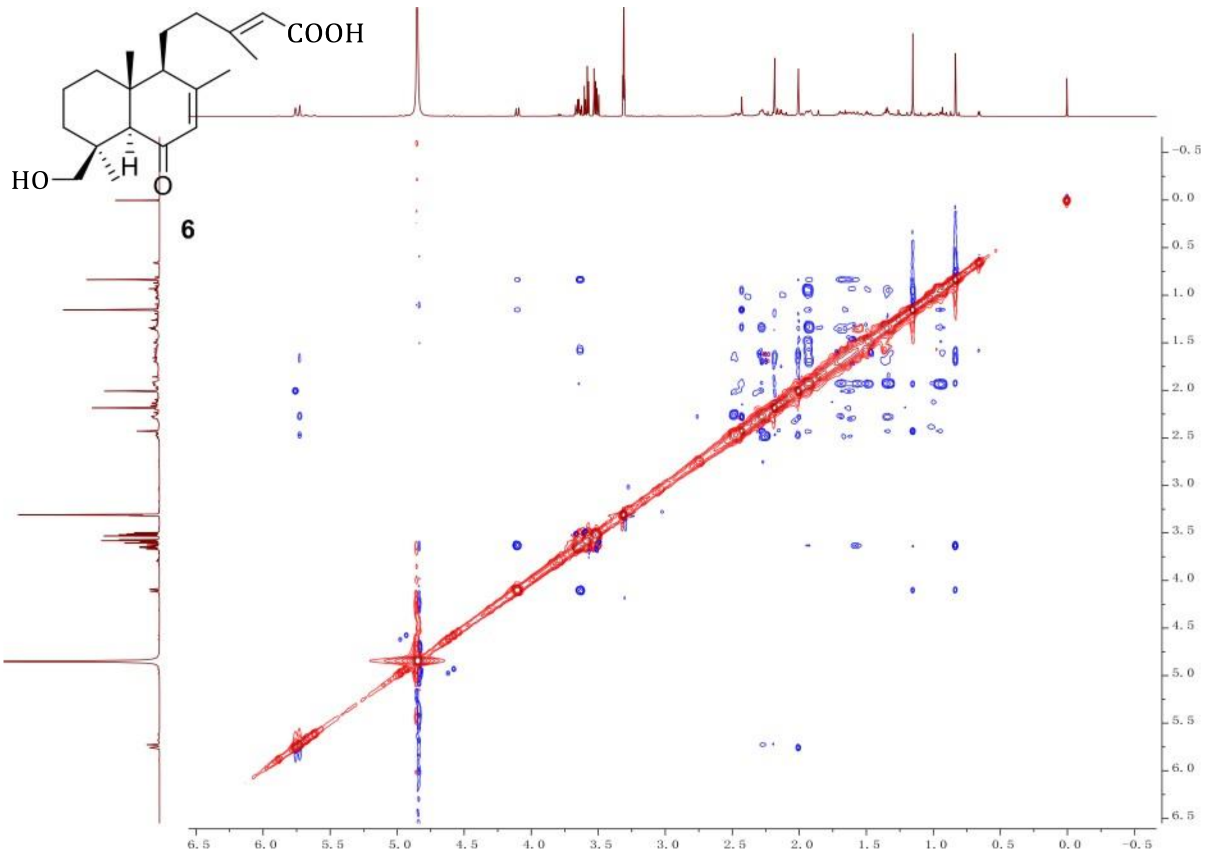


**Figure S42.** HRESIMS of **6**.

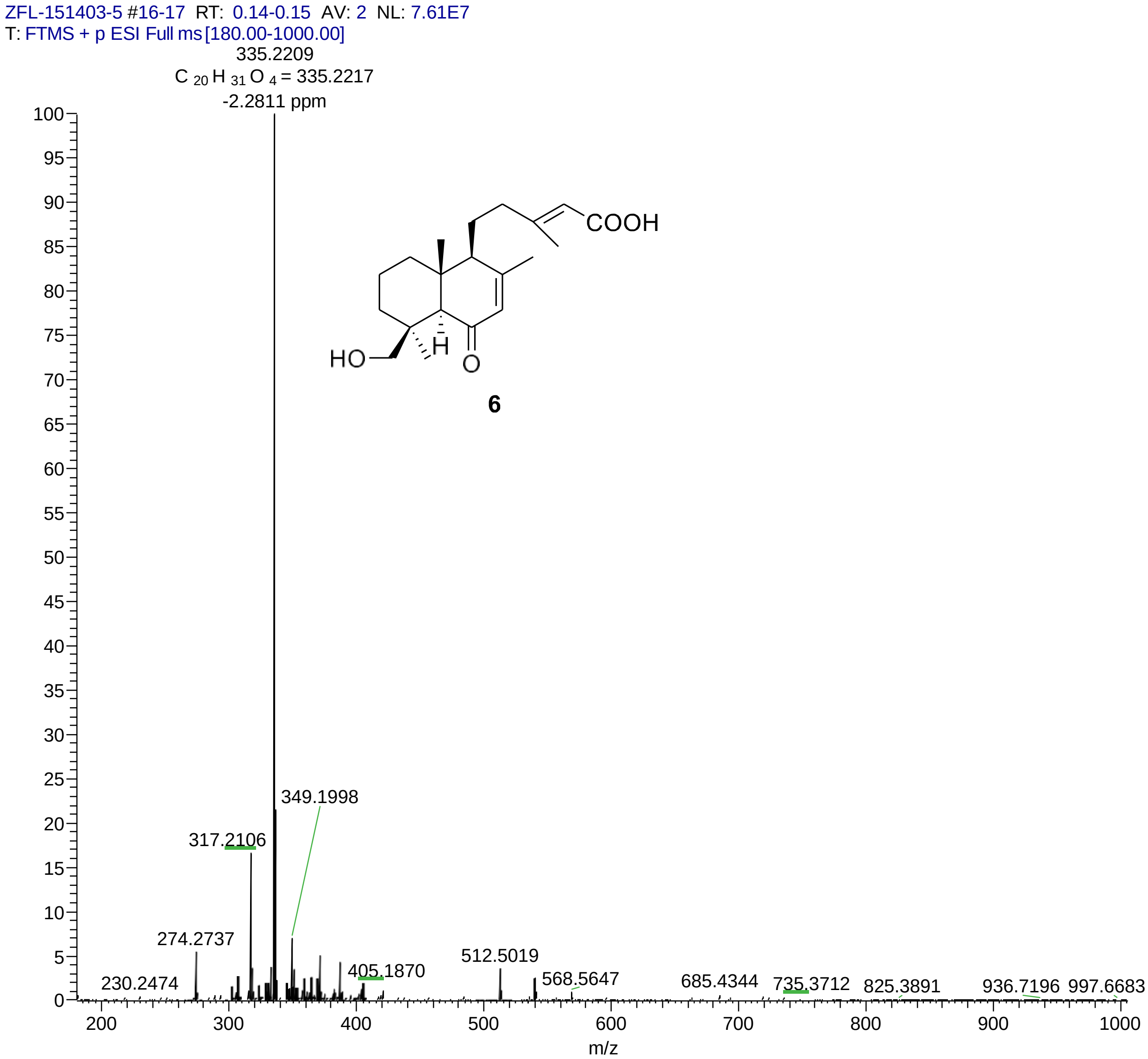



**Figure S43.** UV spectrum of **6**.

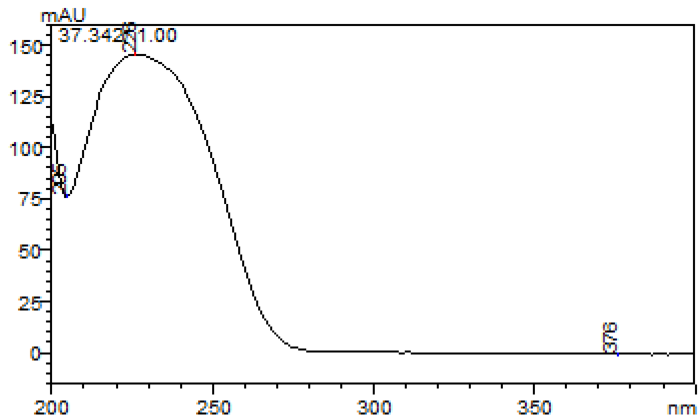
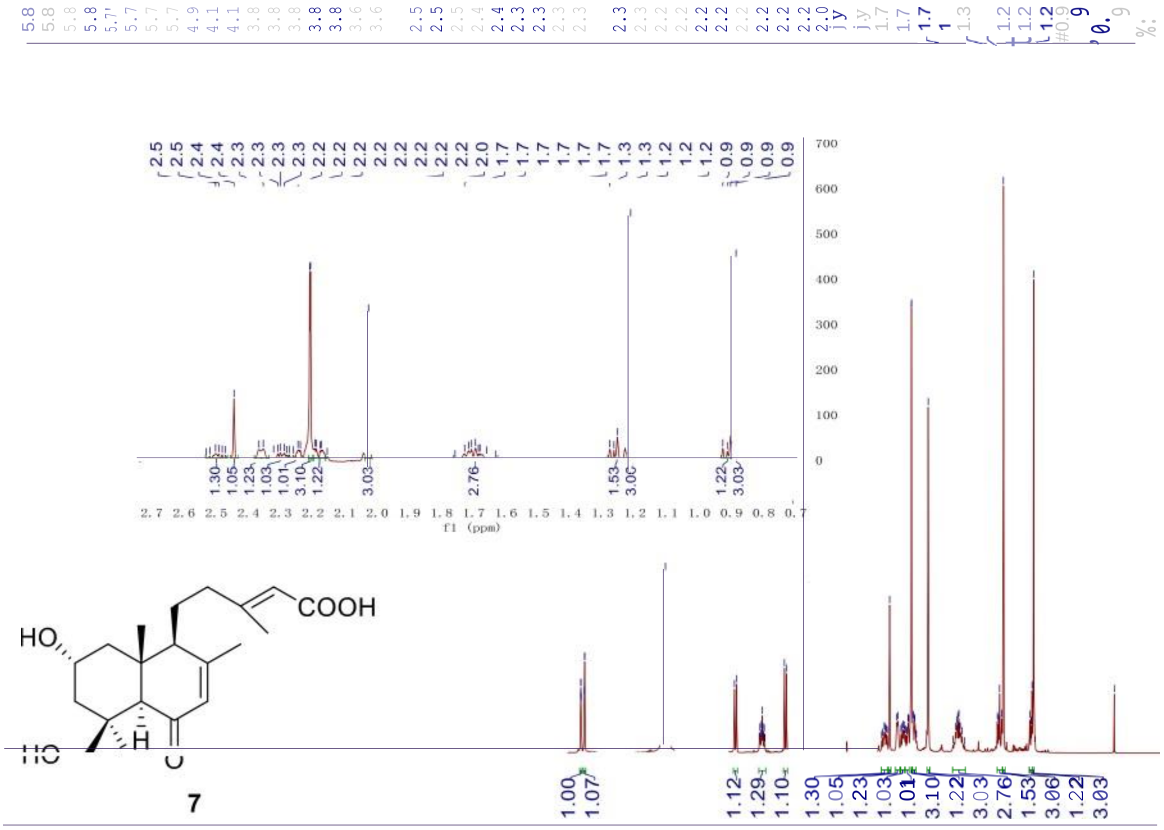


**Figure S44.** $^{1}H$ NMR of **7** in $CD_3OD$.



7

**Figure S45.** $^{13}C$ NMR of **7** in $CD_3OD$.

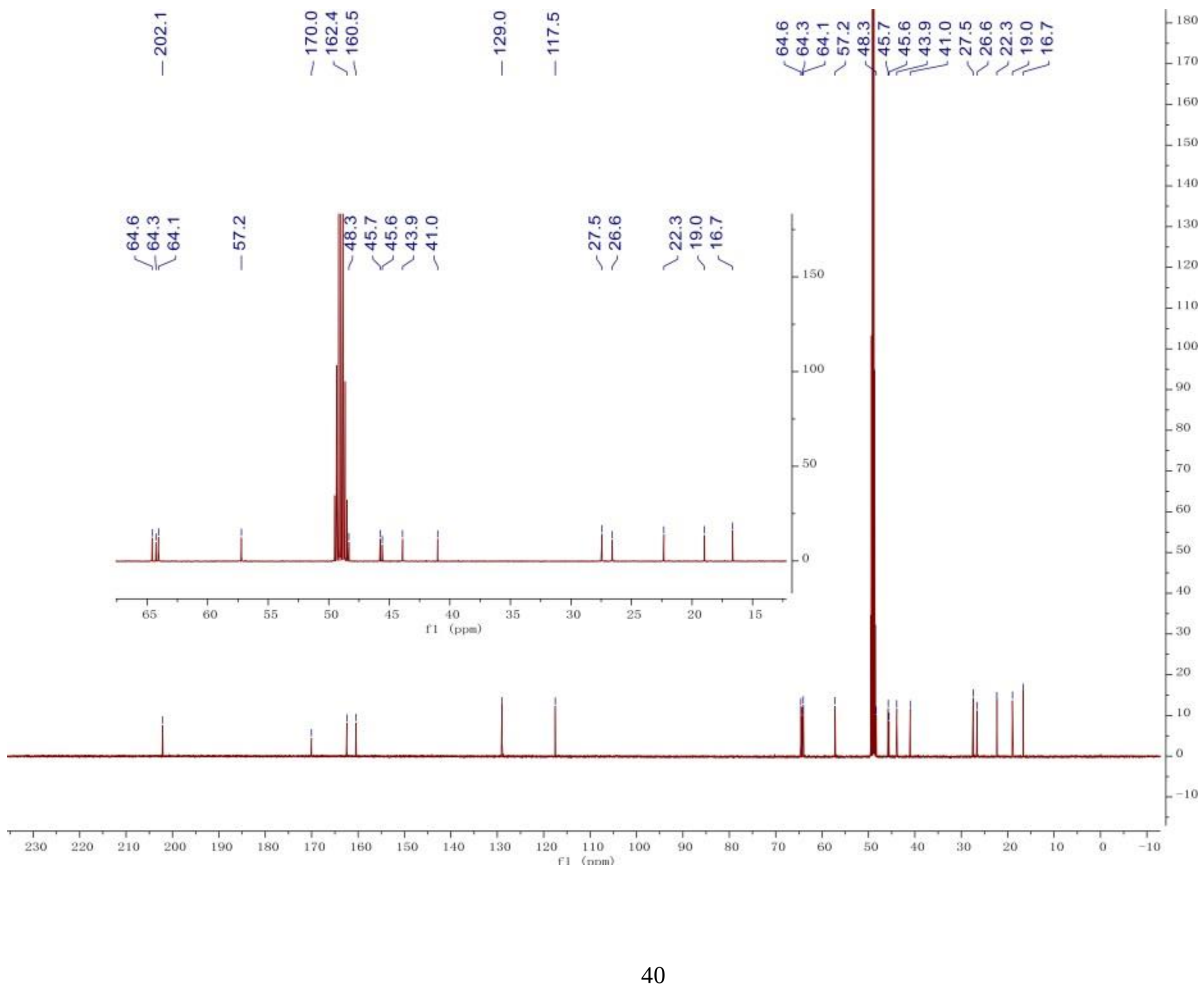


**Figure S46.** HSQC of **7** in $CD_3OD$.

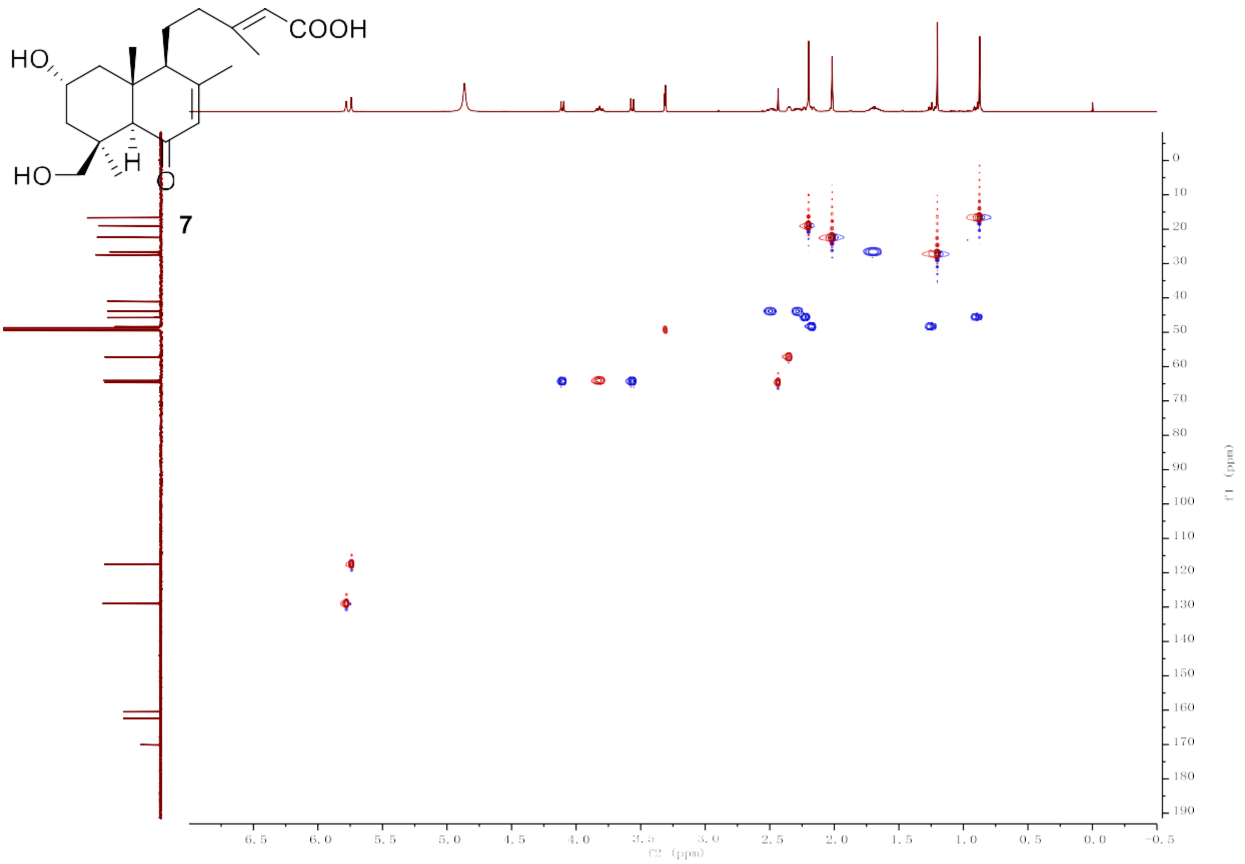



**Figure S47.** HMBC of **7** in $CD_3OD$.

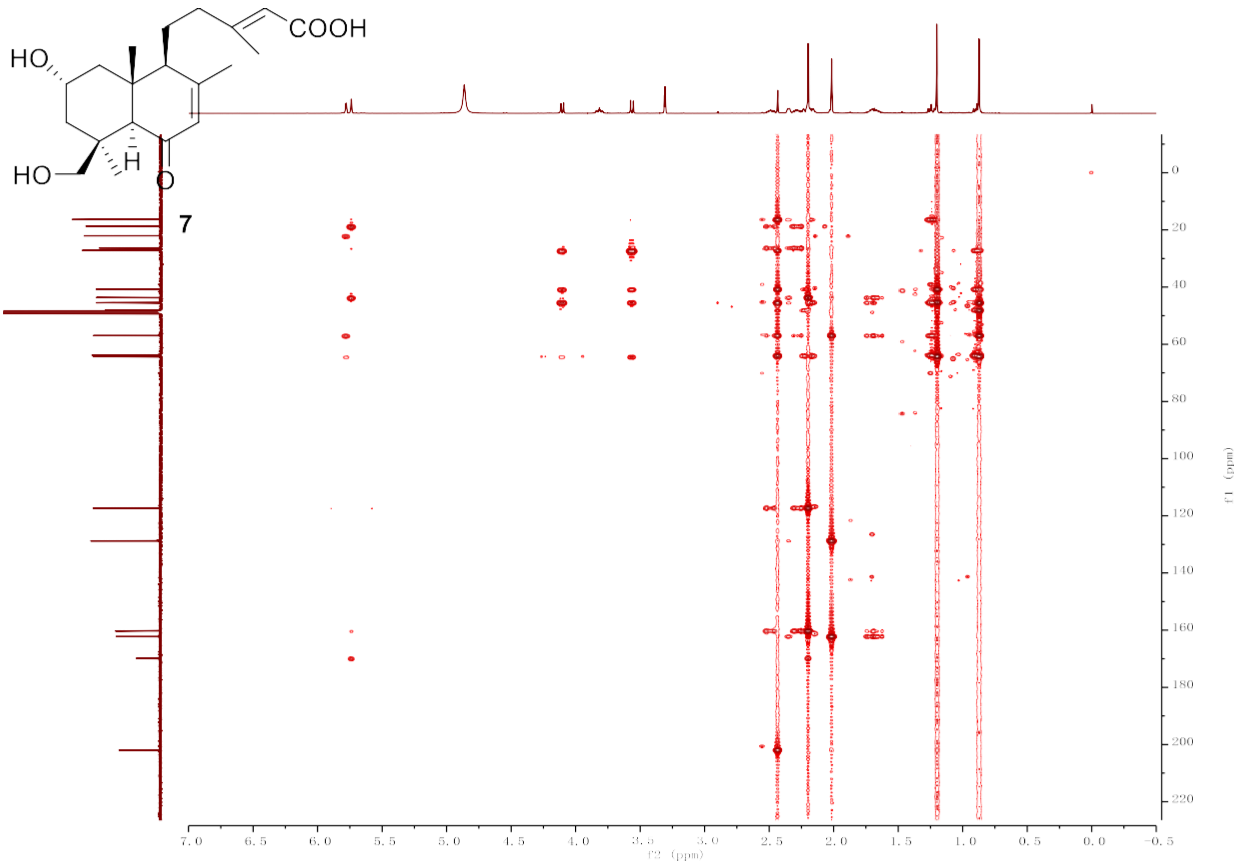


**Figure S48.** $^{1}H$-$^{1}H$ COSY of **7** in $CD_3OD$.

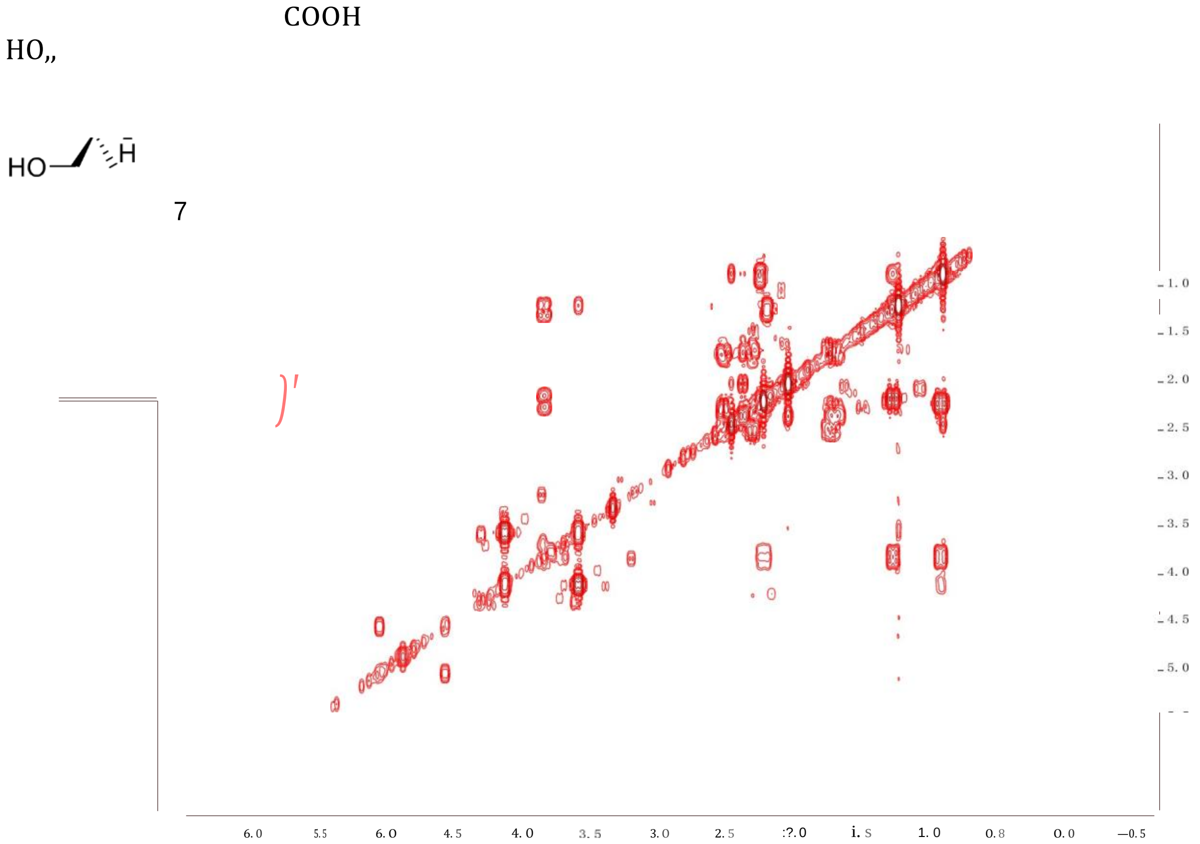


**Figure S49.** ROESY of **7** in $CD_3OD$.

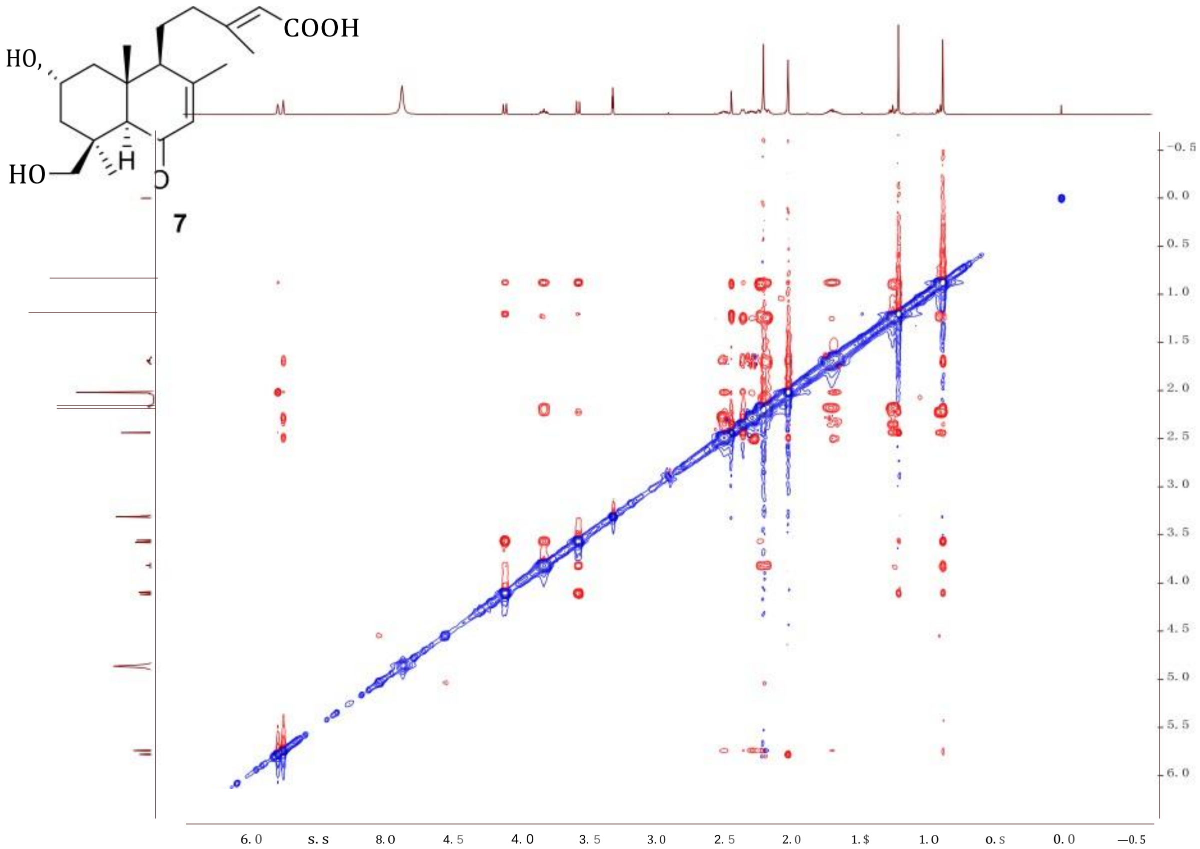


**Figure S50.** HRESIMS of **7**.

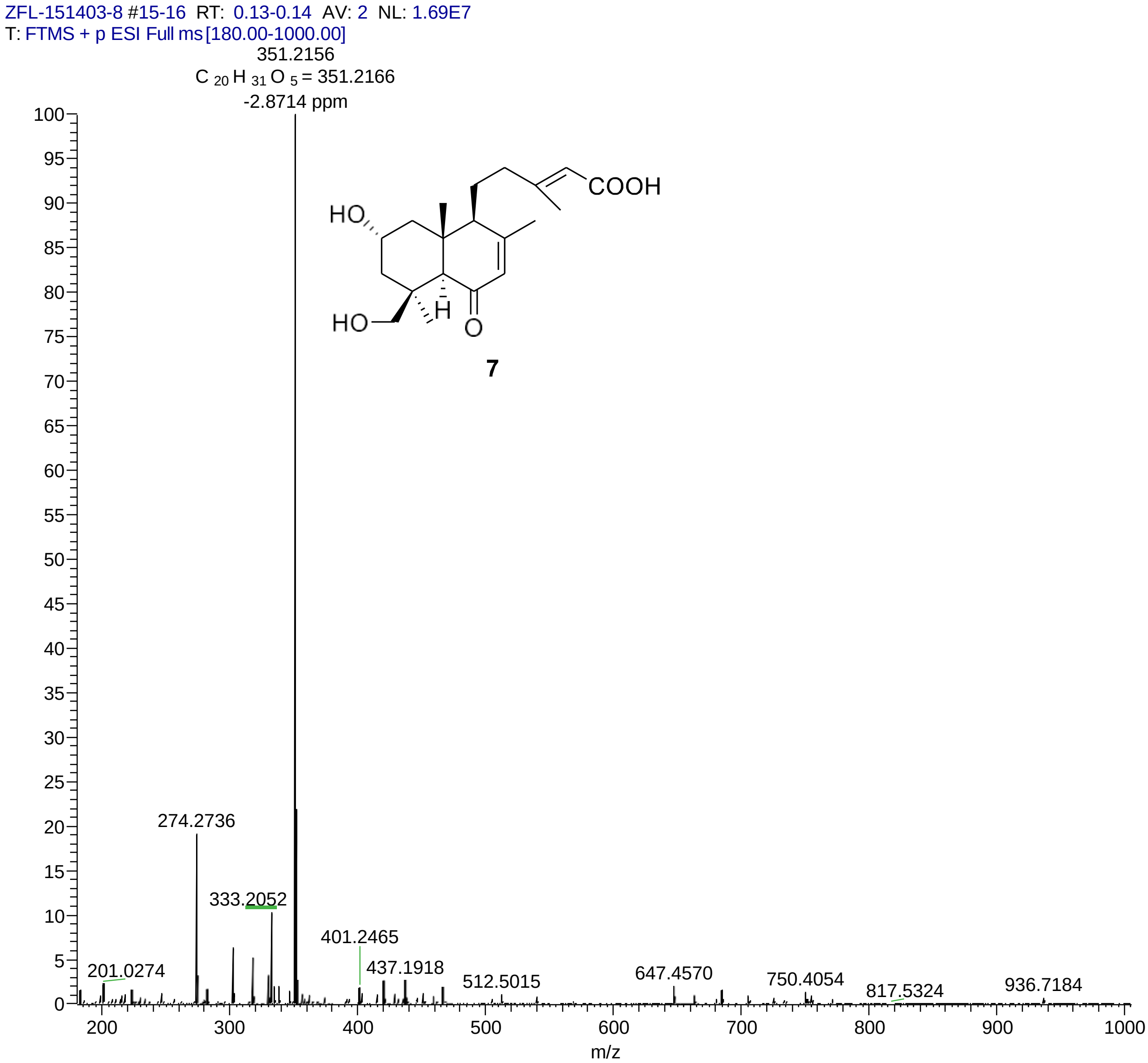



**Figure S51.** UV spectrum of **7**.

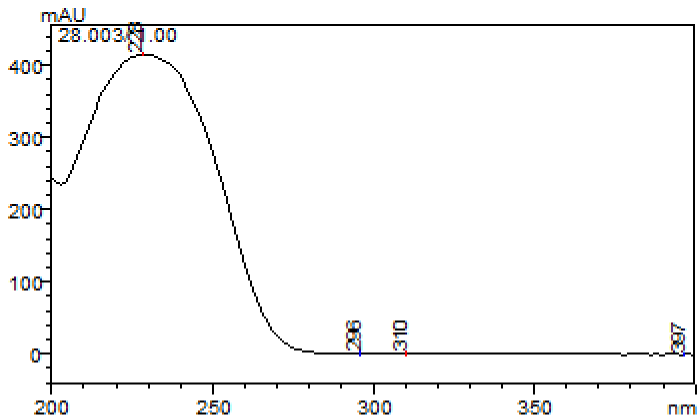


**Figure S52.** $^{1}H$ NMR of **1** in $CD_3OD$.

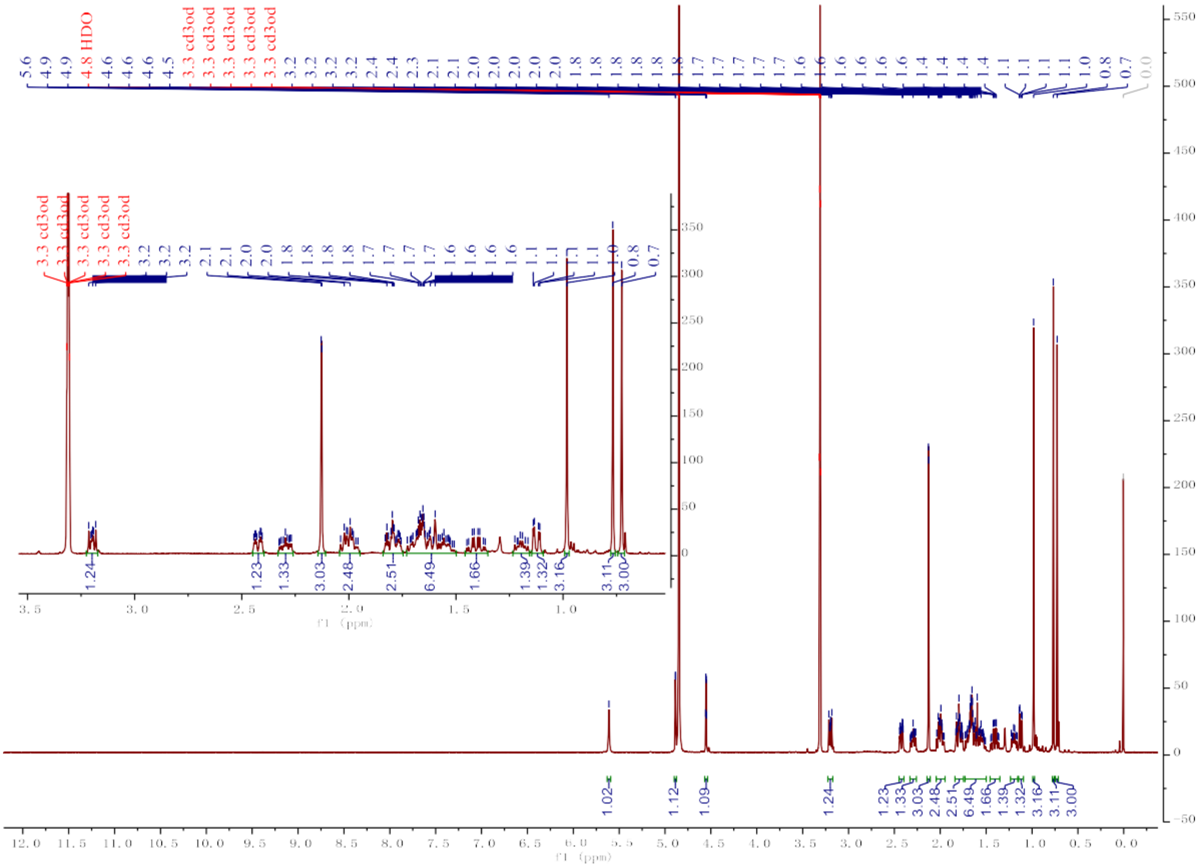


**Figure S53.** $^{13}C$ NMR of **1** in $CD_3OD$.

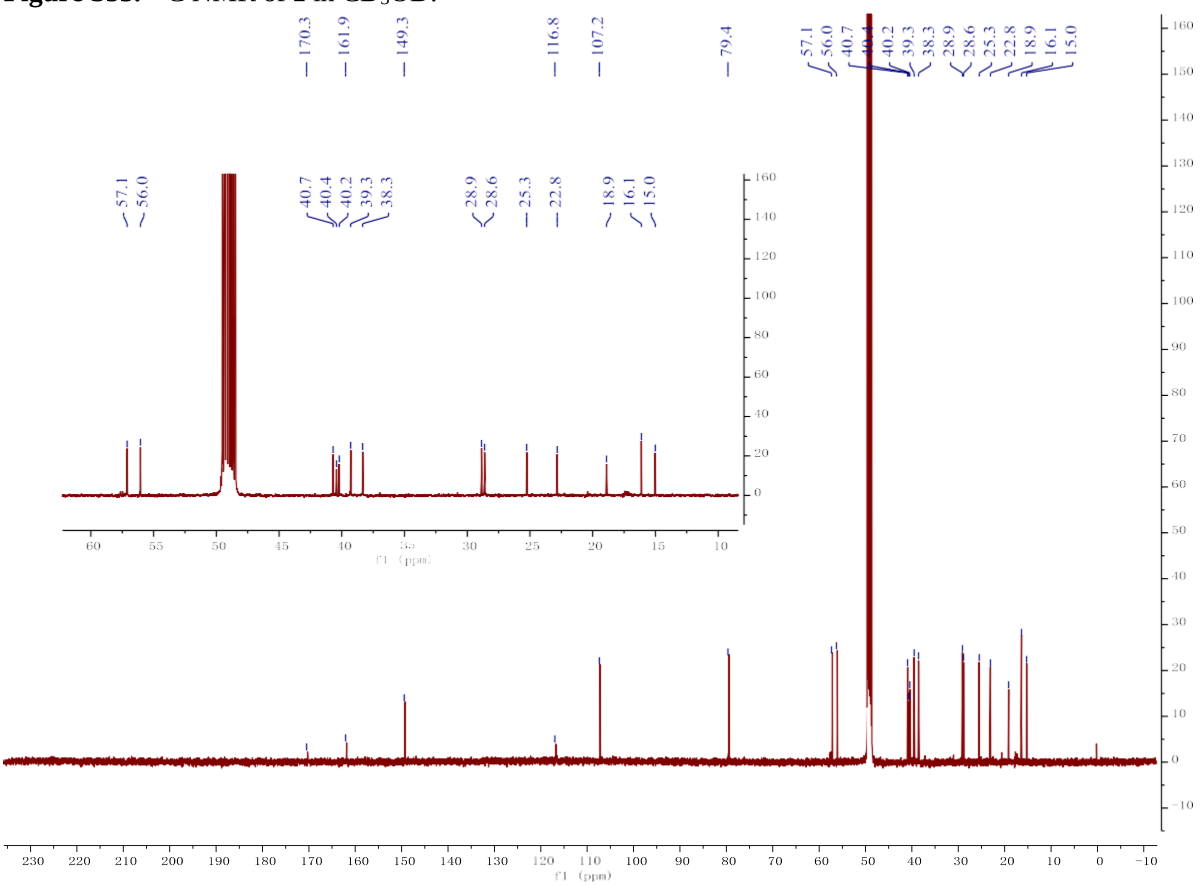


**Figure S54.** $^{1}$H NMR of **2** in $CD_3OD$.

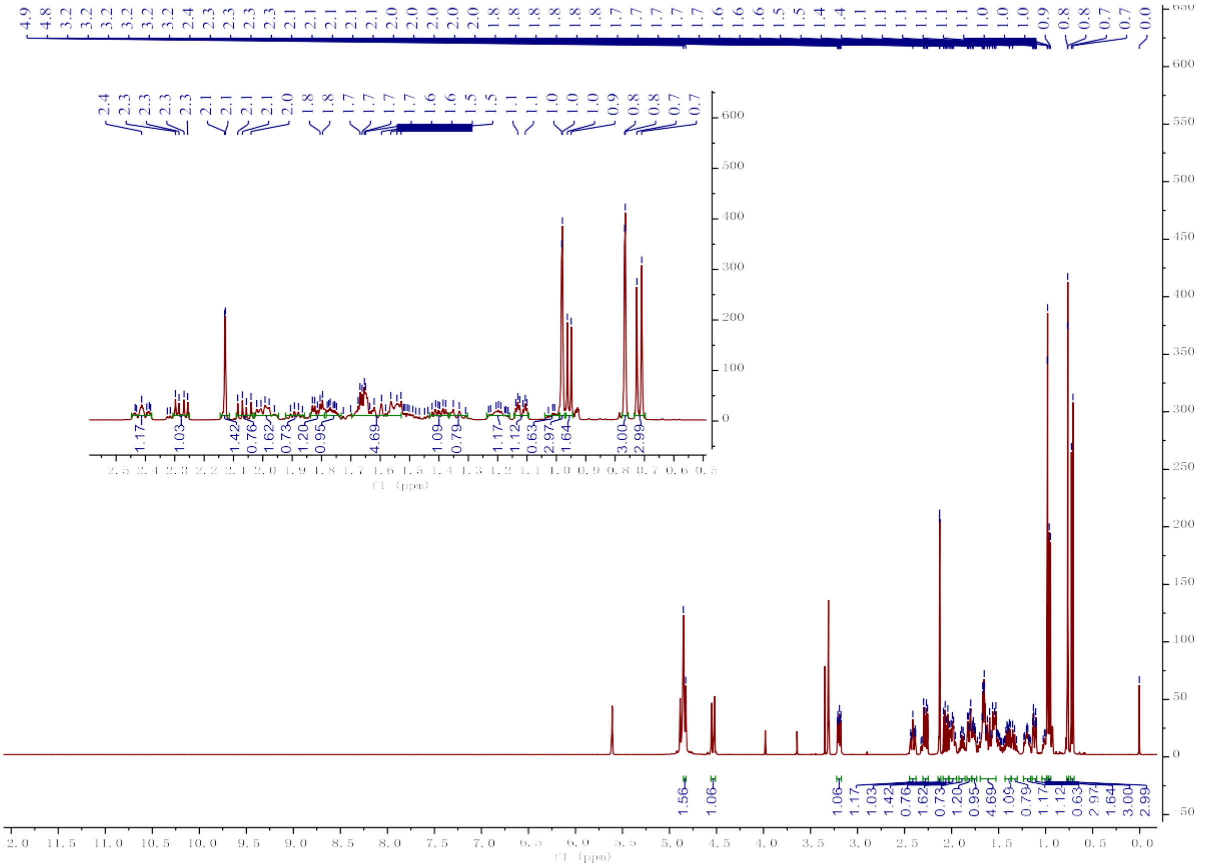


**Figure S55.** $^{13}$C NMR of **2** in $CD_3OD$.

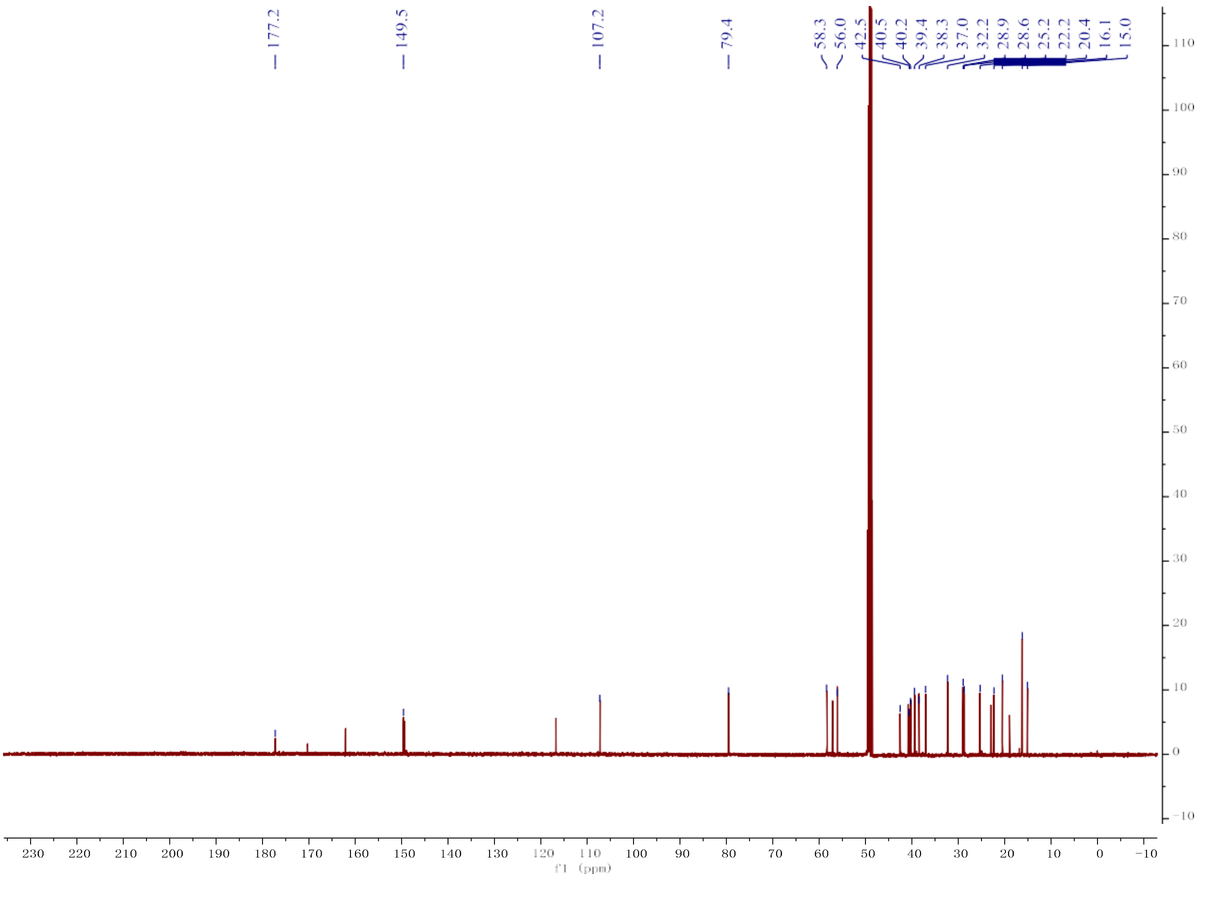


**Figure S56.** $^1$H NMR of **8** in $CD_3OD$.

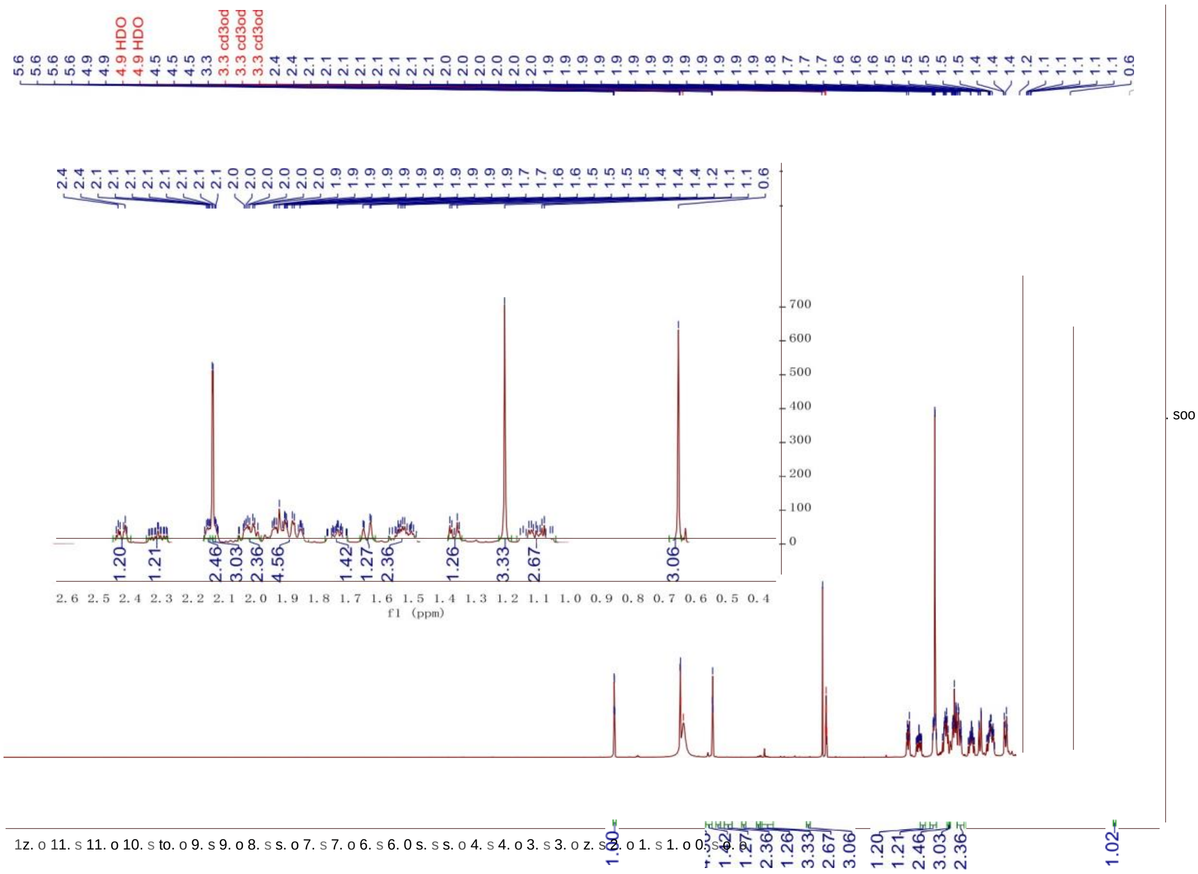


**Figure S57.** $^{13}$C NMR of **8** in $CD_3OD$.

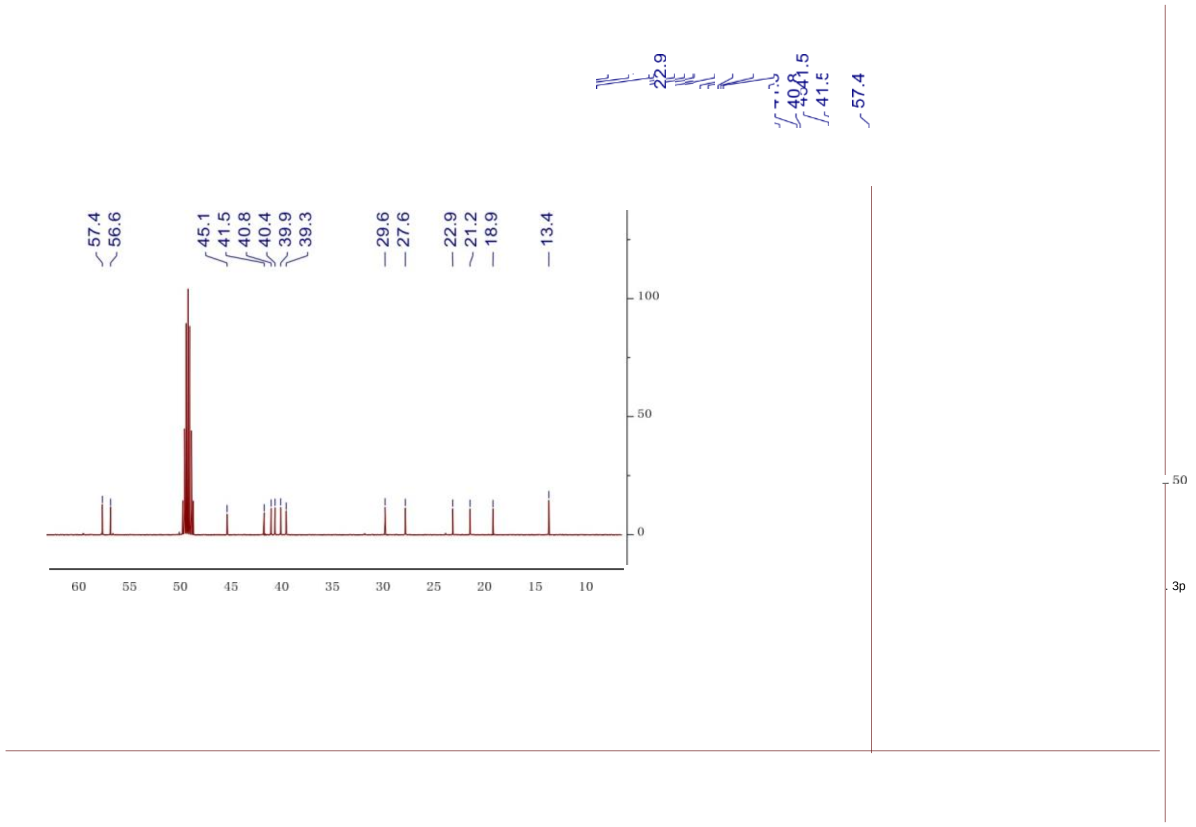


**Figure S58.** $^{1}H$ NMR of **9** in $CD_3OD$.

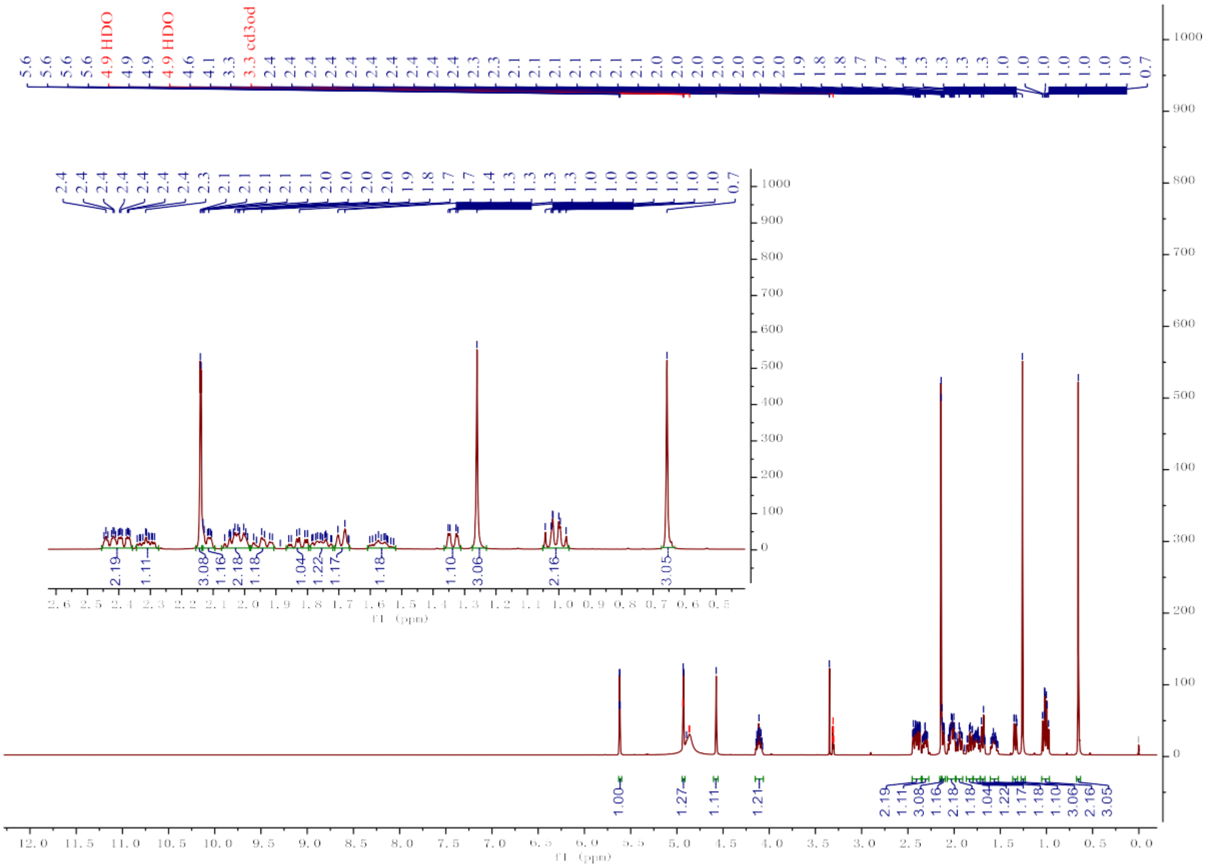


**Figure S59.** $^{13}C$ NMR of **9** in $CD_3OD$.

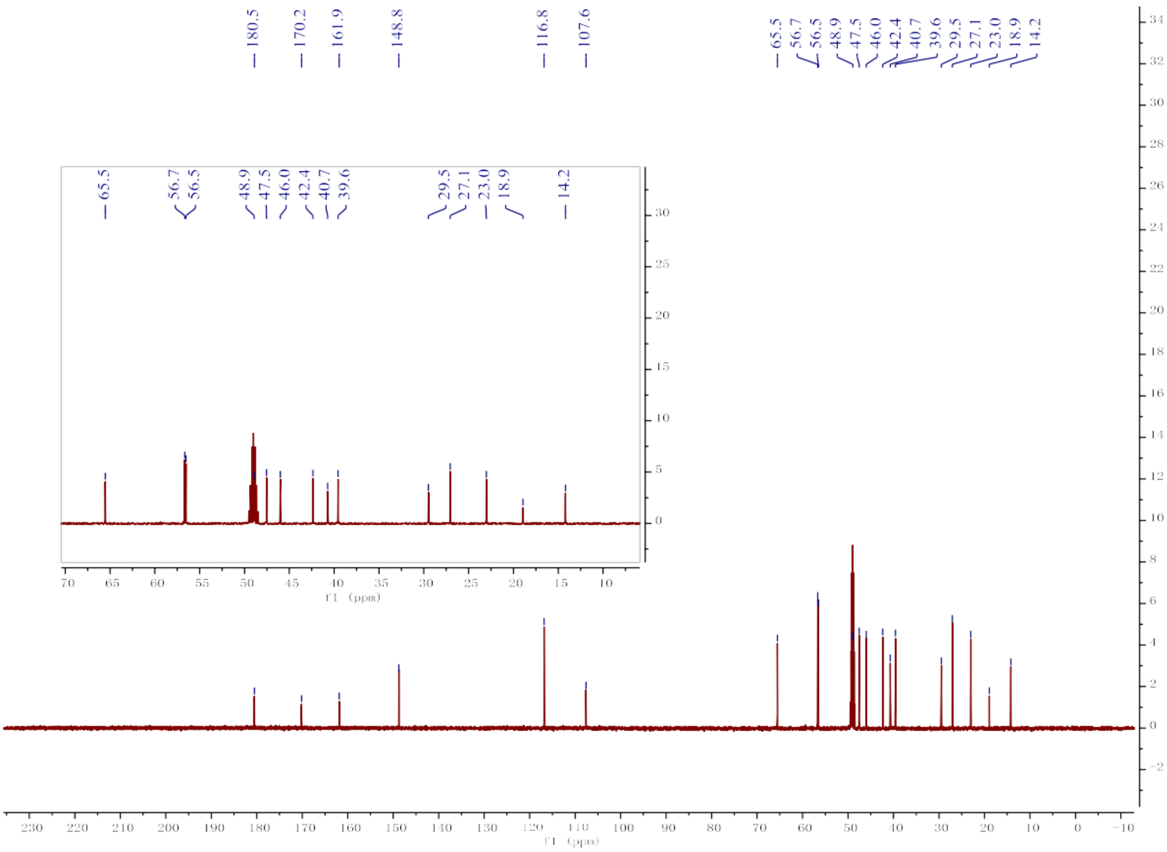


**Figure S60.** $^{1}$H NMR of **10** in $CD_3OD$.

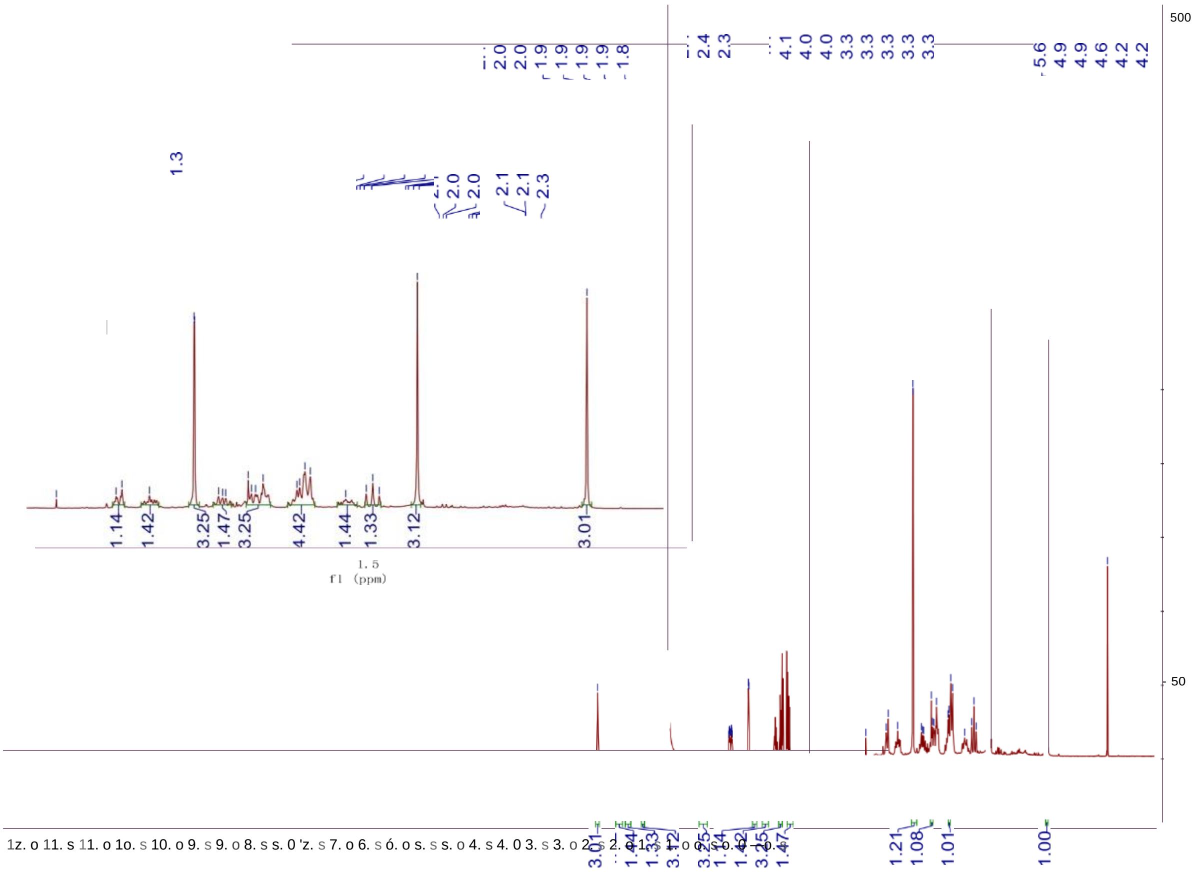


**Figure S61.** $^{13}$C NMR of **10** in $CD_3OD$.

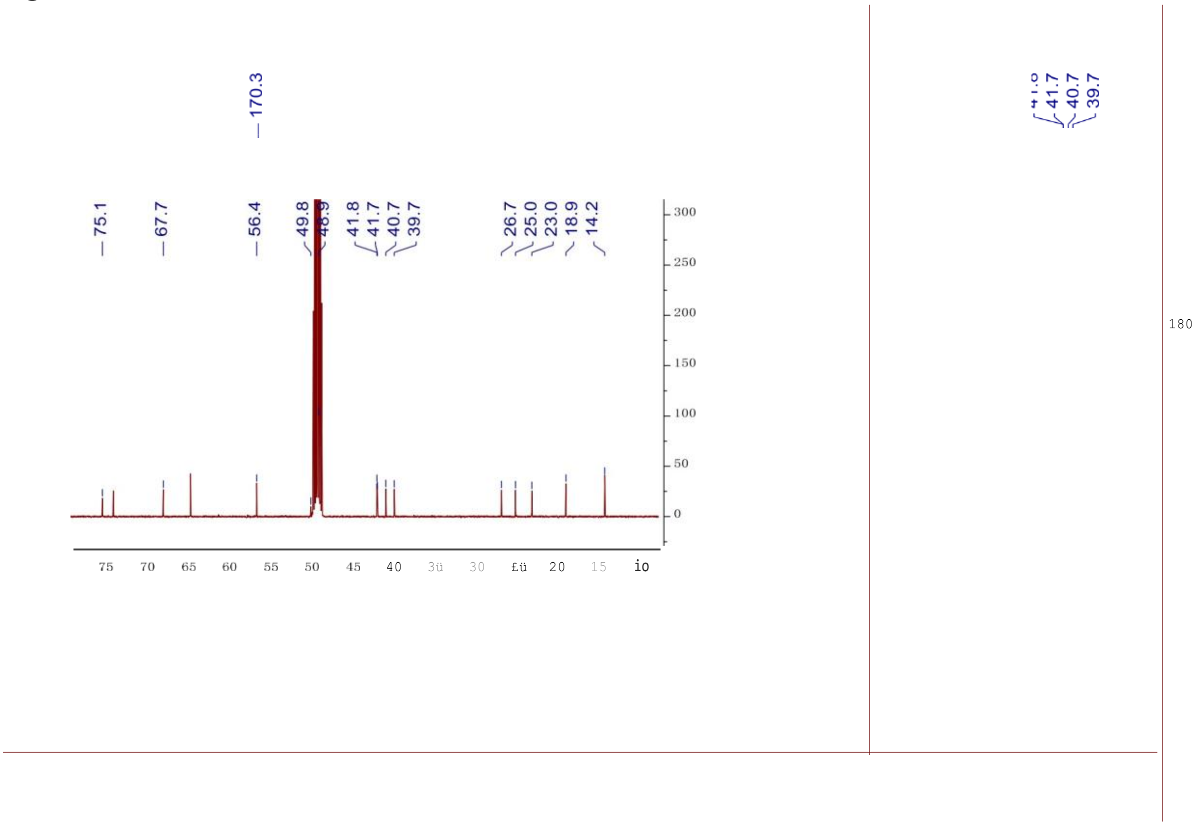


**Figure S62.** $^{1}H$ NMR of **11** in $CD_3OD$.

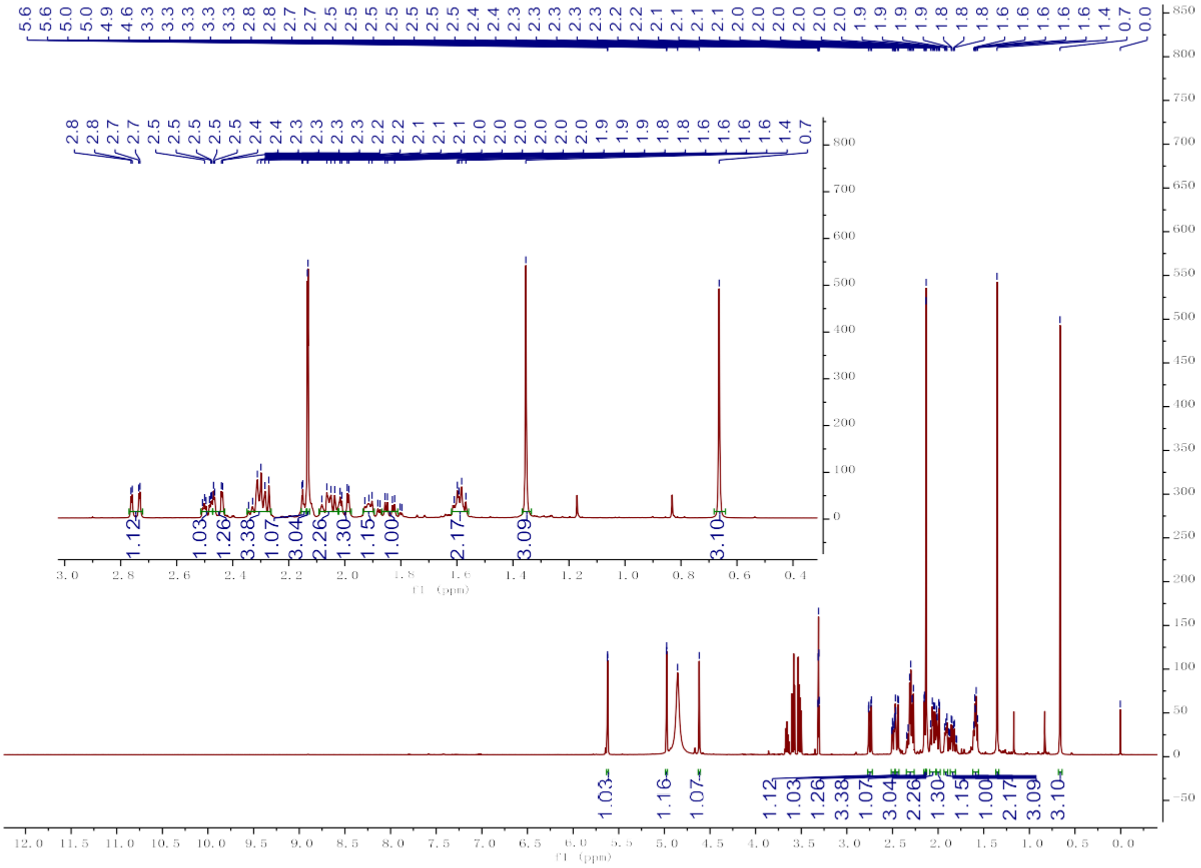


**Figure S63.** $^{13}C$ NMR of **11** in $CD_3OD$.

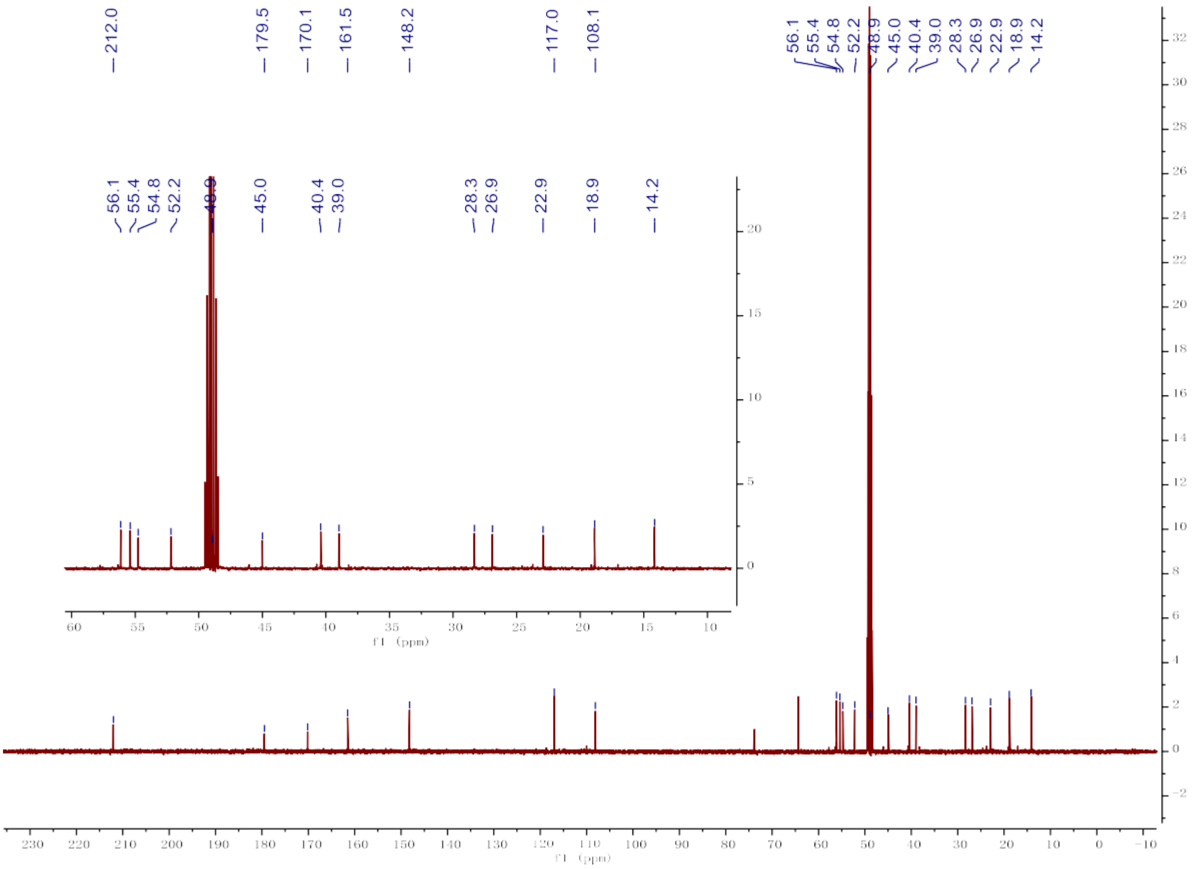


**Figure S64.** $^{1}H$ NMR of **12** in $CD_3OD$.

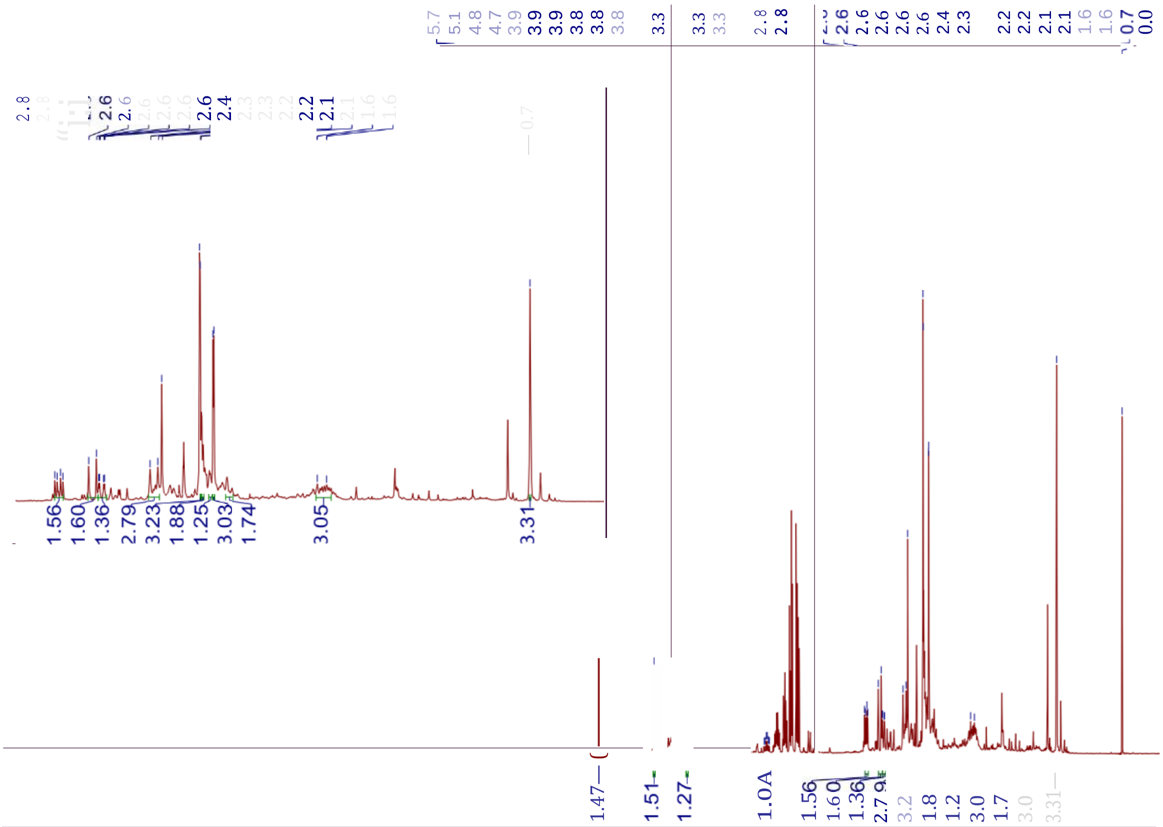


**Figure S65.** $^{13}C$ NMR of **12** in $CD_3OD$.

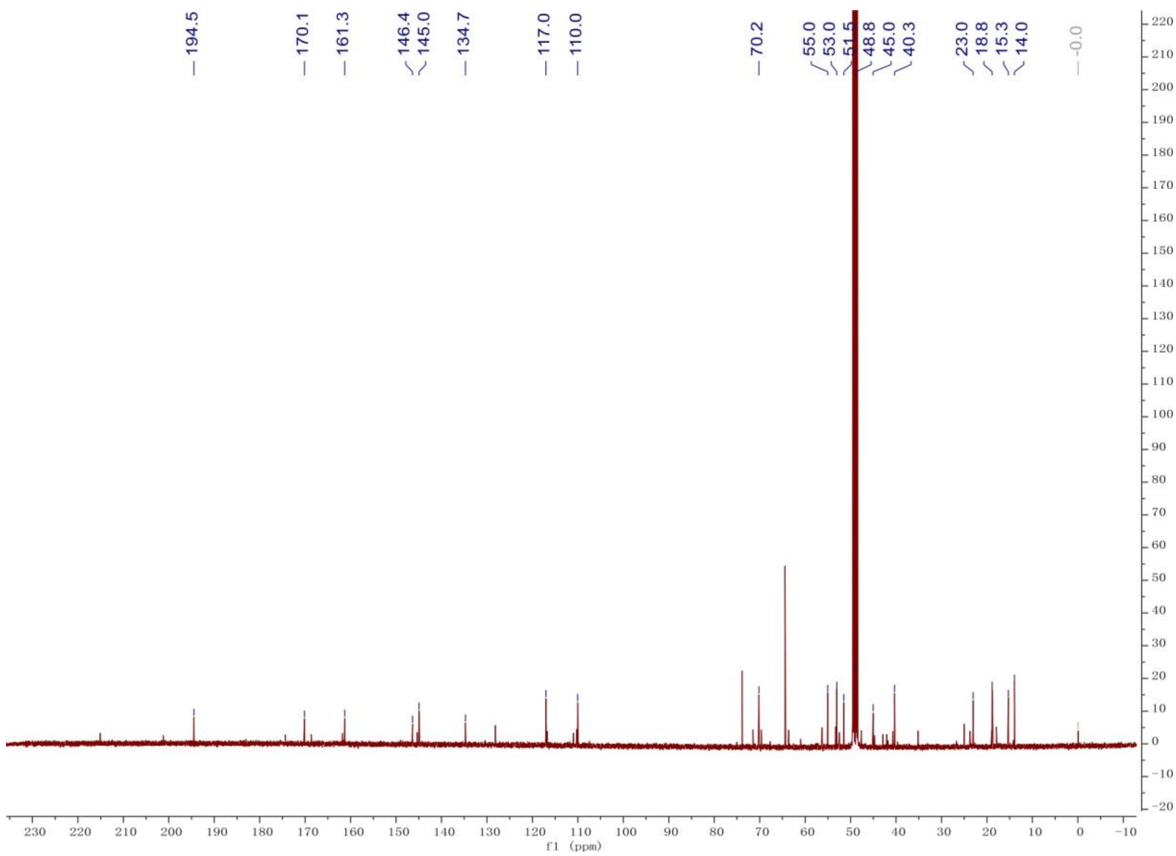


**Figure S66.** $^{1}H$ NMR of **13** in $CD_3OD$.

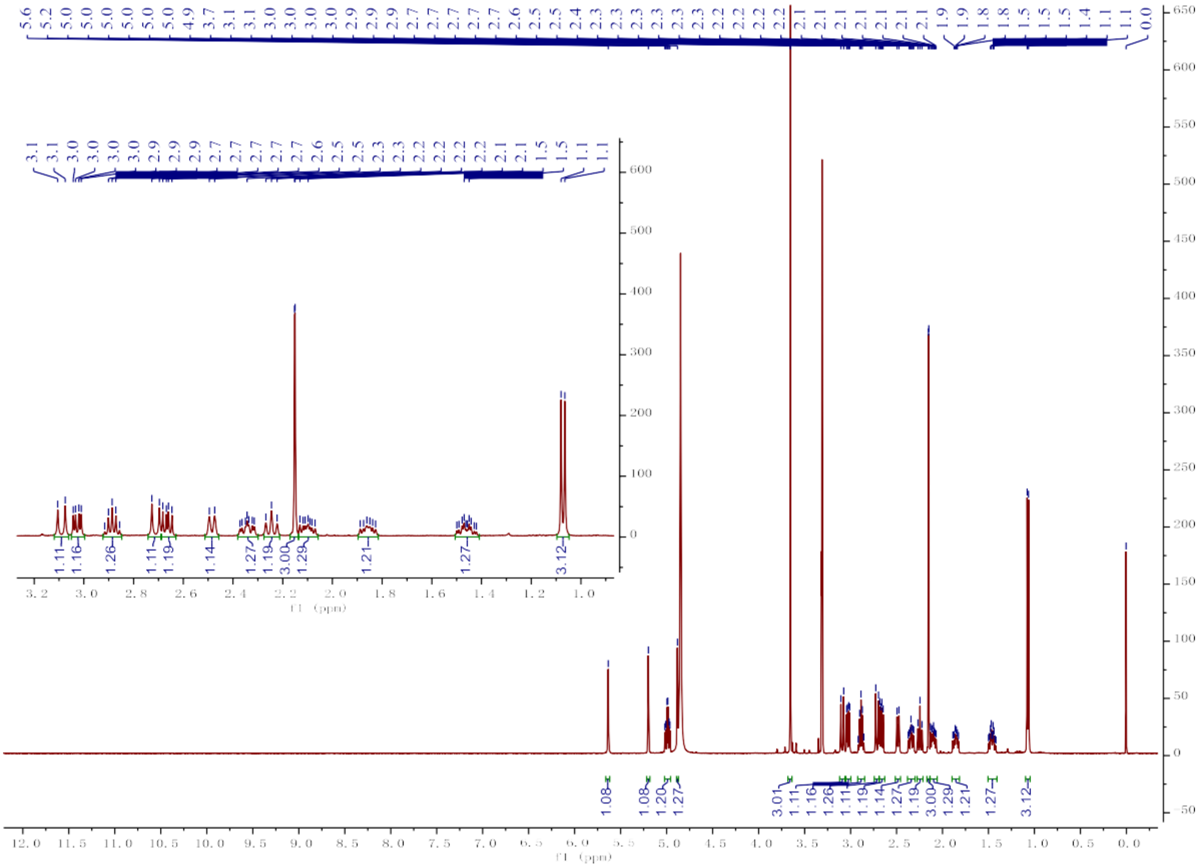


**Figure S67.** $^{13}C$ NMR of **13** in $CD_3OD$.

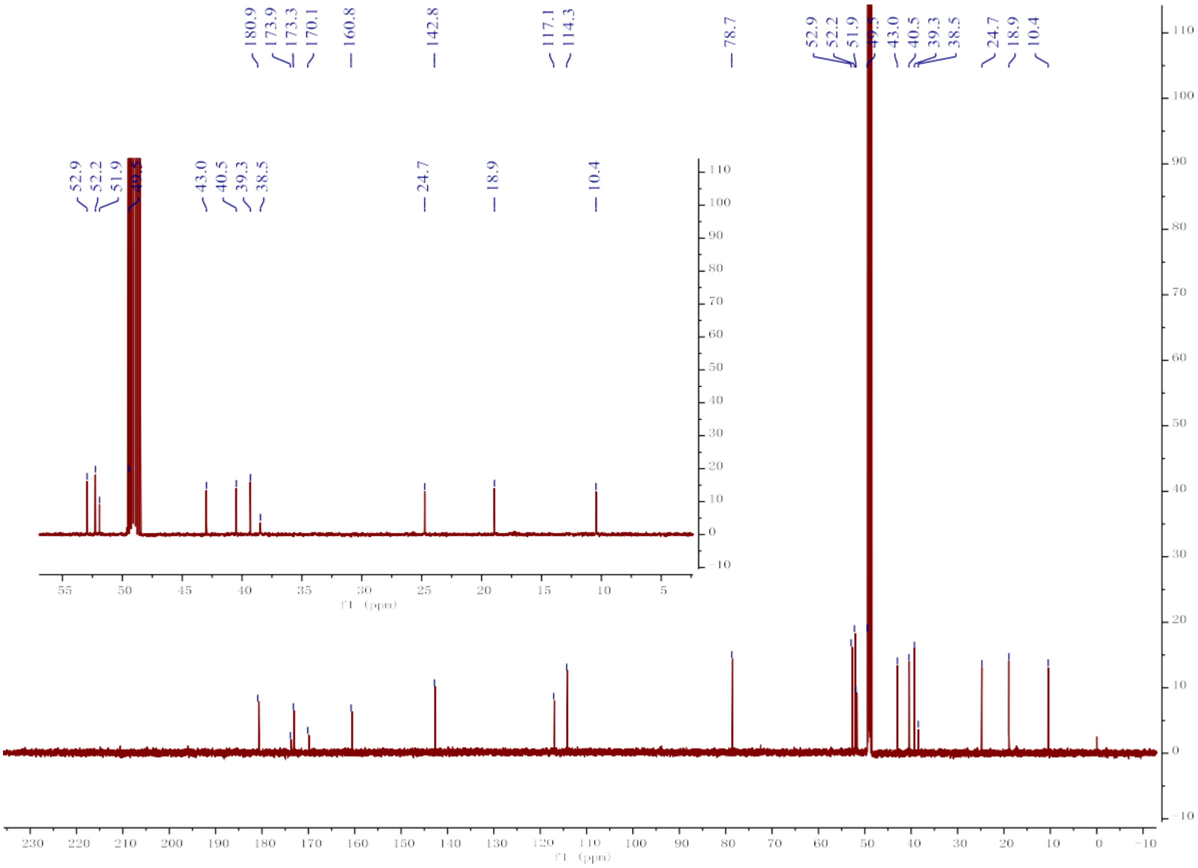
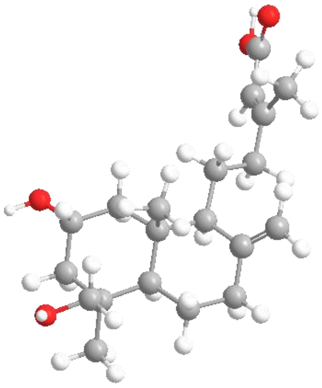
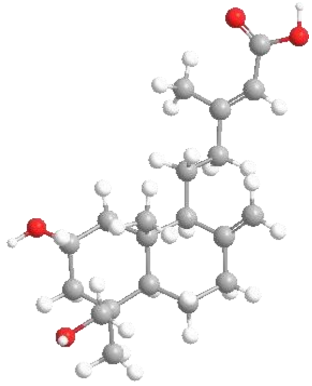
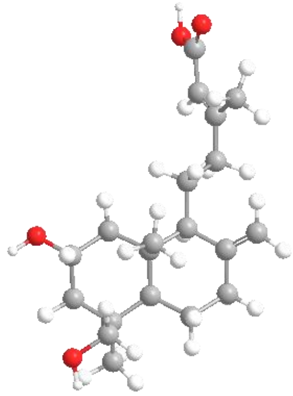
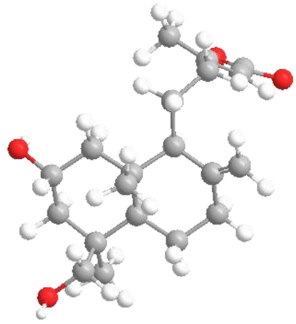
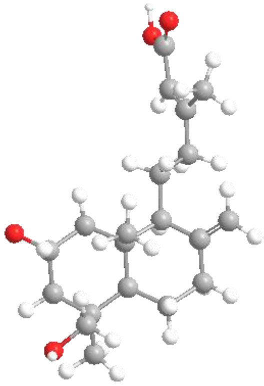
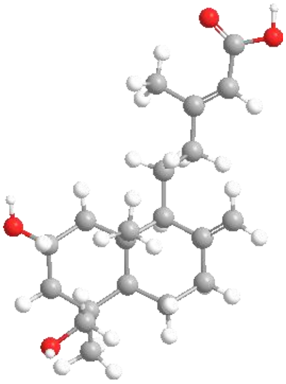
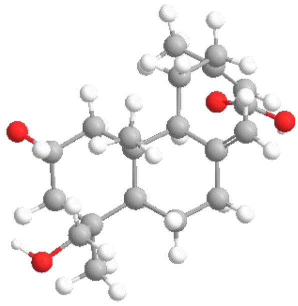
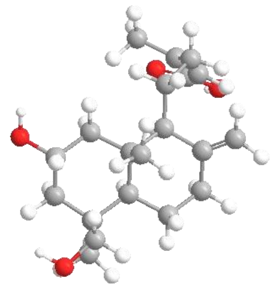
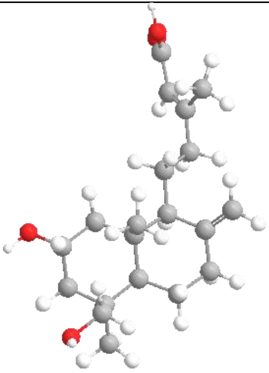
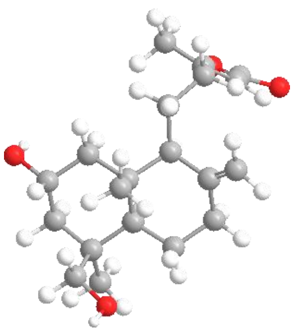
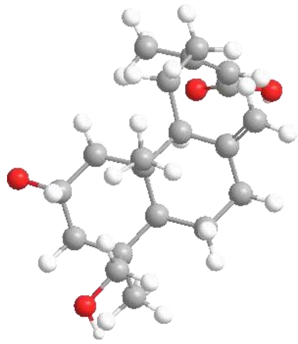
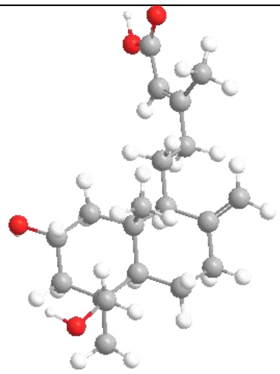
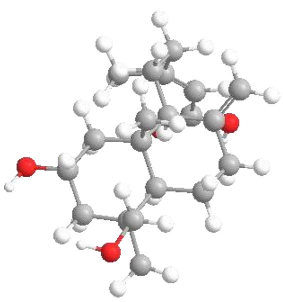
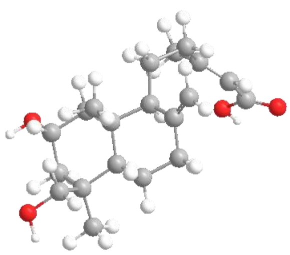


**Figure S68.** Main conformers of (2*R**,4*S**,5*R**,9*S**,10*R**)**-3** in ECD calculations and the energy analysis for optimized geometries of dominant conformers at B3LYP/6-31G(d)-GD3BJ level in the gas phase.

| | | | |
|---|---|---|---|
|  |  |  |  |
| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3A** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3B** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3C** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3D** |
|  |  |  |  |
| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3E** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3F** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3G** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3H** |
|  |  |  |  |
| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3I** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3J** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3K** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3L** |
|  |  | | |
| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3M** | (2*R**,4*S**,5*R**,9*S**,10*R**)-**3N** | | |

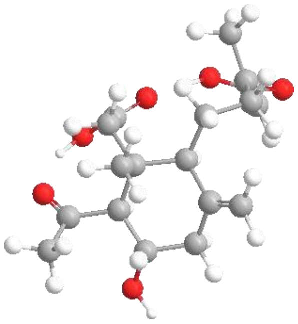
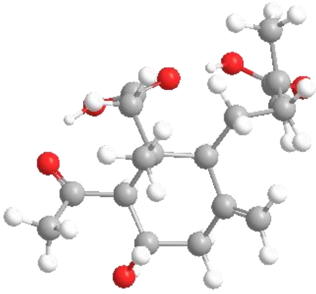
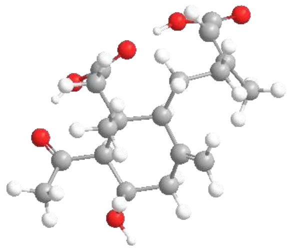
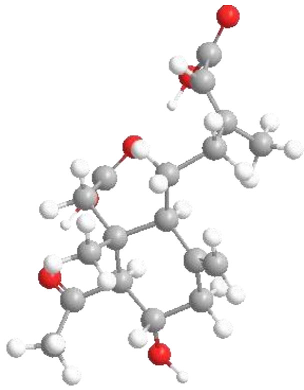
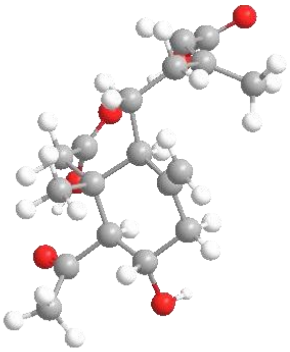
Continued

Energy analysis:

| Species | $E'=E+ZPE$ | $E$ | $H$ | $G$ | $\Delta G$ | $\Delta E$(kcal/mol) | $PE$% |
|---|---|---|---|---|---|---|---|
| **3A** | -1081.878860 | -1081.853347 | -1081.852403 | -1081.934377 | 0.002713 | 1.702433 | 1.44% |
| **3B** | -1081.879043 | -1081.853539 | -1081.852595 | -1081.934699 | 0.002391 | 1.500375 | 2.03% |
| **3C** | -1081.879732 | -1081.854358 | -1081.853414 | -1081.935064 | 0.002026 | 1.271334 | 2.98% |
| **3D** | -1081.881048 | -1081.855650 | -1081.854706 | -1081.936470 | 0.000620 | 0.389056 | 13.24% |
| **3E** | -1081.878262 | -1081.852738 | -1081.851794 | -1081.933940 | 0.003150 | 1.976655 | 0.91% |
| **3F** | -1081.881685 | -1081.856369 | -1081.855425 | -1081.937029 | 0.000061 | 0.038278 | 23.94% |
| **3G** | -1081.881034 | -1081.855742 | -1081.854798 | -1081.936233 | 0.000857 | 0.537776 | 10.30% |
| **3H** | -1081.875604 | -1081.850037 | -1081.849093 | -1081.931337 | 0.005753 | 3.610062 | 0.06% |
| **3I** | -1081.880545 | -1081.855190 | -1081.854245 | -1081.935881 | 0.001209 | 0.758659 | 7.09% |
| **3J** | -1081.881763 | -1081.856494 | -1081.855550 | -1081.937090 | 0 | 0 | 25.54% |
| **3K** | -1081.879436 | -1081.853969 | -1081.853025 | -1081.934992 | 0.002098 | 1.316515 | 2.76% |
| **3L** | -1081.880741 | -1081.855375 | -1081.854431 | -1081.936047 | 0.001043 | 0.654492 | 8.46% |
| **3M** | -1081.878896 | -1081.853615 | -1081.852671 | -1081.934242 | 0.002848 | 1.787147 | 1.25% |
| **3N** | -1081.878860 | -1081.853347 | -1081.852403 | -1081.934377 | 0.002713 | 1.702433 | 1.44% |

$E$, $E'$, $H$, $G$: total energy, total energy with zero point energy ($ZPE$), enthalpy, and Gibbs free energy.

**Figure S69.** Main conformers of (5*S**,6*S**,9*S**,10*R**)-**4** in ECD calculations and the energy analysis for optimized geometries of dominant conformers at B3LYP/6-31G(d)-GD3BJ level in the gas phase.

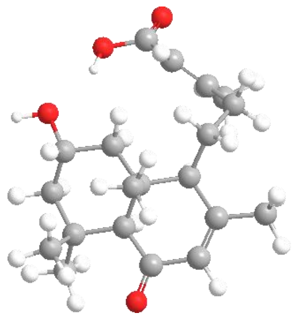
| | | | |
|---|---|---|---|
|  |  |  |  |
| (5*S**,6*S**,9*S**,10*R**)-**4A** | (5*S**,6*S**,9*S**,10*R**)-**4B** | (5*S**,6*S**,9*S**,10*R**)-**4C** | (5*S**,6*S**,9*S**,10*R**)-**4D** |
|  | | | |
| (5*S**,6*S**,9*S**,10*R**)-**4E** | | | |

Energy analysis:

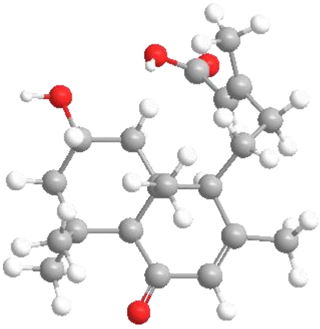
| Species | *E′=E+ZPE* | *E* | *H* | *G* | *ΔG* | *ΔE*(kcal/mol) | *PE*% |
|---|---|---|---|---|---|---|---|
| **4A** | -1152.592400 | -1152.568190 | -1152.567245 | -1152.644168 | 0.000854 | 0.535893 | 15.36% |
| **4B** | -1152.592903 | -1152.568743 | -1152.567799 | -1152.644605 | 0.000417 | 0.261671 | 24.41% |
| **4C** | -1152.592563 | -1152.568277 | -1152.567333 | -1152.644509 | 0.000513 | 0.321912 | 22.05% |
| **4D** | -1152.586308 | -1152.561675 | -1152.560731 | -1152.640050 | 0.004972 | 3.119977 | 0.20% |
| **4E** | -1152.593162 | -1152.568934 | -1152.567989 | -1152.645022 | 0 | 0 | 37.98% |

*E*, *E′*, *H*, *G*: total energy, total energy with zero point energy (*ZPE*), enthalpy, and Gibbs free energy.

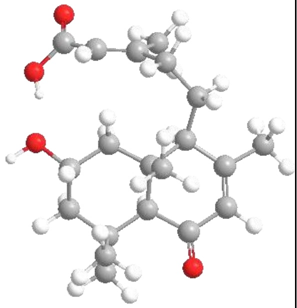
**Figure S70.** Main conformers of (2*S**,5*S**,9*S**,10*R**)-**5** in ECD calculations and the energy analysis for optimized geometries of dominant conformers at B3LYP/6-31G(d)-GD3BJ level in the gas phase.



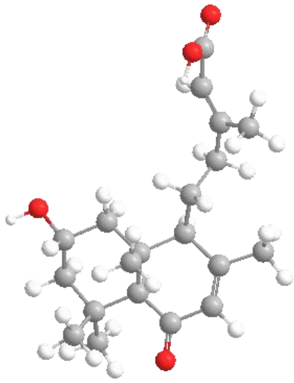
(2*S**,5*S**,9*S**,10*R**)-**5A**



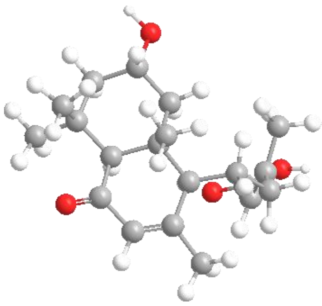
(2*S**,5*S**,9*S**,10*R**)-**5B**



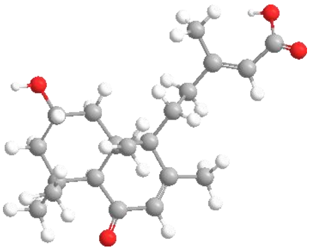
(2*S**,5*S**,9*S**,10*R**)-**5C**



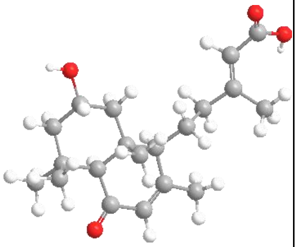
(2*S**,5*S**,9*S**,10*R**)-**5D**



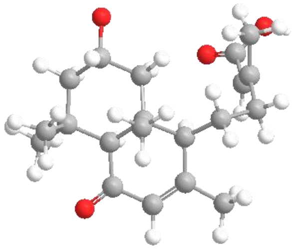
(2*S**,5*S**,9*S**,10*R**)-**5E**



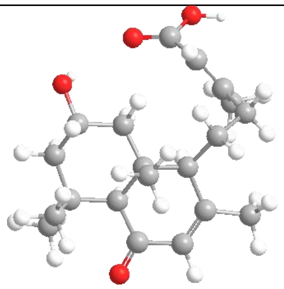
(2*S**,5*S**,9*S**,10*R**)-**5F**



(2*S**,5*S**,9*S**,10*R**)-**5G**



(2*S**,5*S**,9*S**,10*R**)-**5H**



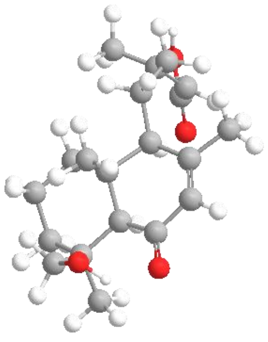
(2*S**,5*S**,9*S**,10*R**)-**5I**

Energy analysis:

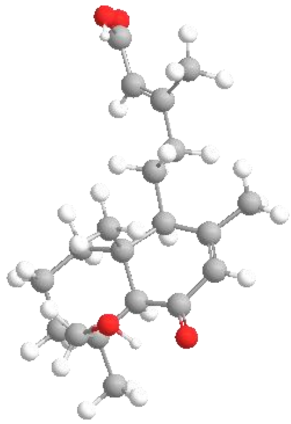
| Species | *E′*=*E*+*ZPE* | *E* | *H* | *G* | *ΔG* | *ΔE*(kcal/mol) | *PE*% |
|---|---|---|---|---|---|---|---|
| **5A** | -1080.717662 | -1080.692943 | -1080.691999 | -1080.769658 | 0 | 0 | 86.88% |
| **5B** | -1080.715230 | -1080.690514 | -1080.689569 | -1080.767185 | 0.002473 | 1.551831 | 6.32% |
| **5C** | -1080.715833 | -1080.691458 | -1080.690514 | -1080.767059 | 0.002599 | 1.630897 | 5.53% |
| **5D** | -1080.706369 | -1080.681167 | -1080.680223 | -1080.761145 | 0.008513 | 5.341988 | 0.01% |
| **5E** | -1080.709286 | -1080.684143 | -1080.683198 | -1080.764062 | 0.005596 | 3.511543 | 0.23% |
| **5F** | -1080.706879 | -1080.681663 | -1080.680719 | -1080.761749 | 0.007909 | 4.962973 | 0.02% |
| **5G** | -1080.706435 | -1080.681248 | -1080.680304 | -1080.760873 | 0.008785 | 5.512671 | 0.01% |
| **5H** | -1080.712743 | -1080.687952 | -1080.687008 | -1080.765247 | 0.004411 | 2.767944 | 0.81% |
| **5I** | -1080.712052 | -1080.687422 | -1080.686478 | -1080.763871 | 0.005787 | 3.631397 | 0.19% |

*E*, *E′*, *H*, *G*: total energy, total energy with zero point energy (*ZPE*), enthalpy, and Gibbs free energy.

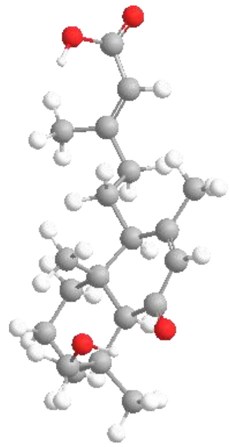
**Figure S71.** Main conformers of (4*S**,5*R**,9*S**,10*R**)-**6** in ECD calculations and the energy analysis for optimized geometries of dominant conformers at B3LYP/6-31G(d)-GD3BJ level in the gas phase.



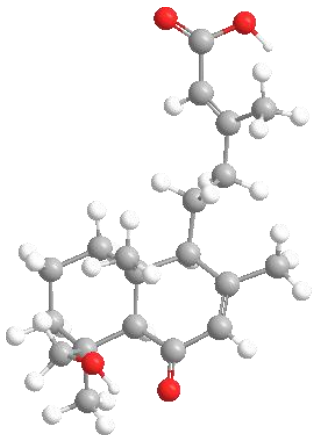
(4*S**,5*R**,9*S**,10*R**)-**6A**



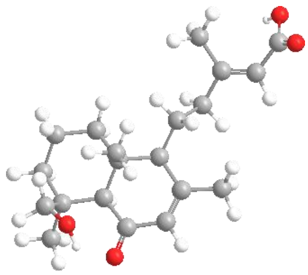
(4*S**,5*R**,9*S**,10*R**)-**6B**



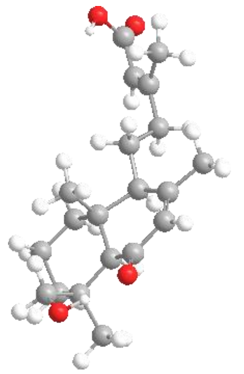
(4*S**,5*R**,9*S**,10*R**)-**6C**



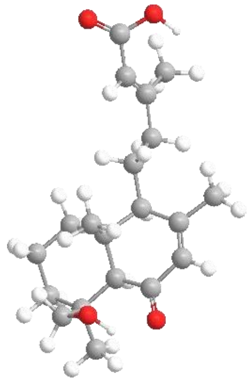
(4*S**,5*R**,9*S**,10*R**)-**6D**



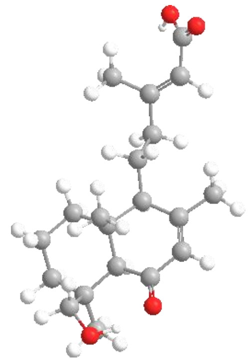
(4*S**,5*R**,9*S**,10*R**)-**6E**



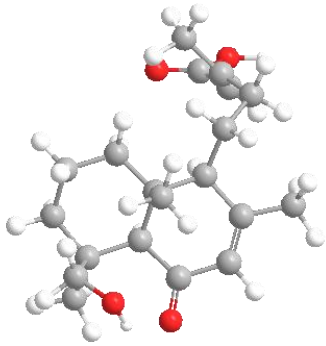
(4*S**,5*R**,9*S**,10*R**)-**6F**



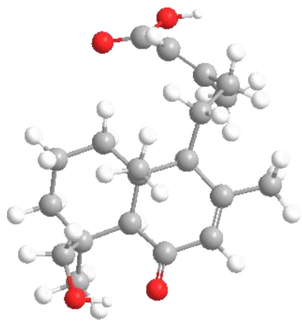
(4*S**,5*R**,9*S**,10*R**)-**6G**



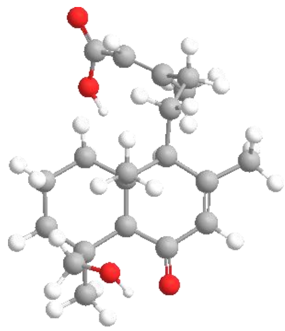
(4*S**,5*R**,9*S**,10*R**)-**6H**



(4*S**,5*R**,9*S**,10*R**)-**6I**



(4*S**,5*R**,9*S**,10*R**)-**6J**



(4*S**,5*R**,9*S**,10*R**)-**6K**

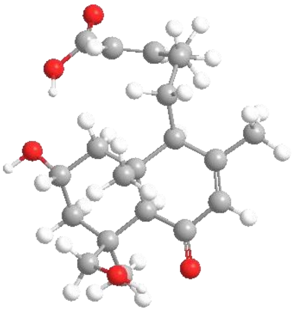
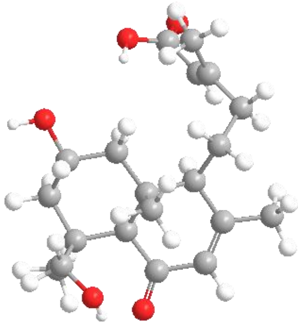
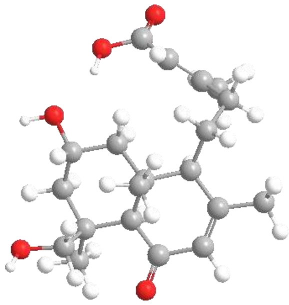
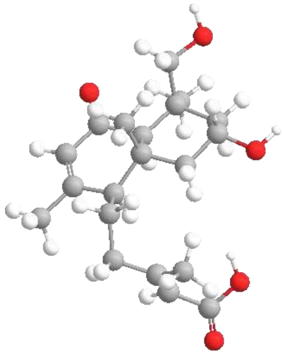
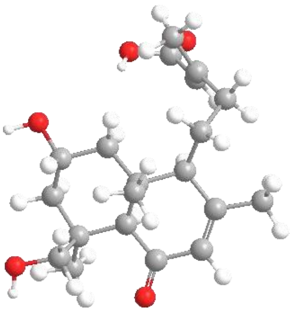
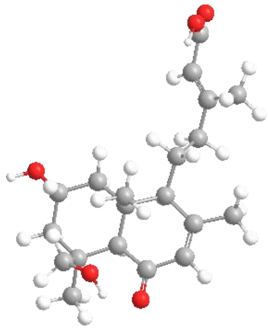
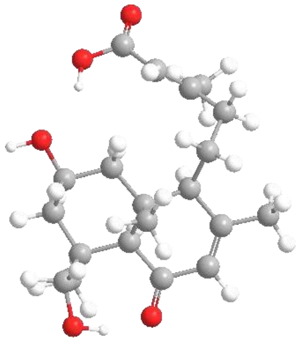
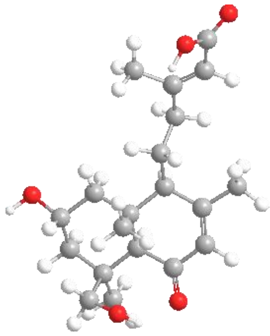
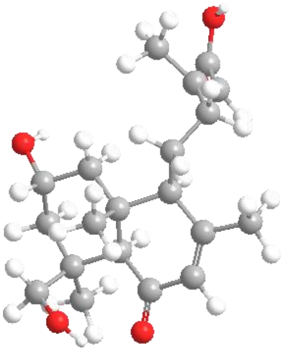
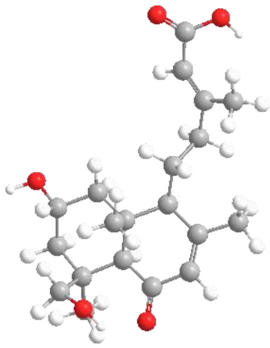
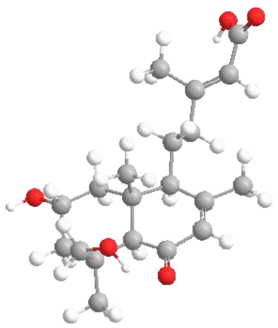
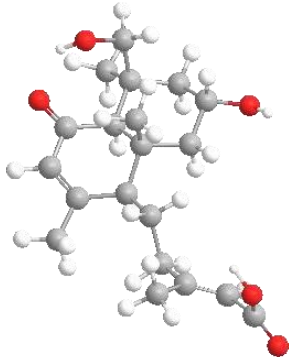
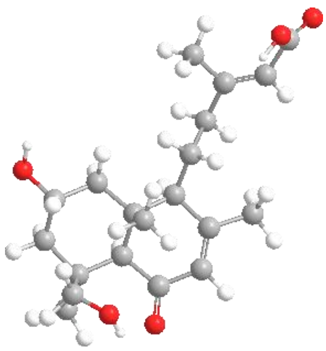
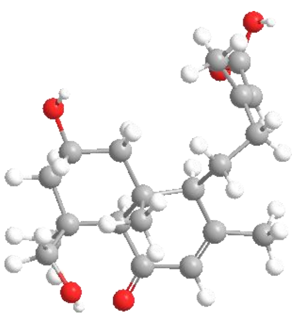
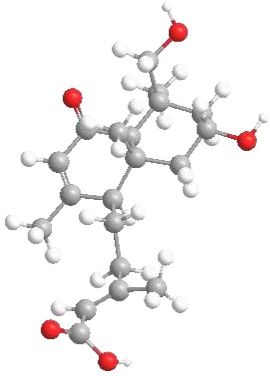
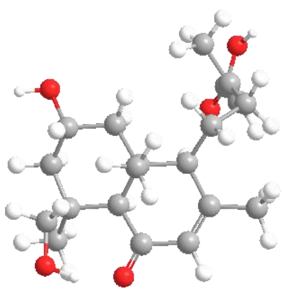
Energy analysis:

| Species | *E'*=*E*+*ZPE* | *E* | *H* | *G* | *ΔG* | *ΔE*(kcal/mol) | *PE*% |
|---|---|---|---|---|---|---|---|
| **6A** | -1080.706544 | -1080.682062 | -1080.681118 | -1080.759902 | 0.003619 | 2.270957 | 2.07% |
| **6B** | -1080.703611 | -1080.679003 | -1080.678059 | -1080.757883 | 0.005638 | 3.537899 | 0.24% |
| **6C** | -1080.703810 | -1080.679219 | -1080.678275 | -1080.758068 | 0.005453 | 3.421809 | 0.30% |
| **6D** | -1080.703715 | -1080.679103 | -1080.678159 | -1080.757812 | 0.005709 | 3.582452 | 0.23% |
| **6E** | -1080.703681 | -1080.679044 | -1080.678100 | -1080.758179 | 0.005342 | 3.352156 | 0.33% |
| **6F** | -1080.703487 | -1080.678861 | -1080.677917 | -1080.757901 | 0.005620 | 3.526603 | 0.25% |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **6G** | -1080.703210 | -1080.678593 | -1080.677649 | -1080.757010 | 0.006511 | 4.085714 | 0.10% |
| **6H** | -1080.703756 | -1080.679099 | -1080.678155 | -1080.758351 | 0.005170 | 3.244224 | 0.40% |
| **6I** | -1080.709757 | -1080.685212 | -1080.684267 | -1080.763521 | 0 | 0 | 95.83% |
| **6J** | -1080.704489 | -1080.680105 | -1080.679161 | -1080.757518 | 0.006003 | 3.766940 | 0.17% |
| **6K** | -1080.703570 | -1080.679112 | -1080.678167 | -1080.756959 | 0.006562 | 4.117717 | 0.09% |

$E$, $E'$, $H$, $G$: total energy, total energy with zero point energy (*ZPE*), enthalpy, and Gibbs free energy.

**Figure S72.** Main conformers of (2R*,4S*,5R*,9S*,10R*)-**7** in ECD calculations and the energy analysis for optimized geometries of dominant conformers at B3LYP/6-31G(d)-GD3BJ level in the gas phase.

| | | | |
|---|---|---|---|
|  |  |  |  |
| (2R*,4S*,5R*,9S*,10R*)-**7A** | (2R*,4S*,5R*,9S*,10R*)-**7B** | (2R*,4S*,5R*,9S*,10R*)-**7C** | (2R*,4S*,5R*,9S*,10R*)-**7D** |
|  |  |  |  |
| (2R*,4S*,5R*,9S*,10R*)-**7E** | (2R*,4S*,5R*,9S*,10R*)-**7F** | (2R*,4S*,5R*,9S*,10R*)-**7G** | (2R*,4S*,5R*,9S*,10R*)-**7H** |
|  |  |  |  |
| (2R*,4S*,5R*,9S*,10R*)-**7I** | (2R*,4S*,5R*,9S*,10R*)-**7J** | (2R*,4S*,5R*,9S*,10R*)-**7K** | (2R*,4S*,5R*,9S*,10R*)-**7L** |
|  |  |  |  |
| (2R*,4S*,5R*,9S*,10R*)-**7M** | (2R*,4S*,5R*,9S*,10R*)-**7N** | (2R*,4S*,5R*,9S*,10R*)-**7O** | (2R*,4S*,5R*,9S*,10R*)-**7P** |

Continued

Energy analysis:

| Species | *E′*=*E*+*ZPE* | *E* | *H* | *G* | *ΔG* | *ΔE*(kcal/mol) | *PE*% |
|---|---|---|---|---|---|---|---|
| **7A** | -1155.922441 | -1155.896965 | -1155.896021 | -1155.975476 | 0.000342 | 0.214608 | 38.16% |
| **7B** | -1155.920260 | -1155.894802 | -1155.893858 | -1155.973178 | 0.002640 | 1.656625 | 3.34% |
| **7C** | -1155.919025 | -1155.893044 | -1155.892100 | -1155.972804 | 0.003014 | 1.891314 | 2.25% |
| **7D** | -1155.916552 | -1155.890566 | -1155.889621 | -1155.970299 | 0.005519 | 3.463225 | 0.16% |
| **7E** | -1155.917810 | -1155.891983 | -1155.891039 | -1155.971399 | 0.004419 | 2.772964 | 0.51% |
| **7F** | -1155.911109 | -1155.885179 | -1155.884235 | -1155.966890 | 0.008928 | 5.602405 | 0.00% |
| **7G** | -1155.922832 | -1155.897425 | -1155.896481 | -1155.975818 | 0 | 0 | 54.83% |
| **7H** | -1155.911435 | -1155.885572 | -1155.884627 | -1155.966966 | 0.008852 | 5.554714 | 0.00% |
| **7I** | -1155.918138 | -1155.892645 | -1155.891701 | -1155.971529 | 0.004289 | 2.691388 | 0.58% |
| **7J** | -1155.911082 | -1155.885170 | -1155.884226 | -1155.966547 | 0.009271 | 5.817641 | 0.00% |
| **7K** | -1155.911489 | -1155.885557 | -1155.884612 | -1155.967380 | 0.008438 | 5.294925 | 0.01% |
| **7L** | -1155.910551 | -1155.884611 | -1155.883667 | -1155.966361 | 0.009457 | 5.934357 | 0.00% |
| **7M** | -1155.910572 | -1155.884697 | -1155.883753 | -1155.966123 | 0.009695 | 6.083705 | 0.00% |
| **7N** | -1155.912793 | -1155.886969 | -1155.886025 | -1155.968347 | 0.007471 | 4.688123 | 0.02% |
| **7O** | -1155.908053 | -1155.881551 | -1155.880606 | -1155.964715 | 0.011103 | 6.967238 | 0.00% |
| **7P** | -1155.914765 | -1155.888920 | -1155.887976 | -1155.970102 | 0.005716 | 3.586844 | 0.13% |

*E*, *E′*, *H*, *G*: total energy, total energy with zero point energy (*ZPE*), enthalpy, and Gibbs free energy.

**Supplementary S1.** The Z-matrices of (2*R**,4*S**,5*R**,9*S**,10*R**)-**3** optimized at B3LYP/6-31G(d)-GD3BJ level by Gaussian.

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3A** | | | |
|---|---|---|---|
| C | -2.5474 | -0.0415 | 1.7368 |
| C | -2.3198 | -1.3761 | 2.4323 |
| C | -0.8514 | -1.6108 | 2.8648 |
| C | 0.0881 | -1.3701 | 1.6265 |
| C | -0.1390 | -0.0335 | 0.7998 |
| C | -1.6550 | 0.1045 | 0.5038 |
| C | 1.5869 | -1.6127 | 1.9169 |
| C | 2.4132 | -1.6394 | 0.6294 |
| C | 2.1650 | -0.4045 | -0.2017 |
| C | 0.6877 | -0.1857 | -0.5536 |
| C | 0.6029 | 1.6028 | -4.0469 |
| C | 0.8994 | 0.5260 | -3.0183 |
| C | 0.4146 | 0.9196 | -1.6108 |
| C | 0.3299 | 1.2521 | 1.5279 |
| C | -0.4824 | -0.7552 | 4.0999 |
| C | -0.7675 | -3.1020 | 3.3002 |
| C | -0.3330 | 1.3880 | -4.9933 |
| C | 3.1879 | 0.4051 | -0.5257 |
| C | 1.4365 | 2.8511 | -3.9255 |
| O | -3.9054 | 0.0334 | 1.3035 |
| O | -1.3643 | -1.0293 | 5.1860 |
| C | -0.7594 | 2.3483 | -6.0273 |
| O | -0.4753 | 3.5236 | -6.1383 |
| O | -1.5758 | 1.7343 | -6.9011 |
| H | -2.3907 | 0.7889 | 2.4313 |
| H | -3.0025 | -1.4616 | 3.2877 |
| H | -2.6363 | -2.1774 | 1.7485 |
| H | -0.1953 | -2.1737 | 0.9253 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3B** | | |
|---|---|---|
| -3.0848 | -0.7996 | 0.2228 |
| -2.9761 | -2.2397 | -0.2574 |
| -1.7116 | -2.9728 | 0.2542 |
| -0.4477 | -2.0958 | -0.0738 |
| -0.5134 | -0.5605 | 0.3263 |
| -1.8586 | 0.0185 | -0.1841 |
| 0.8918 | -2.7389 | 0.3521 |
| 2.0888 | -1.9876 | -0.2343 |
| 2.0144 | -0.5142 | 0.0829 |
| 0.7166 | 0.1537 | -0.3920 |
| 1.6932 | 3.8677 | -1.2041 |
| 1.6406 | 2.3570 | -1.3484 |
| 0.7042 | 1.7053 | -0.3141 |
| -0.4211 | -0.2956 | 1.8507 |
| -1.8394 | -3.3426 | 1.7510 |
| -1.6405 | -4.3075 | -0.5419 |
| 2.8291 | 4.4602 | -0.7838 |
| 3.0117 | 0.0792 | 0.7612 |
| 0.4305 | 4.5947 | -1.5853 |
| -4.2308 | -0.1933 | -0.3744 |
| -2.9970 | -4.1435 | 1.9765 |
| 3.0243 | 5.9030 | -0.5533 |
| 2.1983 | 6.7927 | -0.5494 |
| 4.3243 | 6.1471 | -0.3122 |
| -3.2355 | -0.7626 | 1.3055 |
| -3.8882 | -2.7849 | 0.0183 |
| -2.9816 | -2.2358 | -1.3573 |
| -0.4165 | -2.0871 | -1.1768 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3C** | | |
|---|---|---|
| -2.9689 | -0.7562 | 0.3710 |
| -2.8941 | -2.1813 | -0.1590 |
| -1.6358 | -2.9548 | 0.3064 |
| -0.3607 | -2.0881 | -0.0082 |
| -0.3931 | -0.5658 | 0.4427 |
| -1.7346 | 0.0530 | -0.0288 |
| 0.9726 | -2.7686 | 0.3773 |
| 2.1750 | -2.0197 | -0.2014 |
| 2.1311 | -0.5559 | 0.1628 |
| 0.8391 | 0.1490 | -0.2711 |
| 1.7832 | 3.8785 | -1.0516 |
| 1.7979 | 2.3645 | -1.1646 |
| 0.8545 | 1.6976 | -0.1466 |
| -0.2737 | -0.3521 | 1.9733 |
| -1.7504 | -3.3699 | 1.7929 |
| -1.5964 | -4.2581 | -0.5414 |
| 1.2254 | 4.6196 | -2.0300 |
| 3.1477 | -0.0022 | 0.8459 |
| 2.4454 | 4.4350 | 0.1813 |
| -4.1129 | -0.1135 | -0.1907 |
| -2.9241 | -4.1414 | 2.0367 |
| 1.0979 | 6.0882 | -2.0425 |
| 1.3260 | 6.8800 | -1.1507 |
| 0.6525 | 6.4900 | -3.2456 |
| -3.1026 | -0.7511 | 1.4566 |
| -3.8117 | -2.7191 | 0.1129 |
| -2.9166 | -2.1399 | -1.2580 |
| -0.3436 | -2.0424 | -1.1106 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3D** | | |
|---|---|---|
| -2.9868 | -0.1167 | 0.8082 |
| -2.8894 | -1.5722 | 0.3699 |
| -1.6290 | -2.3011 | 0.9007 |
| -0.3587 | -1.4375 | 0.5587 |
| -0.4157 | 0.1059 | 0.9266 |
| -1.7517 | 0.6833 | 0.3915 |
| 0.9771 | -2.0800 | 0.9993 |
| 2.1809 | -1.3467 | 0.4033 |
| 2.1133 | 0.1317 | 0.6983 |
| 0.8239 | 0.7964 | 0.2009 |
| 1.5238 | 2.7177 | -2.2054 |
| 1.7970 | 3.0244 | -0.7437 |
| 0.8172 | 2.3512 | 0.2385 |
| -0.3323 | 0.3988 | 2.4458 |
| -1.7681 | -2.6362 | 2.4051 |
| -1.5588 | -3.6520 | 0.1321 |
| 2.4226 | 2.0099 | -2.9189 |
| 3.1051 | 0.7276 | 1.3819 |
| 0.2343 | 3.2732 | -2.7495 |
| -4.1388 | 0.4810 | 0.2133 |
| -2.8919 | -3.4832 | 2.6319 |
| 2.2753 | 1.5865 | -4.3226 |
| 1.2869 | 1.6238 | -5.0271 |
| 3.4444 | 1.0979 | -4.7708 |
| -3.1383 | -0.0574 | 1.8893 |
| -3.8063 | -2.0998 | 0.6633 |
| -2.8942 | -1.6027 | -0.7296 |
| -0.3250 | -1.4517 | -0.5442 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3E** | | |
|---|---|---|
| -2.9598 | -0.8698 | 0.3045 |
| -2.8187 | -2.3173 | -0.1480 |
| -1.5449 | -3.0177 | 0.3889 |
| -0.2944 | -2.1168 | 0.0705 |
| -0.3967 | -0.5794 | 0.4513 |
| -1.7426 | -0.0328 | -0.0919 |
| 1.0519 | -2.7276 | 0.5234 |
| 2.2426 | -1.9590 | -0.0531 |
| 2.1338 | -0.4846 | 0.2493 |
| 0.8317 | 0.1522 | -0.2524 |
| 1.6591 | 3.8814 | -1.1583 |
| 1.7403 | 2.3659 | -1.2026 |
| 0.7862 | 1.7041 | -0.1912 |
| -0.3377 | -0.2988 | 1.9744 |
| -1.6920 | -3.3732 | 1.8880 |
| -1.4300 | -4.3578 | -0.3933 |
| 1.1191 | 4.5560 | -2.1931 |
| 3.1067 | 0.1336 | 0.9406 |
| 2.2398 | 4.5180 | 0.0771 |
| -4.1217 | -0.2974 | -0.2958 |
| -2.7953 | -4.2523 | 2.0920 |
| 0.9334 | 6.0162 | -2.2765 |
| 1.0888 | 6.8541 | -1.4116 |
| 0.5257 | 6.3467 | -3.5141 |
| -3.1232 | -0.8259 | 1.3847 |
| -3.7241 | -2.8725 | 0.1297 |
| -2.8108 | -2.3361 | -1.2477 |
| -0.2463 | -2.1195 | -1.0320 |

| | | | |
|---|---|---|---|
| H | -1.9567 | -0.6437 | -0.2425 |
| H | -1.8780 | 1.0764 | 0.0461 |
| H | 1.7340 | -2.5735 | 2.4201 |
| H | 1.9809 | -0.8466 | 2.5935 |
| H | 3.4733 | -1.7459 | 0.8893 |
| H | 2.1488 | -2.5245 | 0.0372 |
| H | 0.3452 | -1.1198 | -1.0256 |
| H | 0.4139 | -0.4158 | -3.3060 |
| H | 1.9745 | 0.3186 | -3.0301 |
| H | 0.8648 | 1.8701 | -1.3041 |
| H | -0.6613 | 1.1047 | -1.6898 |
| H | 1.3453 | 1.1704 | 1.9239 |
| H | 0.3170 | 2.1136 | 0.8518 |
| H | -0.3209 | 1.5357 | 2.3543 |
| H | -0.5536 | 0.3122 | 3.9091 |
| H | 0.5354 | -0.9736 | 4.4390 |
| H | 0.1931 | -3.3368 | 3.7696 |
| H | -1.5490 | -3.3513 | 4.0276 |
| H | -0.8973 | -3.7747 | 2.4449 |
| H | -0.8692 | 0.4436 | -5.0212 |
| H | 3.0590 | 1.3212 | -1.0908 |
| H | 4.2057 | 0.1789 | -0.2192 |
| H | 2.4535 | 2.6006 | -3.6038 |
| H | 1.5459 | 3.3866 | -4.8710 |
| H | 1.0016 | 3.5288 | -3.1846 |
| H | -4.4669 | -0.0847 | 2.0894 |
| H | -1.0443 | -0.5191 | 5.9502 |
| H | -1.8066 | 2.4445 | -7.5352 |

| | | |
|---|---|---|
| -1.8351 | 0.1005 | -1.2798 |
| -2.0082 | 1.0425 | 0.1800 |
| 0.9531 | -3.7747 | 0.0037 |
| 0.9763 | -2.7750 | 1.4436 |
| 3.0130 | -2.4376 | 0.1478 |
| 2.1093 | -2.1153 | -1.3239 |
| 0.6297 | -0.0765 | -1.4654 |
| 1.3001 | 2.1086 | -2.3619 |
| 2.6498 | 1.9388 | -1.2684 |
| 0.9591 | 2.0511 | 0.6942 |
| -0.3040 | 2.0781 | -0.5168 |
| -1.3269 | -0.5750 | 2.3878 |
| 0.4142 | -0.8181 | 2.3236 |
| -0.2903 | 0.7721 | 2.0566 |
| -1.9397 | -2.4713 | 2.3927 |
| -0.9707 | -3.9167 | 2.0893 |
| -0.8664 | -4.9754 | -0.1508 |
| -2.5897 | -4.8540 | -0.4930 |
| -1.4261 | -4.1285 | -1.6016 |
| 3.7032 | 3.8560 | -0.5577 |
| 2.9918 | 1.1259 | 1.0429 |
| 3.8914 | -0.4774 | 1.0731 |
| 0.6069 | 5.6267 | -1.8957 |
| -0.0491 | 4.1028 | -2.4389 |
| -0.2760 | 4.5941 | -0.7496 |
| -5.0032 | -0.7337 | -0.1327 |
| -2.9883 | -4.4014 | 2.9146 |
| 4.3509 | 7.1165 | -0.1726 |

| | | |
|---|---|---|
| -1.7257 | 0.1693 | -1.1216 |
| -1.8596 | 1.0676 | 0.3695 |
| 1.0097 | -3.7935 | -0.0054 |
| 1.0713 | -2.8420 | 1.4658 |
| 3.0960 | -2.4976 | 0.1535 |
| 2.1788 | -2.1131 | -1.2947 |
| 0.7325 | -0.0472 | -1.3494 |
| 1.4973 | 2.0577 | -2.1750 |
| 2.8291 | 2.0157 | -1.0456 |
| 1.1157 | 2.0029 | 0.8725 |
| -0.1462 | 2.0985 | -0.3366 |
| -1.1768 | -0.6312 | 2.5151 |
| 0.5582 | -0.9054 | 2.4165 |
| -0.1193 | 0.7057 | 2.2116 |
| -1.8204 | -2.5133 | 2.4573 |
| -0.8884 | -3.9628 | 2.1162 |
| -0.8418 | -4.9607 | -0.1736 |
| -2.5602 | -4.7799 | -0.5208 |
| -1.3721 | -4.0435 | -1.5925 |
| 0.7922 | 4.1325 | -2.8990 |
| 3.1500 | 1.0347 | 1.1625 |
| 4.0217 | -0.5834 | 1.1276 |
| 2.8222 | 5.4507 | 0.0436 |
| 1.7475 | 4.4289 | 1.0240 |
| 3.3154 | 3.8272 | 0.4540 |
| -4.8956 | -0.6126 | 0.1019 |
| -2.7561 | -5.0444 | 1.7172 |
| 0.5953 | 7.4637 | -3.1536 |

| | | |
|---|---|---|
| -1.7181 | 0.7388 | -0.7055 |
| -1.8962 | 1.7167 | 0.7301 |
| 1.0333 | -3.1224 | 0.6704 |
| 1.0591 | -2.0957 | 2.0916 |
| 3.1013 | -1.7960 | 0.7953 |
| 2.2038 | -1.4917 | -0.6842 |
| 0.7361 | 0.5292 | -0.8619 |
| 2.8286 | 2.7622 | -0.4851 |
| 1.7365 | 4.1117 | -0.6037 |
| 1.0388 | 2.7128 | 1.2491 |
| -0.1818 | 2.7302 | 0.0036 |
| -1.2390 | 0.1248 | 2.9837 |
| 0.5023 | -0.1126 | 2.9321 |
| -0.2060 | 1.4705 | 2.6329 |
| -1.9200 | -1.7517 | 3.0186 |
| -0.8832 | -3.1626 | 2.7757 |
| -0.7955 | -4.3179 | 0.5473 |
| -2.5131 | -4.1897 | 0.1779 |
| -1.3289 | -3.4961 | -0.9280 |
| 3.3416 | 1.6703 | -2.4490 |
| 3.0857 | 1.7761 | 1.6560 |
| 3.9774 | 0.1694 | 1.7114 |
| 0.2545 | 3.4224 | -3.8312 |
| -0.6002 | 2.6103 | -2.5010 |
| 0.0306 | 4.2578 | -2.3143 |
| -4.0744 | 0.3660 | -0.7504 |
| -2.9374 | -3.6513 | 3.5888 |
| 3.2473 | 0.8463 | -5.6969 |

| | | |
|---|---|---|
| -1.6995 | 0.0348 | -1.1878 |
| -1.9185 | 0.9929 | 0.2554 |
| 1.1394 | -3.7659 | 0.1883 |
| 1.1211 | -2.7489 | 1.6164 |
| 3.1697 | -2.3869 | 0.3468 |
| 2.2817 | -2.0964 | -1.1411 |
| 0.7673 | -0.0909 | -1.3245 |
| 1.4919 | 2.0032 | -2.2087 |
| 2.7796 | 2.0673 | -1.0300 |
| 0.9997 | 2.0588 | 0.8230 |
| -0.2211 | 2.0586 | -0.4315 |
| -1.2397 | -0.6080 | 2.5007 |
| 0.5089 | -0.7868 | 2.4640 |
| -0.2488 | 0.7747 | 2.1727 |
| -1.8745 | -2.4999 | 2.5094 |
| -0.7976 | -3.8801 | 2.2632 |
| -0.6538 | -5.0076 | 0.0233 |
| -2.3700 | -4.9212 | -0.3642 |
| -1.1926 | -4.1841 | -1.4490 |
| 0.7486 | 4.0150 | -3.0592 |
| 3.0613 | 1.1813 | 1.2154 |
| 3.9917 | -0.4030 | 1.2723 |
| 2.5850 | 5.5405 | -0.0902 |
| 1.5025 | 4.5221 | 0.8857 |
| 3.1174 | 3.9576 | 0.4181 |
| -4.0495 | -0.4064 | -1.2592 |
| -2.8484 | -4.4309 | 3.0467 |
| 0.4272 | 7.3205 | -3.4689 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3F** | | | |
|---|---|---|---|
| C | -3.1030 | -0.7885 | 0.2104 |
| C | -3.0106 | -2.2323 | -0.2615 |
| C | -1.7534 | -2.9797 | 0.2495 |
| C | -0.4798 | -2.1160 | -0.0786 |
| C | -0.5285 | -0.5809 | 0.3218 |
| C | -1.8649 | 0.0140 | -0.1930 |
| C | 0.8530 | -2.7742 | 0.3467 |
| C | 2.0588 | -2.0357 | -0.2373 |
| C | 2.0001 | -0.5625 | 0.0846 |
| C | 0.7117 | 0.1201 | -0.3925 |
| C | 1.7224 | 3.8255 | -1.2015 |
| C | 1.6668 | 2.3145 | -1.3404 |
| C | 0.7165 | 1.6717 | -0.3133 |
| C | -0.4385 | -0.3196 | 1.8467 |
| C | -1.8861 | -3.3471 | 1.7470 |
| C | -1.6945 | -4.3144 | -0.5477 |
| C | 2.8520 | 4.4159 | -0.7619 |
| C | 3.0015 | 0.0174 | 0.7687 |
| C | 0.4708 | 4.5563 | -1.6108 |
| O | -4.2492 | -0.1949 | -0.3994 |
| O | -3.0206 | -4.1809 | 1.9672 |
| C | 3.0452 | 5.8591 | -0.5324 |
| O | 2.2176 | 6.7475 | -0.5366 |
| O | 4.3428 | 6.1041 | -0.2808 |
| H | -3.2643 | -0.7539 | 1.2919 |
| H | -3.9288 | -2.7642 | 0.0204 |
| H | -3.0189 | -2.2349 | -1.3616 |
| H | -0.4484 | -2.1071 | -1.1816 |
| H | -1.8376 | 0.0951 | -1.2886 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3G** | | |
|---|---|---|
| -2.5212 | 0.7270 | 1.6165 |
| -2.2666 | -0.6009 | 2.3164 |
| -0.7926 | -0.8022 | 2.7464 |
| 0.1323 | -0.5530 | 1.4961 |
| -0.1212 | 0.7767 | 0.6650 |
| -1.6414 | 0.8888 | 0.3764 |
| 1.6378 | -0.7760 | 1.7699 |
| 2.4507 | -0.7969 | 0.4735 |
| 2.1798 | 0.4355 | -0.3545 |
| 0.6975 | 0.6314 | -0.6946 |
| 0.2695 | 0.1607 | -3.7886 |
| 0.8961 | 1.4016 | -3.1780 |
| 0.3961 | 1.7274 | -1.7561 |
| 0.3333 | 2.0703 | 1.3866 |
| -0.4297 | 0.0731 | 3.9714 |
| -0.6747 | -2.2879 | 3.1913 |
| 1.0368 | -0.9176 | -4.0468 |
| 3.1885 | 1.2617 | -0.6802 |
| -1.2040 | 0.2609 | -4.0818 |
| -3.8921 | 0.7917 | 1.2282 |
| -1.2106 | -0.2625 | 5.1159 |
| 0.5656 | -2.2077 | -4.5801 |
| -0.5748 | -2.6074 | -4.7010 |
| 1.6206 | -2.9632 | -4.9298 |
| -2.3644 | 1.5558 | 2.3121 |
| -2.9500 | -0.7001 | 3.1689 |
| -2.5636 | -1.4117 | 1.6348 |
| -0.1475 | -1.3636 | 0.8016 |
| -1.9333 | 0.1345 | -0.3675 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3H** | | |
|---|---|---|
| -2.5226 | 0.7261 | 1.6335 |
| -2.2709 | -0.6041 | 2.3301 |
| -0.7961 | -0.8191 | 2.7510 |
| 0.1204 | -0.5790 | 1.4925 |
| -0.1286 | 0.7525 | 0.6641 |
| -1.6497 | 0.8774 | 0.3869 |
| 1.6265 | -0.8170 | 1.7526 |
| 2.4290 | -0.8412 | 0.4498 |
| 2.1620 | 0.3972 | -0.3703 |
| 0.6792 | 0.6017 | -0.7017 |
| 0.2757 | 0.1320 | -3.7982 |
| 0.8820 | 1.3808 | -3.1837 |
| 0.3771 | 1.6988 | -1.7617 |
| 0.3413 | 2.0409 | 1.3853 |
| -0.4183 | 0.0575 | 3.9713 |
| -0.6863 | -2.3049 | 3.1960 |
| 1.0610 | -0.9332 | -4.0570 |
| 3.1732 | 1.2208 | -0.6949 |
| -1.1987 | 0.2101 | -4.0929 |
| -3.8962 | 0.7665 | 1.2516 |
| -1.1518 | -0.2986 | 5.1407 |
| 0.6169 | -2.2290 | -4.6006 |
| -0.5149 | -2.6351 | -4.7686 |
| 1.6890 | -2.9818 | -4.9019 |
| -2.3655 | 1.5550 | 2.3295 |
| -2.9499 | -0.7007 | 3.1864 |
| -2.5794 | -1.4110 | 1.6487 |
| -0.1730 | -1.3870 | 0.8004 |
| -1.9565 | 0.1249 | -0.3528 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3I** | | |
|---|---|---|
| -2.5637 | -0.0391 | 1.7159 |
| -2.3539 | -1.3769 | 2.4109 |
| -0.8891 | -1.6305 | 2.8448 |
| 0.0548 | -1.4012 | 1.6076 |
| -0.1546 | -0.0616 | 0.7811 |
| -1.6684 | 0.0959 | 0.4836 |
| 1.5501 | -1.6627 | 1.8996 |
| 2.3778 | -1.6986 | 0.6131 |
| 2.1456 | -0.4602 | -0.2175 |
| 0.6715 | -0.2241 | -0.5715 |
| 0.6085 | 1.5630 | -4.0655 |
| 0.8969 | 0.4848 | -3.0359 |
| 0.4124 | 0.8835 | -1.6297 |
| 0.3298 | 1.2178 | 1.5100 |
| -0.5104 | -0.7802 | 4.0806 |
| -0.8247 | -3.1228 | 3.2797 |
| -0.3113 | 1.3443 | -5.0273 |
| 3.1784 | 0.3378 | -0.5390 |
| 1.4433 | 2.8093 | -3.9380 |
| -3.9202 | 0.0541 | 1.2816 |
| -1.3974 | -1.0426 | 5.1654 |
| -0.7656 | 2.2532 | -6.0917 |
| -1.2847 | 1.8835 | -7.1303 |
| -0.6359 | 3.5539 | -5.7993 |
| -2.3967 | 0.7887 | 2.4110 |
| -3.0386 | -1.4542 | 3.2655 |
| -2.6799 | -2.1737 | 1.7262 |
| -0.2379 | -2.2010 | 0.9059 |
| -1.9790 | -0.6484 | -0.2630 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3J** | | |
|---|---|---|
| -3.0103 | -0.1336 | 0.7650 |
| -2.9007 | -1.5892 | 0.3324 |
| -1.6578 | -2.3161 | 0.9038 |
| -0.3769 | -1.4551 | 0.5755 |
| -0.4413 | 0.0941 | 0.9230 |
| -1.7719 | 0.6674 | 0.3675 |
| 0.9657 | -2.0795 | 1.0203 |
| 2.1602 | -1.3514 | 0.4012 |
| 2.0934 | 0.1283 | 0.6908 |
| 0.7999 | 0.7879 | 0.2001 |
| 1.4605 | 2.7296 | -2.2064 |
| 1.7595 | 3.0205 | -0.7464 |
| 0.7908 | 2.3429 | 0.2437 |
| -0.3729 | 0.3966 | 2.4401 |
| -1.9012 | -2.6404 | 2.3984 |
| -1.5674 | -3.6767 | 0.1562 |
| 2.3404 | 2.0181 | -2.9397 |
| 3.0899 | 0.7267 | 1.3655 |
| 0.1695 | 3.3038 | -2.7263 |
| -4.1591 | 0.4477 | 0.1497 |
| -0.8293 | -3.3754 | 2.9675 |
| 2.1655 | 1.6079 | -4.3440 |
| 1.1644 | 1.6566 | -5.0297 |
| 3.3238 | 1.1182 | -4.8181 |
| -3.1794 | -0.0697 | 1.8433 |
| -3.8220 | -2.1193 | 0.6096 |
| -2.8792 | -1.6250 | -0.7665 |
| -0.3355 | -1.4783 | -0.5273 |
| -1.7214 | 0.7217 | -0.7289 |

| | | | |
|---|---|---|---|
| H | -2.0015 | 1.0399 | 0.1705 |
| H | 0.9029 | -3.8103 | -0.0030 |
| H | 0.9372 | -2.8123 | 1.4382 |
| H | 2.9777 | -2.4969 | 0.1442 |
| H | 2.0786 | -2.1605 | -1.3272 |
| H | 0.6249 | -0.1078 | -1.4664 |
| H | 1.3370 | 2.0627 | -2.3566 |
| H | 2.6737 | 1.8935 | -1.2471 |
| H | 0.9688 | 2.0135 | 0.6971 |
| H | -0.2861 | 2.0556 | -0.5221 |
| H | -1.3475 | -0.5948 | 2.3806 |
| H | 0.3920 | -0.8489 | 2.3206 |
| H | -0.3010 | 0.7468 | 2.0550 |
| H | -2.0179 | -2.4747 | 2.3820 |
| H | -1.0058 | -3.8951 | 2.0972 |
| H | -0.9315 | -4.9923 | -0.1522 |
| H | -2.6510 | -4.8486 | -0.5061 |
| H | -1.4713 | -4.1371 | -1.6059 |
| H | 3.7204 | 3.8106 | -0.5173 |
| H | 2.9926 | 1.0632 | 1.0543 |
| H | 3.8736 | -0.5505 | 1.0816 |
| H | 0.6594 | 5.5843 | -1.9280 |
| H | 0.0025 | 4.0595 | -2.4679 |
| H | -0.2497 | 4.5679 | -0.7873 |
| H | -4.3407 | 0.7042 | -0.0408 |
| H | -3.0386 | -4.4002 | 2.9144 |
| H | 4.3694 | 7.0738 | -0.1433 |

| | | |
|---|---|---|
| -1.8848 | 1.8562 | -0.0799 |
| 1.8026 | -1.7329 | 2.2750 |
| 2.0305 | -0.0020 | 2.4381 |
| 3.5146 | -0.8918 | 0.7220 |
| 2.1893 | -1.6852 | -0.1152 |
| 0.3632 | -0.3136 | -1.1461 |
| 1.9883 | 1.3200 | -3.1836 |
| 0.6711 | 2.2562 | -3.8297 |
| 0.8264 | 2.6880 | -1.4505 |
| -0.6821 | 1.8984 | -1.8272 |
| 1.3561 | 2.0079 | 1.7668 |
| 0.2930 | 2.9317 | 0.7114 |
| -0.3091 | 2.3396 | 2.2241 |
| -0.5723 | 1.1372 | 3.7981 |
| 0.6164 | -0.0741 | 4.2562 |
| 0.2911 | -2.4968 | 3.6625 |
| -1.4509 | -2.5503 | 3.9198 |
| -0.7886 | -2.9693 | 2.3406 |
| 2.1008 | -0.8917 | -3.8274 |
| 3.0431 | 2.1804 | -1.2365 |
| 4.2107 | 1.0498 | -0.3778 |
| -1.4557 | 1.2699 | -4.4267 |
| -1.5301 | -0.4163 | -4.8742 |
| -1.7865 | 0.0530 | -3.1789 |
| -4.0649 | 0.0670 | 0.6023 |
| -2.1003 | 0.1096 | 4.9912 |
| 1.2117 | -3.7874 | -5.2664 |

| | | |
|---|---|---|
| -1.8847 | 1.8466 | -0.0701 |
| 1.7863 | -1.7768 | 2.2539 |
| 2.0325 | -0.0483 | 2.4190 |
| 3.4940 | -0.9463 | 0.6893 |
| 2.1552 | -1.7250 | -0.1402 |
| 0.3358 | -0.3410 | -1.1512 |
| 1.9753 | 1.3164 | -3.1893 |
| 0.6451 | 2.2331 | -3.8343 |
| 0.8023 | 2.6604 | -1.4522 |
| -0.7019 | 1.8643 | -1.8353 |
| 1.3670 | 1.9704 | 1.7563 |
| 0.3007 | 2.9046 | 0.7131 |
| -0.2912 | 2.3114 | 2.2298 |
| -0.5953 | 1.1181 | 3.8072 |
| 0.6393 | -0.0630 | 4.2234 |
| 0.2803 | -2.5195 | 3.6630 |
| -1.4612 | -2.5622 | 3.9276 |
| -0.8083 | -2.9860 | 2.3462 |
| 2.1230 | -0.8906 | -3.8306 |
| 3.0296 | 2.1440 | -1.2442 |
| 4.1956 | 1.0016 | -0.3983 |
| -1.4649 | 1.2155 | -4.4377 |
| -1.5150 | -0.4713 | -4.8855 |
| -1.7786 | -0.0061 | -3.1904 |
| -4.0517 | 1.6067 | 0.7869 |
| -2.0806 | -0.0467 | 5.0045 |
| 1.2963 | -3.8105 | -5.2467 |

| | | |
|---|---|---|
| -1.8785 | 1.0706 | 0.0259 |
| 1.6846 | -2.6257 | 2.4022 |
| 1.9527 | -0.9021 | 2.5773 |
| 3.4362 | -1.8181 | 0.8743 |
| 2.1035 | -2.5802 | 0.0200 |
| 0.3186 | -1.1543 | -1.0434 |
| 0.4059 | -0.4544 | -3.3229 |
| 1.9708 | 0.2711 | -3.0457 |
| 0.8713 | 1.8296 | -1.3224 |
| -0.6615 | 1.0791 | -1.7114 |
| 1.3433 | 1.1230 | 1.9077 |
| 0.3290 | 2.0794 | 0.8339 |
| -0.3185 | 1.5097 | 2.3355 |
| -0.5669 | 0.2881 | 3.8899 |
| 0.5039 | -1.0124 | 4.4211 |
| 0.1325 | -3.3701 | 3.7496 |
| -1.6098 | -3.3623 | 4.0064 |
| -0.9624 | -3.7935 | 2.4240 |
| -0.8168 | 0.3834 | -5.0807 |
| 3.0608 | 1.2558 | -1.1033 |
| 4.1929 | 0.0993 | -0.2310 |
| 2.4441 | 2.5640 | -3.5654 |
| 1.5975 | 3.3126 | -4.8962 |
| 0.9807 | 3.5093 | -3.2357 |
| -4.4842 | -0.0616 | 2.0661 |
| -1.0711 | -0.5380 | 5.9306 |
| -1.0157 | 4.0056 | -6.5802 |

| | | |
|---|---|---|
| -1.9252 | 1.7007 | 0.7023 |
| 1.0280 | -3.1288 | 0.7162 |
| 1.0634 | -2.0614 | 2.1103 |
| 3.0864 | -1.7968 | 0.7839 |
| 2.1689 | -1.5032 | -0.6855 |
| 0.7115 | 0.5229 | -0.8633 |
| 2.7935 | 2.7500 | -0.5073 |
| 1.7073 | 4.1068 | -0.5949 |
| 1.0223 | 2.6999 | 1.2539 |
| -0.2105 | 2.7229 | 0.0216 |
| -1.2680 | 0.0854 | 2.9765 |
| 0.4811 | -0.0785 | 2.9295 |
| -0.2898 | 1.4735 | 2.6221 |
| -2.8045 | -3.2540 | 2.5033 |
| -2.0628 | -1.7507 | 3.0038 |
| -0.7766 | -4.3205 | 0.5525 |
| -2.5075 | -4.2343 | 0.2451 |
| -1.3747 | -3.5318 | -0.9129 |
| 3.2627 | 1.6641 | -2.4869 |
| 3.0726 | 1.7754 | 1.6377 |
| 3.9629 | 0.1678 | 1.6921 |
| 0.1763 | 3.4643 | -3.8066 |
| -0.6682 | 2.6467 | -2.4732 |
| -0.0183 | 4.2858 | -2.2780 |
| -4.0331 | 0.4179 | -0.8146 |
| -1.0640 | -3.5562 | 3.8940 |
| 3.1089 | 0.8741 | -5.7421 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3K** | | | |
|---|---|---|---|
| C | -2.8813 | -0.8871 | -0.7626 |
| C | -3.1232 | -0.8220 | 0.7399 |
| C | -2.5623 | 0.4575 | 1.4106 |
| C | -1.0562 | 0.6359 | 0.9886 |
| C | -0.7199 | 0.5142 | -0.5585 |
| C | -1.3942 | -0.7719 | -1.1019 |
| C | -0.3648 | 1.8623 | 1.6284 |
| C | 1.1503 | 1.8332 | 1.4142 |
| C | 1.4865 | 1.6618 | -0.0468 |
| C | 0.8661 | 0.4079 | -0.6748 |
| C | 3.1684 | -1.6513 | -1.3200 |
| C | 2.8683 | -0.4060 | -2.1352 |
| C | 1.3926 | 0.0396 | -2.0911 |
| C | -1.2041 | 1.7145 | -1.4106 |
| C | -3.4434 | 1.6903 | 1.0929 |
| C | -2.6403 | 0.2069 | 2.9437 |
| C | 3.9775 | -1.5671 | -0.2447 |
| C | 2.2226 | 2.5900 | -0.6815 |
| C | 2.5276 | -2.9185 | -1.8208 |
| O | -3.3670 | -2.1330 | -1.2637 |
| O | -4.7909 | 1.5053 | 1.5178 |
| C | 4.3151 | -2.6685 | 0.6738 |
| O | 3.8047 | -3.7669 | 0.7617 |
| O | 5.3192 | -2.2890 | 1.4827 |
| H | -3.4560 | -0.1087 | -1.2719 |
| H | -4.1970 | -0.9350 | 0.9382 |
| H | -2.6637 | -1.7083 | 1.2014 |
| H | -0.5548 | -0.2359 | 1.4429 |
| H | -0.8715 | -1.6565 | -0.7120 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3L** | | |
|---|---|---|
| -2.5447 | -0.0646 | 1.7544 |
| -2.3128 | -1.4034 | 2.4411 |
| -0.8473 | -1.6241 | 2.8896 |
| 0.0991 | -1.3673 | 1.6569 |
| -0.1313 | -0.0268 | 0.8370 |
| -1.6462 | 0.1025 | 0.5283 |
| 1.5982 | -1.6030 | 1.9534 |
| 2.4319 | -1.6164 | 0.6706 |
| 2.1823 | -0.3757 | -0.1514 |
| 0.7071 | -0.1619 | -0.5115 |
| 0.6263 | 1.6551 | -3.9906 |
| 0.9378 | 0.5777 | -2.9671 |
| 0.4347 | 0.9514 | -1.5604 |
| 0.3230 | 1.2550 | 1.5803 |
| -0.4949 | -0.7690 | 4.1319 |
| -0.7498 | -3.1166 | 3.3164 |
| -0.2862 | 1.4220 | -4.9553 |
| 3.2028 | 0.4433 | -0.4590 |
| 1.4205 | 2.9264 | -3.8441 |
| -3.9095 | 0.0182 | 1.3487 |
| -1.3012 | -1.1094 | 5.2572 |
| -0.7232 | 2.3799 | -5.9874 |
| -0.4715 | 3.5638 | -6.0826 |
| -1.5087 | 1.7513 | -6.8790 |
| -2.3892 | 0.7541 | 2.4621 |
| -3.0093 | -1.5066 | 3.2825 |
| -2.6075 | -2.2028 | 1.7452 |
| -0.1748 | -2.1678 | 0.9484 |
| -1.9343 | -0.6406 | -0.2281 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3M** | | |
|---|---|---|
| -2.4845 | 0.7873 | 1.6548 |
| -2.2833 | -0.5750 | 2.3054 |
| -0.8146 | -0.8681 | 2.7012 |
| 0.1033 | -0.6197 | 1.4462 |
| -0.0957 | 0.7513 | 0.6705 |
| -1.6114 | 0.9476 | 0.4103 |
| 1.6000 | -0.9277 | 1.6867 |
| 2.3951 | -0.9331 | 0.3789 |
| 2.1722 | 0.3446 | -0.3925 |
| 0.6965 | 0.6180 | -0.7060 |
| 0.2799 | 0.2611 | -3.8107 |
| 0.9166 | 1.4766 | -3.1608 |
| 0.4292 | 1.7611 | -1.7257 |
| 0.4304 | 1.9926 | 1.4343 |
| -0.3863 | -0.0601 | 3.9510 |
| -0.7670 | -2.3738 | 3.0883 |
| 1.0425 | -0.8081 | -4.1165 |
| 3.2120 | 1.1411 | -0.6930 |
| -1.1966 | 0.3765 | -4.0821 |
| -3.8464 | 0.9173 | 1.2499 |
| -1.1604 | -0.4022 | 5.0984 |
| 0.5696 | -2.0762 | -4.6995 |
| -0.5705 | -2.4596 | -4.8650 |
| 1.6251 | -2.8339 | -5.0445 |
| -2.2904 | 1.5900 | 2.3719 |
| -2.9535 | -0.6699 | 3.1690 |
| -2.6357 | -1.3443 | 1.6023 |
| -0.2270 | -1.3887 | 0.7269 |
| -1.9517 | 0.2353 | -0.3543 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**3N** | | |
|---|---|---|
| -2.7758 | 0.9694 | 0.8485 |
| -2.5831 | -0.0207 | 1.9887 |
| -1.1919 | 0.0681 | 2.6638 |
| -0.0813 | -0.0136 | 1.5523 |
| -0.2543 | 0.9333 | 0.2888 |
| -1.7081 | 0.7904 | -0.2314 |
| 1.3637 | 0.0252 | 2.1013 |
| 2.3884 | -0.3333 | 1.0220 |
| 2.1986 | 0.5180 | -0.2096 |
| 0.7879 | 0.4264 | -0.8048 |
| 0.9683 | -1.1074 | -3.5526 |
| 1.3776 | 0.3399 | -3.3449 |
| 0.6134 | 1.0587 | -2.2148 |
| 0.0118 | 2.4331 | 0.5754 |
| -1.0805 | 1.3268 | 3.5571 |
| -1.0860 | -1.1752 | 3.5920 |
| 1.8589 | -2.0931 | -3.3189 |
| 3.2009 | 1.2962 | -0.6520 |
| -0.4364 | -1.3124 | -4.0532 |
| -4.0495 | 0.7410 | 0.2457 |
| -2.1134 | 1.3713 | 4.5386 |
| 1.6667 | -3.5486 | -3.4102 |
| 2.5705 | -4.3489 | -3.5757 |
| 0.4044 | -3.9502 | -3.2121 |
| -2.7823 | 1.9970 | 1.2230 |
| -3.3879 | 0.1097 | 2.7238 |
| -2.7369 | -1.0350 | 1.5917 |
| -0.1980 | -1.0323 | 1.1443 |
| -1.8396 | -0.1951 | -0.6997 |

| | | | |
|---|---|---|---|
| H | -1.2971 | -0.8350 | -2.1928 |
| H | -0.5427 | 1.8882 | 2.7081 |
| H | -0.7760 | 2.7942 | 1.2253 |
| H | 1.5857 | 2.7521 | 1.8248 |
| H | 1.5899 | 1.0021 | 1.9800 |
| H | 1.1585 | -0.4310 | -0.0273 |
| H | 3.5194 | 0.4186 | -1.8260 |
| H | 3.1394 | -0.6060 | -3.1802 |
| H | 1.2661 | 0.8822 | -2.7804 |
| H | 0.7994 | -0.7769 | -2.5134 |
| H | -0.9112 | 2.6798 | -0.9900 |
| H | -0.7937 | 1.6675 | -2.4248 |
| H | -2.2848 | 1.7328 | -1.5467 |
| H | -3.4979 | 1.8945 | 0.0270 |
| H | -3.0648 | 2.5950 | 1.5795 |
| H | -2.4345 | 1.1171 | 3.5160 |
| H | -3.6343 | -0.1452 | 3.2432 |
| H | -1.9227 | -0.5588 | 3.2599 |
| H | 4.4194 | -0.6126 | 0.0281 |
| H | 2.4555 | 2.5363 | -1.7387 |
| H | 2.6070 | 3.4607 | -0.1570 |
| H | 1.4944 | -2.9879 | -1.4669 |
| H | 2.5158 | -2.9316 | -2.9164 |
| H | 3.0645 | -3.8196 | -1.5164 |
| H | -2.9151 | -2.8487 | -0.7851 |
| H | -4.8181 | 1.6151 | 2.4832 |
| H | 5.4695 | -3.0762 | 2.0461 |

| | | |
|---|---|---|
| -1.8742 | 1.0773 | 0.0797 |
| 1.7483 | -2.5660 | 2.4516 |
| 1.9848 | -0.8384 | 2.6359 |
| 3.4910 | -1.7201 | 0.9357 |
| 2.1749 | -2.4980 | 0.0699 |
| 0.3735 | -1.0935 | -0.9944 |
| 0.4742 | -0.3720 | -3.2648 |
| 2.0172 | 0.3935 | -2.9724 |
| 0.8729 | 1.9028 | -1.2392 |
| -0.6421 | 1.1270 | -1.6482 |
| 1.3413 | 1.1820 | 1.9705 |
| 0.2949 | 2.1252 | 0.9157 |
| -0.3266 | 1.5173 | 2.4143 |
| -0.6200 | 0.2992 | 3.9699 |
| 0.5438 | -0.9339 | 4.4337 |
| 0.2071 | -3.3411 | 3.7983 |
| -1.5387 | -3.3811 | 4.0302 |
| -0.8580 | -3.7857 | 2.4552 |
| -0.7923 | 0.4621 | -5.0031 |
| 3.0734 | 1.3652 | -1.0145 |
| 4.2193 | 0.2205 | -0.1455 |
| 2.4376 | 2.7034 | -3.5031 |
| 1.5335 | 3.4711 | -4.7840 |
| 0.9509 | 3.5861 | -3.1081 |
| -4.0825 | -0.6974 | 0.7130 |
| -2.1788 | -0.7107 | 5.1284 |
| -1.7468 | 2.4601 | -7.5122 |

| | | |
|---|---|---|
| -1.8109 | 1.9412 | -0.0102 |
| 1.7235 | -1.9120 | 2.1493 |
| 2.0395 | -0.2026 | 2.3802 |
| 3.4564 | -1.0877 | 0.6078 |
| 2.0847 | -1.7828 | -0.2421 |
| 0.3142 | -0.2947 | -1.1852 |
| 2.0082 | 1.3891 | -3.1761 |
| 0.6942 | 2.3541 | -3.7824 |
| 0.8884 | 2.6962 | -1.3852 |
| -0.6439 | 1.9657 | -1.7881 |
| 1.4509 | 1.8634 | 1.8038 |
| 0.4306 | 2.8790 | 0.7912 |
| -0.1920 | 2.2638 | 2.2862 |
| -0.4802 | 1.0157 | 3.8210 |
| 0.6564 | -0.2685 | 4.2088 |
| 0.1942 | -2.6499 | 3.5335 |
| -1.5439 | -2.6236 | 3.8204 |
| -0.9301 | -3.0154 | 2.2149 |
| 2.1077 | -0.7915 | -3.9025 |
| 3.0992 | 2.0892 | -1.2059 |
| 4.2270 | 0.8730 | -0.4122 |
| -1.4467 | 1.3958 | -4.3965 |
| -1.5379 | -0.2774 | -4.8873 |
| -1.7684 | 0.1478 | -3.1775 |
| -4.4080 | 0.7780 | 2.0312 |
| -2.0237 | 0.0363 | 5.0217 |
| 1.2133 | -3.6423 | -5.4141 |

| | | |
|---|---|---|
| -1.9130 | 1.5186 | -1.0261 |
| 1.4863 | -0.6906 | 2.9203 |
| 1.5947 | 1.0120 | 2.5168 |
| 3.3970 | -0.2235 | 1.4384 |
| 2.2811 | -1.3893 | 0.7439 |
| 0.5848 | -0.6456 | -0.9396 |
| 2.4569 | 0.4108 | -3.1725 |
| 1.2036 | 0.8844 | -4.2824 |
| 0.9205 | 2.1108 | -2.2063 |
| -0.4439 | 1.0627 | -2.4966 |
| 0.9480 | 2.6040 | 1.1126 |
| 0.0655 | 3.0078 | -0.3553 |
| -0.7844 | 2.9058 | 1.1496 |
| -1.1776 | 2.2474 | 2.9885 |
| -0.1202 | 1.3684 | 4.0815 |
| -0.2110 | -1.1207 | 4.2476 |
| -1.9670 | -1.2709 | 4.2372 |
| -1.0138 | -2.1017 | 3.0111 |
| 2.8734 | -1.8414 | -3.0197 |
| 3.1010 | 1.9574 | -1.5050 |
| 4.1664 | 1.3102 | -0.1535 |
| -0.7226 | -0.5015 | -4.7322 |
| -0.5493 | -2.2358 | -4.6273 |
| -1.1421 | -1.3224 | -3.2170 |
| -4.7227 | 0.8821 | 0.9343 |
| -1.8758 | 0.7476 | 5.2460 |
| 0.4581 | -4.9256 | -3.2714 |

**Supplementary S2.** The Z-matrices of (5$S^*$,6$S^*$,9$S^*$,10$R^*$)-**4** optimized at B3LYP/6-31G(d)-GD3BJ level by Gaussian.

| (5$S^*$,6$S^*$,9$S^*$,10$R^*$)-**4A** | | | |
|---|---|---|---|
| O | 3.4050 | -1.4303 | -1.3344 |
| C | 2.3377 | -1.6695 | -1.9170 |
| C | 1.0138 | -1.4380 | -1.1761 |
| C | 0.6714 | 0.1006 | -1.0195 |
| C | 1.8483 | 0.8452 | -0.3031 |
| C | -0.1396 | -2.2874 | -1.7391 |
| C | -1.4138 | -2.0898 | -0.9164 |
| C | -1.7750 | -0.6297 | -0.8437 |
| C | -0.6851 | 0.2420 | -0.2027 |
| C | -1.3805 | 1.7527 | 2.5886 |
| C | -2.0877 | 1.8705 | 1.2523 |
| C | -1.1253 | 1.7137 | 0.0585 |
| C | 0.5141 | 0.7642 | -2.4114 |
| C | 2.3410 | -2.1241 | -3.3539 |
| C | -1.4884 | 0.6245 | 3.3179 |
| C | -2.9574 | -0.2132 | -1.3295 |
| C | -0.6150 | 2.9758 | 3.0275 |
| O | 0.2344 | -3.6650 | -1.6779 |
| C | 2.1876 | 0.3288 | 1.0787 |
| O | 1.5895 | 0.6640 | 2.0942 |
| O | 3.1936 | -0.5656 | 1.1061 |
| C | -0.8053 | 0.3777 | 4.5984 |
| O | -1.4047 | 0.0502 | 5.6085 |
| O | 0.5334 | 0.4809 | 4.5113 |
| H | 1.2047 | -1.8462 | -0.1715 |
| H | 2.7573 | 0.8390 | -0.9157 |
| H | 1.6467 | 1.9166 | -0.1991 |
| H | -0.3336 | -2.0479 | -2.7903 |

| (5$S^*$,6$S^*$,9$S^*$,10$R^*$)-**4B** | | |
|---|---|---|
| 3.3965 | -1.4316 | -1.3599 |
| 2.3268 | -1.6641 | -1.9407 |
| 1.0092 | -1.4359 | -1.1877 |
| 0.6574 | 0.1016 | -1.0434 |
| 1.8326 | 0.8562 | -0.3341 |
| -0.1391 | -2.3022 | -1.7317 |
| -1.4247 | -2.0977 | -0.9285 |
| -1.7853 | -0.6367 | -0.8648 |
| -0.6989 | 0.2406 | -0.2265 |
| -1.4017 | 1.7409 | 2.5616 |
| -2.1079 | 1.8669 | 1.2253 |
| -1.1444 | 1.7113 | 0.0321 |
| 0.4942 | 0.7552 | -2.4392 |
| 2.3202 | -2.1137 | -3.3791 |
| -1.5134 | 0.6093 | 3.2849 |
| -2.9661 | -0.2244 | -1.3578 |
| -0.6331 | 2.9599 | 3.0066 |
| 0.2315 | -3.6816 | -1.6671 |
| 2.1790 | 0.3414 | 1.0465 |
| 1.5736 | 0.6608 | 2.0626 |
| 3.1942 | -0.5431 | 1.0703 |
| -0.8287 | 0.3482 | 4.5619 |
| -1.4257 | -0.0009 | 5.5661 |
| 0.5096 | 0.4578 | 4.4761 |
| 1.2113 | -1.8326 | -0.1810 |
| 2.7392 | 0.8515 | -0.9505 |
| 1.6260 | 1.9266 | -0.2312 |
| -0.3328 | -2.0769 | -2.7859 |

| (5$S^*$,6$S^*$,9$S^*$,10$R^*$)-**4C** | | |
|---|---|---|
| 1.8292 | 0.3811 | 3.5188 |
| 1.8292 | 1.2674 | 2.6526 |
| 1.3972 | 0.9141 | 1.2235 |
| -0.1667 | 0.6842 | 1.1060 |
| -0.6446 | -0.4032 | 2.1239 |
| 1.9775 | 1.8825 | 0.1732 |
| 1.5669 | 1.4798 | -1.2457 |
| 0.0701 | 1.3469 | -1.3338 |
| -0.4949 | 0.2747 | -0.3959 |
| -1.4907 | -2.0840 | -2.2290 |
| -2.2557 | -0.7944 | -2.0146 |
| -1.9809 | -0.1005 | -0.6617 |
| -0.9313 | 1.9817 | 1.4809 |
| 2.1893 | 2.6850 | 3.0159 |
| -1.7373 | -3.1547 | -1.4507 |
| -0.6321 | 2.1558 | -2.1453 |
| -0.4689 | -2.0530 | -3.3346 |
| 3.4032 | 1.8527 | 0.2646 |
| -0.0113 | -1.7687 | 1.9736 |
| -0.4350 | -2.6337 | 1.2161 |
| 1.0784 | -1.9674 | 2.7379 |
| -1.0070 | -4.4292 | -1.5505 |
| -0.9970 | -5.1408 | -2.5389 |
| -0.3652 | -4.7079 | -0.4000 |
| 1.8944 | -0.0494 | 1.0316 |
| -0.5086 | -0.0696 | 3.1595 |
| -1.7297 | -0.5483 | 2.0669 |
| 1.6607 | 2.9129 | 0.3687 |

| (5$S^*$,6$S^*$,9$S^*$,10$R^*$)-**4D** | | |
|---|---|---|
| -0.4553 | -3.7733 | -1.0983 |
| -1.3909 | -2.9634 | -1.1666 |
| -1.2906 | -1.6416 | -0.3952 |
| -0.2744 | -0.6268 | -1.0637 |
| 1.1305 | -1.2943 | -1.2338 |
| -2.6686 | -1.0344 | -0.0717 |
| -2.5255 | 0.2389 | 0.7657 |
| -1.6101 | 1.2197 | 0.0818 |
| -0.1959 | 0.6732 | -0.1522 |
| 2.1085 | 2.1991 | 1.5361 |
| 1.2337 | 2.7731 | 0.4394 |
| 0.8298 | 1.7388 | -0.6318 |
| -0.7480 | -0.2441 | -2.4893 |
| -2.5829 | -3.2491 | -2.0433 |
| 3.4159 | 1.9687 | 1.3009 |
| -2.0744 | 2.4283 | -0.2793 |
| 1.4397 | 1.9777 | 2.8682 |
| -3.4255 | -1.9893 | 0.6744 |
| 1.7857 | -1.7477 | 0.0523 |
| 2.4408 | -1.0069 | 0.7758 |
| 1.5704 | -3.0405 | 0.3606 |
| 4.3349 | 1.3831 | 2.2886 |
| 5.2530 | 2.0054 | 2.7933 |
| 4.0694 | 0.0850 | 2.5232 |
| -0.8750 | -1.9424 | 0.5791 |
| 1.0921 | -2.1413 | -1.9285 |
| 1.8375 | -0.6198 | -1.7298 |
| -3.2302 | -0.8161 | -0.9866 |

| (5$S^*$,6$S^*$,9$S^*$,10$R^*$)-**4E** | | |
|---|---|---|
| 1.8242 | 0.4097 | 3.5210 |
| 1.8197 | 1.2926 | 2.6516 |
| 1.3933 | 0.9248 | 1.2242 |
| -0.1722 | 0.7099 | 1.1013 |
| -0.6617 | -0.3700 | 2.1220 |
| 1.9926 | 1.8744 | 0.1692 |
| 1.5722 | 1.4931 | -1.2529 |
| 0.0743 | 1.3681 | -1.3375 |
| -0.4972 | 0.2992 | -0.4006 |
| -1.4829 | -2.0481 | -2.2455 |
| -2.2554 | -0.7635 | -2.0263 |
| -1.9833 | -0.0726 | -0.6712 |
| -0.9276 | 2.0147 | 1.4688 |
| 2.1749 | 2.7138 | 3.0050 |
| -1.7165 | -3.1200 | -1.4647 |
| -0.6238 | 2.1829 | -2.1465 |
| -0.4685 | -2.0092 | -3.3575 |
| 3.4194 | 1.8407 | 0.2560 |
| -0.0288 | -1.7366 | 1.9819 |
| -0.4385 | -2.6003 | 1.2156 |
| 1.0522 | -1.9343 | 2.7592 |
| -0.9753 | -4.3884 | -1.5638 |
| -0.9440 | -5.0929 | -2.5569 |
| -0.3450 | -4.6687 | -0.4071 |
| 1.8812 | -0.0457 | 1.0457 |
| -0.5294 | -0.0309 | 3.1565 |
| -1.7468 | -0.5125 | 2.0590 |
| 1.6908 | 2.9093 | 0.3631 |

| | | | |
|---|---|---|---|
| H | -1.2770 | -2.4870 | 0.0982 |
| H | -2.2216 | -2.6913 | -1.3526 |
| H | -0.4975 | -0.2117 | 0.7786 |
| H | -2.9066 | 1.1454 | 1.1855 |
| H | -2.5656 | 2.8569 | 1.1964 |
| H | -1.5990 | 2.1328 | -0.8371 |
| H | -0.2638 | 2.3583 | 0.2420 |
| H | 1.4450 | 0.7124 | -2.9859 |
| H | -0.2697 | 0.2936 | -3.0120 |
| H | 0.2649 | 1.8269 | -2.3199 |
| H | 2.0751 | -3.1806 | -3.4183 |
| H | 1.6539 | -1.5195 | -3.9491 |
| H | 3.3456 | -1.9956 | -3.7683 |
| H | -2.1227 | -0.1974 | 3.0034 |
| H | -3.6681 | -0.9111 | -1.7657 |
| H | -3.2775 | 0.8225 | -1.3149 |
| H | -1.2501 | 3.8647 | 2.9488 |
| H | -0.2815 | 2.9219 | 4.0675 |
| H | 0.2669 | 3.1273 | 2.3983 |
| H | -0.5344 | -4.2020 | -1.9430 |
| H | 3.5440 | -0.8279 | 0.2165 |
| H | 0.8727 | 0.6219 | 3.5911 |

| | | |
|---|---|---|
| -1.3040 | -2.4859 | 0.0916 |
| -2.2248 | -2.7035 | -1.3725 |
| -0.5091 | -0.2104 | 0.7556 |
| -2.9290 | 1.1446 | 1.1545 |
| -2.5825 | 2.8550 | 1.1729 |
| -1.6188 | 2.1280 | -0.8641 |
| -0.2851 | 2.3587 | 0.2159 |
| 1.4267 | 0.7126 | -3.0118 |
| -0.2823 | 0.2709 | -3.0384 |
| 0.2315 | 1.8152 | -2.3542 |
| 2.0547 | -3.1703 | -3.4442 |
| 1.6279 | -1.5088 | -3.9677 |
| 3.3216 | -1.9827 | -3.8003 |
| -2.1530 | -0.2071 | 2.9662 |
| -3.6727 | -0.9270 | -1.7941 |
| -3.2879 | 0.8108 | -1.3527 |
| -1.2660 | 3.8508 | 2.9321 |
| -0.3004 | 2.8999 | 4.0464 |
| 0.2493 | 3.1123 | 2.3784 |
| 0.2008 | -3.9762 | -0.7384 |
| 3.5545 | -0.7914 | 0.1806 |
| 0.8490 | 0.6177 | 3.5593 |

| | | |
|---|---|---|
| 2.0422 | 0.5309 | -1.5267 |
| 1.9562 | 2.2180 | -1.9584 |
| 0.0884 | -0.6346 | -0.5958 |
| -2.0626 | -0.1081 | -2.8455 |
| -3.3301 | -1.0151 | -2.0755 |
| -2.6180 | 0.7892 | -0.5931 |
| -2.3433 | -0.7770 | 0.1169 |
| -0.7550 | 2.2596 | 2.5257 |
| -0.6391 | 2.8364 | 0.8643 |
| -2.0132 | 1.8512 | 1.3722 |
| 2.2498 | 2.7719 | 4.1051 |
| 3.1615 | 2.9494 | 2.5964 |
| 1.4202 | 3.3768 | 2.6670 |
| -2.4752 | -3.1223 | -0.6569 |
| -0.1409 | 2.8968 | -2.7710 |
| -1.7137 | 2.1261 | -2.2191 |
| 0.1247 | -2.9679 | -3.4041 |
| -0.9656 | -1.9034 | -4.2988 |
| 0.2337 | -1.2283 | -3.1776 |
| 3.7669 | 2.3849 | -0.4662 |
| 1.3655 | -1.1821 | 3.2711 |
| -0.3917 | -3.9664 | 0.2570 |

| | | |
|---|---|---|
| -2.1304 | -0.0028 | 1.7613 |
| -3.5206 | 0.6645 | 0.9480 |
| 0.1510 | 0.3286 | 0.8288 |
| 0.3551 | 3.2599 | 0.8752 |
| 1.7892 | 3.5785 | -0.0606 |
| 0.4385 | 2.2733 | -1.5057 |
| 1.7502 | 1.2634 | -0.9795 |
| -0.7737 | -1.1184 | -3.1484 |
| -1.7477 | 0.1993 | -2.4946 |
| -0.0664 | 0.4761 | -2.9545 |
| -3.4540 | -3.4909 | -1.4319 |
| -2.7952 | -2.3967 | -2.6915 |
| -2.3605 | -4.1093 | -2.6821 |
| 3.8834 | 2.2140 | 0.3544 |
| -3.0992 | 2.7270 | -0.0723 |
| -1.4694 | 3.1693 | -0.7900 |
| 2.1364 | 1.6666 | 3.6517 |
| 0.9717 | 2.9072 | 3.2098 |
| 0.6641 | 1.2112 | 2.7943 |
| -4.2578 | -1.5667 | 0.9542 |
| 0.9669 | -3.5235 | -0.2603 |
| 3.3739 | -0.2906 | 1.9250 |

| | | |
|---|---|---|
| 2.0358 | 0.5431 | -1.5495 |
| 1.9668 | 2.2371 | -1.9564 |
| 0.0840 | -0.6121 | -0.5972 |
| -2.0662 | -0.0728 | -2.8545 |
| -3.3286 | -0.9899 | -2.0878 |
| -2.6194 | 0.8178 | -0.6024 |
| -2.3485 | -0.7504 | 0.1051 |
| -0.7603 | 2.2903 | 2.5157 |
| -0.6198 | 2.8667 | 0.8562 |
| -2.0095 | 1.8951 | 1.3485 |
| 2.2318 | 2.8092 | 4.0937 |
| 3.1478 | 2.9768 | 2.5859 |
| 1.4058 | 3.4016 | 2.6482 |
| -2.4513 | -3.0917 | -0.6676 |
| -0.1272 | 2.9229 | -2.7696 |
| -1.7056 | 2.1619 | -2.2189 |
| 0.1337 | -2.9181 | -3.4294 |
| -0.9726 | -1.8658 | -4.3188 |
| 0.2272 | -1.1776 | -3.2062 |
| 3.7406 | 1.0023 | -0.1236 |
| 1.3275 | -1.1519 | 3.3030 |
| -0.3898 | -3.9339 | 0.2559 |

**Supplementary S3.** The Z-matrices of (2*S**,5*S**,9*S**,10*R**)-**5** optimized at B3LYP/6-31G(d)-GD3BJ level by Gaussian.

| (2*S**,5*S**,9*S**,10*R**)-**5A** | | | | (2*S**,5*S**,9*S**,10*R**)-**5B** | | | (2*S**,5*S**,9*S**,10*R**)-**5C** | | | (2*S**,5*S**,9*S**,10*R**)-**5D** | | | (2*S**,5*S**,9*S**,10*R**)-**5E** | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -2.4516 | 0.2773 | 0.6814 | -2.3235 | 0.2063 | 1.2149 | -2.2949 | -0.7981 | -0.1321 | -2.5136 | 1.5740 | 0.9578 | -2.6446 | -0.0297 | 1.1256 |
| C | -2.7153 | 1.0713 | -0.5925 | -2.6128 | 1.5410 | 0.5382 | -2.1677 | -1.1155 | -1.6141 | -2.0365 | 3.0185 | 0.8689 | -2.9181 | 1.3475 | 0.5342 |
| C | -2.2029 | 0.3701 | -1.8806 | -2.4039 | 1.5184 | -0.9967 | -0.9012 | -1.9419 | -1.9514 | -1.2031 | 3.3187 | -0.4011 | -2.5837 | 1.4487 | -0.9742 |
| C | -0.6957 | -0.0208 | -1.6841 | -0.9762 | 0.9463 | -1.3061 | 0.3534 | -1.1995 | -1.3692 | -0.0525 | 2.2575 | -0.5197 | -1.1191 | 0.9348 | -1.2083 |
| C | -0.3203 | -0.7735 | -0.3642 | -0.5561 | -0.3812 | -0.5851 | 0.3102 | -0.7378 | 0.1310 | -0.4350 | 0.7457 | -0.3427 | -0.7093 | -0.4290 | -0.5475 |
| C | -0.9784 | -0.0502 | 0.8262 | -0.9059 | -0.2678 | 0.9204 | -1.0588 | -0.0903 | 0.3919 | -1.3379 | 0.6021 | 0.9128 | -1.1856 | -0.4315 | 0.9307 |
| C | -0.0124 | -0.7265 | -2.8580 | -0.6031 | 0.8438 | -2.7862 | 1.7017 | -1.8615 | -1.6359 | 0.8561 | 2.4017 | -1.7410 | -0.6395 | 0.9479 | -2.6596 |
| C | 1.4037 | -1.1364 | -2.6647 | 0.7389 | 0.2967 | -3.1020 | 2.8963 | -1.1299 | -1.1593 | 1.9380 | 1.4010 | -1.8947 | 0.7305 | 0.4467 | -2.9184 |
| C | 2.0057 | -1.0827 | -1.4620 | 1.5070 | -0.2900 | -2.1666 | 2.7964 | -0.0968 | -0.3043 | 2.0021 | 0.2944 | -1.1333 | 1.4504 | -0.1886 | -1.9766 |
| C | 1.2597 | -0.6654 | -0.1892 | 1.0265 | -0.5219 | -0.7256 | 1.4618 | 0.3595 | 0.3365 | 0.9190 | -0.0702 | -0.1042 | 0.8888 | -0.5201 | -0.5831 |
| C | 2.1503 | 0.7946 | 2.5094 | 2.5993 | -1.0314 | 2.0913 | -0.2052 | 2.6384 | 2.0099 | 1.2583 | -3.7755 | 1.1807 | 2.7665 | -0.9092 | 1.9706 |
| C | 2.7287 | -0.5027 | 1.9602 | 2.8487 | -1.6666 | 0.7320 | 0.6071 | 1.5211 | 2.6451 | 1.5565 | -2.2917 | 1.0577 | 2.7521 | -1.8164 | 0.7525 |
| C | 1.7666 | -1.3610 | 1.1142 | 1.5670 | -1.8468 | -0.1015 | 1.7181 | 0.8650 | 1.7980 | 0.6691 | -1.6059 | 0.0052 | 1.4133 | -1.8747 | -0.0095 |
| C | -0.7638 | -2.2586 | -0.3711 | -1.2572 | -1.6279 | -1.1836 | 0.5120 | -1.9029 | 1.1275 | -1.1818 | 0.1724 | -1.5751 | -1.3194 | -1.6541 | -1.2767 |
| C | -3.1404 | -0.8019 | -2.2299 | -3.5760 | 0.7634 | -1.6551 | -1.0951 | -3.3910 | -1.4636 | -2.1502 | 3.4071 | -1.6152 | -3.6776 | 0.7213 | -1.7823 |
| C | -2.3272 | 1.4085 | -3.0263 | -2.4890 | 2.9922 | -1.4753 | -0.8075 | -1.9912 | -3.4994 | -0.5908 | 4.7309 | -0.2018 | -2.6734 | 2.9533 | -1.3446 |
| C | 1.0786 | 0.8010 | 3.3306 | 2.9757 | 0.2426 | 2.3222 | -1.5536 | 2.5845 | 2.0544 | 0.6996 | -4.2576 | 2.3096 | 3.4549 | 0.2500 | 1.9300 |
| C | 3.4853 | -1.3534 | -1.3774 | 2.9215 | -0.6615 | -2.5329 | 4.0472 | 0.6943 | -0.0064 | 3.2217 | -0.5813 | -1.2607 | 2.8829 | -0.5256 | -2.2948 |
| C | 2.8871 | 2.0388 | 2.0798 | 2.0159 | -1.9517 | 3.1340 | 0.5811 | 3.7611 | 1.3858 | 1.7117 | -4.6218 | 0.0187 | 1.9742 | -1.3986 | 3.1557 |
| O | -0.5294 | -0.9209 | -3.9531 | -1.3013 | 1.2369 | -3.7147 | 1.8645 | -2.9064 | -2.2558 | 0.7948 | 3.3142 | -2.5583 | -1.2771 | 1.3954 | -3.6072 |
| O | -2.7768 | 1.0631 | 1.8343 | -2.4221 | 0.3656 | 2.6300 | -3.3875 | 0.1115 | 0.0819 | -3.1876 | 1.3802 | 2.1998 | -2.9022 | 0.0005 | 2.5284 |
| C | 0.5073 | 2.0186 | 3.9389 | 2.8197 | 0.9939 | 3.5815 | -2.4806 | 3.5218 | 1.3948 | 0.3645 | -5.6682 | 2.5797 | 3.5850 | 1.2329 | 3.0211 |
| O | 1.1590 | 2.8295 | 4.5740 | 3.7231 | 1.6546 | 4.0639 | -2.4413 | 4.7334 | 1.5031 | 0.6762 | -6.2358 | 3.6113 | 3.3883 | 2.4241 | 2.8599 |
| O | -0.8202 | 2.1204 | 3.7381 | 1.5719 | 0.9470 | 4.0827 | -3.3932 | 2.8548 | 0.6566 | -0.3864 | -6.2219 | 1.6086 | 4.0317 | 0.6870 | 4.1674 |
| H | -3.0616 | -0.6300 | 0.7198 | -3.0533 | -0.5545 | 0.9228 | -2.5013 | -1.6994 | 0.4531 | -3.2321 | 1.3442 | 0.1657 | -3.3111 | -0.7836 | 0.6969 |
| H | -3.7901 | 1.2841 | -0.6697 | -3.6357 | 1.8576 | 0.7836 | -3.0733 | -1.6365 | -1.9525 | -2.9026 | 3.6915 | 0.9297 | -3.9668 | 1.6196 | 0.7157 |
| H | -2.2400 | 2.0578 | -0.4925 | -1.9665 | 2.3070 | 0.9908 | -2.1593 | -0.1705 | -2.1762 | -1.4432 | 3.2440 | 1.7669 | -2.3344 | 2.0899 | 1.0975 |
| H | -0.1755 | 0.9515 | -1.6345 | -0.2908 | 1.7217 | -0.9219 | 0.4014 | -0.2691 | -1.9620 | 0.6155 | 2.4925 | 0.3271 | -0.4881 | 1.6984 | -0.7215 |

| | | | |
|---|---|---|---|
| H | -0.4510 | 0.8975 | 0.9965 |
| H | -0.8653 | -0.6273 | 1.7500 |
| H | 1.9223 | -1.4315 | -3.5710 |
| H | 1.4862 | 0.4060 | -0.0932 |
| H | 3.6288 | -0.2882 | 1.3730 |
| H | 3.0759 | -1.1041 | 2.8110 |
| H | 2.2616 | -2.3091 | 0.8738 |
| H | 0.9409 | -1.6513 | 1.7686 |
| H | -1.8465 | -2.3697 | -0.3193 |
| H | -0.4209 | -2.7975 | -1.2588 |
| H | -0.3778 | -2.8038 | 0.4956 |
| H | -4.1324 | -0.4282 | -2.5130 |
| H | -2.7735 | -1.3925 | -3.0731 |
| H | -3.3079 | -1.4807 | -1.3943 |
| H | -2.0934 | 0.9766 | -4.0035 |
| H | -3.3477 | 1.8053 | -3.0877 |
| H | -1.6562 | 2.2603 | -2.8674 |
| H | 0.5861 | -0.1189 | 3.6240 |
| H | 3.6930 | -2.2508 | -0.7885 |
| H | 3.9310 | -1.5095 | -2.3663 |
| H | 4.0016 | -0.5006 | -0.9265 |
| H | 3.8876 | 2.0536 | 2.5239 |
| H | 2.9939 | 2.0561 | 0.9898 |
| H | 2.3782 | 2.9649 | 2.3577 |
| H | -3.7063 | 1.3449 | 1.7367 |
| H | -1.2389 | 1.4958 | 3.1048 |

| | | |
|---|---|---|
| -0.2077 | 0.4272 | 1.4071 |
| -0.7583 | -1.2240 | 1.4350 |
| 1.0688 | 0.4553 | -4.1236 |
| 1.4615 | 0.3126 | -0.1579 |
| 3.5904 | -1.0897 | 0.1701 |
| 3.3078 | -2.6510 | 0.8899 |
| 1.7580 | -2.5827 | -0.8920 |
| 0.8243 | -2.3233 | 0.5438 |
| -2.3353 | -1.6153 | -1.0321 |
| -1.0790 | -1.7342 | -2.2575 |
| -0.9139 | -2.5544 | -0.7133 |
| -4.5099 | 1.3270 | -1.5354 |
| -3.4323 | 0.6186 | -2.7284 |
| -3.7636 | -0.2127 | -1.2086 |
| -2.4631 | 3.0756 | -2.5655 |
| -3.4223 | 3.4608 | -1.1405 |
| -1.6632 | 3.5905 | -1.0741 |
| 3.4972 | 0.8158 | 1.5604 |
| 3.6299 | -0.1349 | -1.8865 |
| 3.0884 | -1.7385 | -2.4478 |
| 3.1657 | -0.3833 | -3.5645 |
| 0.9540 | -2.1280 | 2.9418 |
| 2.5333 | -2.9170 | 3.1207 |
| 2.1182 | -1.5614 | 4.1504 |
| -3.3251 | 0.6721 | 2.8281 |
| 0.9342 | 0.4610 | 3.5257 |

| | | |
|---|---|---|
| -1.0582 | 0.9173 | -0.0414 |
| -1.2154 | 0.0128 | 1.4651 |
| 3.8380 | -1.4559 | -1.5882 |
| 1.1677 | 1.2421 | -0.2489 |
| 1.0889 | 1.9462 | 3.5373 |
| -0.0443 | 0.7344 | 3.0416 |
| 2.5118 | 1.6223 | 1.7598 |
| 2.1454 | 0.0430 | 2.3879 |
| 0.4952 | -1.5471 | 2.1630 |
| -0.2792 | -2.6487 | 1.0646 |
| 1.4649 | -2.4198 | 0.9824 |
| -0.1989 | -4.0016 | -1.5972 |
| -1.3894 | -3.4557 | -0.4164 |
| -1.8978 | -3.8810 | -2.0290 |
| -0.0013 | -2.6447 | -3.8448 |
| -1.7379 | -2.3722 | -3.9373 |
| -0.6342 | -0.9944 | -3.9206 |
| -2.0598 | 1.7680 | 2.5596 |
| 4.8819 | 0.4078 | -0.6561 |
| 3.8693 | 1.7625 | -0.1686 |
| 4.3730 | 0.5345 | 1.0260 |
| 1.1923 | 3.3969 | 0.5556 |
| -0.0443 | 4.5637 | 0.9895 |
| 1.2474 | 4.2069 | 2.1320 |
| -4.1841 | -0.3233 | -0.2814 |
| -3.2617 | 1.8789 | 0.5778 |

| | | |
|---|---|---|
| -0.7337 | 0.7466 | 1.8198 |
| -1.7396 | -0.4140 | 1.0022 |
| 2.6941 | 1.6565 | -2.6301 |
| 1.3200 | 0.2634 | 0.8648 |
| 1.4003 | -1.7949 | 2.0242 |
| 2.6187 | -2.1707 | 0.8292 |
| 0.7969 | -2.0782 | -0.9765 |
| -0.3651 | -1.8142 | 0.2948 |
| -2.1443 | 0.6514 | -1.7448 |
| -0.6028 | 0.2682 | -2.4983 |
| -1.4087 | -0.8914 | -1.4513 |
| -2.8122 | 4.2773 | -1.5212 |
| -1.6138 | 3.5229 | -2.5598 |
| -2.8100 | 2.5454 | -1.7101 |
| -0.0699 | 5.0866 | -1.0953 |
| -1.3694 | 5.4678 | 0.0291 |
| 0.1238 | 4.7425 | 0.6290 |
| 0.4955 | -3.6093 | 3.1573 |
| 3.7557 | -0.6256 | -0.3068 |
| 2.9552 | -1.5936 | -1.5766 |
| 3.9308 | -0.1960 | -2.0025 |
| 1.0341 | -4.4976 | -0.8314 |
| 2.7187 | -4.3271 | -0.2957 |
| 1.7618 | -5.6865 | 0.2634 |
| -3.9390 | 1.9981 | 2.2267 |
| -0.6267 | -5.5882 | 0.9075 |

| | | |
|---|---|---|
| -0.5564 | 0.2481 | 1.5226 |
| -1.0495 | -1.4168 | 1.3910 |
| 1.1191 | 0.6736 | -3.9058 |
| 1.2549 | 0.2845 | 0.0680 |
| 3.5635 | -1.5445 | 0.0714 |
| 3.0012 | -2.8329 | 1.0862 |
| 1.5102 | -2.6055 | -0.8231 |
| 0.6857 | -2.3170 | 0.6755 |
| -2.4066 | -1.6749 | -1.2278 |
| -1.0399 | -1.6960 | -2.3334 |
| -0.9929 | -2.5958 | -0.8236 |
| -4.6393 | 1.2393 | -1.6763 |
| -3.4578 | 0.6867 | -2.8519 |
| -3.8547 | -0.2995 | -1.4458 |
| -2.5592 | 3.1230 | -2.4190 |
| -3.6452 | 3.3717 | -1.0561 |
| -1.9025 | 3.5377 | -0.8297 |
| 3.9367 | 0.5815 | 1.0143 |
| 3.5540 | -0.0299 | -1.5871 |
| 3.0517 | -1.6056 | -2.2658 |
| 3.1748 | -0.1877 | -3.2958 |
| 0.9584 | -1.6737 | 2.8594 |
| 2.4557 | -2.2810 | 3.5890 |
| 1.8712 | -0.6460 | 3.9417 |
| -3.8226 | 0.2905 | 2.6528 |
| 4.2207 | -0.2663 | 4.0874 |

| (2*S**,5*S**,9*S**,10*R**)-**5F** | | | |
|---|---|---|---|
| C | -3.1903 | 0.2455 | -0.0763 |
| C | -3.4145 | 0.8187 | -1.4703 |
| C | -2.5205 | 0.1741 | -2.5578 |
| C | -1.0252 | 0.2171 | -2.0818 |
| C | -0.7127 | -0.2662 | -0.6217 |
| C | -1.7322 | 0.3886 | 0.3503 |
| C | -0.0086 | -0.4022 | -3.0418 |
| C | 1.4084 | -0.4092 | -2.6081 |
| C | 1.7756 | -0.0821 | -1.3564 |
| C | 0.7569 | 0.2408 | -0.2505 |
| C | 2.4923 | 0.3221 | 3.2816 |
| C | 1.9885 | 0.8294 | 1.9425 |
| C | 1.2096 | -0.2425 | 1.1614 |
| C | -0.7875 | -1.8085 | -0.4764 |
| C | -3.0673 | -1.2284 | -2.8935 |
| C | -2.6871 | 1.0418 | -3.8340 |
| C | 3.7800 | -0.0583 | 3.4070 |
| C | 3.2489 | 0.0251 | -1.0574 |
| C | 1.4622 | 0.2669 | 4.3803 |
| O | -0.2702 | -0.8274 | -4.1623 |
| O | -3.9884 | 0.9698 | 0.8585 |
| C | 4.4307 | -0.5558 | 4.6329 |
| O | 5.1067 | -1.5687 | 4.6559 |
| O | 4.2736 | 0.2731 | 5.6821 |
| H | -3.5054 | -0.8006 | -0.0221 |
| H | -4.4759 | 0.7216 | -1.7363 |
| H | -3.2335 | 1.9027 | -1.4328 |
| H | -0.7711 | 1.2912 | -2.0966 |
| H | -1.5053 | 1.4590 | 0.4563 |

| (2*S**,5*S**,9*S**,10*R**)-**5G** | | |
|---|---|---|
| -2.8065 | 0.8214 | 1.1983 |
| -3.4550 | 1.5264 | 0.0131 |
| -3.2200 | 0.8111 | -1.3397 |
| -1.6831 | 0.5452 | -1.5165 |
| -0.9119 | -0.0942 | -0.3086 |
| -1.3031 | 0.6623 | 0.9904 |
| -1.2813 | -0.1761 | -2.8035 |
| 0.1599 | -0.4665 | -2.9890 |
| 1.0552 | -0.3052 | -1.9986 |
| 0.6516 | 0.1060 | -0.5727 |
| 3.6047 | -0.4090 | 1.9772 |
| 2.7589 | 0.2680 | 0.9144 |
| 1.5269 | -0.5675 | 0.5281 |
| -1.2253 | -1.6031 | -0.1349 |
| -4.1206 | -0.4389 | -1.4116 |
| -3.7107 | 1.7860 | -2.4435 |
| 3.4723 | -0.0466 | 3.2694 |
| 2.5150 | -0.4795 | -2.3294 |
| 4.5310 | -1.4842 | 1.4708 |
| -2.0491 | -0.4676 | -3.7146 |
| -3.0005 | 1.6115 | 2.3700 |
| 4.2294 | -0.5980 | 4.4081 |
| 3.6952 | -1.0009 | 5.4255 |
| 5.5624 | -0.5237 | 4.2312 |
| -3.2727 | -0.1501 | 1.3862 |
| -4.5302 | 1.6447 | 0.2051 |
| -3.0649 | 2.5534 | -0.0353 |
| -1.2503 | 1.5530 | -1.6410 |
| -0.8461 | 1.6621 | 0.9864 |

| (2*S**,5*S**,9*S**,10*R**)-**5H** | | |
|---|---|---|
| -2.5147 | 0.0913 | 1.1944 |
| -2.8178 | 1.4375 | 0.5470 |
| -2.5628 | 1.4611 | -0.9805 |
| -1.1154 | 0.9240 | -1.2647 |
| -0.6818 | -0.4109 | -0.5618 |
| -1.0721 | -0.3366 | 0.9400 |
| -0.7079 | 0.8651 | -2.7378 |
| 0.6478 | 0.3469 | -3.0386 |
| 1.4092 | -0.2481 | -2.1032 |
| 0.9084 | -0.5210 | -0.6754 |
| 2.6641 | -0.9520 | 2.0017 |
| 2.7776 | -1.7306 | 0.7020 |
| 1.4547 | -1.8567 | -0.0785 |
| -1.3425 | -1.6596 | -1.2015 |
| -3.7018 | 0.7046 | -1.6939 |
| -2.6625 | 2.9462 | -1.4205 |
| 3.1296 | 0.3117 | 2.0698 |
| 2.8317 | -0.5922 | -2.4608 |
| 2.0027 | -1.6858 | 3.1410 |
| -1.3884 | 1.2733 | -3.6730 |
| -2.7221 | 0.1867 | 2.6028 |
| 3.0695 | 1.1872 | 3.2527 |
| 2.5691 | 2.2973 | 3.2247 |
| 3.6877 | 0.6569 | 4.3238 |
| -3.2077 | -0.6742 | 0.8347 |
| -3.8549 | 1.7216 | 0.7718 |
| -2.2038 | 2.2071 | 1.0369 |
| -0.4555 | 1.7039 | -0.8466 |
| -0.4055 | 0.3655 | 1.4602 |

| (2*S**,5*S**,9*S**,10*R**)-**5I** | | |
|---|---|---|
| -2.4546 | -0.9033 | 0.9835 |
| -3.0910 | -0.6478 | -0.3765 |
| -2.3069 | -1.2839 | -1.5532 |
| -0.8011 | -0.8494 | -1.4616 |
| -0.0888 | -0.9790 | -0.0689 |
| -1.0194 | -0.3895 | 1.0244 |
| 0.1225 | -1.4088 | -2.5454 |
| 1.5555 | -1.0333 | -2.4674 |
| 2.0739 | -0.4074 | -1.3957 |
| 1.2494 | -0.1065 | -0.1354 |
| 1.7735 | 2.2901 | 1.8363 |
| 2.7395 | 1.1340 | 1.6353 |
| 2.0805 | -0.1879 | 1.1849 |
| 0.2573 | -2.4457 | 0.2935 |
| -2.5524 | -2.8062 | -1.5613 |
| -2.9342 | -0.7186 | -2.8553 |
| 0.7690 | 2.1887 | 2.7300 |
| 3.4980 | 0.0768 | -1.4721 |
| 1.9968 | 3.4683 | 0.9233 |
| -0.2439 | -2.0830 | -3.5024 |
| -3.2158 | -0.2432 | 1.9930 |
| -0.3000 | 3.1822 | 2.9215 |
| -1.4786 | 2.9133 | 2.7656 |
| 0.1686 | 4.3743 | 3.3311 |
| -2.4861 | -1.9688 | 1.2269 |
| -4.1291 | -1.0065 | -0.3638 |
| -3.1711 | 0.4386 | -0.5256 |
| -0.8251 | 0.2324 | -1.6799 |
| -1.0466 | 0.7034 | 0.9232 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H | -1.6381 | -0.0198 | 1.3633 | -0.8918 | 0.1695 | 1.8791 | -0.9151 | -1.2989 | 1.4403 | -0.6269 | -0.5782 | 2.0297 |
| H | 2.1226 | -0.6505 | -3.3888 | 0.4383 | -0.7690 | -3.9933 | 0.9924 | 0.5328 | -4.0506 | 2.1341 | -1.2567 | -3.3578 |
| H | 0.7100 | 1.3398 | -0.2159 | 0.8425 | 1.1886 | -0.5220 | 1.3150 | 0.3054 | -0.0783 | 0.9245 | 0.9345 | -0.2633 |
| H | 1.3458 | 1.7029 | 2.1126 | 2.4195 | 1.2471 | 1.2784 | 3.5542 | -1.2931 | 0.0675 | 3.5220 | 1.4222 | 0.9266 |
| H | 2.8318 | 1.1994 | 1.3520 | 3.3925 | 0.4809 | 0.0490 | 3.1397 | -2.7395 | 0.9400 | 3.2657 | 0.9568 | 2.5829 |
| H | 1.8023 | -1.1623 | 1.0795 | 1.8213 | -1.5753 | 0.2118 | 1.5902 | -2.5929 | -0.8811 | 2.8593 | -0.9556 | 1.0929 |
| H | 0.3455 | -0.5116 | 1.7734 | 0.9548 | -0.7111 | 1.4495 | 0.7284 | -2.3158 | 0.5964 | 1.4609 | -0.5271 | 2.0193 |
| H | -1.7891 | -2.1993 | -0.6462 | -2.2682 | -1.7907 | 0.1141 | -2.4255 | -1.6647 | -1.0932 | 0.8039 | -2.5094 | 1.2399 |
| H | -0.1141 | -2.3278 | -1.1644 | -0.9945 | -2.1850 | -1.0319 | -1.1212 | -1.7502 | -2.2689 | -0.6276 | -3.0647 | 0.4316 |
| H | -0.5208 | -2.1333 | 0.5344 | -0.6512 | -2.0438 | 0.6864 | -1.0030 | -2.5859 | -0.7275 | 0.8790 | -2.9304 | -0.4647 |
| H | -4.0507 | -1.1506 | -3.3742 | -5.1775 | -0.1469 | -1.4552 | -4.6508 | 1.2428 | -1.5760 | -1.9681 | -3.3211 | -2.3277 |
| H | -2.4232 | -1.7764 | -3.5851 | -3.9268 | -1.0466 | -2.2985 | -3.5309 | 0.6032 | -2.7681 | -2.3389 | -3.2820 | -0.6050 |
| H | -3.2192 | -1.8528 | -2.0137 | -4.0307 | -1.0846 | -0.5387 | -3.8771 | -0.2914 | -1.2888 | -3.6073 | -3.0224 | -1.7723 |
| H | -2.1827 | 0.6057 | -4.7008 | -3.6936 | 1.3297 | -3.4372 | -2.6066 | 3.0611 | -2.5067 | -2.5212 | -1.1888 | -3.7522 |
| H | -3.7455 | 1.1488 | -4.1008 | -4.7432 | 2.1043 | -2.2557 | -3.6141 | 3.3877 | -1.1006 | -4.0175 | -0.8880 | -2.8751 |
| H | -2.2860 | 2.0508 | -3.6858 | -3.0935 | 2.6908 | -2.4799 | -1.8605 | 3.5483 | -0.9786 | -2.7728 | 0.3620 | -2.9396 |
| H | 4.4428 | -0.0766 | 2.5463 | 2.7167 | 0.6722 | 3.5749 | 3.5279 | 0.8128 | 1.1921 | 0.6158 | 1.2839 | 3.3104 |
| H | 3.5492 | -0.6681 | -0.2672 | 2.9675 | -1.2778 | -1.7350 | 3.5252 | -0.0562 | -1.8058 | 4.1231 | -0.4034 | -0.7144 |
| H | 3.8654 | -0.2094 | -1.9328 | 2.6708 | -0.7430 | -3.3818 | 3.0150 | -1.6671 | -2.3818 | 3.9555 | -0.1392 | -2.4443 |
| H | 3.5005 | 1.0471 | -0.7591 | 3.0558 | 0.4553 | -2.1546 | 3.0801 | -0.3039 | -3.4887 | 3.5354 | 1.1622 | -1.3386 |
| H | 1.1755 | 1.2810 | 4.6764 | 3.9896 | -2.1923 | 0.8355 | 1.0398 | -2.1016 | 2.8311 | 2.0605 | 3.1359 | -0.1182 |
| H | 0.5639 | -0.2595 | 4.0434 | 5.3353 | -1.0372 | 0.8779 | 2.6407 | -2.5105 | 3.4744 | 1.1944 | 4.2088 | 0.9692 |
| H | 1.8138 | -0.2615 | 5.2703 | 4.9845 | -2.0716 | 2.2735 | 1.7991 | -1.0453 | 4.0031 | 2.9350 | 3.9689 | 1.1830 |
| H | -4.9189 | 0.8620 | 0.5948 | -3.9592 | 1.6808 | 2.5220 | -2.1715 | 0.9135 | 2.9436 | -3.0650 | 0.7188 | 1.9236 |
| H | 3.7817 | 1.0843 | 5.4558 | 5.8099 | -0.0843 | 3.3966 | 4.0938 | -0.2109 | 4.1394 | 1.1365 | 4.3799 | 3.4561 |

**Supplementary S4.** The Z-matrices of (4*S**,5*R**,9*S**,10*R**)-**6** optimized at B3LYP/6-31G(d)-GD3BJ level by Gaussian.

| (4*S**,5*R**,9*S**,10*R**)-**6A** | | | |
|---|---|---|---|
| C | -2.6213 | -0.8604 | 0.8885 |
| C | -2.0764 | -1.1379 | 2.2835 |
| C | -1.2086 | 0.0181 | 2.8526 |
| C | -0.0970 | 0.3649 | 1.7959 |
| C | -0.5730 | 0.6261 | 0.3247 |
| C | -1.5078 | -0.5429 | -0.1032 |
| C | 0.9053 | 1.4350 | 2.2252 |
| C | 1.8894 | 1.8982 | 1.2229 |
| C | 1.8423 | 1.5114 | -0.0635 |
| C | 0.7160 | 0.6278 | -0.6224 |
| C | 1.0248 | -1.2914 | -3.1814 |
| C | 1.1822 | 0.2192 | -3.1774 |
| C | 0.3537 | 0.9552 | -2.1065 |
| C | -1.3328 | 1.9686 | 0.1819 |
| C | -2.1526 | 1.1726 | 3.2920 |
| C | -0.5472 | -0.5498 | 4.1412 |
| C | 2.0218 | -2.0688 | -2.7117 |
| C | 2.9832 | 1.9147 | -0.9601 |
| C | -0.2841 | -1.8058 | -3.7237 |
| O | 0.9987 | 1.8733 | 3.3708 |
| O | -1.5317 | 2.4405 | 3.3956 |
| C | 2.0209 | -3.5413 | -2.6567 |
| O | 2.2704 | -4.1632 | -1.6398 |
| O | 1.8001 | -4.1068 | -3.8582 |
| H | -3.3542 | -0.0480 | 0.9095 |
| H | -3.1659 | -1.7459 | 0.5382 |
| H | -2.9147 | -1.3528 | 2.9589 |
| H | -1.4777 | -2.0582 | 2.2388 |

| (4*S**,5*R**,9*S**,10*R**)-**6B** | | |
|---|---|---|
| -2.1854 | -1.8806 | 1.3586 |
| -1.6769 | -1.9430 | 2.7932 |
| -1.0979 | -0.5961 | 3.3075 |
| -0.0239 | -0.0945 | 2.2741 |
| -0.4609 | -0.0378 | 0.7693 |
| -1.1047 | -1.4049 | 0.3939 |
| 0.7110 | 1.1881 | 2.6613 |
| 1.6299 | 1.7826 | 1.6661 |
| 1.7344 | 1.3108 | 0.4119 |
| 0.8481 | 0.1754 | -0.1221 |
| 1.1599 | -0.2251 | -4.0260 |
| 1.5308 | -0.3601 | -2.5597 |
| 0.5081 | 0.3244 | -1.6376 |
| -1.4752 | 1.1007 | 0.4942 |
| -2.2816 | 0.3627 | 3.6188 |
| -0.4074 | -0.9271 | 4.6618 |
| 0.7737 | -1.3122 | -4.7244 |
| 2.8124 | 1.8875 | -0.4694 |
| 1.3487 | 1.1506 | -4.6124 |
| 0.6522 | 1.7067 | 3.7751 |
| -1.9402 | 1.7361 | 3.6418 |
| 0.3946 | -1.3470 | -6.1493 |
| 0.8249 | -2.1814 | -6.9255 |
| -0.5334 | -0.4253 | -6.4685 |
| -3.0696 | -1.2400 | 1.2850 |
| -2.5150 | -2.8820 | 1.0558 |
| -2.4910 | -2.2818 | 3.4470 |
| -0.9011 | -2.7194 | 2.8460 |

| (4*S**,5*R**,9*S**,10*R**)-**6C** | | |
|---|---|---|
| -1.6473 | -2.7805 | 0.4776 |
| -1.2399 | -3.1121 | 1.9076 |
| -1.1209 | -1.8645 | 2.8260 |
| -0.1767 | -0.8223 | 2.1220 |
| -0.5097 | -0.4570 | 0.6339 |
| -0.6938 | -1.7799 | -0.1663 |
| 0.1181 | 0.4439 | 2.9253 |
| 0.8825 | 1.5205 | 2.2584 |
| 1.2058 | 1.4718 | 0.9546 |
| 0.7343 | 0.3413 | 0.0270 |
| 1.4557 | 1.2559 | -3.7314 |
| 1.7068 | 0.6992 | -2.3413 |
| 0.4704 | 0.8179 | -1.4348 |
| -1.7946 | 0.4005 | 0.5128 |
| -2.5531 | -1.3851 | 3.1946 |
| -0.4553 | -2.3722 | 4.1374 |
| 2.0874 | 2.3797 | -4.1275 |
| 2.1194 | 2.5430 | 0.4159 |
| 0.5547 | 0.4237 | -4.6077 |
| -0.1649 | 0.5874 | 4.1136 |
| -2.6356 | -0.0364 | 3.6158 |
| 1.9594 | 3.0374 | -5.4413 |
| 2.9220 | 3.4060 | -6.0903 |
| 0.6794 | 3.2610 | -5.7937 |
| -2.6744 | -2.4048 | 0.4410 |
| -1.6448 | -3.7039 | -0.1144 |
| -1.9591 | -3.8270 | 2.3279 |
| -0.2744 | -3.6357 | 1.8739 |

| (4*S**,5*R**,9*S**,10*R**)-**6D** | | |
|---|---|---|
| -2.5340 | -1.5096 | 1.2668 |
| -2.0245 | -1.8142 | 2.6695 |
| -1.1808 | -0.6657 | 3.2884 |
| -0.0461 | -0.2825 | 2.2692 |
| -0.4882 | 0.0094 | 0.7932 |
| -1.3963 | -1.1608 | 0.3134 |
| 0.9353 | 0.7853 | 2.7506 |
| 1.9327 | 1.2919 | 1.7828 |
| 1.9213 | 0.9386 | 0.4860 |
| 0.8229 | 0.0516 | -0.1198 |
| 0.9876 | -0.0421 | -4.0546 |
| 1.3555 | -0.3655 | -2.6175 |
| 0.4946 | 0.4068 | -1.6032 |
| -1.2612 | 1.3459 | 0.6633 |
| -2.1444 | 0.4705 | 3.7325 |
| -0.5476 | -1.2609 | 4.5790 |
| 0.2127 | -0.8961 | -4.7538 |
| 3.0713 | 1.3904 | -0.3765 |
| 1.5233 | 1.2661 | -4.5765 |
| 1.0045 | 1.1840 | 3.9122 |
| -1.5338 | 1.7383 | 3.8852 |
| -0.2200 | -0.7382 | -6.1544 |
| -1.3786 | -0.8704 | -6.5059 |
| 0.8076 | -0.5281 | -6.9985 |
| -3.2744 | -0.7041 | 1.2864 |
| -3.0609 | -2.3915 | 0.8821 |
| -2.8789 | -2.0505 | 3.3170 |
| -1.4178 | -2.7290 | 2.6202 |

| (4*S**,5*R**,9*S**,10*R**)-**6E** | | |
|---|---|---|
| -2.3396 | -1.7803 | 1.4335 |
| -1.8022 | -1.8606 | 2.8565 |
| -1.1442 | -0.5420 | 3.3489 |
| -0.0705 | -0.1002 | 2.2882 |
| -0.5386 | -0.0301 | 0.7932 |
| -1.2585 | -1.3652 | 0.4416 |
| 0.7369 | 1.1456 | 2.6508 |
| 1.6545 | 1.6947 | 1.6287 |
| 1.7070 | 1.2124 | 0.3751 |
| 0.7595 | 0.1122 | -0.1273 |
| 1.0575 | -0.2915 | -4.0323 |
| 1.3594 | -0.5137 | -2.5613 |
| 0.3985 | 0.2547 | -1.6384 |
| -1.5001 | 1.1567 | 0.5326 |
| -2.2700 | 0.4773 | 3.6809 |
| -0.4406 | -0.9012 | 4.6893 |
| 1.8036 | 0.5811 | -4.7399 |
| 2.7820 | 1.7431 | -0.5386 |
| -0.1060 | -1.0773 | -4.5796 |
| 0.7361 | 1.6659 | 3.7654 |
| -1.8570 | 1.8308 | 3.6976 |
| 1.6554 | 0.8991 | -6.1720 |
| 1.6054 | 2.0410 | -6.5925 |
| 1.6770 | -0.1956 | -6.9554 |
| -3.1918 | -1.0963 | 1.3757 |
| -2.7261 | -2.7654 | 1.1448 |
| -2.6173 | -2.1541 | 3.5307 |
| -1.0657 | -2.6749 | 2.8969 |

| | | | |
|---|---|---|---|
| H | 0.5233 | -0.5469 | 1.7438 |
| H | -1.9793 | -0.3357 | -1.0693 |
| H | -0.9088 | -1.4529 | -0.2424 |
| H | 2.6807 | 2.5259 | 1.6197 |
| H | 1.1190 | -0.3929 | -0.5923 |
| H | 2.2393 | 0.4862 | -3.0922 |
| H | 0.8796 | 0.5934 | -4.1647 |
| H | 0.4457 | 2.0356 | -2.2779 |
| H | -0.6956 | 0.7315 | -2.3137 |
| H | -0.7293 | 2.8235 | 0.5010 |
| H | -1.6321 | 2.1569 | -0.8540 |
| H | -2.2582 | 1.9897 | 0.7563 |
| H | -2.6037 | 0.9476 | 4.2661 |
| H | -2.9970 | 1.2921 | 2.6101 |
| H | 0.1881 | -1.3268 | 3.9038 |
| H | -0.0443 | 0.2203 | 4.7315 |
| H | -1.2984 | -1.0057 | 4.7978 |
| H | 2.9081 | -1.6321 | -2.2599 |
| H | 2.6354 | 2.5242 | -1.7985 |
| H | 3.7355 | 2.5100 | -0.4297 |
| H | 3.4963 | 1.0265 | -1.3405 |
| H | -0.3473 | -1.6083 | -4.7985 |
| H | -0.4207 | -2.8791 | -3.5672 |
| H | -1.1290 | -1.3134 | -3.2343 |
| H | -0.6776 | 2.3304 | 3.8650 |
| H | 1.7067 | -3.4526 | -4.5756 |

| | | |
|---|---|---|
| 0.7731 | -0.8573 | 2.3171 |
| -1.5478 | -1.3712 | -0.6070 |
| -0.3221 | -2.1745 | 0.3560 |
| 2.2503 | 2.5886 | 2.0447 |
| 1.4541 | -0.7367 | -0.0139 |
| 1.5952 | -1.4207 | -2.2833 |
| 2.5364 | 0.0445 | -2.4183 |
| 0.4004 | 1.3848 | -1.8965 |
| -0.4609 | -0.1281 | -1.8679 |
| -2.4154 | 0.9628 | 1.0268 |
| -1.0821 | 2.0831 | 0.7721 |
| -1.7492 | 1.1535 | -0.5643 |
| -2.7271 | 0.1183 | 4.5908 |
| -3.0955 | 0.2537 | 2.8990 |
| 0.4847 | -1.5462 | 4.5147 |
| -0.1086 | -0.0316 | 5.2125 |
| -1.0842 | -1.4865 | 5.3193 |
| 0.7647 | -2.2979 | -4.2674 |
| 3.3835 | 2.6738 | 0.0378 |
| 3.5283 | 1.1089 | -0.7489 |
| 2.3928 | 2.3385 | -1.3727 |
| 0.5441 | 1.8176 | -4.2884 |
| 2.3034 | 1.5758 | -4.2842 |
| 1.3708 | 1.1462 | -5.7057 |
| -1.1150 | 1.8424 | 4.1612 |
| -0.8384 | 0.0908 | -5.6995 |

| | | |
|---|---|---|
| 0.8056 | -1.3249 | 2.0856 |
| -1.0591 | -1.5813 | -1.1794 |
| 0.2822 | -2.2697 | -0.2839 |
| 1.2087 | 2.3203 | 2.9155 |
| 1.5748 | -0.3682 | -0.0113 |
| 1.9990 | -0.3553 | -2.4275 |
| 2.5647 | 1.2041 | -1.8888 |
| 0.0901 | 1.8472 | -1.4394 |
| -0.3159 | 0.2189 | -1.9012 |
| -1.7298 | 1.3290 | 1.0877 |
| -1.9998 | 0.6809 | -0.5252 |
| -2.6855 | -0.1293 | 0.8478 |
| -2.9704 | -2.0061 | 3.9966 |
| -3.2483 | -1.4961 | 2.3599 |
| 0.5878 | -2.6631 | 3.9696 |
| -0.4723 | -1.6253 | 4.9352 |
| -0.9786 | -3.2549 | 4.5251 |
| 2.8105 | 2.8730 | -3.4839 |
| 1.6507 | 3.0972 | -0.4016 |
| 2.3868 | 3.2803 | 1.1816 |
| 3.0560 | 2.0998 | 0.0652 |
| -0.4903 | 0.5479 | -4.3079 |
| 0.6396 | 0.6795 | -5.6675 |
| 0.8154 | -0.6368 | -4.5224 |
| -1.9153 | 0.1326 | 4.2597 |
| 0.0423 | 2.9927 | -5.1060 |

| | | |
|---|---|---|
| 0.5843 | -1.1869 | 2.2103 |
| -1.8411 | -0.9412 | -0.6629 |
| -0.7825 | -2.0608 | 0.1743 |
| 2.7029 | 1.9239 | 2.2131 |
| 1.2412 | -0.9662 | -0.1158 |
| 1.2315 | -1.4415 | -2.4366 |
| 2.4214 | -0.1654 | -2.4805 |
| 0.5838 | 1.4884 | -1.7597 |
| -0.5460 | 0.1677 | -1.8406 |
| -0.6779 | 2.1996 | 1.0209 |
| -1.5338 | 1.5571 | -0.3757 |
| -2.2024 | 1.3414 | 1.2116 |
| -2.6194 | 0.2175 | 4.6883 |
| -2.9714 | 0.6023 | 3.0317 |
| 0.2016 | -2.0244 | 4.3410 |
| -0.0683 | -0.5019 | 5.2025 |
| -1.3110 | -1.7409 | 5.2035 |
| -0.2137 | -1.7774 | -4.2823 |
| 2.7272 | 1.9995 | -1.2166 |
| 3.7899 | 2.0022 | 0.1810 |
| 3.6222 | 0.5243 | -0.7550 |
| 2.6106 | 1.2075 | -4.6889 |
| 1.0951 | 1.5494 | -5.5415 |
| 1.2936 | 2.0821 | -3.8843 |
| -0.6948 | 1.6223 | 4.3794 |
| 1.6752 | -0.5482 | -6.5538 |

| | | |
|---|---|---|
| 0.6881 | -0.9018 | 2.3181 |
| -1.7223 | -1.3152 | -0.5492 |
| -0.5164 | -2.1733 | 0.3913 |
| 2.3167 | 2.4771 | 1.9856 |
| 1.3256 | -0.8254 | -0.0184 |
| 1.2987 | -1.5882 | -2.3448 |
| 2.3970 | -0.2348 | -2.3562 |
| 0.3570 | 1.3132 | -1.9242 |
| -0.6035 | -0.1335 | -1.8353 |
| -2.4362 | 1.0665 | 1.0823 |
| -1.0544 | 2.1191 | 0.8007 |
| -1.7893 | 1.2210 | -0.5211 |
| -2.7097 | 0.2558 | 4.6610 |
| -3.1016 | 0.4114 | 2.9762 |
| 0.4161 | -1.5646 | 4.5257 |
| -0.0854 | -0.0196 | 5.2288 |
| -1.1294 | -1.4234 | 5.3647 |
| 2.5691 | 1.1818 | -4.2563 |
| 3.3912 | 2.5149 | -0.0539 |
| 3.4649 | 0.9385 | -0.8265 |
| 2.3576 | 2.1988 | -1.4371 |
| 0.1434 | -2.1427 | -4.6117 |
| -0.9905 | -0.9505 | -3.9479 |
| -0.3980 | -0.7653 | -5.5857 |
| -1.0140 | 1.8935 | 4.1947 |
| 1.8209 | -1.0194 | -6.4539 |

| (4*S**,5*R**,9*S**,10*R**)-**6F** | | | |
|---|---|---|---|
| C | -2.1124 | -2.2946 | 0.6529 |
| C | -1.7875 | -2.5414 | 2.1163 |
| C | -1.5534 | -1.2396 | 2.9310 |
| C | -0.4850 | -0.3693 | 2.1712 |
| C | -0.6384 | -0.1808 | 0.6164 |
| C | -0.9746 | -1.5497 | -0.0360 |
| C | -0.1829 | 0.9934 | 2.7840 |
| C | 0.8615 | 1.8087 | 2.1228 |
| C | 1.3317 | 1.4989 | 0.9011 |
| C | 0.7735 | 0.3334 | 0.0644 |
| C | 1.9501 | 0.5060 | -3.6880 |
| C | 2.0253 | 0.2286 | -2.1969 |
| C | 0.7362 | 0.6375 | -1.4645 |
| C | -1.7520 | 0.8326 | 0.2358 |
| C | -2.9243 | -0.5513 | 3.1847 |
| C | -0.9673 | -1.6906 | 4.2979 |
| C | 1.9041 | -0.5208 | -4.5611 |
| C | 2.4926 | 2.2974 | 0.3671 |
| C | 2.0266 | 1.9607 | -4.0757 |
| O | -0.7197 | 1.4360 | 3.7946 |
| O | -2.9582 | 0.2693 | 4.3436 |
| C | 1.8433 | -0.4172 | -6.0312 |
| O | 2.5587 | -1.0721 | -6.7679 |
| O | 0.8637 | 0.4008 | -6.4601 |
| H | -3.0573 | -1.7511 | 0.5534 |
| H | -2.2587 | -3.2593 | 0.1522 |
| H | -2.5909 | -3.1368 | 2.5688 |
| H | -0.8885 | -3.1717 | 2.1636 |
| H | 0.4546 | -0.9326 | 2.3065 |

| (4*S**,5*R**,9*S**,10*R**)-**6G** | | |
|---|---|---|
| -2.1735 | -2.3308 | 0.7254 |
| -1.9458 | -2.4802 | 2.2241 |
| -1.6907 | -1.1318 | 2.9523 |
| -0.5294 | -0.3793 | 2.2049 |
| -0.6737 | -0.2181 | 0.6517 |
| -1.0147 | -1.6109 | 0.0445 |
| -0.0895 | 0.9405 | 2.8368 |
| 0.8948 | 1.7631 | 2.1003 |
| 1.3099 | 1.4512 | 0.8605 |
| 0.7331 | 0.2675 | 0.0683 |
| 1.9999 | 0.3068 | -3.7179 |
| 1.9468 | 0.0780 | -2.2119 |
| 0.6730 | 0.5274 | -1.4704 |
| -1.7801 | 0.7957 | 0.2656 |
| -3.0452 | -0.3812 | 3.0897 |
| -1.2296 | -1.5129 | 4.3885 |
| 0.9843 | 0.8404 | -4.4279 |
| 2.4290 | 2.2683 | 0.2680 |
| 3.2891 | -0.1819 | -4.3380 |
| -0.4346 | 1.3179 | 3.9555 |
| -2.9297 | 1.0138 | 3.3003 |
| 0.9831 | 1.0907 | -5.8823 |
| 0.0897 | 0.7120 | -6.6181 |
| 2.0208 | 1.8518 | -6.2792 |
| -3.1154 | -1.8116 | 0.5232 |
| -2.2804 | -3.3285 | 0.2822 |
| -2.8080 | -2.9952 | 2.6674 |
| -1.0842 | -3.1458 | 2.3729 |
| 0.3528 | -1.0272 | 2.3493 |

| (4*S**,5*R**,9*S**,10*R**)-**6H** | | |
|---|---|---|
| -2.1605 | -1.3748 | 2.0302 |
| -1.6610 | -0.8021 | 3.3455 |
| -1.2880 | 0.7040 | 3.2686 |
| -0.3002 | 0.9060 | 2.0604 |
| -0.6442 | 0.2185 | 0.6871 |
| -1.0978 | -1.2445 | 0.9450 |
| 0.1147 | 2.3456 | 1.7779 |
| 1.0825 | 2.5615 | 0.6779 |
| 1.3859 | 1.5873 | -0.1989 |
| 0.7004 | 0.2087 | -0.1811 |
| 1.4699 | -1.7775 | -3.4914 |
| 1.6553 | -1.2704 | -2.0728 |
| 0.4841 | -0.3900 | -1.6044 |
| -1.7685 | 0.9523 | -0.0935 |
| -2.5947 | 1.5448 | 3.2140 |
| -0.5467 | 1.0277 | 4.5957 |
| 2.1096 | -1.1620 | -4.5066 |
| 2.4817 | 1.8528 | -1.1988 |
| 0.5344 | -2.9492 | -3.6422 |
| -0.2706 | 3.3184 | 2.4188 |
| -2.4577 | 2.8649 | 3.7205 |
| 2.0493 | -1.5344 | -5.9319 |
| 1.8269 | -0.7265 | -6.8157 |
| 2.3549 | -2.8277 | -6.1477 |
| -3.0947 | -0.8909 | 1.7283 |
| -2.3959 | -2.4368 | 2.1699 |
| -2.4177 | -0.9696 | 4.1225 |
| -0.7819 | -1.3832 | 3.6573 |
| 0.6329 | 0.4260 | 2.4026 |

| (4*S**,5*R**,9*S**,10*R**)-**6I** | | |
|---|---|---|
| -2.2517 | -1.8364 | -0.4763 |
| -3.2325 | -0.7131 | -0.1680 |
| -2.9047 | 0.6161 | -0.9018 |
| -1.4049 | 0.9853 | -0.6061 |
| -0.3345 | -0.1325 | -0.8608 |
| -0.8145 | -1.4372 | -0.1608 |
| -0.9312 | 2.3154 | -1.1890 |
| 0.5050 | 2.6474 | -1.0713 |
| 1.4085 | 1.7777 | -0.5877 |
| 1.0437 | 0.3363 | -0.1954 |
| 2.6647 | -1.3616 | 1.9834 |
| 3.2319 | -0.8298 | 0.6813 |
| 2.1978 | -0.6859 | -0.4521 |
| -0.1202 | -0.4119 | -2.3694 |
| -3.3154 | 0.4700 | -2.3940 |
| -3.8425 | 1.6846 | -0.2697 |
| 2.5804 | -0.5624 | 3.0652 |
| 2.8134 | 2.2754 | -0.3736 |
| 2.2609 | -2.8143 | 1.9714 |
| -1.6802 | 3.1629 | -1.6726 |
| -2.6895 | 1.3856 | -3.2739 |
| 1.9782 | -0.9768 | 4.3477 |
| 0.9235 | -1.5744 | 4.4573 |
| 2.7391 | -0.5875 | 5.3887 |
| -2.3373 | -2.1548 | -1.5198 |
| -2.5163 | -2.7135 | 0.1270 |
| -4.2481 | -1.0461 | -0.4186 |
| -3.2267 | -0.5438 | 0.9177 |
| -1.3789 | 1.1702 | 0.4820 |

| (4*S**,5*R**,9*S**,10*R**)-**6J** | | |
|---|---|---|
| -2.3314 | -1.6469 | -0.4243 |
| -3.1918 | -0.5010 | 0.0801 |
| -2.8873 | 0.8573 | -0.6097 |
| -1.3389 | 1.1218 | -0.5131 |
| -0.3523 | -0.0539 | -0.8618 |
| -0.8537 | -1.3592 | -0.1850 |
| -0.8368 | 2.3812 | -1.2094 |
| 0.6068 | 2.6863 | -1.0847 |
| 1.4837 | 1.7786 | -0.6197 |
| 1.0789 | 0.3384 | -0.2572 |
| 2.7043 | -1.4653 | 1.8083 |
| 3.2433 | -0.9657 | 0.4799 |
| 2.1757 | -0.7158 | -0.6041 |
| -0.2265 | -0.3074 | -2.3884 |
| -3.4783 | 0.8343 | -2.0475 |
| -3.6428 | 1.9350 | 0.2166 |
| 2.1253 | -2.6806 | 1.8875 |
| 2.9054 | 2.2203 | -0.3936 |
| 2.8446 | -0.5012 | 2.9578 |
| -1.5488 | 3.1652 | -1.8293 |
| -3.7907 | 2.1179 | -2.5703 |
| 1.5471 | -3.2877 | 3.0991 |
| 0.4201 | -3.7482 | 3.1304 |
| 2.4206 | -3.3455 | 4.1214 |
| -2.5293 | -1.8419 | -1.4830 |
| -2.6055 | -2.5626 | 0.1134 |
| -4.2504 | -0.7636 | -0.0422 |
| -3.0326 | -0.4072 | 1.1635 |
| -1.1766 | 1.3317 | 0.5583 |

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H | -1.2453 | -1.4282 | -1.0904 | -1.2583 | -1.5292 | -1.0199 | -1.4957 | -1.7010 | 0.0322 | -0.1751 | -2.2846 | -0.4286 | -0.2843 | -2.2278 | -0.5330 |
| H | -0.0834 | -2.1911 | -0.0201 | -0.1298 | -2.2584 | 0.1069 | -0.2299 | -1.8503 | 1.2377 | -0.7279 | -1.3162 | 0.9273 | -0.6879 | -1.2960 | 0.8985 |
| H | 1.2384 | 2.6395 | 2.7103 | 1.2952 | 2.6019 | 2.6607 | 1.5475 | 3.5417 | 0.6591 | 0.7601 | 3.6633 | -1.3552 | 0.8891 | 3.6974 | -1.3590 |
| H | 1.4857 | -0.4925 | 0.2122 | 1.4422 | -0.5585 | 0.2295 | 1.4048 | -0.4552 | 0.3427 | 0.8656 | 0.3742 | 0.8876 | 0.9546 | 0.3460 | 0.8335 |
| H | 2.2029 | -0.8405 | -2.0209 | 2.0776 | -0.9976 | -2.0330 | 1.7637 | -2.1303 | -1.3991 | 3.7479 | 0.1184 | 0.8530 | 3.8520 | -0.0712 | 0.6392 |
| H | 2.9000 | 0.7448 | -1.7927 | 2.8201 | 0.5741 | -1.7794 | 2.6007 | -0.7248 | -2.0018 | 4.0189 | -1.5178 | 0.3447 | 3.9489 | -1.7154 | 0.0957 |
| H | 0.5169 | 1.6993 | -1.6308 | 0.4676 | 1.5870 | -1.6657 | 0.2943 | 0.4106 | -2.3305 | 2.7283 | -0.4177 | -1.3750 | 2.6854 | -0.4279 | -1.5328 |
| H | -0.0776 | 0.0914 | -1.9510 | -0.1555 | -0.0255 | -1.9209 | -0.4095 | -1.0185 | -1.6263 | 1.8010 | -1.6874 | -0.6388 | 1.7246 | -1.6879 | -0.8221 |
| H | -1.6374 | 1.7965 | 0.7395 | -2.7725 | 0.4728 | 0.5777 | -1.9056 | 0.5346 | -1.0959 | 0.1867 | 0.4831 | -2.9187 | 0.0316 | 0.5963 | -2.9475 |
| H | -1.7635 | 1.0376 | -0.8394 | -1.6062 | 1.7851 | 0.6989 | -2.7427 | 0.8551 | 0.3859 | 0.6523 | -1.1699 | -2.5342 | 0.5457 | -1.0498 | -2.6135 |
| H | -2.7514 | 0.4598 | 0.4597 | -1.8482 | 0.9289 | -0.8187 | -1.5679 | 2.0196 | -0.2218 | -1.0139 | -0.8020 | -2.8550 | -1.1397 | -0.7146 | -2.8220 |
| H | -3.7000 | -1.3095 | 3.3408 | -3.6277 | -0.7922 | 3.9232 | -3.3686 | 1.0740 | 3.8307 | -4.3992 | 0.5961 | -2.5060 | -4.4227 | 0.2784 | -2.0545 |
| H | -3.2565 | 0.0551 | 2.3462 | -3.6775 | -0.5147 | 2.2095 | -3.0088 | 1.6215 | 2.2120 | -3.1055 | -0.5295 | -2.7801 | -2.8294 | 0.3395 | -2.7655 |
| H | -0.0462 | -2.2699 | 4.1641 | -0.2409 | -1.9854 | 4.3786 | 0.3327 | 0.3865 | 4.7267 | -3.5655 | 1.8947 | 0.7695 | -3.3297 | 1.9227 | 1.2671 |
| H | -0.7223 | -0.8466 | 4.9490 | -1.1842 | -0.6514 | 5.0595 | -0.1965 | 2.0630 | 4.6400 | -3.8348 | 2.6302 | -0.8178 | -3.4698 | 2.9485 | -0.1567 |
| H | -1.6790 | -2.3280 | 4.8356 | -1.9248 | -2.2279 | 4.8455 | -1.2029 | 0.8630 | 5.4584 | -4.8828 | 1.3367 | -0.2629 | -4.7240 | 1.7547 | 0.1956 |
| H | 1.9642 | -1.5504 | -4.2193 | 0.0309 | 1.0910 | -3.9751 | 2.6974 | -0.2646 | -4.3344 | 2.9095 | 0.4702 | 3.0243 | 1.9855 | -3.2948 | 1.0025 |
| H | 2.2319 | 2.8052 | -0.5655 | 2.1262 | 2.7450 | -0.6680 | 2.8998 | 2.8607 | -1.0944 | 2.9301 | 3.3247 | -0.6684 | 3.0506 | 3.2811 | -0.6282 |
| H | 2.8171 | 3.0740 | 1.0693 | 2.7527 | 3.0725 | 0.9389 | 3.3079 | 1.1514 | -1.0489 | 3.0771 | 2.2162 | 0.6866 | 3.1795 | 2.0891 | 0.6573 |
| H | 3.3539 | 1.6442 | 0.1982 | 3.3041 | 1.6367 | 0.0892 | 2.1158 | 1.7691 | -2.2256 | 3.5336 | 1.7029 | -0.9643 | 3.5997 | 1.6594 | -1.0254 |
| H | 1.0728 | 2.4592 | -3.8783 | 4.1176 | 0.4705 | -4.0444 | -0.4174 | -2.7520 | -3.1395 | 1.3125 | -2.9454 | 1.4439 | 3.8962 | -0.4177 | 3.2501 |
| H | 2.8075 | 2.4673 | -3.4982 | 3.5118 | -1.1982 | -3.9950 | 0.2926 | -3.1726 | -4.6846 | 3.0235 | -3.4146 | 1.4635 | 2.4890 | 0.4932 | 2.6695 |
| H | 2.2773 | 2.1059 | -5.1302 | 3.2555 | -0.2237 | -5.4298 | 0.9797 | -3.8440 | -3.1959 | 2.1551 | -3.2371 | 2.9741 | 2.2665 | -0.7960 | 3.8375 |
| H | -2.1993 | 0.8905 | 4.2986 | -2.2445 | 1.1693 | 3.9844 | -1.6946 | 3.2857 | 3.2683 | -2.7166 | 2.2766 | -2.8652 | -2.9995 | 2.6892 | -2.4649 |
| H | 0.3228 | 0.7618 | -5.7337 | 2.5867 | 2.1383 | -5.5385 | 2.6007 | -3.3023 | -5.3321 | 3.6013 | -0.2102 | 5.1347 | 3.3059 | -3.0109 | 3.8858 |

| (4*S**,5*R**,9*S**,10*R**)-**6K** | | | |
|---|---|---|---|
| C | -2.6742 | -0.7617 | 0.6753 |
| C | -2.2270 | -1.0861 | 2.0948 |
| C | -1.3378 | 0.0159 | 2.7342 |
| C | -0.1520 | 0.3266 | 1.7489 |
| C | -0.5302 | 0.6342 | 0.2583 |
| C | -1.4889 | -0.4860 | -0.2432 |
| C | 0.8748 | 1.3383 | 2.2558 |
| C | 1.9335 | 1.7725 | 1.3188 |
| C | 1.9413 | 1.4112 | 0.0243 |
| C | 0.8092 | 0.5947 | -0.6155 |
| C | 1.2537 | -1.2738 | -3.1567 |
| C | 1.4051 | 0.2371 | -3.1544 |
| C | 0.5441 | 0.9701 | -2.1077 |
| C | -1.2213 | 2.0114 | 0.0989 |
| C | -2.2474 | 1.2084 | 3.1434 |
| C | -0.7796 | -0.6065 | 4.0464 |
| C | 0.0979 | -1.8317 | -3.5716 |
| C | 3.1471 | 1.7777 | -0.8005 |
| C | 2.4933 | -2.0400 | -2.7728 |
| O | 0.9283 | 1.7434 | 3.4158 |
| O | -1.5704 | 2.4418 | 3.2971 |
| C | -0.2087 | -3.2723 | -3.6419 |
| O | -0.7199 | -3.7914 | -4.6178 |
| O | 0.0459 | -3.9187 | -2.4885 |
| H | -3.3666 | 0.0856 | 0.6676 |
| H | -3.2391 | -1.6141 | 0.2784 |
| H | -3.1133 | -1.2684 | 2.7163 |
| H | -1.6730 | -2.0347 | 2.0688 |
| H | 0.4262 | -0.6134 | 1.7138 |

| | | | |
|---|---|---|---|
| H | -1.8892 | -0.2490 | -1.2344 |
| H | -0.9241 | -1.4210 | -0.3559 |
| H | 2.7291 | 2.3563 | 1.7710 |
| H | 1.1608 | -0.4449 | -0.5887 |
| H | 2.4589 | 0.5074 | -3.0481 |
| H | 1.1235 | 0.6113 | -4.1486 |
| H | 0.6736 | 2.0513 | -2.2460 |
| H | -0.4975 | 0.7774 | -2.3792 |
| H | -0.5977 | 2.8331 | 0.4635 |
| H | -1.4571 | 2.2279 | -0.9478 |
| H | -2.1739 | 2.0664 | 0.6243 |
| H | -2.7587 | 0.9935 | 4.0896 |
| H | -3.0484 | 1.3778 | 2.4208 |
| H | -0.0688 | -1.4133 | 3.8352 |
| H | -0.2766 | 0.1279 | 4.6806 |
| H | -1.5882 | -1.0377 | 4.6493 |
| H | -0.7125 | -1.2145 | -3.9505 |
| H | 2.8746 | 2.4292 | -1.6353 |
| H | 3.9013 | 2.3155 | -0.2145 |
| H | 3.6313 | 0.8740 | -1.1829 |
| H | 2.7078 | -1.9098 | -1.7079 |
| H | 2.4163 | -3.1112 | -2.9765 |
| H | 3.3537 | -1.6758 | -3.3447 |
| H | -0.7577 | 2.2869 | 3.8238 |
| H | 0.3687 | -3.3286 | -1.7833 |

**Supplementary S5.** The Z-matrices of (2*R**,4*S**,5*R**,9*S**,10*R**)-**7** optimized at B3LYP/6-31G(d)-GD3BJ level by Gaussian.

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7A** | | | |
|---|---|---|---|
| C | -2.2338 | -0.2594 | -1.1926 |
| C | -1.5608 | -1.1612 | -2.2232 |
| C | -0.6772 | -2.2774 | -1.5908 |
| C | 0.3368 | -1.6007 | -0.5970 |
| C | -0.2718 | -0.6348 | 0.4713 |
| C | -1.2200 | 0.3489 | -0.2435 |
| C | 1.3591 | -2.5245 | 0.0678 |
| C | 2.2407 | -1.9387 | 1.1083 |
| C | 2.0761 | -0.6834 | 1.5638 |
| C | 0.9225 | 0.2113 | 1.0985 |
| C | 0.6252 | 3.3627 | 0.6866 |
| C | 0.9933 | 2.6632 | 1.9882 |
| C | 0.4294 | 1.2391 | 2.1669 |
| C | -1.0474 | -1.3851 | 1.5809 |
| C | -1.6078 | -3.3726 | -1.0029 |
| C | 0.1021 | -2.9201 | -2.7724 |
| C | -0.6602 | 3.6018 | 0.3502 |
| C | 3.1136 | -0.1077 | 2.4924 |
| C | 1.8056 | 3.7757 | -0.1569 |
| O | 1.5418 | -3.6944 | -0.2636 |
| O | -2.8588 | 0.8545 | -1.8405 |
| O | -1.0097 | -4.1777 | -0.0061 |
| C | -1.0781 | 4.3225 | -0.8684 |
| O | -0.6559 | 5.4207 | -1.1863 |
| O | -1.9985 | 3.6424 | -1.5781 |
| H | -3.0120 | -0.7930 | -0.6395 |
| H | -2.3283 | -1.5989 | -2.8757 |
| H | -0.9493 | -0.5342 | -2.8880 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7B** | | |
|---|---|---|
| -2.1406 | 0.2354 | -1.4603 |
| -1.3793 | -0.1897 | -2.7124 |
| -0.5073 | -1.4594 | -2.5107 |
| 0.4179 | -1.2253 | -1.2611 |
| -0.2832 | -0.7523 | 0.0577 |
| -1.2028 | 0.4505 | -0.2791 |
| 1.4145 | -2.3432 | -0.9523 |
| 2.2249 | -2.2183 | 0.2807 |
| 2.0064 | -1.2481 | 1.1854 |
| 0.8468 | -0.2495 | 1.0626 |
| 0.3320 | 2.7446 | 2.2705 |
| 0.8644 | 1.5075 | 2.9775 |
| 0.2647 | 0.1945 | 2.4421 |
| -1.1214 | -1.8777 | 0.7127 |
| -1.4429 | -2.6994 | -2.4759 |
| 0.3664 | -1.5789 | -3.7918 |
| 1.1158 | 3.4195 | 1.4055 |
| 2.9908 | -1.0932 | 2.3170 |
| -1.0499 | 3.1797 | 2.6894 |
| 1.6399 | -3.2898 | -1.7040 |
| -2.7878 | 1.4832 | -1.7079 |
| -0.8967 | -3.8313 | -1.8278 |
| 0.7563 | 4.6363 | 0.6538 |
| 1.4969 | 5.6015 | 0.5811 |
| -0.4117 | 4.5334 | -0.0062 |
| -2.9205 | -0.4864 | -1.2015 |
| -2.0915 | -0.3374 | -3.5357 |
| -0.7465 | 0.6497 | -3.0355 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7C** | | |
|---|---|---|
| -2.0878 | 0.5837 | -1.2113 |
| -1.4268 | 0.0760 | -2.4841 |
| -0.8130 | -1.3454 | -2.3321 |
| 0.1542 | -1.3416 | -1.0963 |
| -0.3864 | -0.7279 | 0.2413 |
| -1.0942 | 0.6050 | -0.0648 |
| 0.8420 | -2.6647 | -0.7649 |
| 1.7607 | -2.6657 | 0.4043 |
| 1.8112 | -1.6345 | 1.2689 |
| 0.8823 | -0.4182 | 1.1543 |
| 1.1528 | 2.6741 | 1.9279 |
| 1.3080 | 1.4933 | 2.8770 |
| 0.4942 | 0.2333 | 2.5198 |
| -1.3761 | -1.6613 | 0.9874 |
| -1.9168 | -2.4284 | -2.2677 |
| 0.0058 | -1.5949 | -3.6293 |
| -0.0480 | 3.2478 | 1.6997 |
| 2.8771 | -1.6294 | 2.3337 |
| 2.4418 | 3.1472 | 1.3033 |
| 0.7127 | -3.6970 | -1.4135 |
| -2.5002 | 1.9458 | -1.3736 |
| -2.8474 | -2.2581 | -3.3352 |
| -0.2520 | 4.4291 | 0.8383 |
| 0.3671 | 5.4720 | 0.9608 |
| -1.2180 | 4.2377 | -0.0798 |
| -2.9752 | -0.0050 | -0.9605 |
| -2.1466 | 0.1176 | -3.3113 |
| -0.6402 | 0.7885 | -2.7734 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7D** | | |
|---|---|---|
| 2.0301 | 1.1650 | -1.0620 |
| 2.1071 | 0.0523 | -2.0967 |
| 0.7520 | -0.2246 | -2.7988 |
| -0.3335 | -0.4789 | -1.6954 |
| -0.4149 | 0.5339 | -0.4969 |
| 1.0150 | 0.8249 | 0.0245 |
| -1.7504 | -0.7354 | -2.2026 |
| -2.7835 | -1.0148 | -1.1757 |
| -2.5544 | -0.8041 | 0.1335 |
| -1.2490 | -0.1826 | 0.6597 |
| 0.2085 | -0.2522 | 3.5778 |
| -1.2525 | 0.0166 | 3.2522 |
| -1.4573 | 0.7339 | 1.9056 |
| -1.0874 | 1.8778 | -0.8855 |
| 0.3985 | 0.9055 | -3.7970 |
| 0.9600 | -1.5233 | -3.6279 |
| 0.6937 | -1.5090 | 3.5207 |
| -3.5914 | -1.2678 | 1.1246 |
| 0.9936 | 0.9458 | 4.0500 |
| -2.0747 | -0.7643 | -3.3844 |
| 3.2969 | 1.2990 | -0.4188 |
| 1.5067 | 1.1842 | -4.6515 |
| 2.0721 | -1.9385 | 3.8218 |
| 2.3155 | -2.9094 | 4.5170 |
| 3.0110 | -1.2144 | 3.1861 |
| 1.7979 | 2.1261 | -1.5302 |
| 2.8971 | 0.2809 | -2.8234 |
| 2.4582 | -0.8617 | -1.5951 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7E** | | |
|---|---|---|
| -2.2002 | 0.4045 | -1.2682 |
| -1.5367 | -0.0945 | -2.5447 |
| -0.8188 | -1.4591 | -2.3726 |
| 0.1680 | -1.3471 | -1.1578 |
| -0.3816 | -0.7373 | 0.1803 |
| -1.1818 | 0.5503 | -0.1419 |
| 0.9571 | -2.6128 | -0.8314 |
| 1.9008 | -2.5372 | 0.3101 |
| 1.9053 | -1.4928 | 1.1586 |
| 0.8846 | -0.3458 | 1.0687 |
| 0.9107 | 2.7404 | 2.1304 |
| 1.3042 | 1.4747 | 2.8763 |
| 0.4848 | 0.2401 | 2.4592 |
| -1.2958 | -1.7188 | 0.9608 |
| -1.8544 | -2.6045 | -2.2506 |
| -0.0065 | -1.6823 | -3.6791 |
| 1.7310 | 3.2546 | 1.1918 |
| 3.0047 | -1.4119 | 2.1871 |
| -0.3695 | 3.3887 | 2.5941 |
| 0.8995 | -3.6535 | -1.4775 |
| -2.7482 | 1.7015 | -1.5017 |
| -2.7482 | -2.6129 | -3.3627 |
| 1.5078 | 4.4751 | 0.3945 |
| 2.3780 | 5.3116 | 0.2257 |
| 0.2976 | 4.5207 | -0.1913 |
| -3.0247 | -0.2484 | -0.9674 |
| -2.2810 | -0.1348 | -3.3505 |
| -0.8140 | 0.6648 | -2.8784 |

| | | | |
|---|---|---|---|
| H | 0.9660 | -0.9675 | -1.2468 |
| H | -0.6160 | 1.0579 | -0.8250 |
| H | -1.7795 | 0.9530 | 0.4782 |
| H | 3.0565 | -2.5781 | 1.4298 |
| H | 1.3583 | 0.7886 | 0.2709 |
| H | 2.0833 | 2.6344 | 2.0981 |
| H | 0.6364 | 3.2862 | 2.8191 |
| H | 0.6737 | 0.8890 | 3.1764 |
| H | -0.6597 | 1.3276 | 2.1750 |
| H | -0.4392 | -2.1510 | 2.0708 |
| H | -1.3946 | -0.7071 | 2.3665 |
| H | -1.9459 | -1.8724 | 1.2013 |
| H | -1.9673 | -4.0393 | -1.7960 |
| H | -2.5095 | -2.9443 | -0.5597 |
| H | 0.6382 | -3.8262 | -2.4785 |
| H | -0.5811 | -3.2081 | -3.5808 |
| H | 0.8301 | -2.2206 | -3.1984 |
| H | -1.4781 | 3.2982 | 0.9935 |
| H | 3.5288 | 0.8136 | 2.0732 |
| H | 2.6921 | 0.1040 | 3.4786 |
| H | 3.9538 | -0.7946 | 2.6453 |
| H | 2.4746 | 2.9225 | -0.3128 |
| H | 1.5270 | 4.1384 | -1.1492 |
| H | 2.3689 | 4.5666 | 0.3489 |
| H | -3.4905 | 0.4942 | -2.4917 |
| H | -0.1215 | -4.4560 | -0.3165 |
| H | -2.1814 | 2.7118 | -1.3199 |

| | | |
|---|---|---|
| 1.0722 | -0.3885 | -1.5621 |
| -0.5845 | 1.3331 | -0.4940 |
| -1.8143 | 0.7366 | 0.5839 |
| 3.0412 | -2.9285 | 0.3650 |
| 1.3023 | 0.6355 | 0.5964 |
| 1.9575 | 1.4766 | 2.9242 |
| 0.6296 | 1.5924 | 4.0464 |
| 0.4178 | -0.5959 | 3.1865 |
| -0.8198 | 0.3248 | 2.4021 |
| -0.5234 | -2.7675 | 0.9308 |
| -1.5703 | -1.5573 | 1.6577 |
| -1.9591 | -2.1900 | 0.0895 |
| -1.7192 | -3.0020 | -3.4932 |
| -2.3900 | -2.4804 | -1.9779 |
| 0.9062 | -2.5279 | -3.8454 |
| -0.2534 | -1.5198 | -4.6949 |
| 1.1018 | -0.7687 | -3.8512 |
| 2.1456 | 3.1174 | 1.2353 |
| 3.4459 | -0.0988 | 2.2894 |
| 2.5133 | -1.2443 | 3.2886 |
| 3.8102 | -1.8181 | 2.2513 |
| -1.1421 | 3.1521 | 3.7805 |
| -1.2829 | 4.2042 | 2.3864 |
| -1.8084 | 2.5174 | 2.2633 |
| -3.4113 | 1.3519 | -2.4445 |
| 0.0179 | -3.9690 | -2.1554 |
| -0.8387 | 3.6586 | 0.0675 |

| | | |
|---|---|---|
| 0.9858 | -0.6893 | -1.4143 |
| -0.3343 | 1.3586 | -0.3087 |
| -1.6221 | 0.9836 | 0.8171 |
| 2.4102 | -3.5317 | 0.4785 |
| 1.4843 | 0.3198 | 0.6052 |
| 2.3666 | 1.2232 | 2.9634 |
| 1.0121 | 1.8266 | 3.8807 |
| 0.5995 | -0.4936 | 3.3335 |
| -0.5611 | 0.5162 | 2.5502 |
| -1.5497 | -1.3358 | 2.0174 |
| -2.3642 | -1.6712 | 0.5247 |
| -1.0260 | -2.6958 | 1.0428 |
| -2.4949 | -2.3864 | -1.3484 |
| -1.5003 | -3.4355 | -2.3563 |
| 0.4287 | -2.6035 | -3.6602 |
| -0.6178 | -1.4774 | -4.5231 |
| 0.8364 | -0.8854 | -3.7187 |
| -0.9492 | 2.8833 | 2.1790 |
| 3.4817 | -0.7204 | 2.2605 |
| 2.4406 | -1.6901 | 3.3341 |
| 3.5629 | -2.4781 | 2.2314 |
| 2.9676 | 2.3050 | 0.8406 |
| 2.2981 | 3.8936 | 0.5184 |
| 3.0927 | 3.5802 | 2.0698 |
| -3.0821 | 1.9716 | -2.1579 |
| -3.3763 | -3.0741 | -3.3817 |
| -1.5707 | 3.3273 | -0.1969 |

| | | |
|---|---|---|
| -0.0362 | -1.4438 | -1.2494 |
| 1.3884 | -0.0463 | 0.5801 |
| 1.0124 | 1.6451 | 0.7518 |
| -3.7061 | -1.4418 | -1.5550 |
| -0.6485 | -1.0448 | 0.9823 |
| -1.8283 | -0.9142 | 3.2789 |
| -1.6749 | 0.6399 | 4.0509 |
| -2.4638 | 1.1693 | 1.8855 |
| -0.7834 | 1.5947 | 1.8909 |
| -1.2932 | 2.5010 | -0.0101 |
| -0.4513 | 2.4933 | -1.5218 |
| -2.0408 | 1.7406 | -1.4031 |
| 0.1492 | 1.8412 | -3.3044 |
| -0.4423 | 0.6306 | -4.4392 |
| 0.0765 | -1.7770 | -4.2214 |
| 1.8003 | -1.4213 | -4.3244 |
| 1.1794 | -2.3793 | -2.9796 |
| 0.0430 | -2.3464 | 3.2836 |
| -4.4435 | -1.7505 | 0.6325 |
| -3.1589 | -2.0065 | 1.8061 |
| -3.9925 | -0.4332 | 1.7054 |
| 0.4103 | 1.5194 | 4.7783 |
| 1.9267 | 0.6717 | 4.5499 |
| 1.2365 | 1.6023 | 3.2099 |
| 3.9532 | 1.4893 | -1.1138 |
| 1.1698 | 1.7363 | -5.3791 |
| 2.6534 | -0.5345 | 2.5838 |

| | | |
|---|---|---|
| 0.9419 | -0.6422 | -1.5079 |
| -0.4862 | 1.3559 | -0.4143 |
| -1.7112 | 0.9198 | 0.7438 |
| 2.6122 | -3.3542 | 0.3735 |
| 1.4135 | 0.4453 | 0.5188 |
| 2.3748 | 1.2779 | 2.7588 |
| 1.1588 | 1.6477 | 3.9504 |
| 0.5856 | -0.5301 | 3.2334 |
| -0.5704 | 0.5246 | 2.4896 |
| -1.5143 | -1.3600 | 1.9710 |
| -2.2722 | -1.8422 | 0.4927 |
| -0.8531 | -2.7127 | 1.0702 |
| -2.4850 | -2.4972 | -1.3722 |
| -1.3903 | -3.5923 | -2.1946 |
| 0.4415 | -2.6794 | -3.7189 |
| -0.6392 | -1.5760 | -4.5678 |
| 0.8031 | -0.9496 | -3.7749 |
| 2.6961 | 2.7991 | 0.9870 |
| 3.5876 | -0.4969 | 2.0461 |
| 2.6048 | -1.4312 | 3.2042 |
| 3.7059 | -2.2504 | 2.1061 |
| -0.4072 | 3.4155 | 3.6885 |
| -0.4671 | 4.4245 | 2.2573 |
| -1.2371 | 2.8292 | 2.2335 |
| -3.4110 | 1.6098 | -2.2104 |
| -2.3036 | -3.0953 | -4.0823 |
| -0.2507 | 3.7267 | -0.0433 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7F** | | | |
|---|---|---|---|
| C | 2.6778 | 0.8501 | -1.2788 |
| C | 2.8194 | -0.1771 | -2.3977 |
| C | 1.4798 | -0.5119 | -3.1072 |
| C | 0.4272 | -0.9135 | -2.0091 |
| C | 0.2519 | 0.0710 | -0.8015 |
| C | 1.6608 | 0.4015 | -0.2331 |
| C | -0.9387 | -1.3507 | -2.5372 |
| C | -2.0077 | -1.6100 | -1.5485 |
| C | -1.8546 | -1.3464 | -0.2393 |
| C | -0.5956 | -0.6743 | 0.3292 |
| C | -1.0666 | 0.4581 | 4.0701 |
| C | -0.8213 | -0.4768 | 2.8991 |
| C | -0.8920 | 0.2540 | 1.5477 |
| C | -0.4576 | 1.3856 | -1.2116 |
| C | 1.1102 | 0.6731 | -4.0428 |
| C | 1.7807 | -1.7378 | -4.0162 |
| C | -0.0627 | 0.7435 | 4.9242 |
| C | -2.9439 | -1.7940 | 0.7012 |
| C | -2.4886 | 0.9328 | 4.2278 |
| O | -1.1773 | -1.5781 | -3.7221 |
| O | 3.9360 | 0.9973 | -0.6235 |
| O | -0.2630 | 0.7611 | -4.3691 |
| C | -0.1500 | 1.6195 | 6.1075 |
| O | 0.2718 | 1.2943 | 7.2028 |
| O | -0.6626 | 2.8320 | 5.8237 |
| H | 2.4078 | 1.8342 | -1.6721 |
| H | 3.5624 | 0.1791 | -3.1244 |
| H | 3.2572 | -1.0928 | -1.9744 |
| H | 0.8315 | -1.8429 | -1.5713 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7G** | | |
|---|---|---|
| -2.1661 | 0.1847 | -1.3196 |
| -1.3566 | -0.1032 | -2.5756 |
| -0.4464 | -1.3622 | -2.4620 |
| 0.4309 | -1.2205 | -1.1630 |
| -0.2882 | -0.7970 | 0.1656 |
| -1.2490 | 0.3691 | -0.1267 |
| 1.3622 | -2.3831 | -0.8322 |
| 2.2194 | -2.2368 | 0.3720 |
| 2.0114 | -1.2570 | 1.2717 |
| 0.8431 | -0.2685 | 1.1575 |
| 0.4185 | 2.7615 | 2.0774 |
| 0.7748 | 1.5919 | 2.9849 |
| 0.2649 | 0.2106 | 2.5269 |
| -1.0900 | -1.9518 | 0.8221 |
| -1.3345 | -2.6337 | -2.5330 |
| 0.4785 | -1.3356 | -3.7096 |
| -0.8648 | 3.0841 | 1.8087 |
| 3.0104 | -1.0660 | 2.3834 |
| 1.6062 | 3.5221 | 1.5423 |
| 1.4565 | -3.4033 | -1.5071 |
| -2.8624 | 1.4280 | -1.4518 |
| -0.6531 | -3.7981 | -2.9714 |
| -1.2745 | 4.2371 | 0.9829 |
| -0.8896 | 5.3781 | 1.1709 |
| -2.1419 | 3.8918 | 0.0125 |
| -2.9095 | -0.5969 | -1.1368 |
| -2.0353 | -0.1905 | -3.4346 |
| -0.7420 | 0.7808 | -2.8002 |
| 1.1221 | -0.3952 | -1.4067 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7H** | | |
|---|---|---|
| -2.2583 | -0.5307 | -2.1504 |
| -1.5066 | -1.4022 | -3.1517 |
| -0.5342 | -2.4141 | -2.4879 |
| 0.4069 | -1.6225 | -1.5065 |
| -0.2876 | -0.6706 | -0.4721 |
| -1.2984 | 0.2285 | -1.2387 |
| 1.4860 | -2.4560 | -0.8161 |
| 2.3103 | -1.7940 | 0.2183 |
| 2.0538 | -0.5481 | 0.6528 |
| 0.8357 | 0.2600 | 0.1792 |
| 0.3455 | 3.4787 | 2.3888 |
| 0.8725 | 2.6064 | 1.2632 |
| 0.2548 | 1.1984 | 1.2818 |
| -1.0341 | -1.4520 | 0.6379 |
| -1.3717 | -3.5755 | -1.8833 |
| 0.3078 | -3.0124 | -3.6509 |
| 1.1614 | 3.8279 | 3.4042 |
| 3.0470 | 0.0882 | 1.5915 |
| -1.0712 | 3.9651 | 2.2183 |
| 1.7631 | -3.6138 | -1.1250 |
| -3.0313 | 0.4325 | -2.8639 |
| -0.7246 | -4.2950 | -0.8520 |
| 0.8088 | 4.6716 | 4.5614 |
| 1.5145 | 5.5854 | 4.9497 |
| -0.3134 | 4.2662 | 5.1851 |
| -2.9594 | -1.1215 | -1.5543 |
| -2.2304 | -1.9256 | -3.7913 |
| -0.9514 | -0.7442 | -3.8360 |
| 0.9923 | -0.9587 | -2.1665 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7I** | | |
|---|---|---|
| -2.3622 | 0.6182 | -1.2606 |
| -1.9103 | -0.0969 | -2.5302 |
| -1.3367 | -1.5163 | -2.2716 |
| -0.2142 | -1.4011 | -1.1753 |
| -0.5879 | -0.6435 | 0.1462 |
| -1.2360 | 0.7177 | -0.2355 |
| 0.5242 | -2.6993 | -0.8486 |
| 1.4991 | -2.6749 | 0.2642 |
| 1.6484 | -1.6051 | 1.0643 |
| 0.7606 | -0.3569 | 0.9511 |
| 1.4274 | 2.6792 | 1.8417 |
| 1.5066 | 1.4332 | 2.7077 |
| 0.4946 | 0.3354 | 2.3260 |
| -1.5695 | -1.4534 | 1.0293 |
| -2.5199 | -2.4794 | -1.9740 |
| -0.7062 | -1.9669 | -3.6203 |
| 2.3542 | 2.8927 | 0.8859 |
| 2.7829 | -1.6164 | 2.0562 |
| 0.2638 | 3.5944 | 2.1290 |
| 0.4212 | -3.7342 | -1.5051 |
| -2.7988 | 1.9343 | -1.5956 |
| -2.1609 | -3.6496 | -1.2639 |
| 2.3833 | 4.0378 | -0.0397 |
| 2.4133 | 3.9040 | -1.2500 |
| 2.4459 | 5.2205 | 0.5987 |
| -3.2272 | 0.1153 | -0.8201 |
| -2.7496 | -0.1408 | -3.2377 |
| -1.1530 | 0.5243 | -3.0302 |
| 0.5687 | -0.7860 | -1.6525 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7J** | | |
|---|---|---|
| -2.3010 | 0.7749 | -1.9692 |
| -1.8178 | 0.1231 | -3.2609 |
| -1.1710 | -1.2723 | -3.0506 |
| -0.0527 | -1.1368 | -1.9523 |
| -0.4605 | -0.4412 | -0.6076 |
| -1.1734 | 0.8979 | -0.9482 |
| 0.7476 | -2.4076 | -1.6693 |
| 1.7173 | -2.3762 | -0.5528 |
| 1.8155 | -1.3291 | 0.2842 |
| 0.8730 | -0.1179 | 0.2098 |
| 1.2495 | 2.2167 | 3.3572 |
| 1.5585 | 1.6205 | 1.9961 |
| 0.5699 | 0.5091 | 1.6057 |
| -1.4033 | -1.3228 | 0.2488 |
| -2.3032 | -2.3032 | -2.7847 |
| -0.5224 | -1.6444 | -4.4147 |
| 0.5704 | 3.3788 | 3.4402 |
| 2.9393 | -1.3323 | 1.2884 |
| 1.7270 | 1.4076 | 4.5354 |
| 0.6958 | -3.4218 | -2.3631 |
| -2.7638 | 2.0914 | -2.2646 |
| -1.8872 | -3.4766 | -2.1137 |
| 0.2098 | 4.0893 | 4.6809 |
| -0.9184 | 4.4847 | 4.9132 |
| 1.2727 | 4.3256 | 5.4732 |
| -3.1449 | 0.2295 | -1.5375 |
| -2.6557 | 0.0573 | -3.9685 |
| -1.0968 | 0.7999 | -3.7421 |
| 0.6985 | -0.4693 | -2.4095 |

| | | | |
|---|---|---|---|
| H | 2.0637 | -0.4801 | 0.2856 |
| H | 1.6095 | 1.1802 | 0.5366 |
| H | -2.8985 | -2.0795 | -1.9535 |
| H | 0.0297 | -1.5020 | 0.6965 |
| H | 0.1673 | -0.9453 | 2.9919 |
| H | -1.5442 | -1.2951 | 2.9529 |
| H | -1.8661 | 0.7418 | 1.4208 |
| H | -0.1662 | 1.0705 | 1.6039 |
| H | -0.5991 | 2.0543 | -0.3566 |
| H | 0.1159 | 1.9632 | -1.9358 |
| H | -1.4463 | 1.2061 | -1.6443 |
| H | 1.6700 | 0.6095 | -4.9838 |
| H | 1.3910 | 1.6360 | -3.6106 |
| H | 0.9596 | -1.9660 | -4.7005 |
| H | 2.6650 | -1.5553 | -4.6391 |
| H | 1.9842 | -2.6357 | -3.4219 |
| H | 0.9149 | 0.2817 | 4.8171 |
| H | -3.7733 | -2.2775 | 0.1721 |
| H | -2.5517 | -2.5289 | 1.4104 |
| H | -3.3715 | -0.9502 | 1.2494 |
| H | -3.1852 | 0.0997 | 4.0842 |
| H | -2.6921 | 1.3399 | 5.2222 |
| H | -2.7173 | 1.7059 | 3.4880 |
| H | 4.5763 | 1.3239 | -1.2795 |
| H | -0.5782 | -0.1297 | -4.6338 |
| H | -0.8501 | 2.9518 | 4.8742 |

| | | |
|---|---|---|
| -0.6591 | 1.2773 | -0.3058 |
| -1.8812 | 0.5878 | 0.7407 |
| 3.0377 | -2.9453 | 0.4470 |
| 1.2911 | 0.6098 | 0.6715 |
| 1.8610 | 1.5462 | 3.1228 |
| 0.3658 | 1.8016 | 3.9822 |
| 0.4853 | -0.5225 | 3.3117 |
| -0.8266 | 0.2645 | 2.5109 |
| -1.4023 | -1.7063 | 1.8416 |
| -2.0165 | -2.1675 | 0.2875 |
| -0.5200 | -2.8827 | 0.8869 |
| -2.1459 | -2.4797 | -3.2535 |
| -1.8129 | -2.8700 | -1.5860 |
| 1.1932 | -2.1635 | -3.7207 |
| -0.1106 | -1.3955 | -4.6323 |
| 1.0608 | -0.4079 | -3.7530 |
| -1.6890 | 2.5168 | 2.2256 |
| 3.4079 | -0.0468 | 2.3644 |
| 2.5596 | -1.2567 | 3.3609 |
| 3.8657 | -1.7443 | 2.2871 |
| 2.3182 | 2.8312 | 1.0779 |
| 1.3446 | 4.2589 | 0.7791 |
| 2.1157 | 4.0438 | 2.3589 |
| -3.4199 | 1.3655 | -2.2508 |
| 0.1772 | -3.8892 | -2.4555 |
| -2.2947 | 2.9344 | -0.1474 |

| | | |
|---|---|---|
| -0.7498 | 0.9615 | -1.8473 |
| -1.9008 | 0.8315 | -0.5495 |
| 3.1667 | -2.3695 | 0.5550 |
| 1.2157 | 0.9055 | -0.6271 |
| 0.6533 | 3.0919 | 0.3035 |
| 1.9630 | 2.5480 | 1.3189 |
| 0.3716 | 0.7429 | 2.2733 |
| -0.8224 | 1.3289 | 1.1510 |
| -0.3706 | -2.1240 | 1.1904 |
| -1.4908 | -0.7797 | 1.3711 |
| -1.8555 | -2.0522 | 0.2480 |
| -1.6512 | -4.2947 | -2.6628 |
| -2.3193 | -3.2223 | -1.4708 |
| 0.9141 | -3.8656 | -3.3360 |
| -0.3411 | -3.3716 | -4.4591 |
| 0.9793 | -2.2630 | -4.0849 |
| 2.2068 | 3.5317 | 3.4096 |
| 3.4948 | 0.9712 | 1.1261 |
| 2.5797 | 0.3732 | 2.5378 |
| 3.8718 | -0.5895 | 1.8406 |
| -1.7798 | 3.1596 | 2.4335 |
| -1.3091 | 4.8131 | 2.8665 |
| -1.2355 | 4.3049 | 1.1900 |
| -3.6718 | -0.0502 | -3.4150 |
| 0.1865 | -4.5099 | -1.1461 |
| -0.6932 | 3.4561 | 4.7977 |

| | | |
|---|---|---|
| -0.4653 | 1.3929 | -0.6330 |
| -1.6337 | 1.2314 | 0.6469 |
| 2.1216 | -3.5604 | 0.3436 |
| 1.3433 | 0.3379 | 0.3325 |
| 2.5249 | 1.0328 | 2.6995 |
| 1.3250 | 1.7297 | 3.7492 |
| 0.4753 | -0.4177 | 3.1238 |
| -0.4982 | 0.7906 | 2.3566 |
| -1.7995 | -0.9340 | 1.9647 |
| -2.5327 | -1.6137 | 0.5461 |
| -1.1706 | -2.4356 | 1.2996 |
| -3.0033 | -2.7944 | -2.9067 |
| -3.3082 | -1.9923 | -1.3963 |
| -0.4174 | -3.0210 | -3.6188 |
| -1.4166 | -1.8387 | -4.4463 |
| 0.1825 | -1.3738 | -3.8639 |
| 3.1270 | 2.1586 | 0.6768 |
| 3.4773 | -0.7979 | 1.8442 |
| 2.4191 | -1.5269 | 3.0831 |
| 3.3641 | -2.5444 | 2.0075 |
| 0.3902 | 4.0619 | 3.1108 |
| 0.1503 | 4.3897 | 1.3876 |
| -0.6783 | 3.0391 | 2.1332 |
| -2.0585 | 2.4057 | -2.0168 |
| -1.3618 | -4.0348 | -1.6826 |
| 2.4816 | 5.1291 | 1.5694 |

| | | |
|---|---|---|
| -0.4371 | 1.6190 | -1.3311 |
| -1.5875 | 1.3707 | -0.0502 |
| 2.3768 | -3.2364 | -0.4983 |
| 1.4231 | 0.6370 | -0.3720 |
| 1.5234 | 2.4069 | 1.2302 |
| 2.5914 | 1.2618 | 2.0004 |
| 0.5384 | -0.2741 | 2.3725 |
| -0.4242 | 0.9654 | 1.6227 |
| -1.6587 | -0.8413 | 1.1980 |
| -2.3573 | -1.5152 | -0.2409 |
| -0.9580 | -2.2922 | 0.4917 |
| -2.7719 | -2.6108 | -3.7274 |
| -3.1140 | -1.8741 | -2.1921 |
| -0.1811 | -2.6821 | -4.4496 |
| -1.2405 | -1.5241 | -5.2350 |
| 0.3348 | -0.9995 | -4.6388 |
| 0.1749 | 3.8608 | 2.5501 |
| 3.6125 | -0.4899 | 1.1044 |
| 2.5619 | -1.2795 | 2.3131 |
| 3.5474 | -2.2420 | 1.2241 |
| 2.8202 | 1.4312 | 4.5877 |
| 1.3318 | 1.7664 | 5.4894 |
| 1.4107 | 0.3641 | 4.4410 |
| -3.5336 | 2.0093 | -2.8541 |
| -1.0684 | -3.8074 | -2.5410 |
| 2.1124 | 4.0212 | 5.0817 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7K** | | | |
|---|---|---|---|
| C | 2.6729 | 0.9586 | -1.4113 |
| C | 2.8093 | -0.0909 | -2.5097 |
| C | 1.4593 | -0.4797 | -3.1703 |
| C | 0.4508 | -0.8820 | -2.0319 |
| C | 0.2843 | 0.1270 | -0.8433 |
| C | 1.6999 | 0.5085 | -0.3252 |
| C | -0.9174 | -1.3694 | -2.5080 |
| C | -1.9525 | -1.6260 | -1.4829 |
| C | -1.7689 | -1.3260 | -0.1855 |
| C | -0.5085 | -0.6134 | 0.3287 |
| C | -0.9744 | 0.5273 | 4.0677 |
| C | -0.6163 | -0.3719 | 2.8982 |
| C | -0.7862 | 0.3295 | 1.5401 |
| C | -0.4732 | 1.4115 | -1.2631 |
| C | 1.0292 | 0.6709 | -4.1225 |
| C | 1.7679 | -1.7191 | -4.0582 |
| C | -2.1746 | 0.3919 | 4.6675 |
| C | -2.8242 | -1.7681 | 0.7961 |
| C | 0.0744 | 1.5402 | 4.4486 |
| O | -1.1811 | -1.6398 | -3.6785 |
| O | 3.9464 | 1.1534 | -0.7988 |
| O | -0.3534 | 0.7078 | -4.4169 |
| C | -2.6707 | 1.1665 | 5.8198 |
| O | -3.7709 | 1.6888 | 5.8387 |
| O | -1.8232 | 1.1495 | 6.8657 |
| H | 2.3649 | 1.9257 | -1.8188 |
| H | 3.5201 | 0.2677 | -3.2668 |
| H | 3.2850 | -0.9840 | -2.0788 |
| H | 0.8933 | -1.7891 | -1.5842 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7L** | | |
|---|---|---|
| 2.7043 | 0.8329 | -1.3124 |
| 2.8340 | -0.1961 | -2.4304 |
| 1.4905 | -0.5202 | -3.1361 |
| 0.4408 | -0.9173 | -2.0342 |
| 0.2762 | 0.0666 | -0.8239 |
| 1.6894 | 0.3916 | -0.2606 |
| -0.9297 | -1.3463 | -2.5574 |
| -1.9946 | -1.6039 | -1.5638 |
| -1.8343 | -1.3437 | -0.2548 |
| -0.5705 | -0.6768 | 0.3092 |
| -1.0605 | 0.4474 | 4.0500 |
| -0.7874 | -0.4808 | 2.8796 |
| -0.8611 | 0.2514 | 1.5292 |
| -0.4286 | 1.3852 | -1.2295 |
| 1.1246 | 0.6690 | -4.0677 |
| 1.7797 | -1.7461 | -4.0489 |
| -0.0642 | 0.7675 | 4.9006 |
| -2.9210 | -1.7907 | 0.6892 |
| -2.4982 | 0.8706 | 4.2117 |
| -1.1769 | -1.5683 | -3.7414 |
| 3.9813 | 0.9648 | -0.6916 |
| -0.2521 | 0.7698 | -4.3782 |
| -0.1691 | 1.6402 | 6.0853 |
| 0.2984 | 1.3385 | 7.1688 |
| -0.7475 | 2.8257 | 5.8159 |
| 2.4438 | 1.8154 | -1.7160 |
| 3.5785 | 0.1541 | -3.1586 |
| 3.2652 | -1.1157 | -2.0085 |
| 0.8417 | -1.8495 | -1.5993 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7M** | | |
|---|---|---|
| -3.1401 | -0.2695 | 0.5265 |
| -3.4785 | -1.4848 | -0.3304 |
| -2.3911 | -2.5913 | -0.2970 |
| -1.0092 | -1.9325 | -0.6575 |
| -0.6036 | -0.6492 | 0.1480 |
| -1.8010 | 0.3436 | 0.1240 |
| 0.1739 | -2.8960 | -0.7479 |
| 1.5190 | -2.3157 | -0.9516 |
| 1.7421 | -0.9904 | -0.9234 |
| 0.6408 | 0.0281 | -0.5907 |
| 2.2109 | 3.5858 | 0.0085 |
| 1.5974 | 2.4241 | -0.7528 |
| 1.1738 | 1.2761 | 0.1787 |
| -0.2341 | -0.9702 | 1.6180 |
| -2.4878 | -3.3353 | 1.0642 |
| -2.7909 | -3.6075 | -1.4048 |
| 3.5219 | 3.8656 | -0.1388 |
| 3.1175 | -0.5011 | -1.2994 |
| 1.2449 | 4.4067 | 0.8238 |
| 0.0667 | -4.1211 | -0.7434 |
| -4.1669 | 0.7008 | 0.3315 |
| -1.3006 | -3.9969 | 1.4576 |
| 4.2610 | 4.9604 | 0.5174 |
| 5.0081 | 5.7073 | -0.0887 |
| 4.0886 | 4.9830 | 1.8525 |
| -3.1454 | -0.5287 | 1.5890 |
| -4.4508 | -1.8886 | -0.0159 |
| -3.6362 | -1.1477 | -1.3653 |
| -1.1324 | -1.5944 | -1.7013 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7N** | | |
|---|---|---|
| -2.6300 | 0.7840 | 0.8454 |
| -3.2478 | 0.0347 | -0.3297 |
| -2.7069 | -1.4100 | -0.4967 |
| -1.1362 | -1.3434 | -0.5496 |
| -0.4191 | -0.5486 | 0.5976 |
| -1.1082 | 0.8393 | 0.7353 |
| -0.4321 | -2.6783 | -0.7881 |
| 1.0443 | -2.7005 | -0.7107 |
| 1.7608 | -1.6349 | -0.3133 |
| 1.1083 | -0.3306 | 0.1718 |
| 2.5872 | 2.4952 | -0.0695 |
| 3.0472 | 1.3398 | 0.8018 |
| 1.9288 | 0.3957 | 1.2856 |
| -0.4860 | -1.2866 | 1.9578 |
| -3.3419 | -2.3028 | 0.6060 |
| -3.2555 | -1.9089 | -1.8641 |
| 2.8636 | 2.4861 | -1.3897 |
| 3.2604 | -1.7226 | -0.4173 |
| 1.8301 | 3.5859 | 0.6430 |
| -1.0092 | -3.7139 | -1.1153 |
| -3.1429 | 2.1146 | 0.8347 |
| -2.6102 | -3.4757 | 0.9083 |
| 2.5024 | 3.5317 | -2.3638 |
| 1.9326 | 3.2866 | -3.4119 |
| 2.9473 | 4.7514 | -2.0086 |
| -2.9338 | 0.3361 | 1.7957 |
| -4.3410 | 0.0282 | -0.2194 |
| -3.0617 | 0.6118 | -1.2473 |
| -0.9182 | -0.7804 | -1.4739 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7O** | | |
|---|---|---|
| 2.4849 | 1.0166 | -1.5908 |
| 2.6890 | -0.1658 | -2.5259 |
| 1.3654 | -0.6984 | -3.1325 |
| 0.3651 | -0.9961 | -1.9601 |
| 0.1838 | 0.1003 | -0.8478 |
| 1.5801 | 0.6298 | -0.4224 |
| -1.0159 | -1.4900 | -2.3827 |
| -1.9761 | -1.7968 | -1.2962 |
| -1.7441 | -1.4376 | -0.0205 |
| -0.5137 | -0.6137 | 0.4014 |
| -0.9051 | 0.7222 | 4.0827 |
| -0.5370 | -0.2247 | 2.9548 |
| -0.8062 | 0.3801 | 1.5665 |
| -0.6802 | 1.3026 | -1.3154 |
| 0.8184 | 0.2693 | -4.2116 |
| 1.7322 | -2.0284 | -3.8498 |
| -2.0719 | 0.5545 | 4.7376 |
| -2.7060 | -1.9178 | 1.0358 |
| 0.0939 | 1.8160 | 4.3598 |
| -1.3626 | -1.6886 | -3.5418 |
| 3.7450 | 1.4089 | -1.0497 |
| 1.8431 | 0.6133 | -5.1437 |
| -2.5720 | 1.3702 | 5.8594 |
| -3.7000 | 1.8288 | 5.8890 |
| -1.6884 | 1.4679 | 6.8704 |
| 2.0825 | 1.8802 | -2.1284 |
| 3.4095 | 0.1044 | -3.3084 |
| 3.1893 | -0.9682 | -1.9638 |
| 0.8089 | -1.8665 | -1.4468 |

| | | | |
|---|---|---|---|
| H | 2.1418 | -0.3494 | 0.2014 |
| H | 1.6502 | 1.3038 | 0.4274 |
| H | -2.8447 | -2.1226 | -1.8508 |
| H | 0.1477 | -1.4192 | 0.6911 |
| H | 0.4227 | -0.7069 | 3.0134 |
| H | -1.2213 | -1.2825 | 2.9396 |
| H | -1.7867 | 0.7727 | 1.4600 |
| H | -0.0978 | 1.1778 | 1.5363 |
| H | -0.6132 | 2.0946 | -0.4194 |
| H | 0.0648 | 1.9889 | -2.0141 |
| H | -1.4667 | 1.1945 | -1.6666 |
| H | 1.5680 | 0.6028 | -5.0754 |
| H | 1.2897 | 1.6520 | -3.7194 |
| H | 0.9346 | -1.9861 | -4.7131 |
| H | 2.6289 | -1.5283 | -4.7106 |
| H | 2.0128 | -2.5963 | -3.4488 |
| H | -2.9174 | -0.2998 | 4.2796 |
| H | -3.6611 | -2.2745 | 0.3014 |
| H | -2.4019 | -2.4819 | 1.5094 |
| H | -3.2489 | -0.9198 | 1.3393 |
| H | 0.4033 | 2.1062 | 3.5717 |
| H | -0.2842 | 2.2757 | 5.1735 |
| H | 0.9453 | 1.0347 | 4.8777 |
| H | 4.5525 | 1.4951 | -1.4792 |
| H | -0.6489 | -0.1992 | -4.6461 |
| H | -1.0319 | 0.6025 | 6.7053 |

| | | |
|---|---|---|
| 2.0908 | -0.4906 | 0.2579 |
| 1.6432 | 1.1720 | 0.5077 |
| -2.8887 | -2.0697 | -1.9658 |
| 0.0533 | -1.5066 | 0.6742 |
| 0.2096 | -0.9299 | 2.9789 |
| -1.4932 | -1.3142 | 2.9265 |
| -1.8343 | 0.7417 | 1.4053 |
| -0.1331 | 1.0661 | 1.5841 |
| -0.5641 | 2.0532 | -0.3730 |
| 0.1457 | 1.9611 | -1.9545 |
| -1.4195 | 1.2111 | -1.6591 |
| 1.6735 | 0.6006 | -5.0147 |
| 1.4183 | 1.6292 | -3.6381 |
| 0.9542 | -1.9674 | -4.7302 |
| 2.6626 | -1.5679 | -4.6751 |
| 1.9799 | -2.6466 | -3.4574 |
| 0.9270 | 0.3361 | 4.7896 |
| -3.7550 | -2.2684 | 0.1621 |
| -2.5286 | -2.5303 | 1.3933 |
| -3.3424 | -0.9476 | 1.2430 |
| -3.1652 | 0.0136 | 4.0687 |
| -2.7138 | 1.2683 | 5.2073 |
| -2.7563 | 1.6359 | 3.4734 |
| 3.9266 | 1.6946 | -0.0507 |
| -0.5725 | -0.1160 | -4.6533 |
| -0.9709 | 2.9365 | 4.8735 |

| | | |
|---|---|---|
| -1.9054 | 0.7699 | -0.8838 |
| -1.6184 | 1.2056 | 0.7759 |
| 2.2960 | -3.0382 | -1.1807 |
| 0.2729 | 0.3822 | -1.5656 |
| 0.7237 | 2.7854 | -1.3103 |
| 2.2992 | 2.0649 | -1.5105 |
| 2.0031 | 0.9933 | 0.8394 |
| 0.4039 | 1.6809 | 0.8408 |
| 0.5865 | -1.6899 | 1.6921 |
| 0.0766 | -0.0738 | 2.1639 |
| -1.0744 | -1.3732 | 2.1825 |
| -3.2905 | -4.0822 | 1.0398 |
| -2.7532 | -2.6599 | 1.8804 |
| -2.1970 | -4.5243 | -1.3688 |
| -3.8398 | -3.9101 | -1.2980 |
| -2.6805 | -3.1728 | -2.4047 |
| 4.1421 | 3.3006 | -0.8293 |
| 3.8028 | -1.3272 | -1.5219 |
| 3.0658 | 0.1163 | -2.2009 |
| 3.5744 | 0.0746 | -0.4900 |
| 0.3313 | 4.5985 | 0.2509 |
| 0.9726 | 3.8759 | 1.7411 |
| 1.6481 | 5.3847 | 1.1011 |
| -4.0059 | 1.4325 | 0.9519 |
| -0.9715 | -4.5203 | 0.6956 |
| 3.5399 | 4.2460 | 2.1785 |

| | | |
|---|---|---|
| -0.8457 | 1.4688 | -0.1265 |
| -0.7337 | 1.3843 | 1.6090 |
| 1.5026 | -3.6242 | -1.0496 |
| 1.0894 | 0.3222 | -0.7107 |
| 3.8296 | 0.7721 | 0.2906 |
| 3.5459 | 1.7612 | 1.6851 |
| 2.3728 | -0.3490 | 1.9592 |
| 1.2751 | 0.9930 | 1.9260 |
| 0.0376 | -0.7330 | 2.7439 |
| -1.5066 | -1.4057 | 2.3203 |
| -0.0358 | -2.2826 | 1.9130 |
| -4.3543 | -2.6101 | 0.3173 |
| -3.4667 | -1.7629 | 1.5470 |
| -3.0857 | -2.9771 | -2.0212 |
| -4.3390 | -1.7515 | -1.9318 |
| -2.7979 | -1.3678 | -2.6999 |
| 3.3431 | 1.6299 | -1.8559 |
| 3.6374 | -0.9559 | -1.1005 |
| 3.7338 | -1.6080 | 0.5617 |
| 3.5921 | -2.6887 | -0.8150 |
| 2.4980 | 4.1209 | 1.3256 |
| 1.3860 | 4.3155 | -0.0392 |
| 1.0050 | 3.1690 | 1.2271 |
| -2.8102 | 2.5678 | 1.6281 |
| -2.3700 | -3.9154 | 0.0646 |
| 3.4648 | 4.7430 | -1.1821 |

| | | |
|---|---|---|
| 2.0960 | -0.1307 | 0.1806 |
| 1.4926 | 1.5007 | 0.2381 |
| -2.8492 | -2.3639 | -1.6021 |
| 0.2084 | -1.3515 | 0.7828 |
| 0.5250 | -0.4877 | 3.0440 |
| -1.0809 | -1.1661 | 3.0765 |
| -1.8375 | 0.7497 | 1.5046 |
| -0.1757 | 1.2686 | 1.4828 |
| -0.9140 | 1.9804 | -0.4884 |
| -0.1698 | 1.9249 | -2.0499 |
| -1.6352 | 0.9943 | -1.7498 |
| 0.4568 | 1.2053 | -3.7948 |
| 0.0025 | -0.1798 | -4.7836 |
| 0.8765 | -2.4601 | -4.3776 |
| 2.5264 | -1.8764 | -4.5900 |
| 2.0937 | -2.7788 | -3.1374 |
| -2.7850 | -0.2023 | 4.4224 |
| -3.5244 | -2.5093 | 0.6095 |
| -2.1893 | -2.5637 | 1.7517 |
| -3.1668 | -1.0815 | 1.5681 |
| 0.3559 | 2.3443 | 3.4380 |
| -0.2817 | 2.5731 | 5.0531 |
| 1.0089 | 1.3894 | 4.7831 |
| 4.3217 | 1.6370 | -1.8005 |
| 1.4048 | 1.0526 | -5.8937 |
| -0.8716 | 0.9588 | 6.7129 |

| (2*R**,4*S**,5*R**,9*S**,10*R**)-**7P** | | | |
|---|---|---|---|
| C | -2.6300 | 0.7322 | 0.8115 |
| C | -3.1532 | -0.0215 | -0.4015 |
| C | -2.6066 | -1.4698 | -0.5155 |
| C | -1.0363 | -1.4114 | -0.4277 |
| C | -0.3782 | -0.5230 | 0.6926 |
| C | -1.1092 | 0.8434 | 0.7559 |
| C | -0.3223 | -2.7578 | -0.4392 |
| C | 1.1577 | -2.7313 | -0.4177 |
| C | 1.8402 | -1.6078 | -0.1311 |
| C | 1.1490 | -0.2899 | 0.2665 |
| C | 2.5103 | 2.5670 | -0.1554 |
| C | 3.0194 | 1.4888 | 0.7855 |
| C | 1.9416 | 0.5315 | 1.3318 |
| C | -0.4372 | -1.1740 | 2.1008 |
| C | -3.3059 | -2.3547 | 0.5539 |
| C | -3.0217 | -1.9744 | -1.9252 |
| C | 2.7949 | 2.4913 | -1.4717 |
| C | 3.3392 | -1.6395 | -0.2687 |
| C | 1.6948 | 3.6595 | 0.4874 |
| O | -0.8901 | -3.8443 | -0.4911 |
| O | -3.1598 | 2.0553 | 0.8098 |
| O | -3.3714 | -3.7322 | 0.2178 |
| C | 2.3888 | 3.4521 | -2.5132 |
| O | 1.8556 | 3.1076 | -3.5527 |
| O | 2.7536 | 4.7164 | -2.2305 |
| H | -2.9557 | 0.2559 | 1.7410 |
| H | -4.2516 | -0.0217 | -0.3887 |
| H | -2.8903 | 0.5507 | -1.3033 |
| H | -0.7389 | -0.9467 | -1.3836 |

| | | | |
|---|---|---|---|
| H | -0.8347 | 1.4524 | -0.1169 |
| H | -0.7849 | 1.4289 | 1.6240 |
| H | 1.6396 | -3.6666 | -0.6831 |
| H | 1.1188 | 0.3022 | -0.6575 |
| H | 3.8225 | 0.9206 | 0.3073 |
| H | 3.5019 | 1.9852 | 1.6383 |
| H | 2.4181 | -0.1540 | 2.0447 |
| H | 1.2652 | 1.1391 | 1.9383 |
| H | -1.4515 | -1.2230 | 2.4971 |
| H | -0.0259 | -2.1871 | 2.1173 |
| H | 0.1249 | -0.5923 | 2.8384 |
| H | -4.3464 | -2.0348 | 0.6810 |
| H | -2.8435 | -2.2801 | 1.5348 |
| H | -2.6517 | -2.9820 | -2.1363 |
| H | -4.1132 | -1.9946 | -2.0260 |
| H | -2.6328 | -1.3186 | -2.7128 |
| H | 3.3196 | 1.6327 | -1.8816 |
| H | 3.6667 | -0.9018 | -1.0071 |
| H | 3.8287 | -1.4421 | 0.6890 |
| H | 3.7021 | -2.6145 | -0.6139 |
| H | 2.3328 | 4.2726 | 1.1318 |
| H | 1.2125 | 4.3178 | -0.2398 |
| H | 0.8928 | 3.2388 | 1.0999 |
| H | -4.1306 | 1.9881 | 0.8097 |
| H | -2.4669 | -4.0315 | -0.0202 |
| H | 3.2493 | 4.7929 | -1.3942 |