BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

# Supporting Information

for

# Anti-inflammatory aromadendrane- and cadinane-type sesquiterpenoids from the South China Sea sponge *Acanthella cavernosa*

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## HPLC chromatograms of 4 and 5, chiral separation of 4 and 5, X-ray crystallographic data for 2, spectra of compounds (+)-1, 4 and 5, TDDFT-ECD calculation of compound (+)-1

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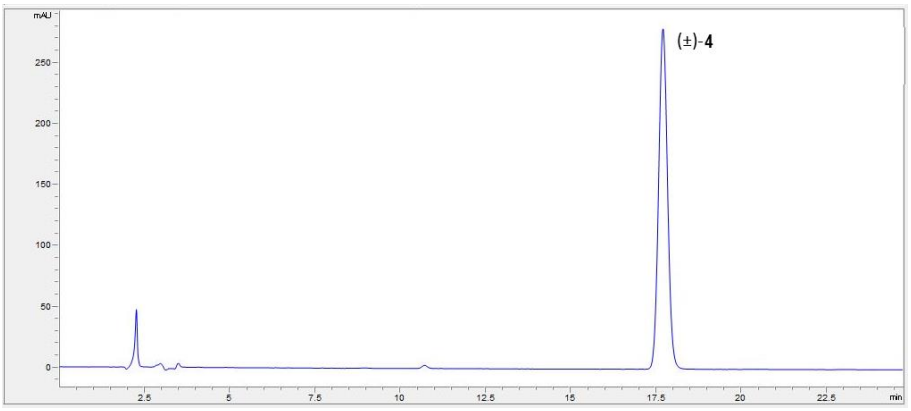
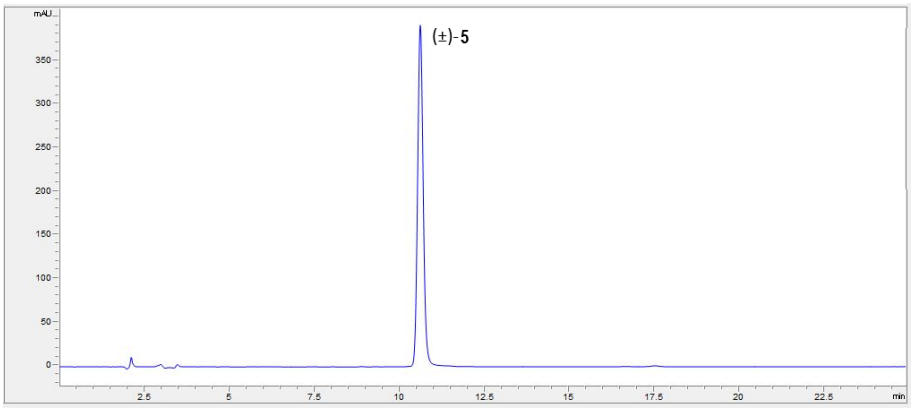
## 1. HPLC chromatograms of compounds 4 and 5.

Chromatographic conditions: An Agilent Eclipse XDB-$C_{18}$ column (5 μm, 9.4 × 250 mm), MeCN:$H_2O$ (35:65), 3.0 mL/min, 210 nm, (±)-**4** ($t_R$ = 17.6 min), (±)-**5** ($t_R$ = 10.6 min).

A




B




C

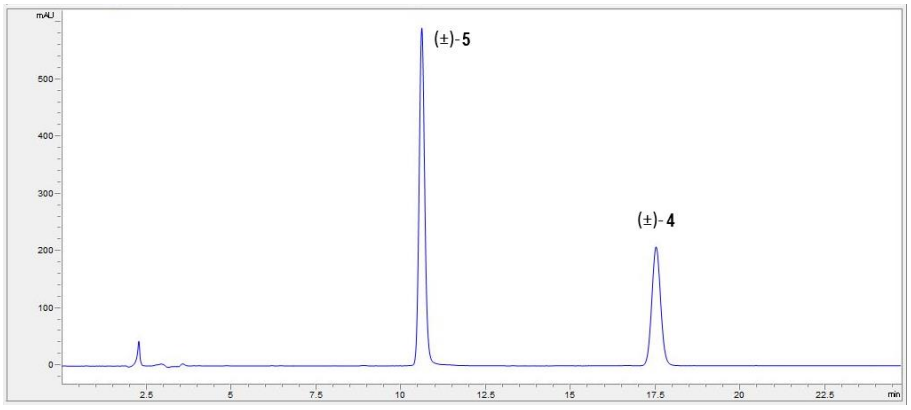



**Figure S1**. RP-HPLC chromatograms of compounds (±)-**4** (A), (±)-**5** (B) and mixture of (±)-**4** and (±)-**5** (C).

## 2. Chiral separation of compounds 4 and 5.

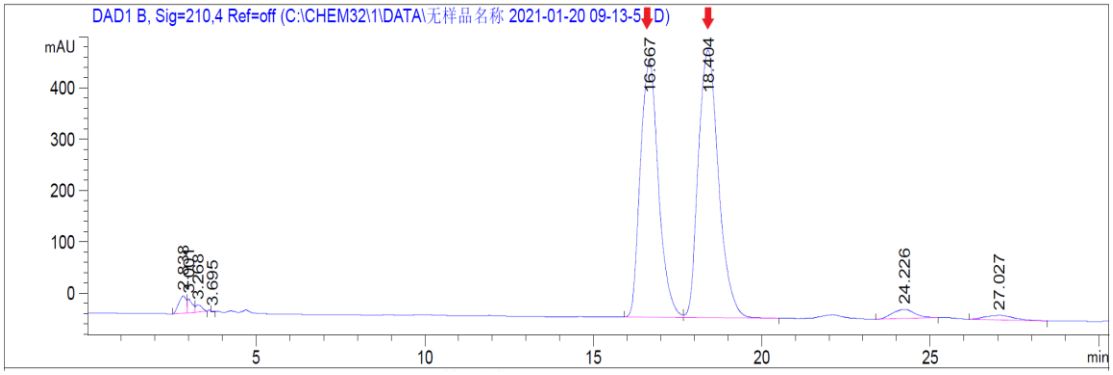



**Figure S2**. Chiral HPLC separation chromatography of compound **4**, (−)-**4**, $t_R$ = 16.7 min and (+)-**4**, $t_R$ = 18.4 min.

| n | Average | Std.Dev. | Maximum | Minimum |
|---|---|---|---|---|
| 6 | 26.042 | 0.4658 | 26.250 | 25.000 |

| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | JD5D-2 | 08:25:52 PM | 25.000 | SR | 0.020 | 589 | 100.00 | 0.080 | 20.0 | |
| 2 | JD5D-2 | 08:26:04 PM | 26.250 | SR | 0.021 | 589 | 100.00 | 0.080 | 20.0 | |
| 3 | JD5D-2 | 08:26:12 PM | 26.250 | SR | 0.021 | 589 | 100.00 | 0.080 | 20.0 | |
| 4 | JD5D-2 | 08:26:20 PM | 26.250 | SR | 0.021 | 589 | 100.00 | 0.080 | 19.9 | |
| 5 | JD5D-2 | 08:26:27 PM | 26.250 | SR | 0.021 | 589 | 100.00 | 0.080 | 19.9 | |
| 6 | JD5D-2 | 08:26:35 PM | 26.250 | SR | 0.021 | 589 | 100.00 | 0.080 | 19.9 | |

**Figure S3**. Specific optical rotation of (+)-**4**.

| n | Average | Std.Dev. | Maximum | Minimum |
|---|---|---|---|---|
| 6 | -24.167 | 0.5893 | -23.750 | -25.000 |

| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | JD5D-1 | 08:53:26 PM | -23.750 | SR | -0.019 | 589 | 100.00 | 0.080 | 19.8 | |
| 2 | JD5D-1 | 08:53:34 PM | -23.750 | SR | -0.019 | 589 | 100.00 | 0.080 | 19.8 | |
| 3 | JD5D-1 | 08:53:42 PM | -23.750 | SR | -0.019 | 589 | 100.00 | 0.080 | 19.8 | |
| 4 | JD5D-1 | 08:53:49 PM | -23.750 | SR | -0.019 | 589 | 100.00 | 0.080 | 19.8 | |
| 5 | JD5D-1 | 08:53:57 PM | -25.000 | SR | -0.020 | 589 | 100.00 | 0.080 | 19.8 | |
| 6 | JD5D-1 | 08:54:05 PM | -25.000 | SR | -0.020 | 589 | 100.00 | 0.080 | 19.8 | |

**Figure S4**. Specific optical rotation of (−)-**4**.

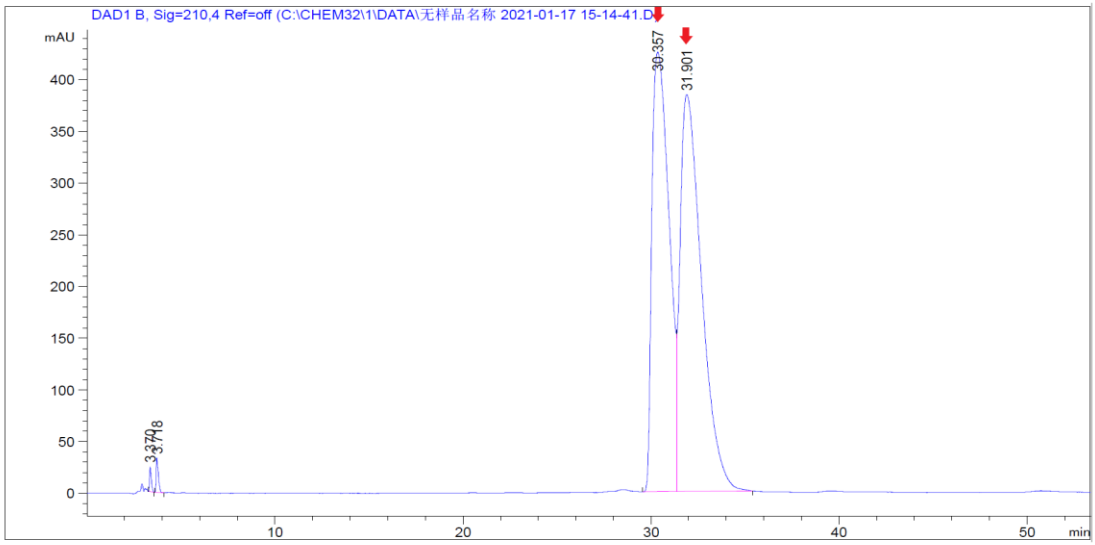



**Figure S5**. Chiral HPLC separation chromatography of compound **5**, (+)-**5**, $t_R$ = 30.4 min, (−)-**5**, $t_R$ = 31.9 min.

| n | Average | Std.Dev. | Maximum | Minimum |
|---|---|---|---|---|
| 6 | 8.750 | 0.0000 | 8.750 | 8.750 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | JD4B5A1 | 06:56:24 PM | 8.750 | SR | 0.007 | 589 | 100.00 | 0.080 | 20.2 | |
| 2 | JD4B5A1 | 06:56:31 PM | 8.750 | SR | 0.007 | 589 | 100.00 | 0.080 | 20.1 | |
| 3 | JD4B5A1 | 06:56:38 PM | 8.750 | SR | 0.007 | 589 | 100.00 | 0.080 | 20.1 | |
| 4 | JD4B5A1 | 06:56:45 PM | 8.750 | SR | 0.007 | 589 | 100.00 | 0.080 | 20.1 | |
| 5 | JD4B5A1 | 06:56:51 PM | 8.750 | SR | 0.007 | 589 | 100.00 | 0.080 | 20.0 | |
| 6 | JD4B5A1 | 06:56:58 PM | 8.750 | SR | 0.007 | 589 | 100.00 | 0.080 | 20.0 | |

**Figure S6**. Specific optical rotation of (+)-**5**.

| n | Average | Std.Dev. | Maximum | Minimum |
|---|---|---|---|---|
| 6 | -8.333 | 0.5322 | -7.143 | -8.571 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | JD4B5A2 | 07:16:56 PM | -8.571 | SR | -0.006 | 589 | 100.00 | 0.070 | 19.8 | |
| 2 | JD4B5A2 | 07:17:03 PM | -8.571 | SR | -0.006 | 589 | 100.00 | 0.070 | 19.8 | |
| 3 | JD4B5A2 | 07:17:10 PM | -8.571 | SR | -0.006 | 589 | 100.00 | 0.070 | 19.8 | |
| 4 | JD4B5A2 | 07:17:23 PM | -8.571 | SR | -0.006 | 589 | 100.00 | 0.070 | 19.8 | |
| 5 | JD4B5A2 | 07:17:29 PM | -8.571 | SR | -0.006 | 589 | 100.00 | 0.070 | 19.8 | |
| 6 | JD4B5A2 | 07:17:36 PM | -7.143 | SR | -0.005 | 589 | 100.00 | 0.070 | 19.8 | |

**Figure S7**. Specific optical rotation of (−)-**5**.

**3. X-ray crystallographic data for 2**.

The crystal of **2** was recrystallized from MeCN at 4 °C. X-ray analysis was carried out on a Bruker D8 Venture diffractometer with Cu Kα radiation (λ = 1.54178 Å) at 170 K. $C_{15}H_{26}O_2$, $M_r$ = 238.36, orthorhombic, crystal size 0.15 × 0.08 × 0.05 $mm^3$, space group $C222_1$, $a$ = 10.6819(3) Å, $b$ = 16.0392(3) Å, $c$ = 16.6572(4) Å, $V$ = 2853.86(12) $Å^3$, $Z$ = 8, $\rho_{calcd}$ = 1.110 $g/cm^3$, F(000) = 1056.0, 15570 collected reflections, 2865 independent reflections ($R_{int}$ = 0.0397, $R_{sigma}$ = 0.0243), final $R$ indexes [I ≥ 2σ (I)]: $R_1$ = 0.0501, $wR_2$ = 0.1269), final $R$ indexes (all data): $R_1$ = 0.0557, $wR_2$ = 0.1329, Flack parameter = 0.00(11). Crystallographic data (excluding structure factors) for the structure in this paper have been deposited with the Cambridge Crystallographic Data Center as supplementary publication CCDC 2173439.

## 4. NMR, MS and IR spectra of compounds (+)-1, 4, and 5.

### 4.1. Original spectra of (+)-**1**.

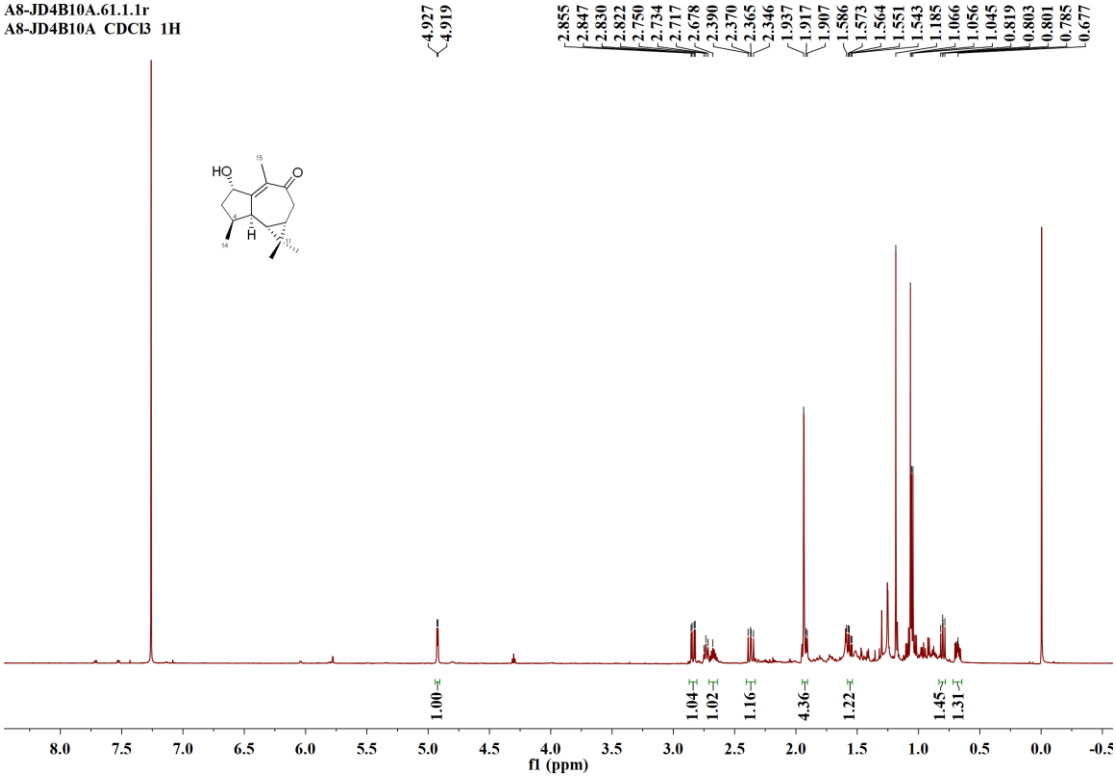



**Figure S8.** $^{1}$H NMR spectrum (600 MHz) of (+)-**1** in $CDCl_3$.

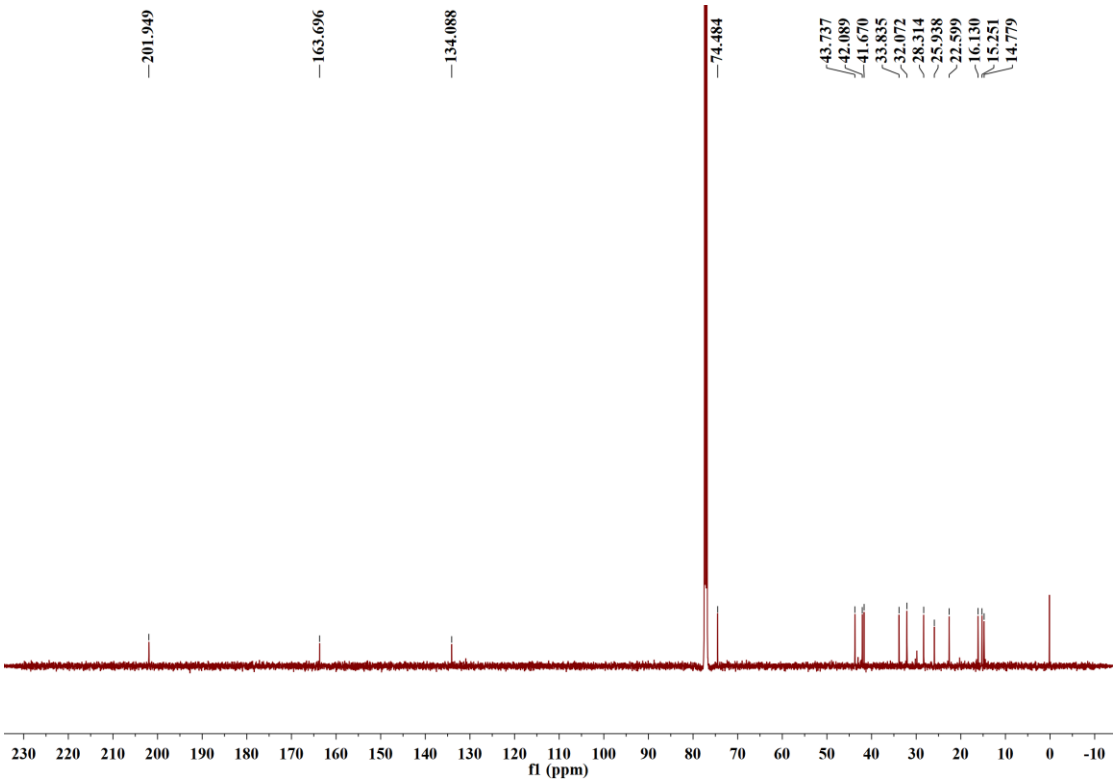



**Figure S9.** $^{13}$C NMR spectrum (125 MHz) of (+)-**1** in $CDCl_3$.

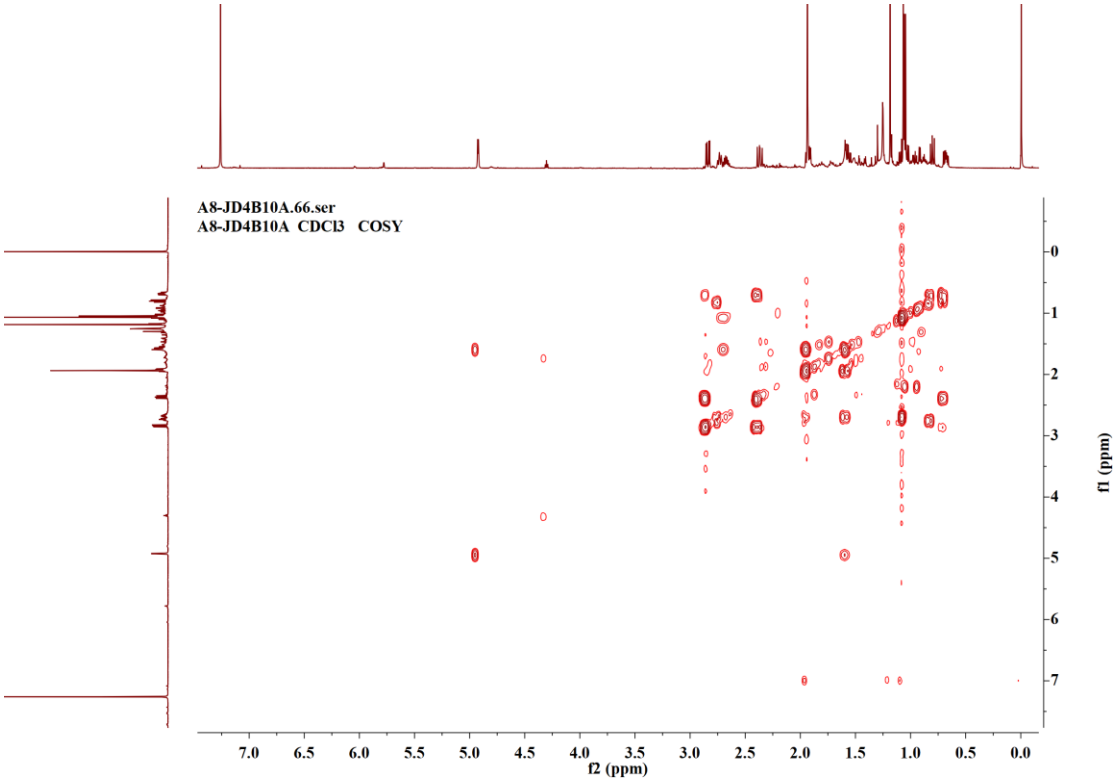



**Figure S10.** $^{1}H$-$^{1}H$ COSY spectrum of (+)-**1** in $CDCl_3$.

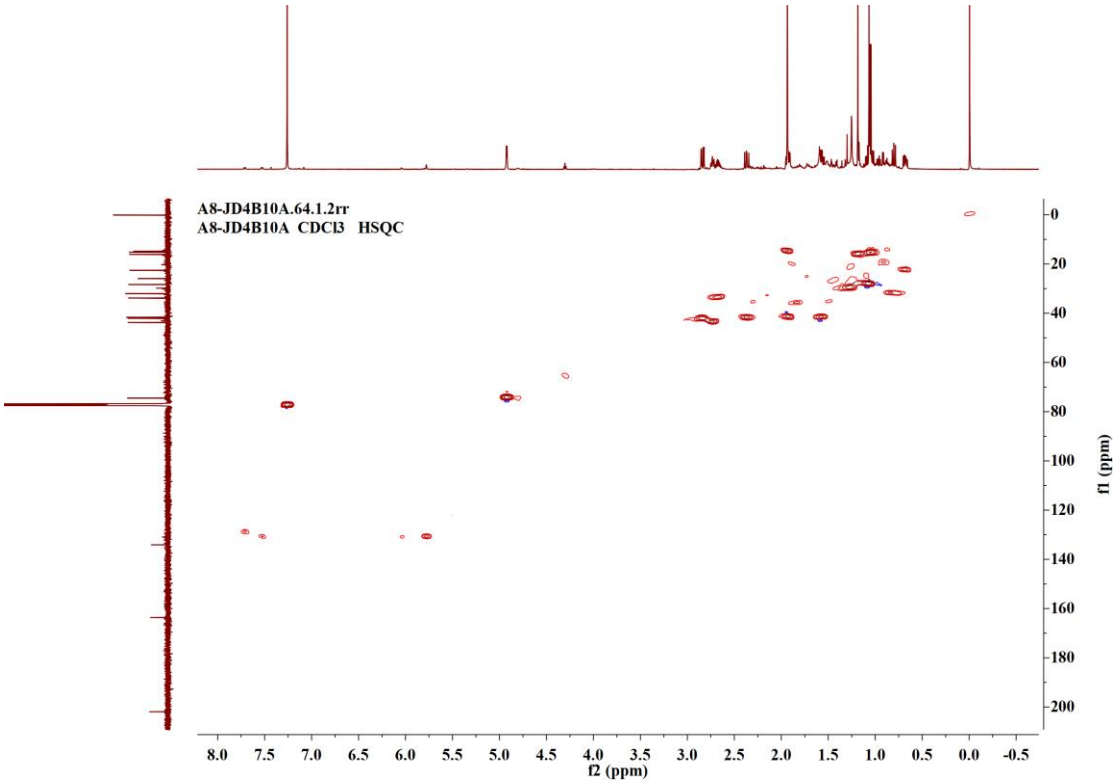



**Figure S11.** HSQC spectrum of (+)-**1** in $CDCl_3$.

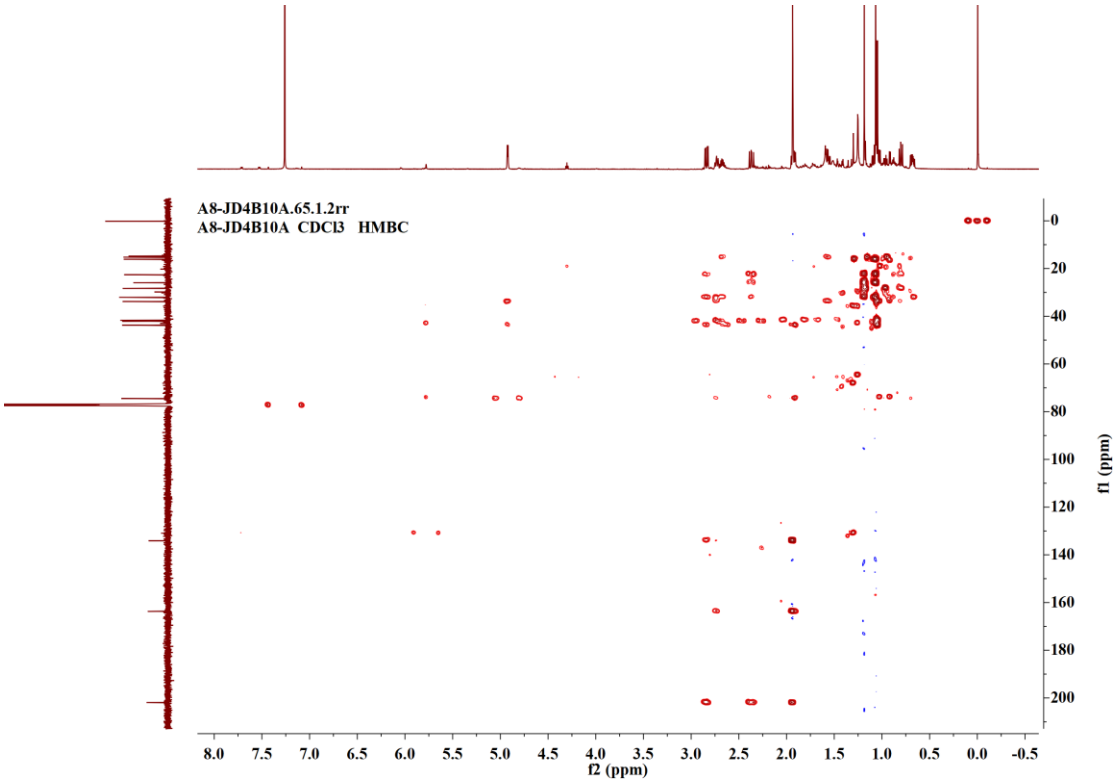



**Figure S12.** HMBC spectrum of (+)-**1** in $CDCl_3$.

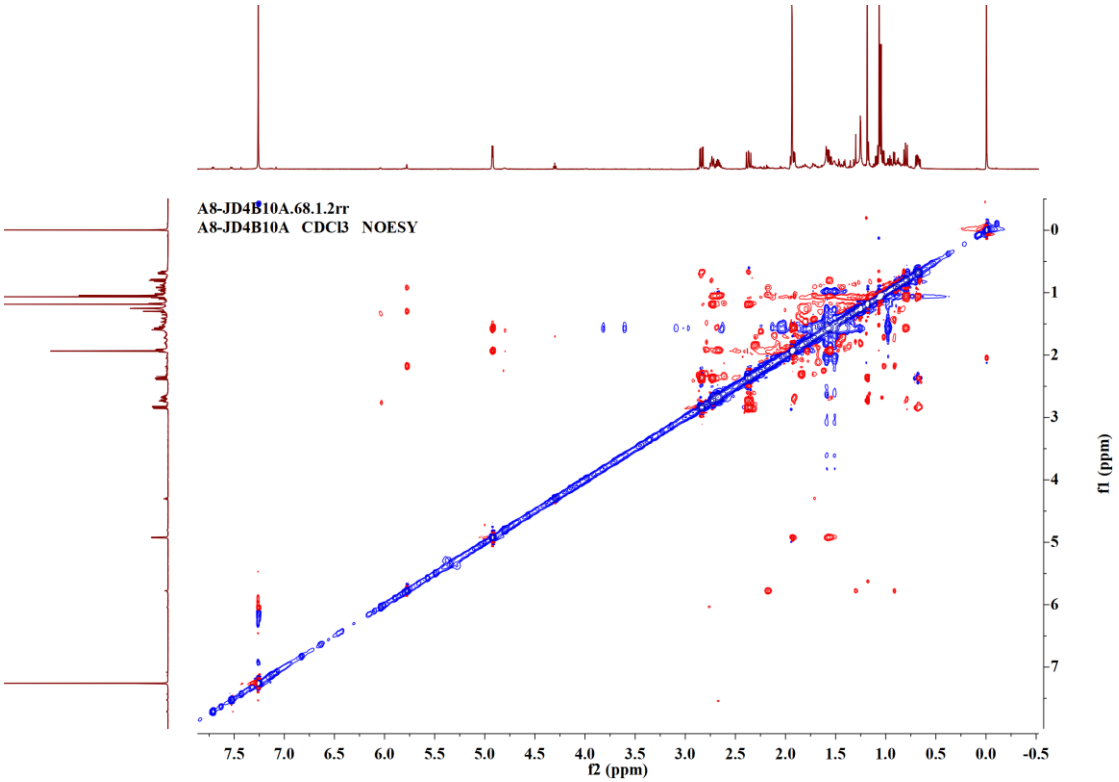


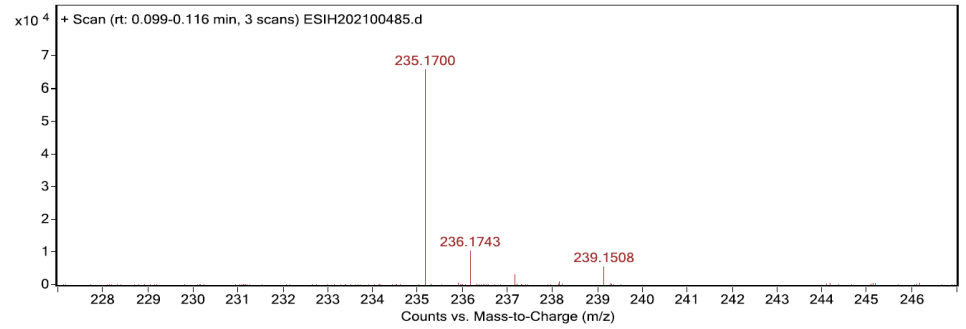

**Figure S13.** NOESY spectrum of (+)-**1** in $CDCl_3$.

**Qualitative Analysis Report**

| | | | |
|---|---|---|---|
| **Data Filename** | ESIH202100485.d | **Sample Name** | A8-JD4B10A |
| **Sample ID** | | **Position** | P1-A1 |
| **Instrument Name** | Agilent G6520 Q-TOF | **Acq Method** | 20160322_MS_ESIH_POS_1min.m |
| **Acquired Time** | 1/22/2021 17:18:11 | **IRM Calibration Status** | Success |
| **DA Method** | small molecular data analysis method.m | **Comment** | ESIH by ZZY |

**User Spectra**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 135 | 0 | ESI |




**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 235.17 | 235.1693 | -0.71 | -3.03 | C15 H23 O2 | (M+H)+ |

--- End Of Report ---

**Figure S14.** HRESIMS of (+)-**1**.

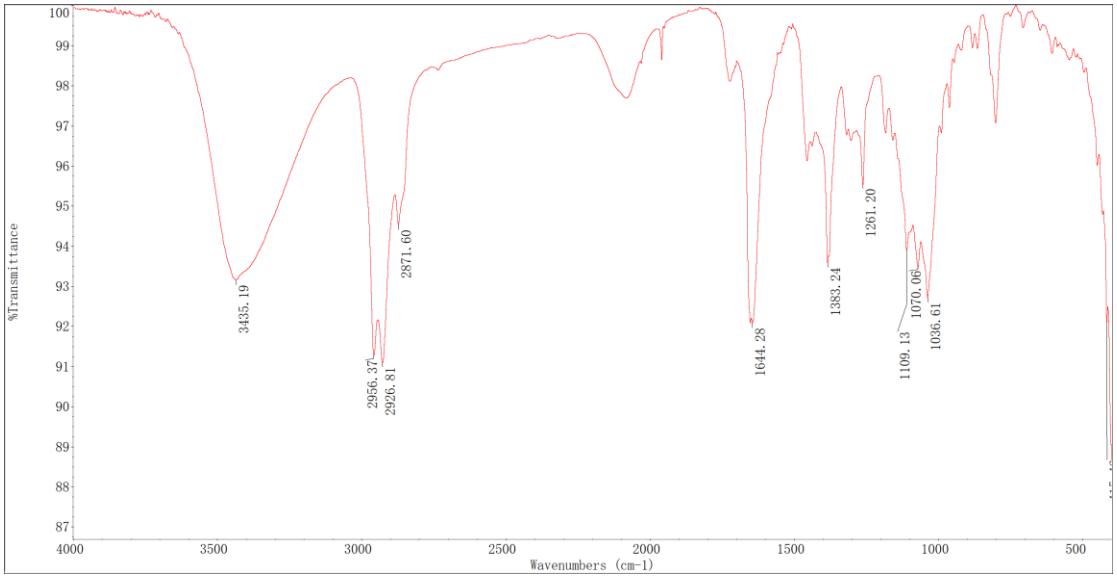



**Figure S15.** IR spectrum of (+)-**1**.

**4.2.** original spectra of **4**.

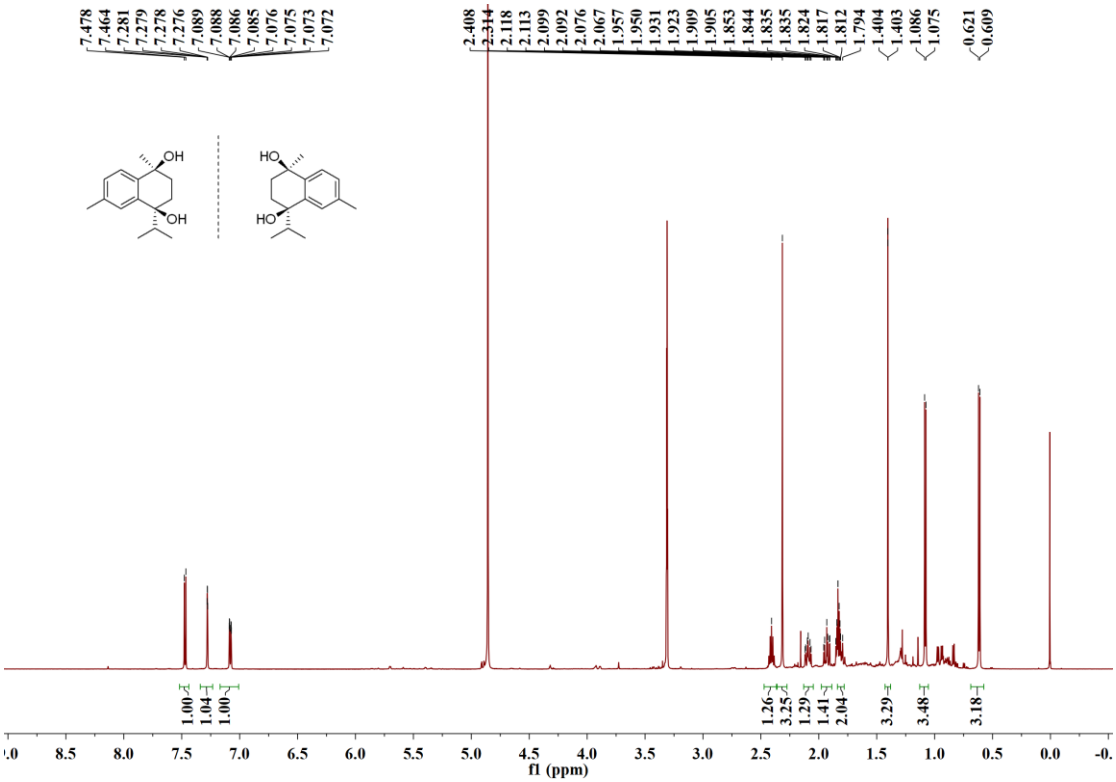



**Figure S16.** $^{1}$H NMR spectrum (600 MHz) of **4** in $CD_3OD$.

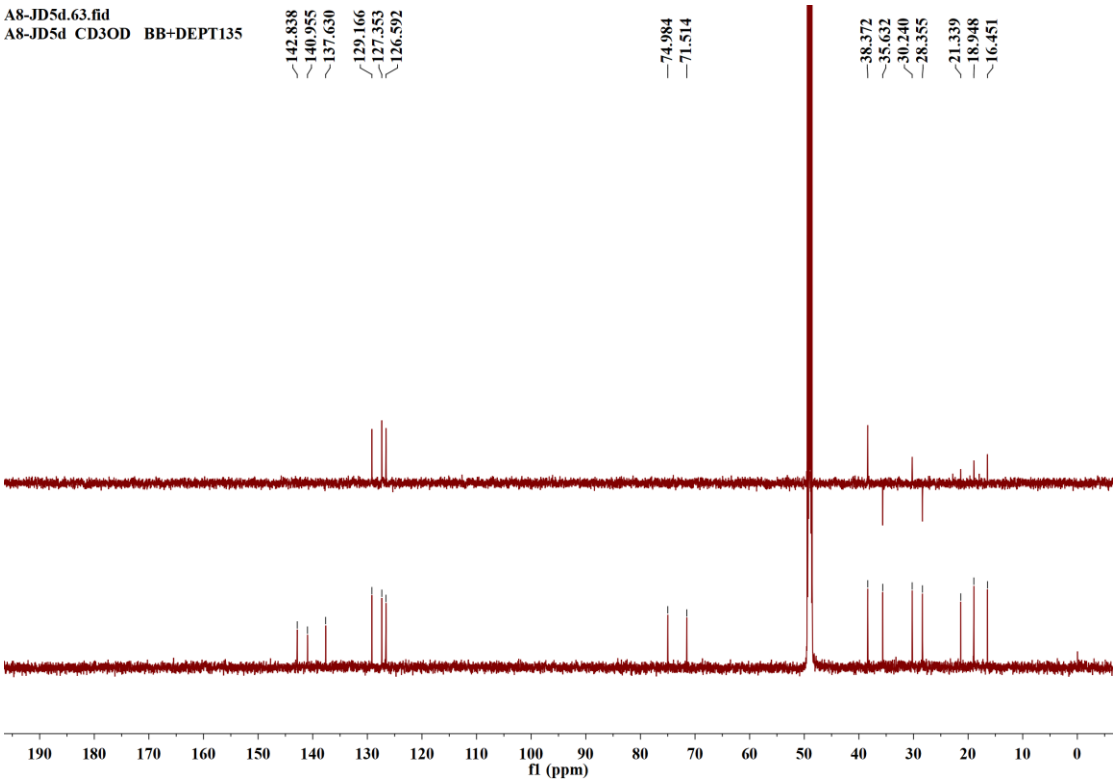



**Figure S17.** $^{13}$C NMR spectrum (125 MHz) of **4** in $CD_3OD$.

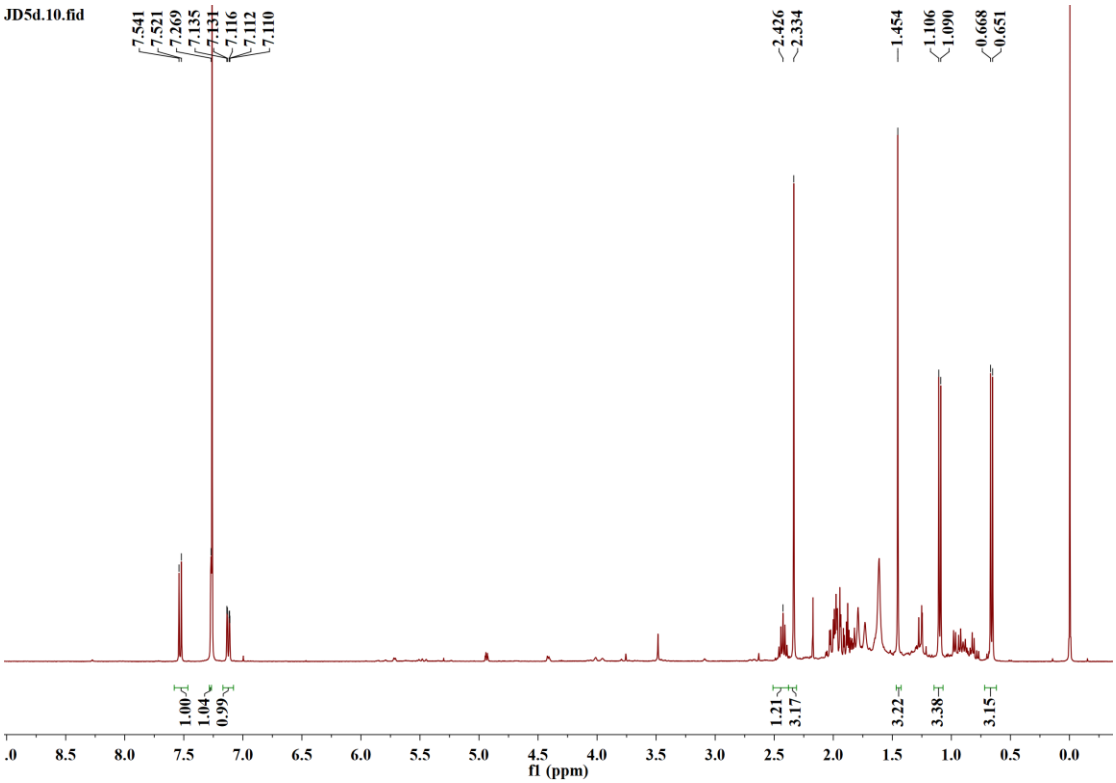



**Figure S18.** $^{1}$H NMR spectrum (400 MHz) of **4** in $CDCl_3$.

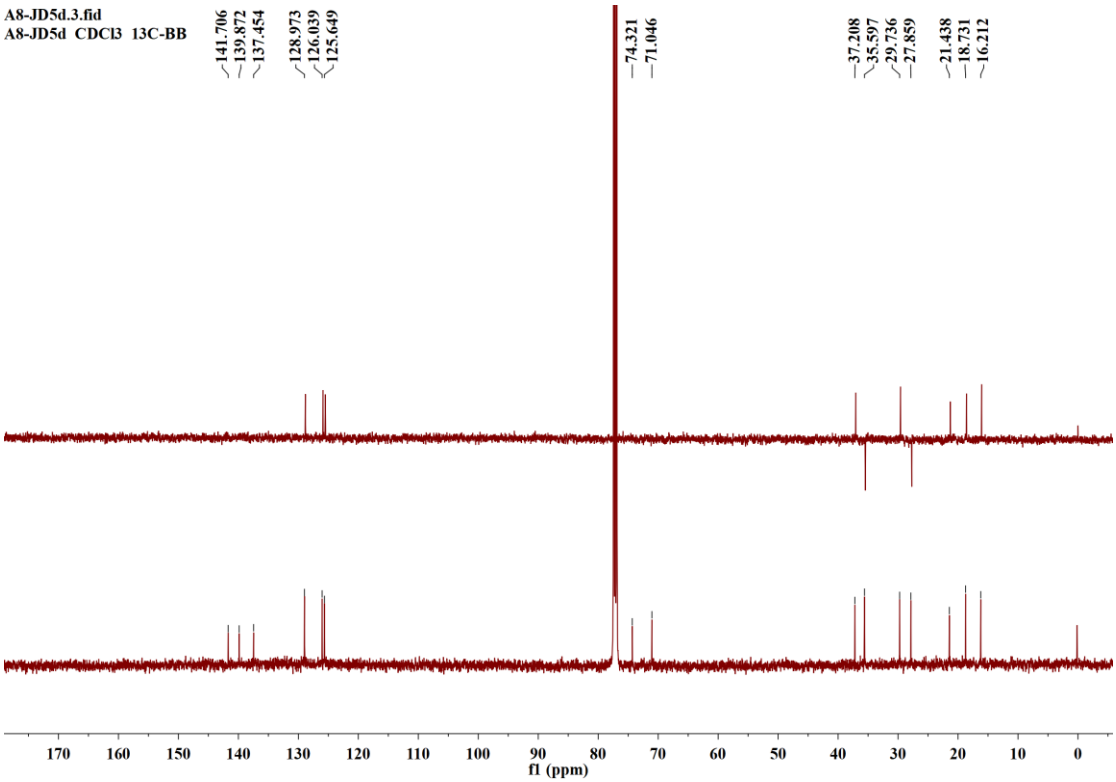



**Figure S19.** $^{13}$C NMR spectrum (150 MHz) of **4** in $CDCl_3$.

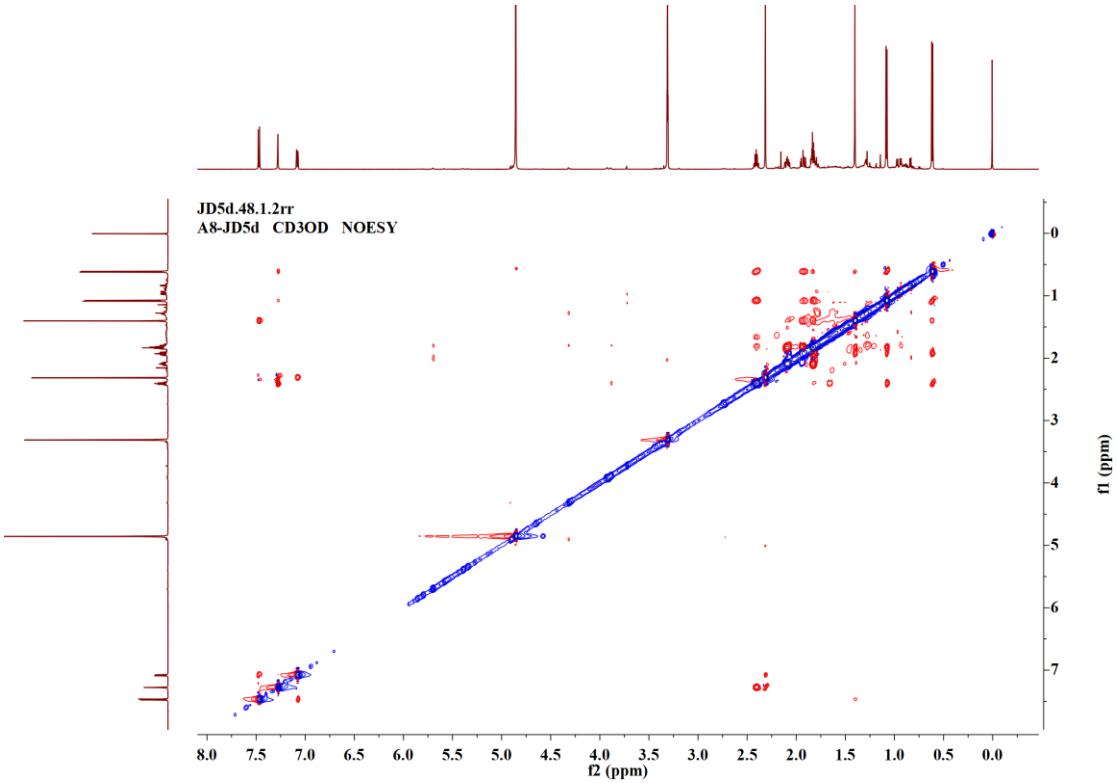



**Figure S20.** NOESY spectrum of **4** in $CD_3OD$.

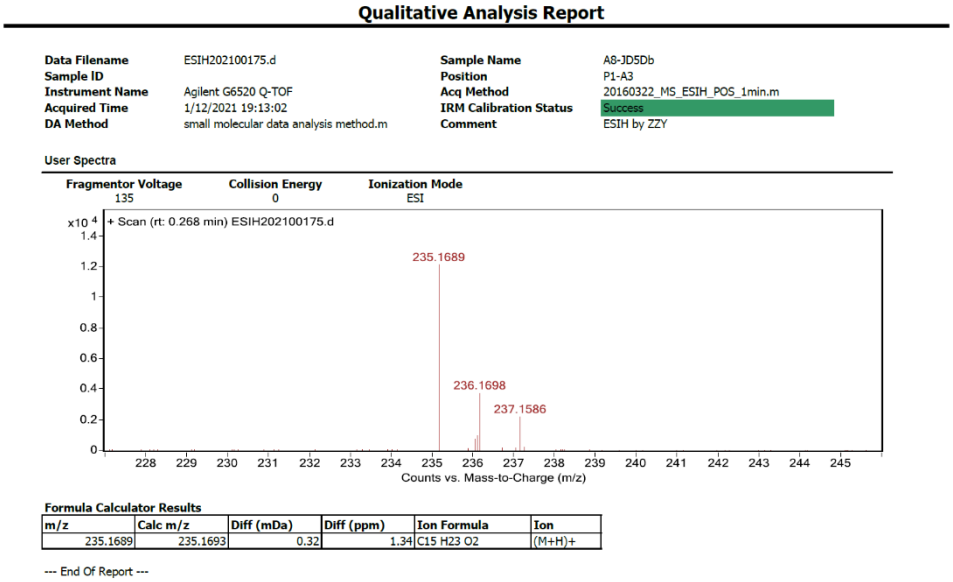



**Figure S21.** HRESIMS of **4**.

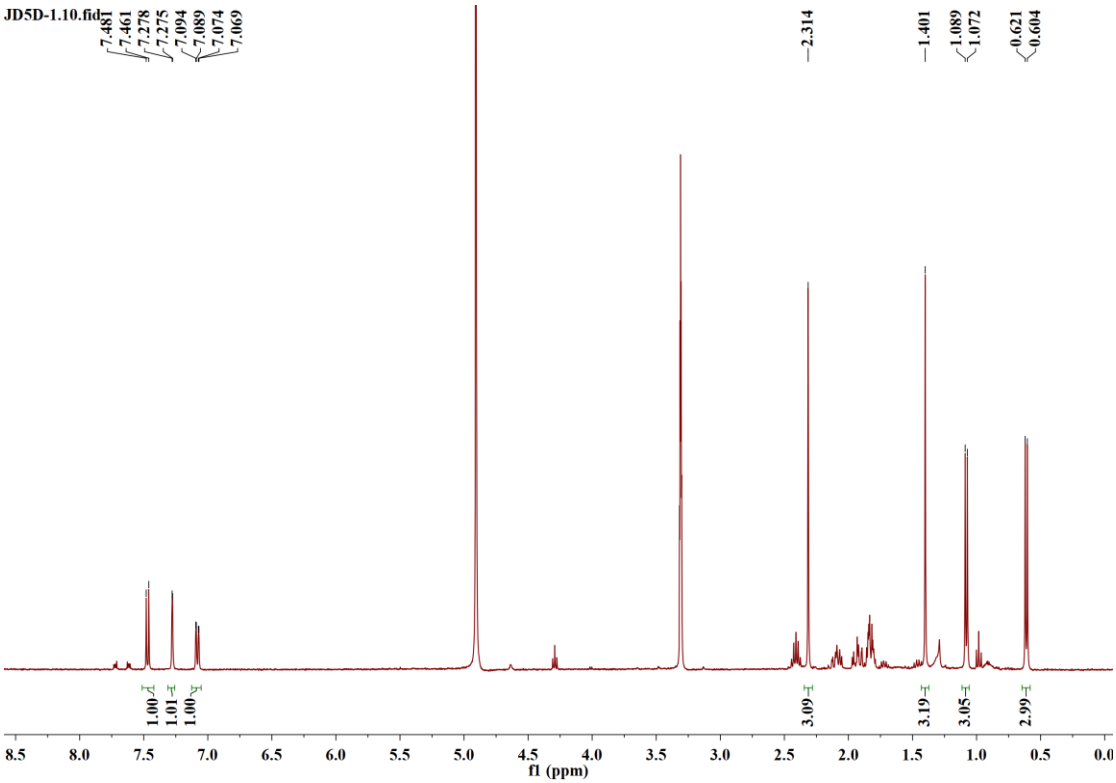



**Figure S22.** $^{1}$H NMR spectrum (400 MHz) of (+)-**4** in $CD_3OD$.

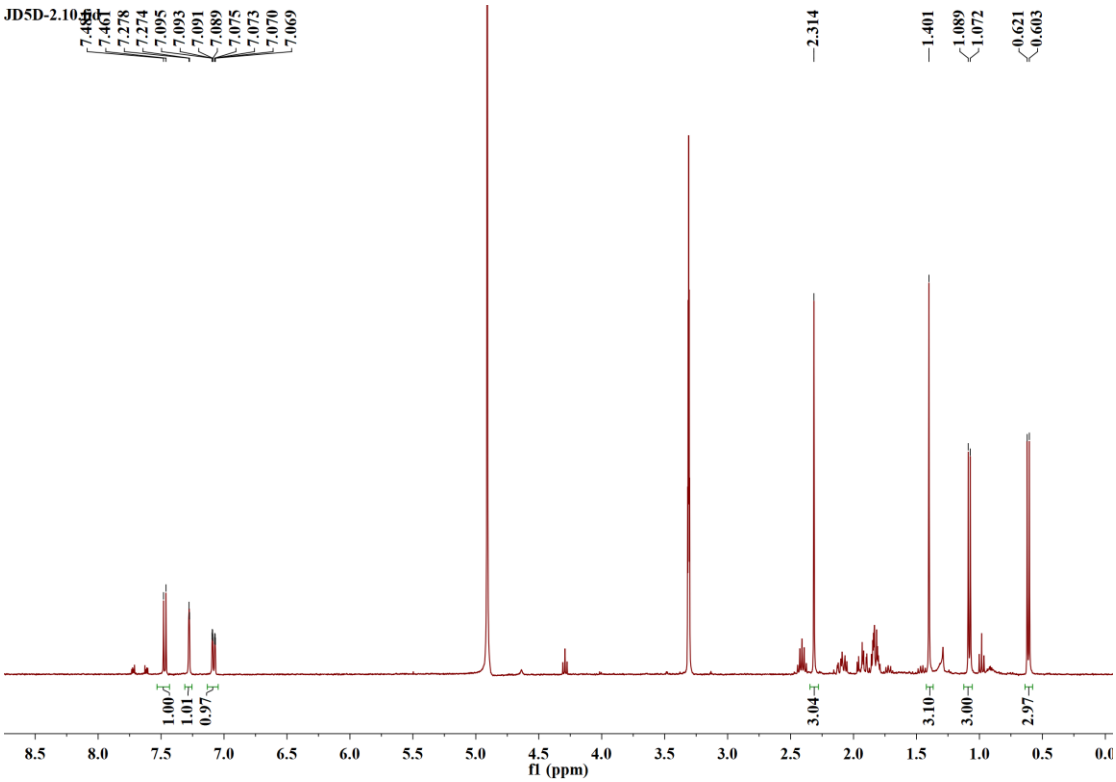



**Figure S23.** $^{1}$H NMR spectrum (400 MHz) of (−)-**4** in $CD_3OD$.

**4.3.** original spectra of **5**.

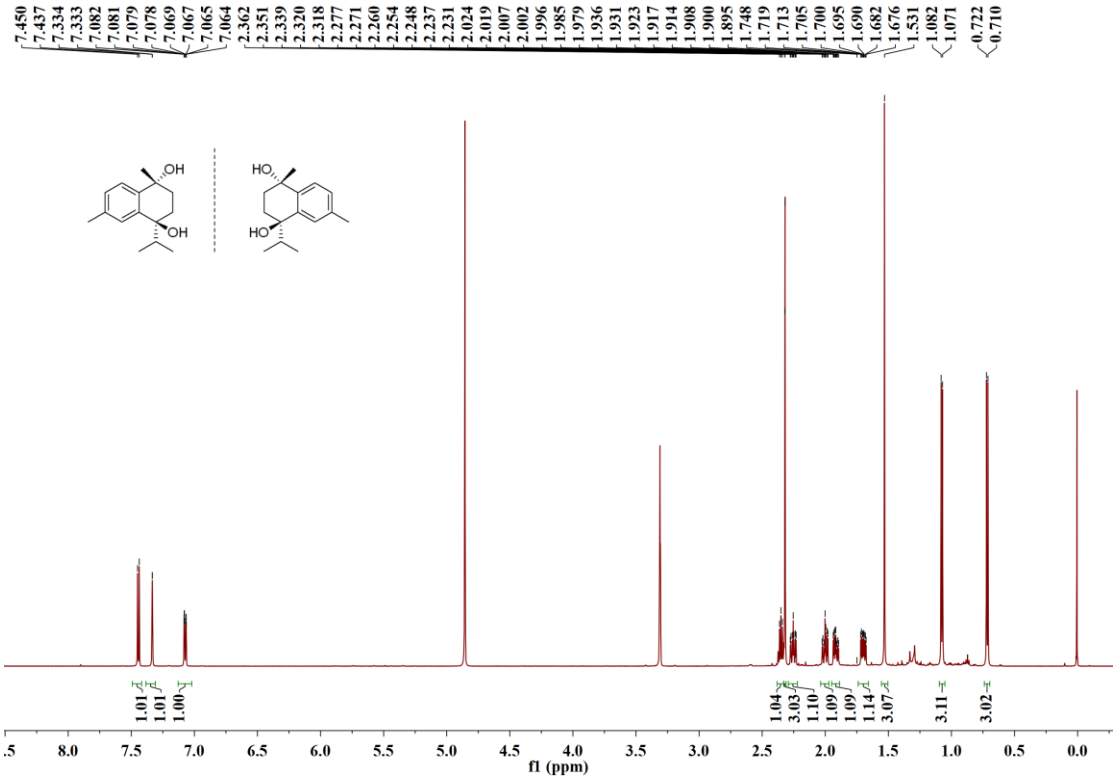



**Figure S24.** $^{1}$H NMR spectrum (600 MHz) of **5** in $CD_3OD$.

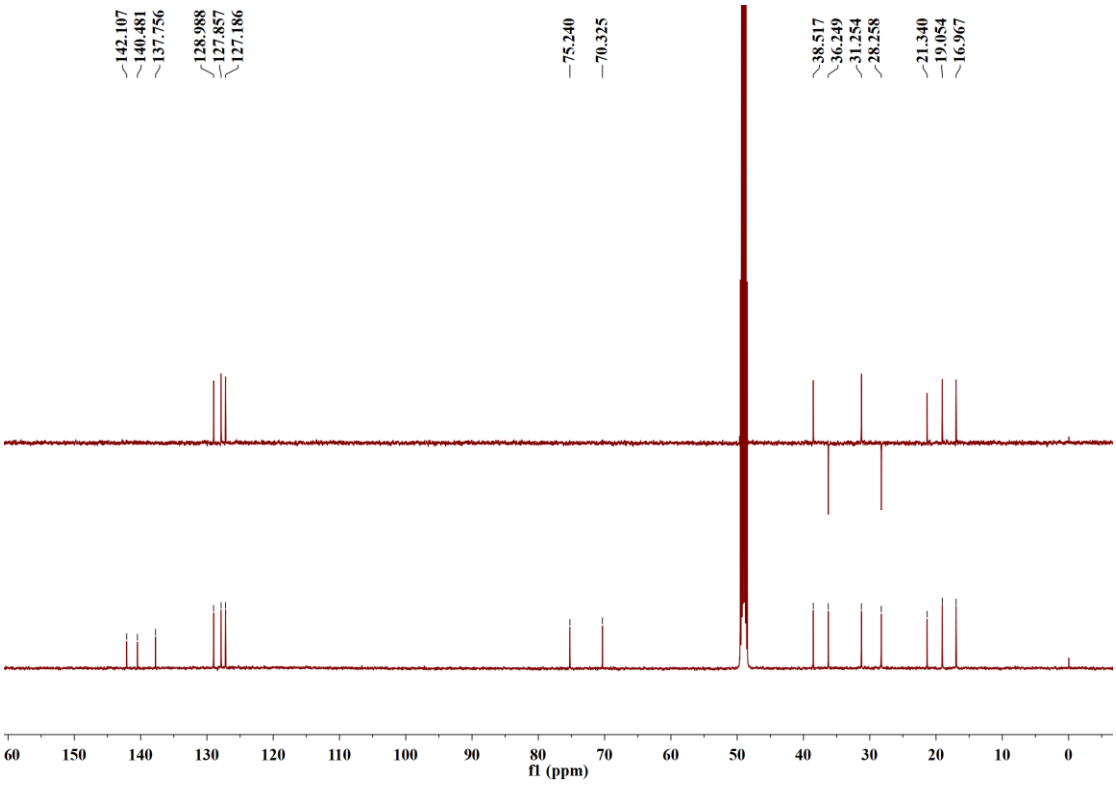



**Figure S25.** $^{13}$C NMR spectrum (125 MHz) of **5** in $CD_3OD$.

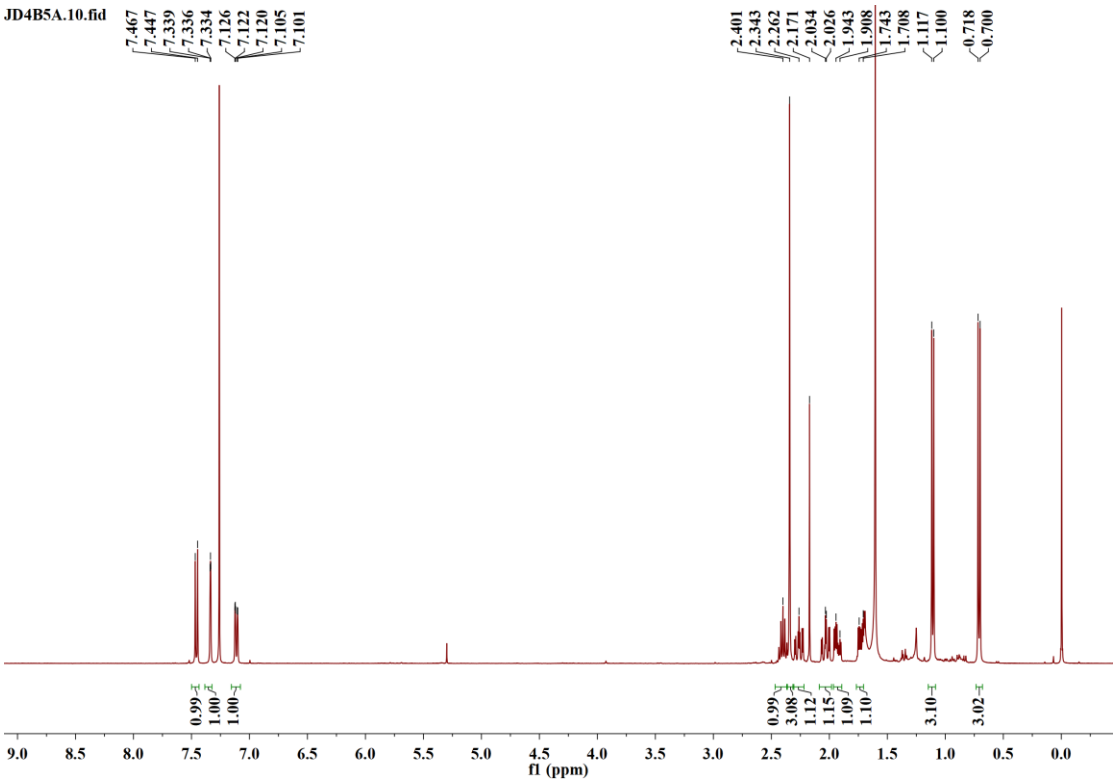



**Figure S26.** $^{1}$H NMR spectrum (400 MHz) of **5** in $CDCl_3$.

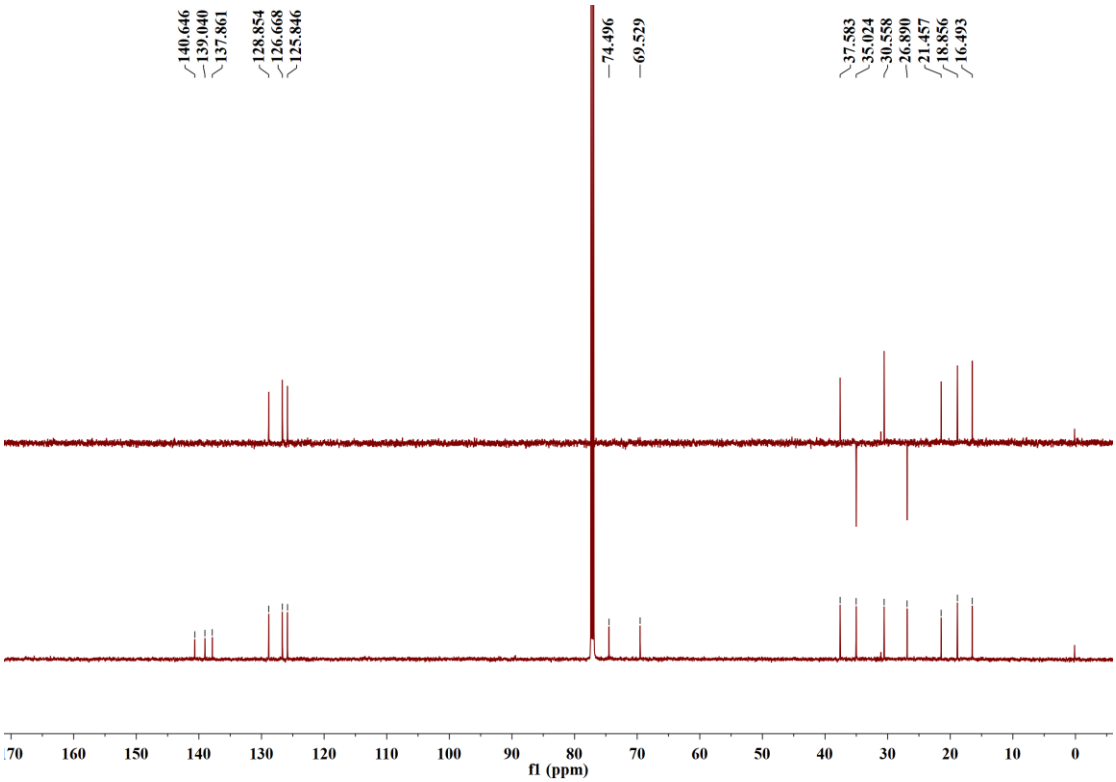



**Figure S27.** $^{13}$C NMR spectrum (150 MHz) of **5** in $CDCl_3$.

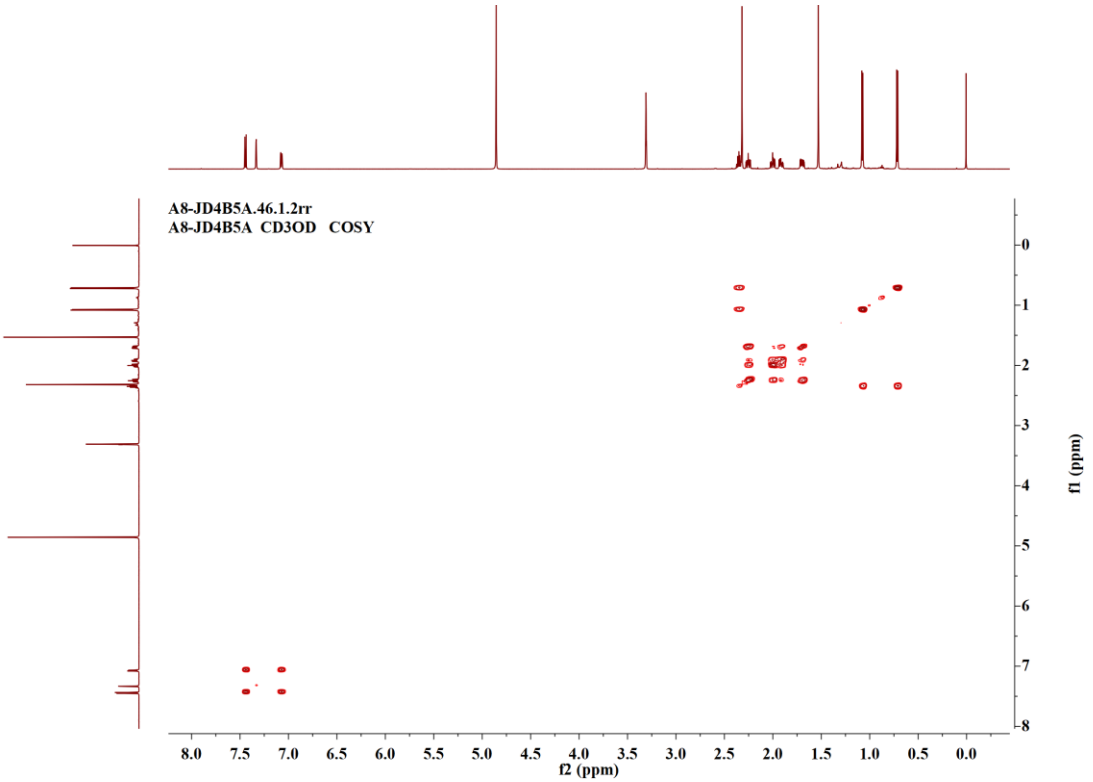



**Figure S28.** $^{1}$H-$^{1}$H COSY spectrum of **5** in $CD_3OD$.

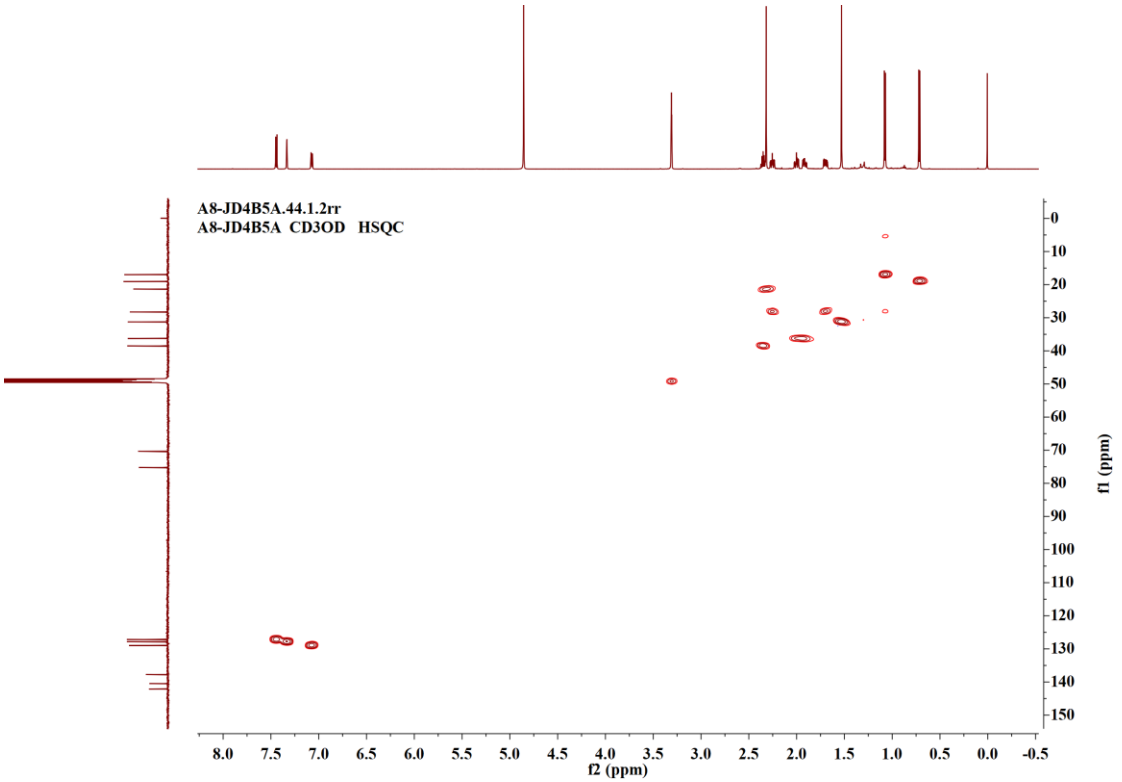



**Figure S29.** HSQC spectrum of **5** in $CD_3OD$.

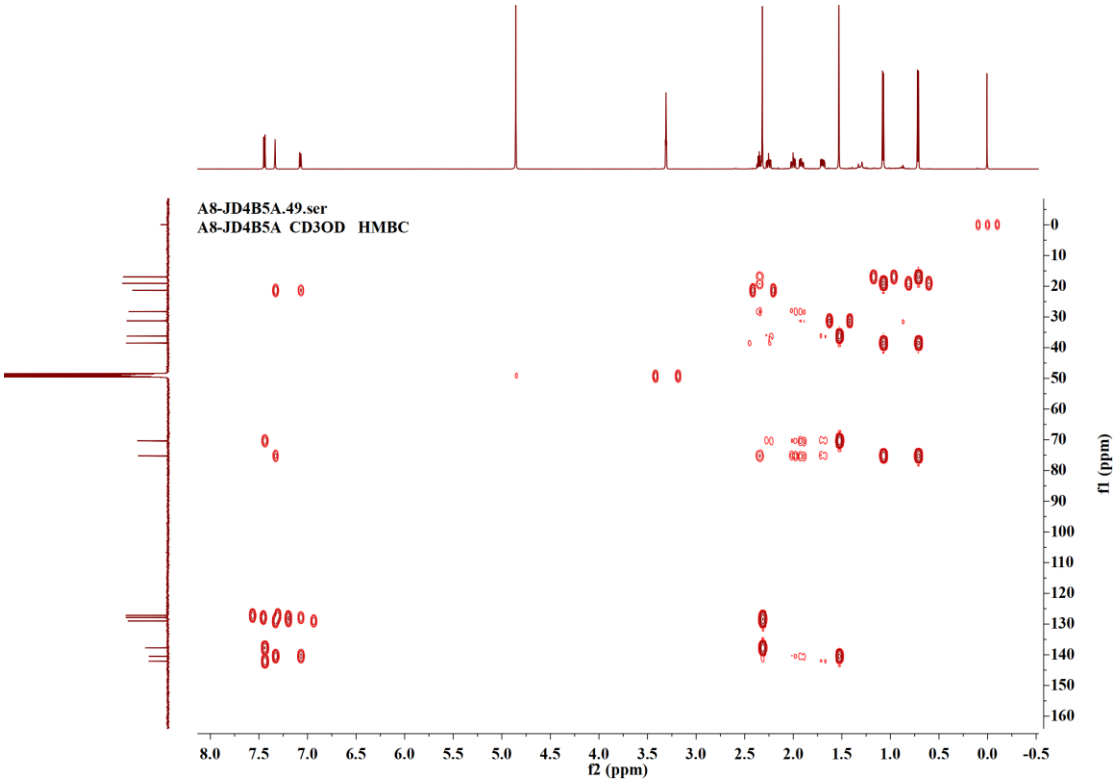



**Figure S30.** HMBC spectrum of **5** in $CD_3OD$.

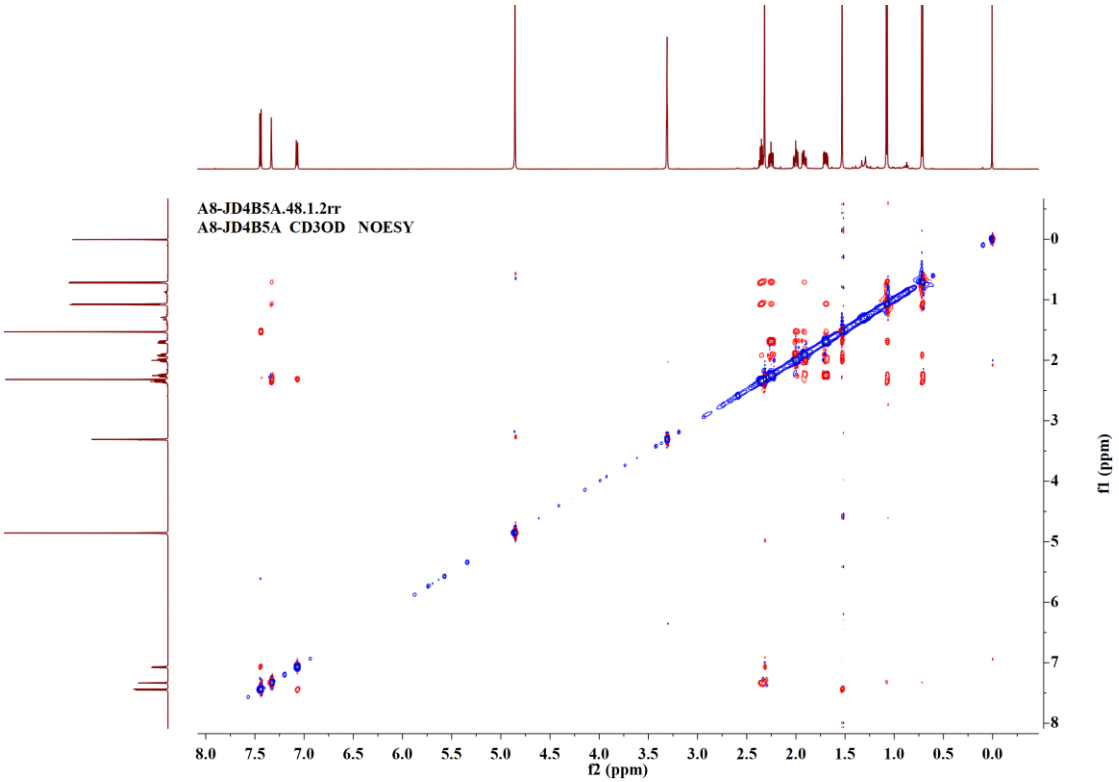



**Figure S31.** NOESY spectrum of **5** in $CD_3OD$.

EIH2020-12-25-05-GYW1 A8-JD4B5A -c1#4 RT: 0.62
T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 173.0963 | 1330209.0 | 100.00 | 173.0961 | 0.24 | 6.5 | $C_{12}H_{13}O_1$ |
| 173.1332 | 11638.0 | 0.87 | 173.1325 | 0.72 | 5.5 | $C_{13}H_{17}$ |
| 174.0995 | 183363.0 | 13.78 | 174.1039 | -4.42 | 6.0 | $C_{12}H_{14}O_1$ |
| 175.0749 | 36995.0 | 2.78 | 175.0754 | -0.48 | 6.5 | $C_{11}H_{11}O_2$ |
| 175.1078 | 25658.0 | 1.93 | 175.1117 | -3.96 | 5.5 | $C_{12}H_{15}O_1$ |
| 176.0819 | 18183.0 | 1.37 | 176.0832 | -1.33 | 6.0 | $C_{11}H_{12}O_2$ |
| 176.1184 | 7558.0 | 0.57 | 176.1196 | -1.19 | 5.0 | $C_{12}H_{16}O_1$ |
| 177.0906 | 19059.0 | 1.43 | 177.0910 | -0.43 | 5.5 | $C_{11}H_{13}O_2$ |
| 177.1279 | 10981.0 | 0.83 | 177.1274 | 0.51 | 4.5 | $C_{12}H_{17}O_1$ |
| 178.0781 | 23030.0 | 1.73 | 178.0777 | 0.41 | 10.0 | $C_{14}H_{10}$ |
| 179.0835 | 16512.0 | 1.24 | 179.0855 | -1.98 | 9.5 | $C_{14}H_{11}$ |
| 180.0927 | 8598.0 | 0.65 | 180.0934 | -0.63 | 9.0 | $C_{14}H_{12}$ |
| 181.1011 | 40637.0 | 3.05 | 181.1012 | -0.08 | 8.5 | $C_{14}H_{13}$ |
| 182.1087 | 15964.0 | 1.20 | 182.1090 | -0.29 | 8.0 | $C_{14}H_{14}$ |
| 183.0824 | 7804.0 | 0.59 | 183.0804 | 1.95 | 8.5 | $C_{13}H_{11}O_1$ |
| 183.1174 | 504990.0 | 37.96 | 183.1168 | 0.56 | 7.5 | $C_{14}H_{15}$ |
| 184.1204 | 85986.0 | 6.46 | 184.1247 | -4.24 | 7.0 | $C_{14}H_{16}$ |
| 185.0937 | 8215.0 | 0.62 | 185.0961 | -2.35 | 7.5 | $C_{13}H_{13}O_1$ |
| 187.0760 | 9611.0 | 0.72 | 187.0754 | 0.61 | 7.5 | $C_{12}H_{11}O_2$ |
| 187.1100 | 12076.0 | 0.91 | 187.1117 | -1.71 | 6.5 | $C_{13}H_{15}O_1$ |
| 189.0910 | 17607.0 | 1.32 | 189.0910 | -0.06 | 6.5 | $C_{12}H_{13}O_2$ |
| 191.1060 | 185773.0 | 13.97 | 191.1067 | -0.65 | 5.5 | $C_{12}H_{15}O_2$ |
| 193.0963 | 7667.0 | 0.58 | 193.1012 | -4.87 | 9.5 | $C_{15}H_{13}$ |
| 194.1264 | 8215.0 | 0.62 | 194.1301 | -3.71 | 4.0 | $C_{12}H_{18}O_2$ |
| 196.1233 | 8516.0 | 0.64 | 196.1247 | -1.31 | 8.0 | $C_{15}H_{16}$ |
| 198.1397 | 208666.0 | 15.69 | 198.1403 | -0.64 | 7.0 | $C_{15}H_{18}$ |
| 199.1437 | 35982.0 | 2.70 | 199.1481 | -4.42 | 6.5 | $C_{15}H_{19}$ |
| 201.1280 | 35298.0 | 2.65 | 201.1274 | 0.59 | 6.5 | $C_{14}H_{17}O_1$ |
| 202.1327 | 7968.0 | 0.60 | 202.1352 | -2.51 | 6.0 | $C_{14}H_{18}O_1$ |
| 216.1504 | 8406.0 | 0.63 | 216.1509 | -0.42 | 6.0 | $C_{15}H_{20}O_1$ |
| 234.1618 | 11227.0 | 0.84 | 234.1614 | 0.36 | 5.0 | $C_{15}H_{22}O_2$ |

**Figure S32.** HRESIMS of **5**.

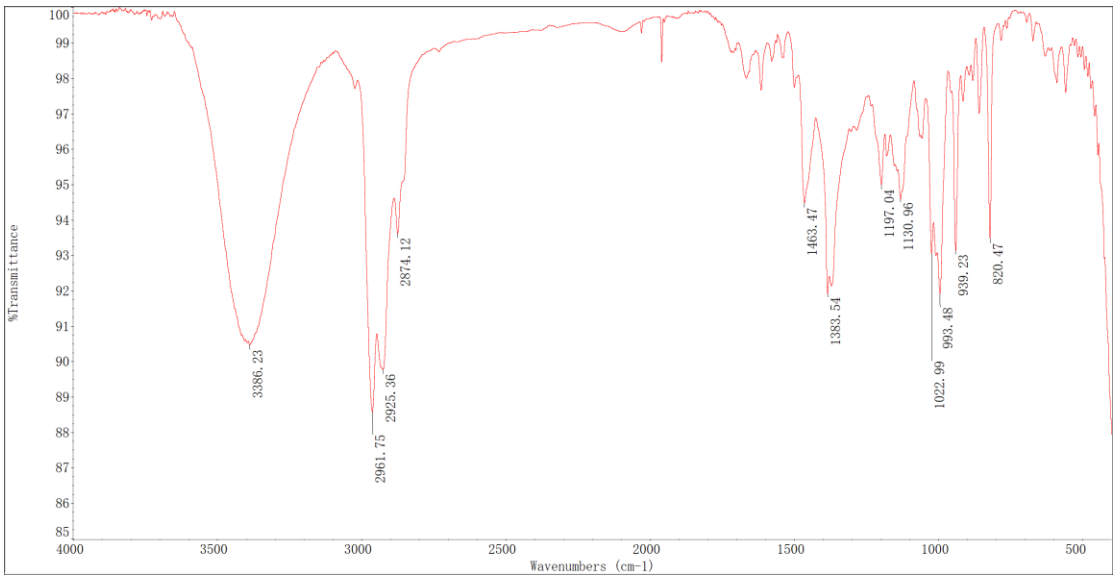



**Figure S33.** IR spectrum of **5**.

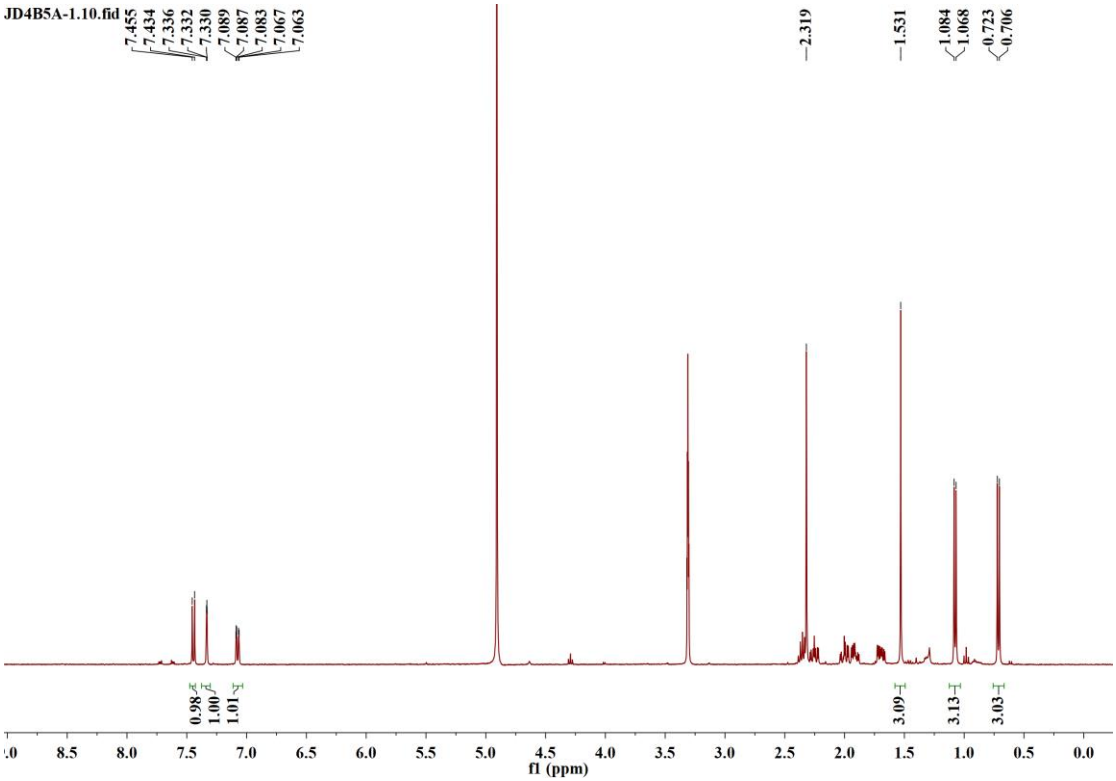



**Figure S34.** $^{1}$H NMR spectrum (400 MHz) of (+)-**5** in $CD_3OD$.

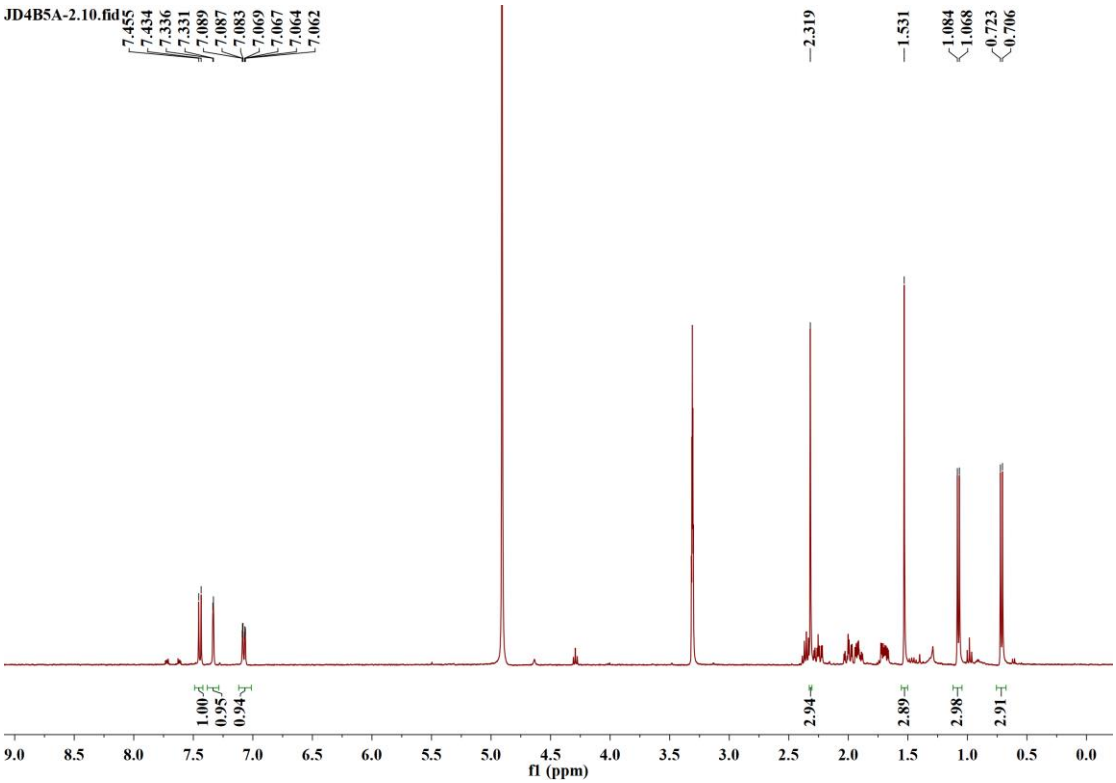



**Figure S35.** $^{1}$H NMR spectrum (400 MHz) of (−)-**5** in $CD_3OD$.

## 5. TDDFT-ECD calculation of compound (+)-1.

**5.1** Computational section.

Conformational searches were carried out using the torsional sampling (MCMM) method and OPLS_2005 force field. Conformers above 1% population were re-optimized at the B3LYP/6-311G(d,p) level of theory with IEFPCM (Polarizable Continuum Model using the Integral Equation Formalism variant) solvent model for acetonitrile. For the resulting geometries, ECD spectra were obtained by TDDFT calculations performed with the B3LYP/6-311G(d,p) level of theory with IEFPCM solvent model for acetonitrile. Finally, the Boltzmann-averaged ECD spectra were obtained with SpecDis1.62.

**5.2** Computational data of (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**].

Torsional sampling (MCMM) conformational searches using OPLS_2005 force field were carried out by means of the conformational search module in the Macromodel1 applying an energy window of 21 kJ/mol, which afforded 4 conformers for (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**]. The Boltzmann populations of the conformers were obtained based on the potential energy provided by the MMFFs force field, giving 2 conformers for (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**] above 1% population for re-optimization. The re-optimization and the following TDDFT calculations of the re-optimized geometries (Fig. S36, Table S1) were all performed with Gaussian 09 at the B3LYP/6-311G(d,p) level with IEFPCM solvent model for acetonitrile. Frequency analysis was performed as well to confirm that the re-optimized geometries were at the energy minima. Finally, the SpecDis1.62 software was used to obtain the Boltzmann-averaged ECD spectra of (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**].

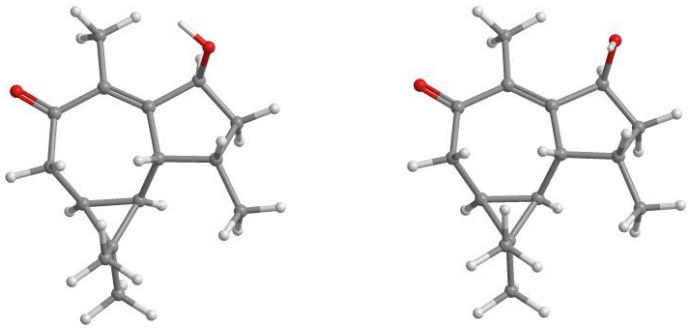



**Figure S36.** Re-optimized conformers above 1% population (OPLS_2005) of (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**] calculated at the B3LYP/6-311G(d,p) level of theory with IEFPCM solvent model for acetonitrile.

**Table S1.** Cartesian coordinates for the re-optimized conformers of (2*S*, 4*S*, 5*R*, 6*S*, 7*S*)-[(+)-**1**] at the B3LYP/6-311G(d,p) level of theory with IEFPCM solvent model for acetonitrile.

| (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**] Conf. 1 | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|
| I | atom | X | Y | Z |
| 1 | C | 1.25990900 | 0.18648400 | 0.02654900 |
| 2 | C | -0.12807500 | 0.68897800 | -0.37935400 |
| 3 | C | -1.18193500 | 0.10330200 | 0.55657000 |
| 4 | C | -1.42037000 | -1.38409000 | 0.45942000 |
| 5 | C | -0.62223300 | -2.17151600 | -0.56766000 |
| 6 | C | 0.84828800 | -2.29679600 | -0.18979200 |
| 7 | C | 1.69007400 | -1.09370200 | 0.11371400 |
| 8 | C | 2.12908300 | 1.39560900 | 0.36861900 |
| 9 | C | 1.12224600 | 2.50526200 | 0.64998300 |
| 10 | C | -0.00847200 | 2.24547500 | -0.35807800 |
| 11 | C | -2.53634700 | -0.41257400 | 0.09680800 |
| 12 | C | -1.29824300 | 3.01750700 | -0.08795600 |
| 13 | C | 3.09954700 | -1.45788900 | 0.52766500 |
| 14 | C | -3.66810900 | -0.30045900 | 1.10608700 |
| 15 | C | -3.01762700 | -0.25874700 | -1.33498800 |
| 16 | H | -0.34812300 | 0.37207900 | -1.39955800 |
| 17 | O | 2.90675800 | 1.80235700 | -0.77521800 |
| 18 | O | 1.35455800 | -3.40977600 | -0.11344700 |
| 19 | H | -1.15650300 | 0.51384700 | 1.56219000 |
| 20 | H | -1.55241300 | -1.91604400 | 1.39755800 |
| 21 | H | -1.00390000 | -3.18969700 | -0.66765600 |
| 22 | H | -0.68312700 | -1.70927300 | -1.55603200 |
| 23 | H | 2.78957500 | 1.20930400 | 1.21959800 |
| 24 | H | 1.57848600 | 3.49262800 | 0.54857700 |
| 25 | H | 0.75269800 | 2.40854400 | 1.67710100 |
| 26 | H | 0.36689300 | 2.54318300 | -1.34217200 |
| 27 | H | -1.11100200 | 4.09442400 | -0.13214900 |
| 28 | H | -2.06614400 | 2.78417600 | -0.83042100 |
| 29 | H | -1.70686000 | 2.79093900 | 0.90038500 |
| 30 | H | 3.08604700 | -2.12304100 | 1.39496100 |
| 31 | H | 3.59975000 | -2.00913800 | -0.27325500 |
| 32 | H | 3.70664500 | -0.58839000 | 0.77252100 |
| 33 | H | -4.42980800 | -1.06627800 | 0.92412100 |
| 34 | H | -3.30646100 | -0.42386800 | 2.13004900 |
| 35 | H | -4.15547800 | 0.67785600 | 1.03702200 |
| 36 | H | -3.74274200 | -1.04331300 | -1.57576600 |
| 37 | H | -3.52180700 | 0.70468300 | -1.46231200 |
| 38 | H | -2.22150800 | -0.30972900 | -2.07759100 |
| 39 | H | 3.42882600 | 1.04539000 | -1.06337000 |

B3LYP/6-311G(d,p) Energy = -735.45333014 a.u.

| (2*S*,4*S*,5*R*,6*S*,7*S*)-[(+)-**1**] Conf. 2 | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|
| I | atom | X | Y | Z |
| 1 | C | 1.25398300 | 0.16943300 | 0.01380600 |
| 2 | C | -0.12925000 | 0.68372000 | -0.39005400 |
| 3 | C | -1.18359800 | 0.12458400 | 0.56151000 |
| 4 | C | -1.43475500 | -1.36216100 | 0.47748100 |
| 5 | C | -0.65850400 | -2.16592300 | -0.55511300 |
| 6 | C | 0.81881600 | -2.30712300 | -0.20624400 |
| 7 | C | 1.68004800 | -1.11274900 | 0.07338400 |
| 8 | C | 2.12908900 | 1.36085500 | 0.41178300 |
| 9 | C | 1.12786600 | 2.49983600 | 0.62964500 |
| 10 | C | 0.01685900 | 2.23702000 | -0.39866300 |
| 11 | C | -2.54674700 | -0.38401000 | 0.12009900 |
| 12 | C | -1.26574200 | 3.03612400 | -0.17784100 |
| 13 | C | 3.09570100 | -1.46990800 | 0.46757300 |
| 14 | C | -3.66565000 | -0.25548300 | 1.14188000 |
| 15 | C | -3.04416700 | -0.23646300 | -1.30674100 |
| 16 | H | -0.36126600 | 0.35304500 | -1.40314600 |
| 17 | O | 3.11862000 | 1.66965900 | -0.58796700 |
| 18 | O | 1.30955300 | -3.42693500 | -0.12741300 |
| 19 | H | -1.14325800 | 0.54313800 | 1.56340800 |
| 20 | H | -1.56068300 | -1.88662400 | 1.42060500 |
| 21 | H | -1.05370900 | -3.18039500 | -0.63928700 |
| 22 | H | -0.73252600 | -1.71279800 | -1.54688400 |
| 23 | H | 2.70844600 | 1.15286700 | 1.31120900 |
| 24 | H | 1.60475000 | 3.47627300 | 0.52032500 |
| 25 | H | 0.72040700 | 2.43735900 | 1.64576400 |
| 26 | H | 0.40851100 | 2.51045400 | -1.38684500 |
| 27 | H | -1.06034700 | 4.10850700 | -0.24259000 |
| 28 | H | -2.02063300 | 2.79621600 | -0.93139800 |
| 29 | H | -1.69821300 | 2.83859700 | 0.80656600 |
| 30 | H | 3.12122200 | -1.94215700 | 1.45519300 |
| 31 | H | 3.50325100 | -2.20175000 | -0.23300800 |
| 32 | H | 3.74754800 | -0.59990000 | 0.47194500 |
| 33 | H | -4.43591400 | -1.01582400 | 0.97348600 |
| 34 | H | -3.29325200 | -0.37588100 | 2.16232500 |
| 35 | H | -4.14534200 | 0.72659400 | 1.07232100 |
| 36 | H | -3.77518600 | -1.01944100 | -1.53450700 |
| 37 | H | -3.54596500 | 0.72824000 | -1.43333500 |
| 38 | H | -2.25723200 | -0.29470200 | -2.05854500 |
| 39 | H | 2.68031400 | 1.70988100 | -1.44558800 |

B3LYP/6-311G(d,p) Energy = -735.45290767 a.u.