

## Supplementary Materials

### Lipids and Terpenoids from the Deep-Sea Fungus *Trichoderma lixii* R22 and Their Antagonism against Two Wheat Pathogens

Chang-Peng Li<sup>1,2,†</sup>, Zhen-Zhen Shi<sup>1,†</sup>, Sheng-Tao Fang<sup>1</sup>, Yin-Ping Song<sup>1</sup>, and Nai-Yun Ji<sup>1,2,3,\*</sup>

<sup>1</sup> Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, Yantai 264003, China; cpli@yic.ac.cn (C.-P.L.); zzshi@yic.ac.cn (Z.-Z.S.); stfang@yic.ac.cn (S.-T.F.); ypsong@yic.ac.cn (Y.-P.S.)

<sup>2</sup> University of Chinese Academy of Sciences, Beijing 100049, China

<sup>3</sup> Shandong Saline-Alkaline Land Modern Agriculture Company, Dongying 257345, China

\* Correspondence: nyji@yic.ac.cn; Tel.: +86-535-210-9176

† These authors contributed equally to this work.

## Table of Contents

- Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{DMSO-}d_6$ .
- Figure S2.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **1** in  $\text{DMSO-}d_6$ .
- Figure S3.** HSQC spectrum of compound **1** in  $\text{DMSO-}d_6$ .
- Figure S4.** HMBC spectrum of compound **1** in  $\text{DMSO-}d_6$ .
- Figure S5.** COSY spectrum of compound **1** in  $\text{DMSO-}d_6$ .
- Figure S6.** NOESY spectrum of compound **1** in  $\text{DMSO-}d_6$ .
- Figure S7.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{CDCl}_3$ .
- Figure S8.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **1** in  $\text{CDCl}_3$ .
- Figure S9.** HSQC spectrum of compound **1** in  $\text{CDCl}_3$ .
- Figure S10.** HMBC spectrum of compound **1** in  $\text{CDCl}_3$ .
- Figure S11.** COSY spectrum of compound **1** in  $\text{CDCl}_3$ .
- Figure S12.** NOESY spectrum of compound **1** in  $\text{CDCl}_3$ .
- Figure S13.** HRESI(-)MS spectrum of compound **1**.
- Figure S14.** IR spectrum of compound **1**.
- Figure S15.** UV spectrum of compound **1** (0.2 mg/mL in MeOH).
- Figure S16.**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{DMSO-}d_6$ .
- Figure S17.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **2** in  $\text{DMSO-}d_6$ .
- Figure S18.** HSQC spectrum of compound **2** in  $\text{DMSO-}d_6$ .
- Figure S19.** HMBC spectrum of compound **2** in  $\text{DMSO-}d_6$ .
- Figure S20.** COSY spectrum of compound **2** in  $\text{DMSO-}d_6$ .
- Figure S21.** NOESY spectrum of compound **2** in  $\text{DMSO-}d_6$ .
- Figure S22.**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .
- Figure S23.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **2** in  $\text{CD}_3\text{OD}$ .
- Figure S24.** HSQC spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .
- Figure S25.** HMBC spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .
- Figure S26.** COSY spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .
- Figure S27.** NOESY spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .
- Figure S28.** HRESI(+)MS spectrum of compound **2**.
- Figure S29.** IR spectrum of compound **2**.
- Figure S30.** UV spectrum of compound **2** (0.4 mg/mL in MeOH).
- Figure S31.**  $^1\text{H}$  NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .

**Figure S32.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **3** in  $\text{CD}_3\text{OD}$ .

**Figure S33.** HSQC spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .

**Figure S34.** HMBC spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .

**Figure S35.** COSY spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .

**Figure S36.** NOESY spectrum of compound **3** in  $\text{CD}_3\text{OD}$ .

**Figure S37.** HRESI(+)MS spectrum of compound **3**.

**Figure S38.** IR spectrum of compound **3**.

**Figure S39.** UV spectrum of compound **3** (0.2 mg/mL in MeOH).

**Figure S40.**  $^1\text{H}$  NMR spectrum of compound **4** in  $\text{DMSO}-d_6$ .

**Figure S41.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **4** in  $\text{DMSO}-d_6$ .

**Figure S42.** HSQC spectrum of compound **4** in  $\text{DMSO}-d_6$ .

**Figure S43.** HMBC spectrum of compound **4** in  $\text{DMSO}-d_6$ .

**Figure S44.** COSY spectrum of compound **4** in  $\text{DMSO}-d_6$ .

**Figure S45.** NOESY spectrum of compound **4** in  $\text{DMSO}-d_6$ .

**Figure S46.** HRESI(+)MS spectrum of compound **4**.

**Figure S47.** IR spectrum of compound **4**.

**Figure S48.** UV spectrum of compound **4** (0.4 mg/mL in MeOH).

**Figure S49.**  $^1\text{H}$  NMR spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S50.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S51.** HSQC spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S52.** HMBC spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S53.** COSY spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S54.** NOESY spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S55.** HRESI(-)MS spectrum of compound **5**.

**Figure S56.** IR spectrum of compound **5**.

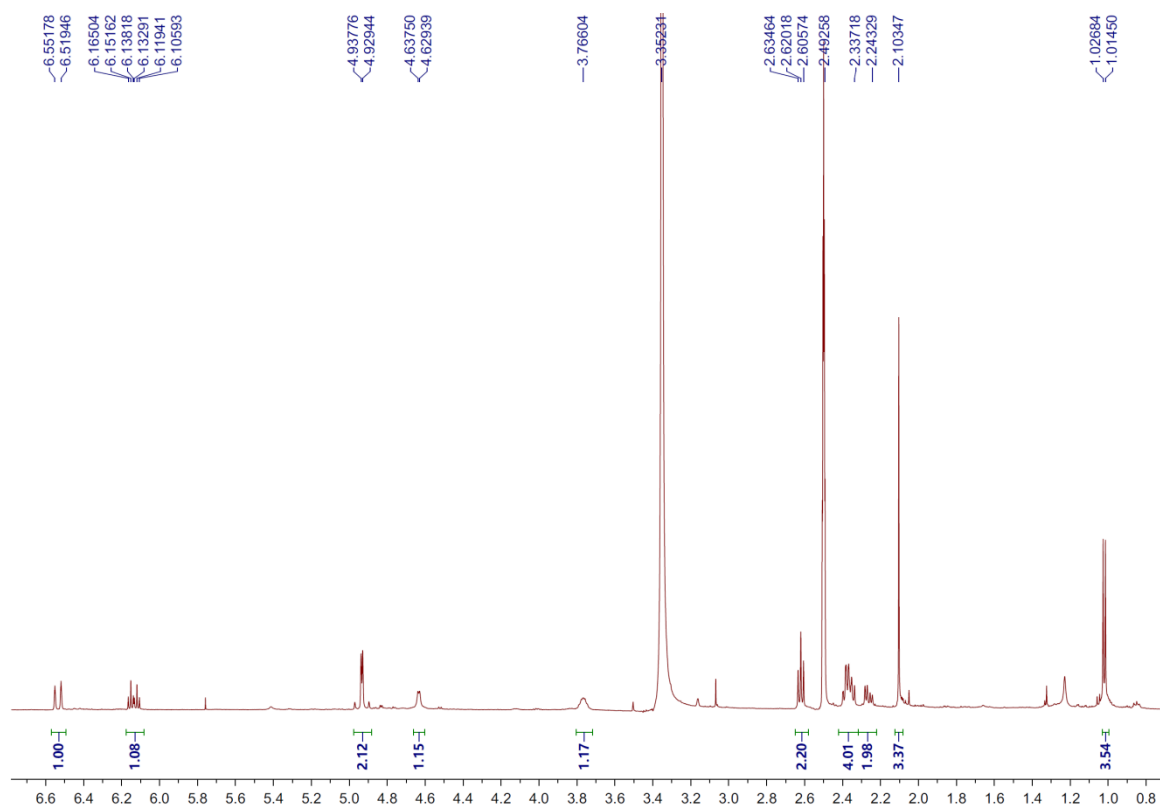
**Figure S57.** UV spectrum of compound **5** (0.1 mg/mL in MeOH).

**Figure S58.**  $^1\text{H}$  NMR spectrum of compound **6** in  $\text{CD}_3\text{OD}$ .

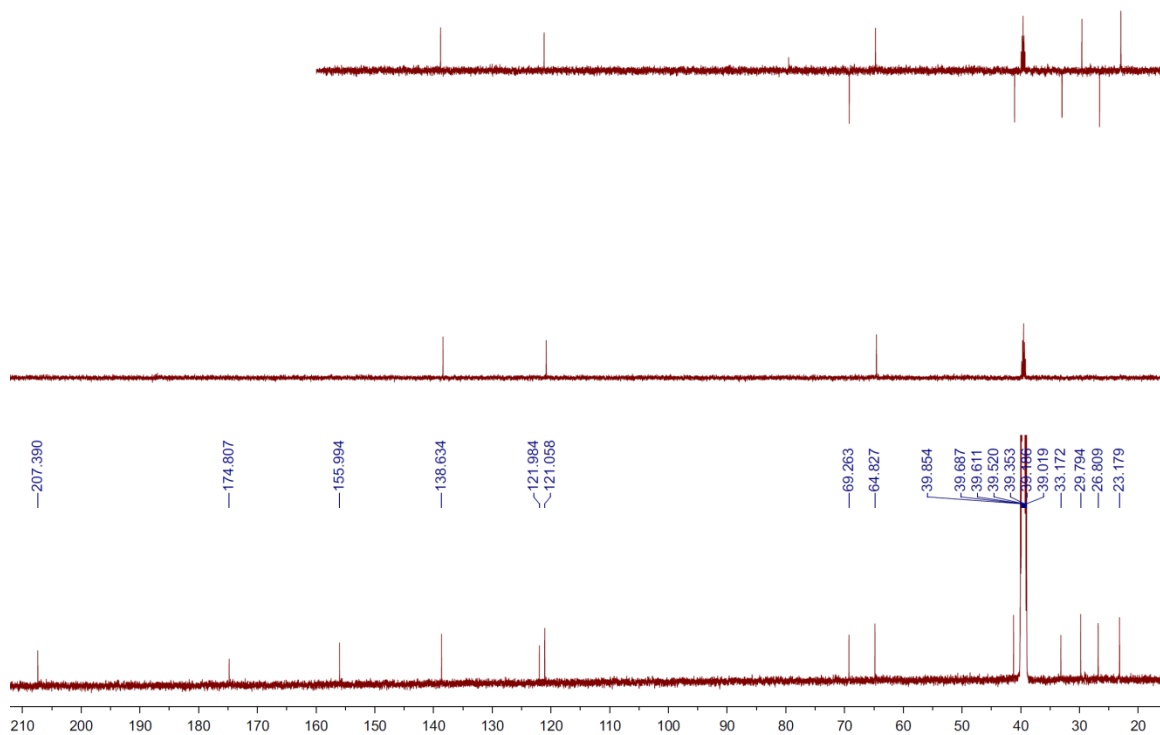
**Figure S59.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **6** in  $\text{CD}_3\text{OD}$ .

**Figure S60.**  $^1\text{H}$  NMR spectrum of compound **7** in  $\text{CDCl}_3$ .

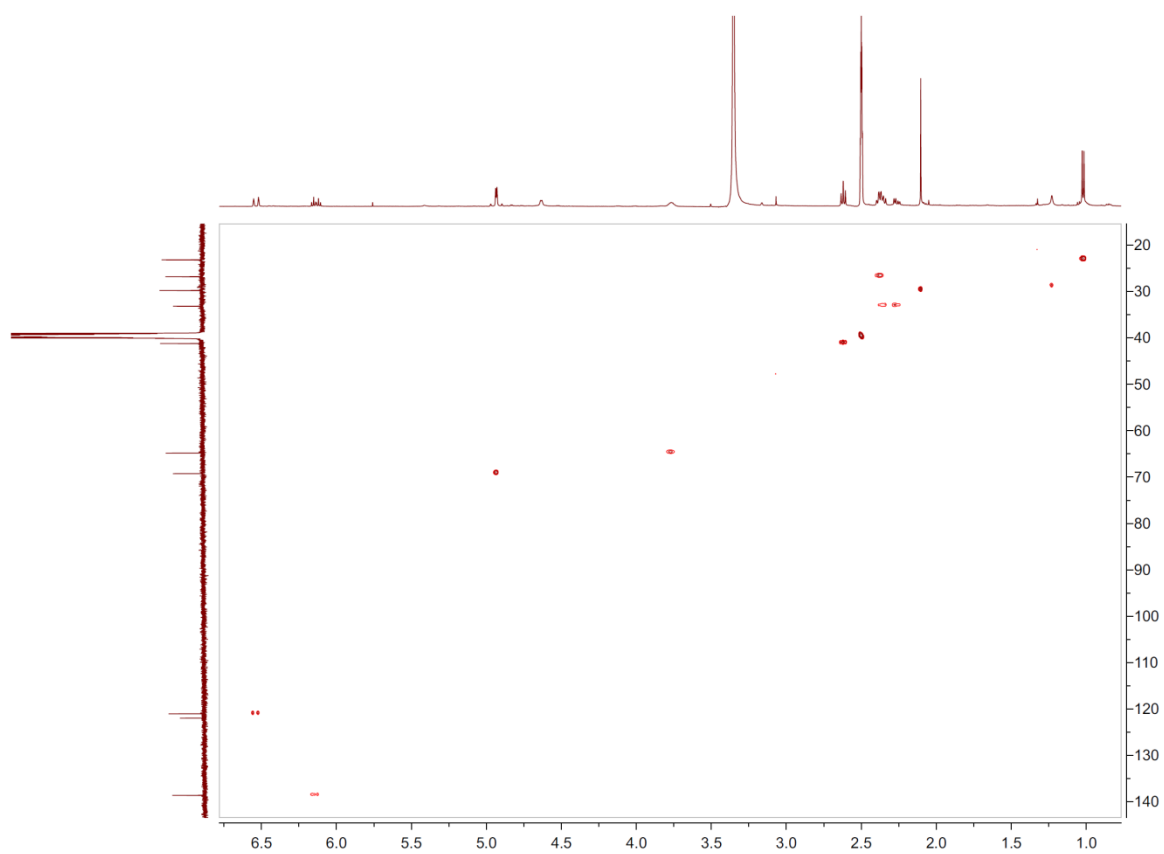
**Figure S61.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **7** in  $\text{CDCl}_3$ .



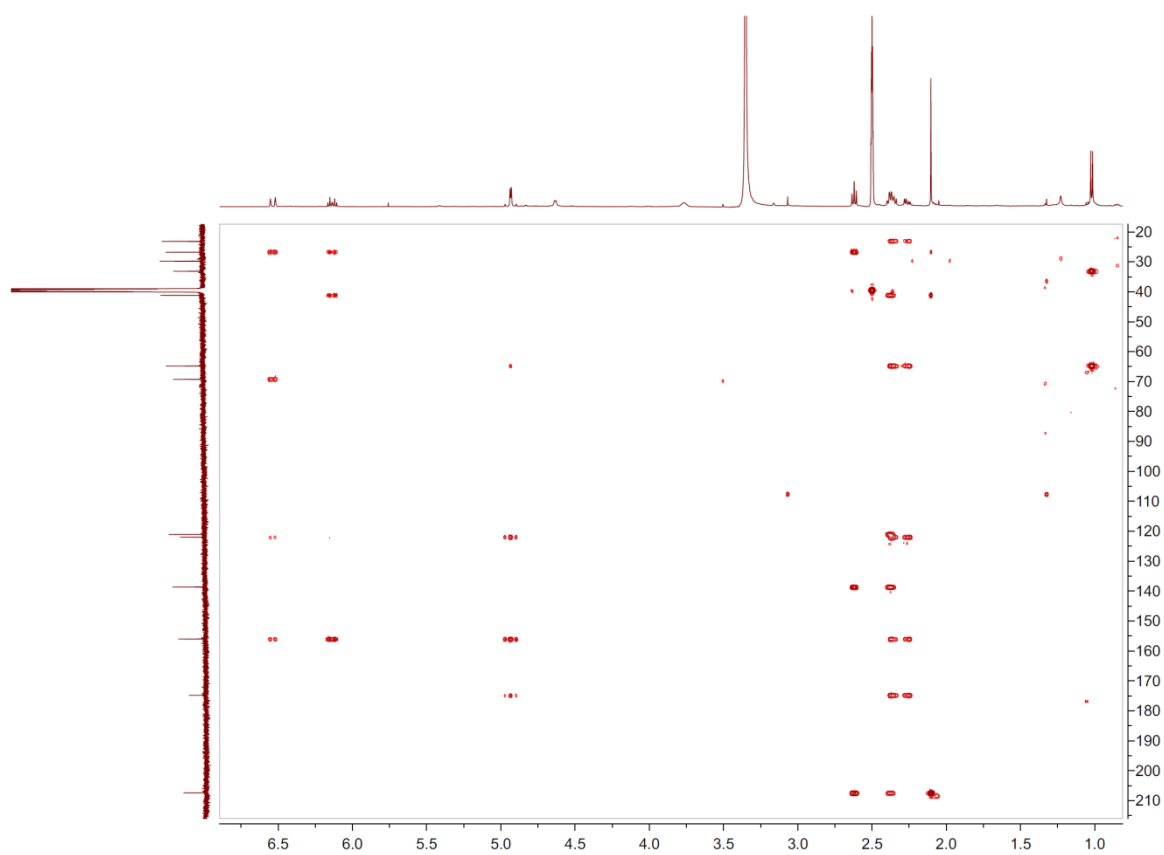
**Figure S1.** <sup>1</sup>H NMR spectrum of compound **1** in DMSO-*d*<sub>6</sub>.



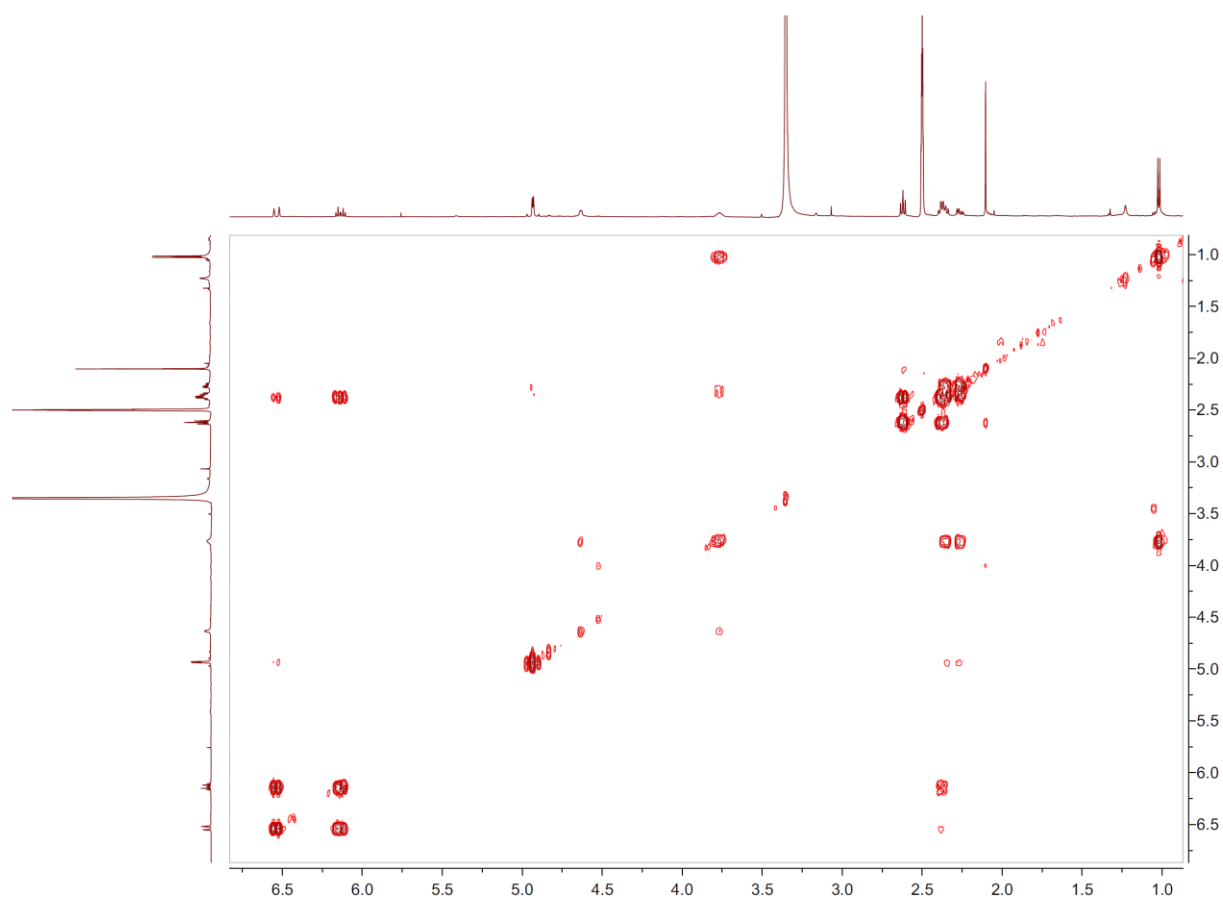
**Figure S2.** <sup>13</sup>C NMR and DEPT spectra of compound **1** in DMSO-*d*<sub>6</sub>.



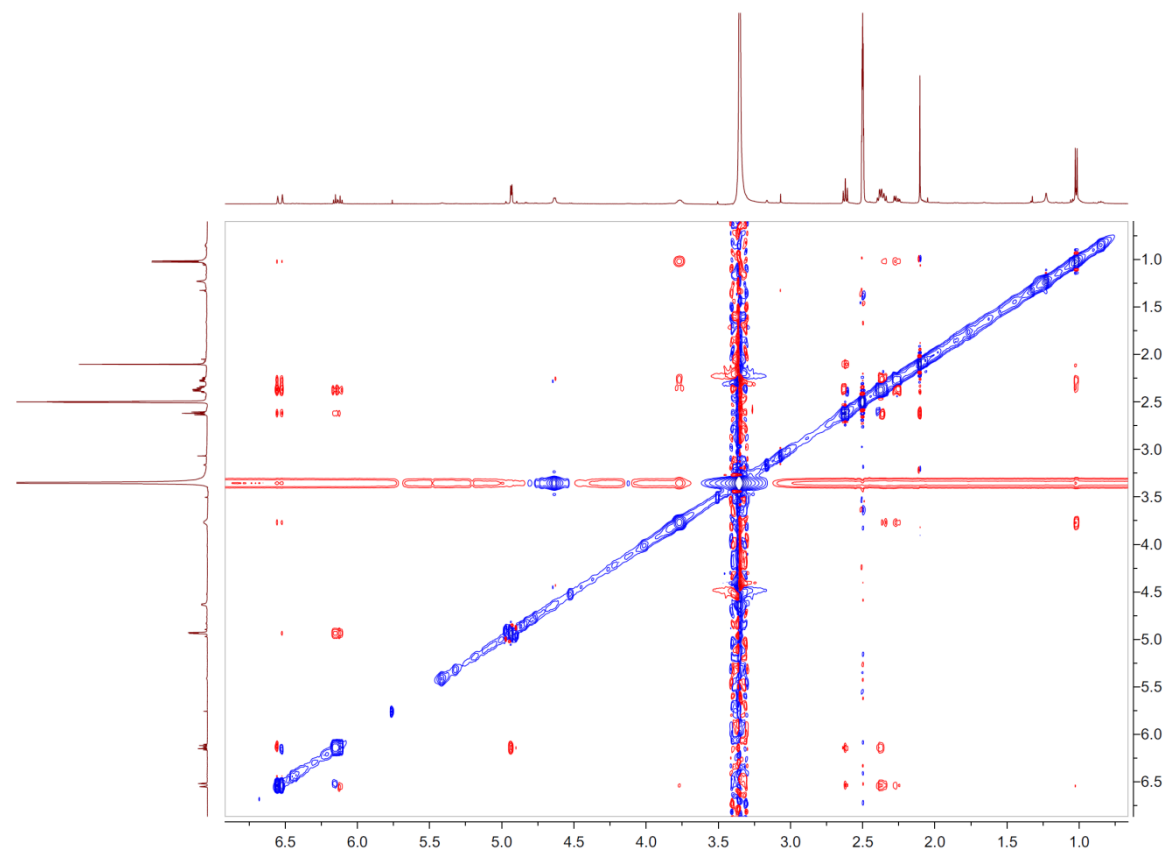
**Figure S3.** HSQC spectrum of compound **1** in DMSO- $d_6$ .



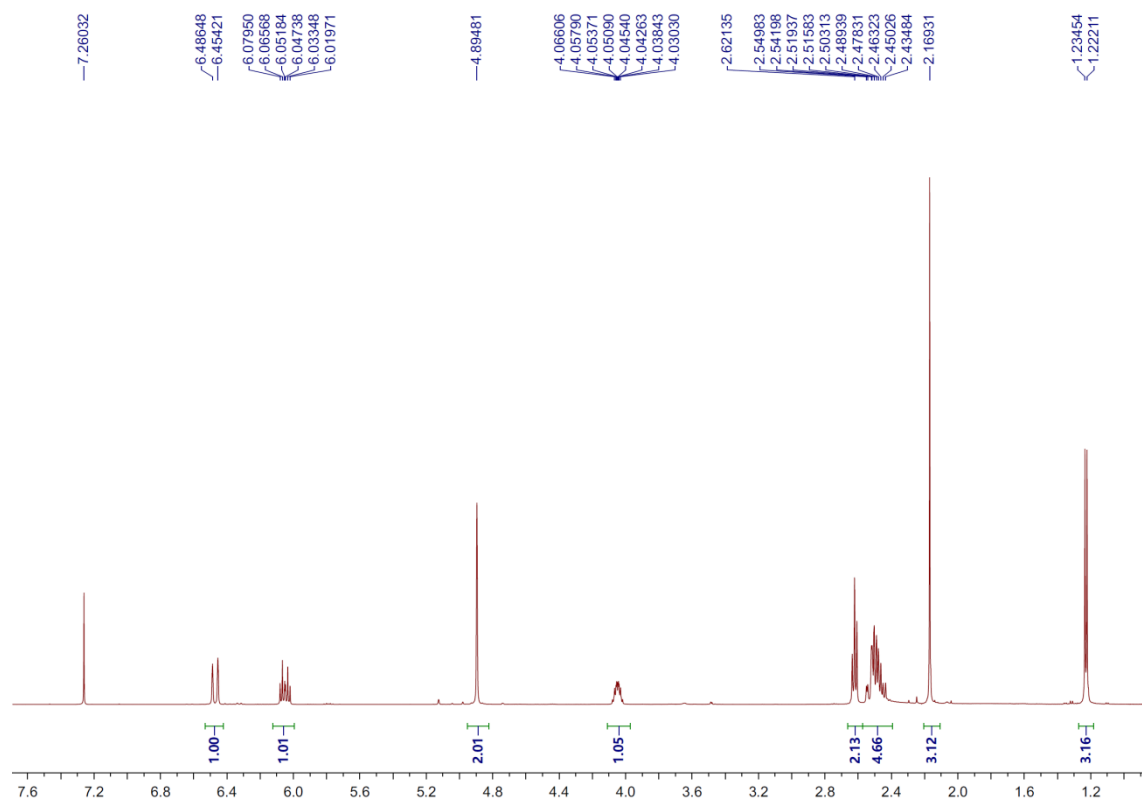
**Figure S4.** HMBC spectrum of compound **1** in DMSO- $d_6$ .



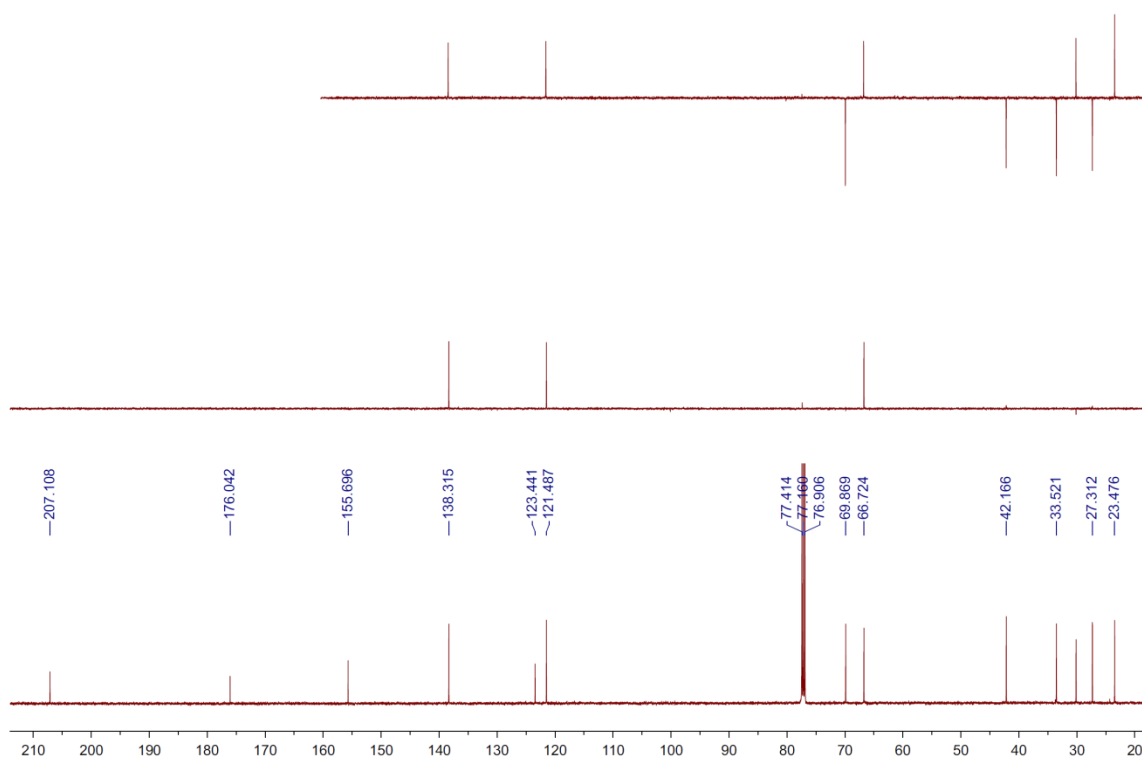
**Figure S5.** COSY spectrum of compound **1** in DMSO- $d_6$ .



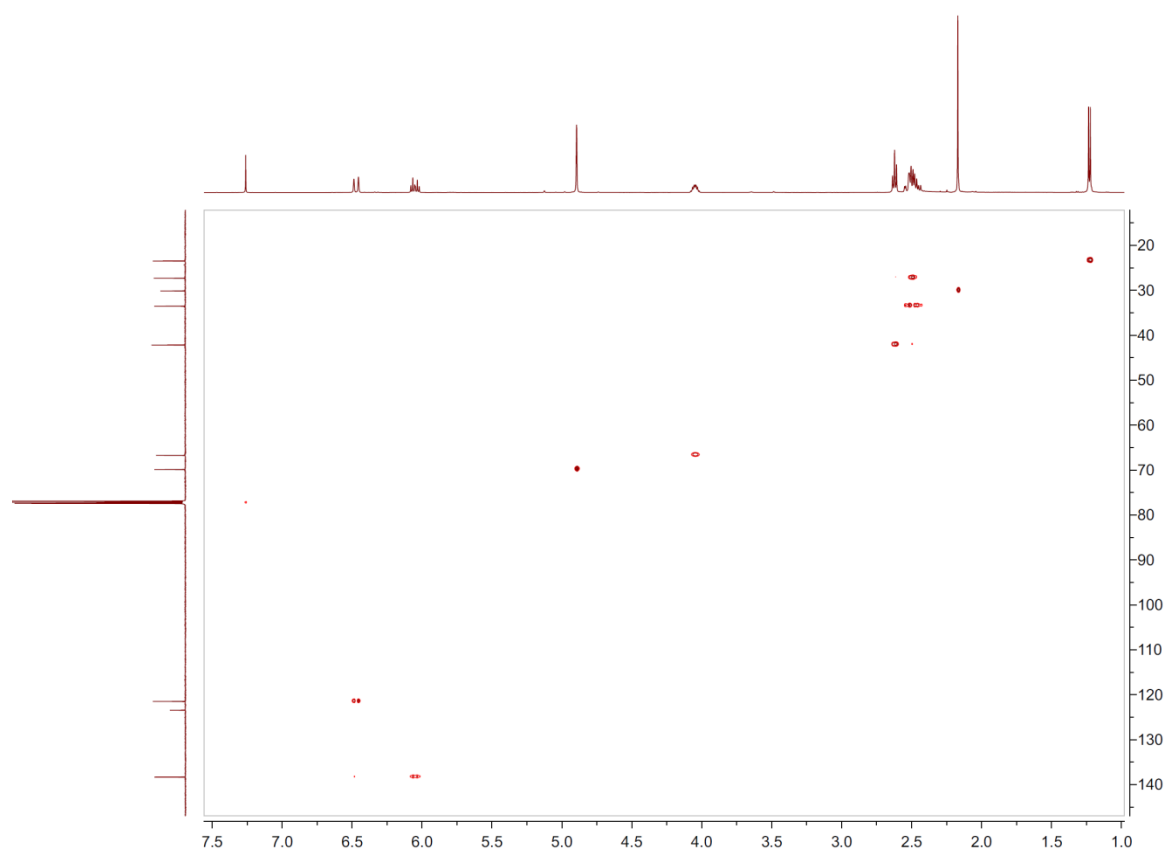
**Figure S6.** NOESY spectrum of compound **1** in DMSO- $d_6$ .



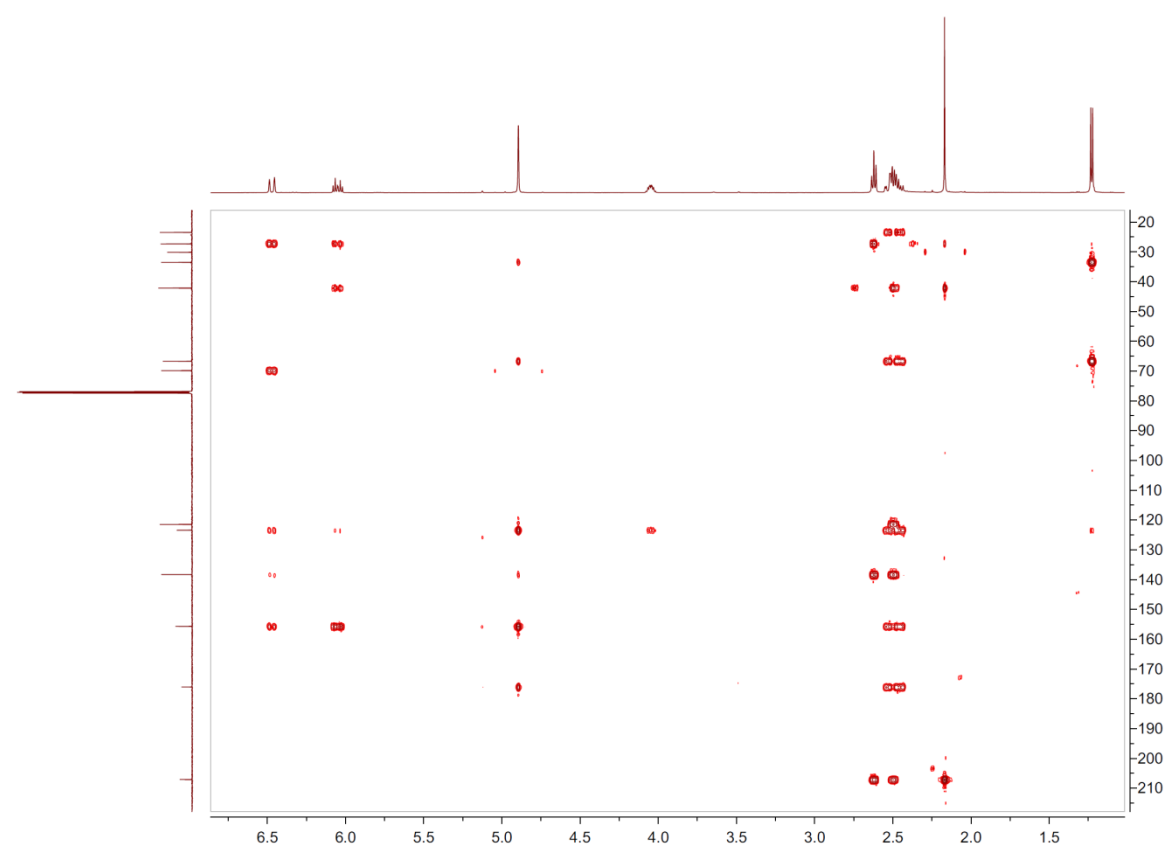
**Figure S7.** <sup>1</sup>H NMR spectrum of compound **1** in CDCl<sub>3</sub>.



**Figure S8.** <sup>13</sup>C NMR and DEPT spectra of compound **1** in CDCl<sub>3</sub>.

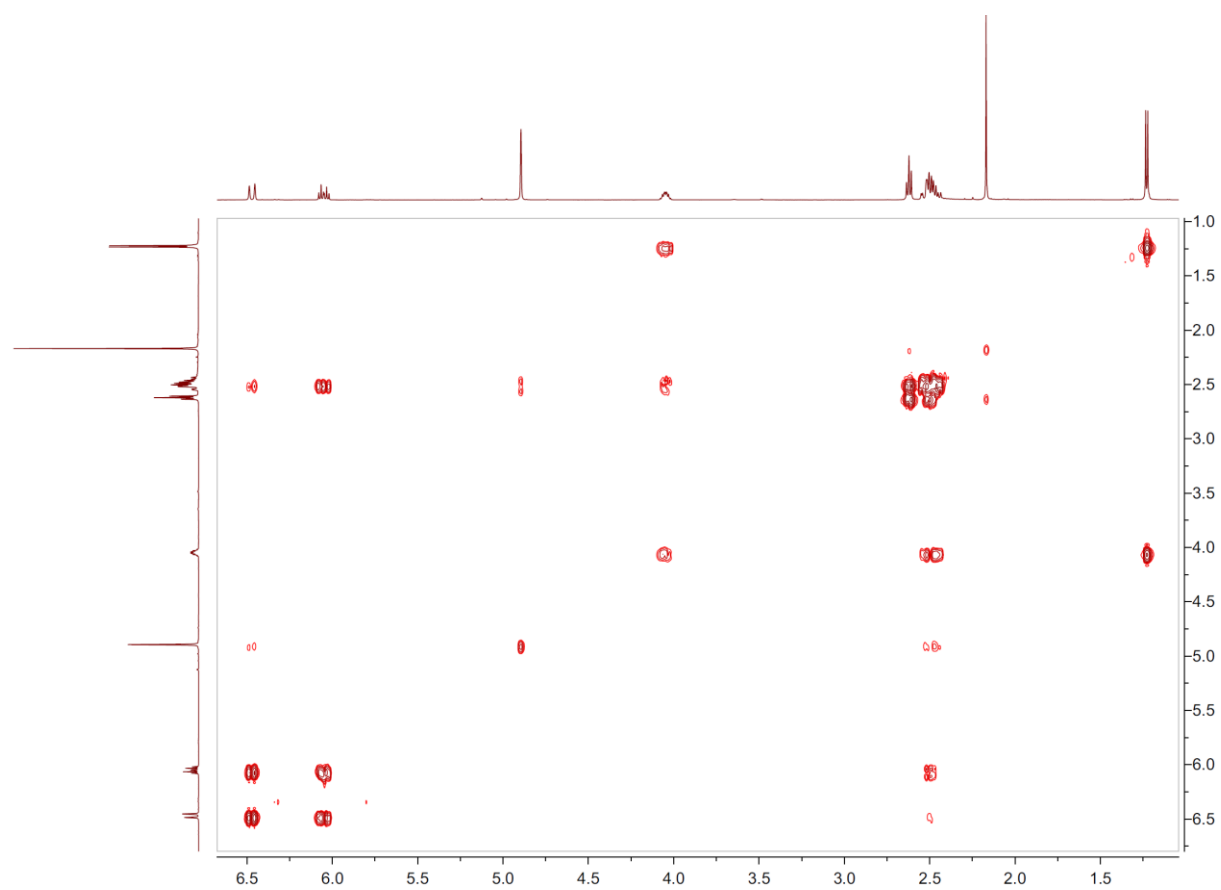


**Figure S9.** HSQC spectrum of compound **1** in CDCl<sub>3</sub>.

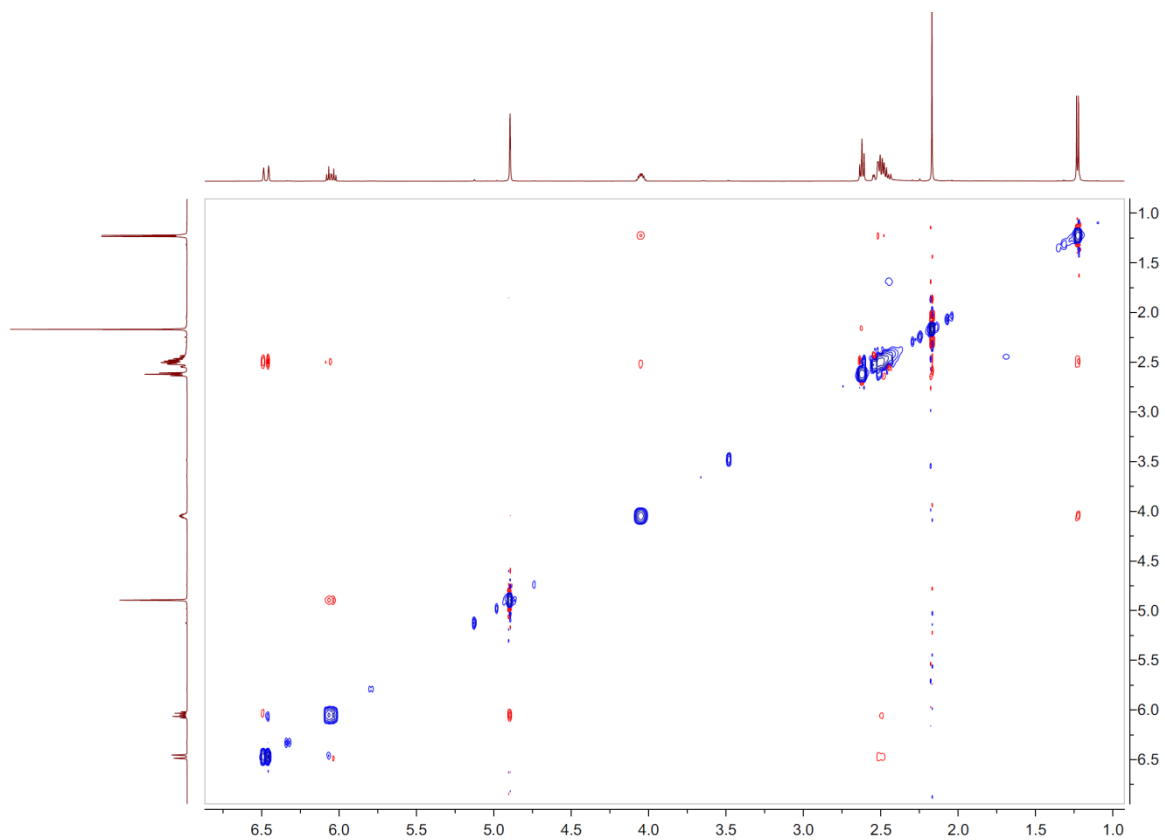


**Figure S10.** HMBC spectrum of compound **1** in CDCl<sub>3</sub>.

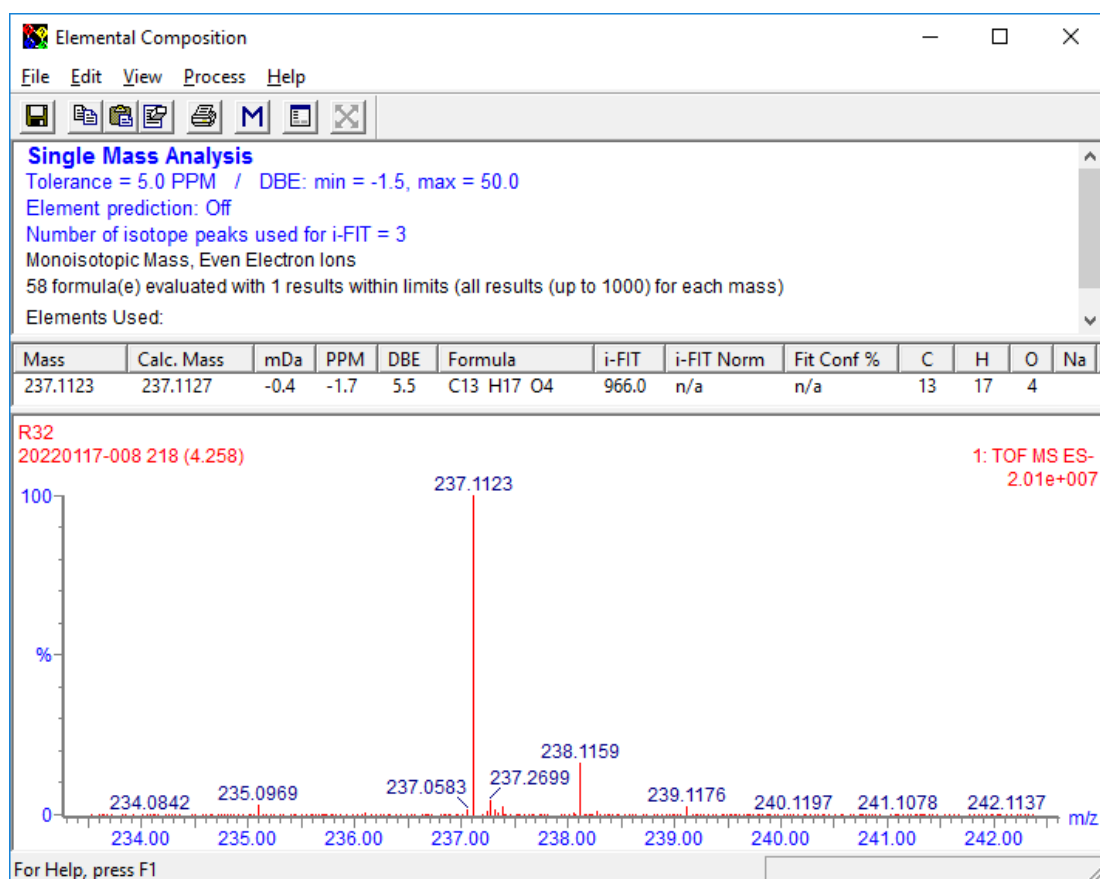




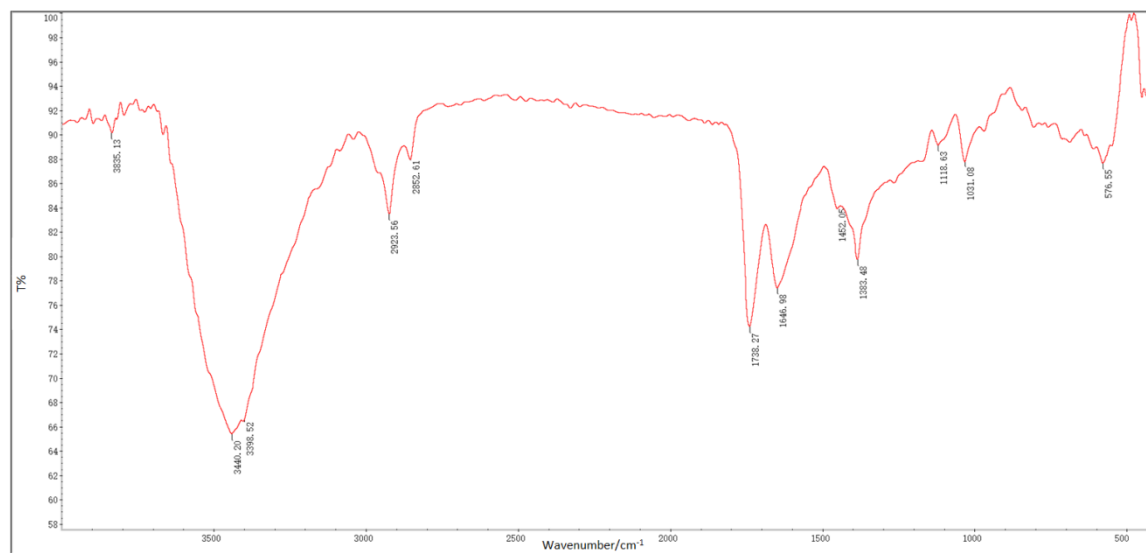
**Figure S11.** COSY spectrum of compound **1** in CDCl<sub>3</sub>.



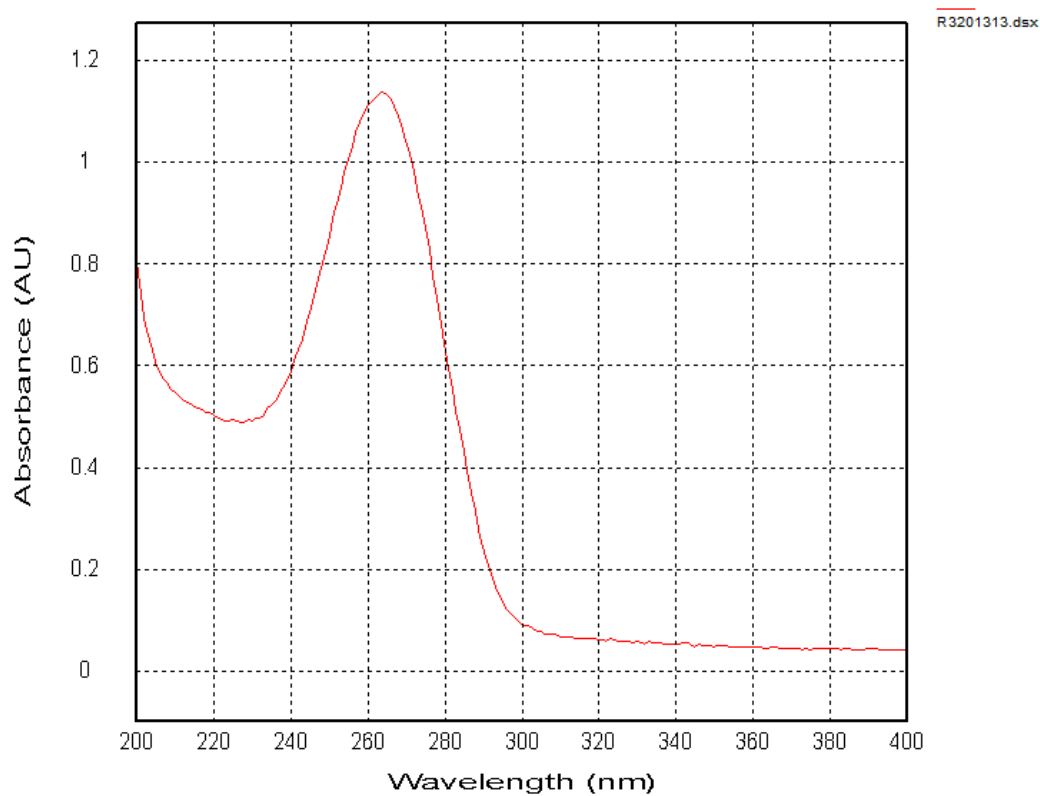
**Figure S12.** NOESY spectrum of compound **1** in CDCl<sub>3</sub>.



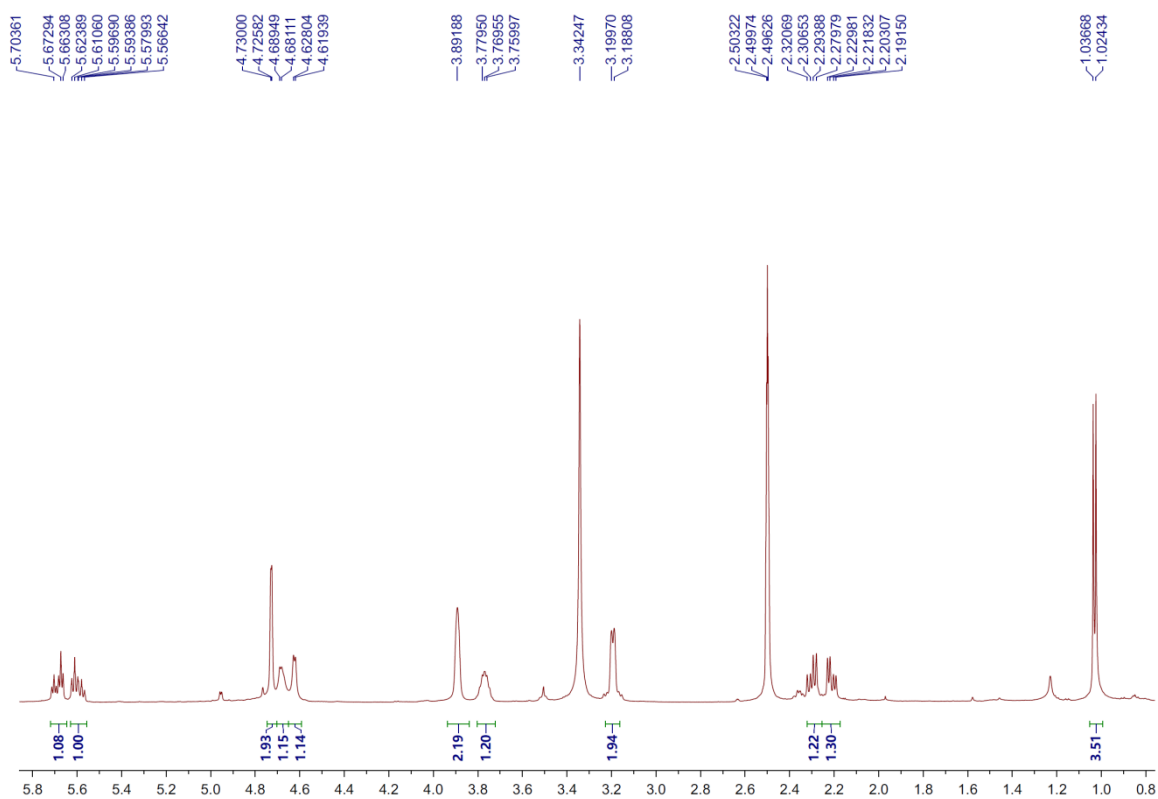
**Figure S13.** HRESI(-)MS spectrum of compound **1**.



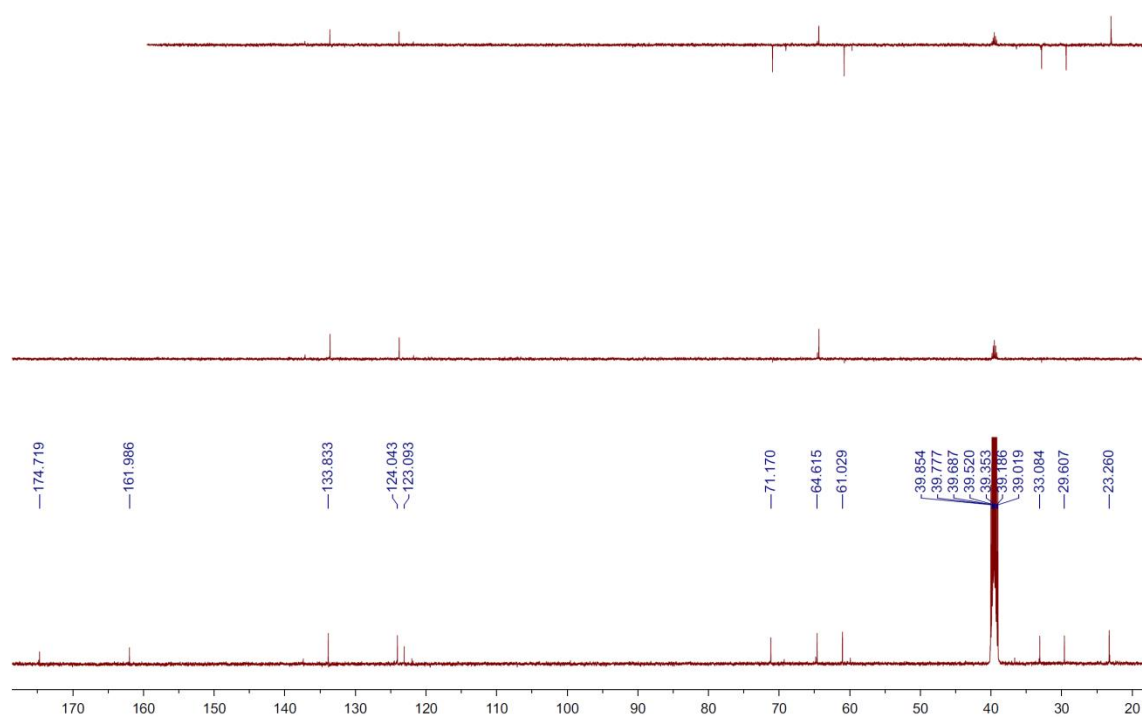
**Figure S14.** IR spectrum of compound **1**.



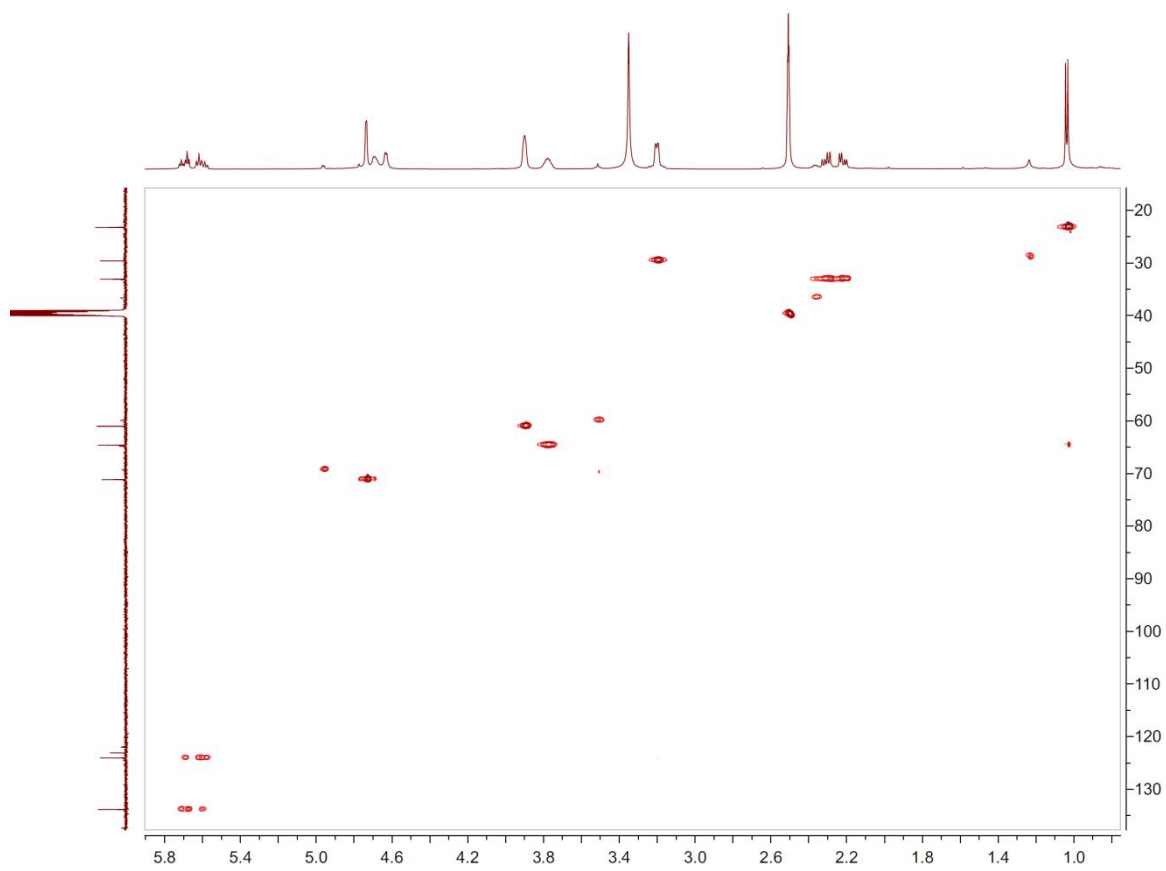
**Figure S15.** UV spectrum of compound **1** (0.2 mg/mL in MeOH).



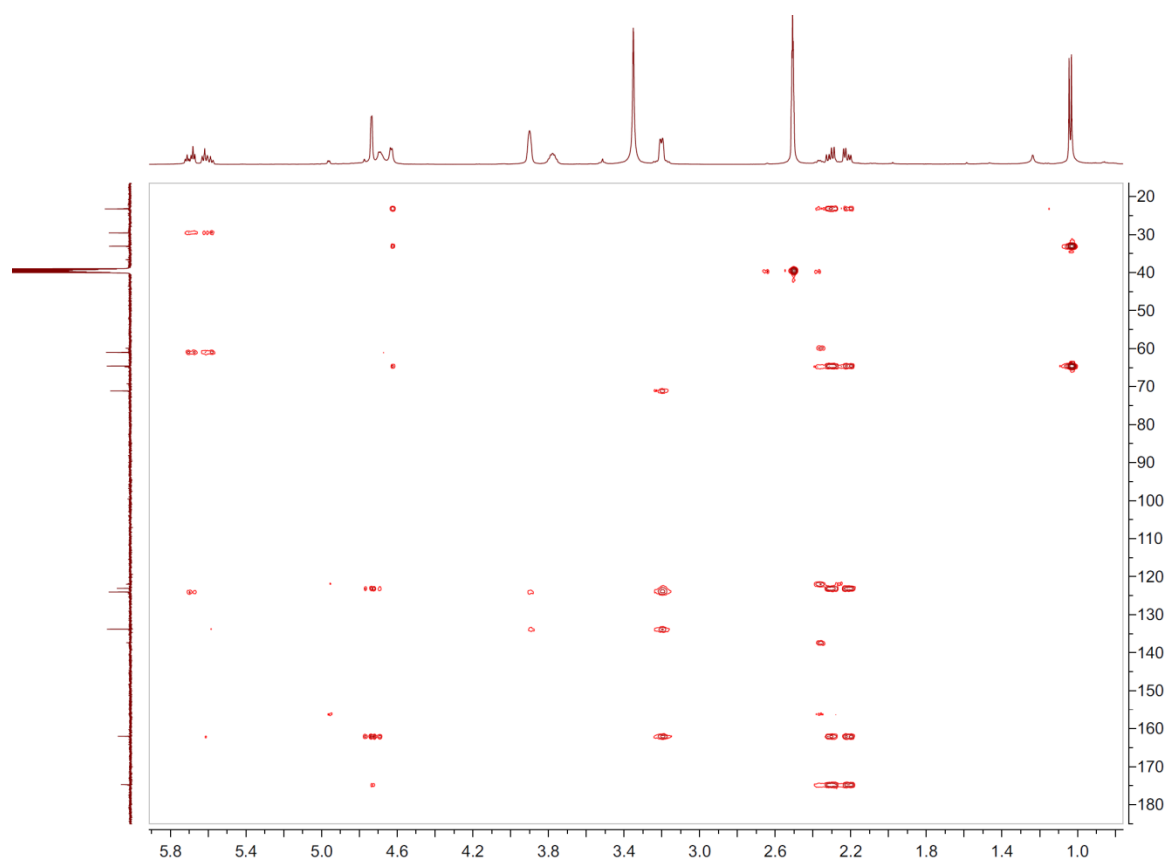
**Figure S16.**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{DMSO}-d_6$ .



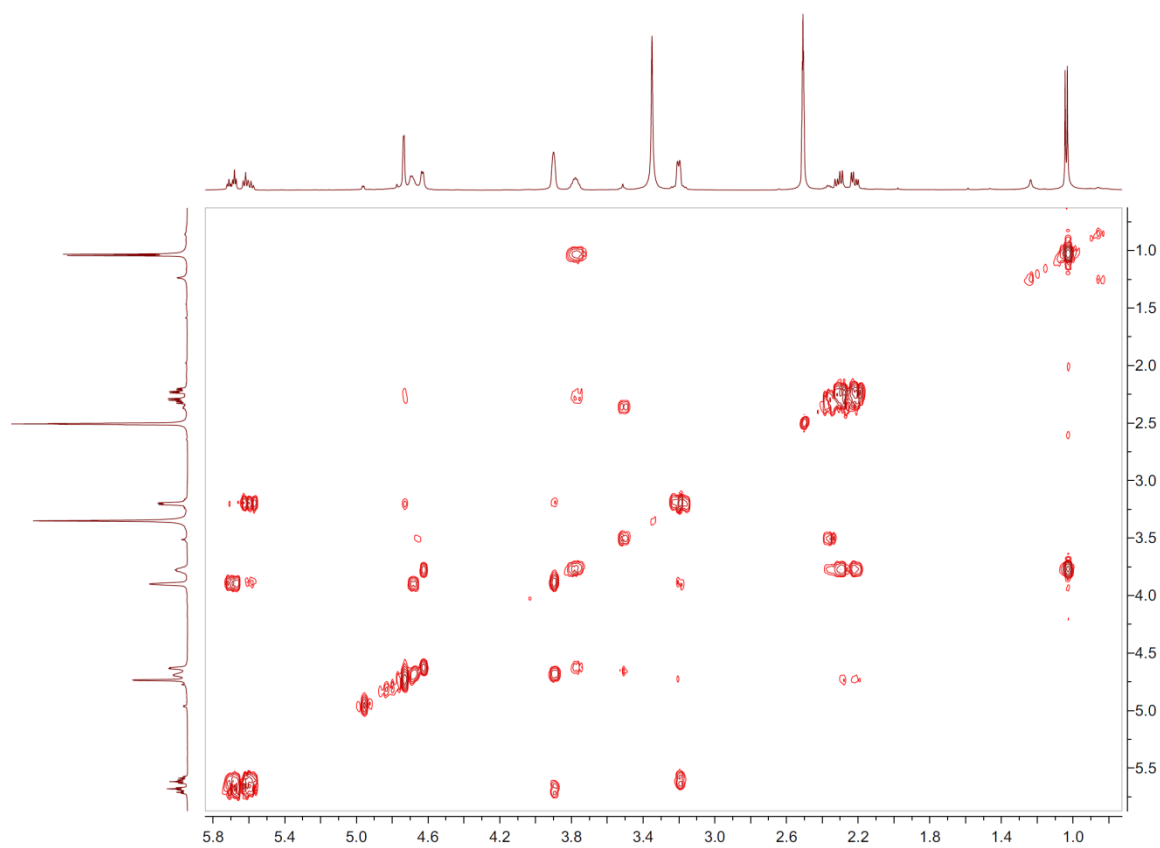
**Figure S17.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **2** in  $\text{DMSO}-d_6$ .



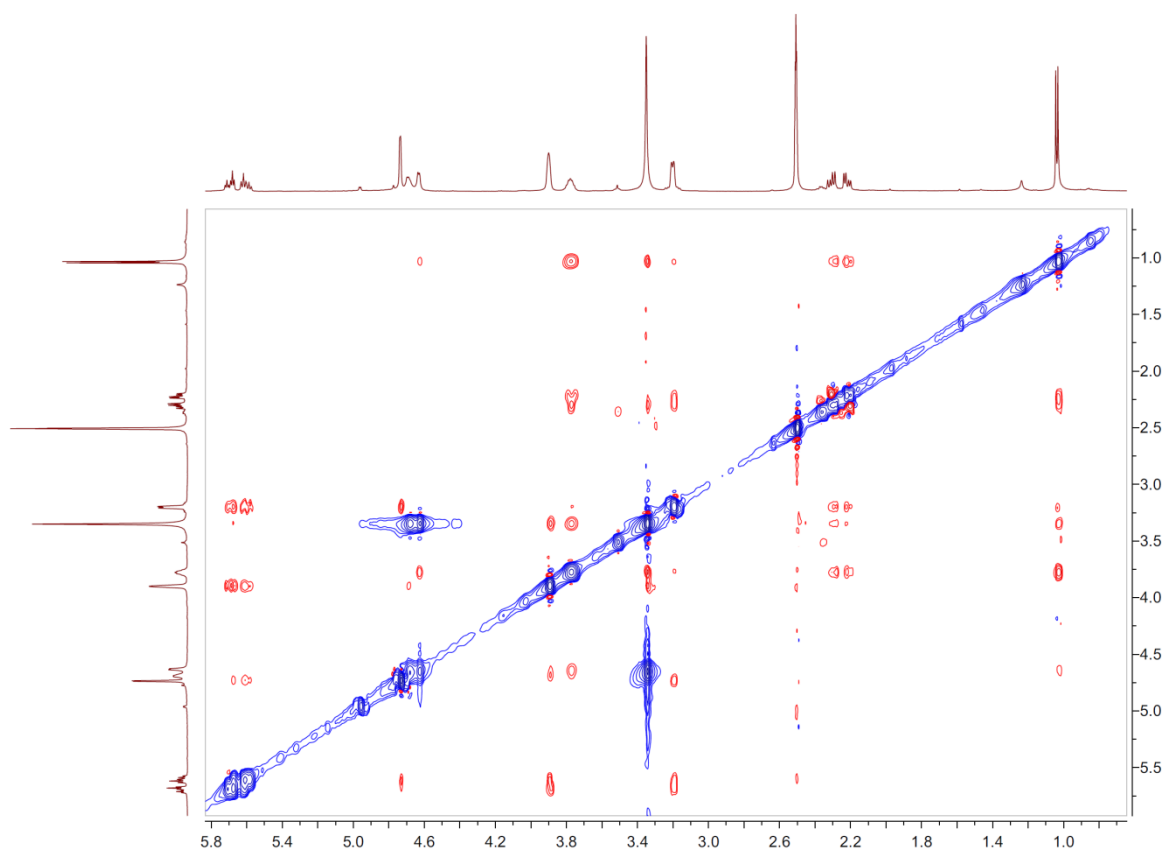
**Figure S18.** HSQC spectrum of compound **2** in  $\text{DMSO}-d_6$ .



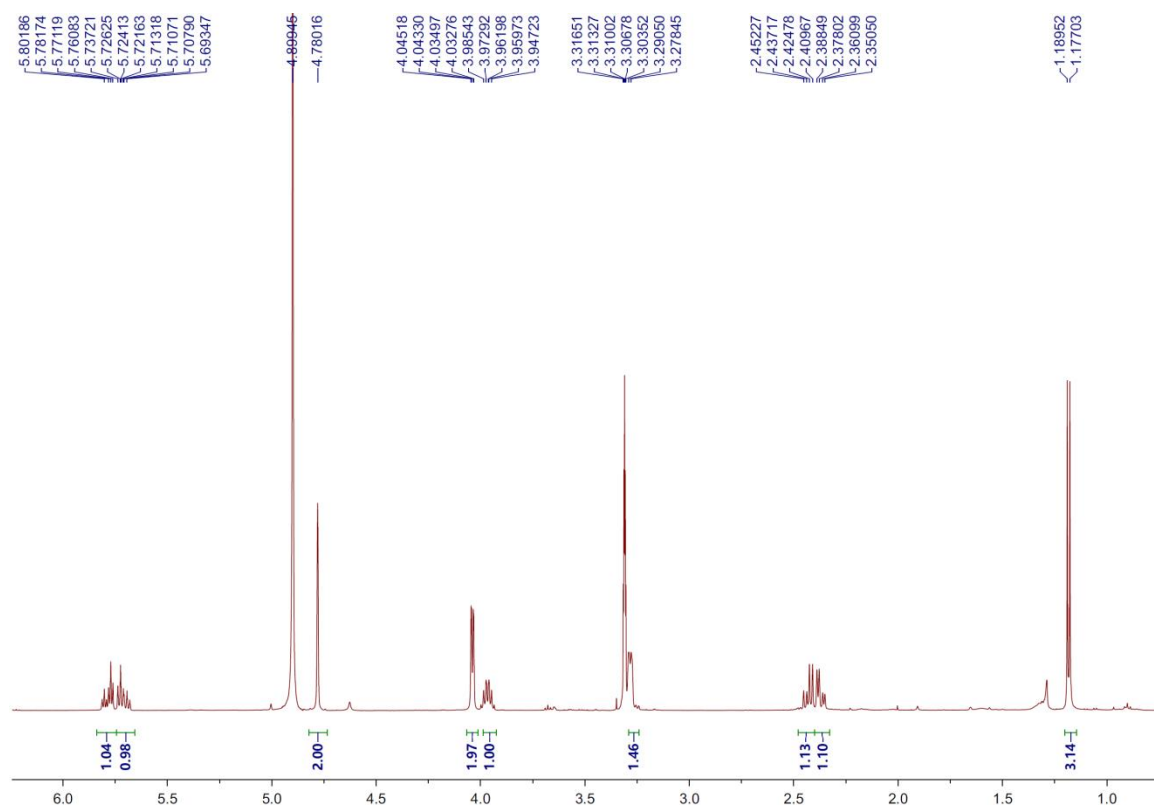
**Figure S19.** HMBC spectrum of compound **2** in DMSO- $d_6$ .



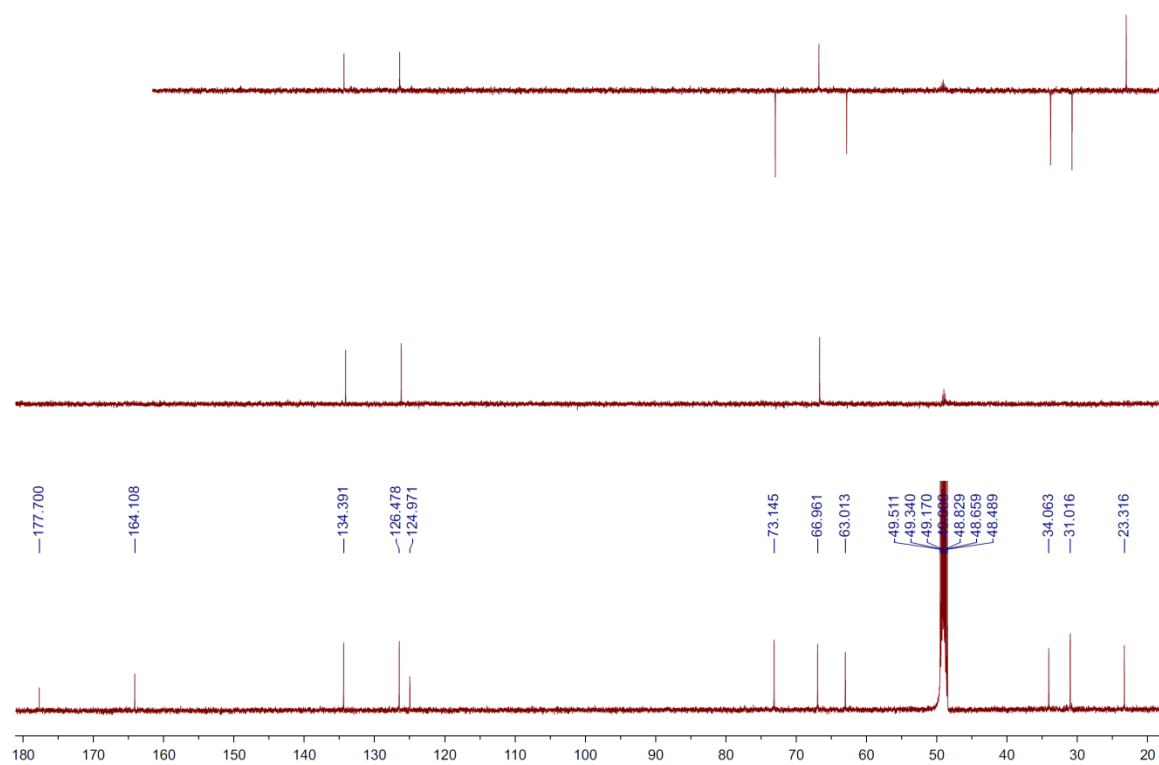
**Figure S20.** COSY spectrum of compound **2** in DMSO- $d_6$ .



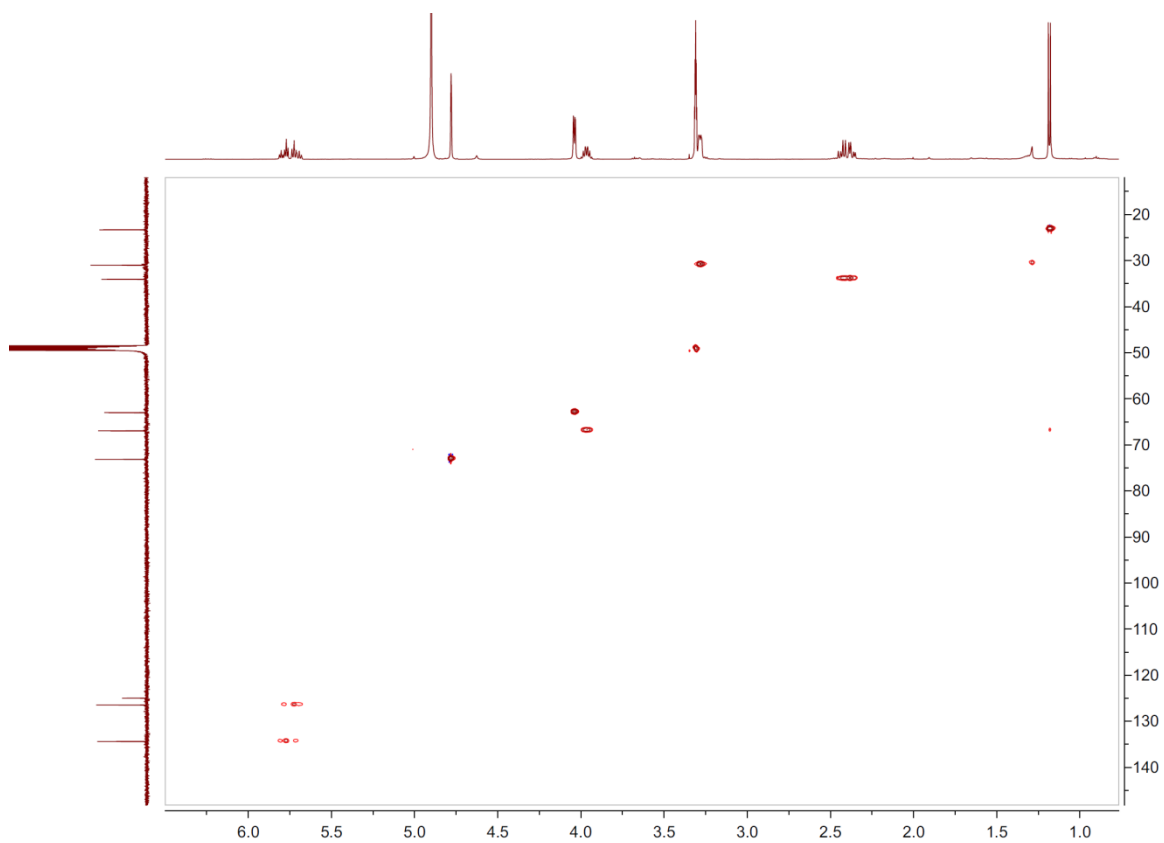
**Figure S21.** NOESY spectrum of compound **2** in DMSO- $d_6$ .



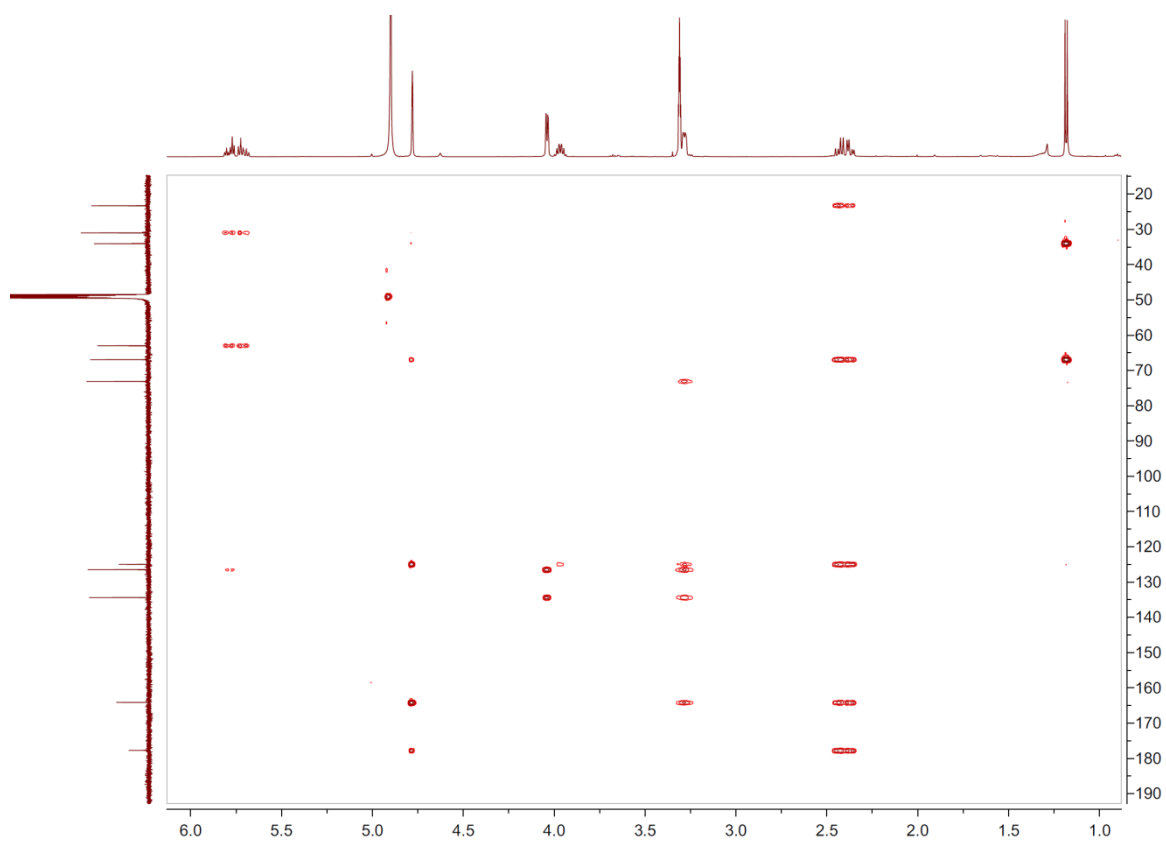
**Figure S22.**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .



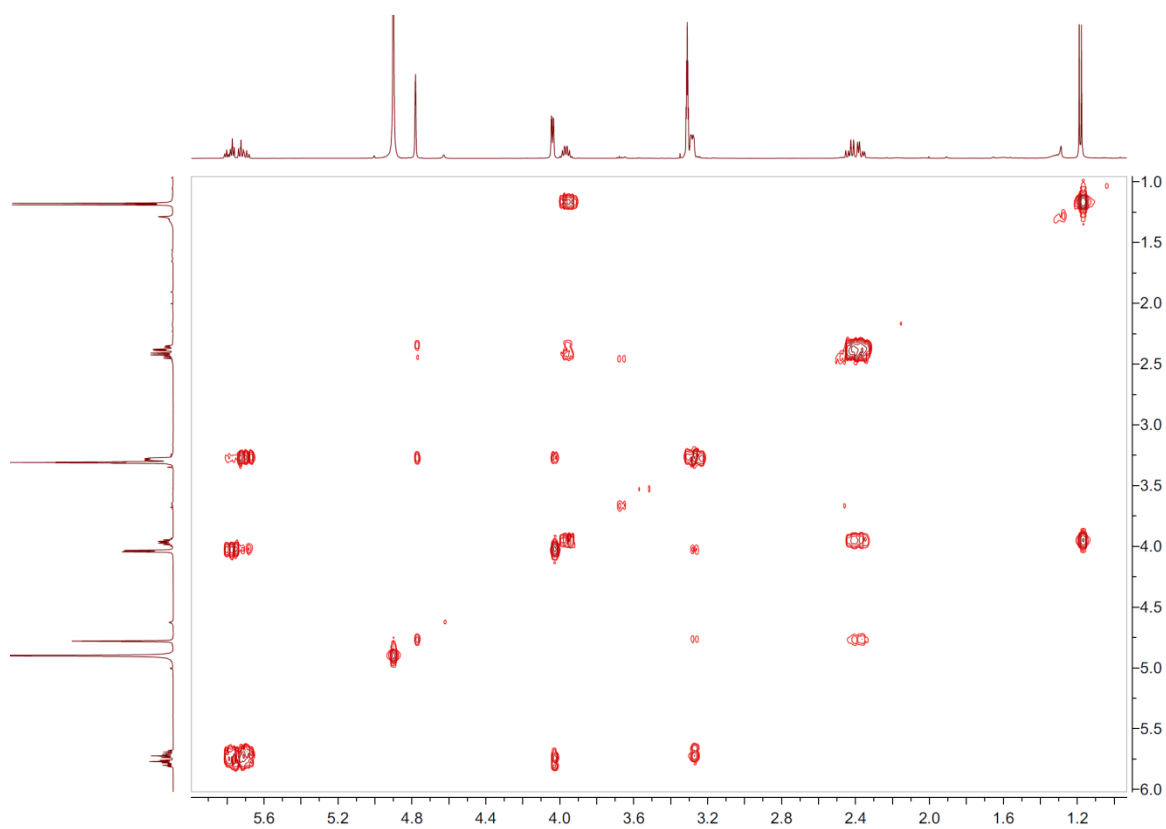
**Figure S23.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **2** in  $\text{CD}_3\text{OD}$ .



**Figure S24.** HSQC spectrum of compound **2** in  $\text{CD}_3\text{OD}$ .

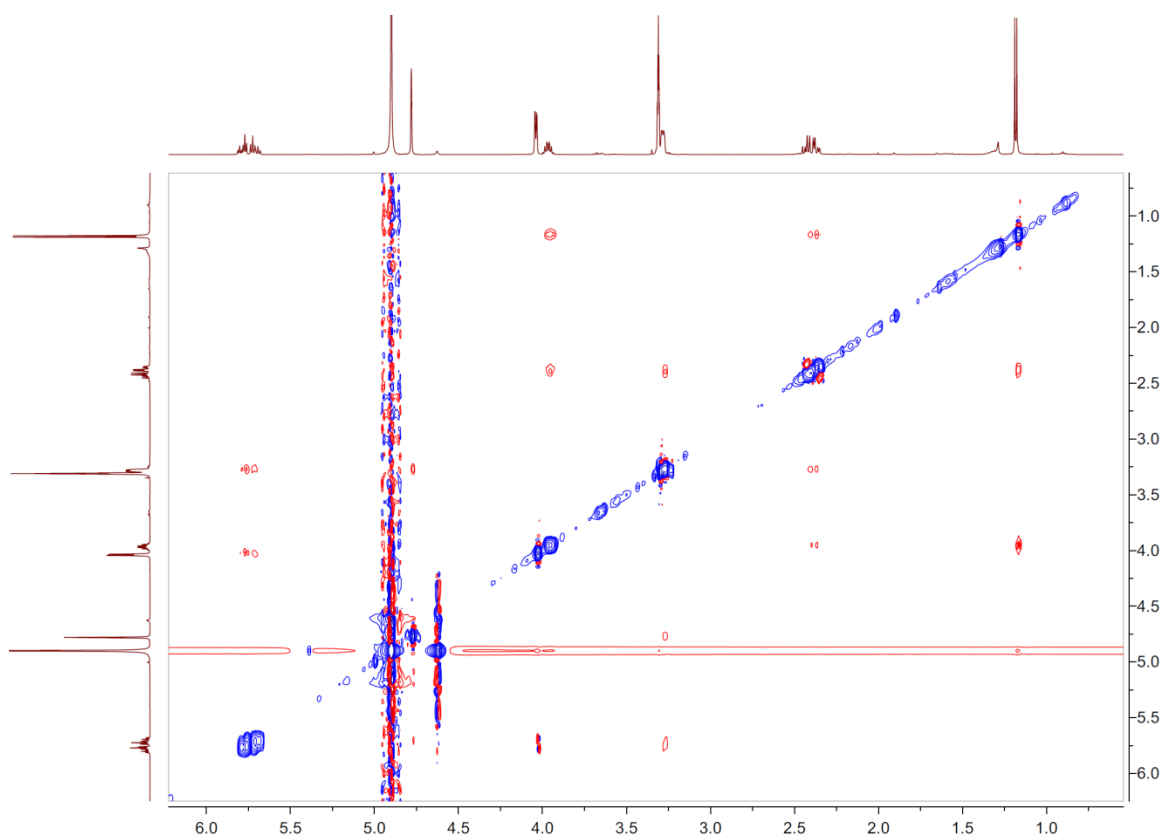


**Figure S25.** HMBC spectrum of compound **2** in CD<sub>3</sub>OD.

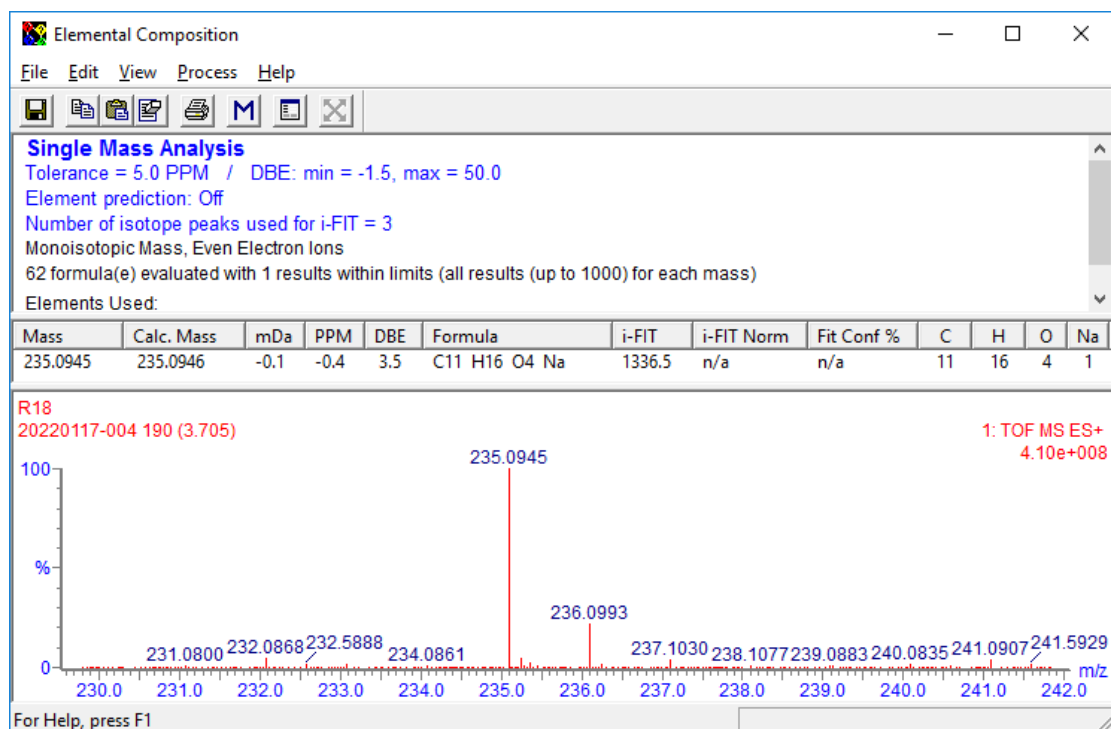


**Figure S26.** COSY spectrum of compound **2** in CD<sub>3</sub>OD.

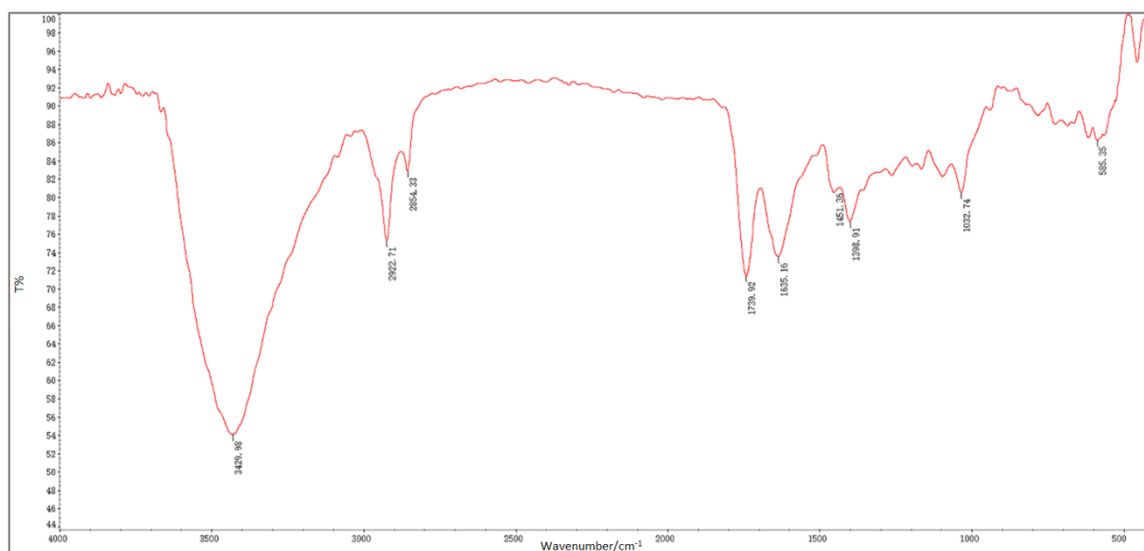




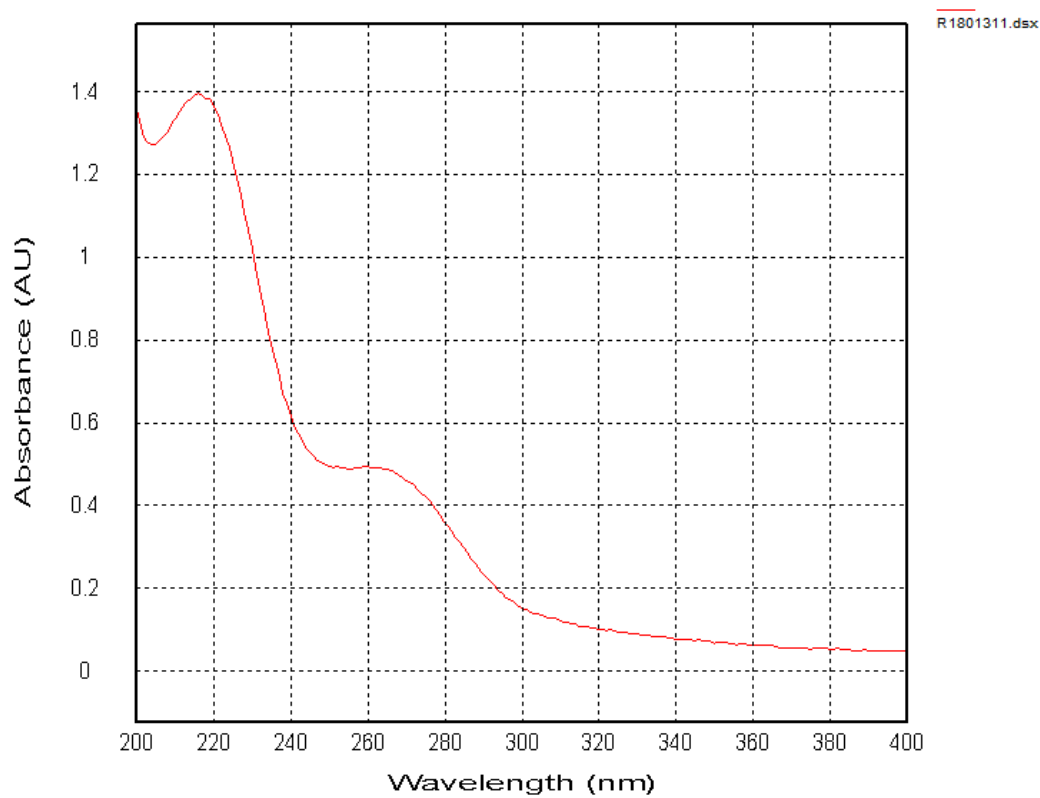
**Figure S27.** NOESY spectrum of compound **2** in CD<sub>3</sub>OD.



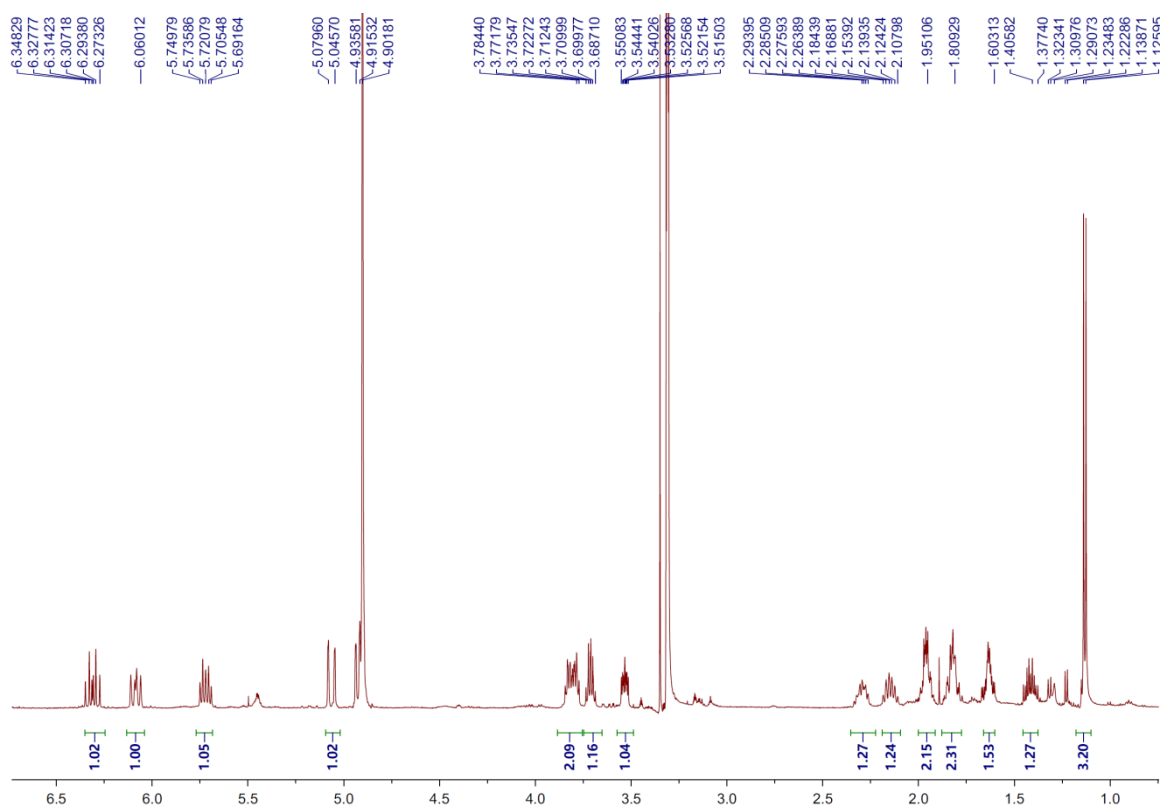
**Figure S28.** HRESI(+)MS spectrum of compound **2**.



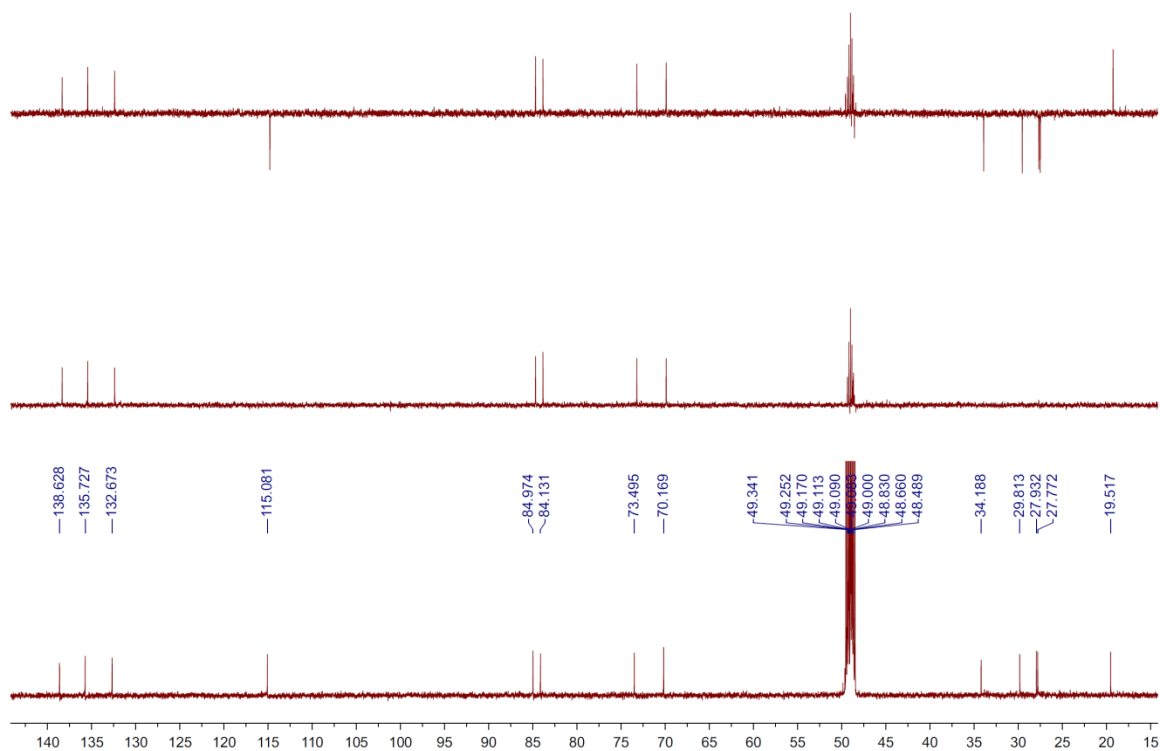
**Figure S29.** IR spectrum of compound **2**.



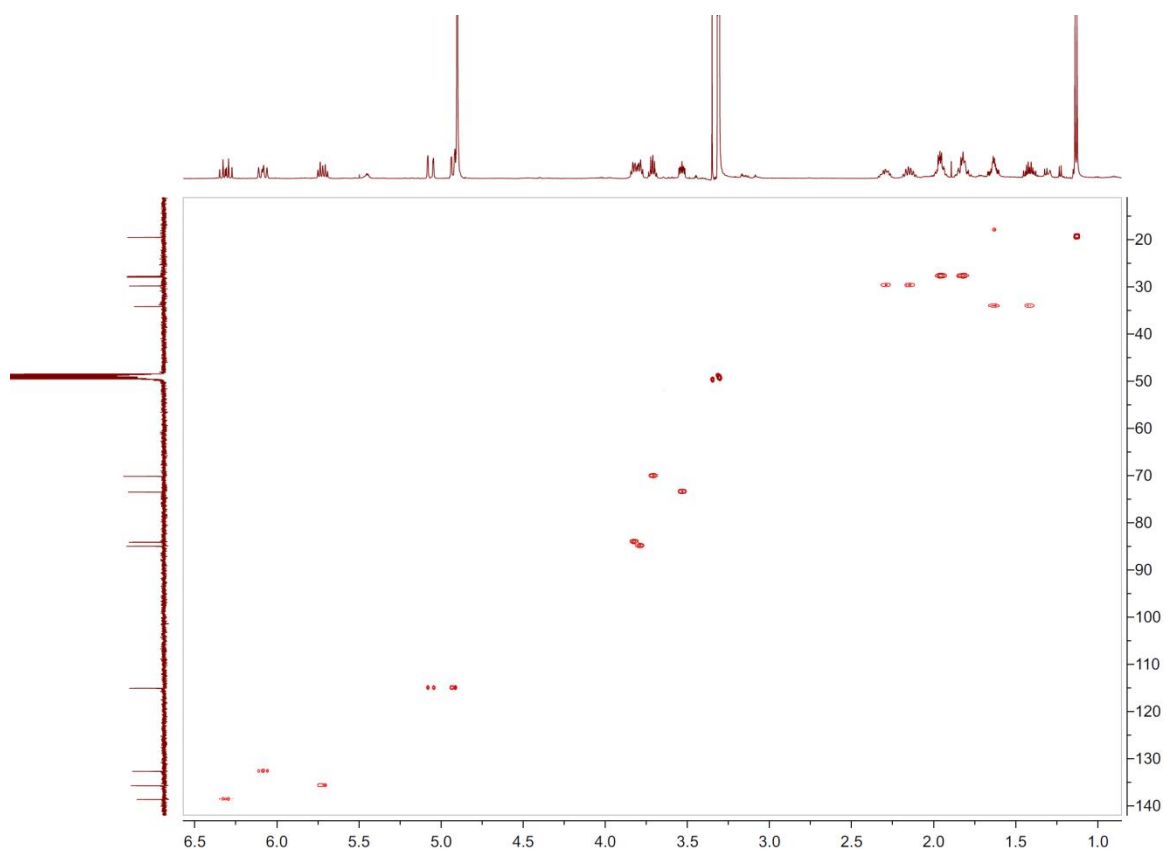
**Figure S30.** UV spectrum of compound **2** (0.4 mg/mL in MeOH).



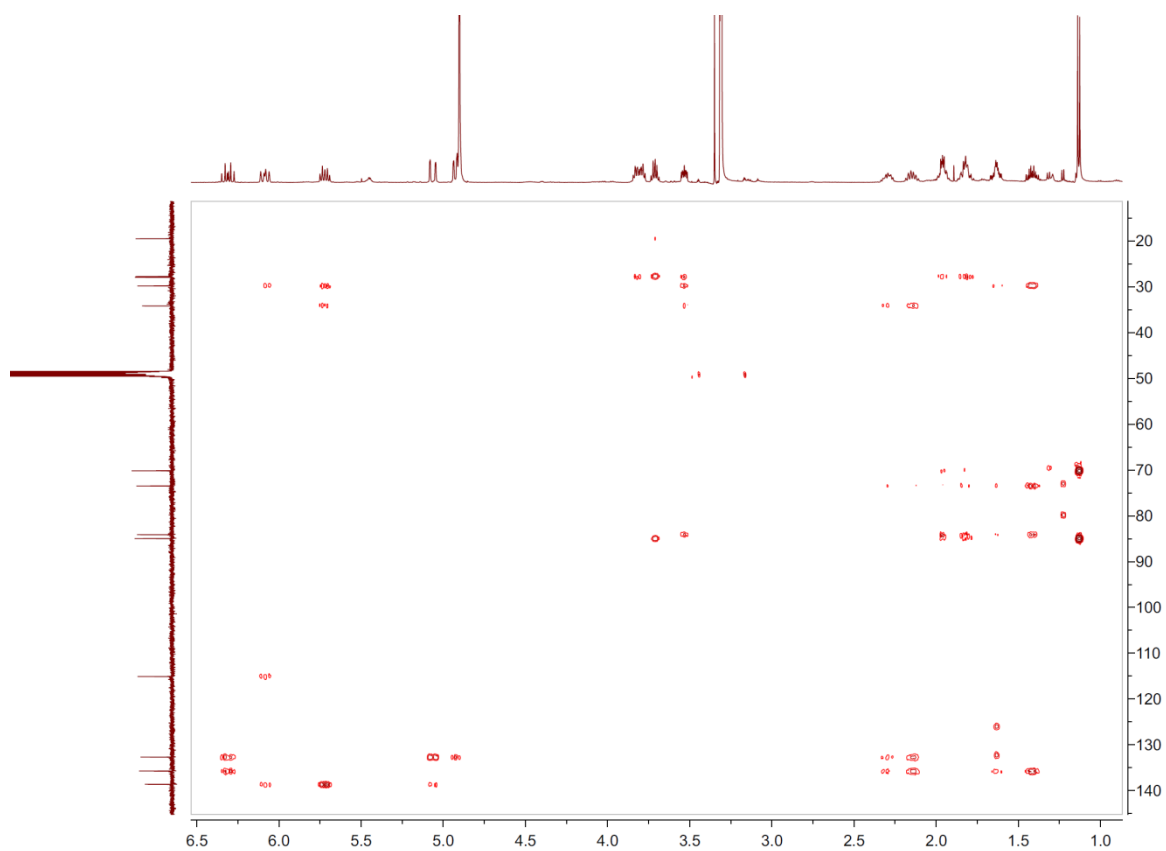
**Figure S31.** <sup>1</sup>H NMR spectrum of compound **3** in CD<sub>3</sub>OD.



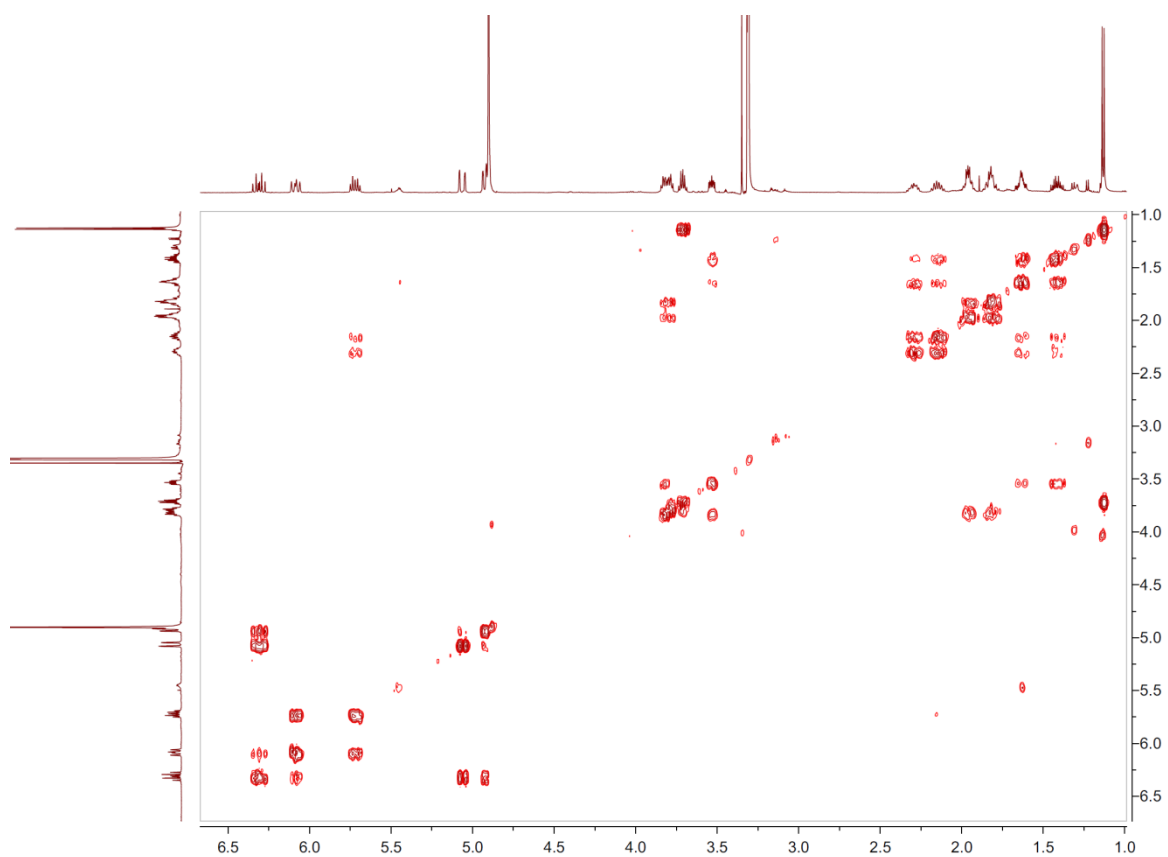
**Figure S32.** <sup>13</sup>C NMR and DEPT spectra of compound **3** in CD<sub>3</sub>OD.



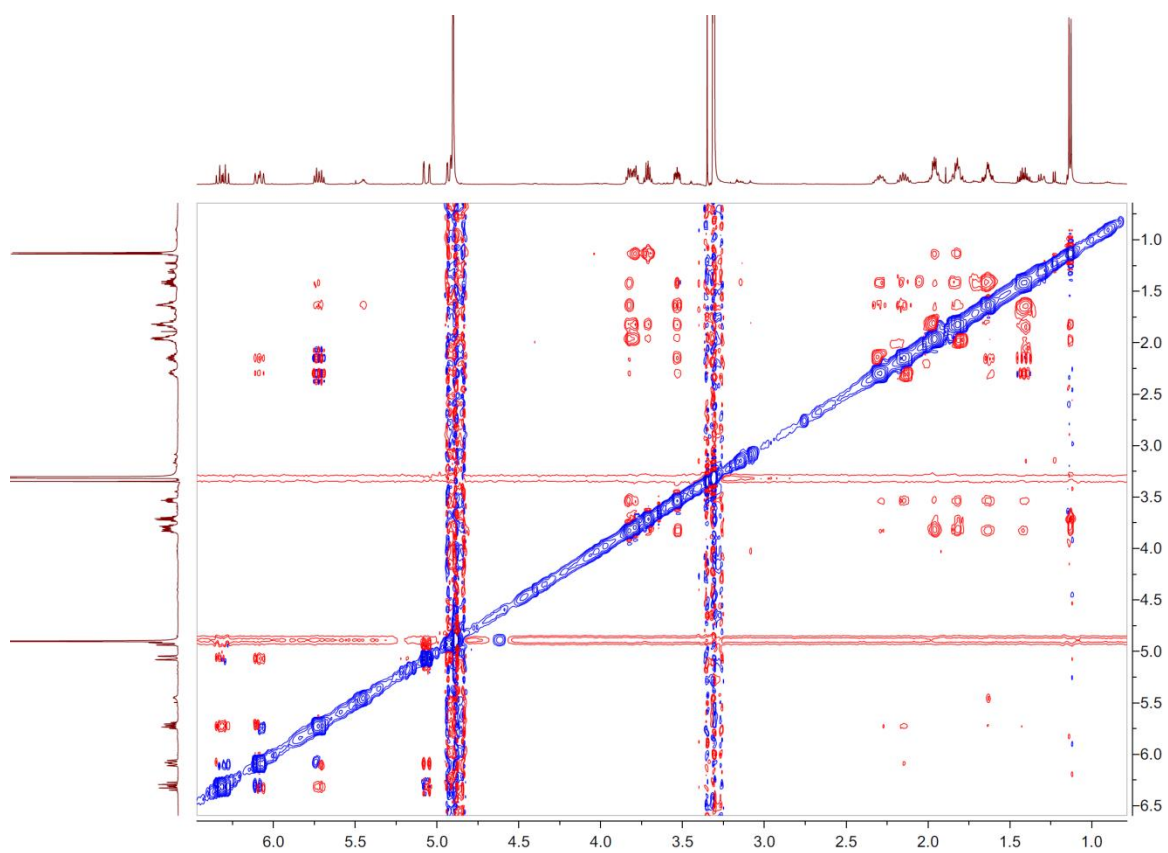
**Figure S33.** HSQC spectrum of compound **3** in CD<sub>3</sub>OD.



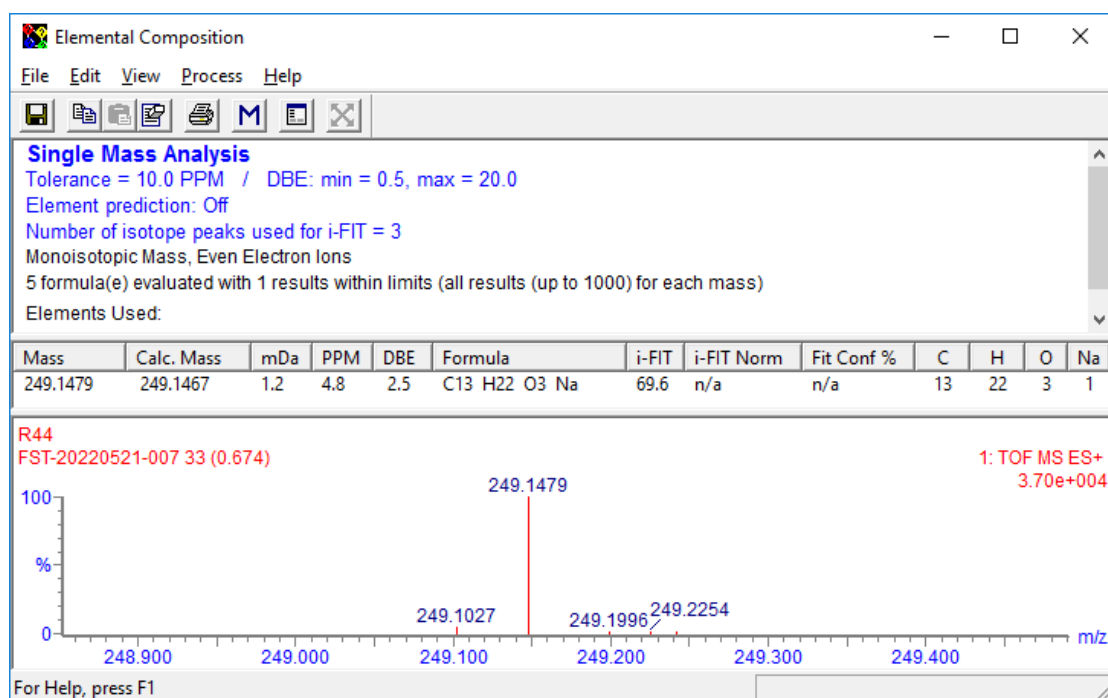
**Figure S34.** HMBC spectrum of compound **3** in CD<sub>3</sub>OD.



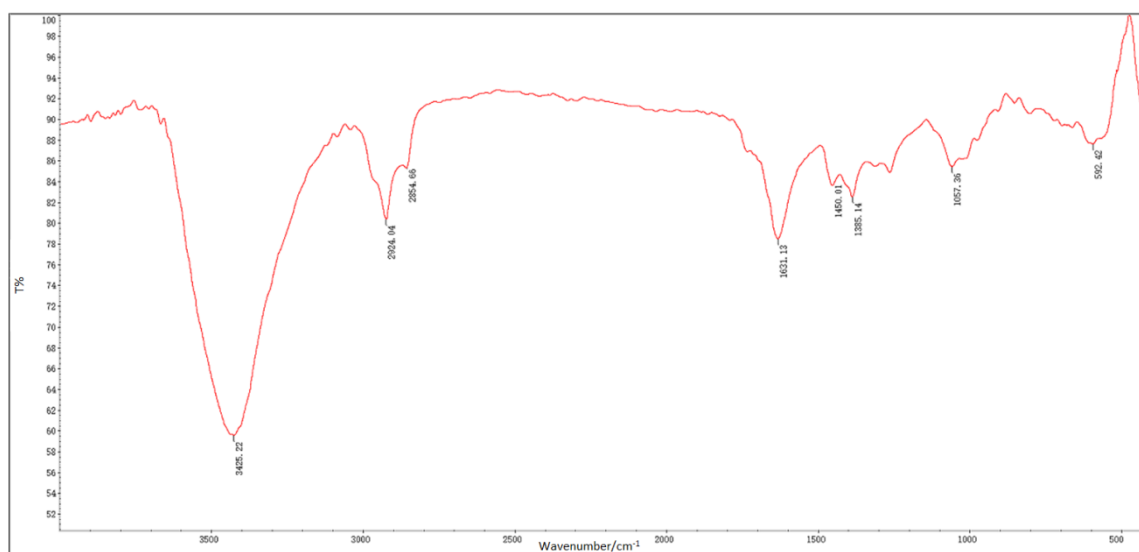
**Figure S35.** COSY spectrum of compound **3** in CD<sub>3</sub>OD.



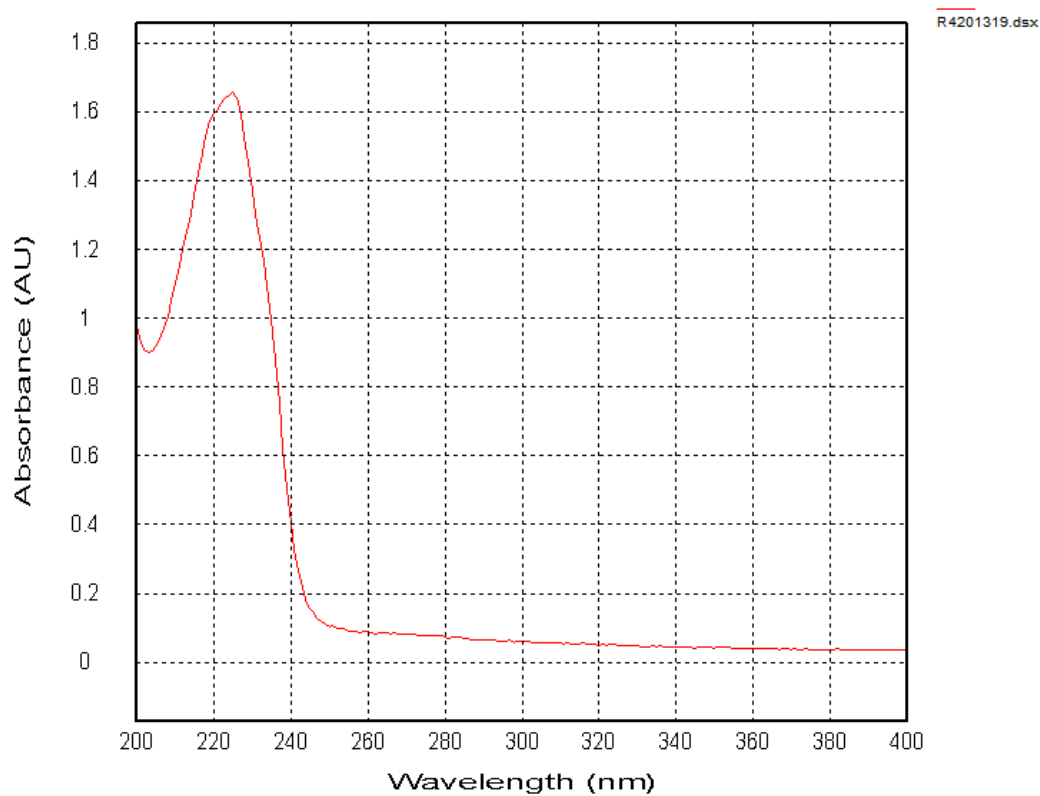
**Figure S36.** NOESY spectrum of compound **3** in CD<sub>3</sub>OD.



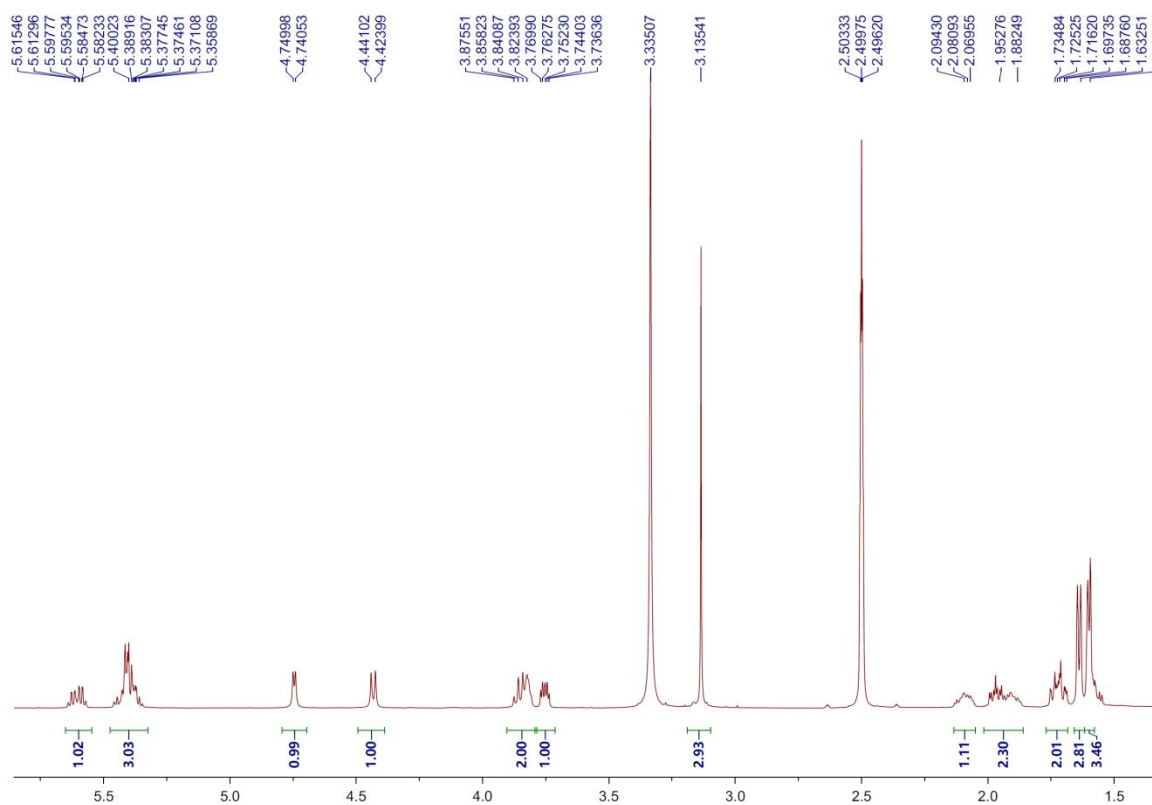
**Figure S37.** HRESI(+)MS spectrum of compound **3**.



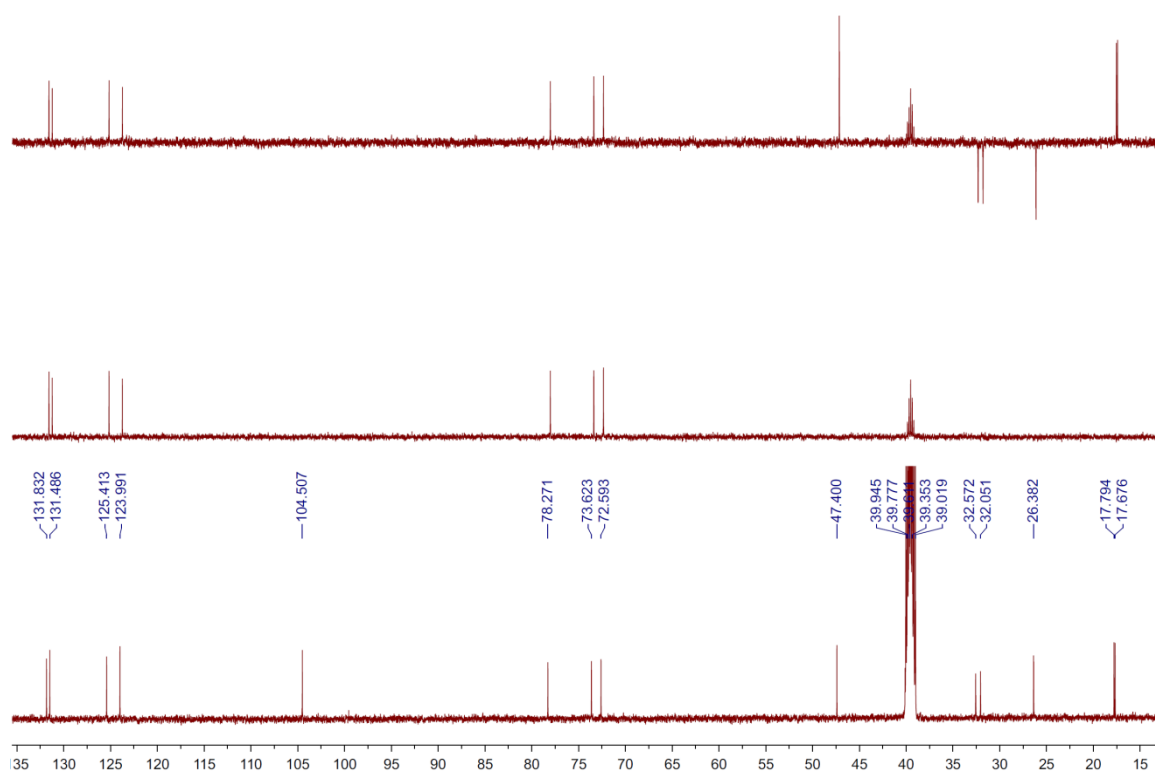
**Figure S38.** IR spectrum of compound **3**.



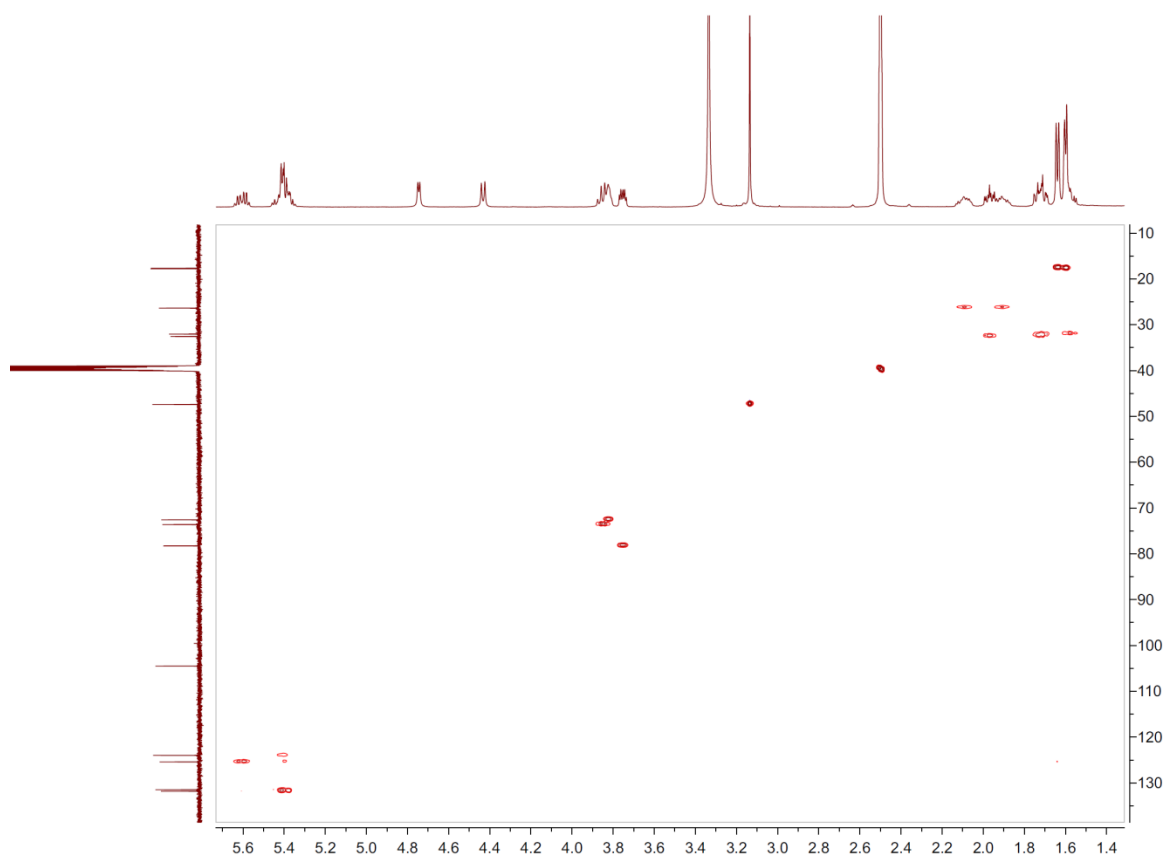
**Figure S39.** UV spectrum of compound **3** (0.2 mg/mL in MeOH).



**Figure S40.**  $^1\text{H}$  NMR spectrum of compound **4** in  $\text{DMSO}-d_6$ .

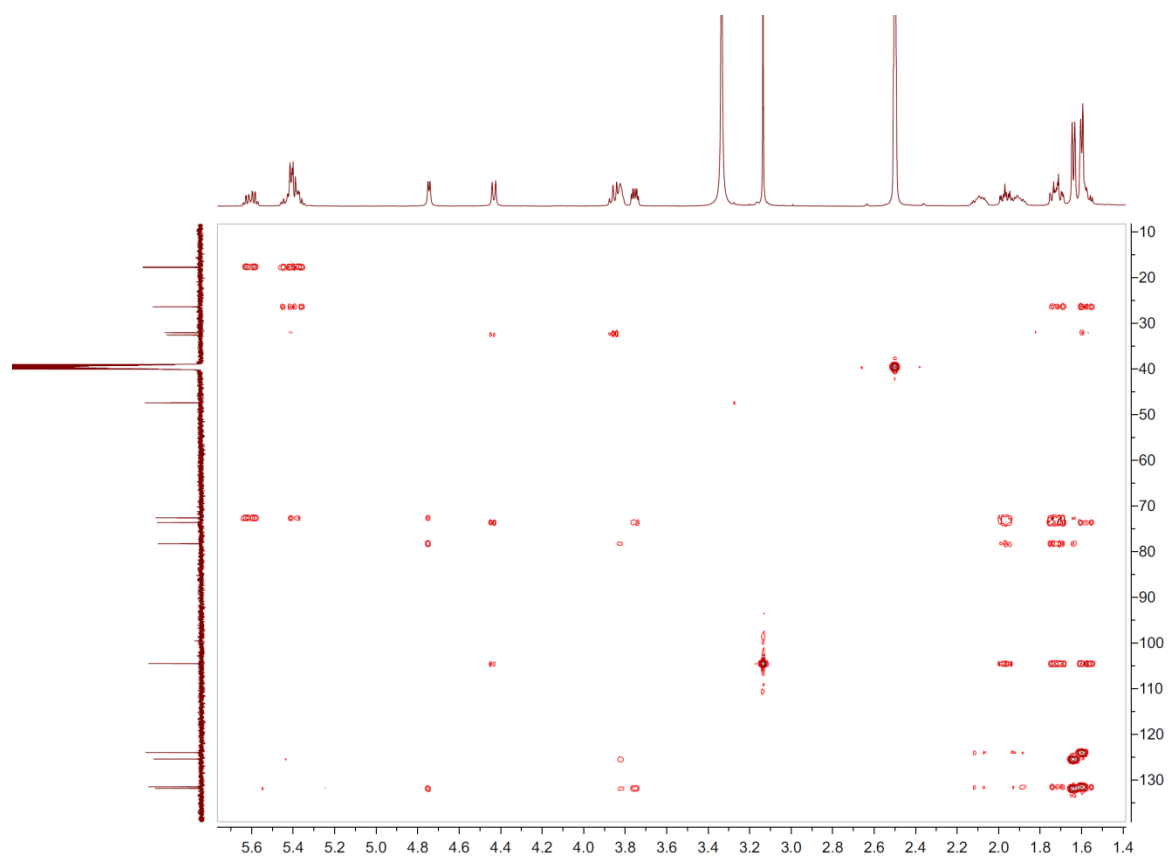


**Figure S41.**  $^{13}\text{C}$  NMR and DEPT spectra of compound **4** in  $\text{DMSO-}d_6$ .

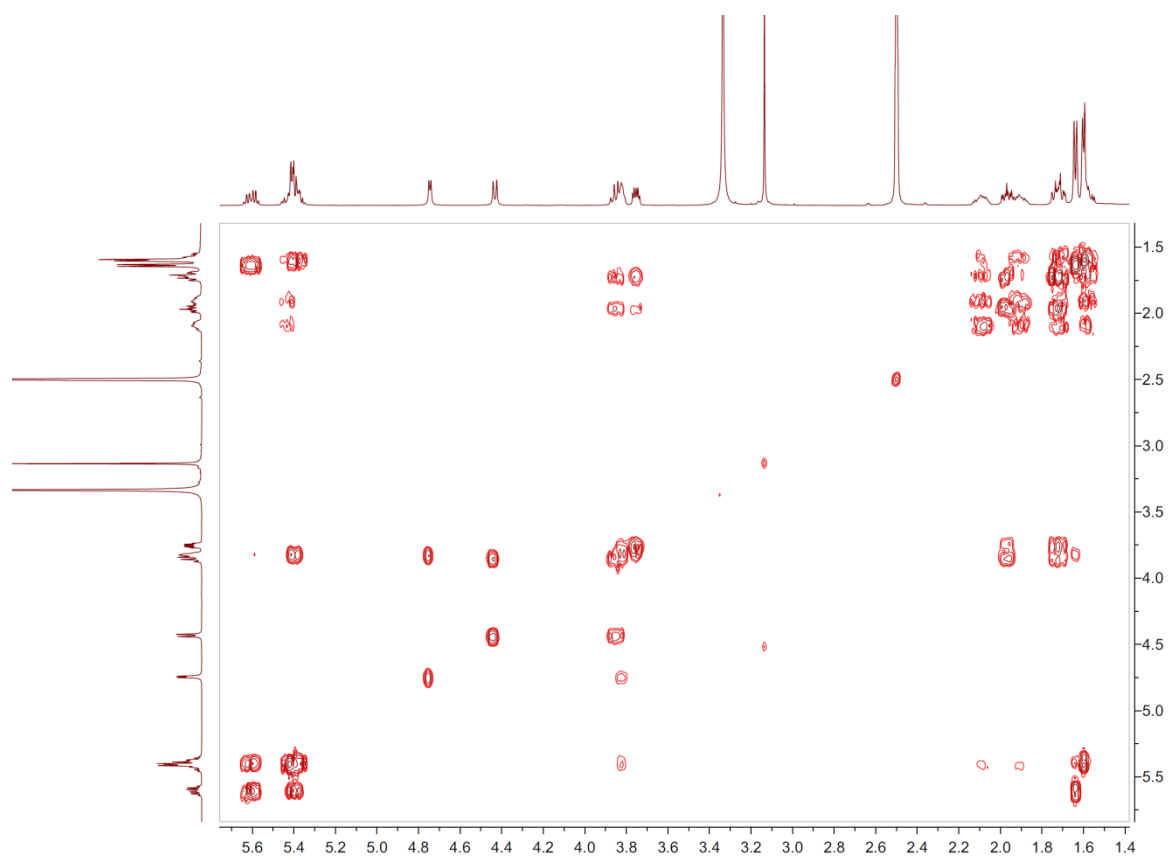


**Figure S42.** HSQC spectrum of compound **4** in  $\text{DMSO-}d_6$ .

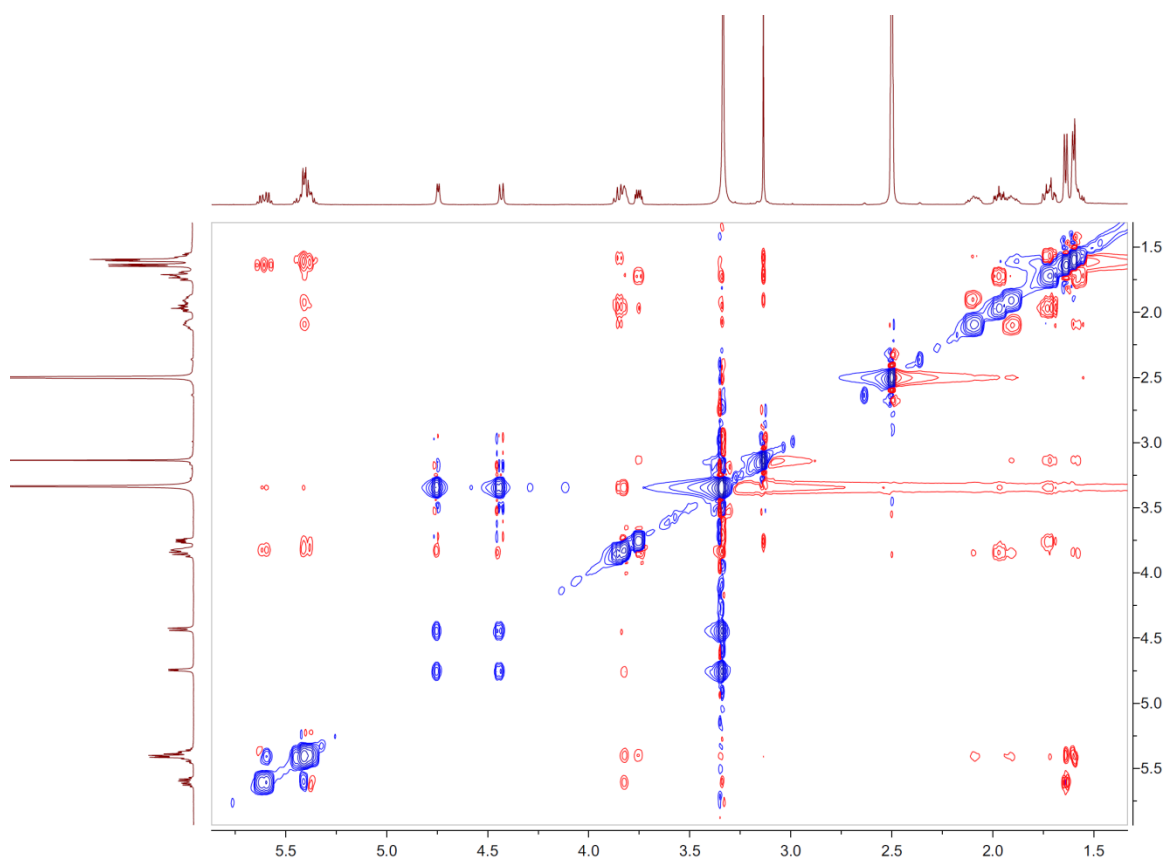




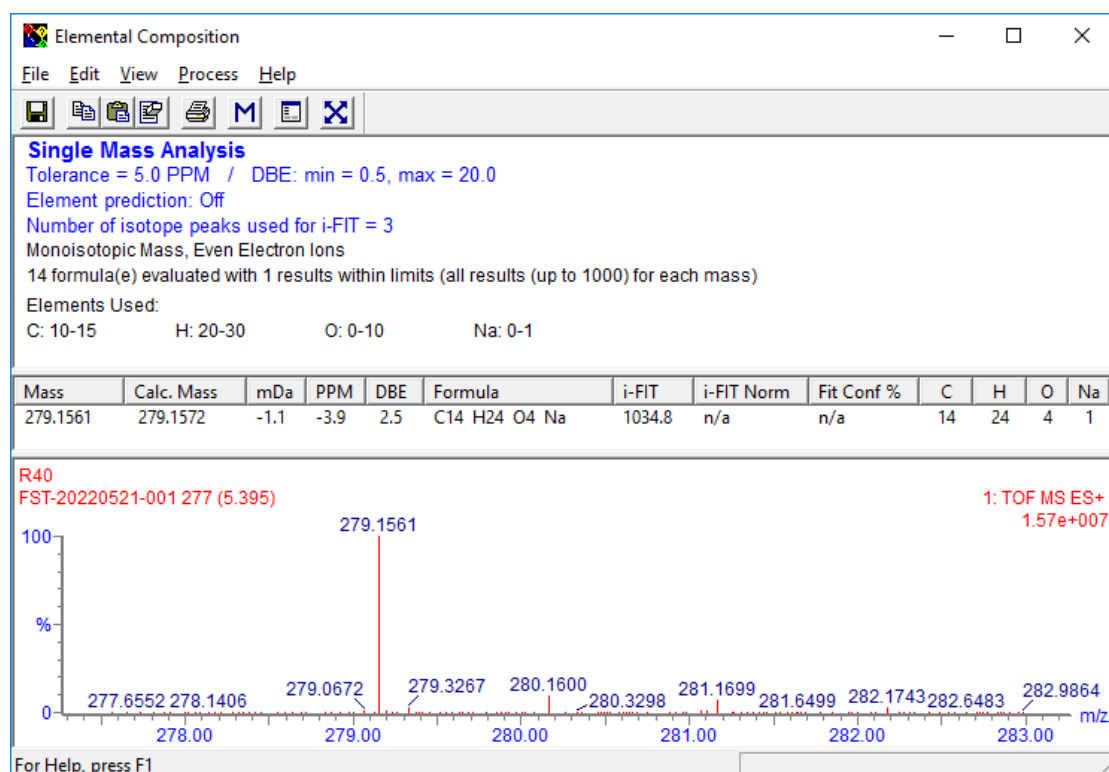
**Figure S43.** HMBC spectrum of compound **4** in DMSO- $d_6$ .



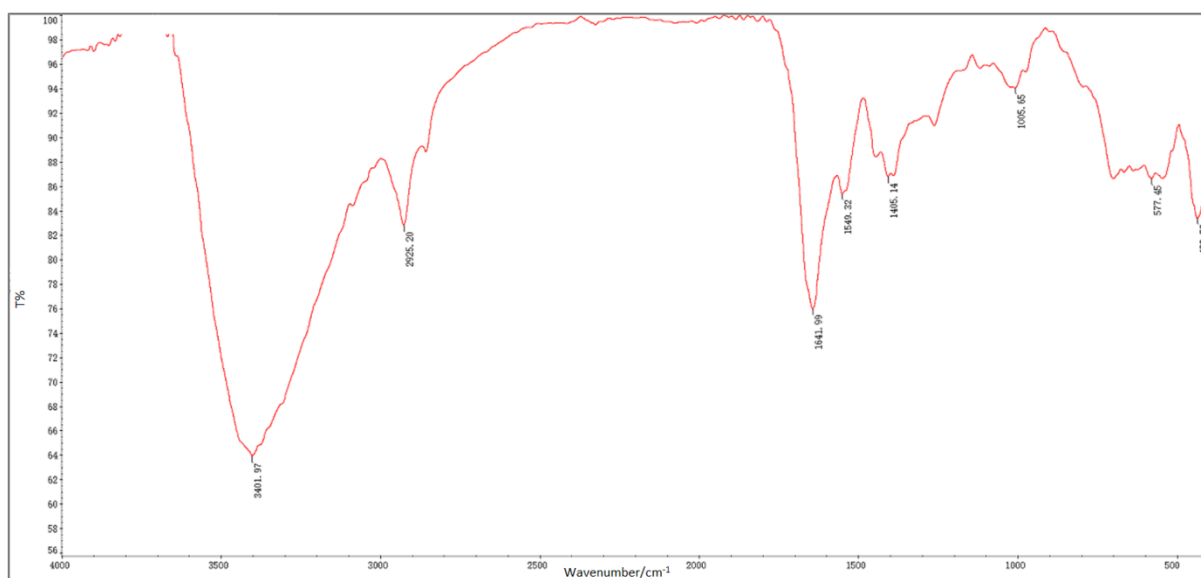
**Figure S44.** COSY spectrum of compound **4** in DMSO- $d_6$ .



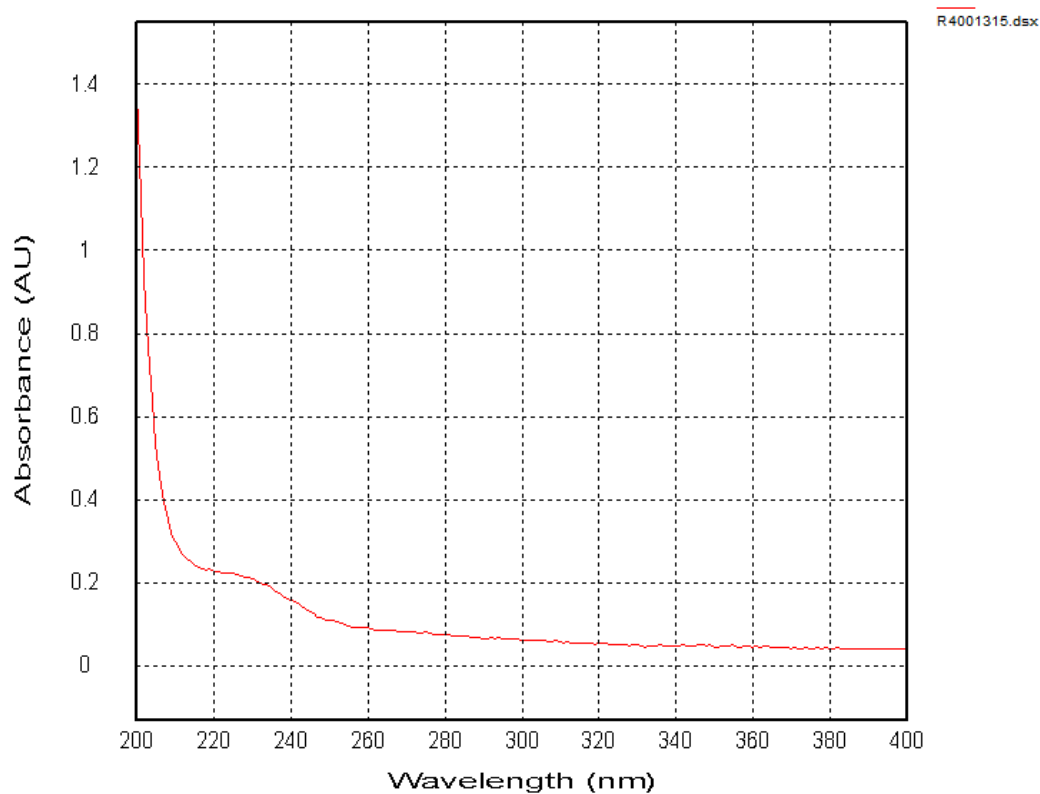
**Figure S45.** NOESY spectrum of compound **4** in DMSO- $d_6$ .



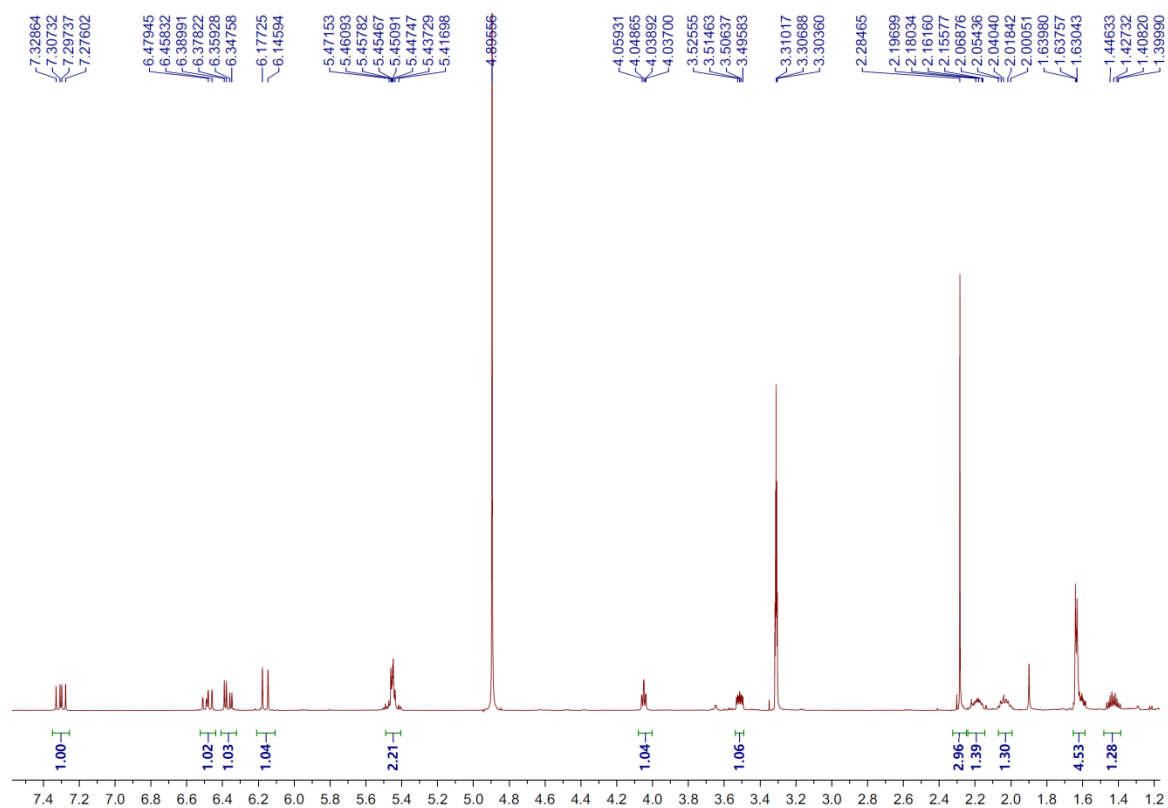
**Figure S46.** HRESI(+)MS spectrum of compound **4**.



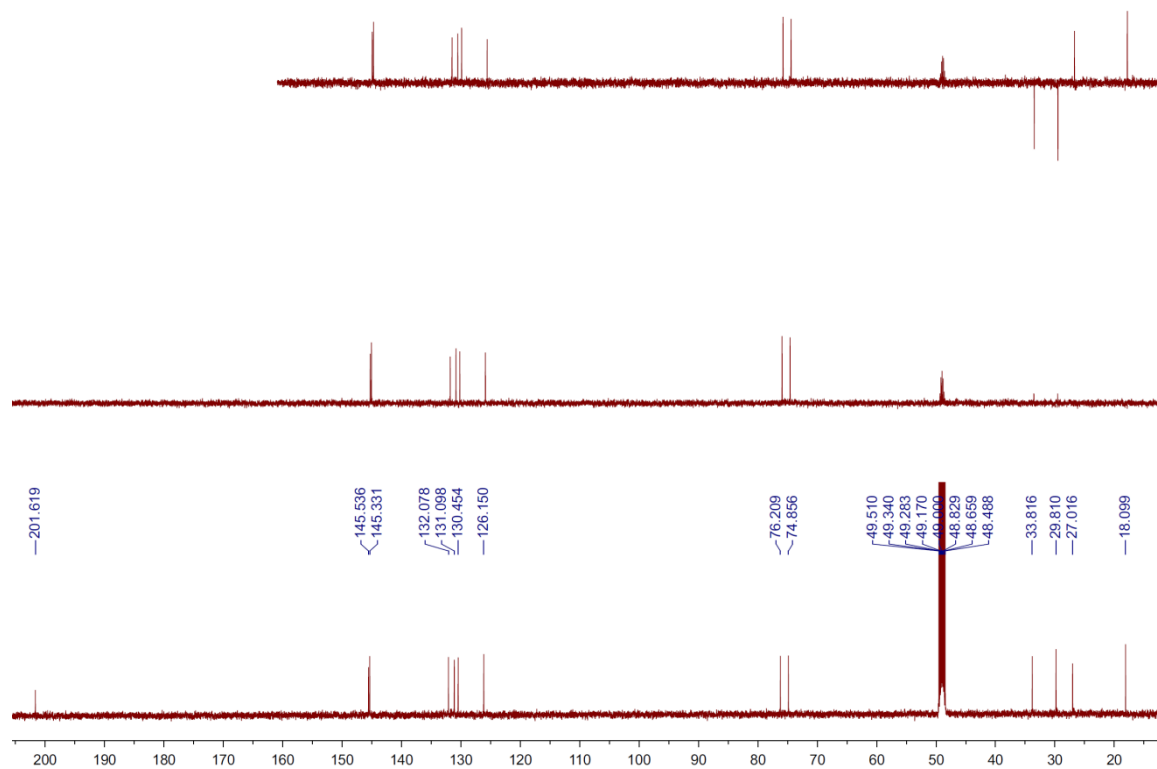
**Figure S47.** IR spectrum of compound **4**.



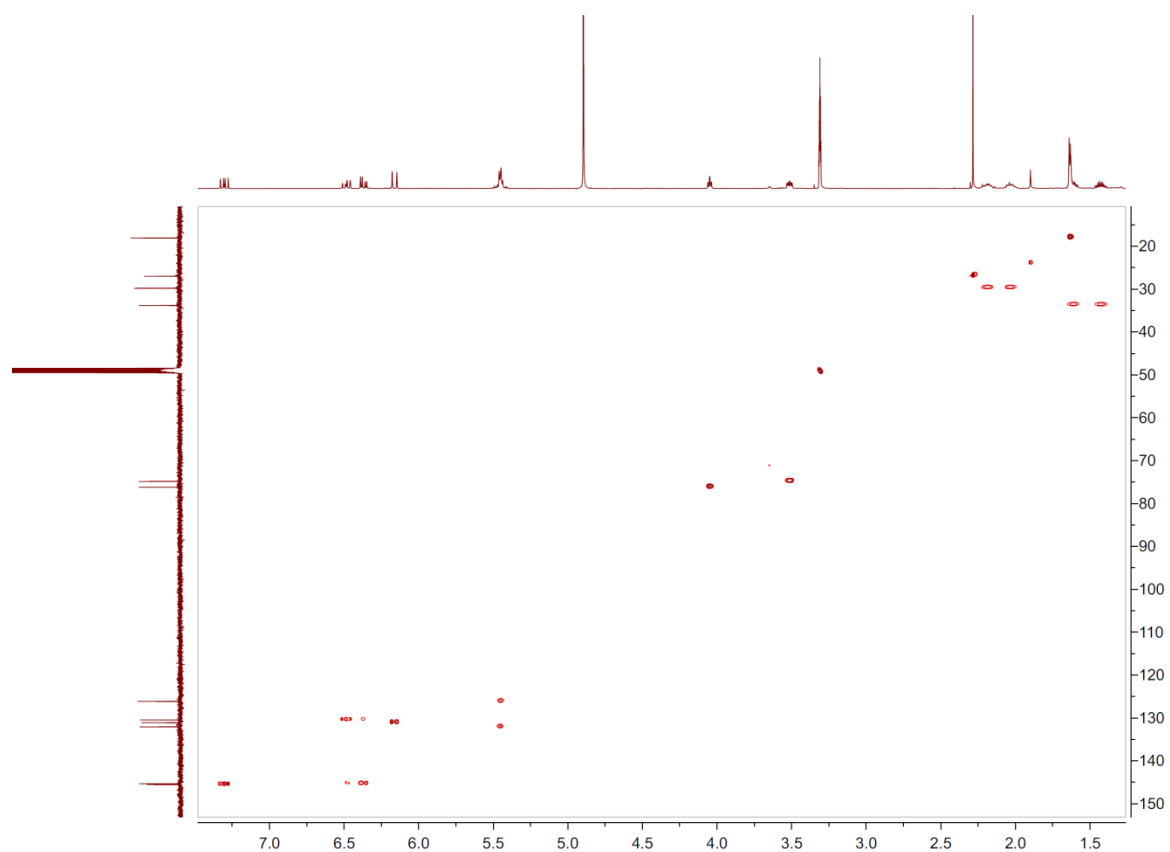
**Figure S48.** UV spectrum of compound **4** (0.4 mg/mL in MeOH).



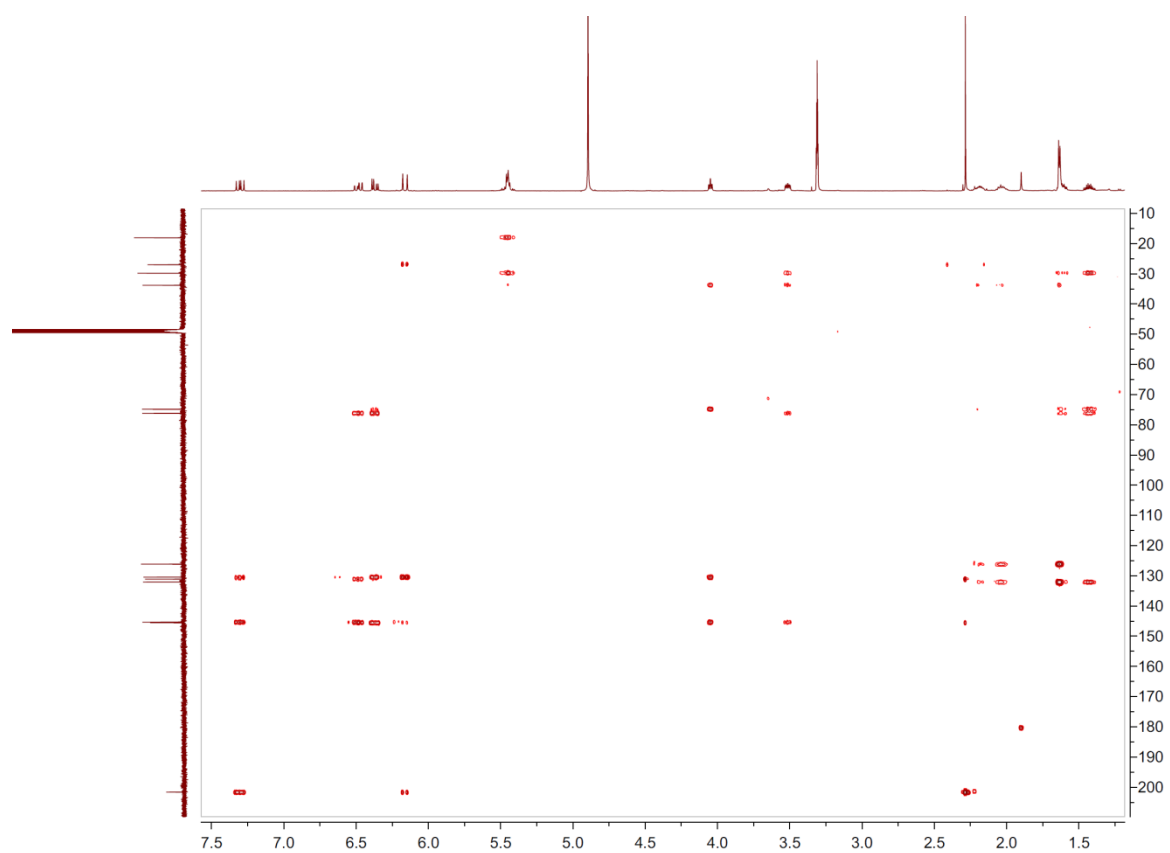
**Figure S49.** <sup>1</sup>H NMR spectrum of compound **5** in CD<sub>3</sub>OD.



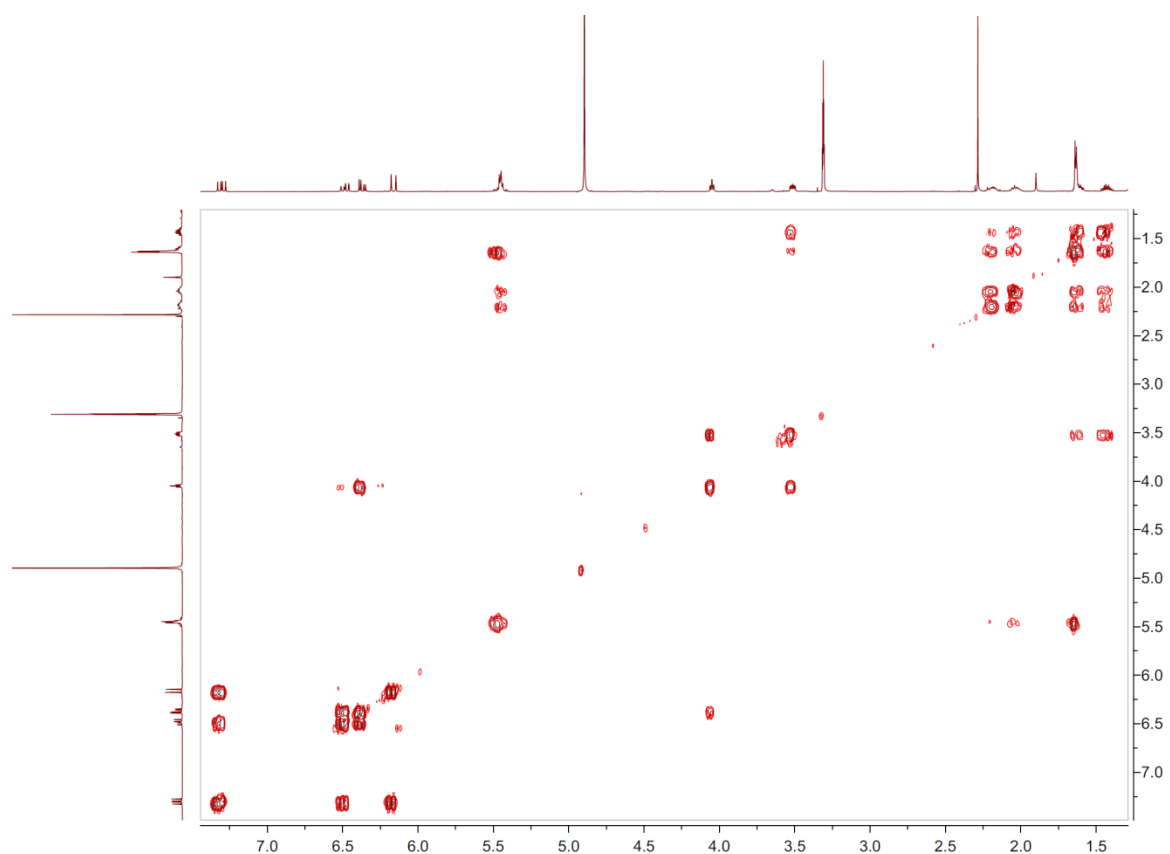
**Figure S50.** <sup>13</sup>C NMR and DEPT spectra of compound **5** in CD<sub>3</sub>OD.



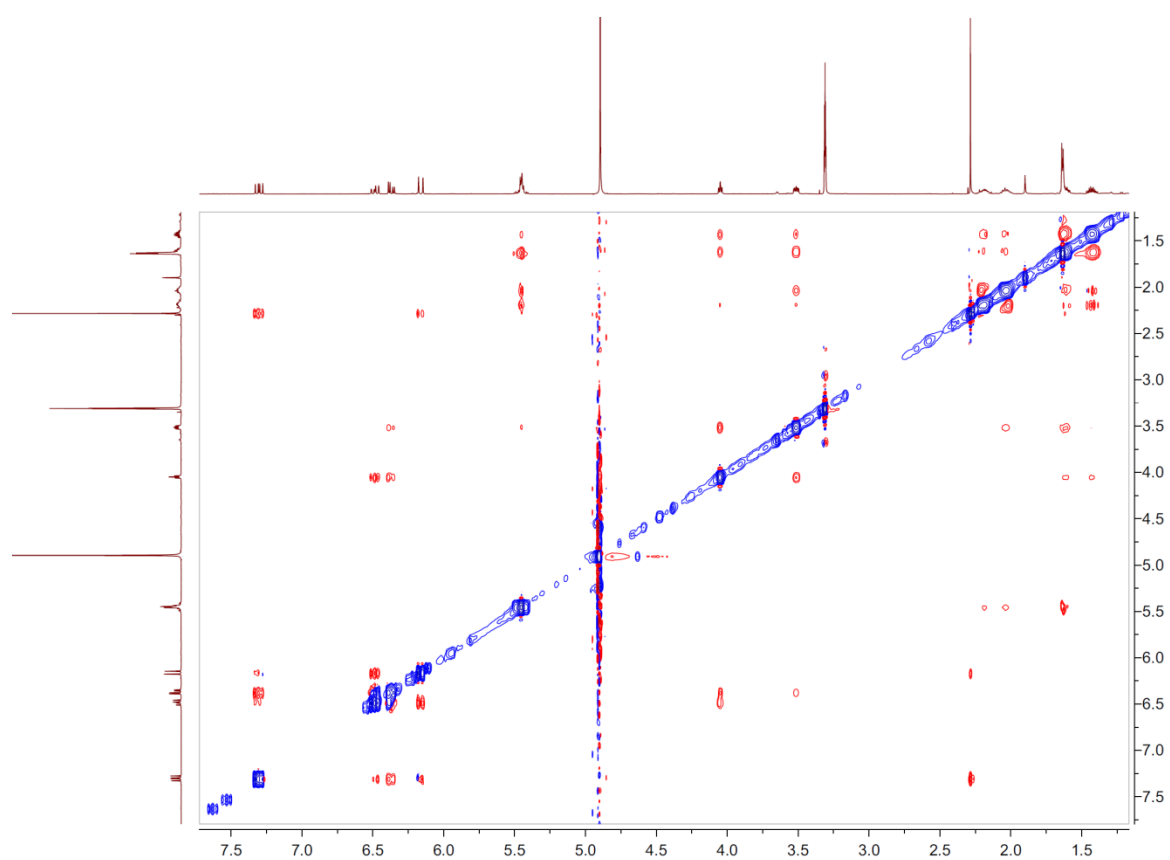
**Figure S51.** HSQC spectrum of compound **5** in CD<sub>3</sub>OD.



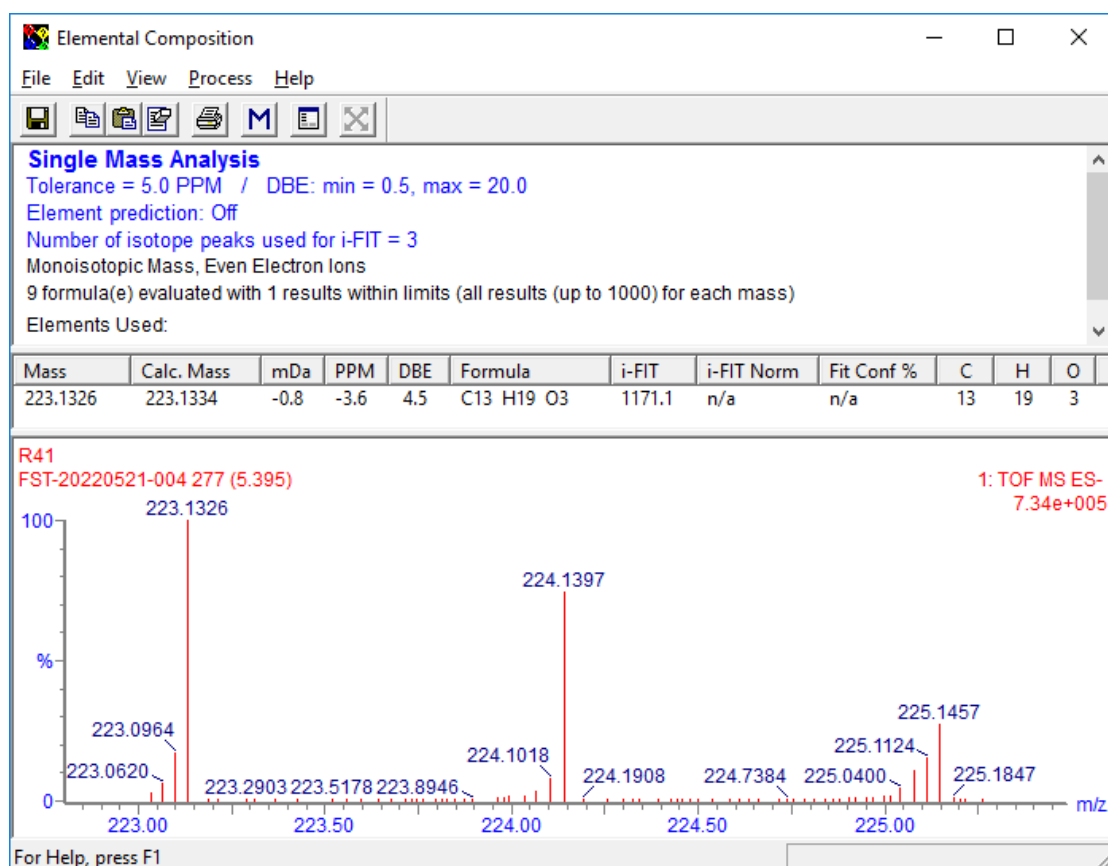
**Figure S52.** HMBC spectrum of compound **5** in CD<sub>3</sub>OD.



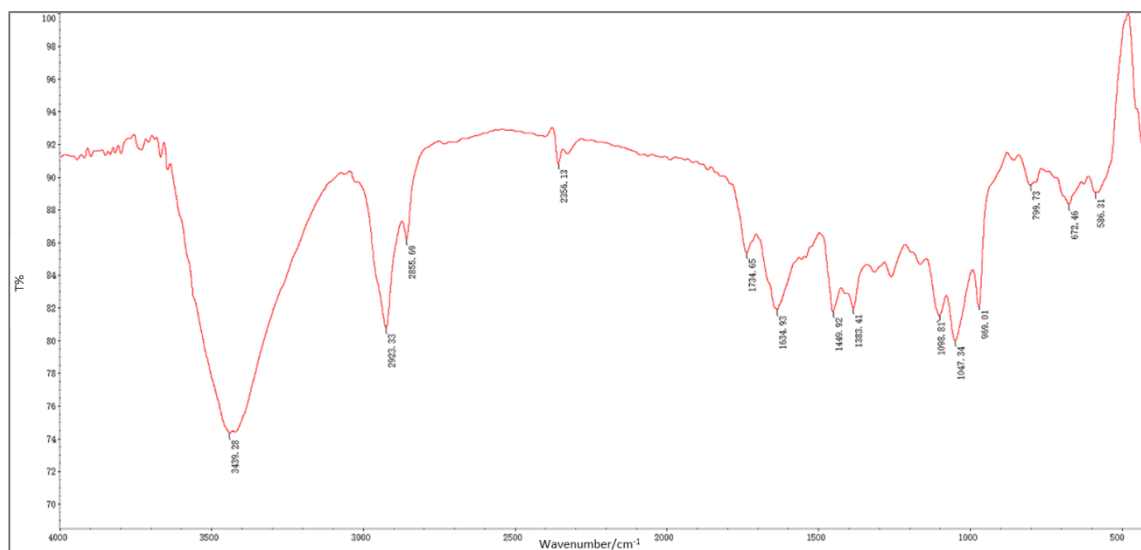
**Figure S53.** COSY spectrum of compound **5** in CD<sub>3</sub>OD.



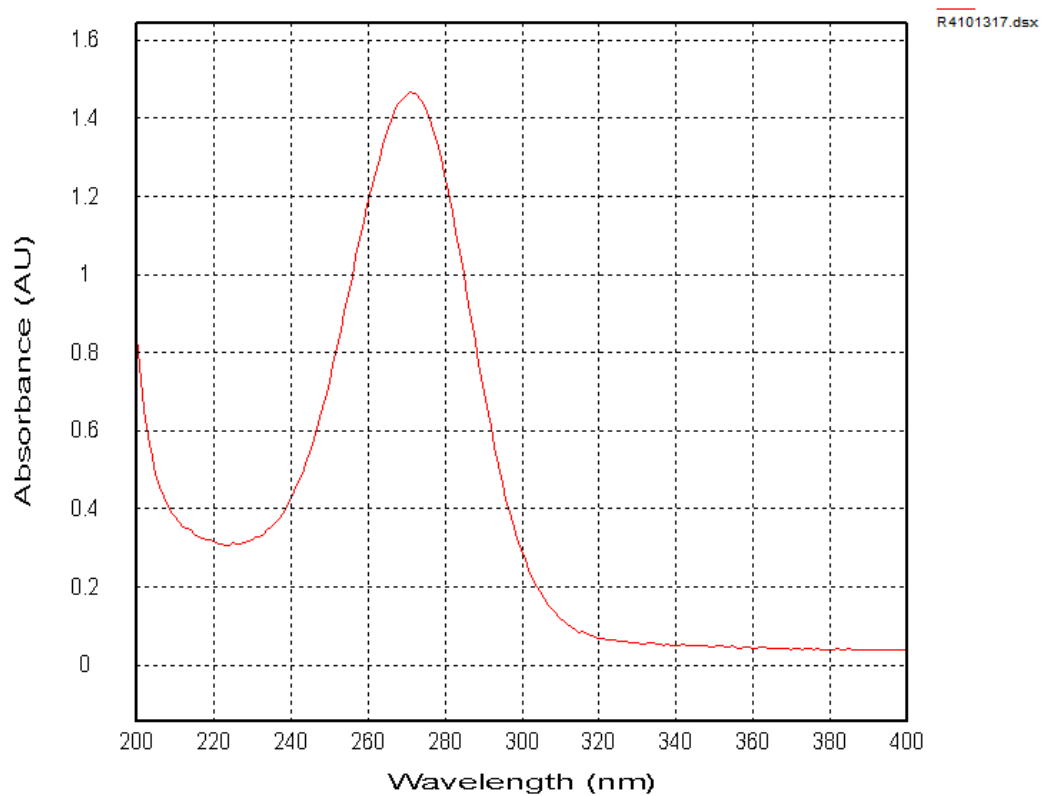
**Figure S54.** NOESY spectrum of compound **5** in CD<sub>3</sub>OD.



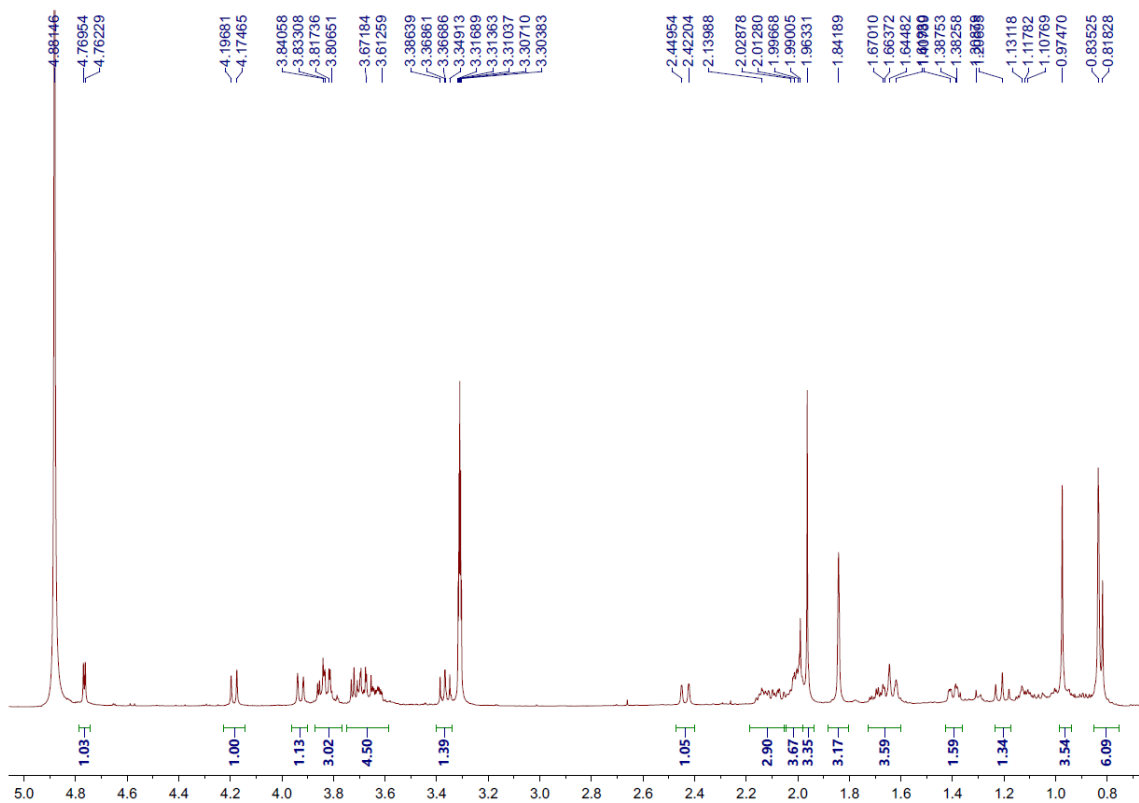
**Figure S55.** HRESI(-)MS spectrum of compound **5**.



**Figure S56.** IR spectrum of compound **5**.

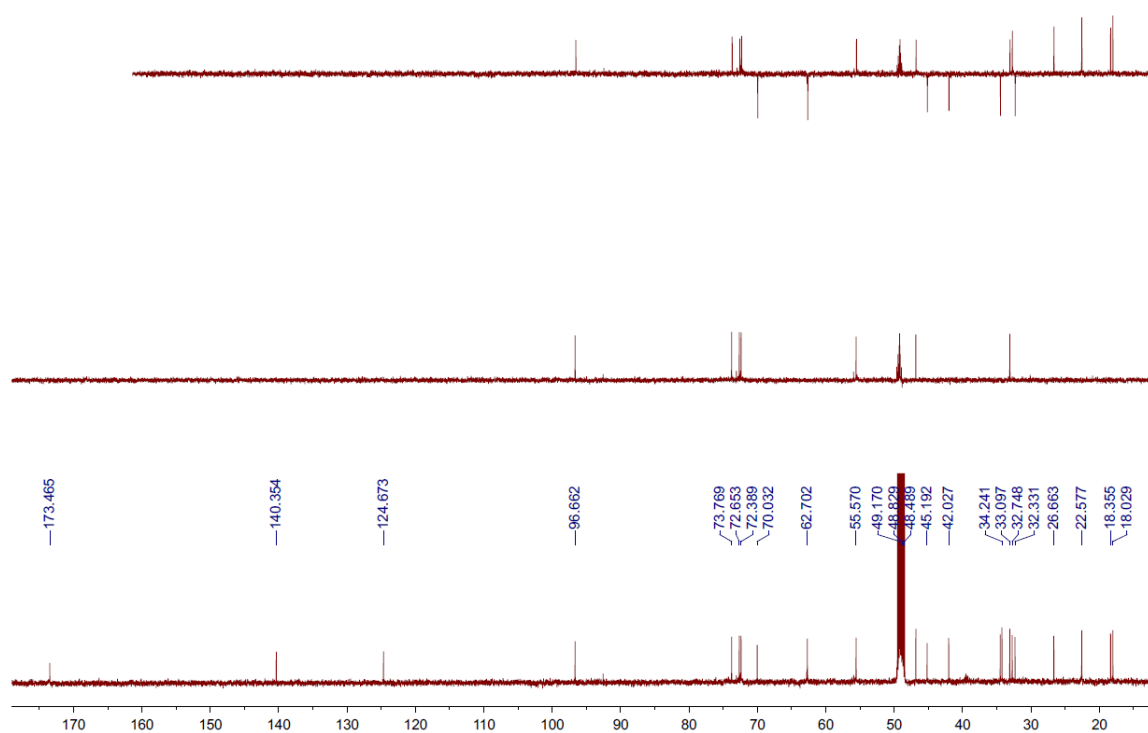


**Figure S57.** UV spectrum of compound **5** (0.1 mg/mL in MeOH).

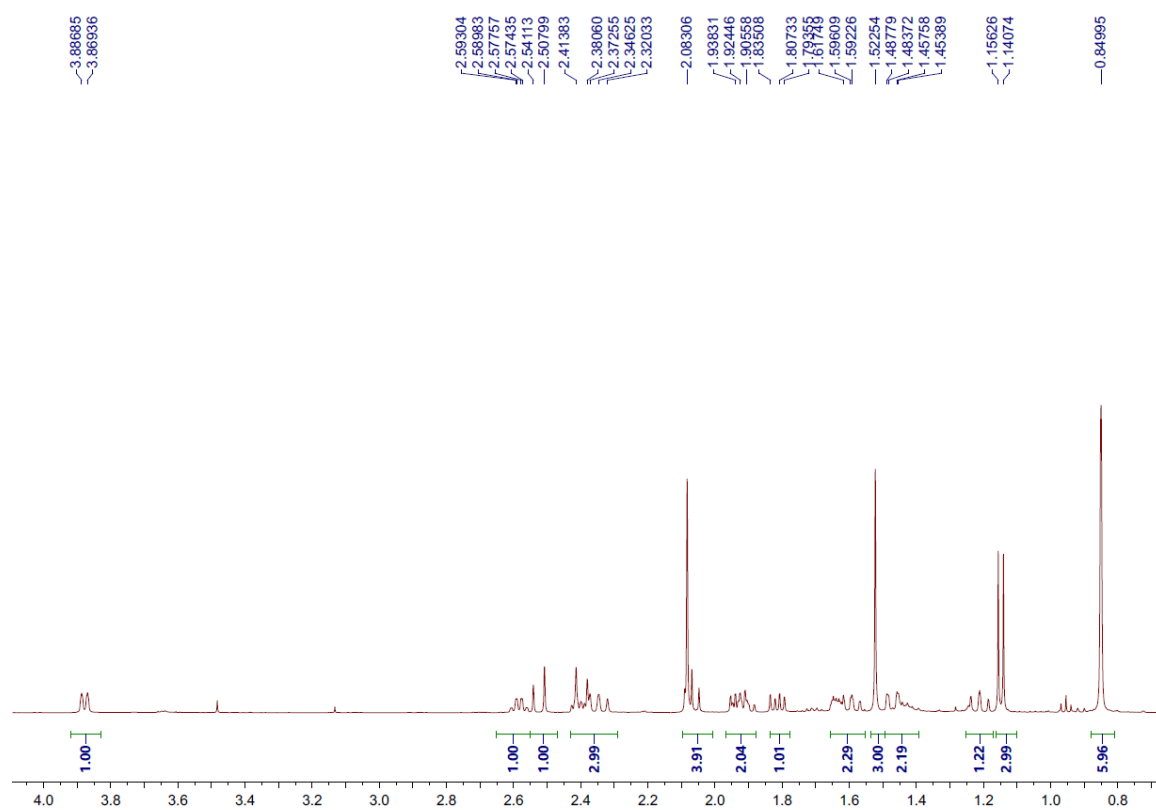


**Figure S58.**  $^1\text{H}$  NMR spectrum of compound **6** in  $\text{CD}_3\text{OD}$ .

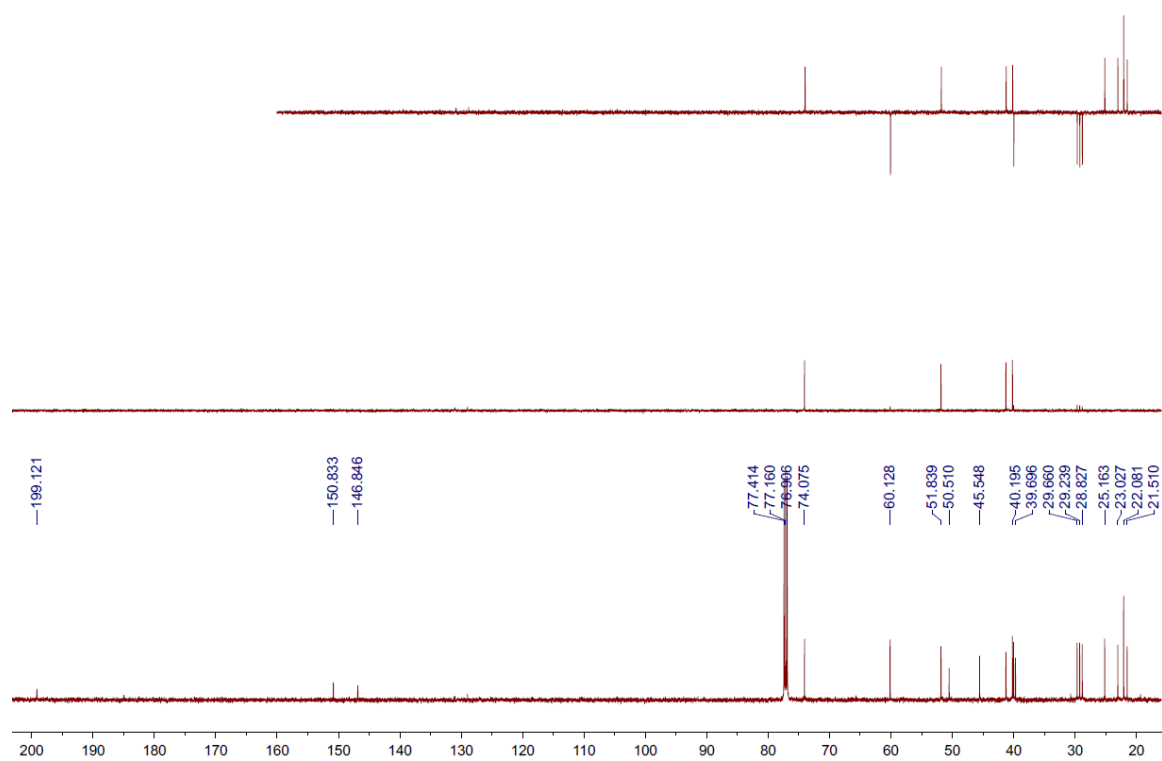




**Figure S59.** <sup>13</sup>C NMR and DEPT spectra of compound **6** in CD<sub>3</sub>OD.



**Figure S60.** <sup>1</sup>H NMR spectrum of compound **7** in CDCl<sub>3</sub>.



**Figure S61.** <sup>13</sup>C NMR and DEPT spectra of compound **7** in CDCl<sub>3</sub>.