

## Supporting Information

*Rec. Nat. Prod.* 16:5 (2022) 443-453

### Brochodilator Phenylpropanoid Glycosides from the Seeds of *Prunus mahaleb* L.

Maged S. Abdel-Kader <sup>\*1,2</sup>, Najeeb Ur Rehman <sup>\*3</sup>,  
Mohammed A. Alghafis <sup>1</sup> and Mubarak A. Almatri <sup>4</sup>

<sup>1</sup>Department of Pharmacognosy, College of Pharmacy, Prince Sattam Bin Abdulaziz University, P. O. Box 173, Al-Kharj 11942, Saudi Arabia

<sup>2</sup>Department of Pharmacognosy, College of Pharmacy, Alexandria University, Alexandria 21215, Egypt

<sup>3</sup>Department of Pharmacology, College of Pharmacy, Prince Sattam bin Abdulaziz University, Al-Kharj 11942, Kingdom of Saudi Arabia

<sup>4</sup>College of Pharmacy, Prince Sattam bin Abdulaziz University, Al-Kharj 11942, Kingdom of Saudi Arabia

Table of Contents	Page
<b>Table S1:</b> NMR data of <b>1</b> and <b>5</b> ( $\delta$ , $J$ values in Hz).	3
<b>Table S2:</b> NMR data of <b>2- 4</b> ( $\delta$ , $J$ values in Hz).	3
<b>Figure S1:</b> <sup>1</sup> H NMR Spectrum of <b>1</b> in CD <sub>3</sub> OD.	4
<b>Figure S2:</b> <sup>13</sup> C NMR Spectrum of <b>1</b> in CD <sub>3</sub> OD.	4
<b>Figure S3:</b> DEPT135 Spectrum of <b>1</b> in CD <sub>3</sub> OD.	5
<b>Figure S4:</b> COSY Spectrum of <b>1</b> in CD <sub>3</sub> OD.	5
<b>Figure S5:</b> HSQC Spectrum of <b>1</b> in CD <sub>3</sub> OD.	6
<b>Figure S6:</b> <sup>1</sup> H NMR Spectrum of <b>1</b> in DMSO.	6
<b>Figure S7:</b> <sup>13</sup> C NMR Spectrum of <b>1</b> in DMSO.	7
<b>Figure S8:</b> DEPT135 of <b>1</b> in DMSO.	7
<b>Figure S9:</b> COSY Spectrum of <b>1</b> in DMSO.	8
<b>Figure S9:</b> HSQC Spectrum of <b>1</b> in DMSO.	8
<b>Figure S11:</b> ESIHRMS Spectra of <b>1</b> .	9
<b>Figure S12:</b> <sup>1</sup> H NMR Spectrum of <b>2</b> .	10
<b>Figure S13:</b> <sup>13</sup> C NMR Spectrum of <b>2</b> .	10
<b>Figure S14:</b> DEPT135 Spectrum of <b>2</b> .	11
<b>Figure S15:</b> COSY Spectrum of <b>3</b> .	11
<b>Figure S16:</b> HSQC Spectrum of <b>2</b> .	12
<b>Figure S17:</b> HMBC Spectrum of <b>2</b> .	12
<b>Figure S18:</b> ESIHRMS Spectra of <b>2</b> .	13
<b>Figure S19:</b> <sup>1</sup> H NMR Spectrum of <b>3</b> .	14
<b>Figure S20:</b> <sup>13</sup> C NMR Spectrum of <b>3</b> .	14
<b>Figure S21:</b> DEPT135 Spectrum of <b>3</b> .	15
<b>Figure S22:</b> COSY Spectrum of <b>3</b> .	15
<b>Figure S23:</b> HSQC Spectrum of <b>3</b> .	16
<b>Figure S24:</b> HMBC Spectrum of <b>3</b> .	16
<b>Figure S25:</b> ESIHRMS Spectra of <b>3</b> .	17
<b>Figure S26:</b> <sup>1</sup> H NMR Spectrum of <b>4</b> .	18
<b>Figure S27:</b> <sup>13</sup> C NMR Spectrum of <b>4</b> .	18

---

<b>Figure S28:</b> DEPT135 Spectrum of <b>4</b> .	19
<b>Figure S29:</b> COSY Spectrum of <b>4</b> .	19
<b>Figure S30:</b> HSQC Spectrum of <b>4</b> .	20
<b>Figure S31:</b> HMBC Spectrum of <b>4</b> .	20
<b>Figure S32:</b> ESIHRMS Spectra of <b>4</b> .	21
<b>Figure S33:</b> <sup>1</sup> H NMR Spectrum of <b>5</b> .	22
<b>Figure S34:</b> <sup>13</sup> C NMR Spectrum of <b>5</b> .	22
<b>Figure S35:</b> DEPT135 Spectrum of <b>5</b> .	23
<b>Figure S36:</b> COSY Spectrum of <b>5</b> .	23
<b>Figure S37:</b> HSQC Spectrum of <b>5</b> .	24
<b>Figure S38:</b> HMBC Spectrum of <b>5</b> .	24
<b>Figure S39:</b> ESIHRMS Spectra of <b>5</b> .	25

---

**Table S1:** NMR data of **1** and **5** ( $\delta$ ,  $J$  values in Hz).

Pos.	<b>1</b> *		<b>1</b> **		<b>5</b> *	
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
<b>1</b>	-	127.89	-	126.86	-	125.70
<b>2</b>	-	155.90	-	154.92	-	157.62
<b>3</b>	7.15 (d, $J=8.25$ )	116.33	7.07 (d, $J=8.25$ )	114.86	7.24 (d, $J=8.3$ )	116.95
<b>4</b>	7.23 (t, $J=7.5$ )	130.17	7.15 (t, $J=7.5$ )	128.64	7.36 (t, $J=8.3$ )	132.93
<b>5</b>	6.97 (bt, $J=6.6$ )	123.14	6.88 (m)	121.46	7.05 (t, $J=7.6$ )	123.70
<b>6</b>	7.60 (bs)	130.96	7.81 (bs)	130.29	7.62 (d, $J=7.6$ )	128.85
<b>7</b>	6.84 (d, $J=12.3$ )	128.75	6.60 (d, $J=12.6$ )	123.50	8.10 (d, $J=16$ )	141.21
<b>8</b>	6.12 (bs)	128.21	5.92 (bd, $J=11.6$ )	130.29	6.52 (d, $J=16$ )	119.96
<b>9</b>	-	170.42	-	171.76	-	171.52
<b>1'</b>	4.98 (d, $J=7$ )	102.19	4.85 (d, $J=6.6$ )	101.09	4.98 (d, $J=7.9$ )	102.41
<b>2'</b>	3.57 m	74.72	3.30 (m)	73.76	7.05 (t, $J=8.8$ )	74.95
<b>3'</b>	3.57 m	77.71	3.30 (m)	77.05	3.45 (m)	78.17
<b>4'</b>	3.46 m	71.12	3.21 (t, $J=8.5$ )	70.07	3.45 (m)	71.32
<b>5'</b>	3.46 m	77.93	3.30 (m)	77.53	3.45 (m)	78.34
<b>6'</b>	3.74 (bd, $J=9.5$ ) 3.68 (d, $J=11.75$ )	62.25	3.49 (dd, $J=11.3, 5.1$ ) 3.68 (d, $J=11.3$ )	61.08	3.49 (dd, $J=12, 5.2$ ) 3.68 (d, $J=12$ )	62.56

\* Spectra were measured in CD<sub>3</sub>OD.

\*\* Spectra were measured in DMSO.

**Table S2:** NMR data of **2-4** ( $\delta$ ,  $J$  values in Hz).

Pos	<b>2</b> *		<b>3</b> *		<b>4</b> **	
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
<b>1</b>	-	119.89	-	123.75	-	118.34
<b>2</b>	-	157.74	-	157.69	-	156.27
<b>3</b>	6.72 (d, $J=2.3$ )	101.02	6.79 bs	103.16	7.28 (bs)	101.73
<b>4</b>	-	162.56	-	160.77	-	159.35
<b>5</b>	6.50 (dd, $J=8.6, 2.3$ )	108.66	6.52 (d, $J=7.7$ )	108.43	6.66 (bd, $J=7$ )	107.00
<b>6</b>	7.57 (d, $J=8.6$ )	132.15	7.06 (d, $J=7.9$ )	131.34	7.68 (d, $J=8.1$ )	129.92
<b>7</b>	6.93 (d, $J=12.7$ )	132.56	2.90 (q, $J=7.2$ )	26.86	8.76 (d, $J=16$ )	139.20
<b>8</b>	5.85 (d, $J=12.7$ )	123.34	2.56 (bt, $J=7.2$ )	36.86	7.04 (d, $J=16$ )	117.45
<b>9</b>	-	173.83	-	179.20	-	169.96
<b>1'</b>	4.87 (d, $J=7.2$ )	102.70	4.91 (d, $J=6.7$ )	102.73	4.87 (bs)	101.88
<b>2'</b>	3.43 (m)	74.94	3.53 (t, $J=6.4$ )	74.95	4.34 (m)	74.39
<b>3'</b>	3.34 (bd, $J=8.6$ )	78.11	3.45 (m)	78.09	4.34 (m)	78.59
<b>4'</b>	3.43 (m)	71.46	3.45 (m)	71.42	4.25 (bs)	70.99
<b>5'</b>	3.38 (dd, $J=2, 5.7$ )	78.35	3.73 (m)	78.18	4.12 (bs)	78.90
<b>6'</b>	3.64 (dd, $J=5.8, 12.1$ ) 3.84 (d, $J=1.9, 12.1$ )	62.58	3.73 (m) 3.93 (d, $J=11.9$ )	62.56	4.34 (m) 4.53 (bd, $J=11.4$ )	62.16
OCH <sub>3</sub>	3.73 (s)	55.98	3.75 (s)	55.89	3.70 (s)	55.20

\* Spectra were measured in CD<sub>3</sub>OD.\*\* Spectra were measured in Pyridine d<sub>6</sub>.

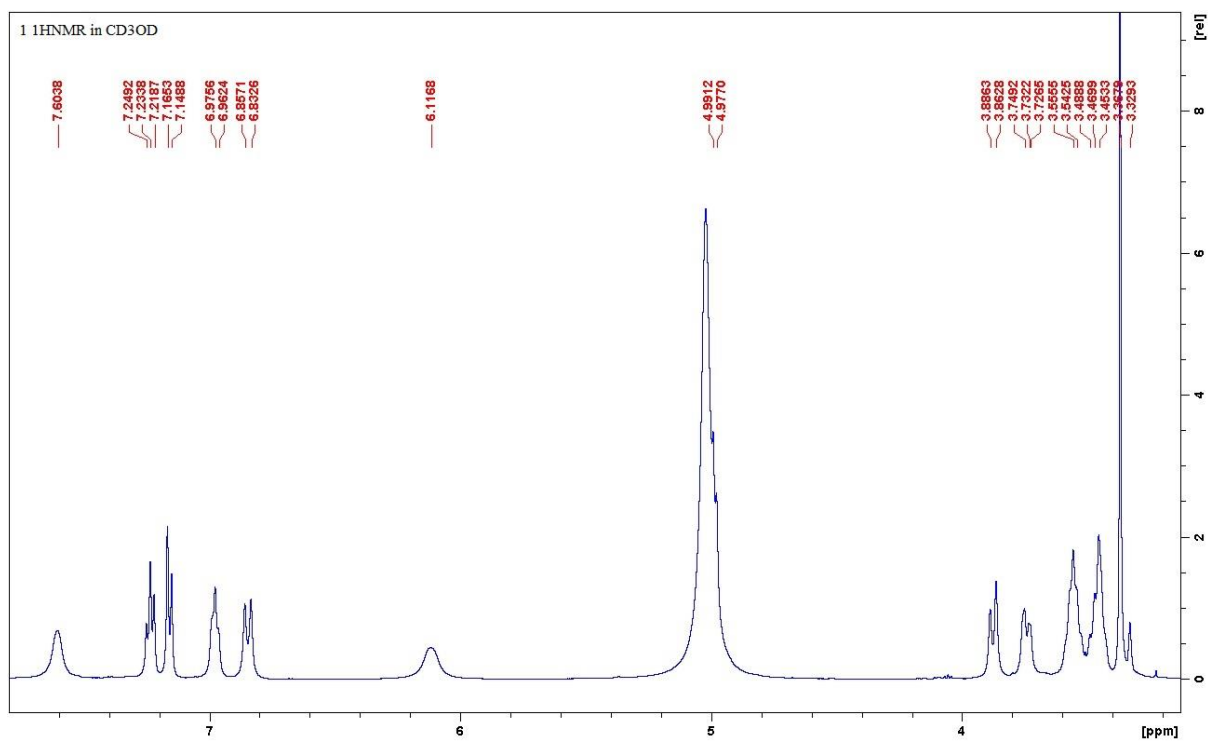


Figure S1: <sup>1</sup>H NMR spectrum of **1** in CD<sub>3</sub>OD.

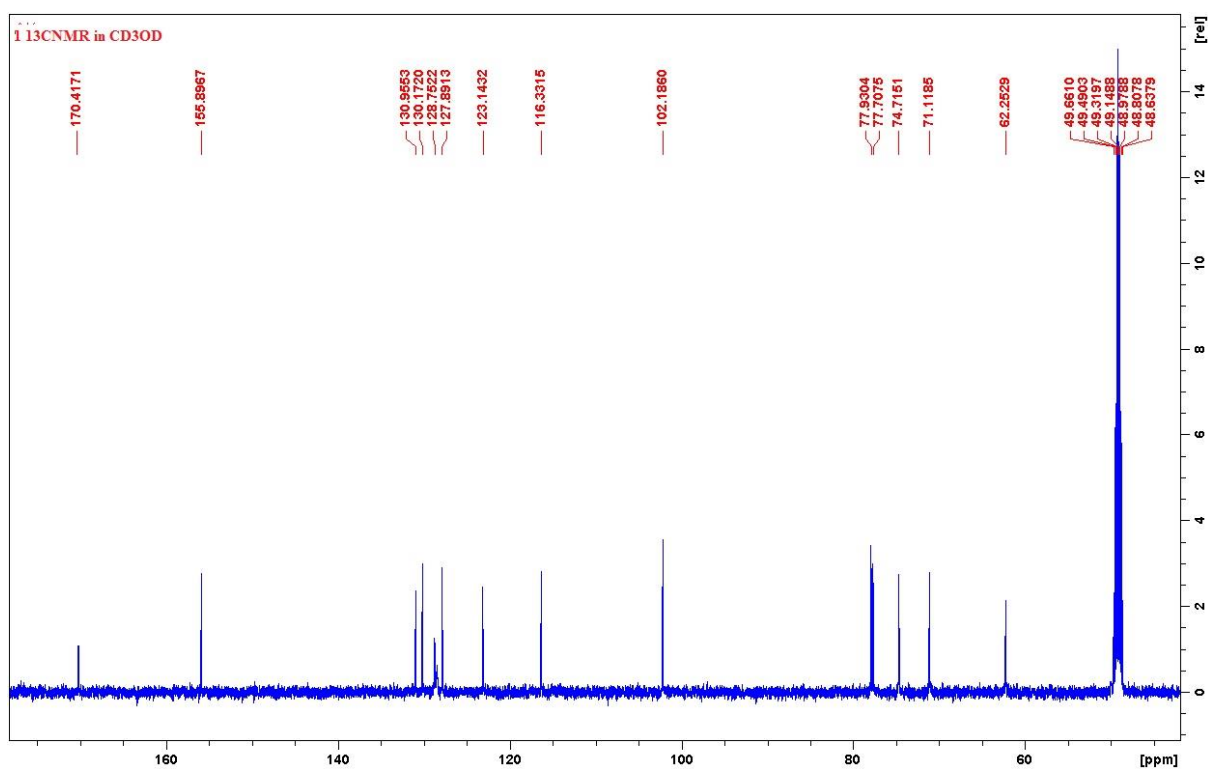
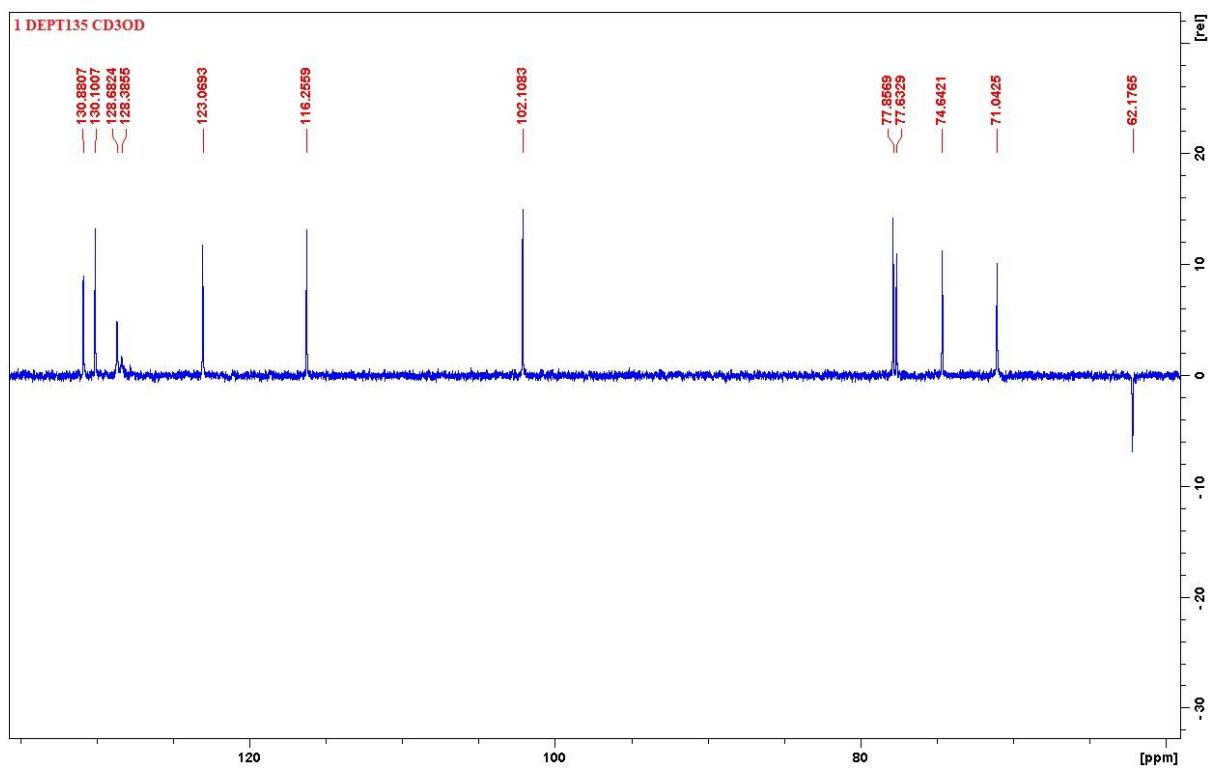
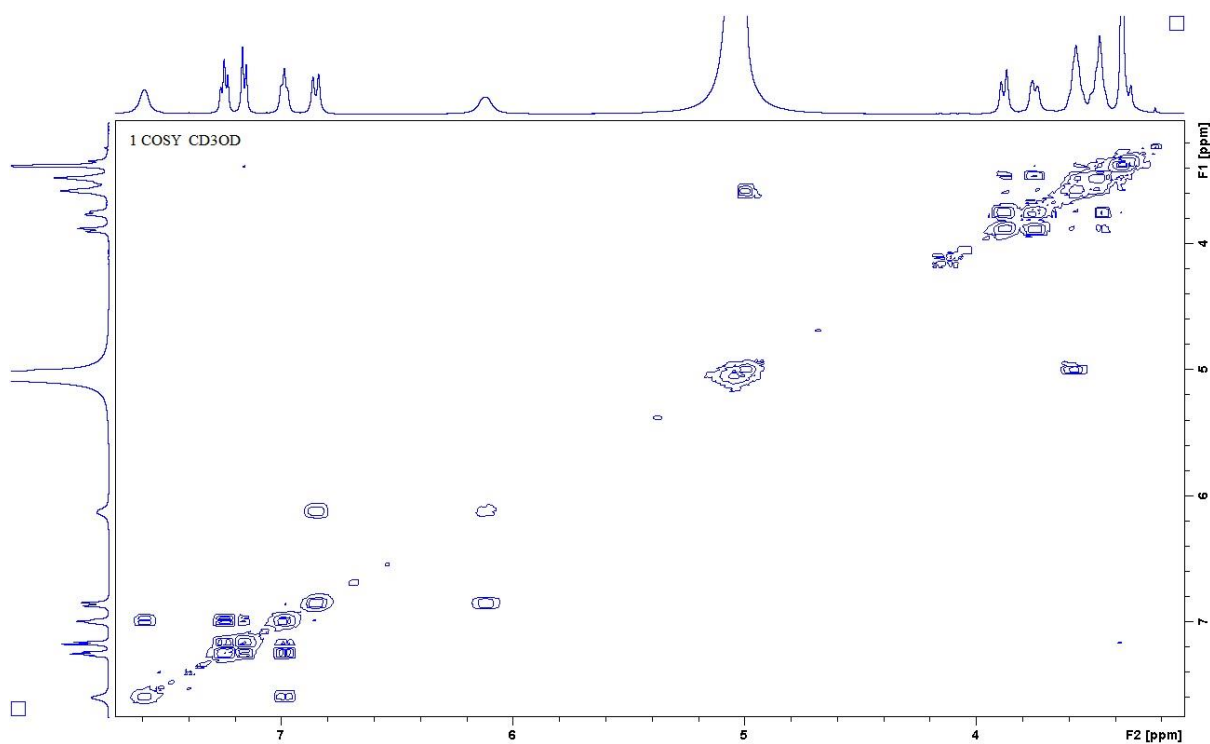


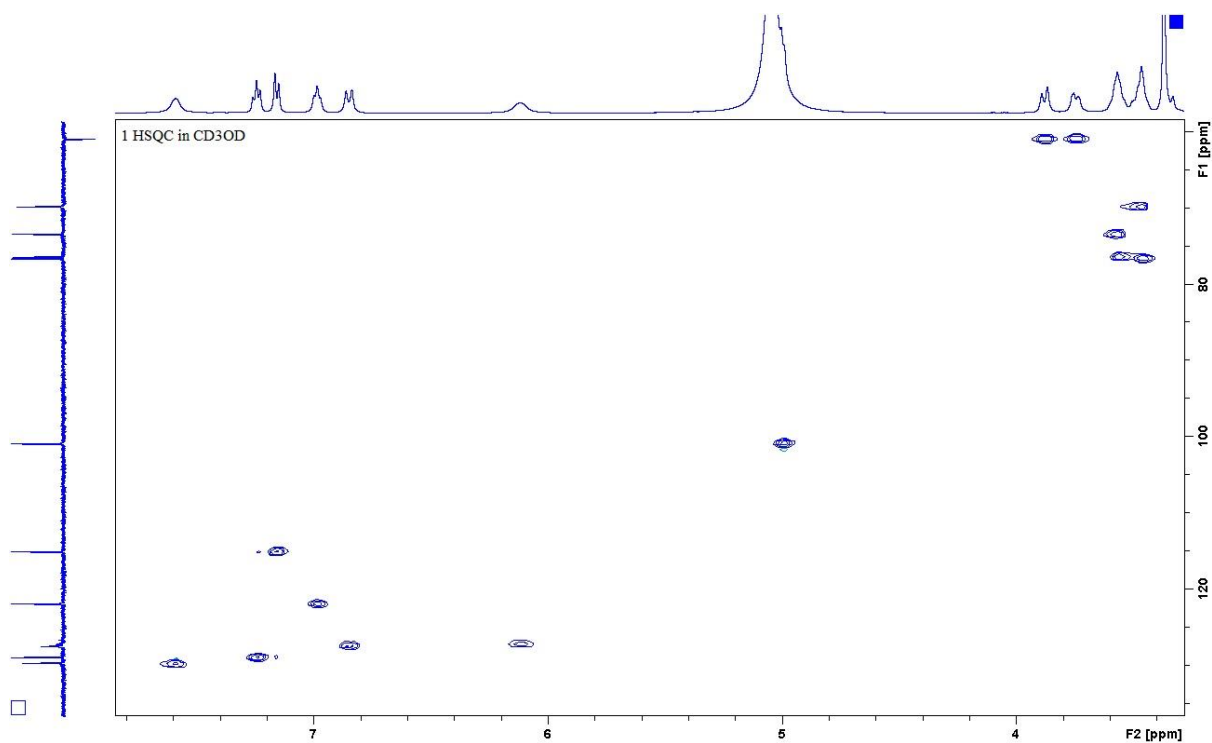
Figure S2: <sup>13</sup>C NMR spectrum of **1** in CD<sub>3</sub>OD.



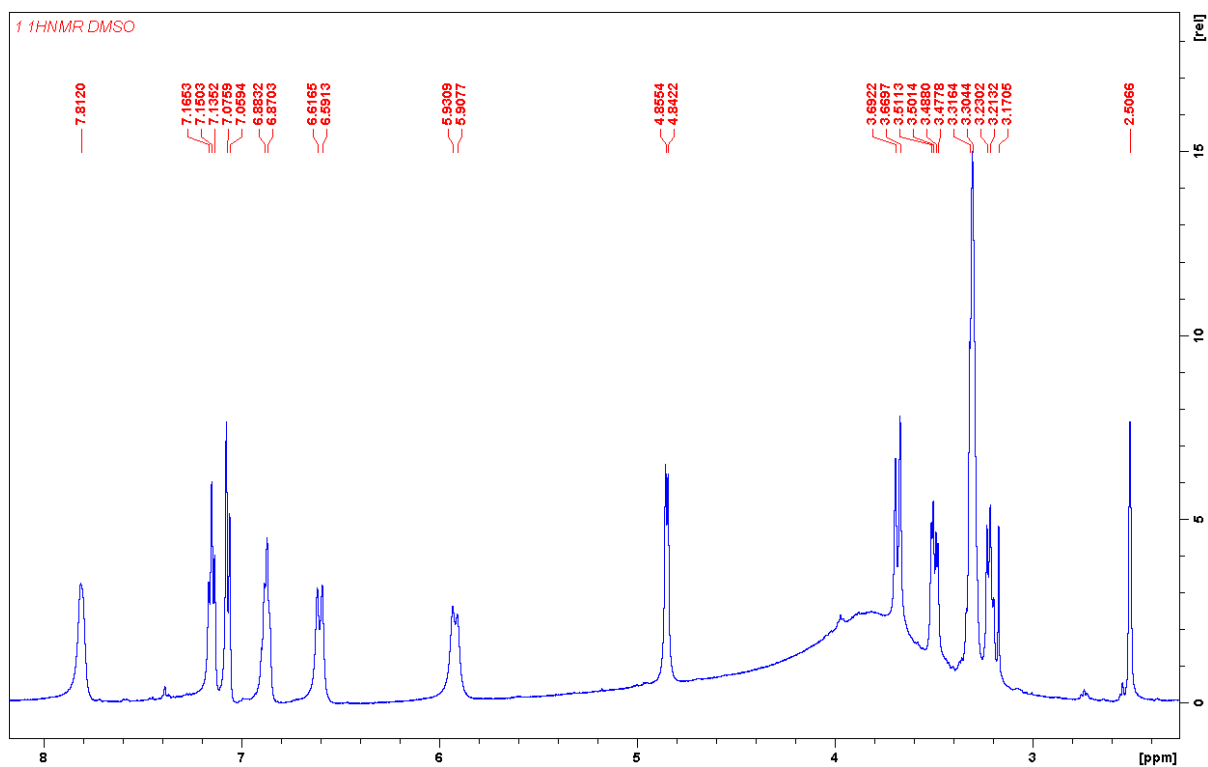
**Figure S3:** DEPT135 spectrum of **1** in CD<sub>3</sub>OD.



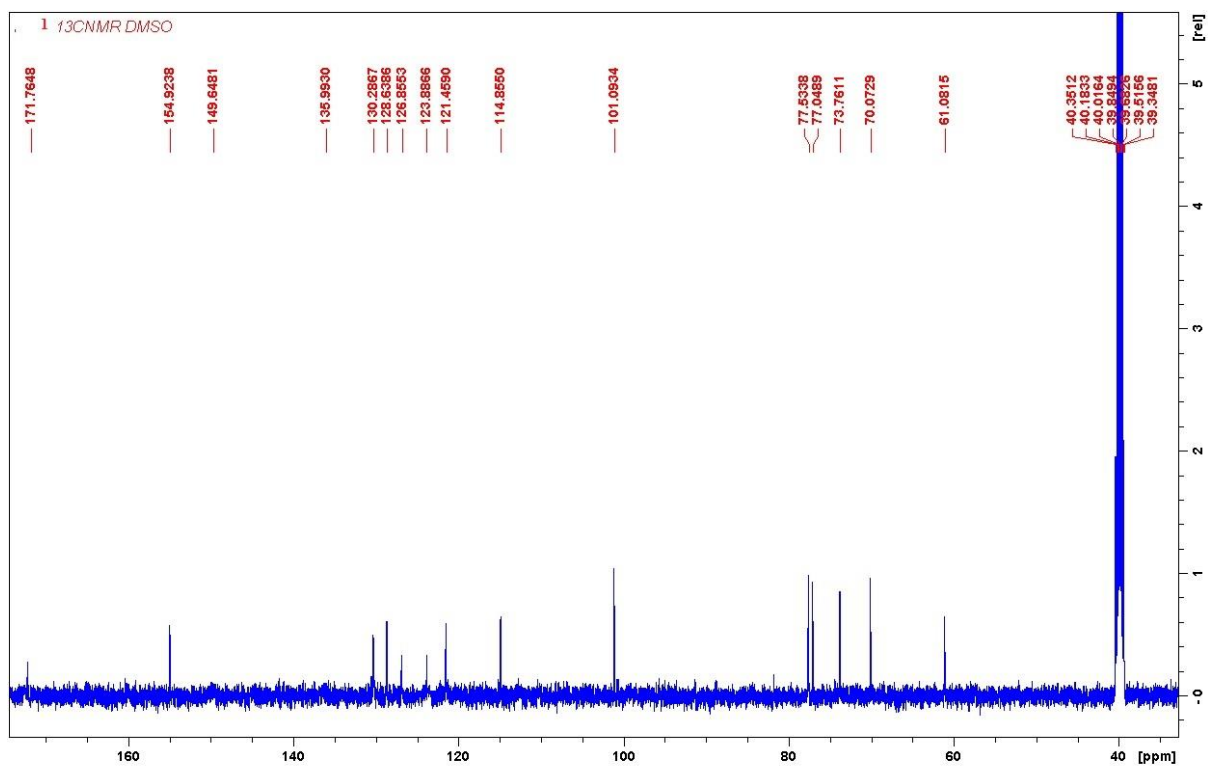
**Figure S4:** COSY spectrum of **1** in CD<sub>3</sub>OD.



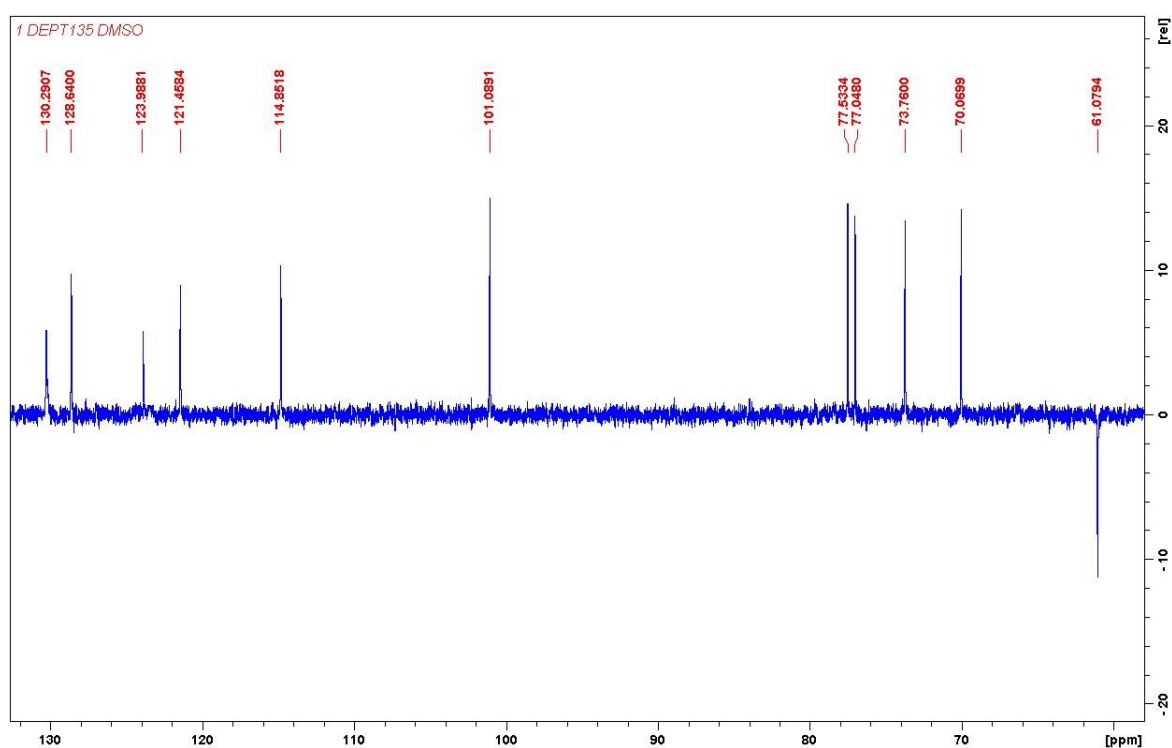
**Figure S5:** HSQC spectrum of **1** in CD<sub>3</sub>OD.



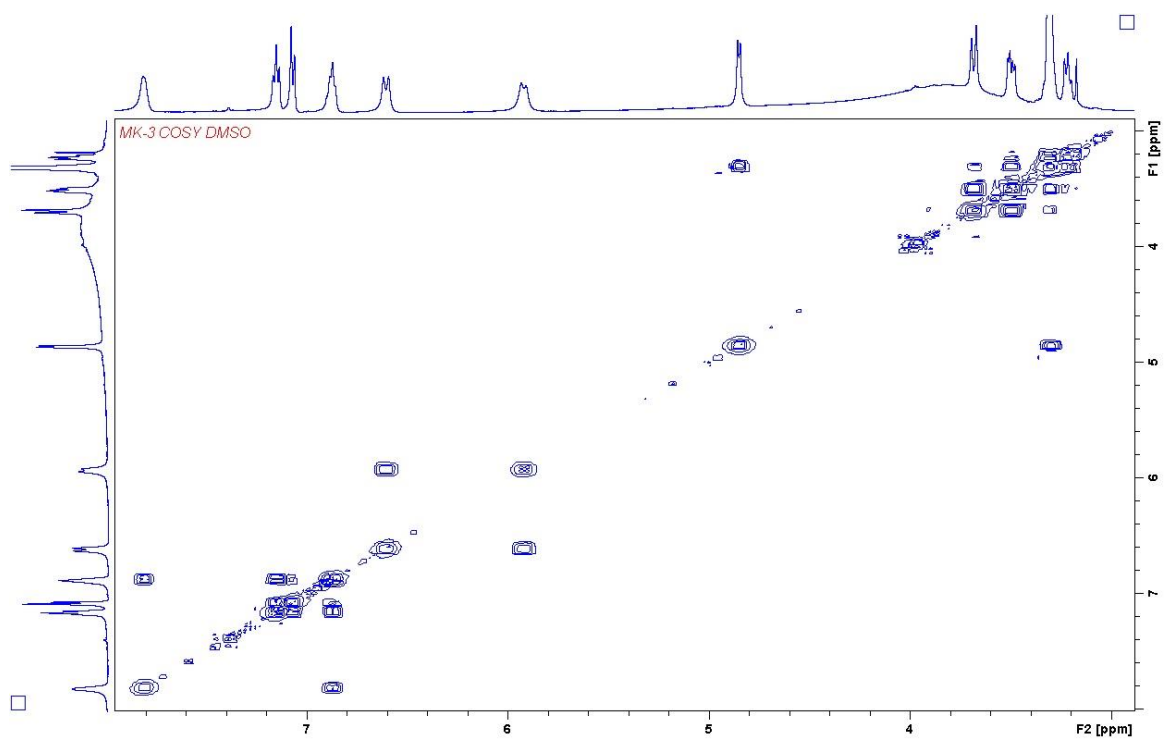
**Figure S6:** <sup>1</sup>H NMR spectrum of **1** in DMSO.



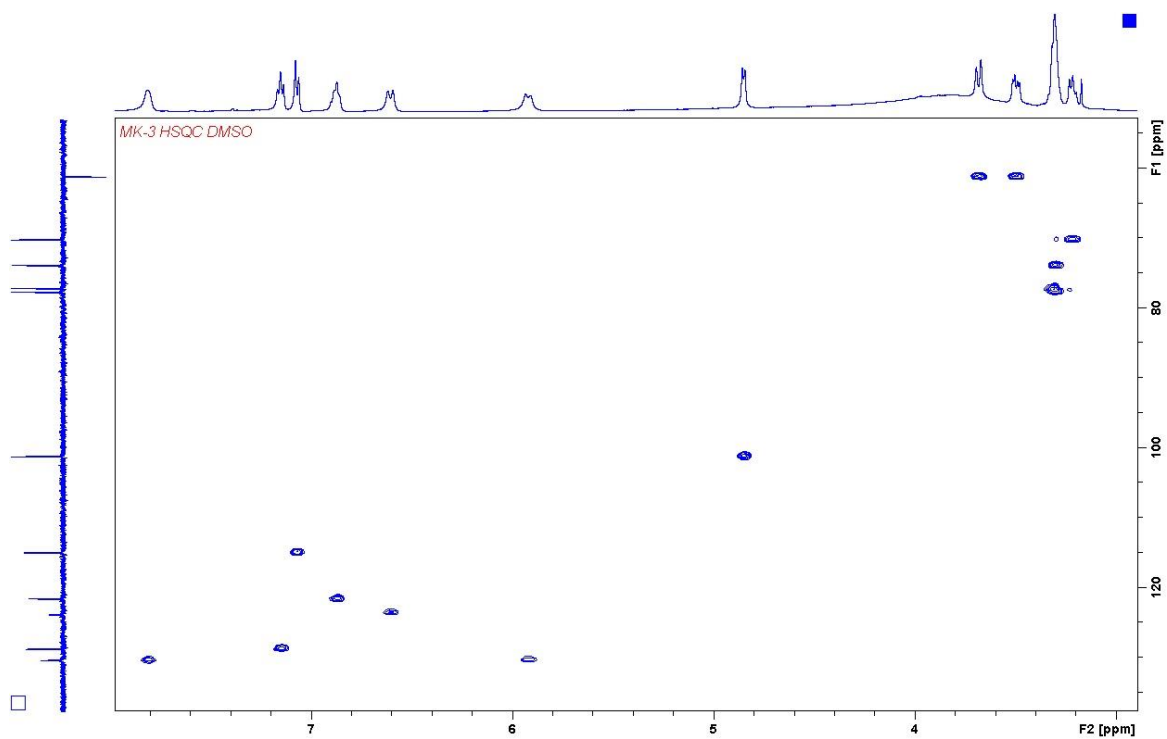
**Figure S7:** <sup>13</sup>C NMR spectrum of **1** in DMSO.



**Figure S8:** DEPT135 of **1** in DMSO.

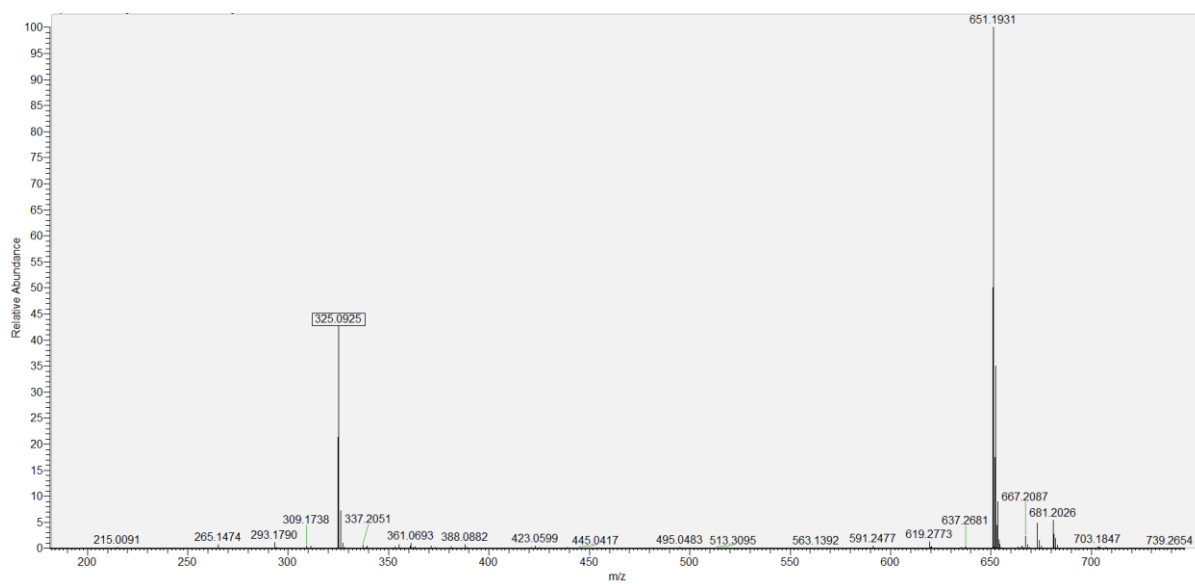


**Figure S9:** COSY Spectrum of **1** in DMSO.

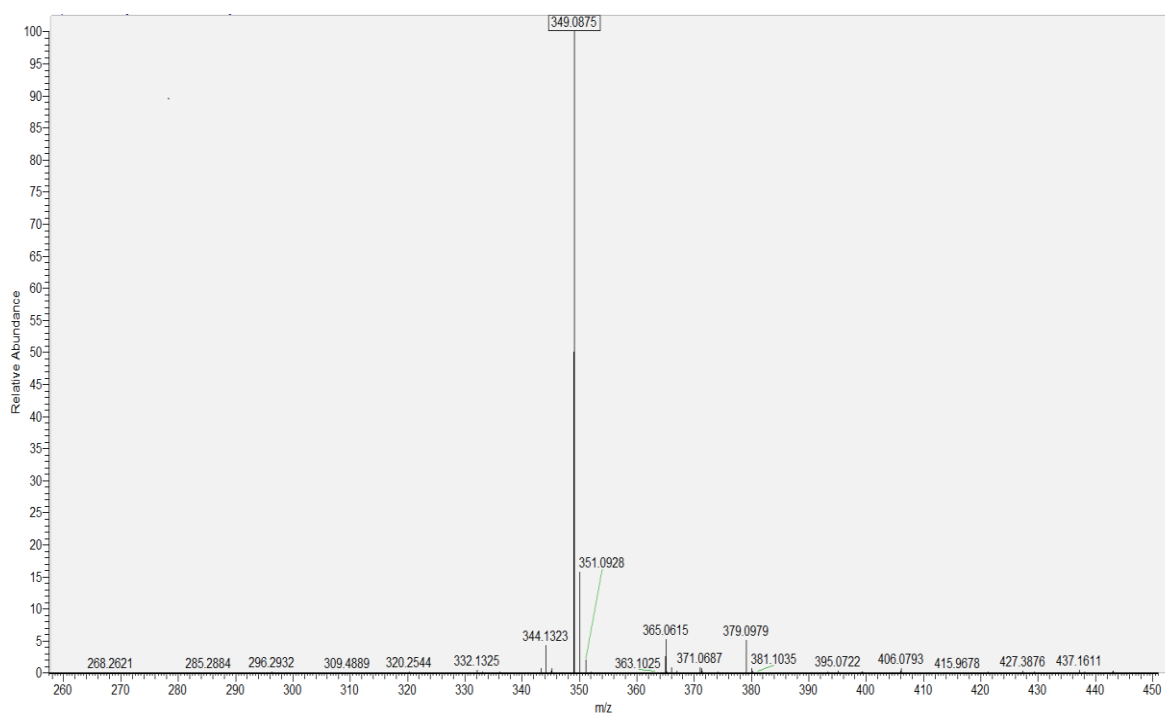


**Figure S10:** HSQC Spectrum of **1** in DMSO.





**A: Negative mode**



**B: Positive mode**

**Figure S11: ESIHRMS spectra of 1.**

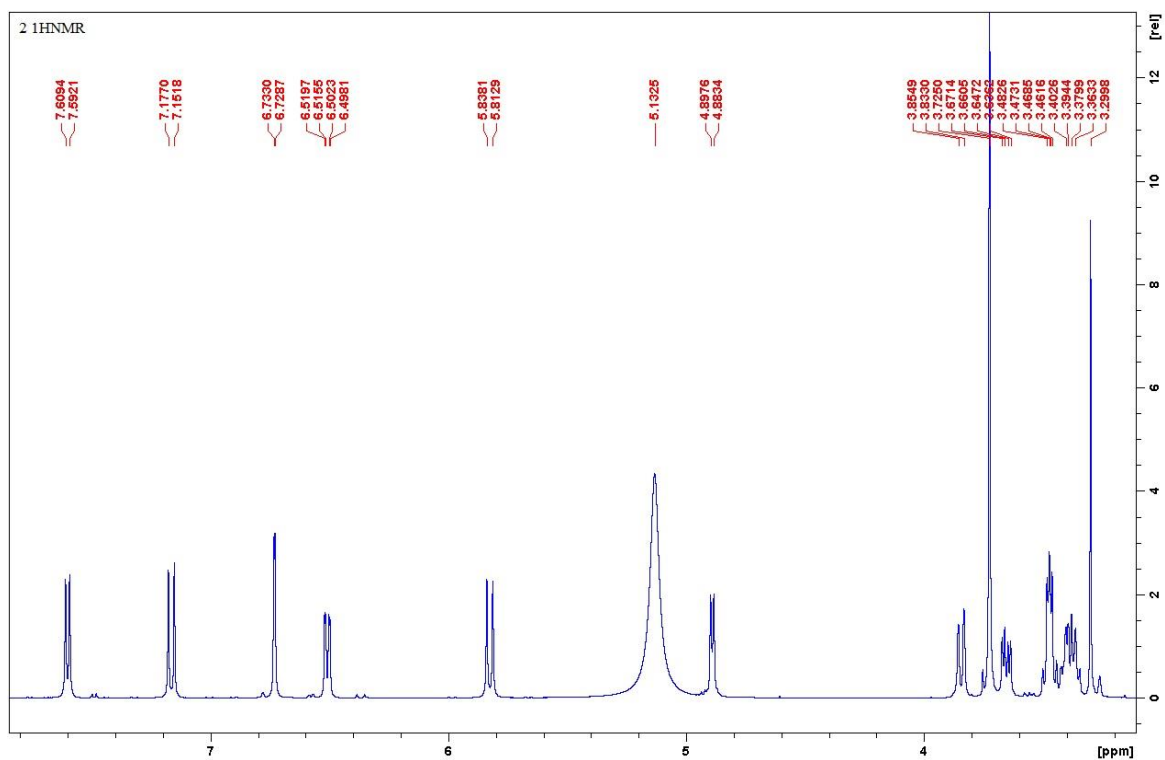


Figure S12: <sup>1</sup>H NMR spectrum of 2.

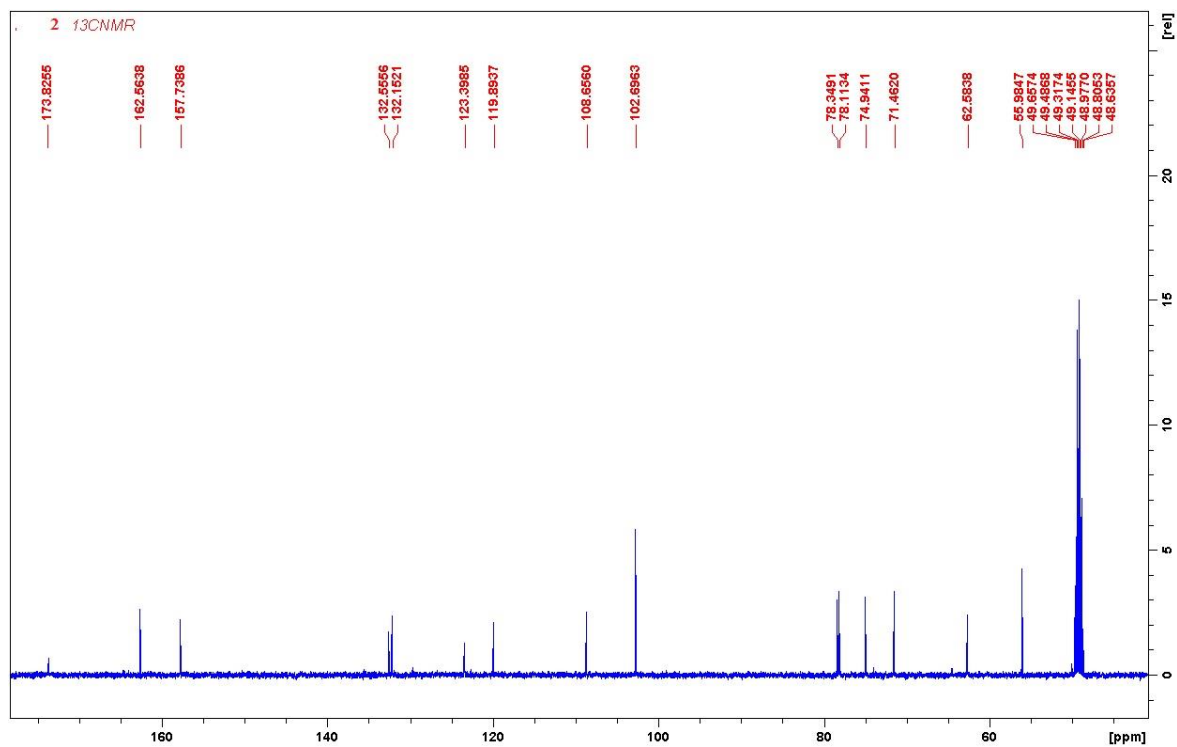


Figure S13: <sup>13</sup>C NMR spectrum of 2.

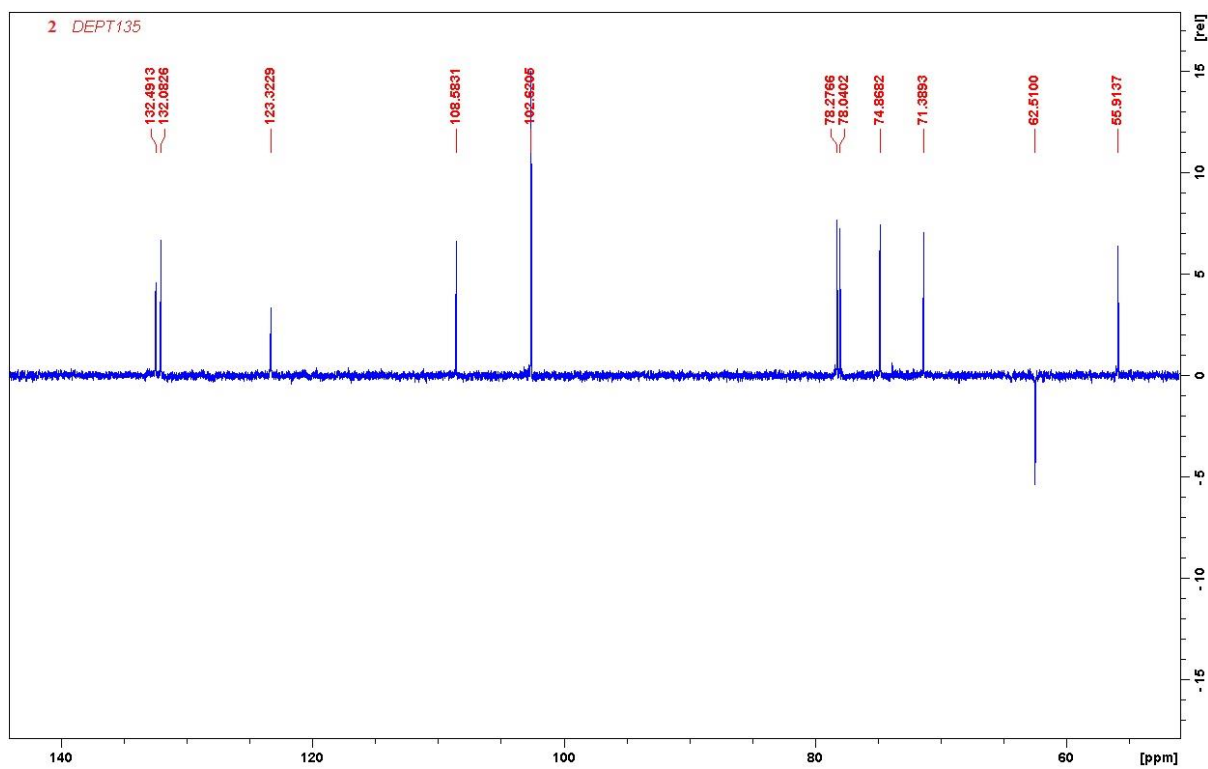


Figure S14: DEPT135 spectrum of **2**.

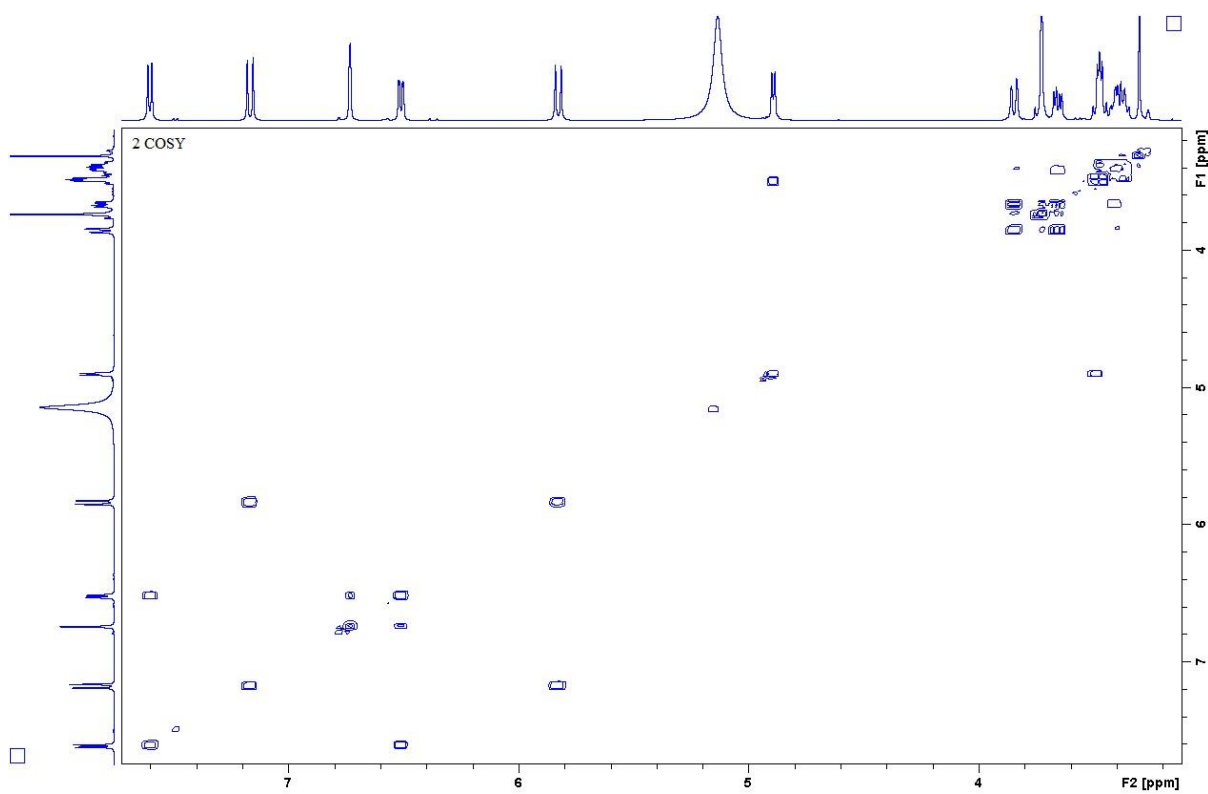
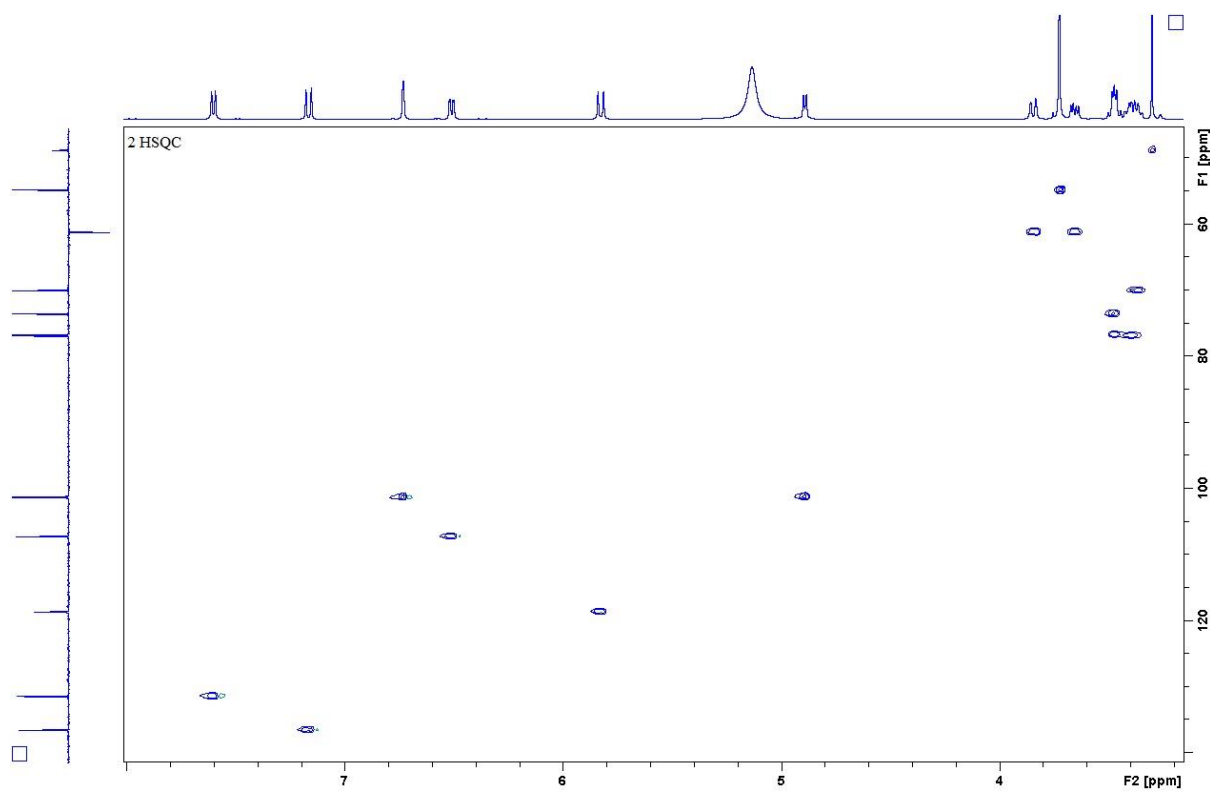
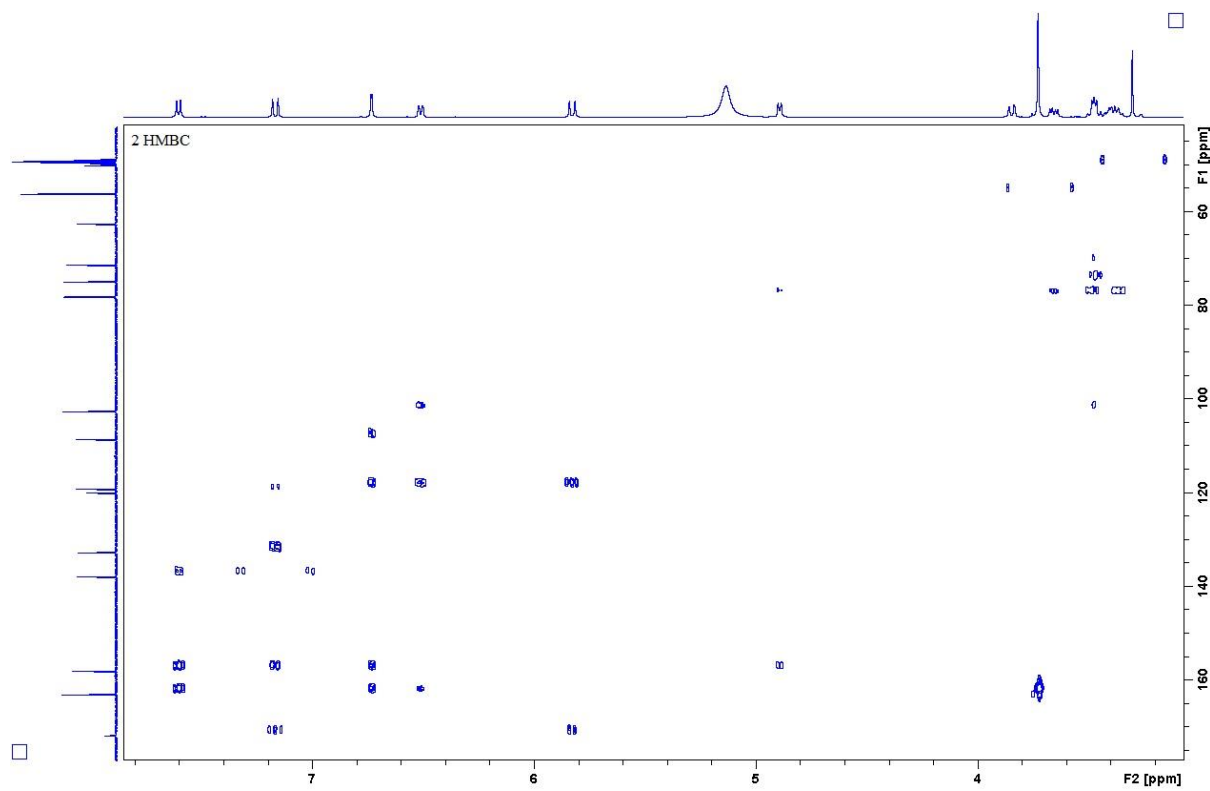


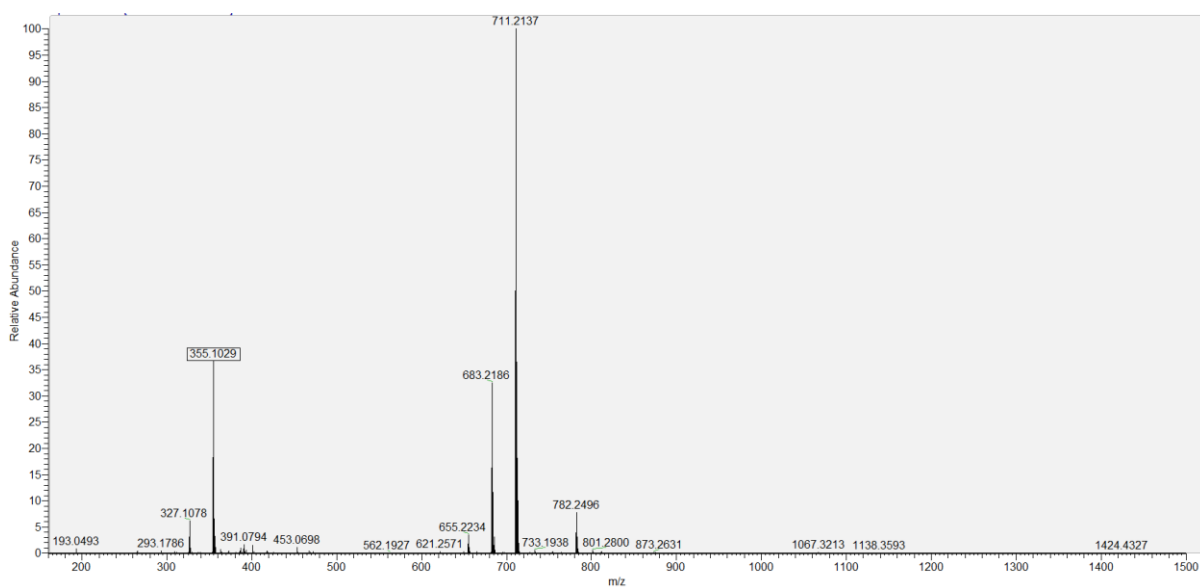
Figure S15: COSY spectrum of **2**.



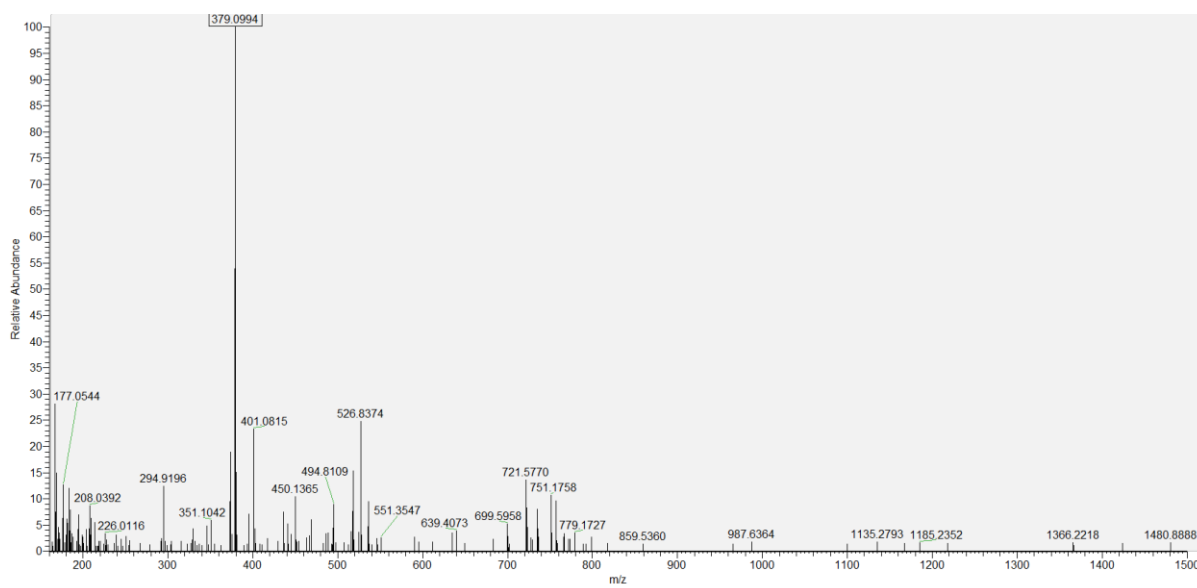
**Figure S16:** HSQC spectrum of **2**.



**Figure S17:** HMBC spectrum of **2**.



**A:** Negative mode.



**B:** Positive mode

**Figure S18:** ESIHRMS spectra of **2**.

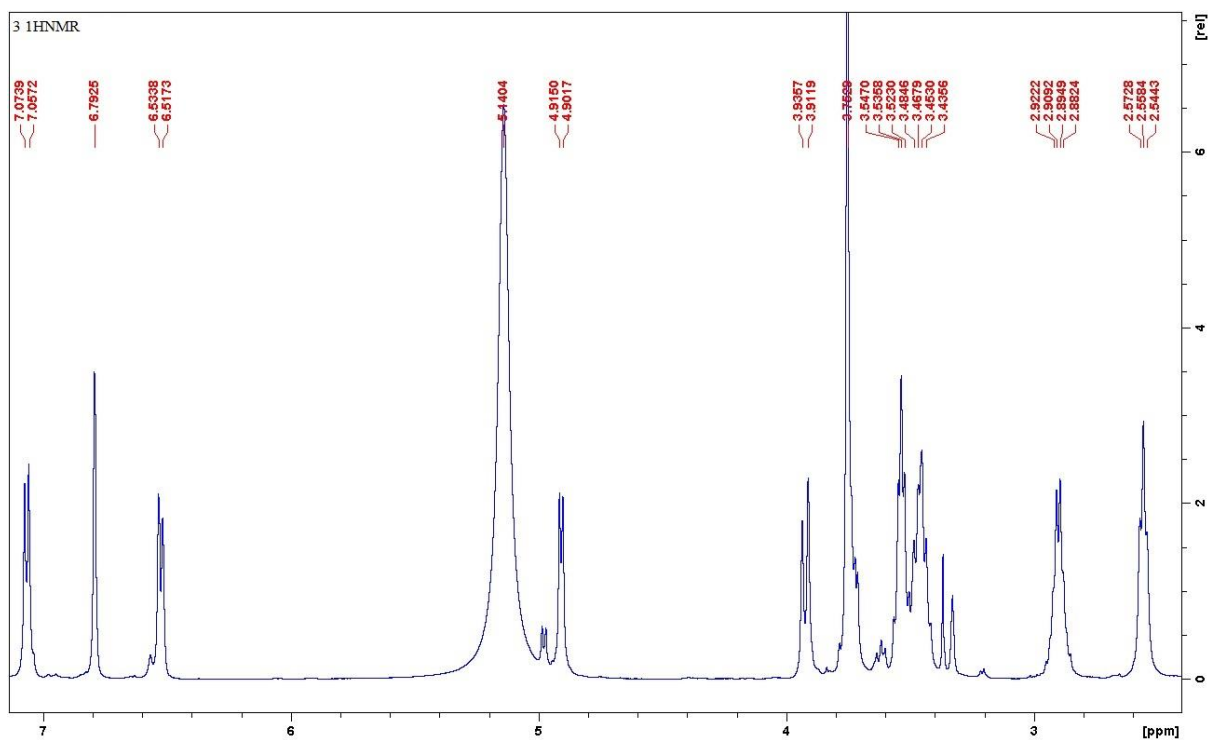


Figure S19: <sup>1</sup>H NMR spectrum of 3.

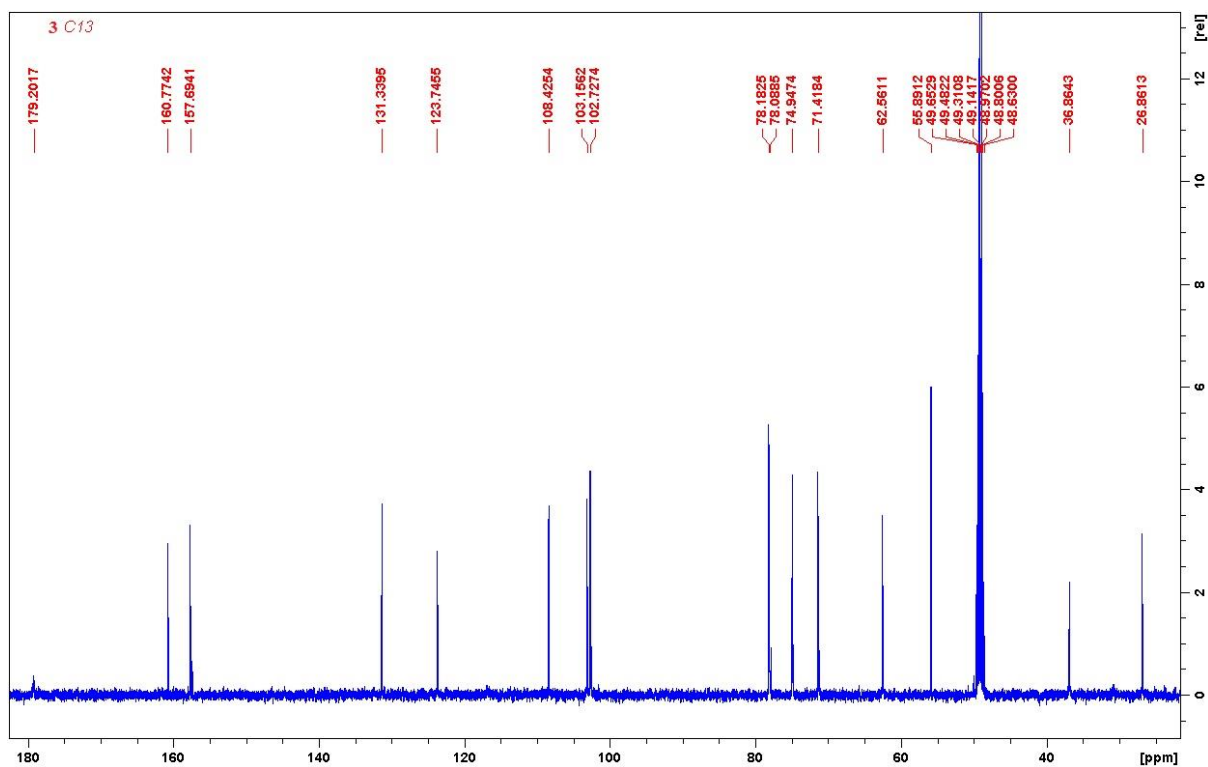


Figure S20: <sup>13</sup>C NMR spectrum of 3.

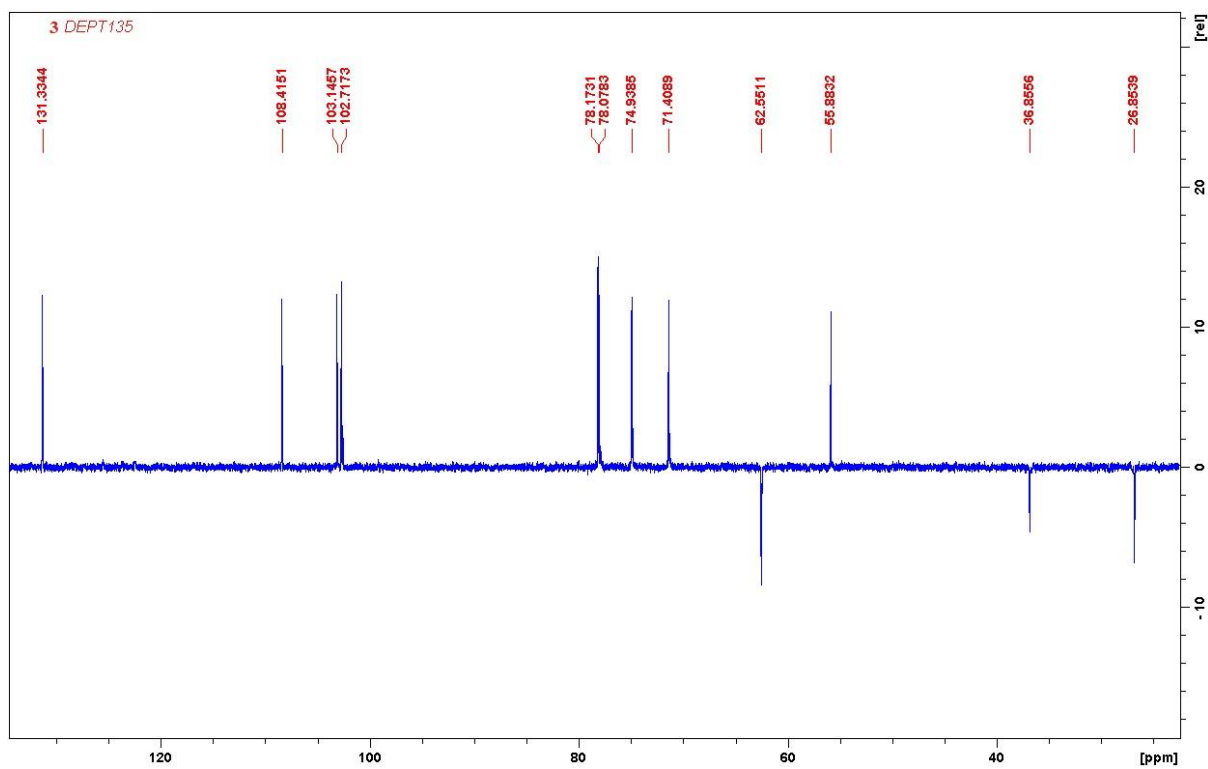


Figure S21: DEPT135 spectrum of 3.

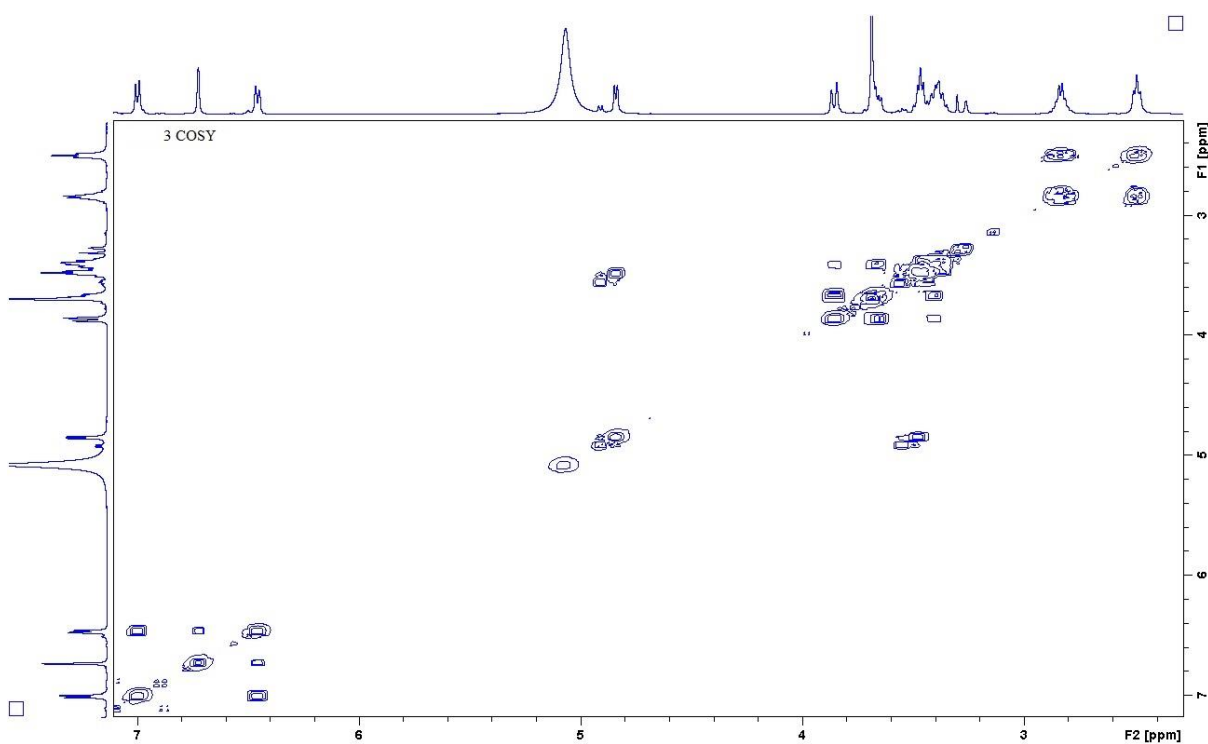
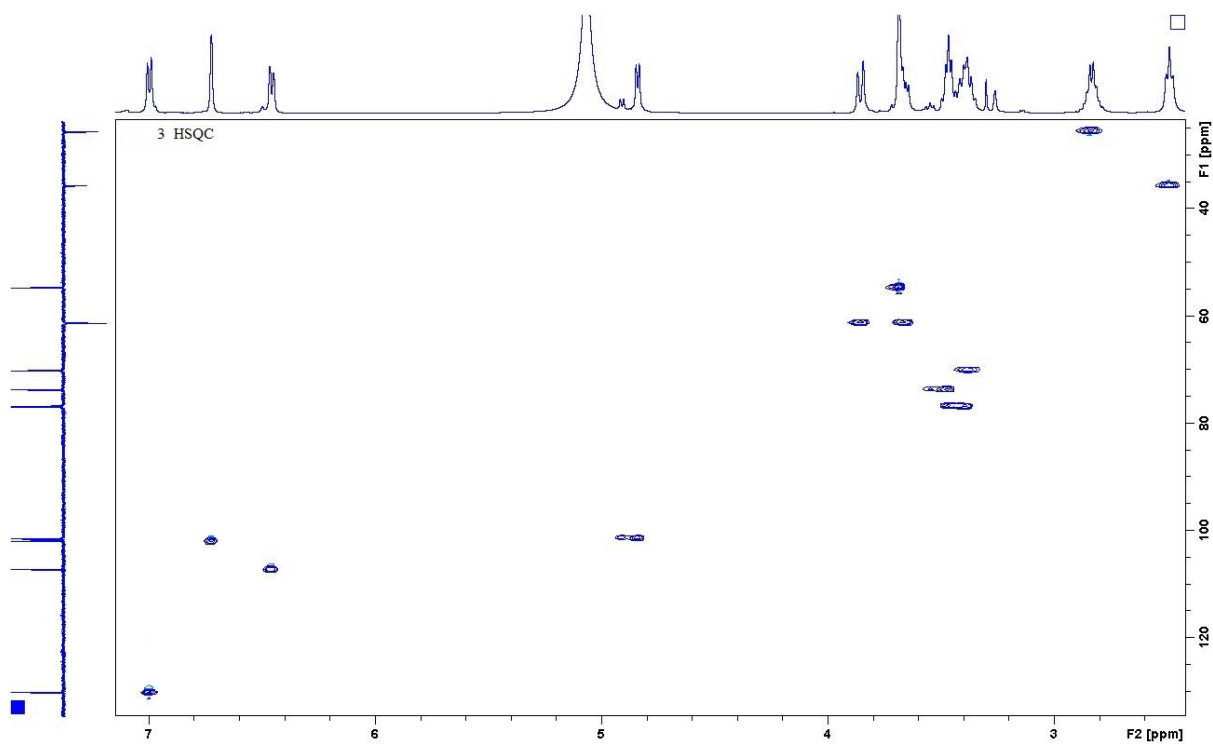
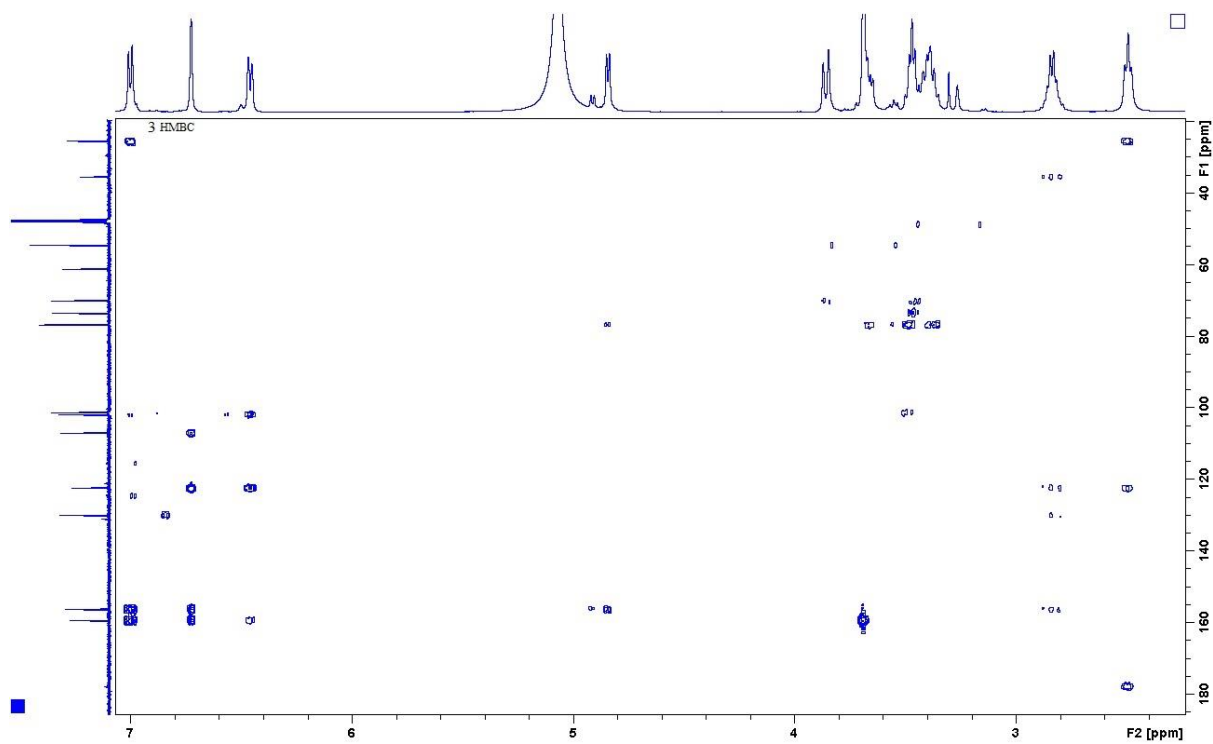


Figure S22: COSY spectrum of 3.

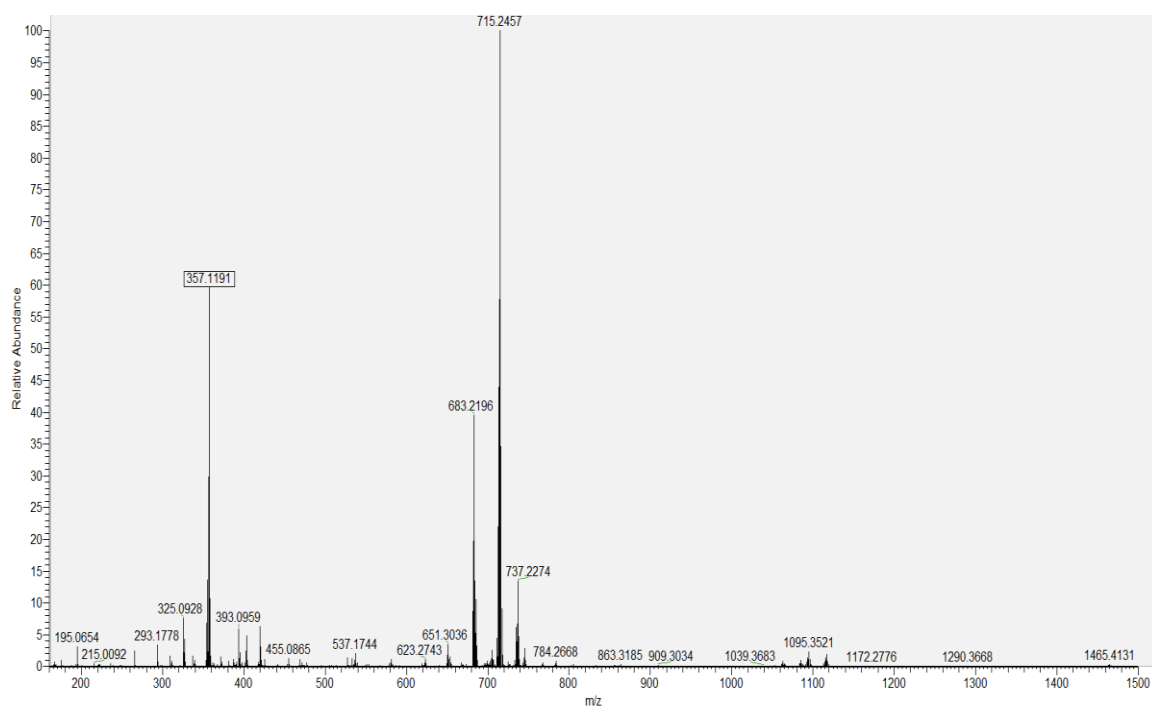


**Figure S23:** HSQC spectrum of **3**.

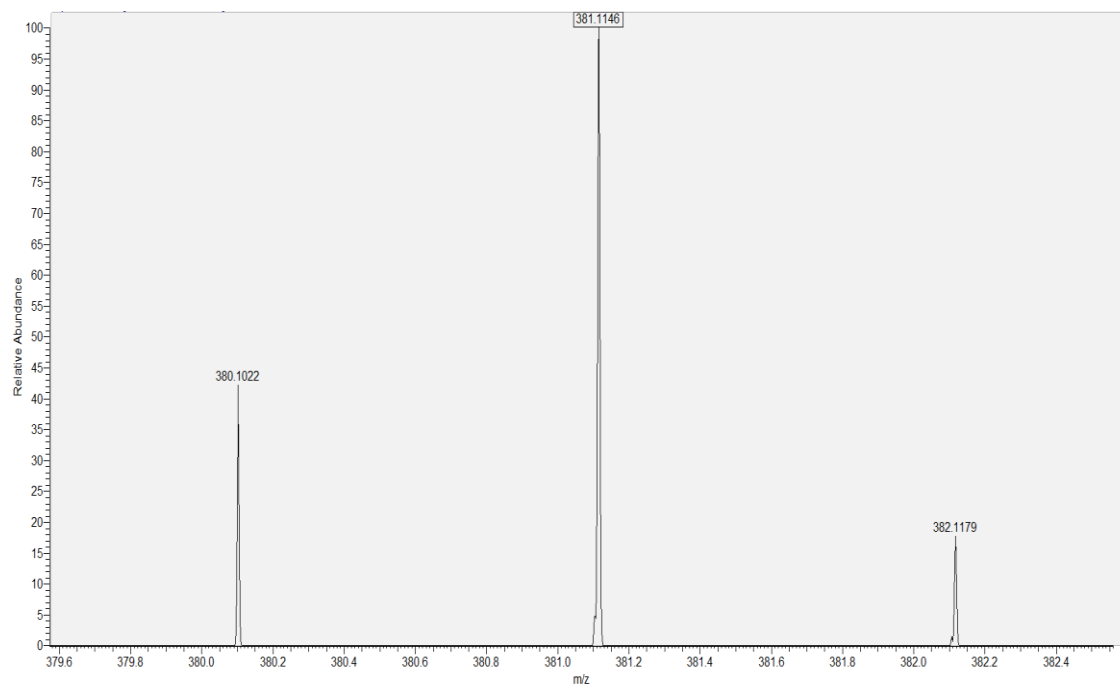


**Figure S24:** HMBC spectrum of **3**.





**A: Negative mode**



**B: Positive mode**

**Figure S25: ESIHRMS spectra of 3.**

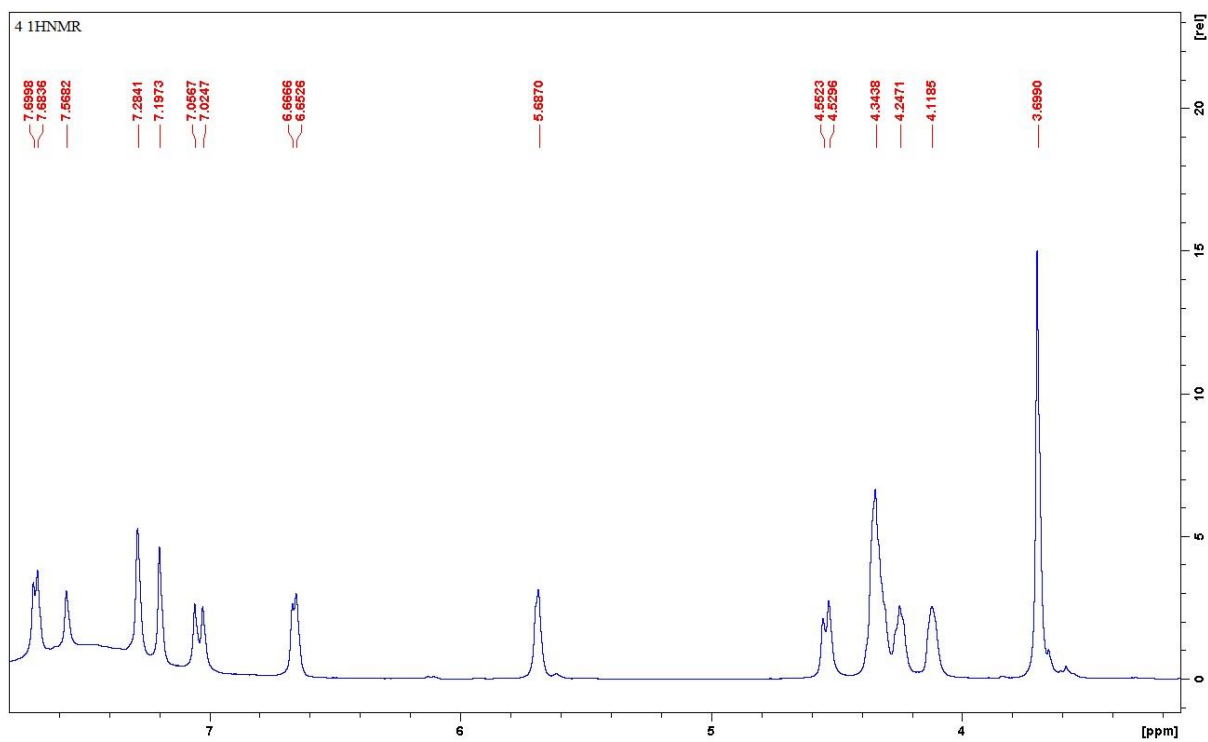


Figure S26: <sup>1</sup>H NMR spectrum of 4.

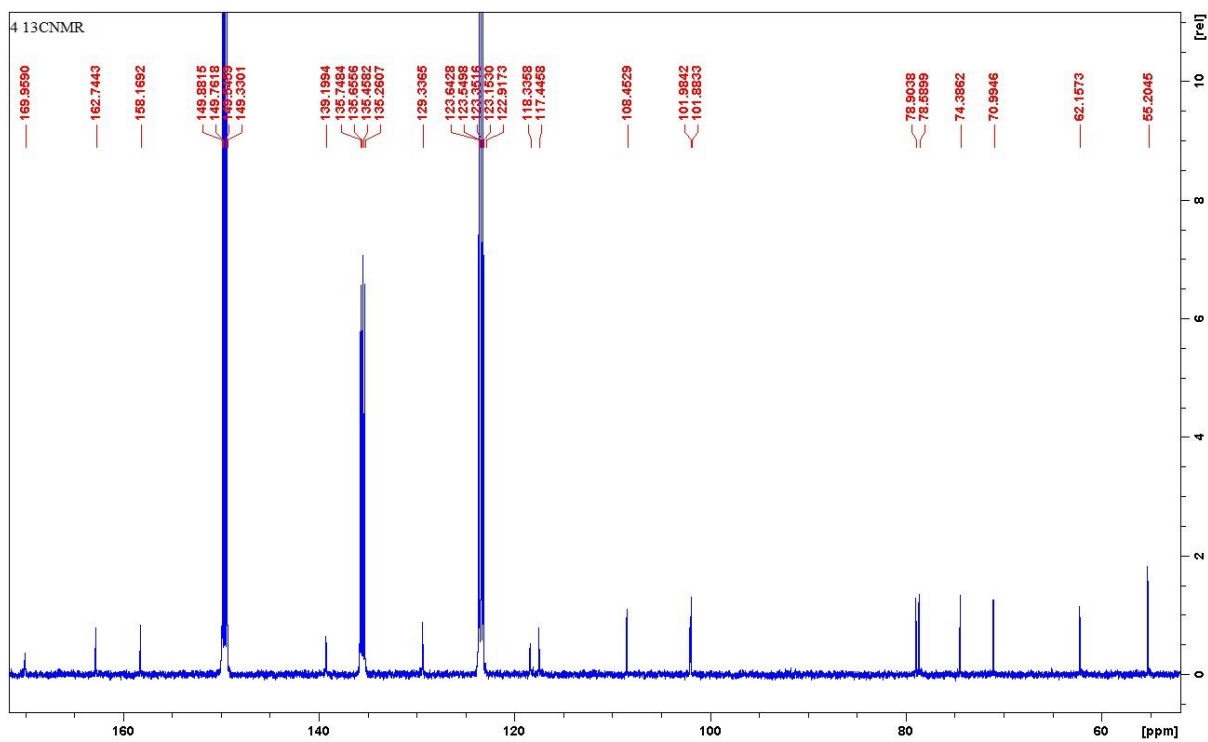


Figure S27: <sup>13</sup>C NMR spectrum of 4.

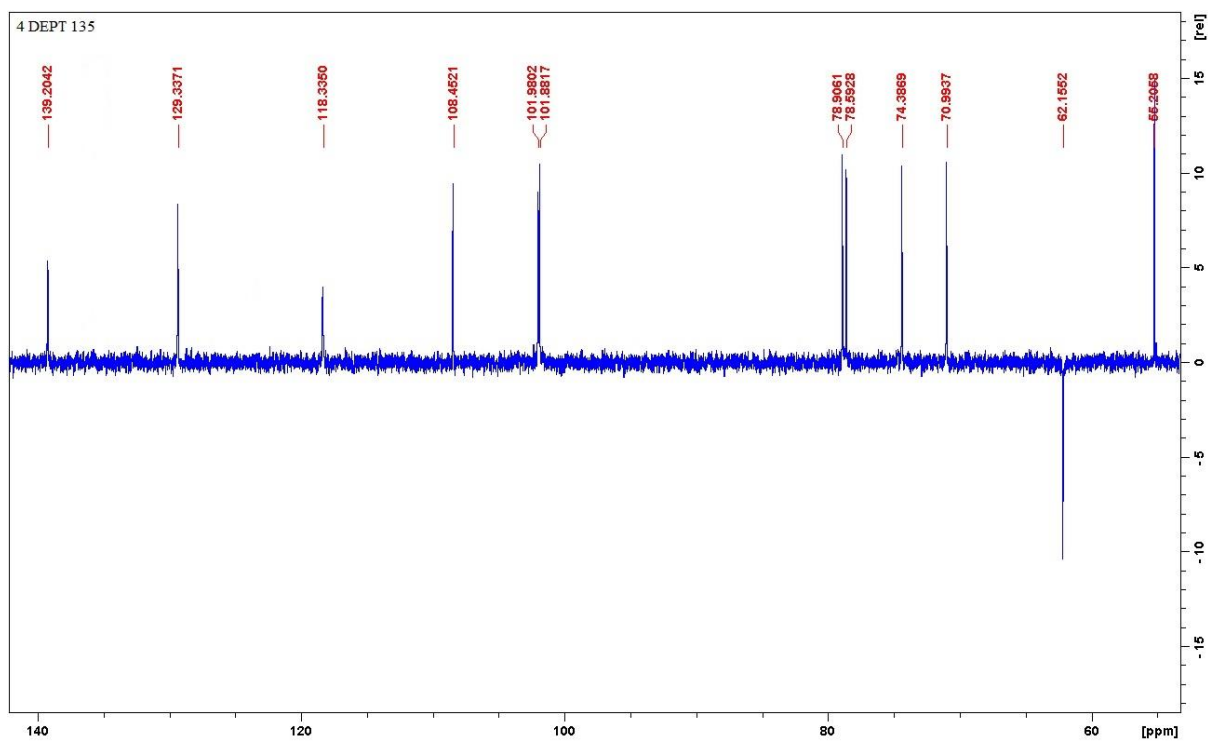


Figure S28: DEPT135 spectrum of 4.

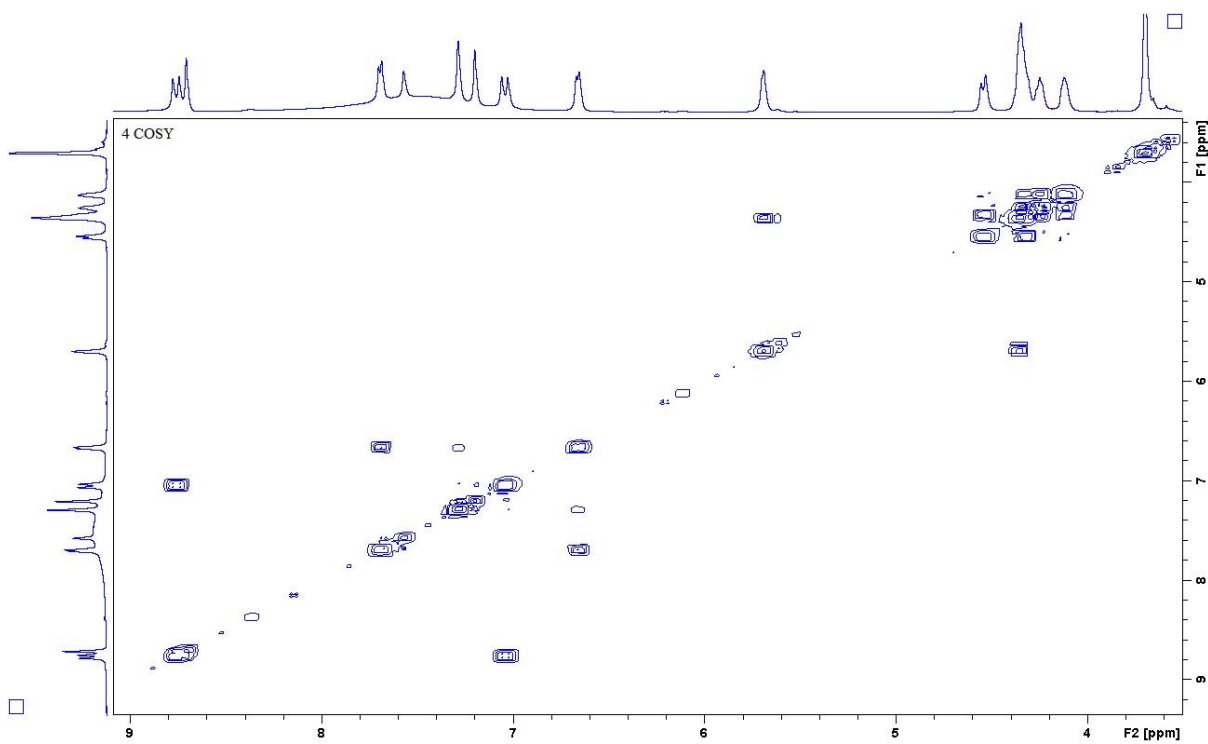
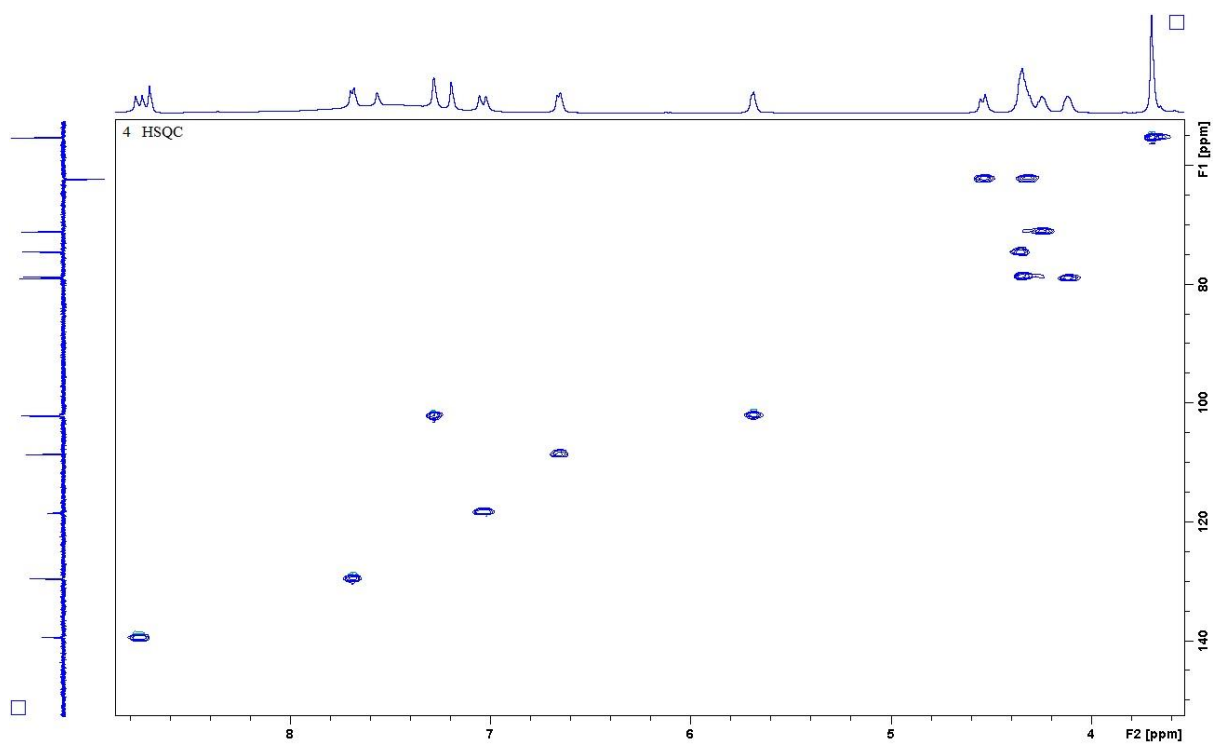
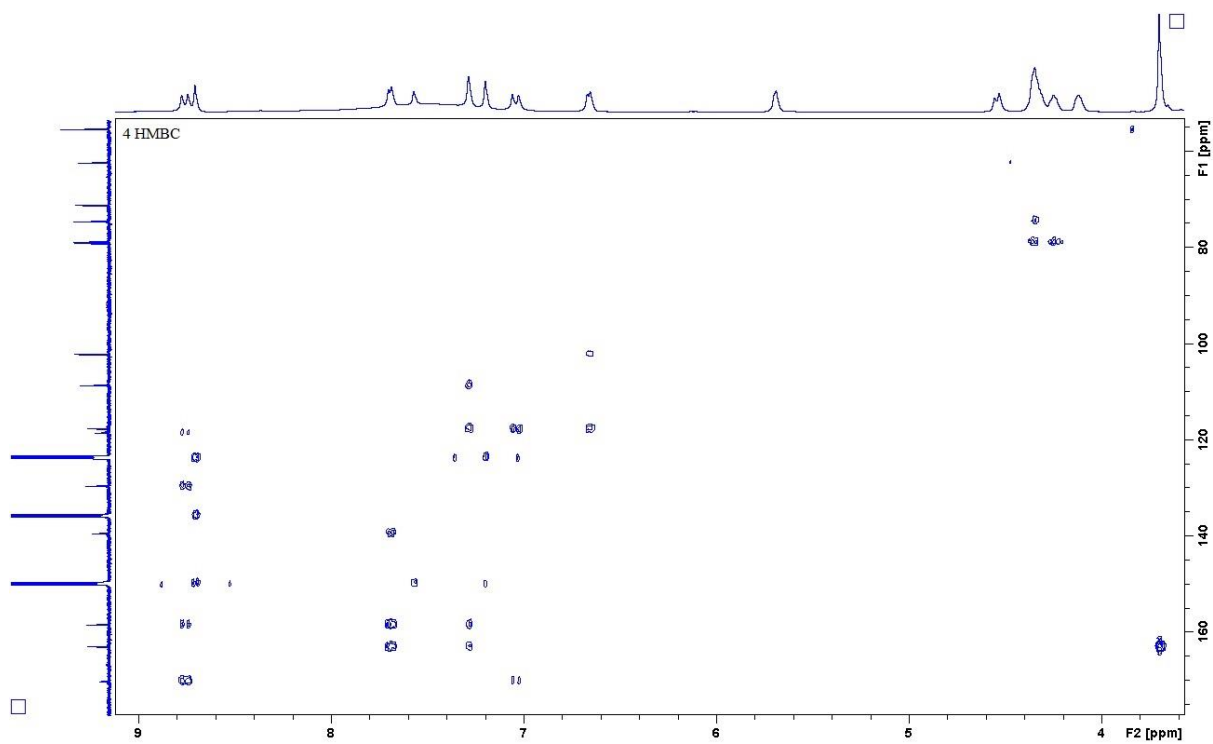


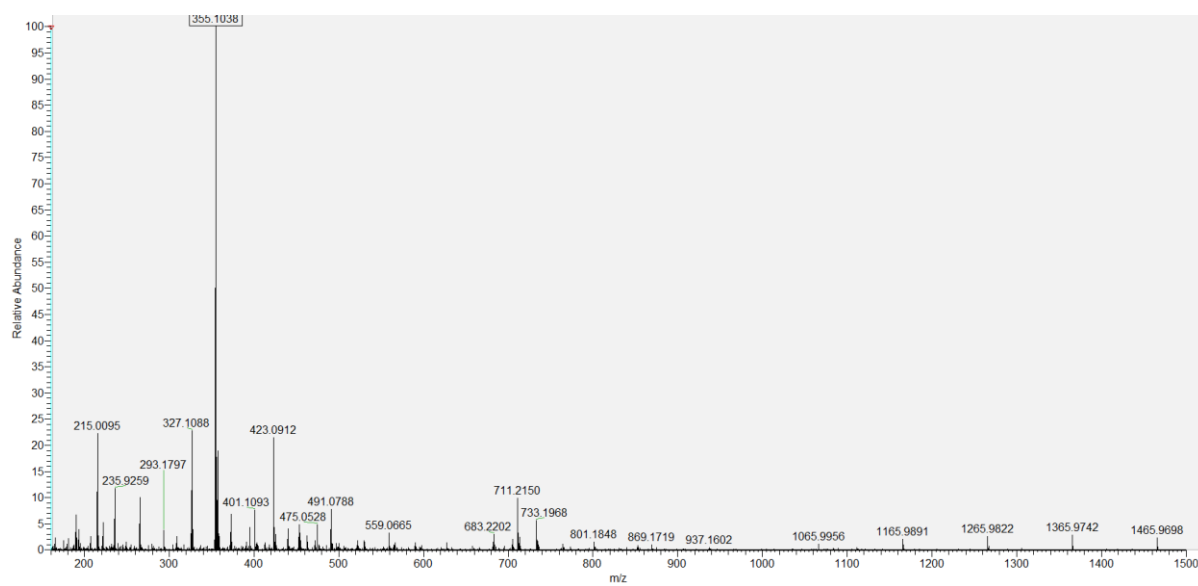
Figure S29: COSY spectrum of 4.



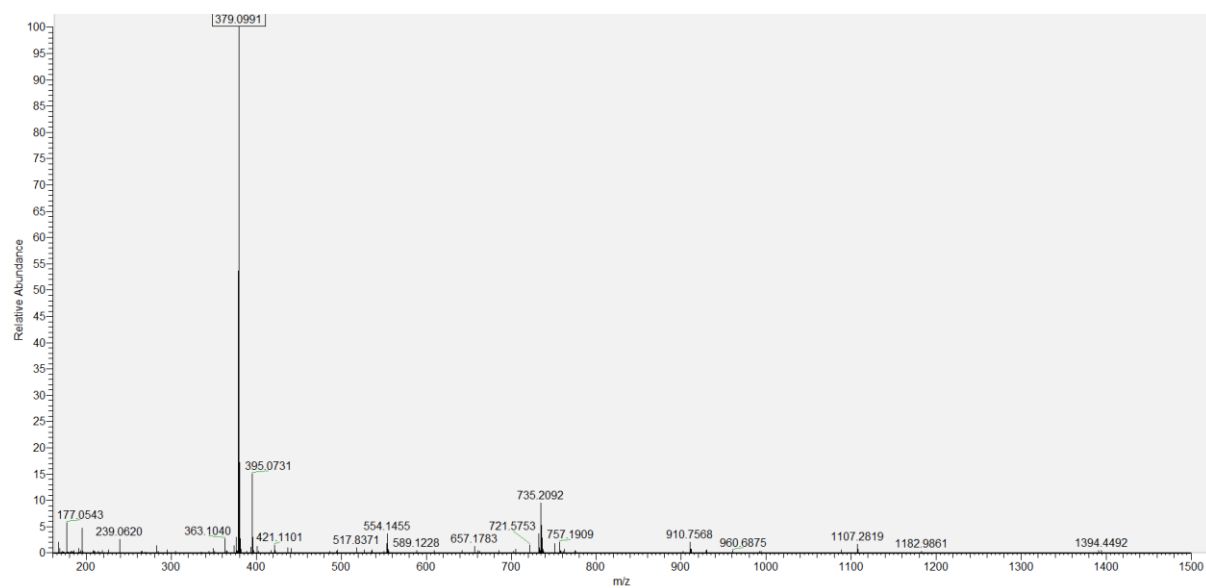
**Figure S30:** HSQC spectrum of **4**.



**Figure S31:** HMBC spectrum of **4**.



**A: Negative mode**



**B: Positive mode**

**Figure S32: ESIHRMS spectra of 4.**

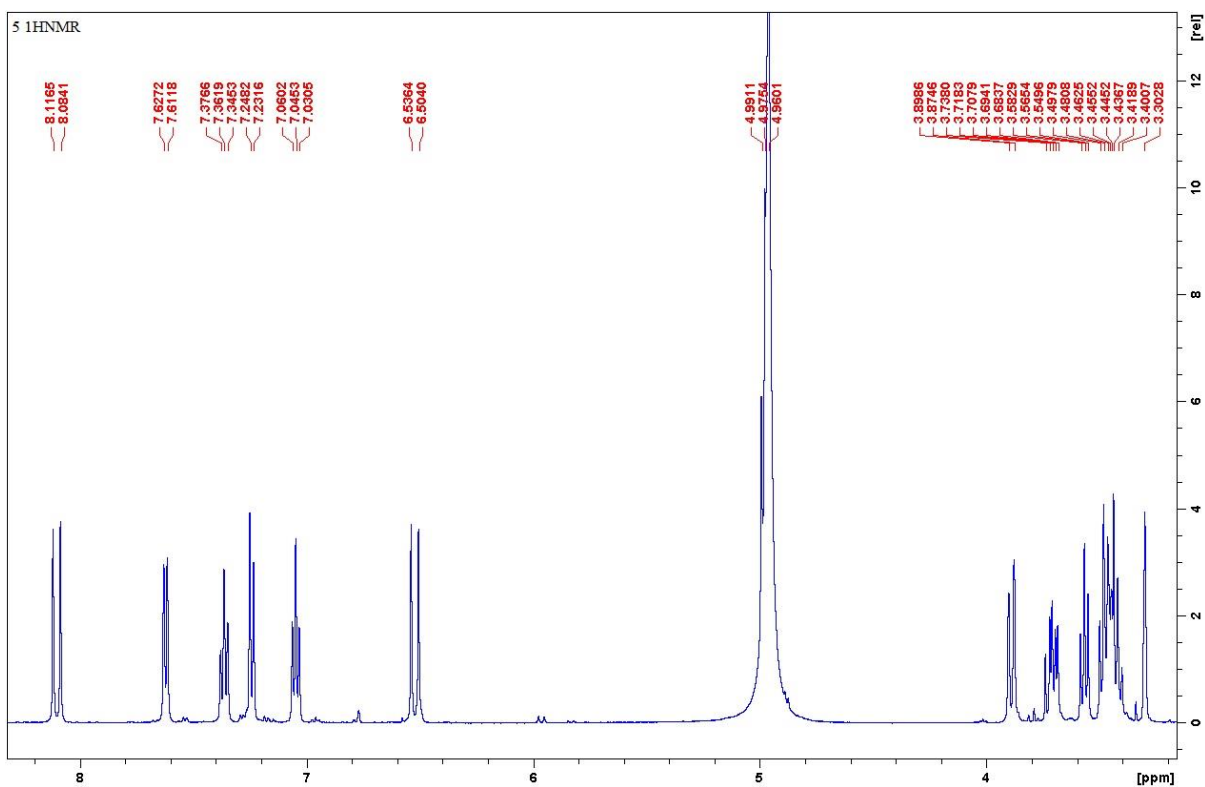


Figure S33: <sup>1</sup>H NMR spectrum of **5**.

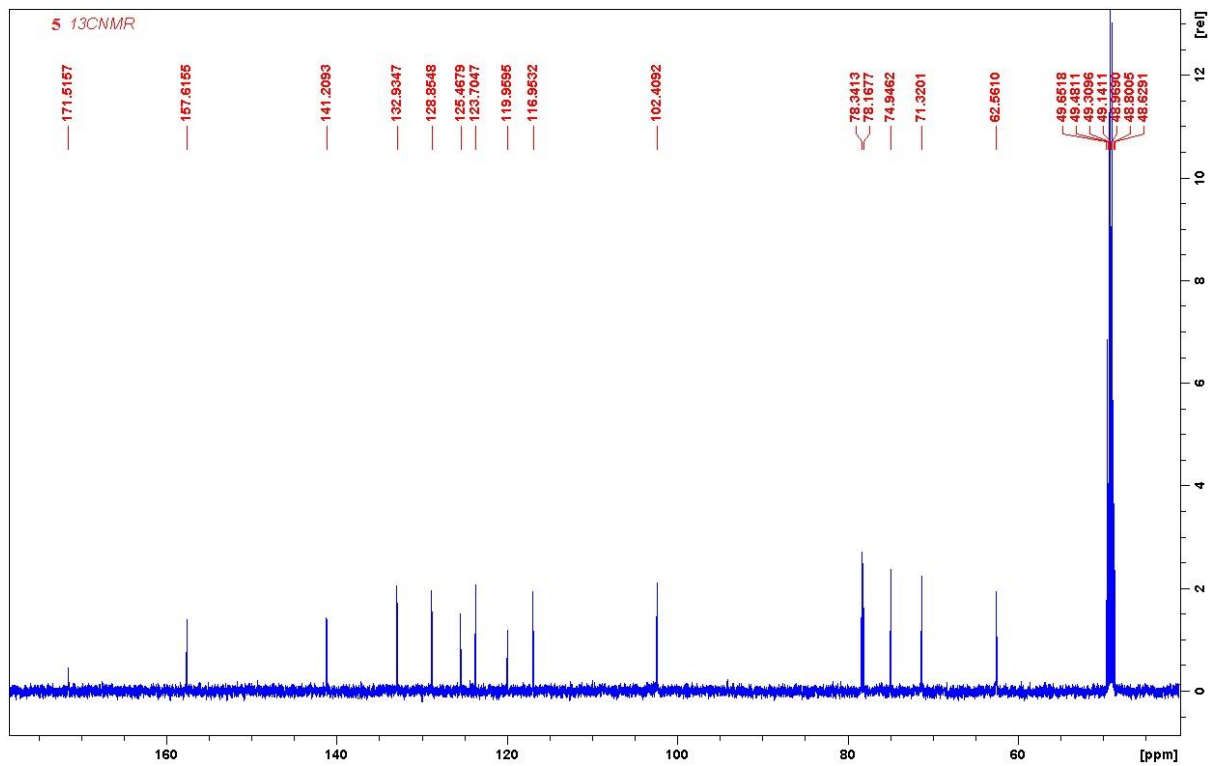


Figure S34: <sup>13</sup>C NMR spectrum of **5**.

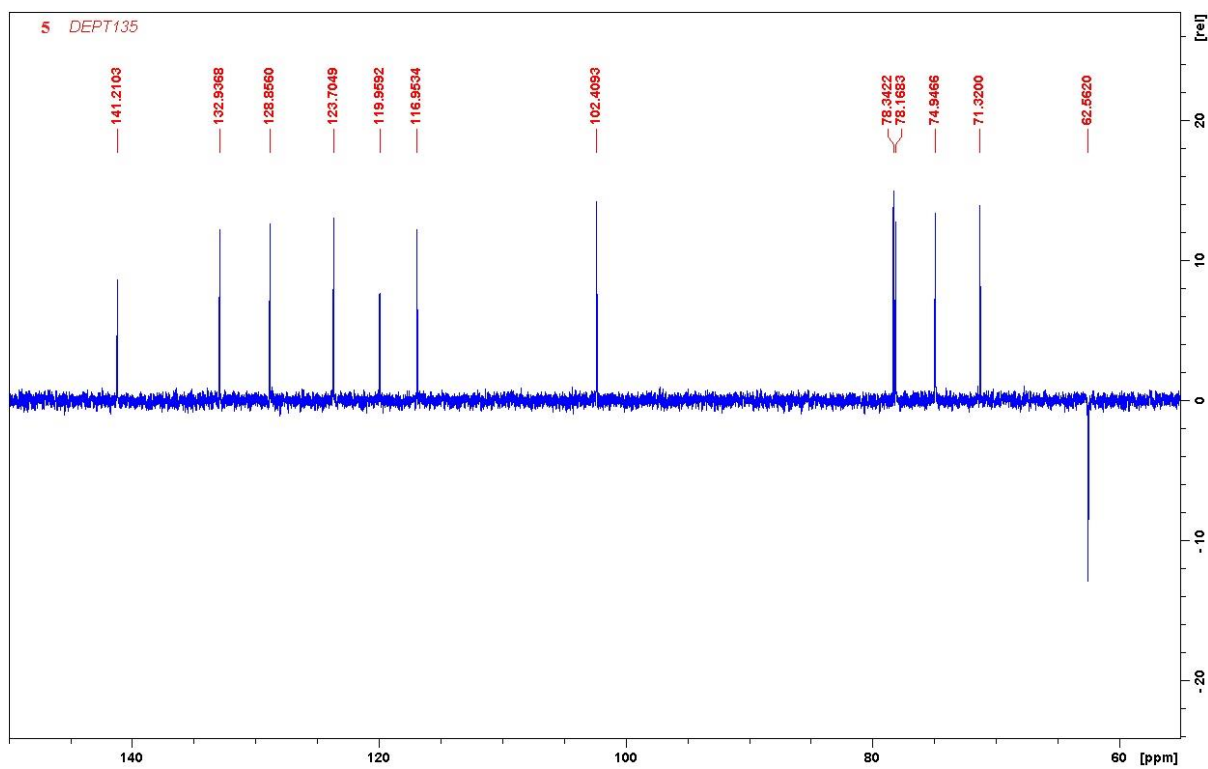


Figure S35: DEPT135 spectrum of 5.

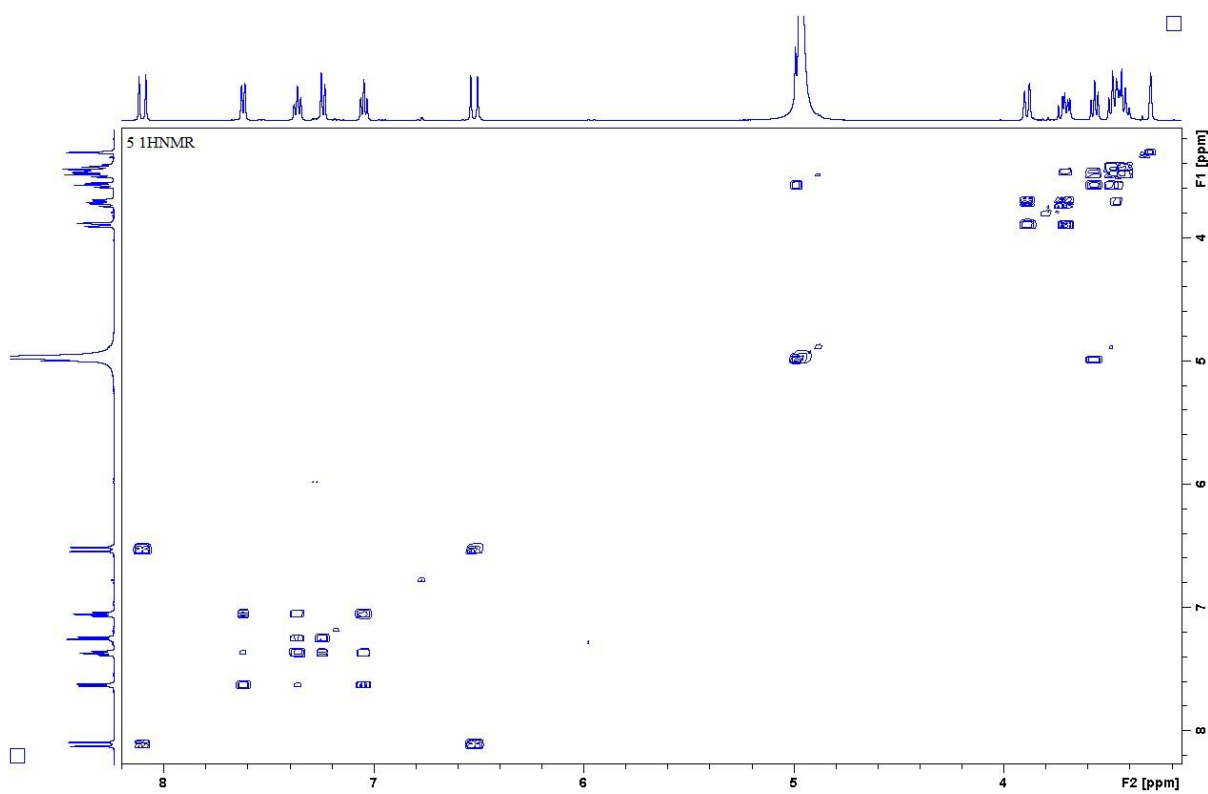
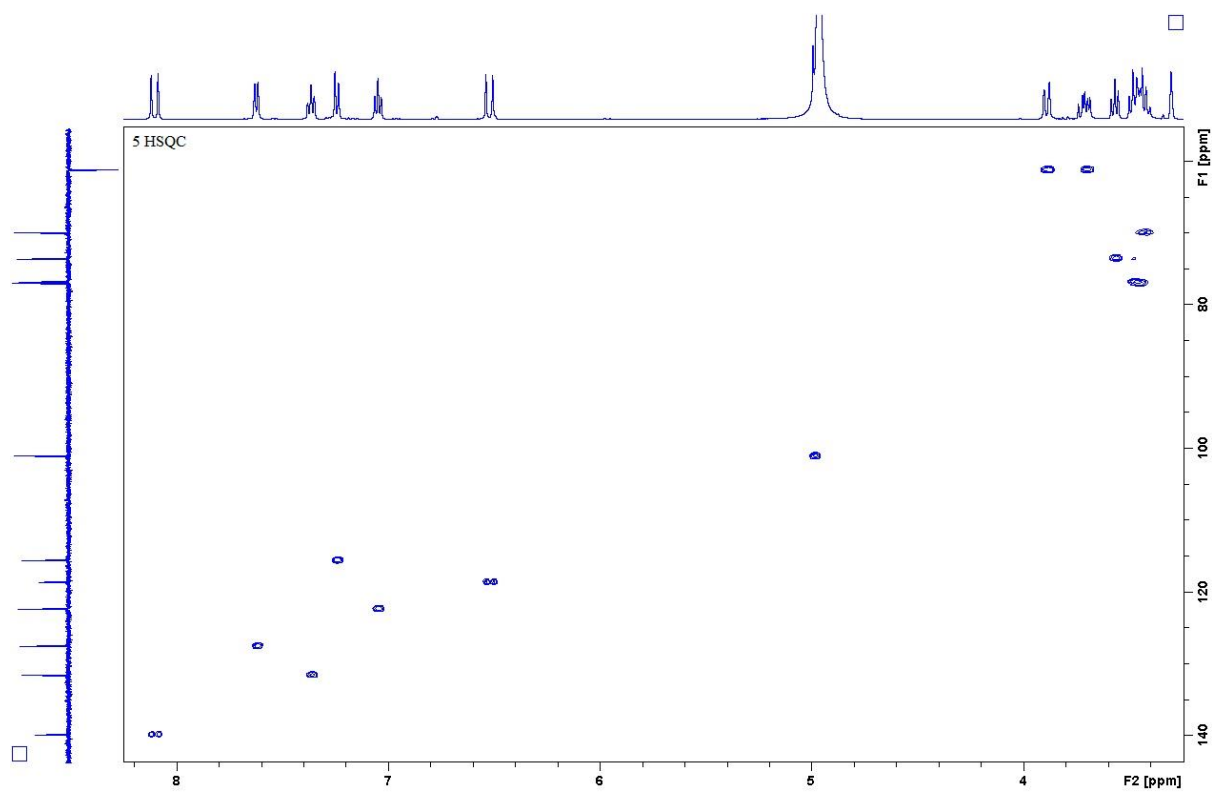
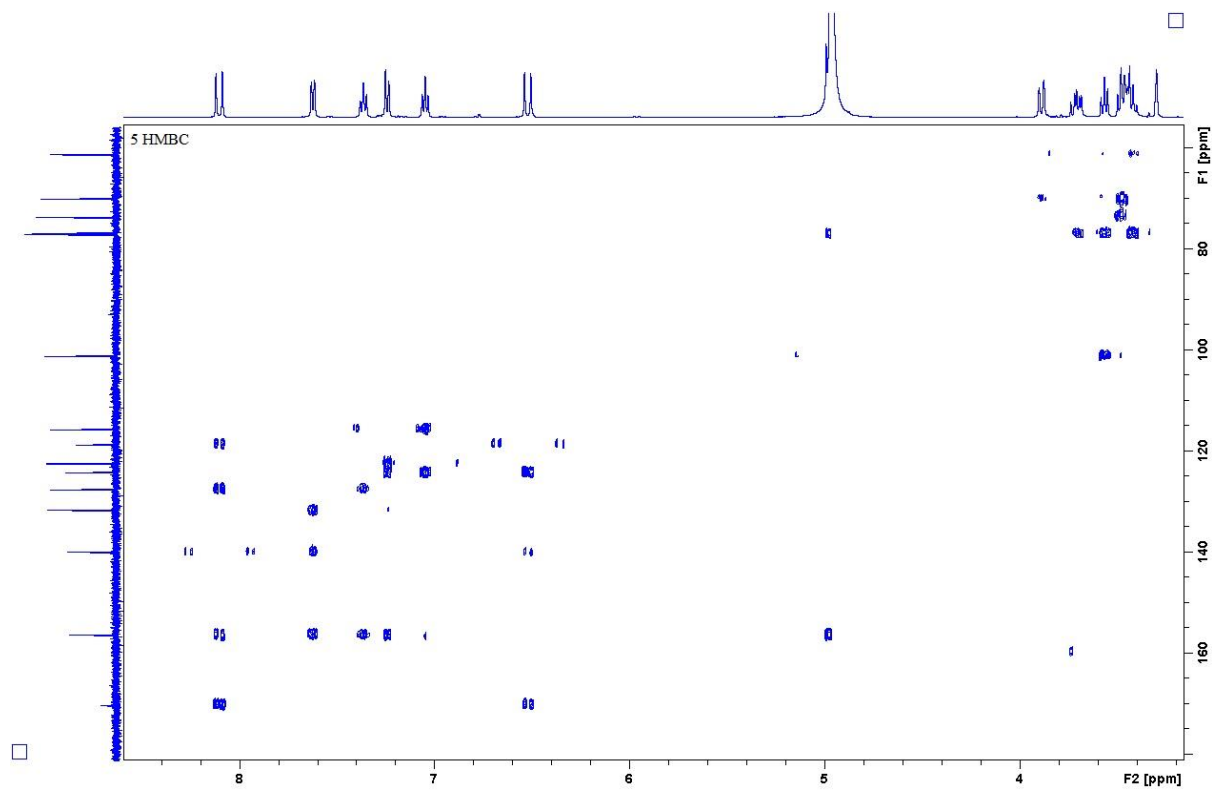


Figure S36: COSY spectrum of 5.

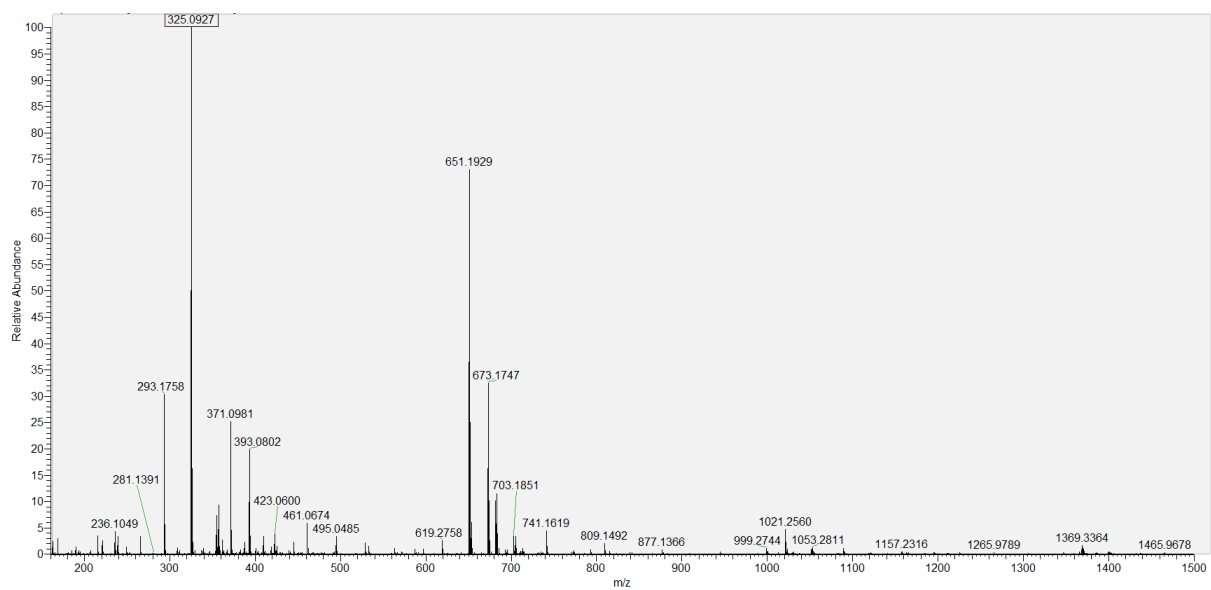


**Figure S37:** HSQC spectrum of **5**.

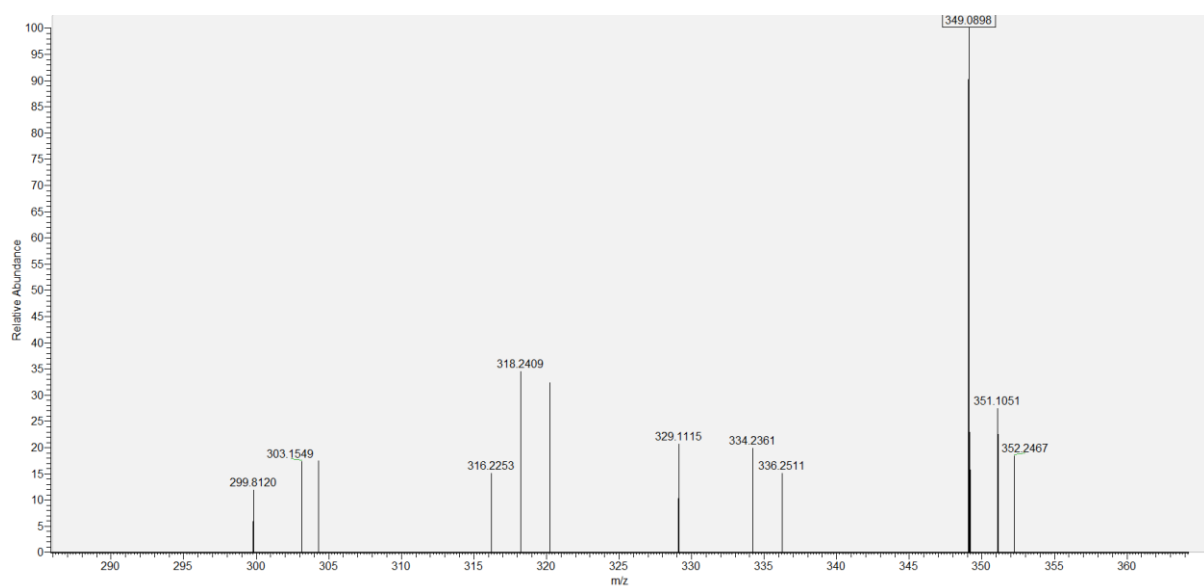


**Figure S38:** HMBC spectrum of **5**.





**A: Negative mode**



**B: Positive mode**

**Figure S39: ESIHRMS spectra of 5.**