

## Supporting Information

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### New Flavonoids from Saudi collection of *Tephrosia purpurea* L. (Pers.)

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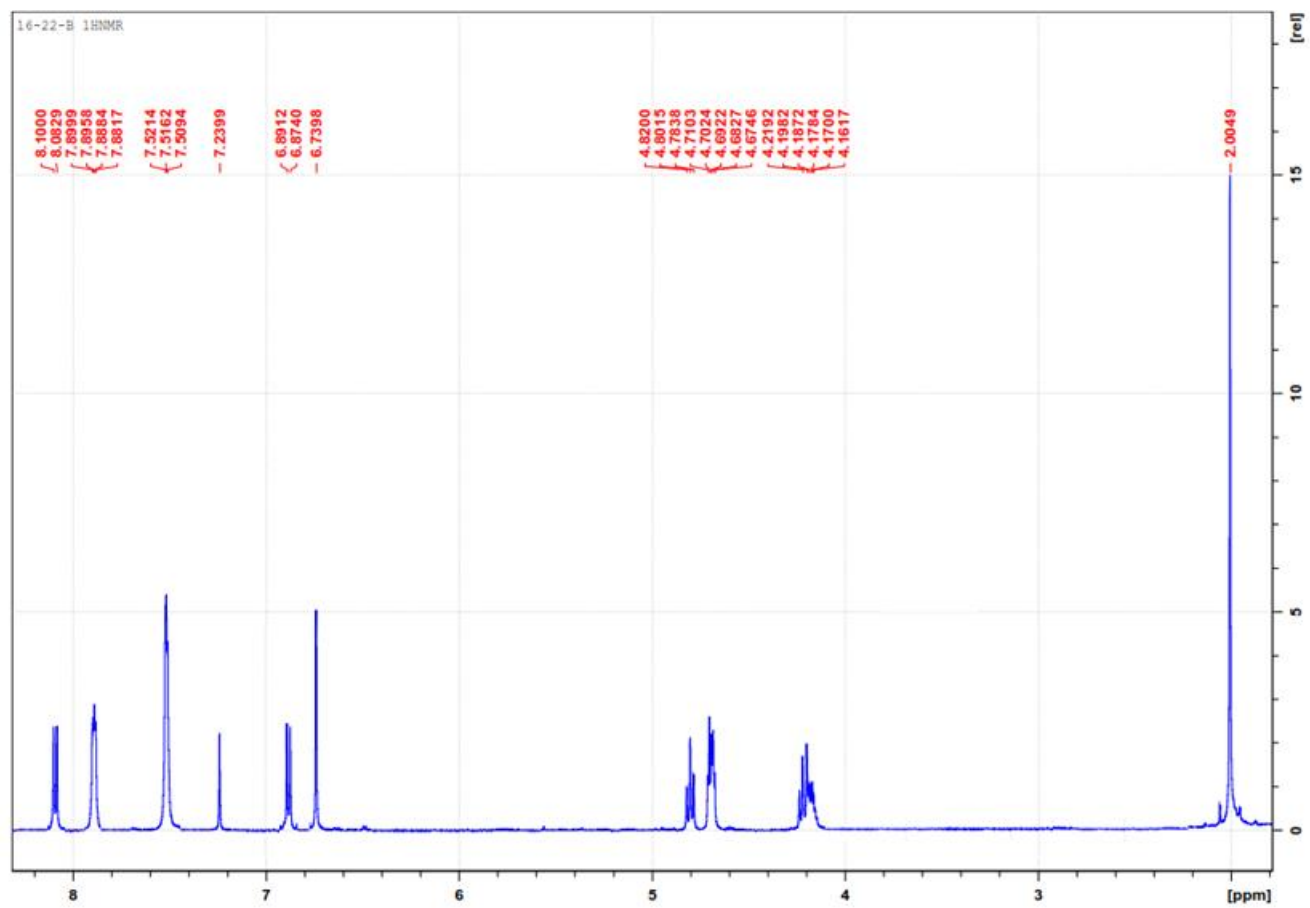
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**Figure S1:**  $^1\text{H}$ NMR Spectrum of **1**  $\text{CDCl}_3$ .

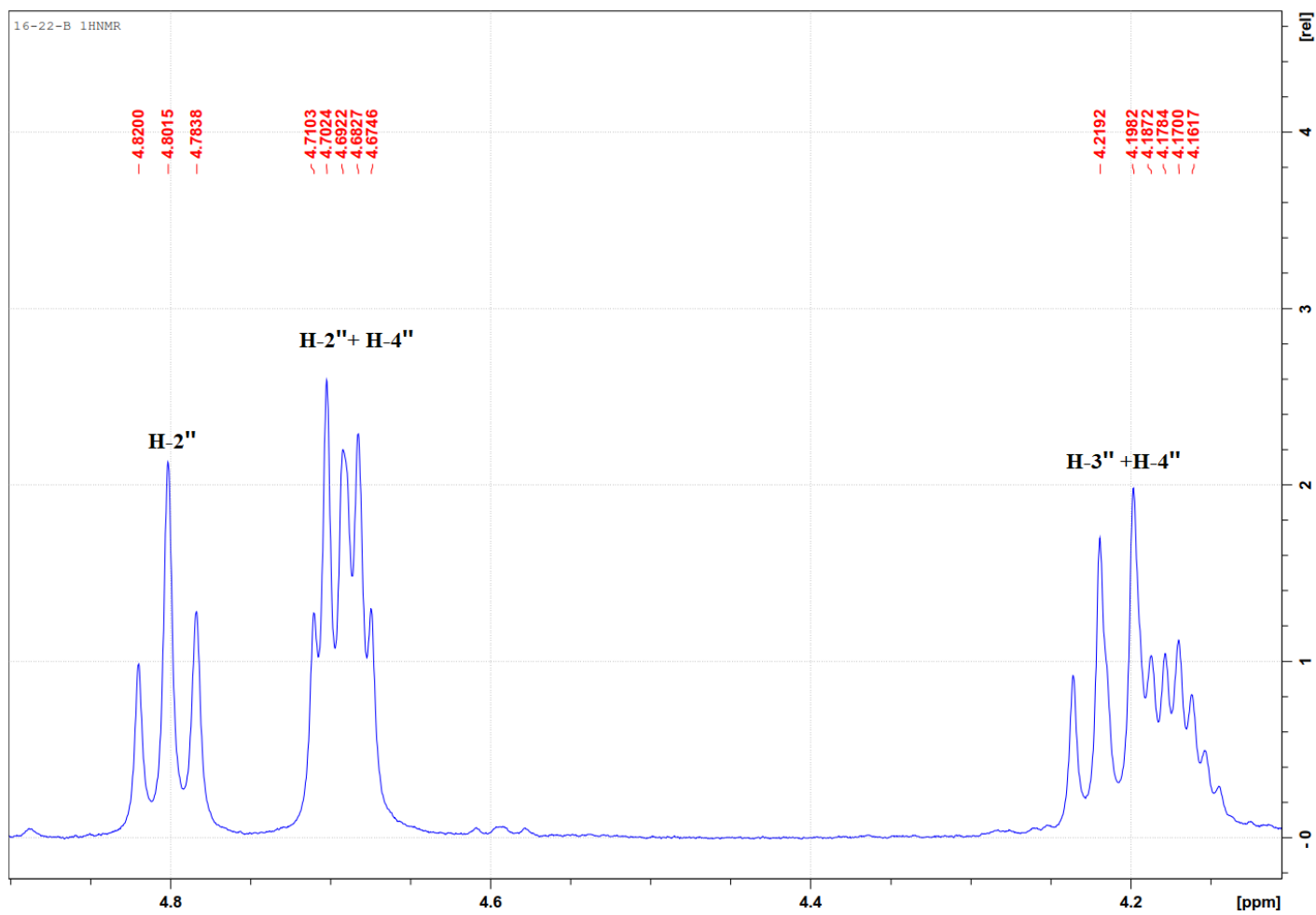


Figure S2 :<sup>1</sup>HNMR Spectrum of **1** CDCl<sub>3</sub> (expansion).

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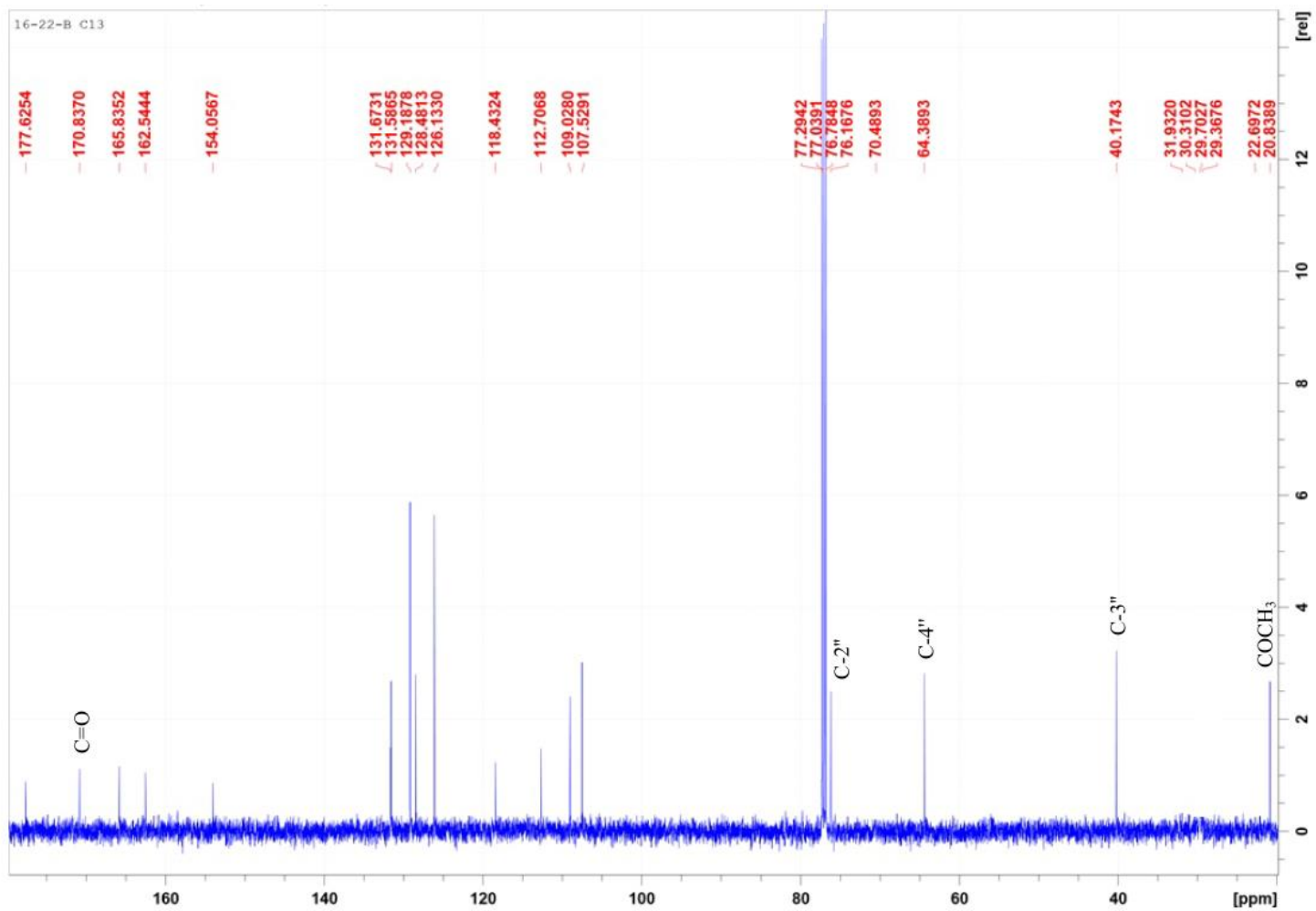
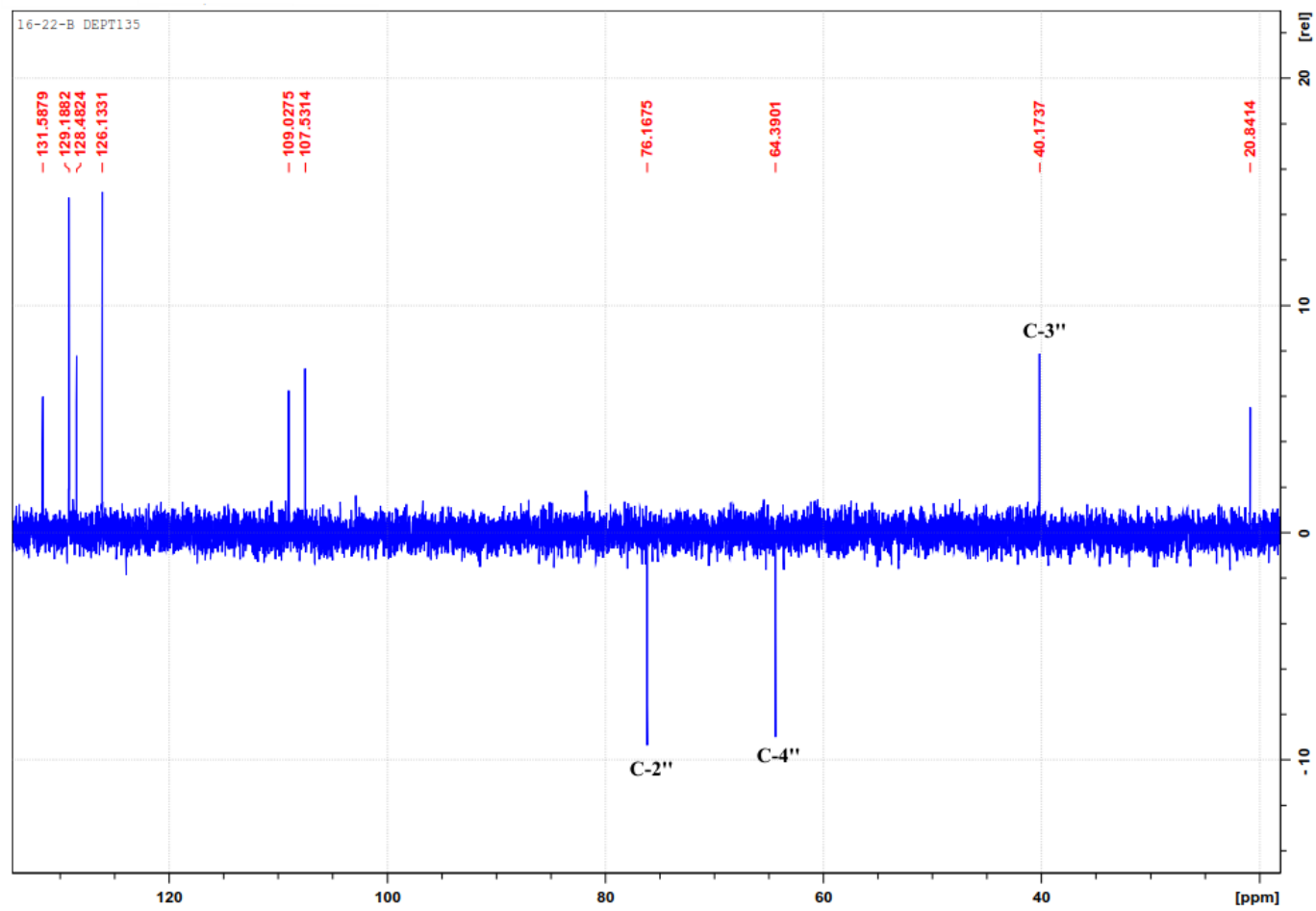


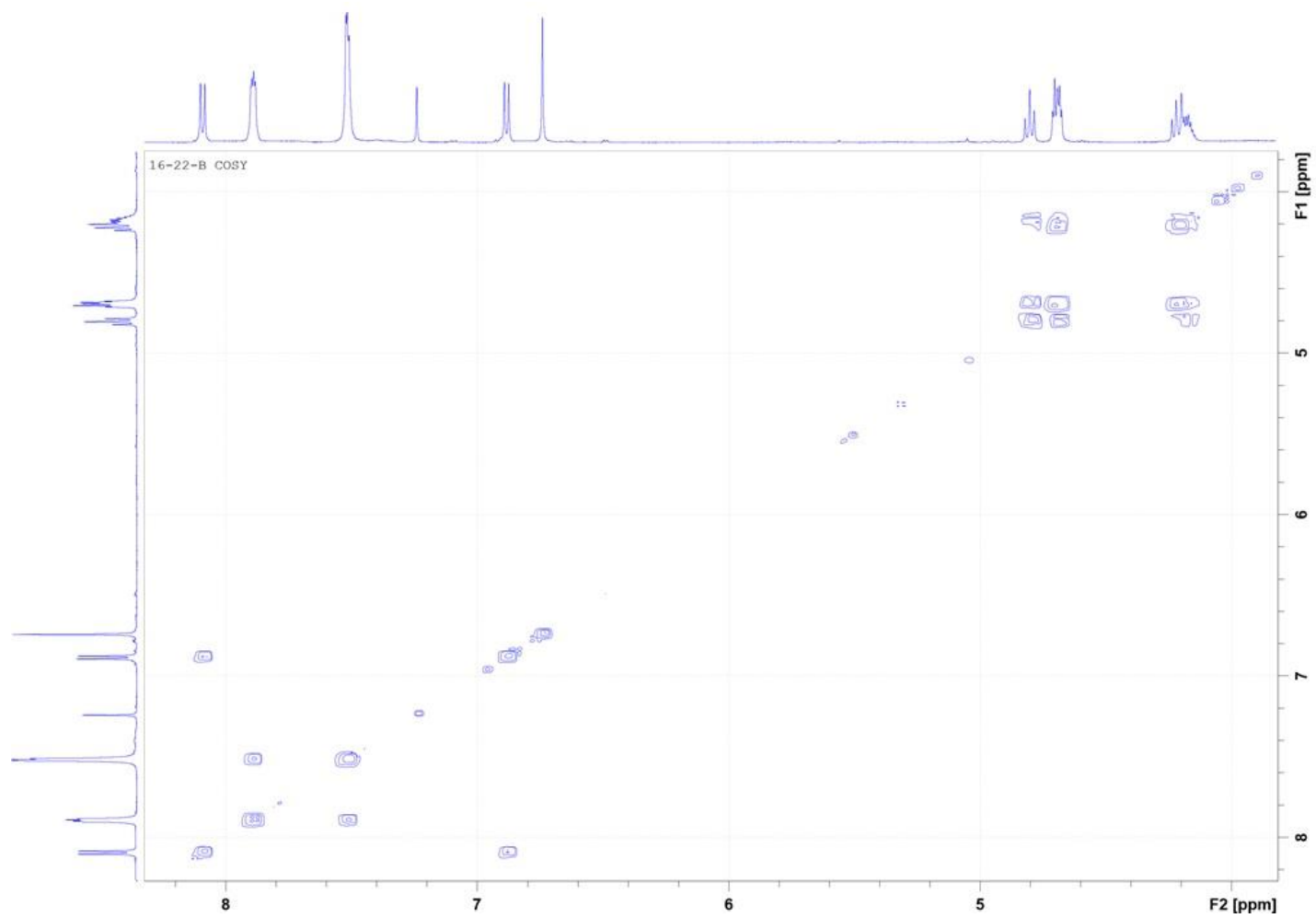
Figure S3 : <sup>13</sup>CNMR Spectrum of 1 CDCl<sub>3</sub>.

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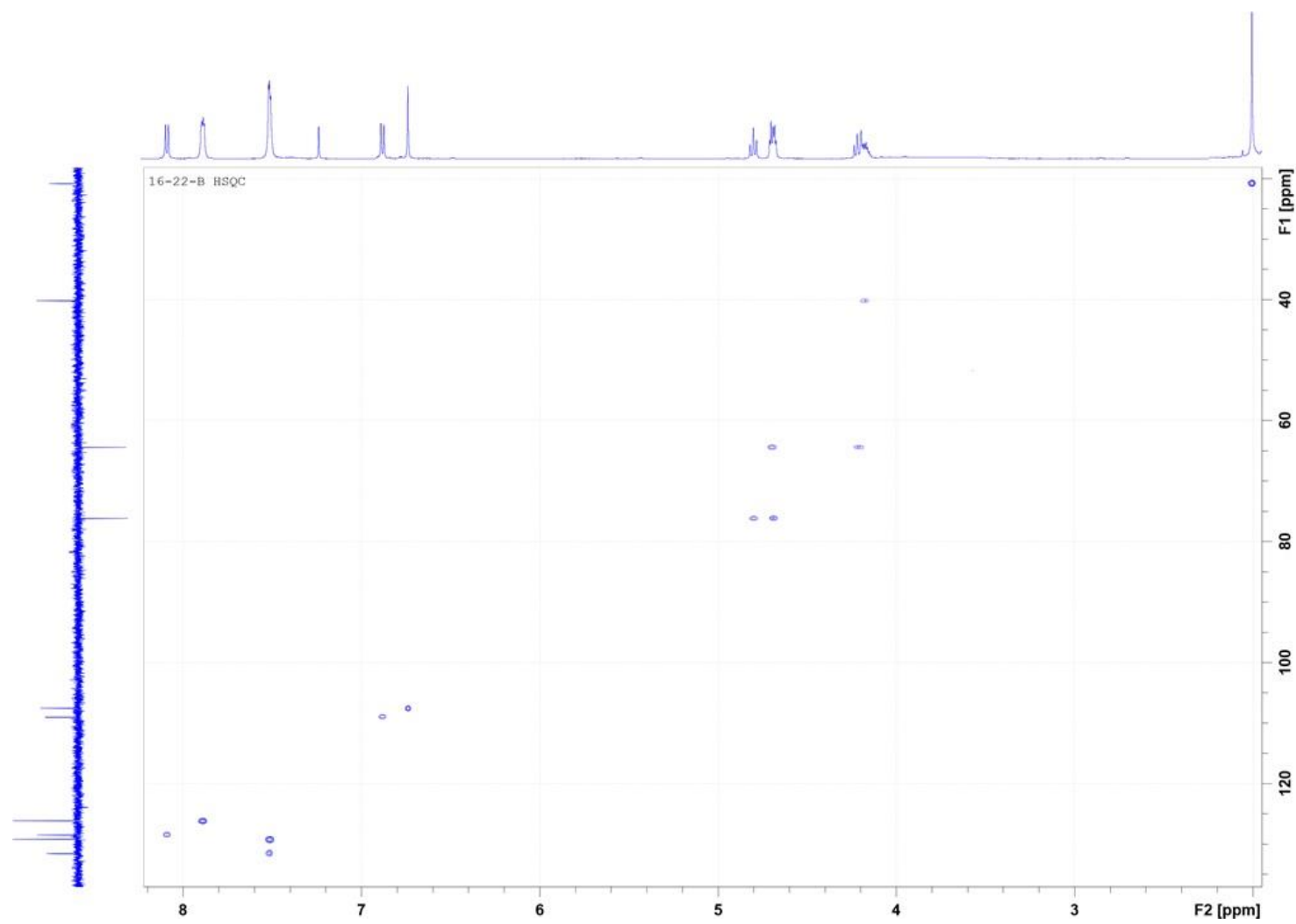


**Figure S4:** DEPT135 Spectrum of **1** CDCl<sub>3</sub>.

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**Figure S5:** COSY Spectrum of **1** CDCl<sub>3</sub>.



**Figure S6:** HSQC Spectrum of **1** CDCl<sub>3</sub>.

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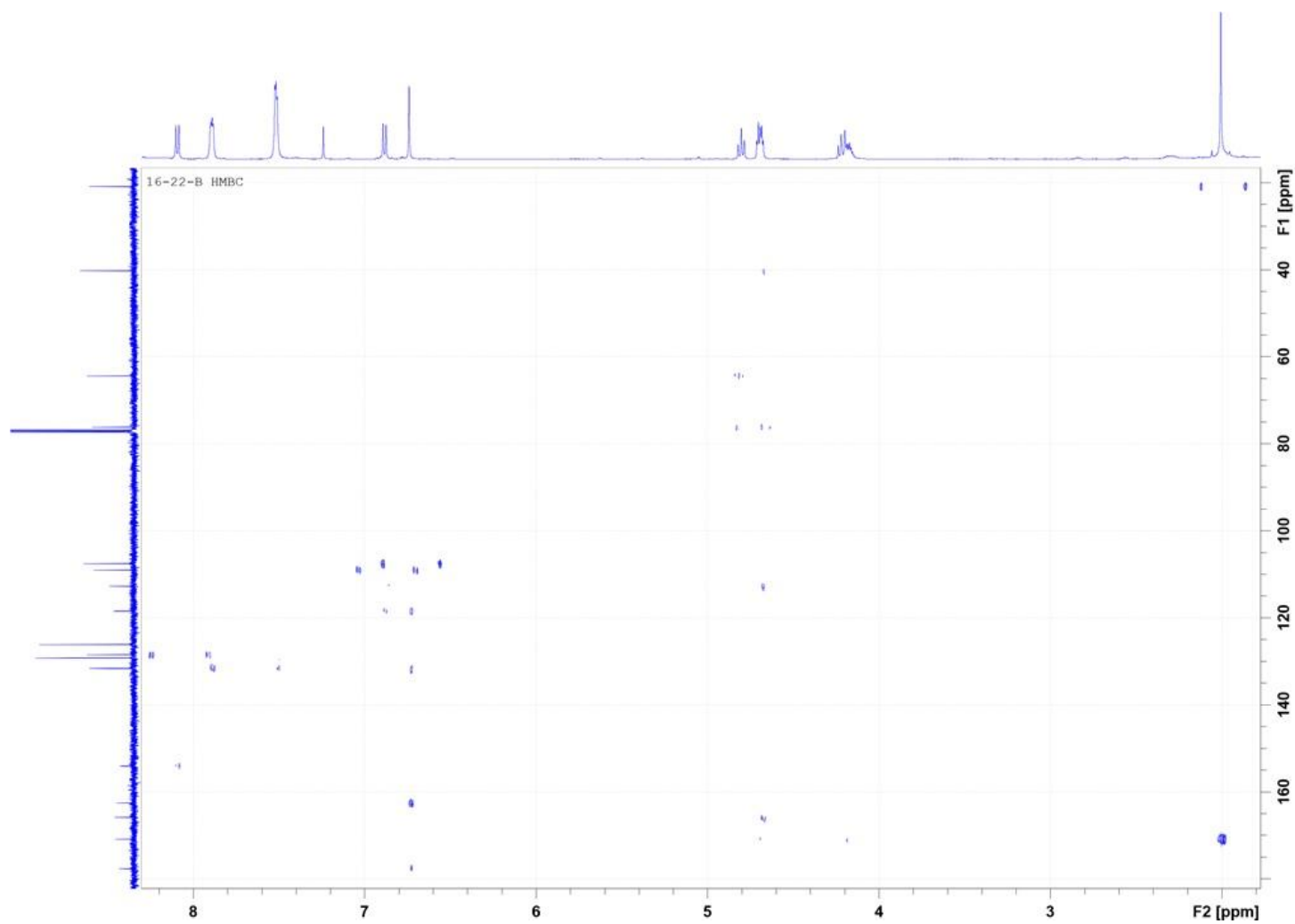


Figure S7: HMBC Spectrum of **1** CDCl<sub>3</sub>.

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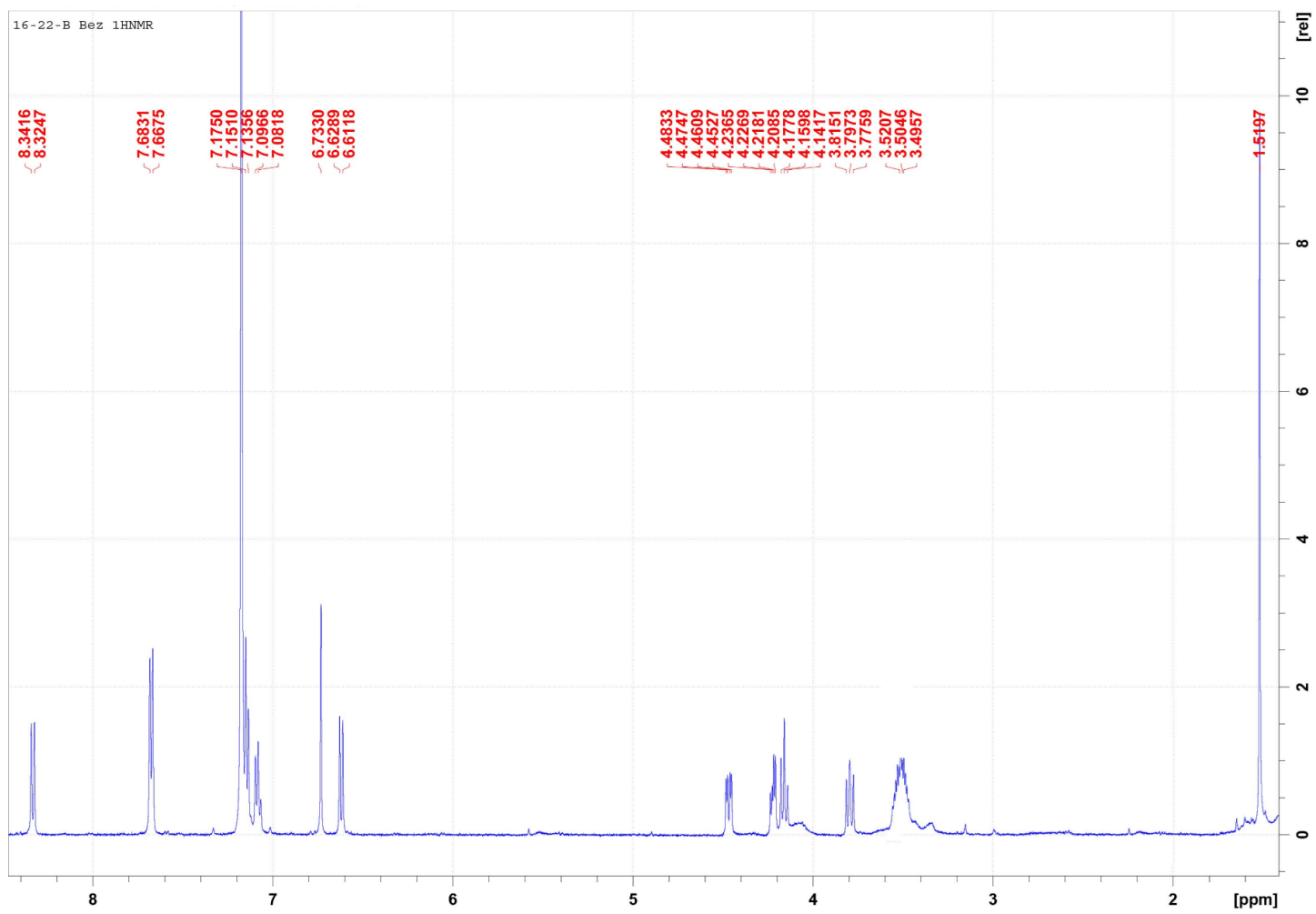
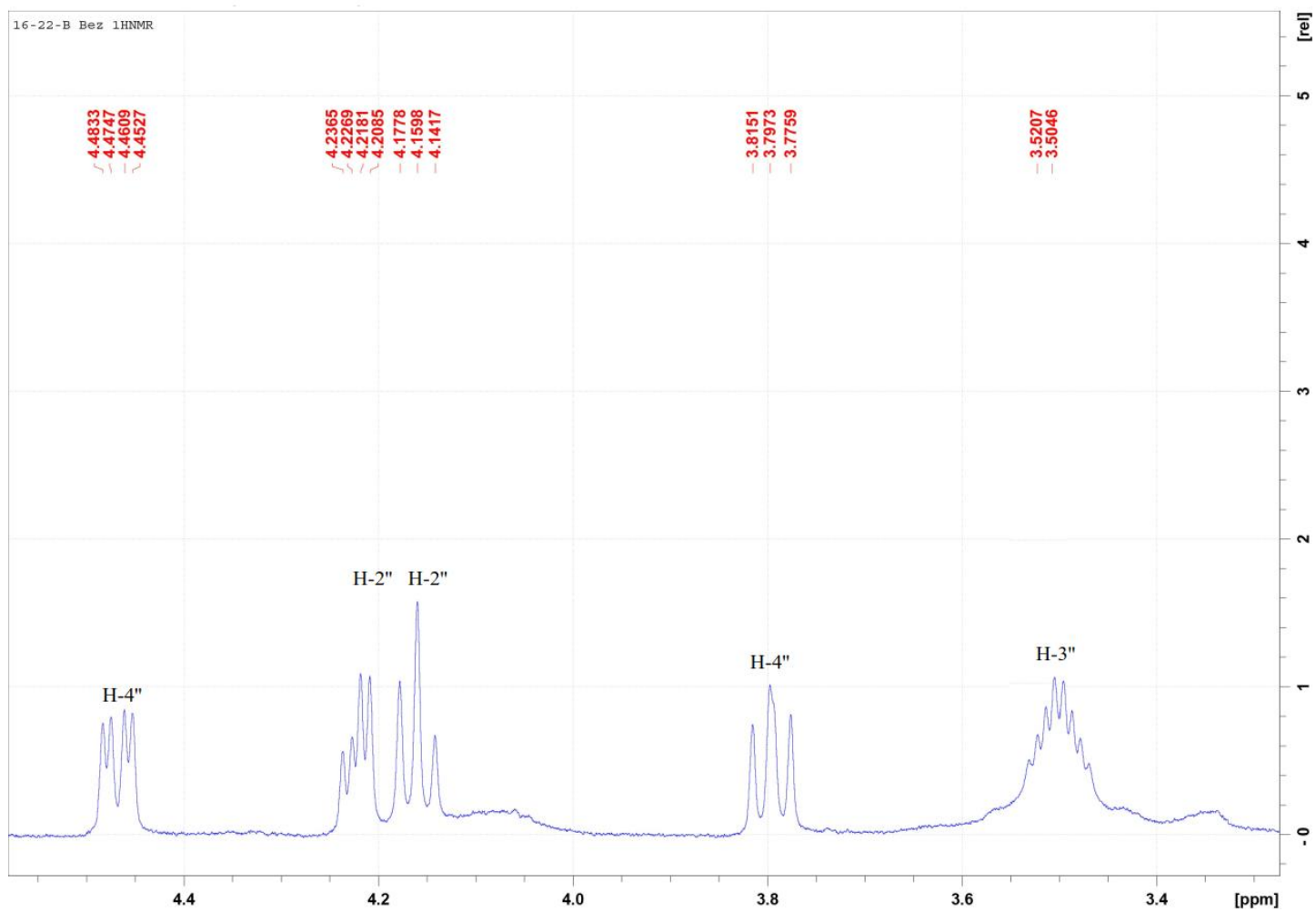
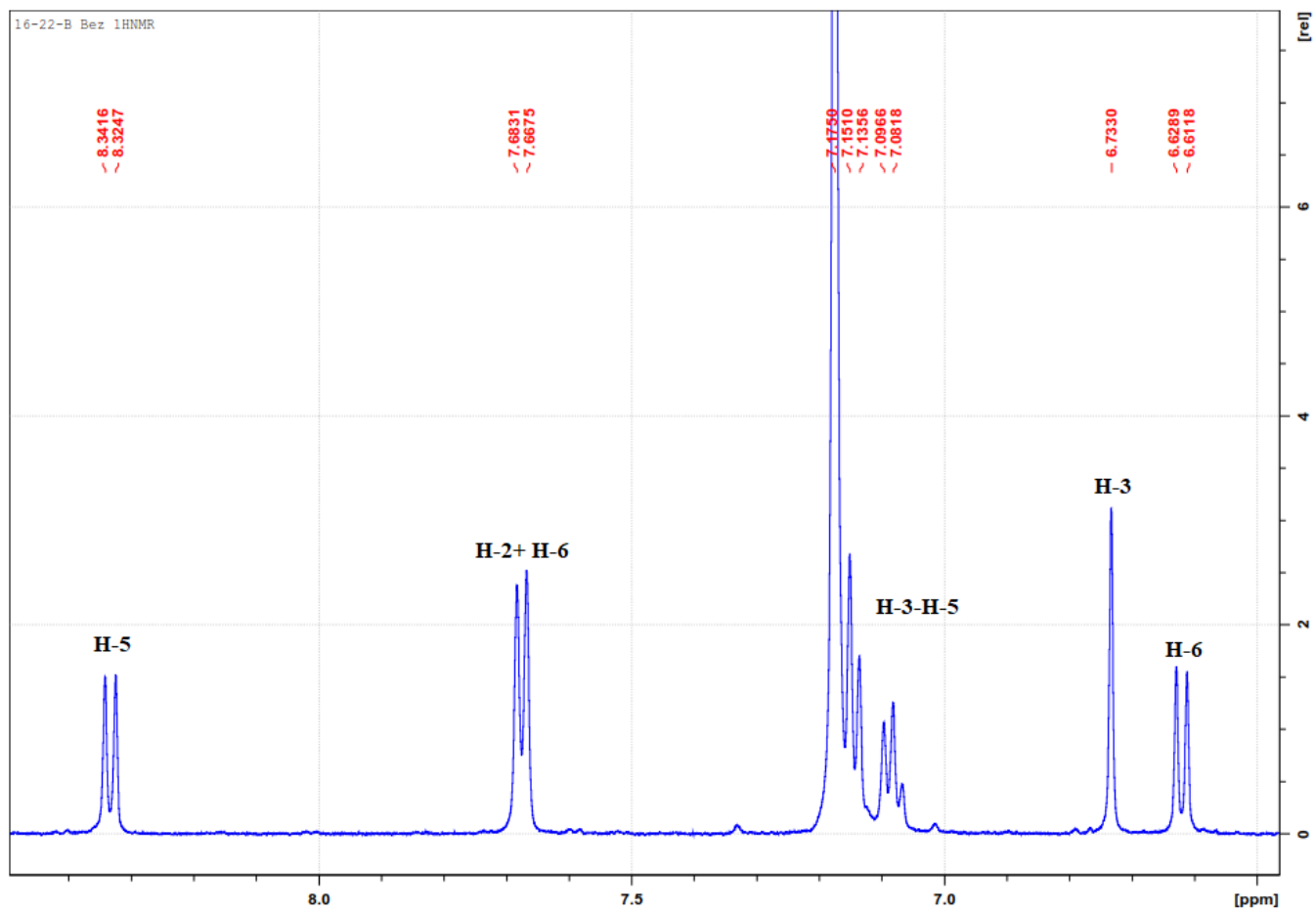


Figure S8:  $^1\text{H}$ NMR Spectrum of **1**  $\text{C}_6\text{D}_6$ .

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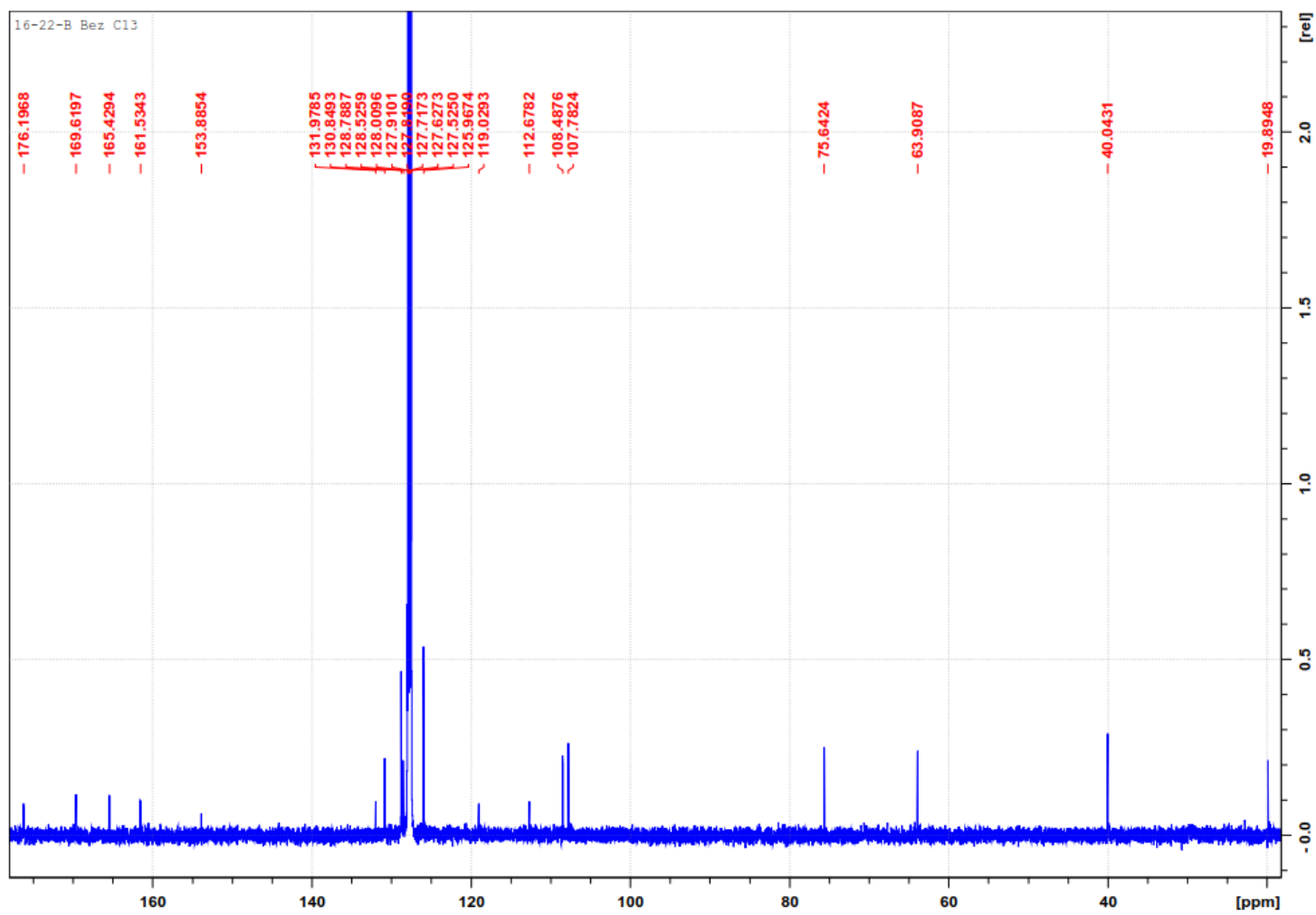


**Figure S9:**  $^1\text{H}$ NMR Spectrum of **1**  $\text{C}_6\text{D}_6$  (expansion).



**Figure S10:**  $^1\text{H}$ NMR Spectrum of **1**  $\text{C}_6\text{D}_6$  (expansion).

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**Figure S11:**  $^{13}\text{C}$ NMR Spectrum of **1**  $\text{C}_6\text{D}_6$ .

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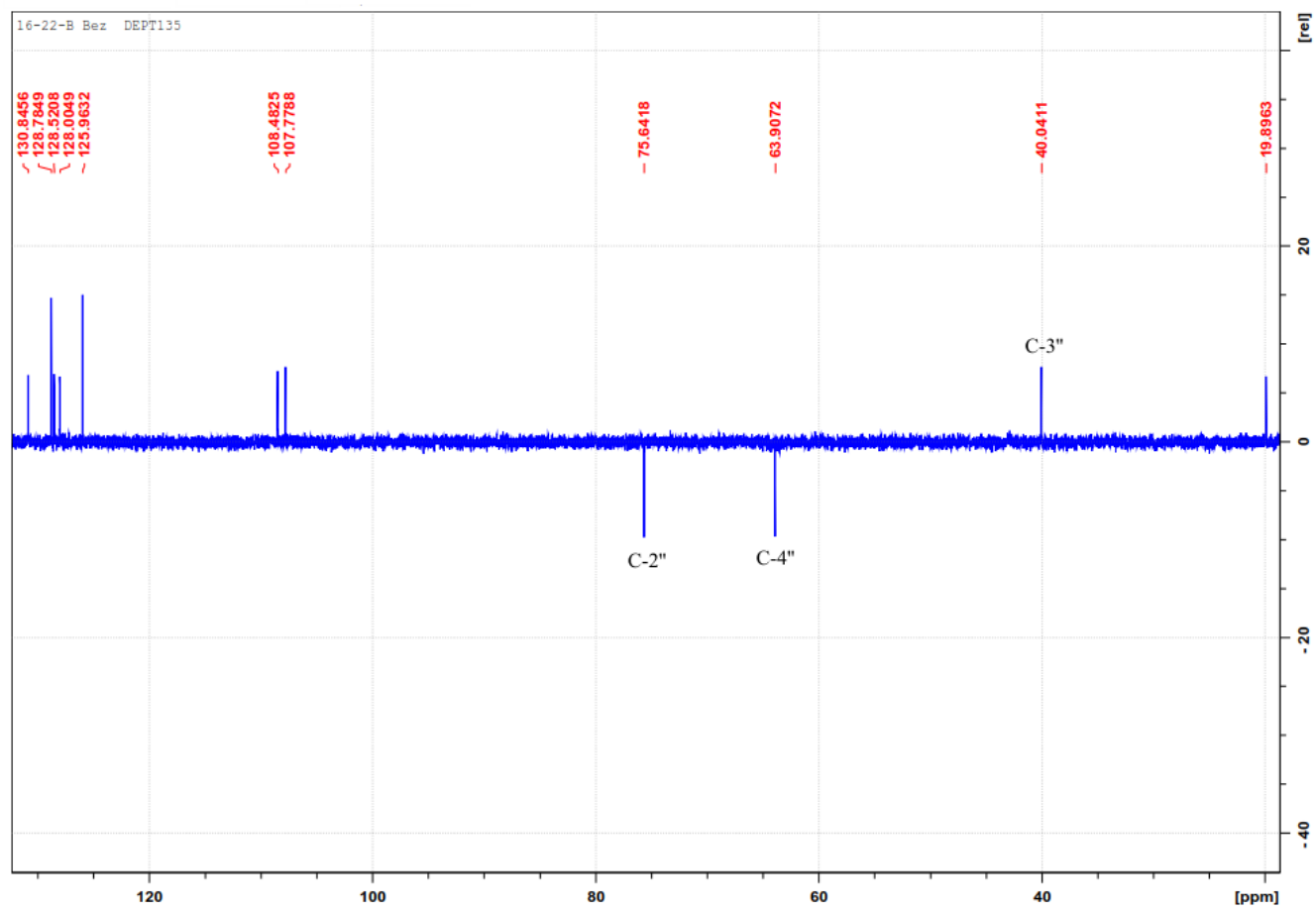
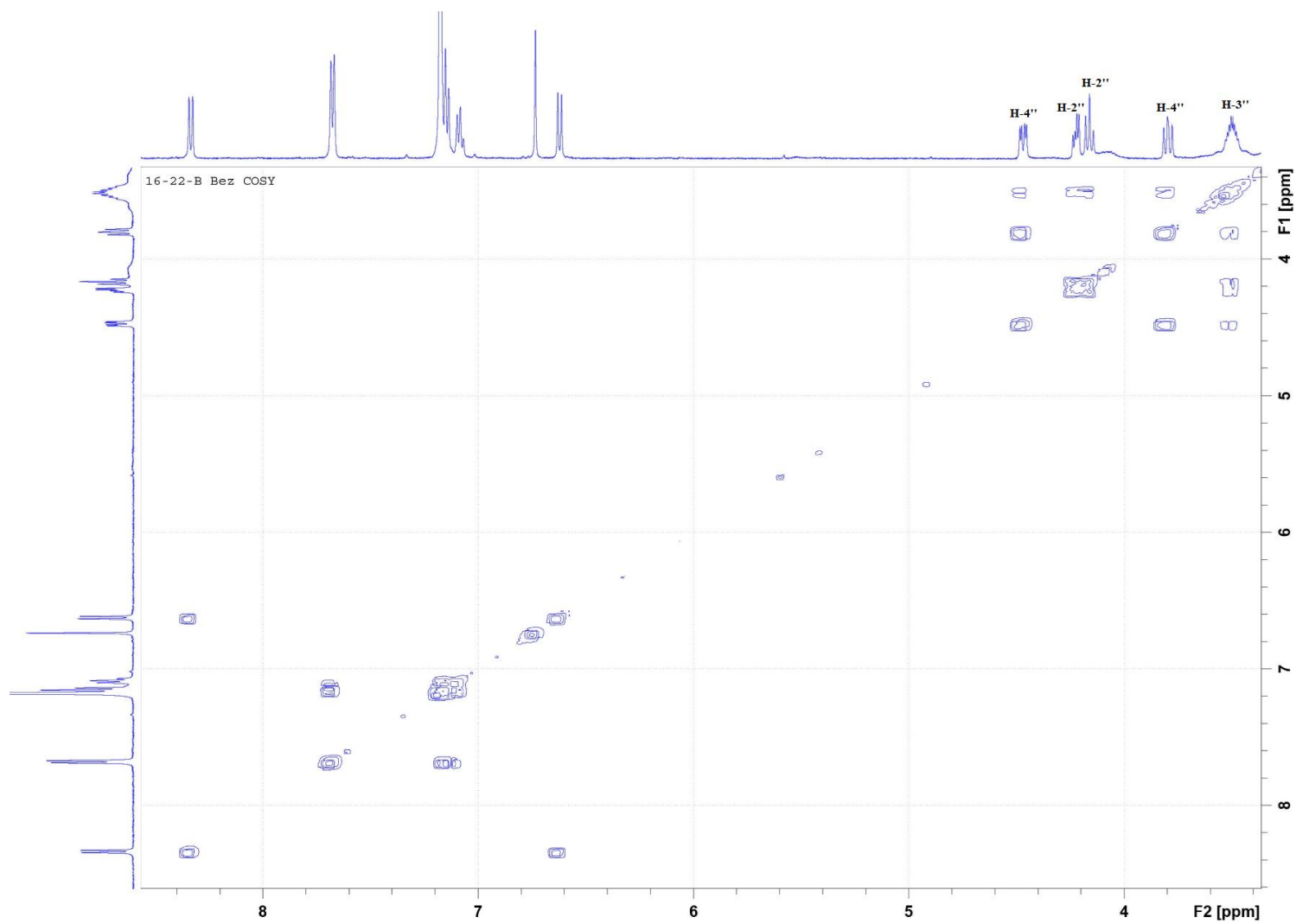


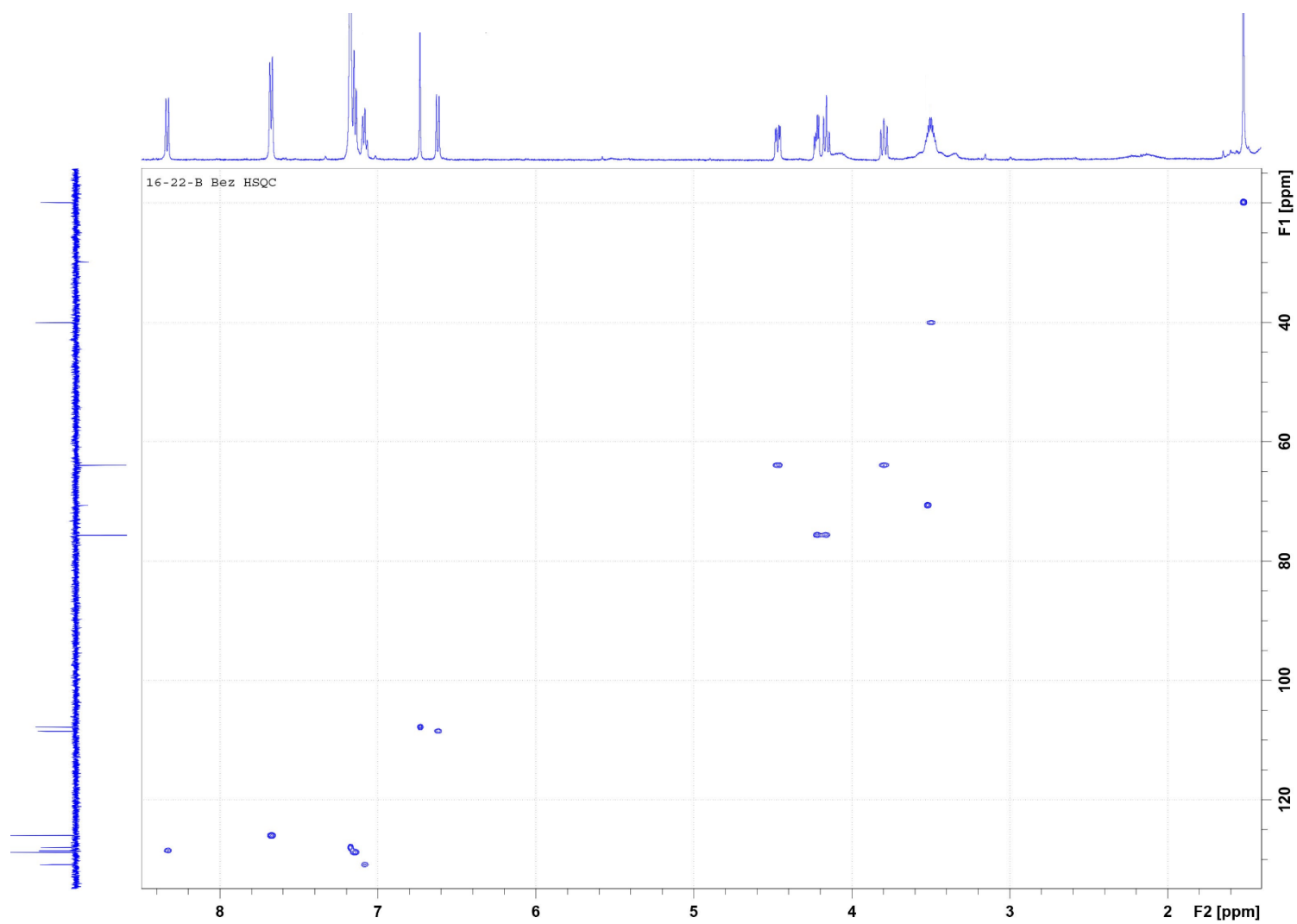
Figure S12: DEPT135 Spectrum of **1** C<sub>6</sub>D<sub>6</sub>.

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**Figure S13:** COSY Spectrum of **1** C<sub>6</sub>D<sub>6</sub>.

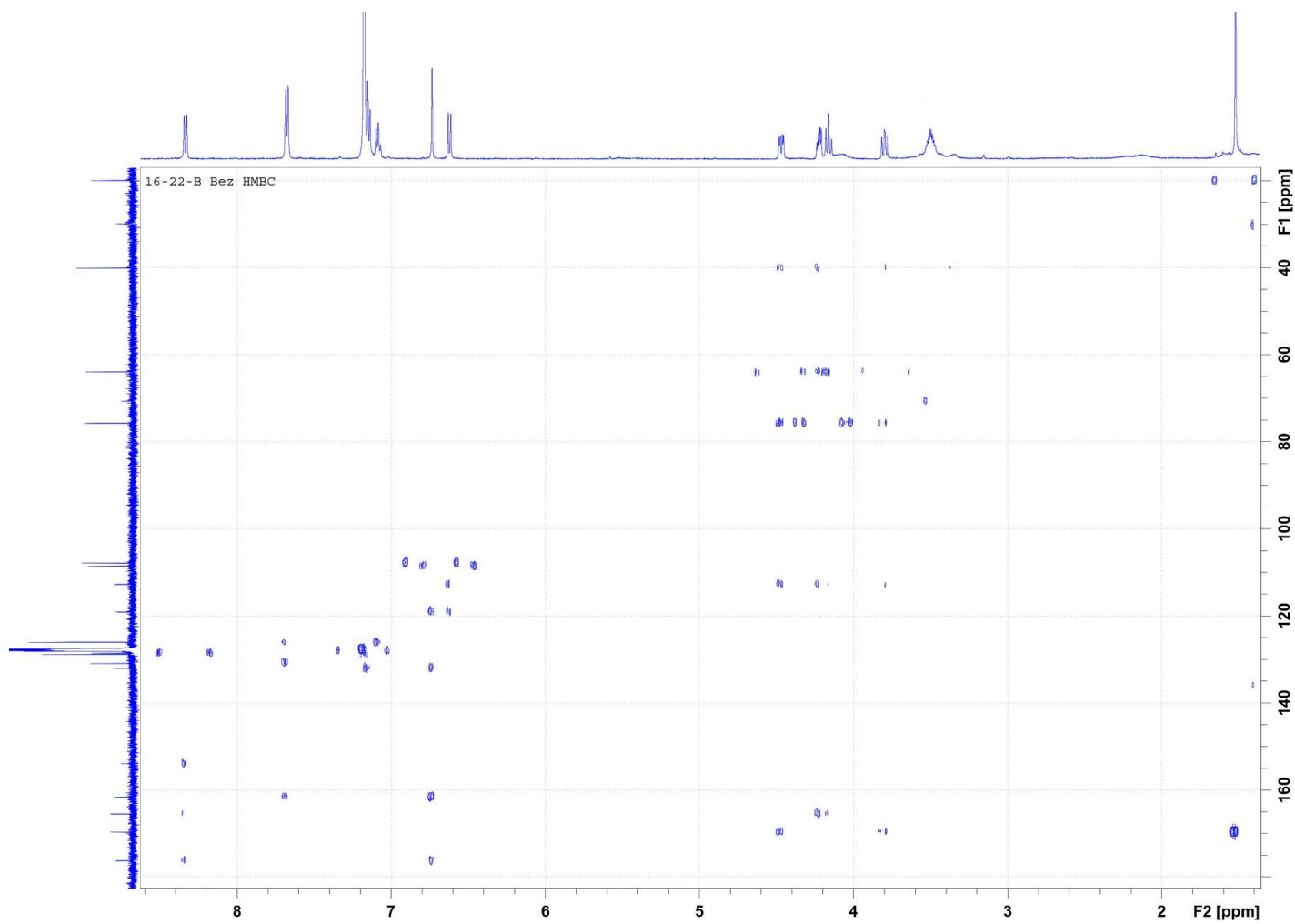
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**Figure S14:** HSQC Spectrum of **1** C<sub>6</sub>D<sub>6</sub>.

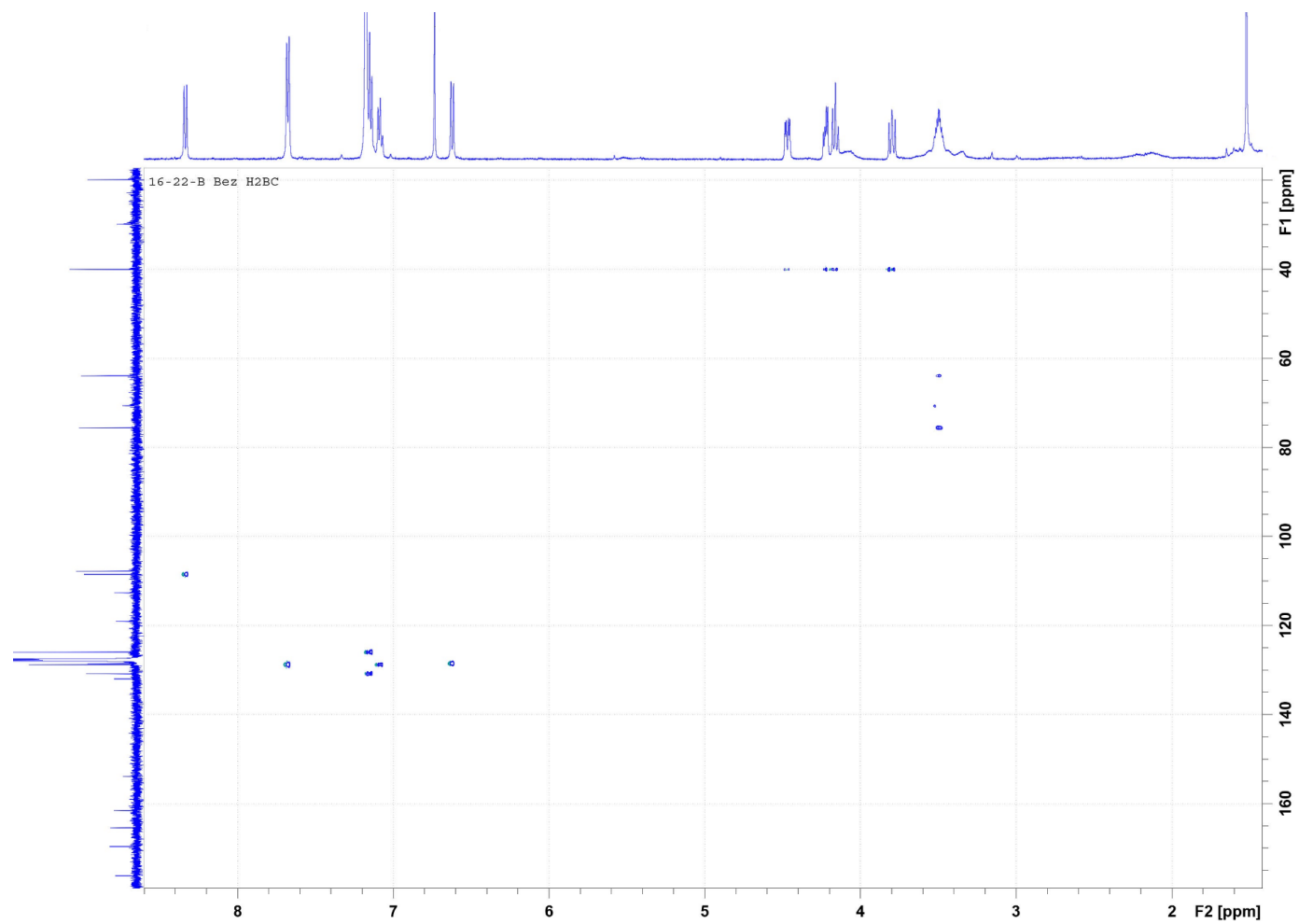
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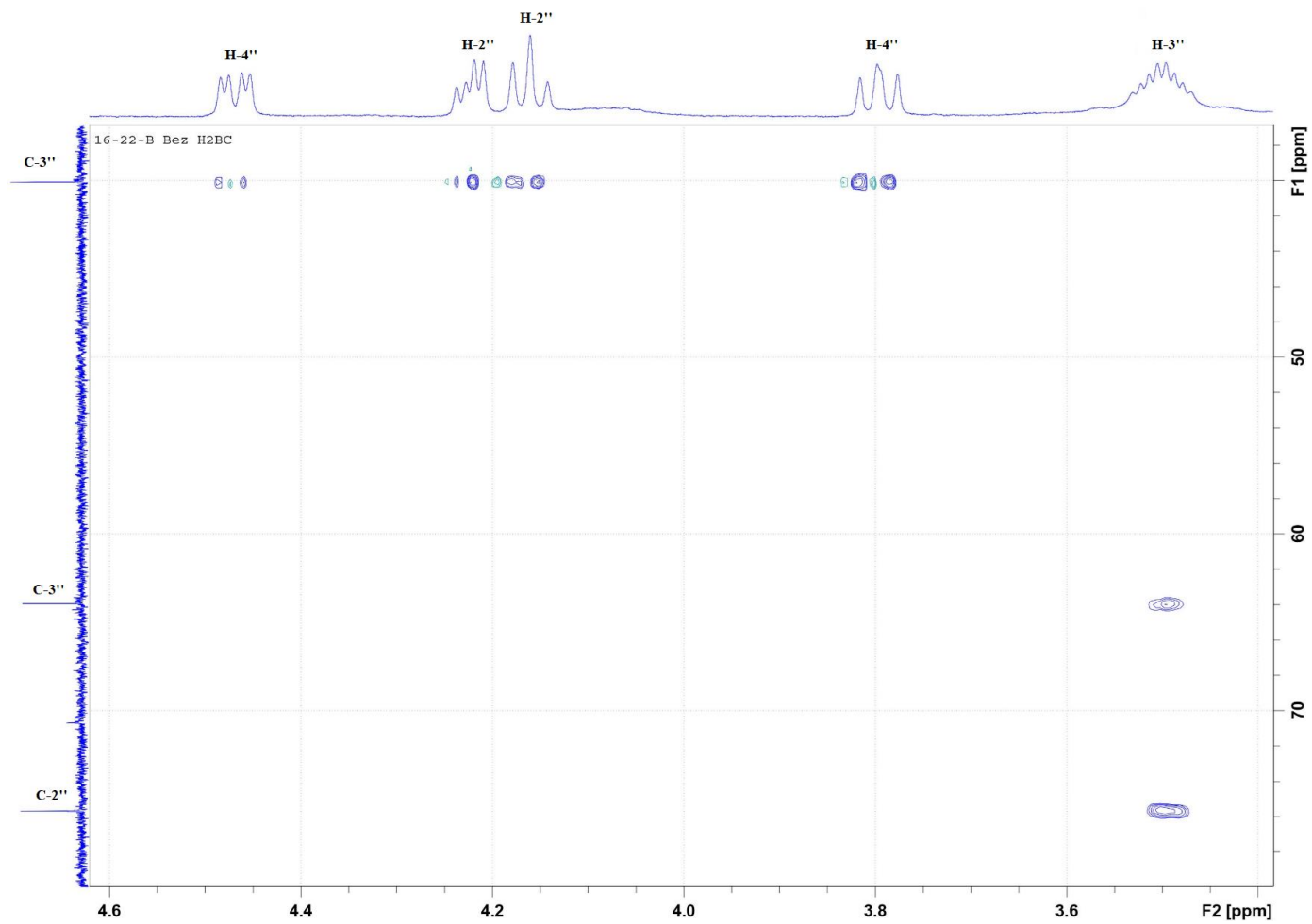
**Figure S15:** HMBC Spectrum of **1** C<sub>6</sub>D<sub>6</sub>.

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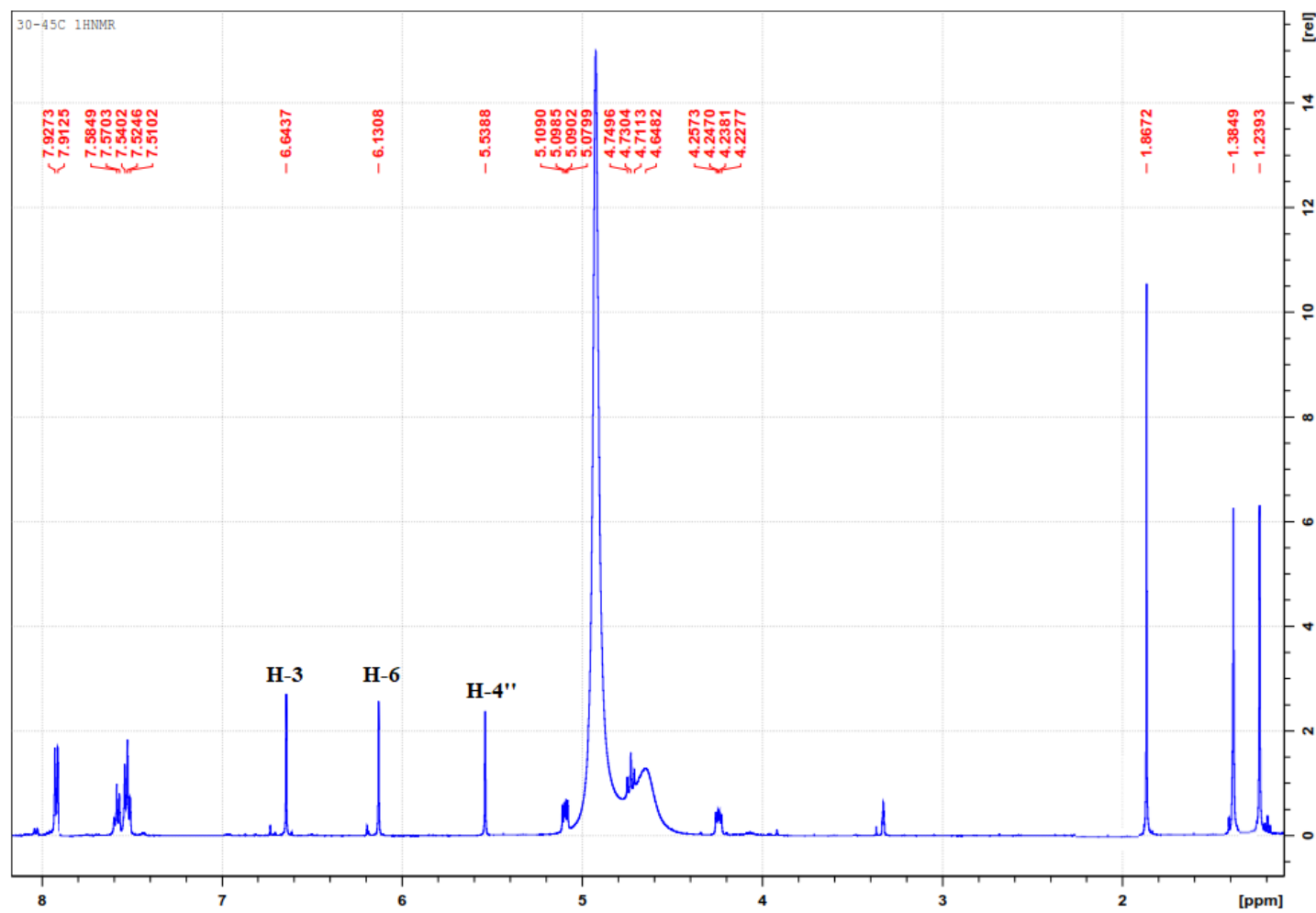
**Figure S16:** H2BC Spectrum of **1** C<sub>6</sub>D<sub>6</sub>.

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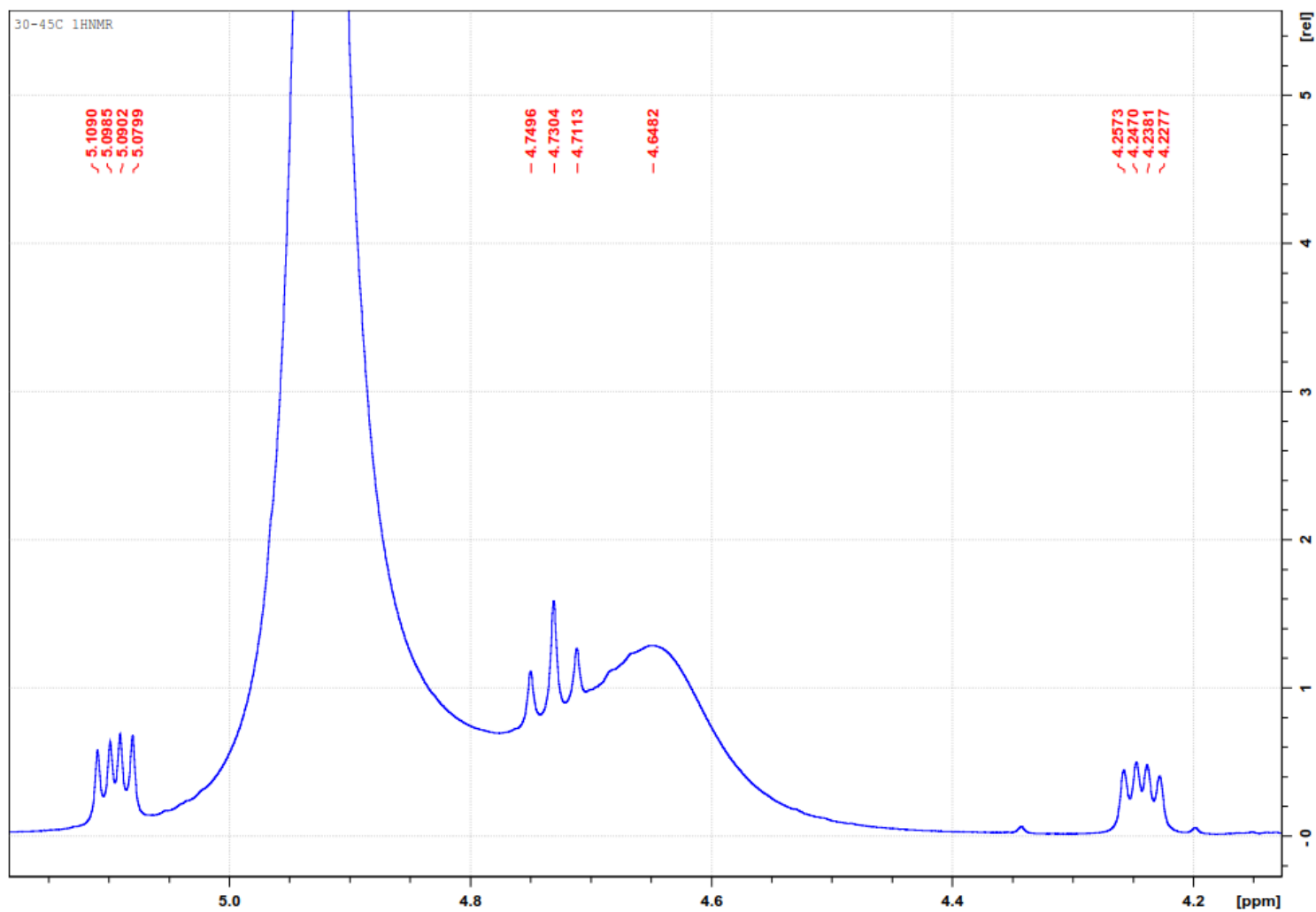
**Figure S17:** H2BC Spectrum of **1** C<sub>6</sub>D<sub>6</sub> (expansion).

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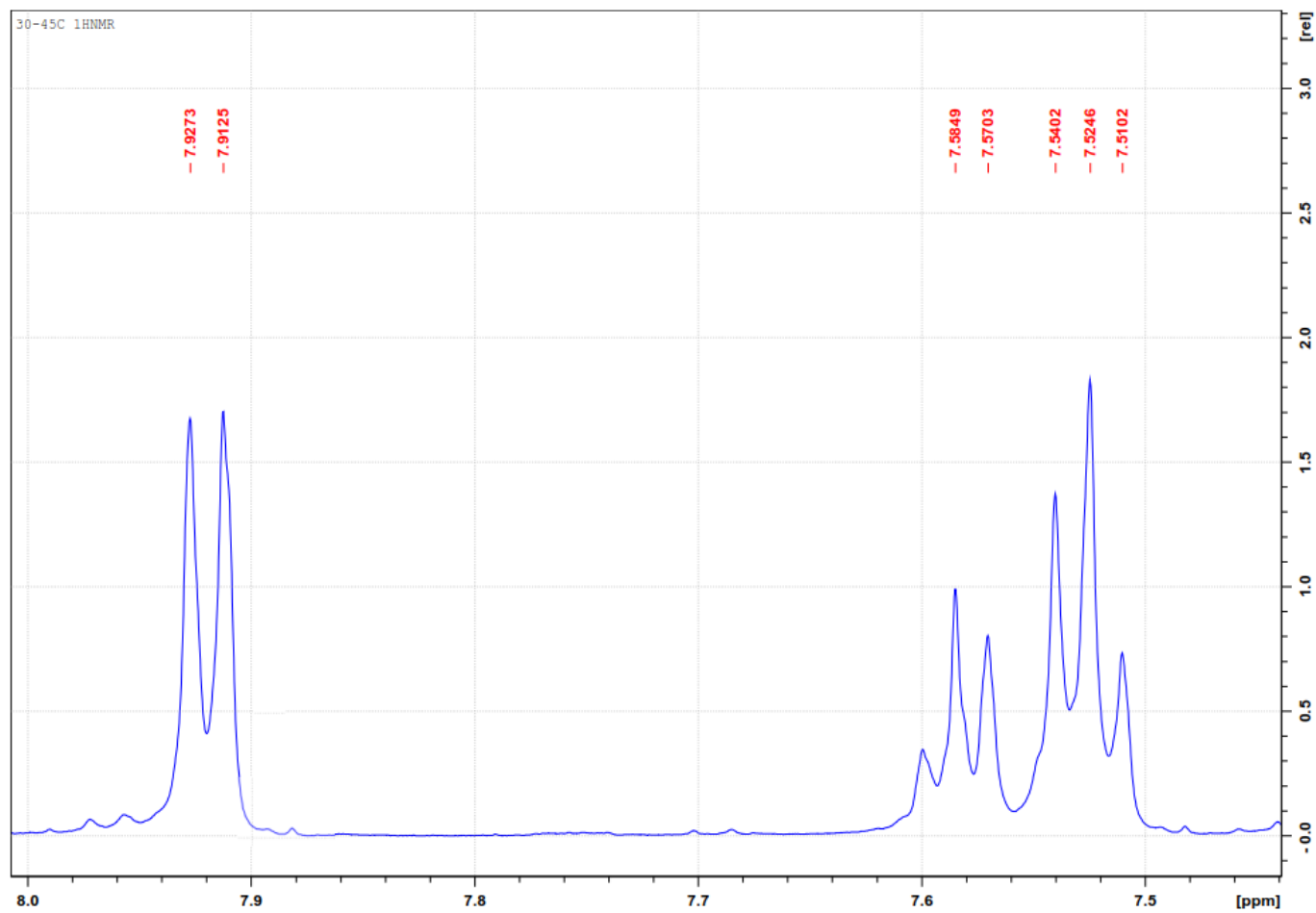


**Figure S18:**  $^1\text{H}$ NMR Spectrum of **2** in  $\text{CD}_3\text{OD}$

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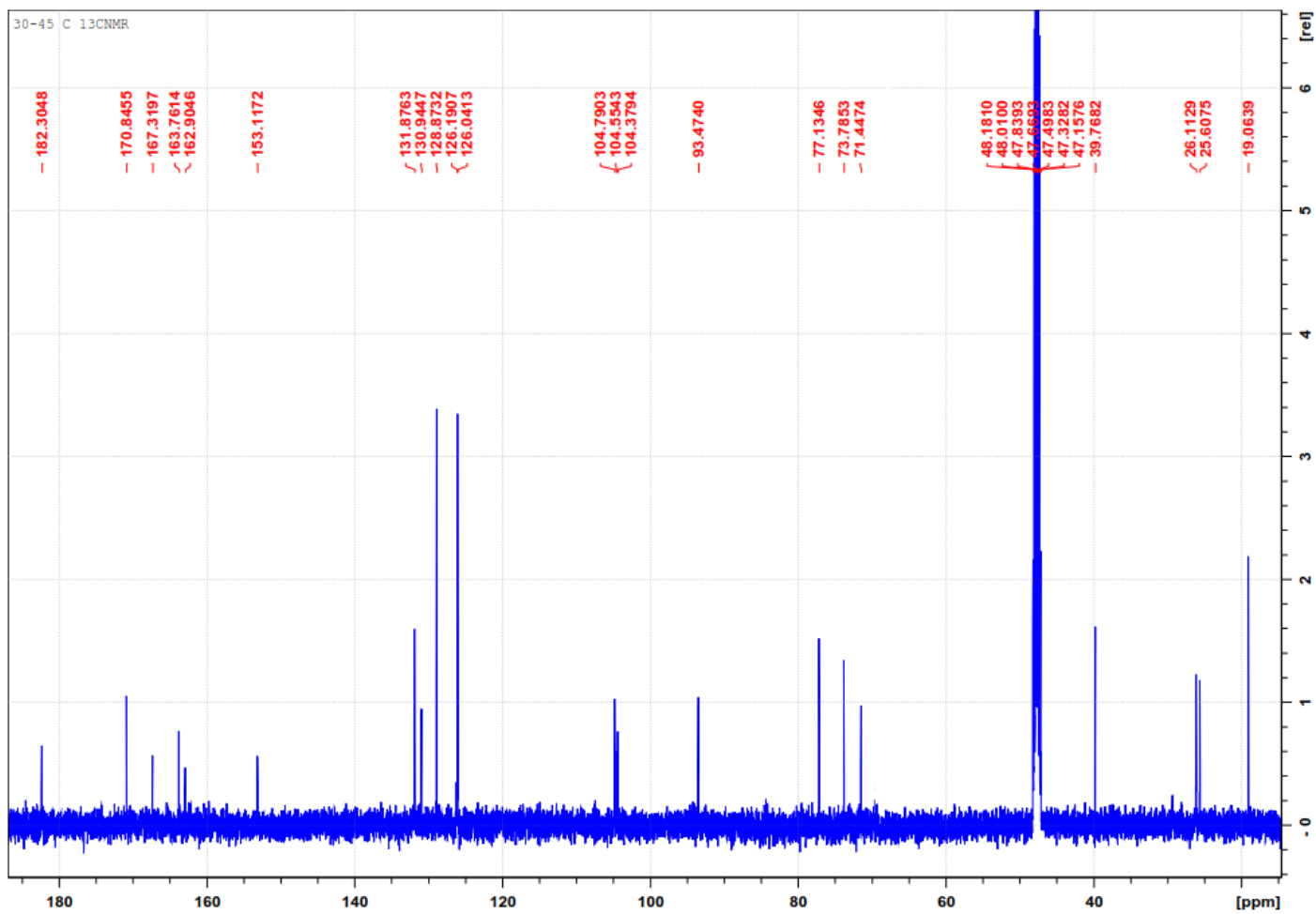


**Figure S19:**  $^1\text{H}$ NMR Spectrum of **2** in  $\text{CD}_3\text{OD}$  (expansion).



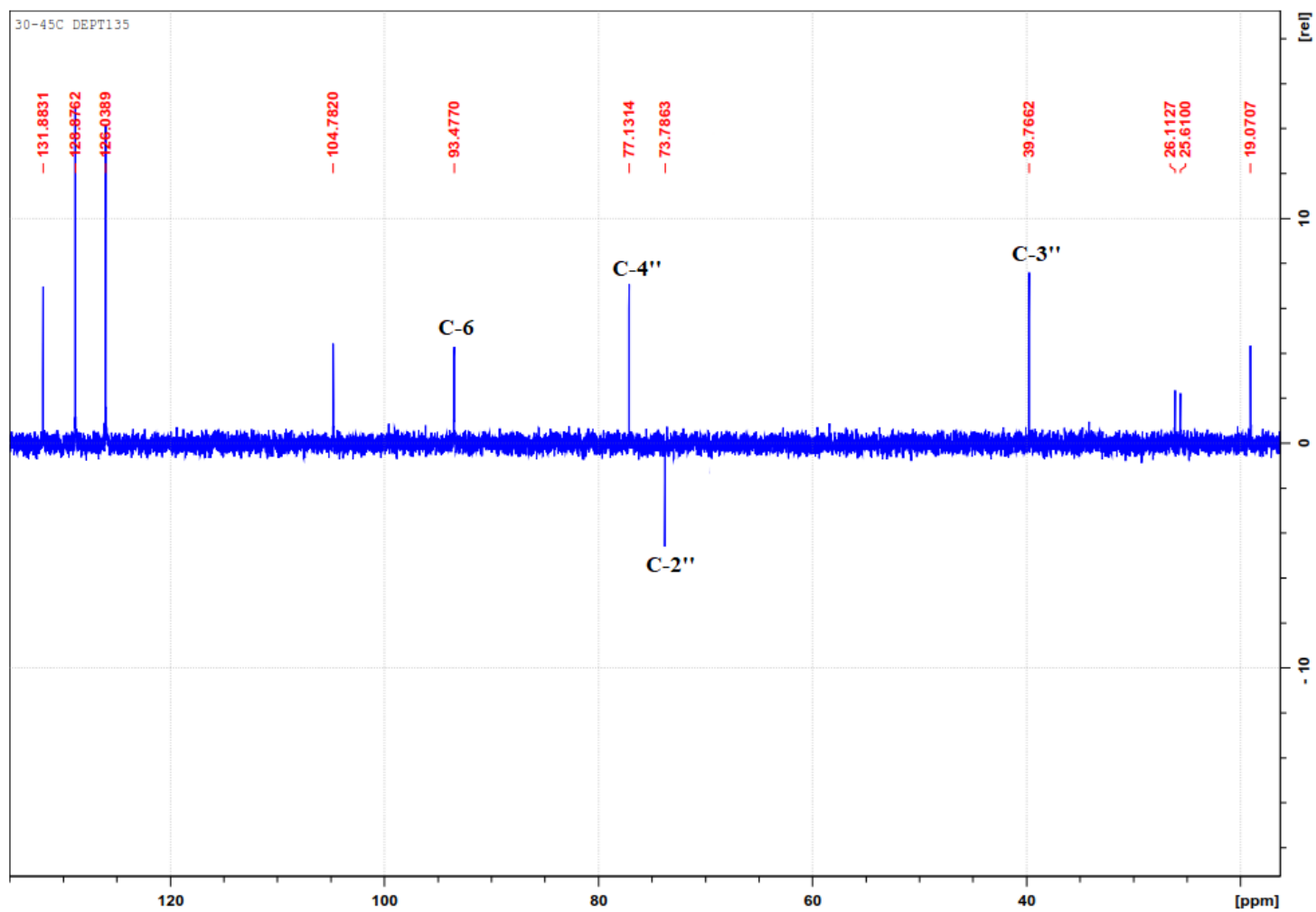
**Figure S20:**  $^1\text{H}$ NMR Spectrum of **2** in  $\text{CD}_3\text{OD}$  (expansion).

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**Figure S21:**  $^{13}\text{C}$ NMR Spectrum of **2** in  $\text{CD}_3\text{OD}$ .

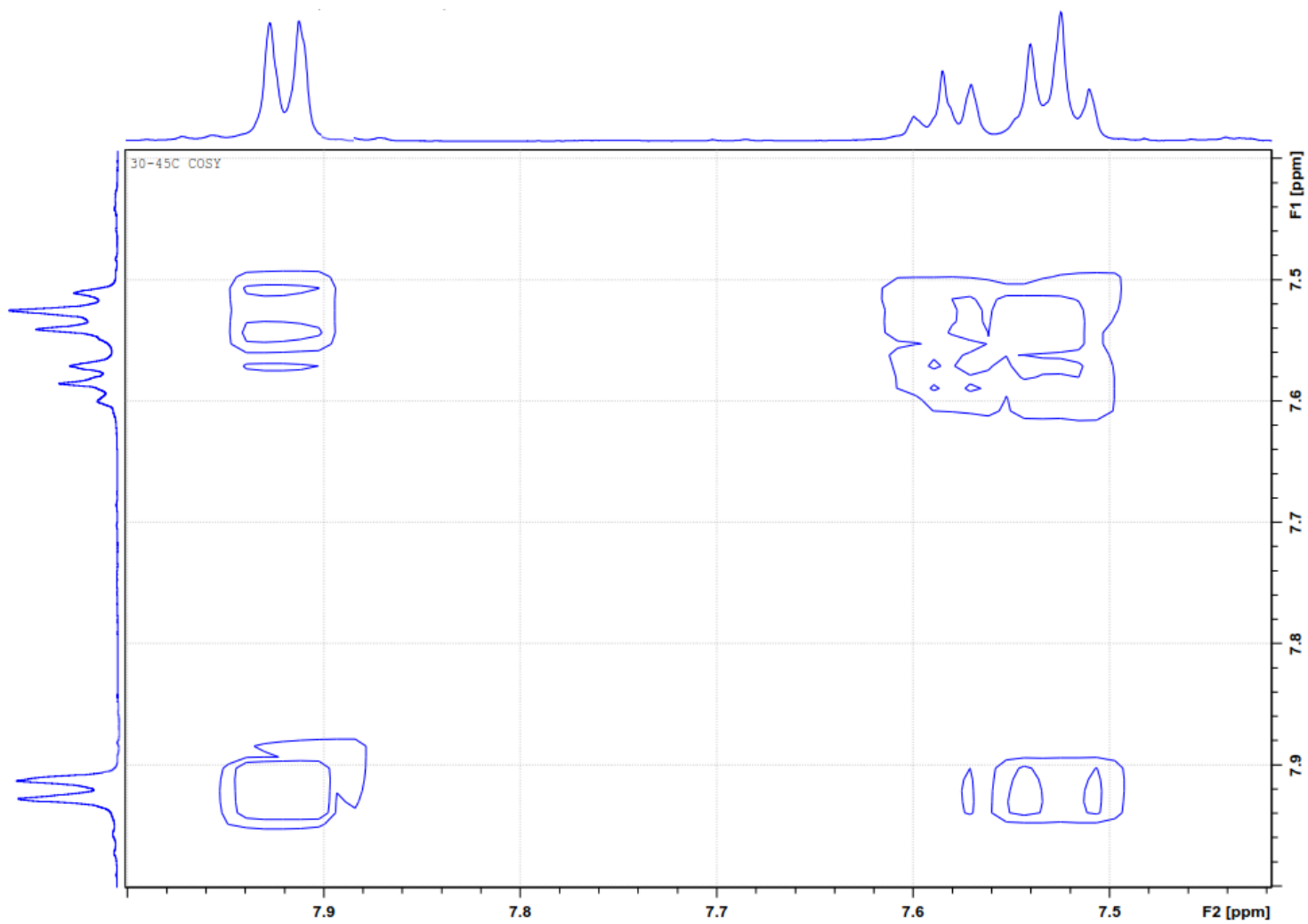
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**Figure S22:** DEPT135 Spectrum of **2** in CD<sub>3</sub>OD.

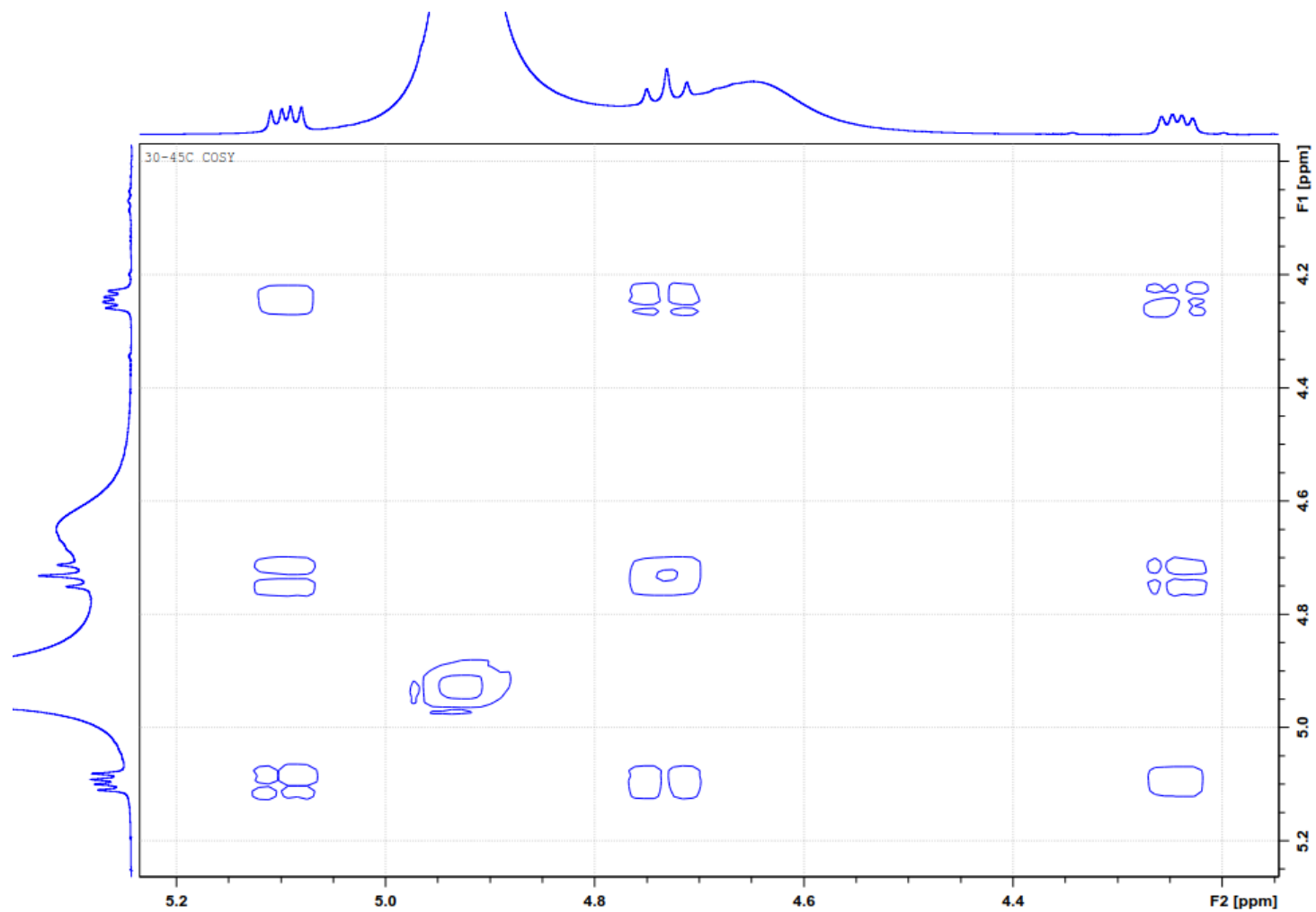
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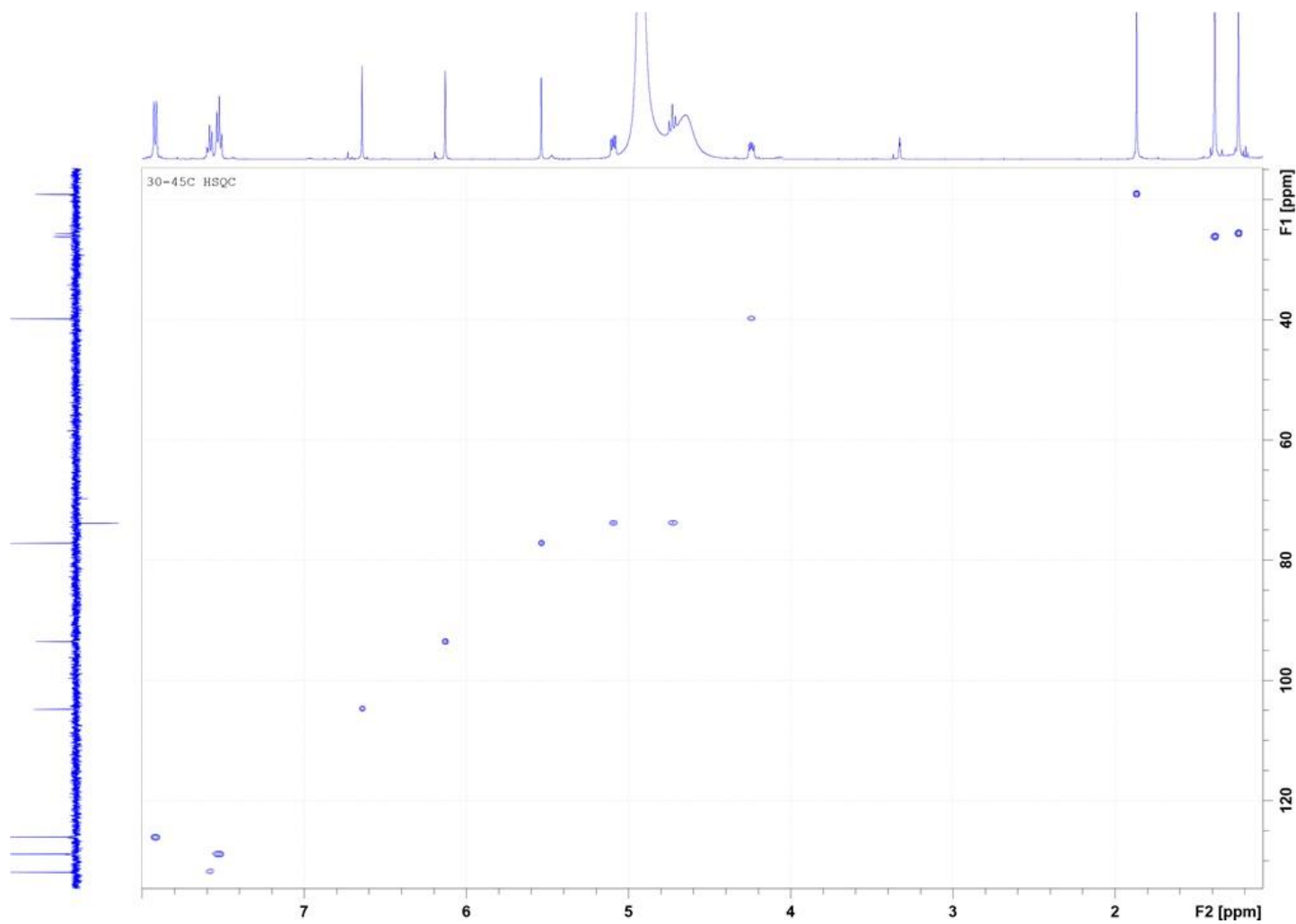


**Figure S23:** COSY Spectrum of **2** in CD<sub>3</sub>OD (expansion).

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**Figure S24:** COSY Spectrum of **2** in CD<sub>3</sub>OD (expansion).



**Figure S25:** HSQC Spectrum of **2** in CD<sub>3</sub>OD.

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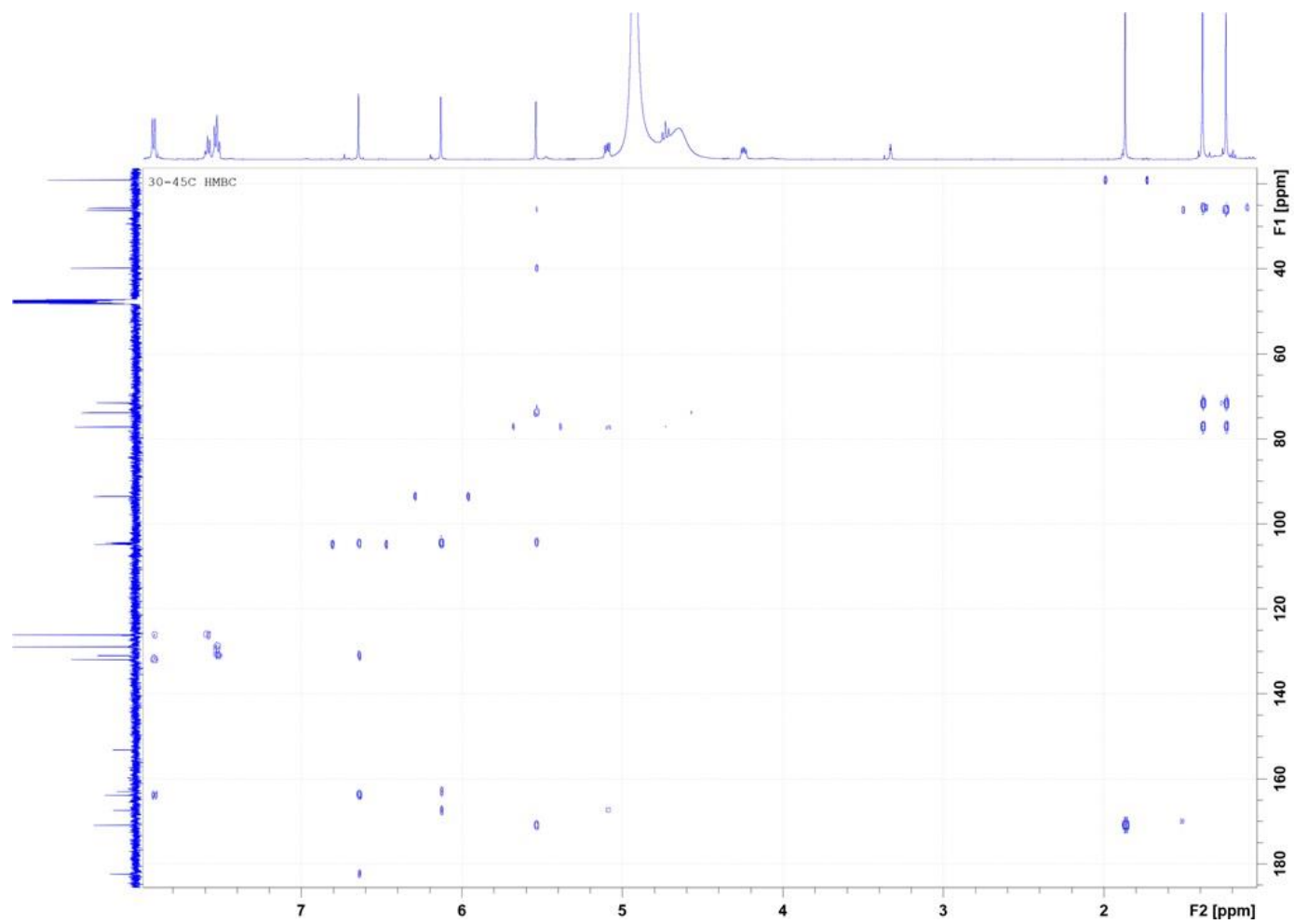


Figure S26: HMBC Spectrum of 2 in CD<sub>3</sub>OD.

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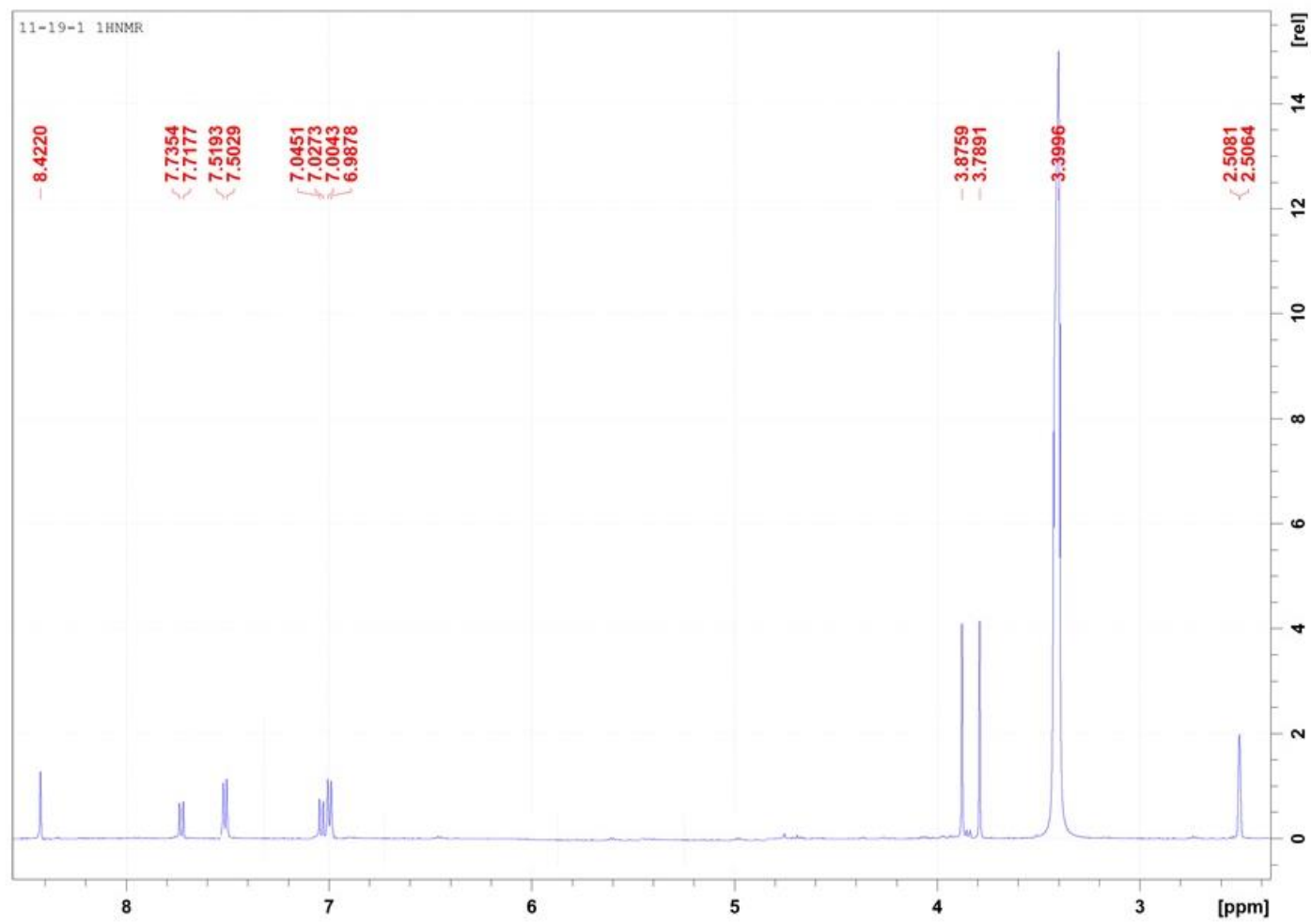
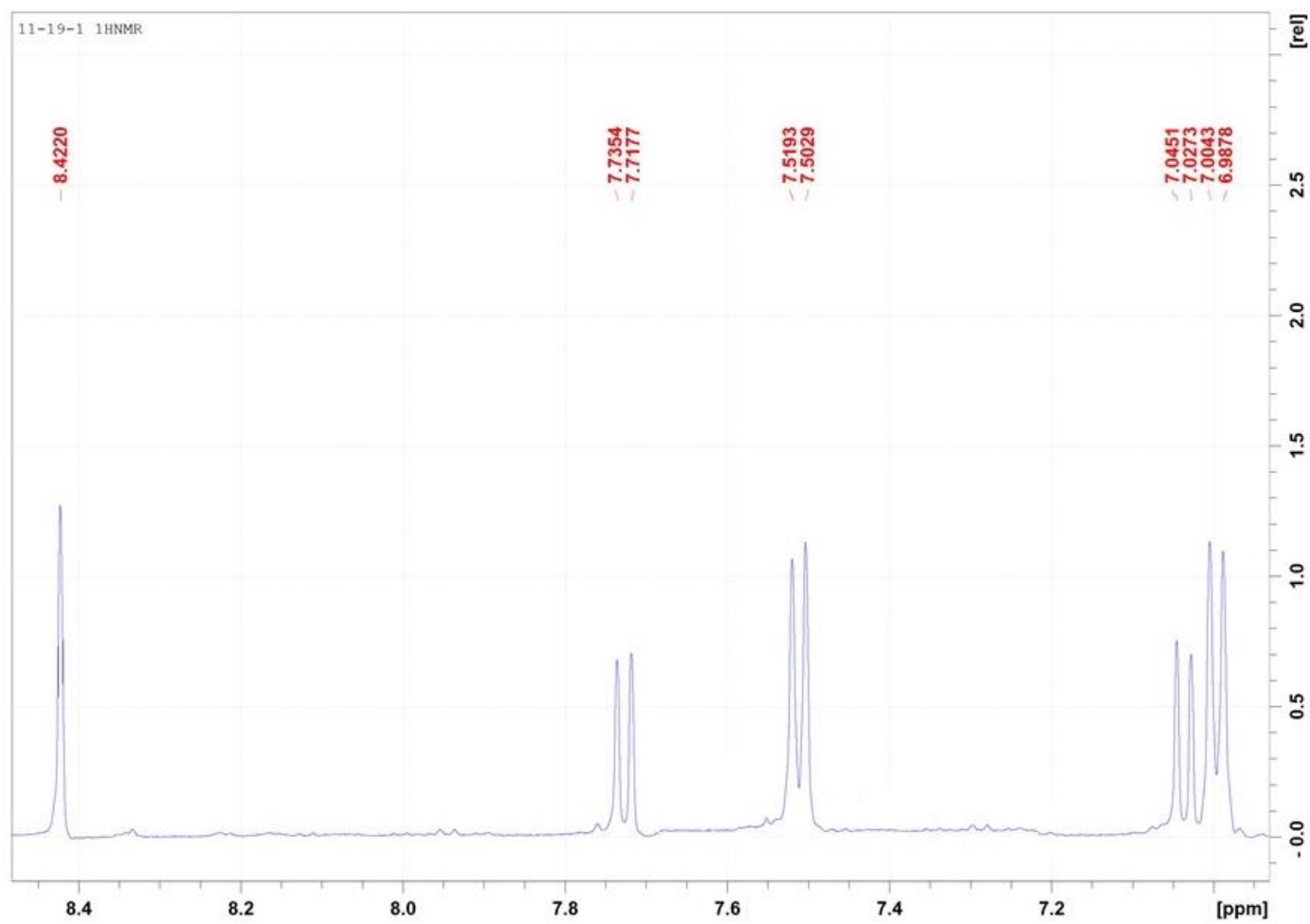


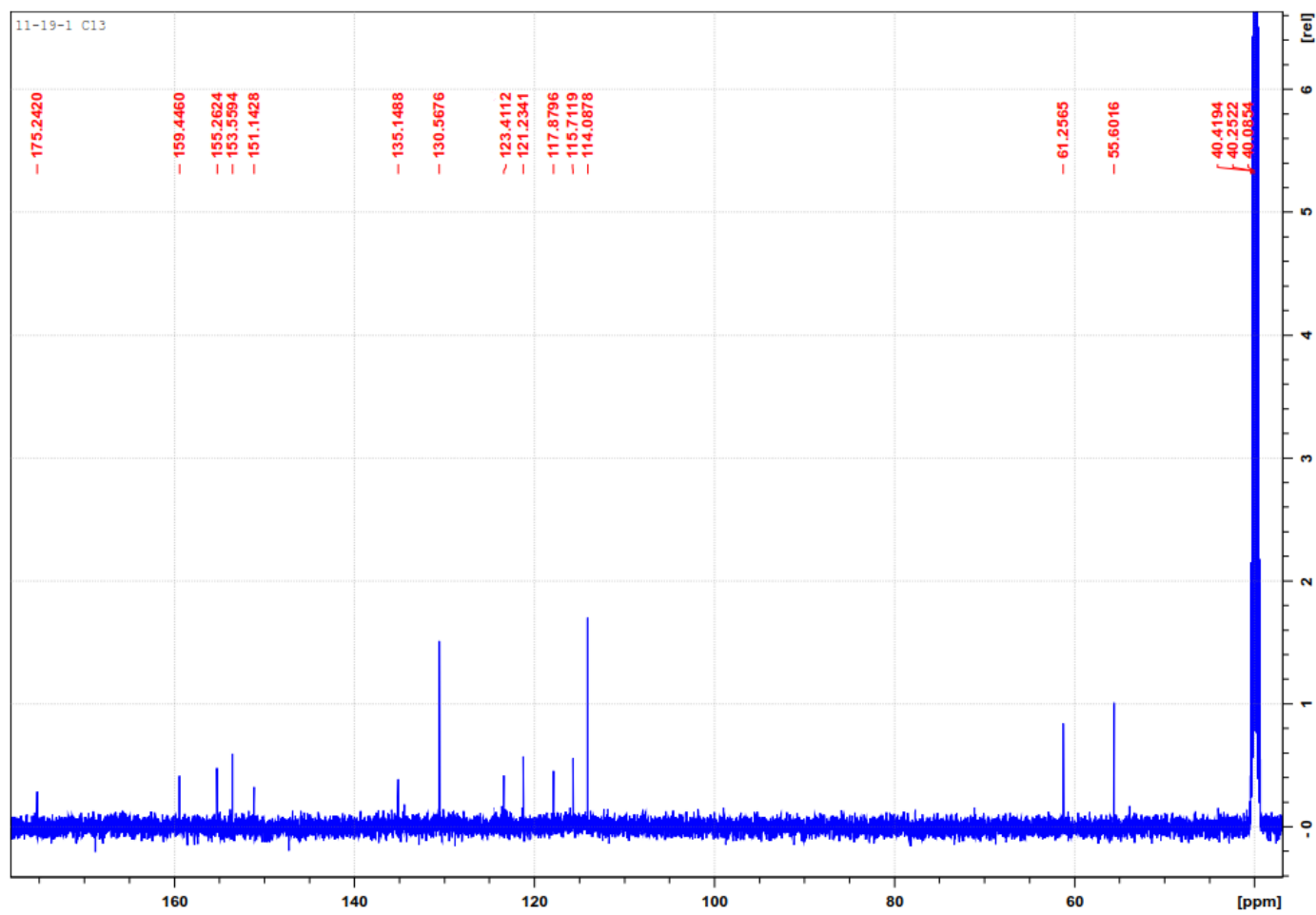
Figure S27: <sup>1</sup>H NMR Spectrum of **3** in DMSO.

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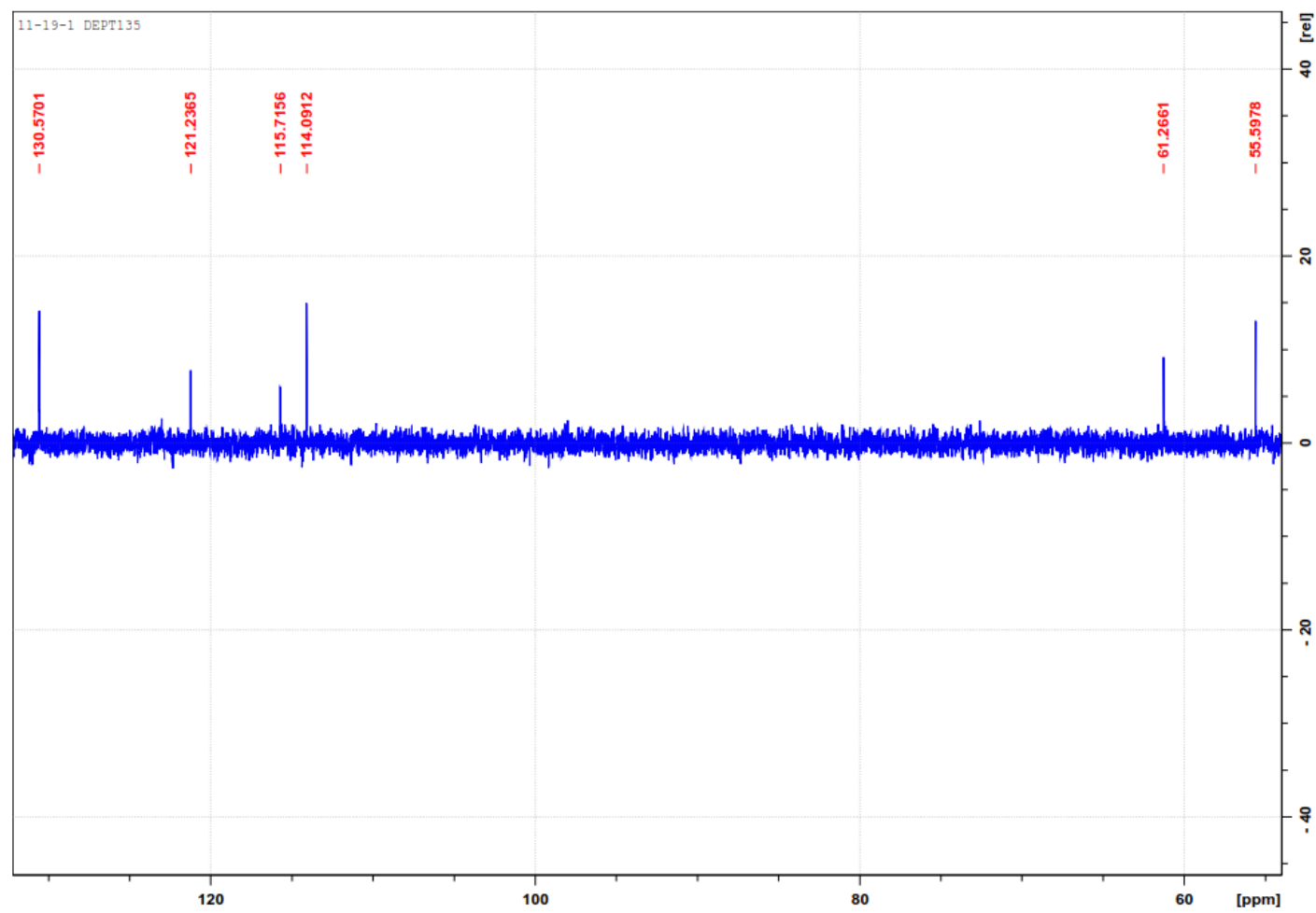
**Figure S28:** <sup>1</sup>H NMR Spectrum of **3** in DMSO.

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**Figure S29:**  $^{13}\text{C}$ NMR Spectrum of **3** in DMSO.

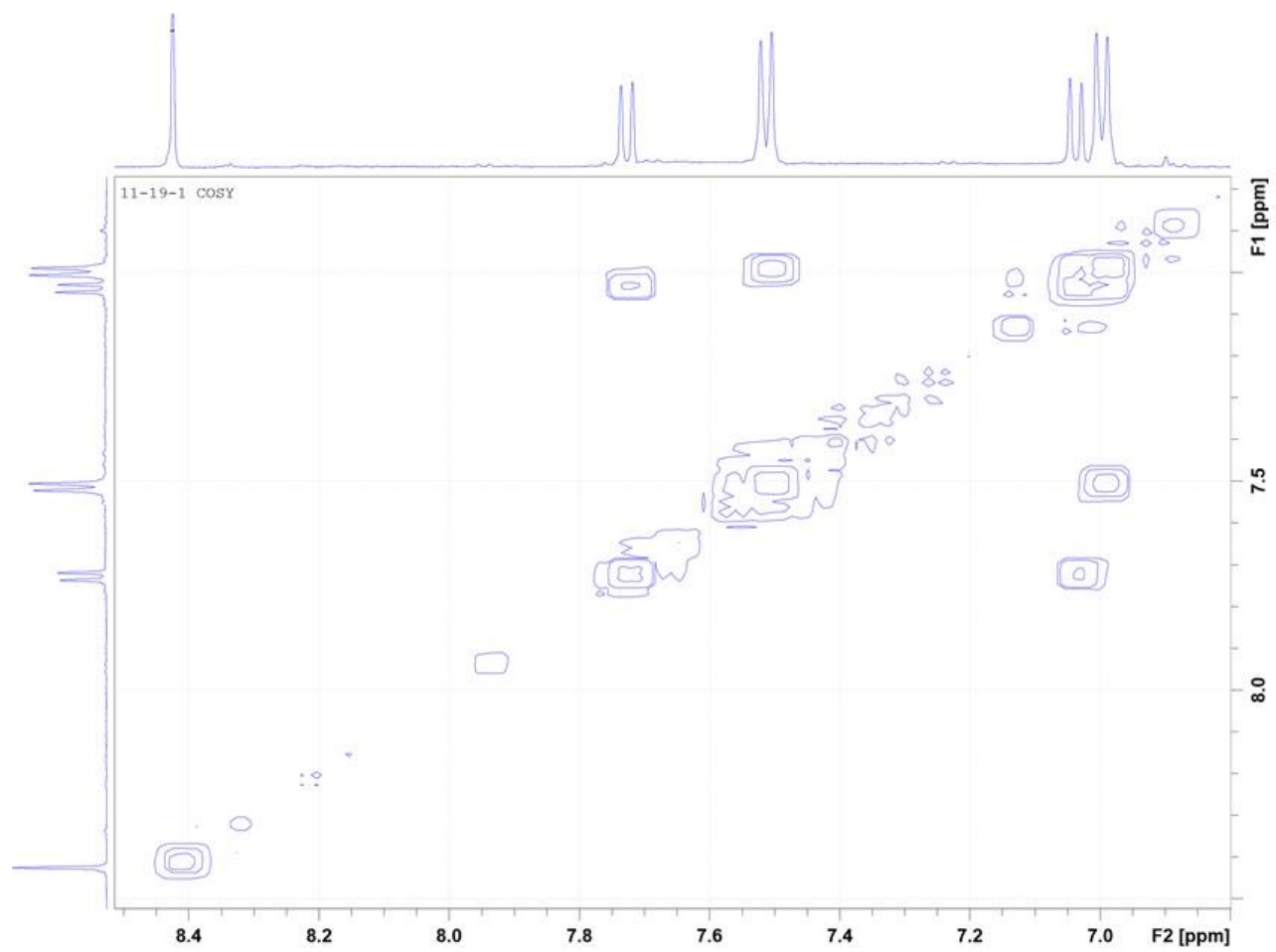
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**Figure S30:** DEPT135 Spectrum of **3** in DMSO.

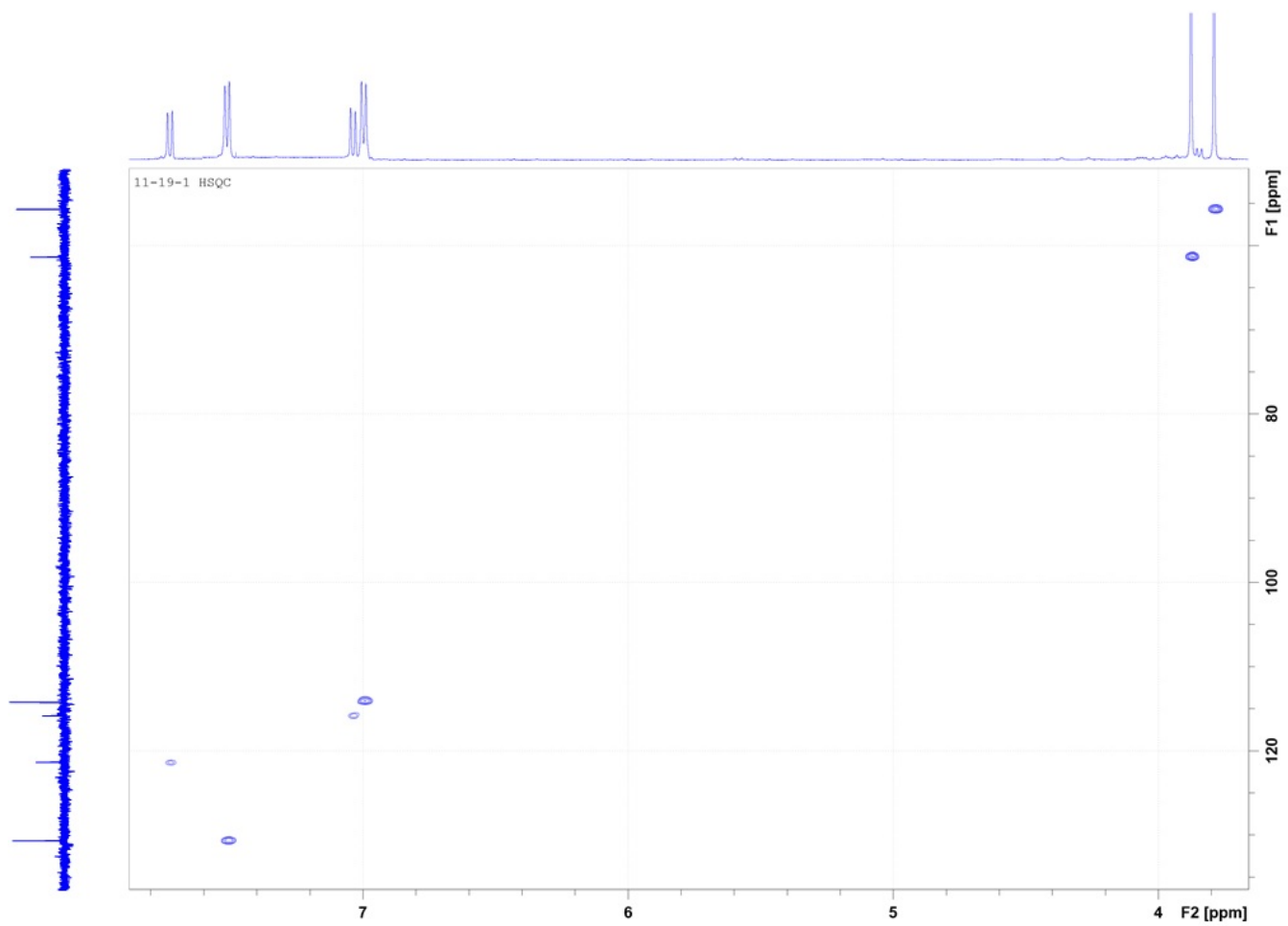
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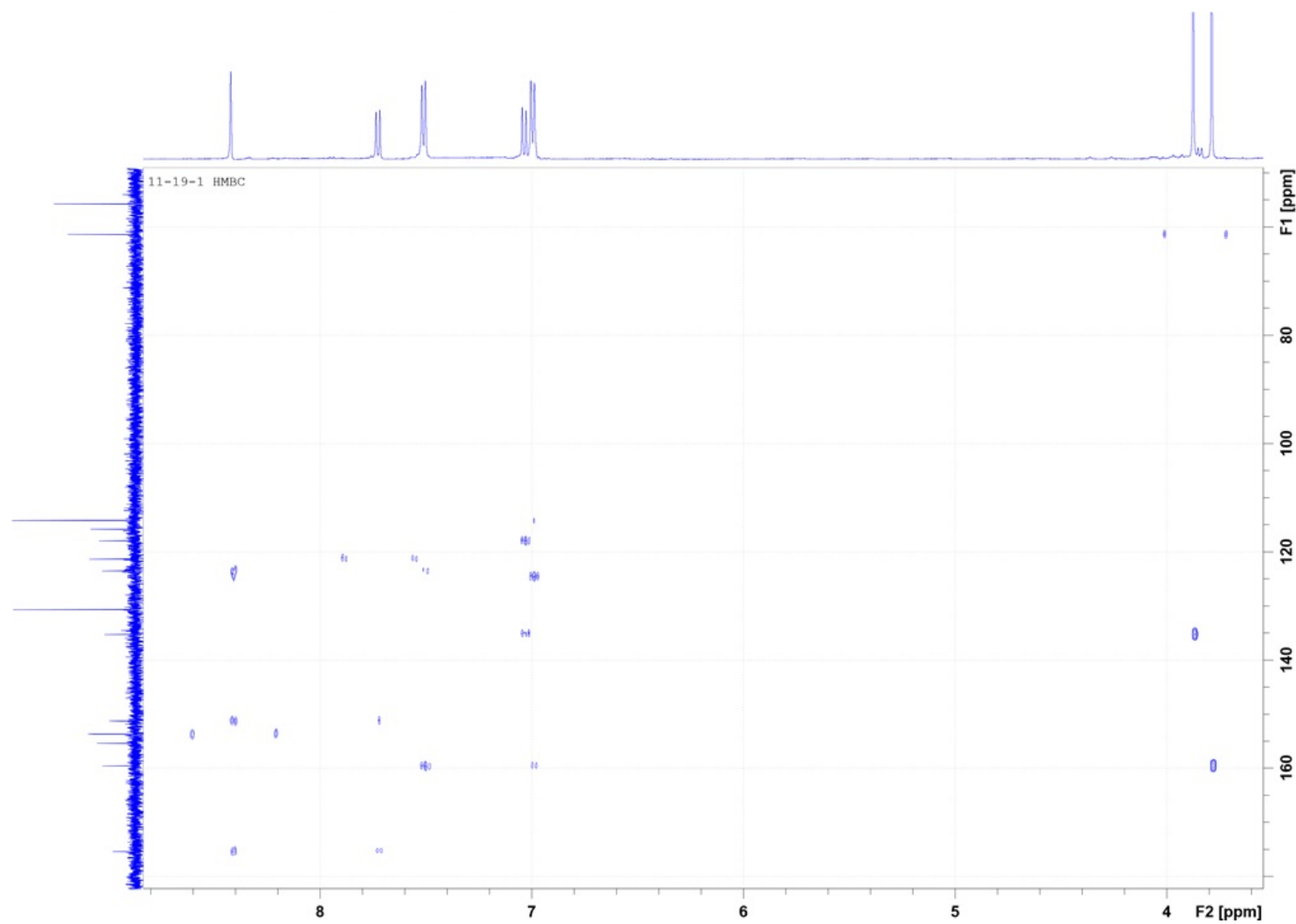
**Figure S31:** COSY Spectrum of **3** in DMSO.

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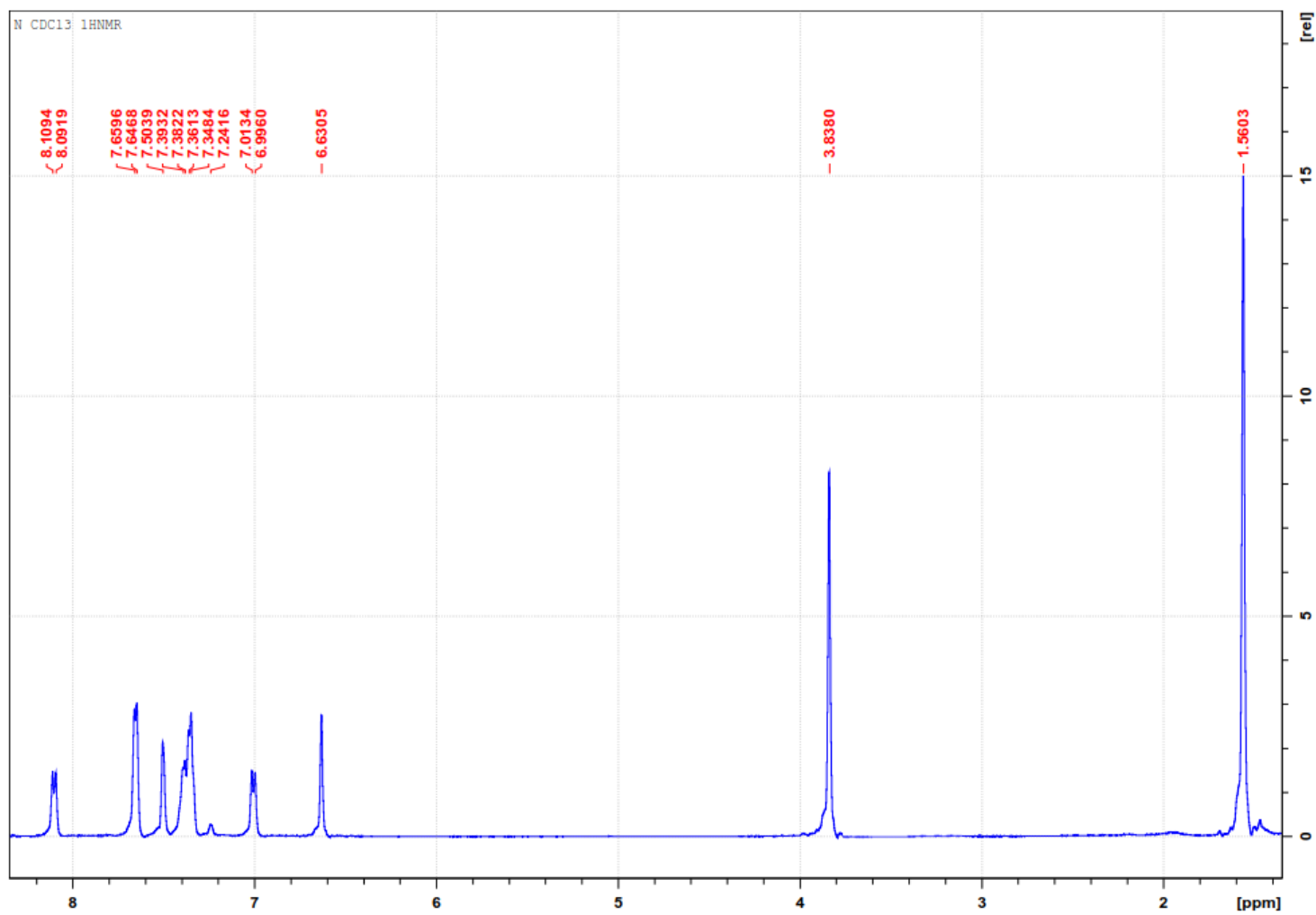
**Figure S32:** HSQC Spectrum of **3** in DMSO.

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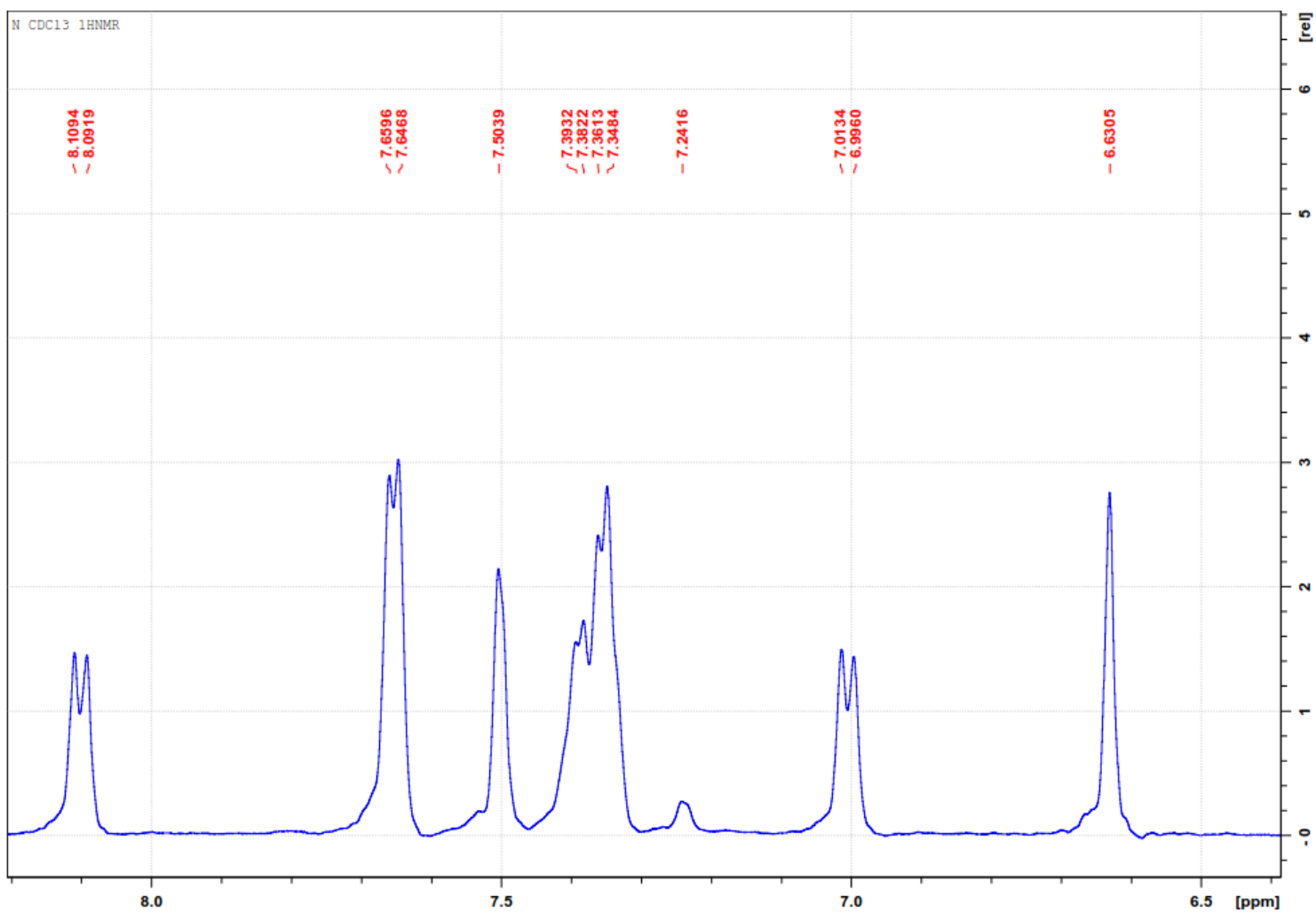
**Figure S33:** HMBC Spectrum of **3** in DMSO.

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**Figure S34:**  $^1\text{H}$ NMR Spectrum of **4** in  $\text{CDCl}_3$ .

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**Figure S35:**  $^1\text{H}$ NMR Spectrum of **4** in  $\text{CDCl}_3$  (expansion).

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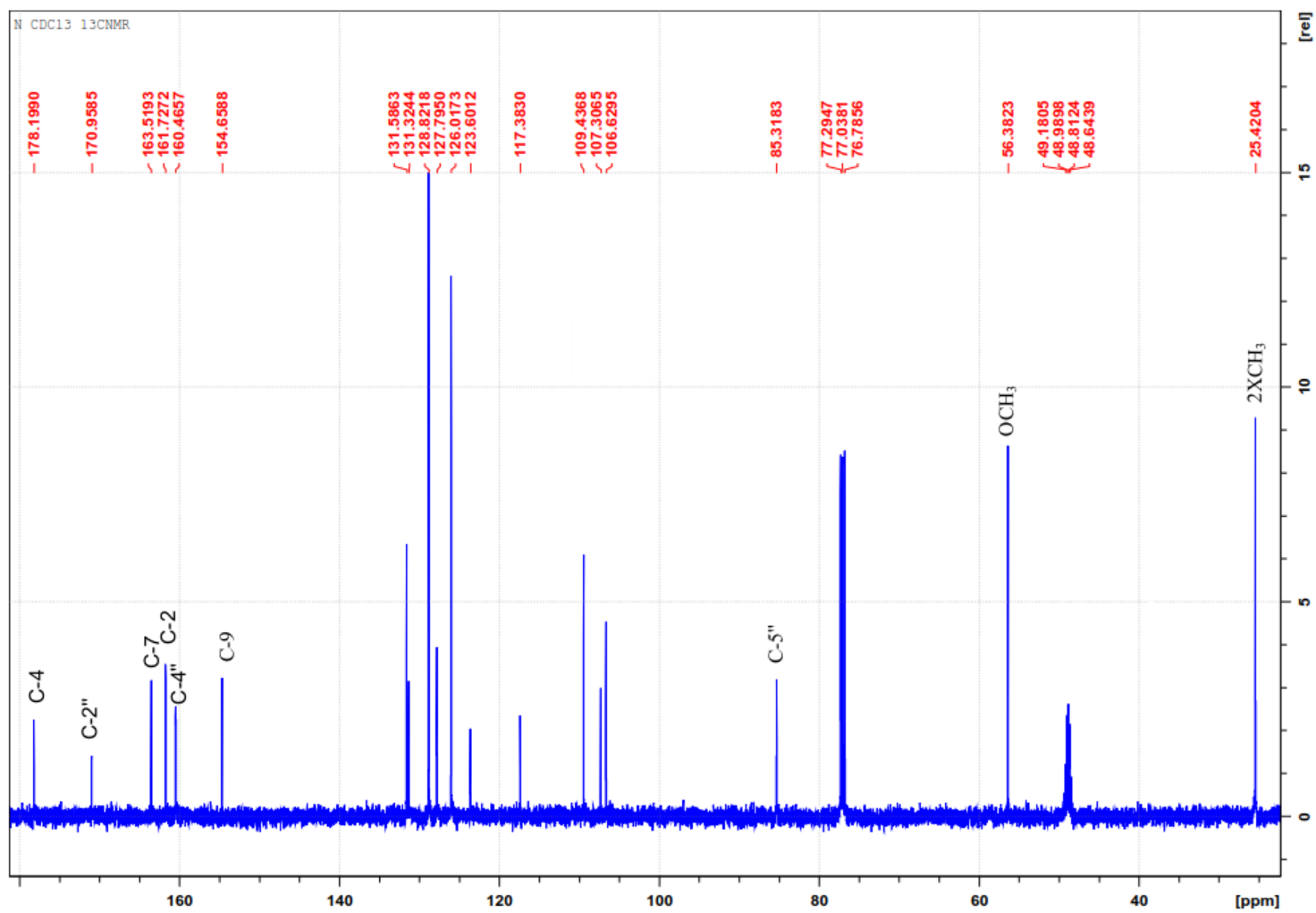
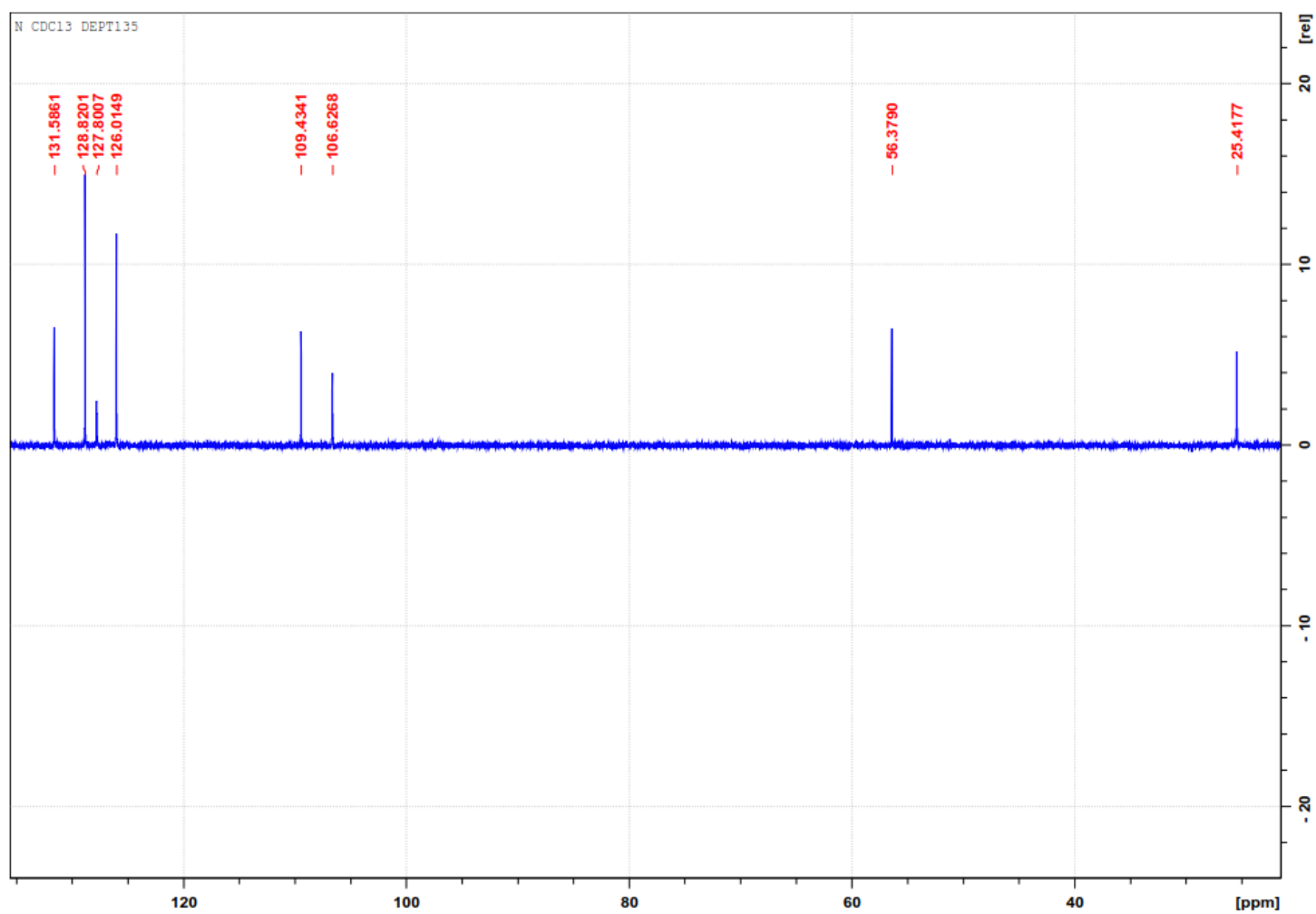


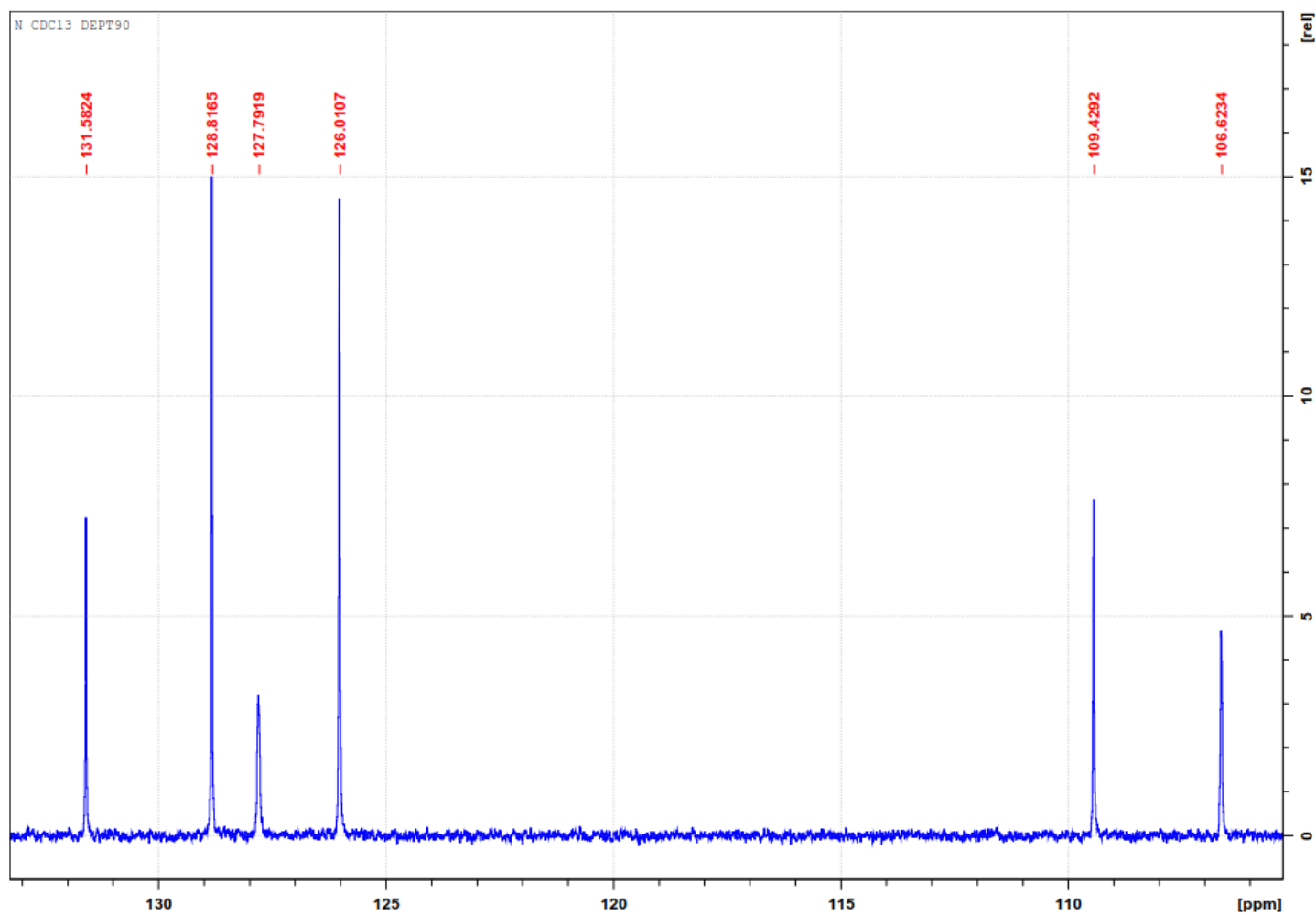
Figure S36: <sup>13</sup>CNMR Spectrum of **4** in CDCl<sub>3</sub>.

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**Figure S37:** DEPT135 Spectrum of **4** in  $\text{CDCl}_3$ .

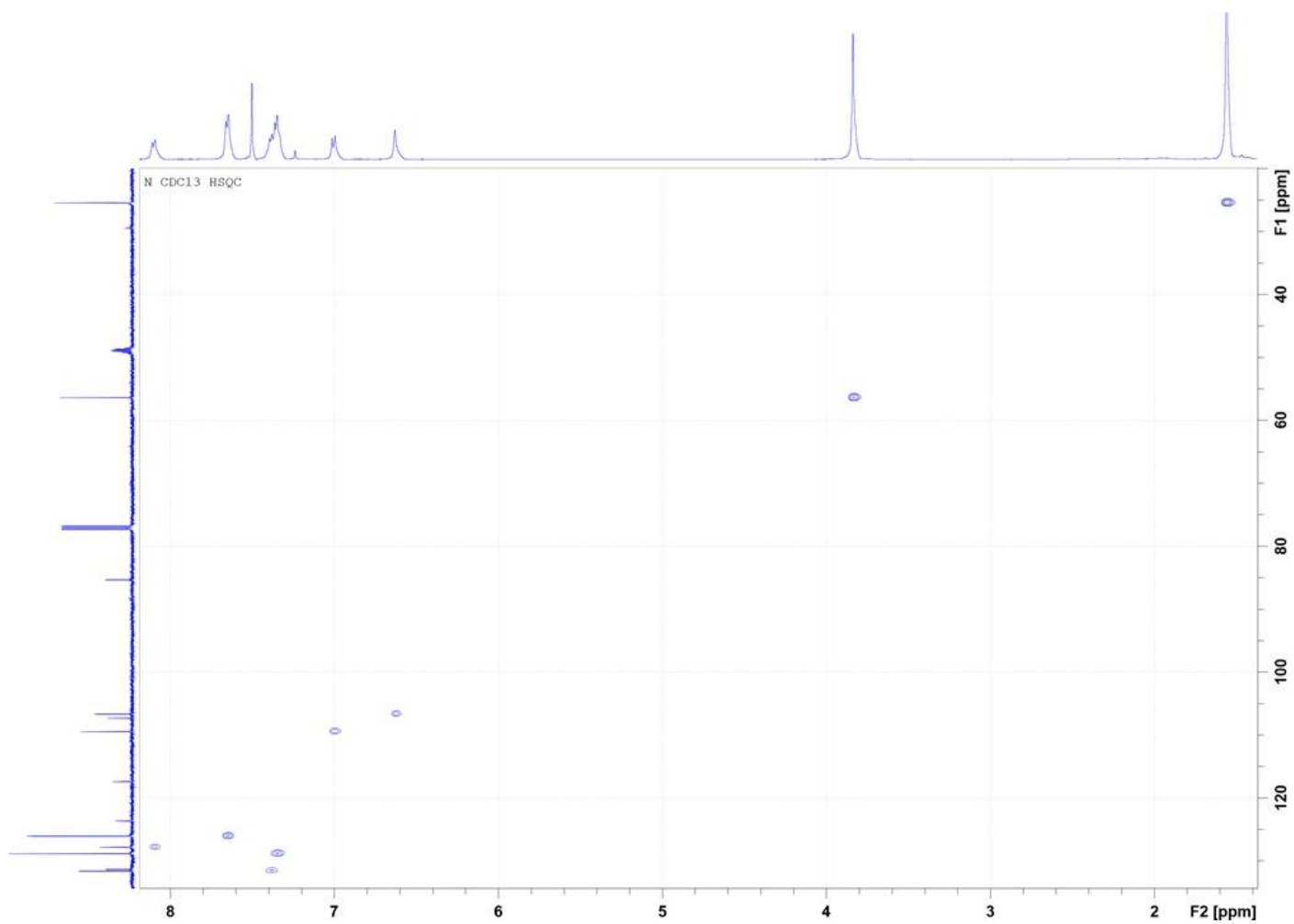
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**Figure S38:** DEPT90 Spectrum of **4** in CDCl<sub>3</sub>.

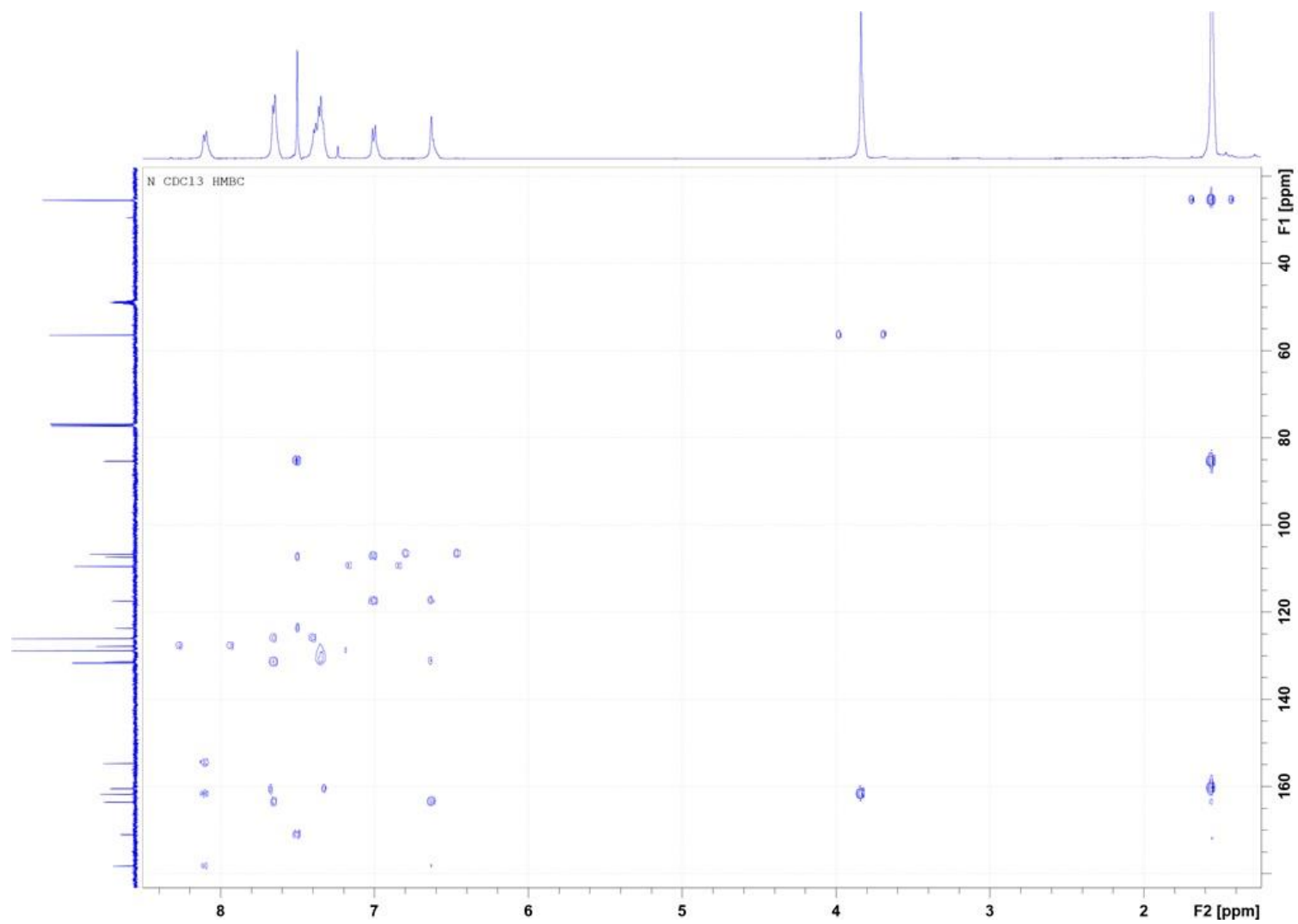
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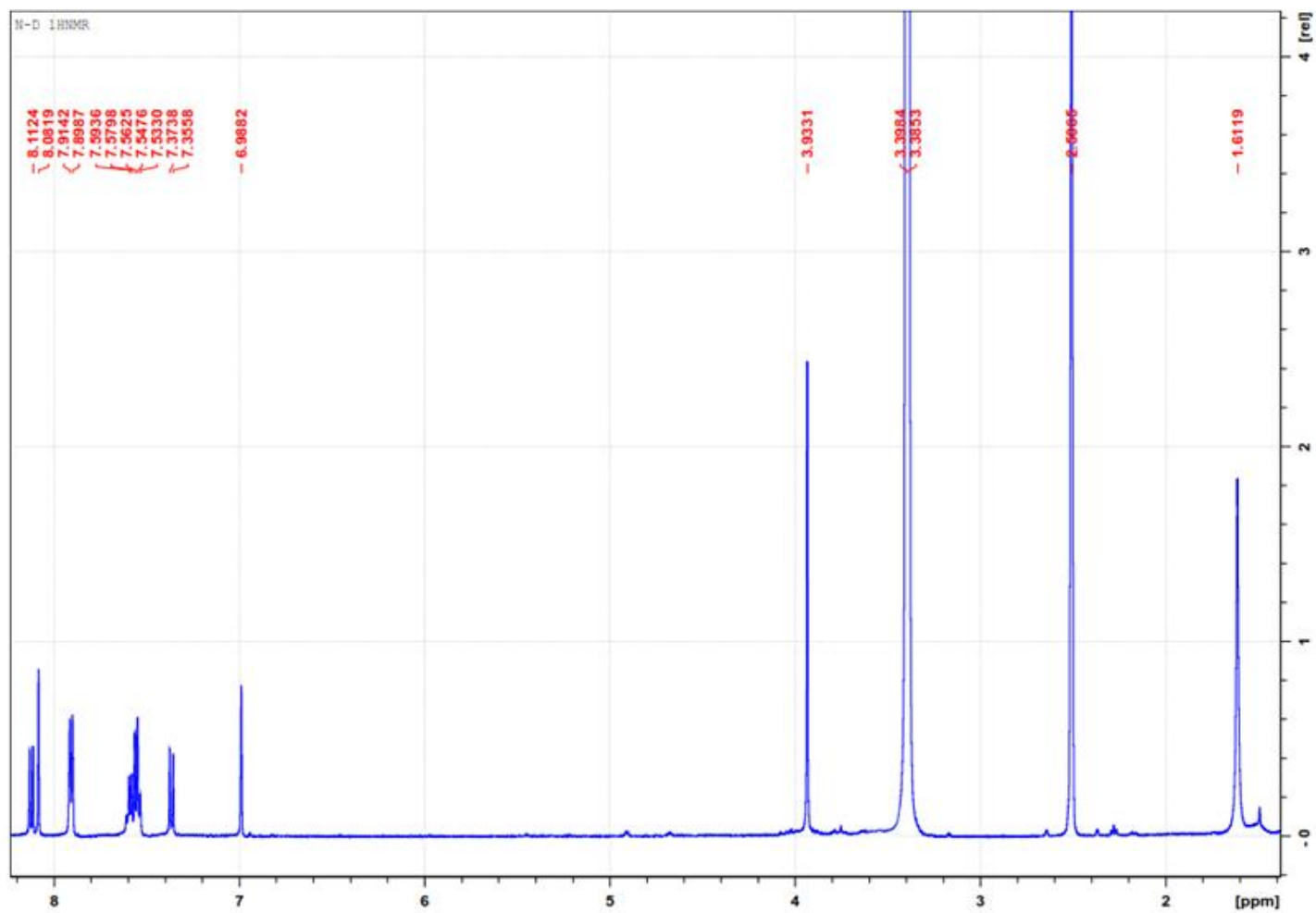
**Figure S39:** HSQC Spectrum of **4** in CDCl<sub>3</sub>.

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**Figure S40:** HMBC Spectrum of **4** in  $\text{CDCl}_3$ .

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**Figure S41:**  $^1\text{H}$ NMR Spectrum of **4** in DMSO.

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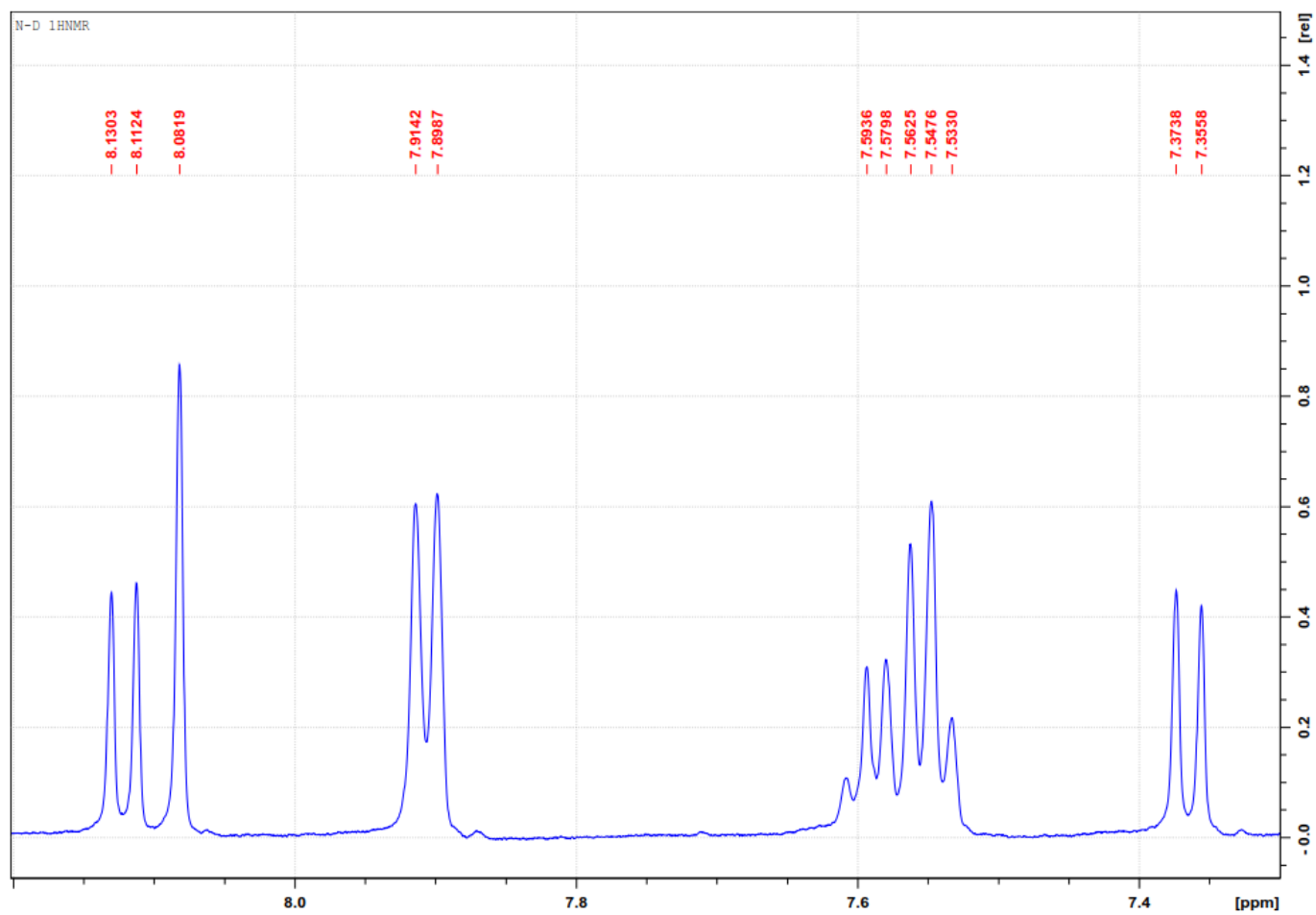
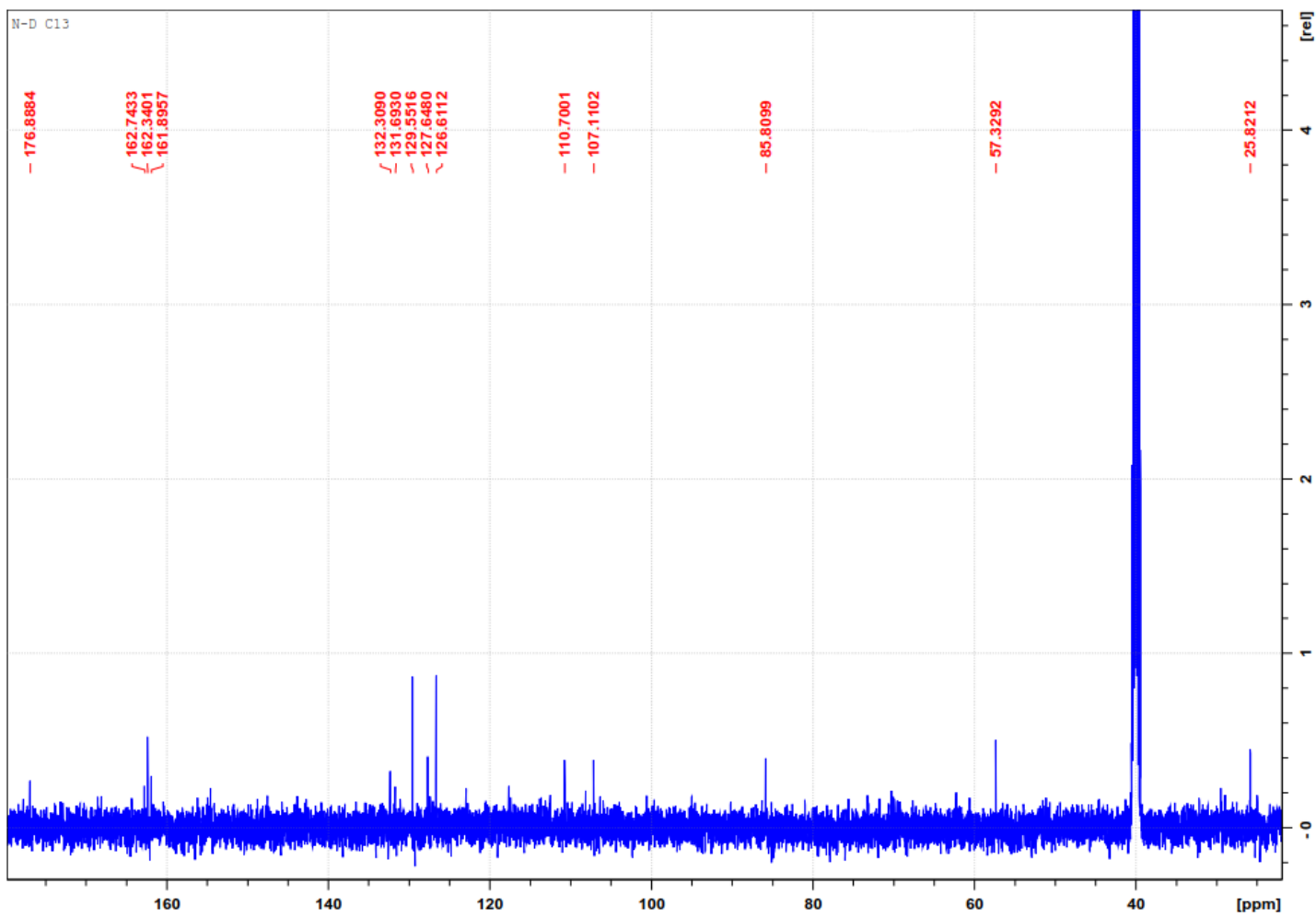


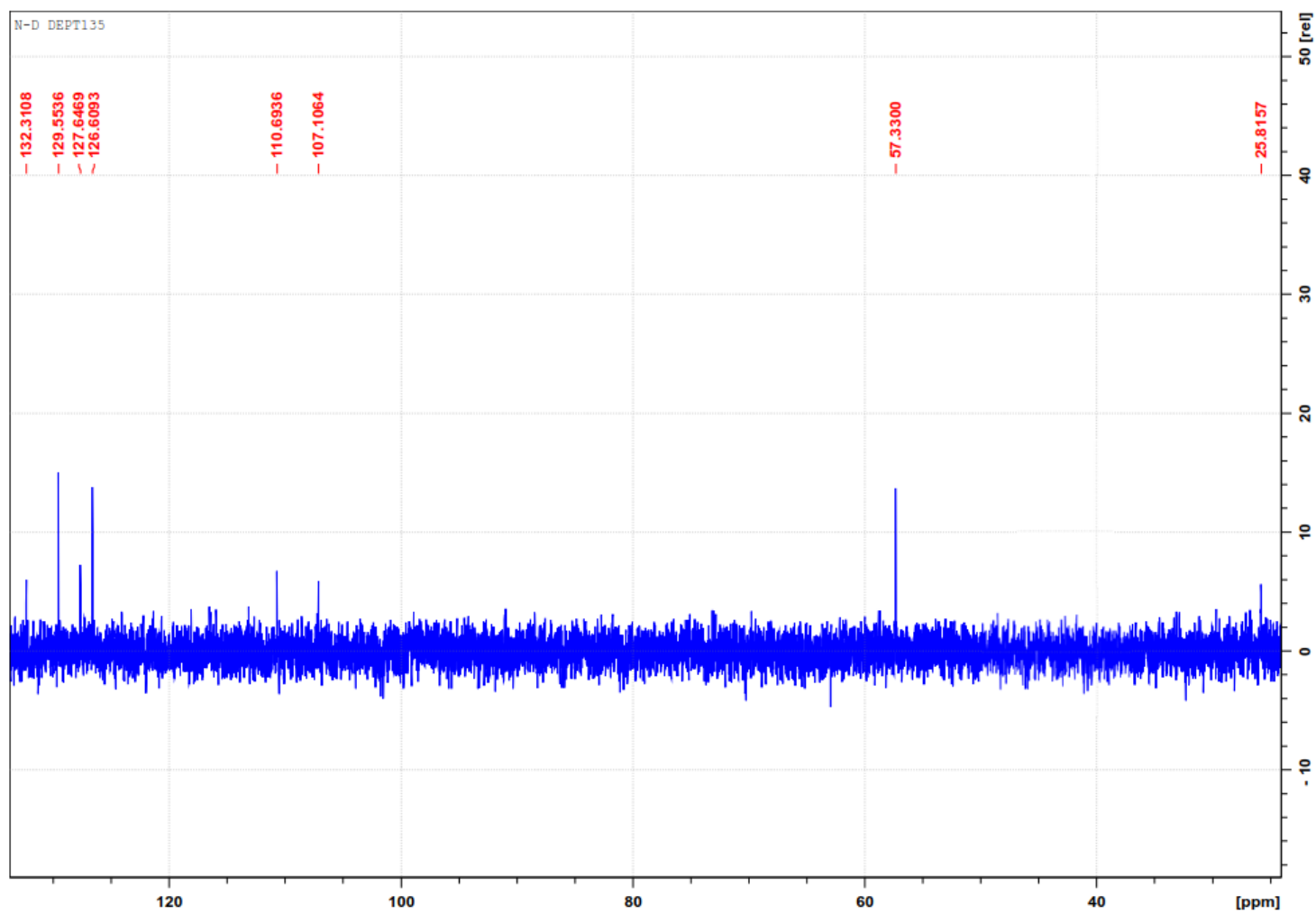
Figure S42: <sup>1</sup>H NMR Spectrum of **4** in DMSO (expansion).

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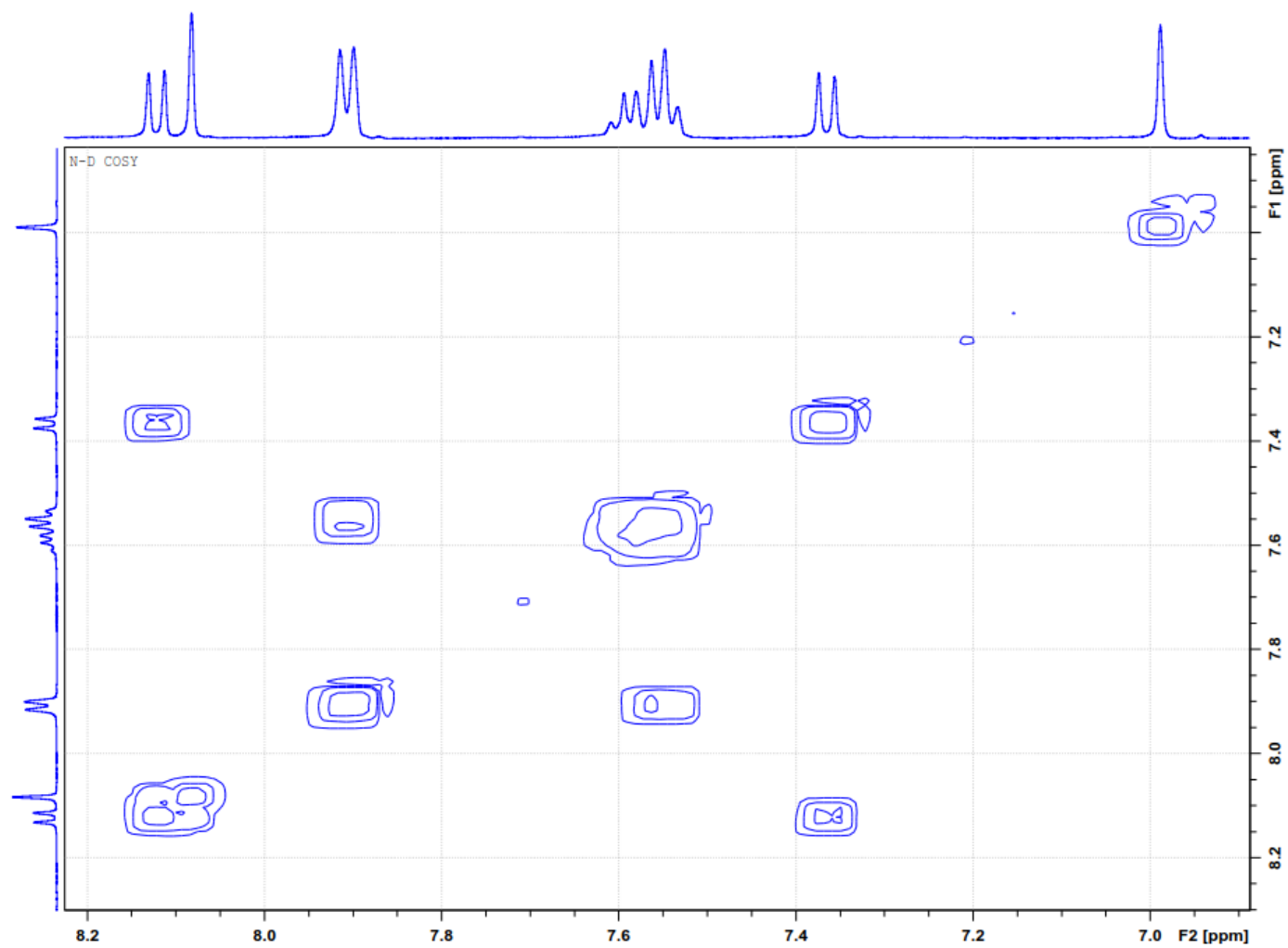
**Figure S43:**  $^{13}\text{C}$ NMR Spectrum of **4** in DMSO.

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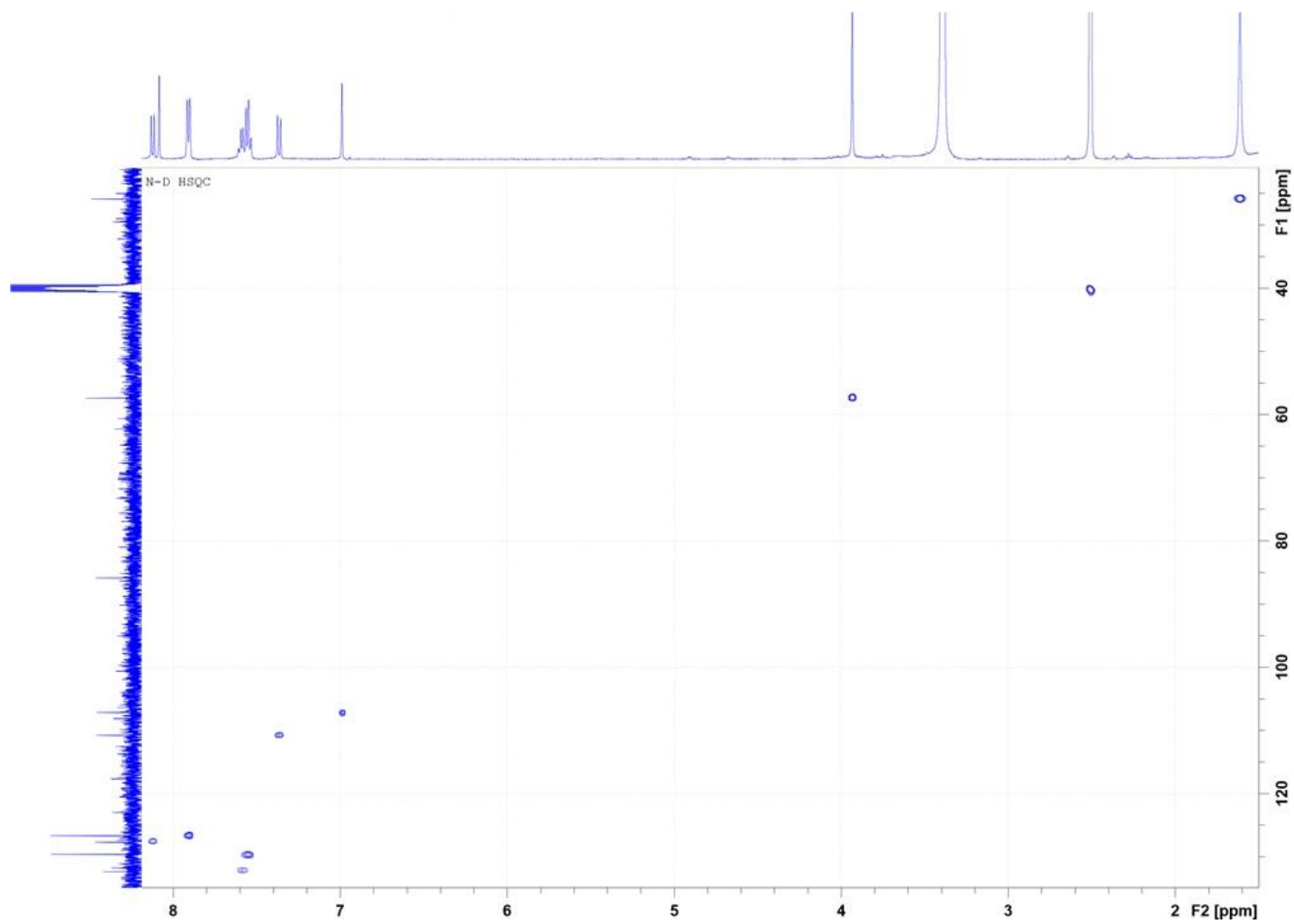
**Figure S44:** DEPT135 Spectrum of **4** in DMSO.

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**Figure S45:** COSY Spectrum of **4** in DMSO.

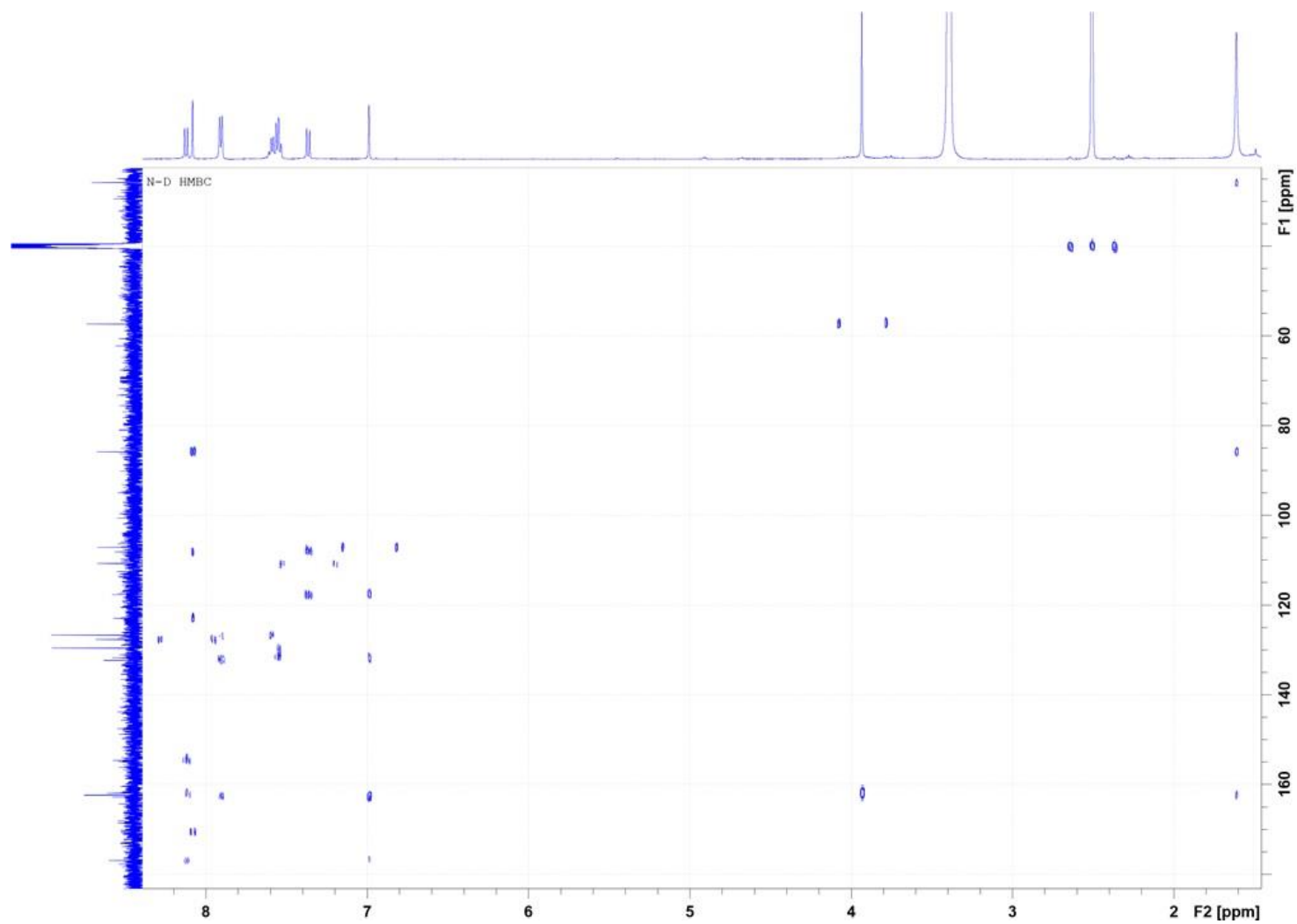
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**Figure S47:** HSQC Spectrum of **4** in DMSO.

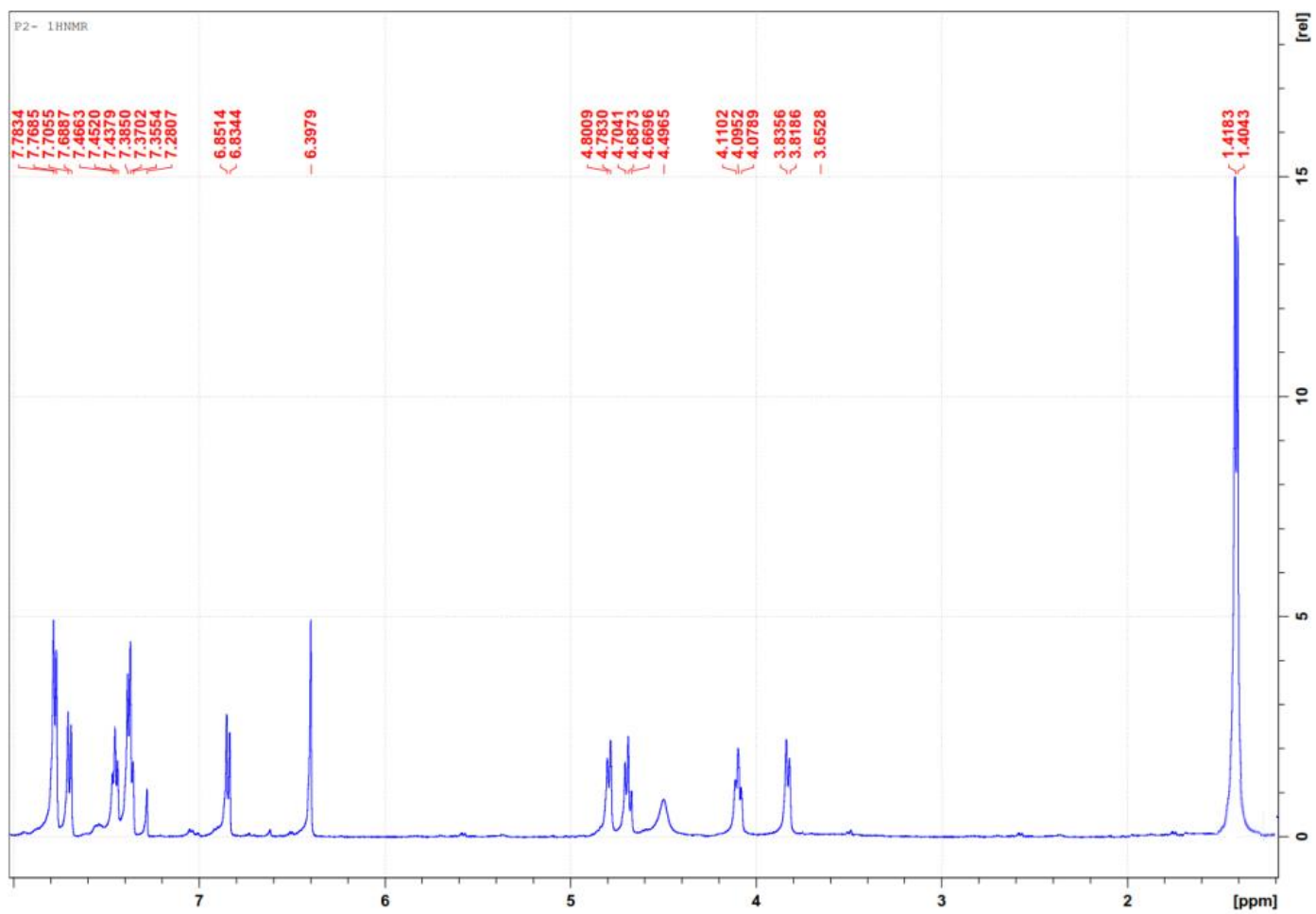
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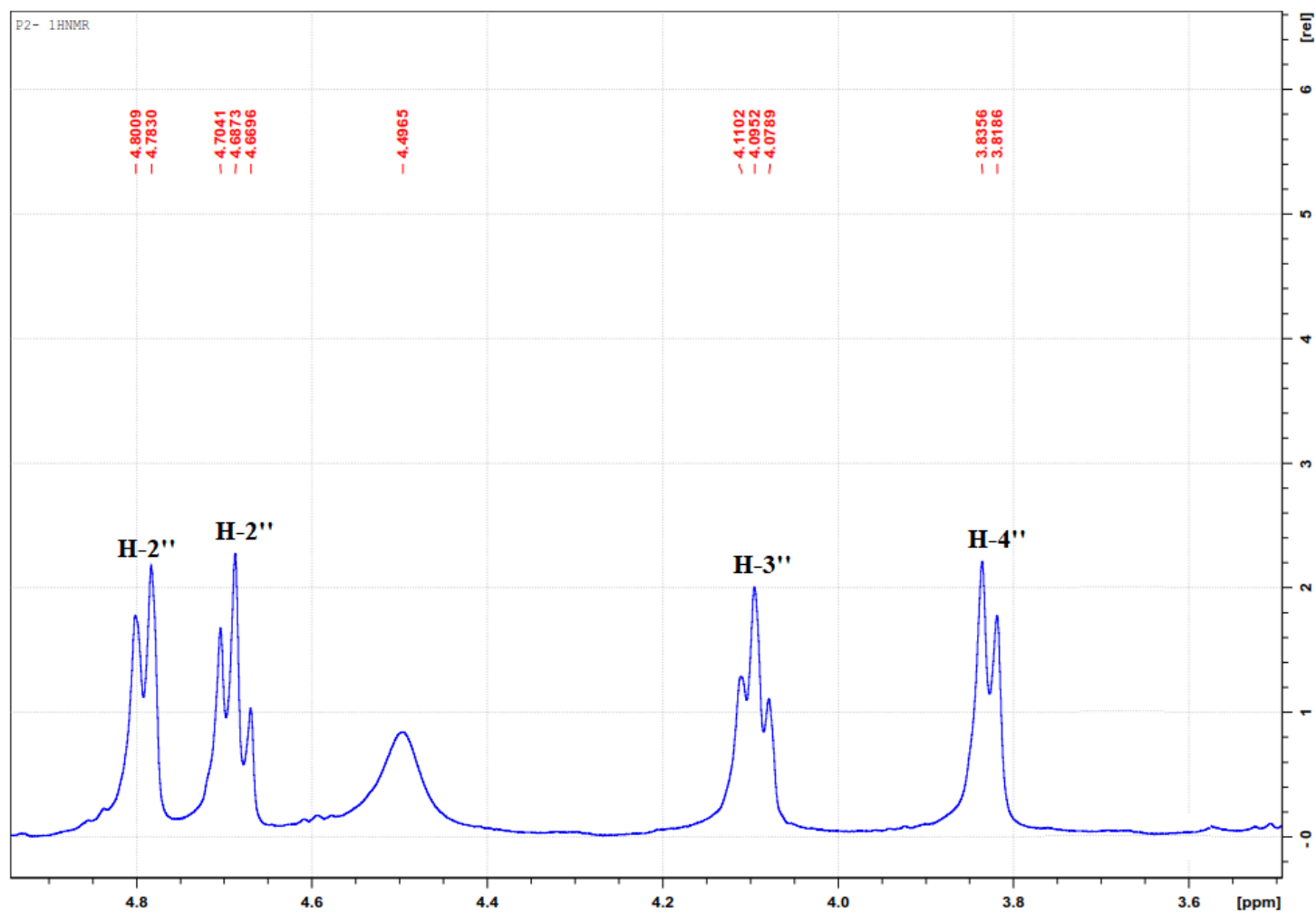
**Figure S48:** HMBC Spectrum of **4** in DMSO.

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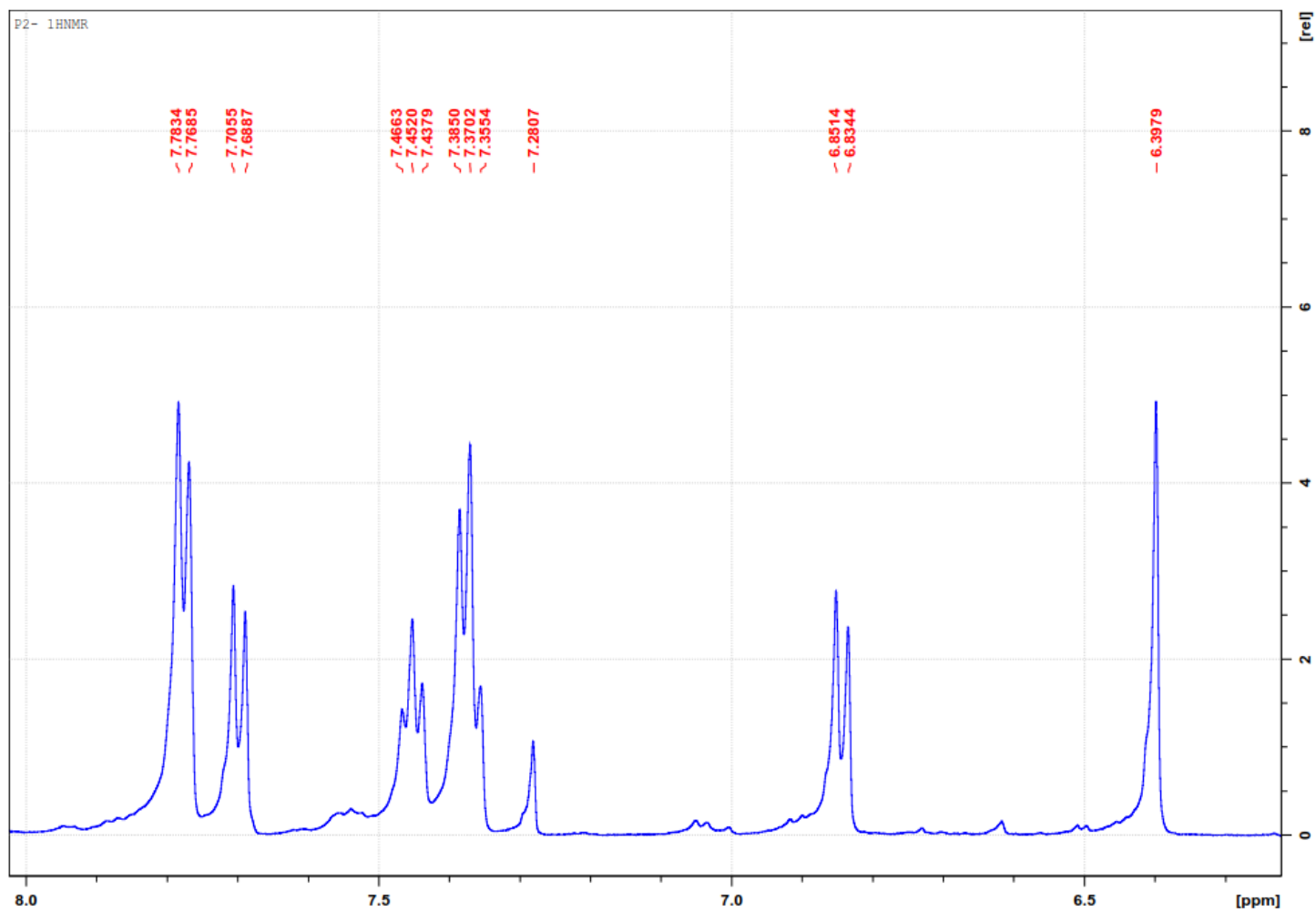
**Figure S49:** <sup>1</sup>HNMR Spectrum of **5** in CDCl<sub>3</sub>.

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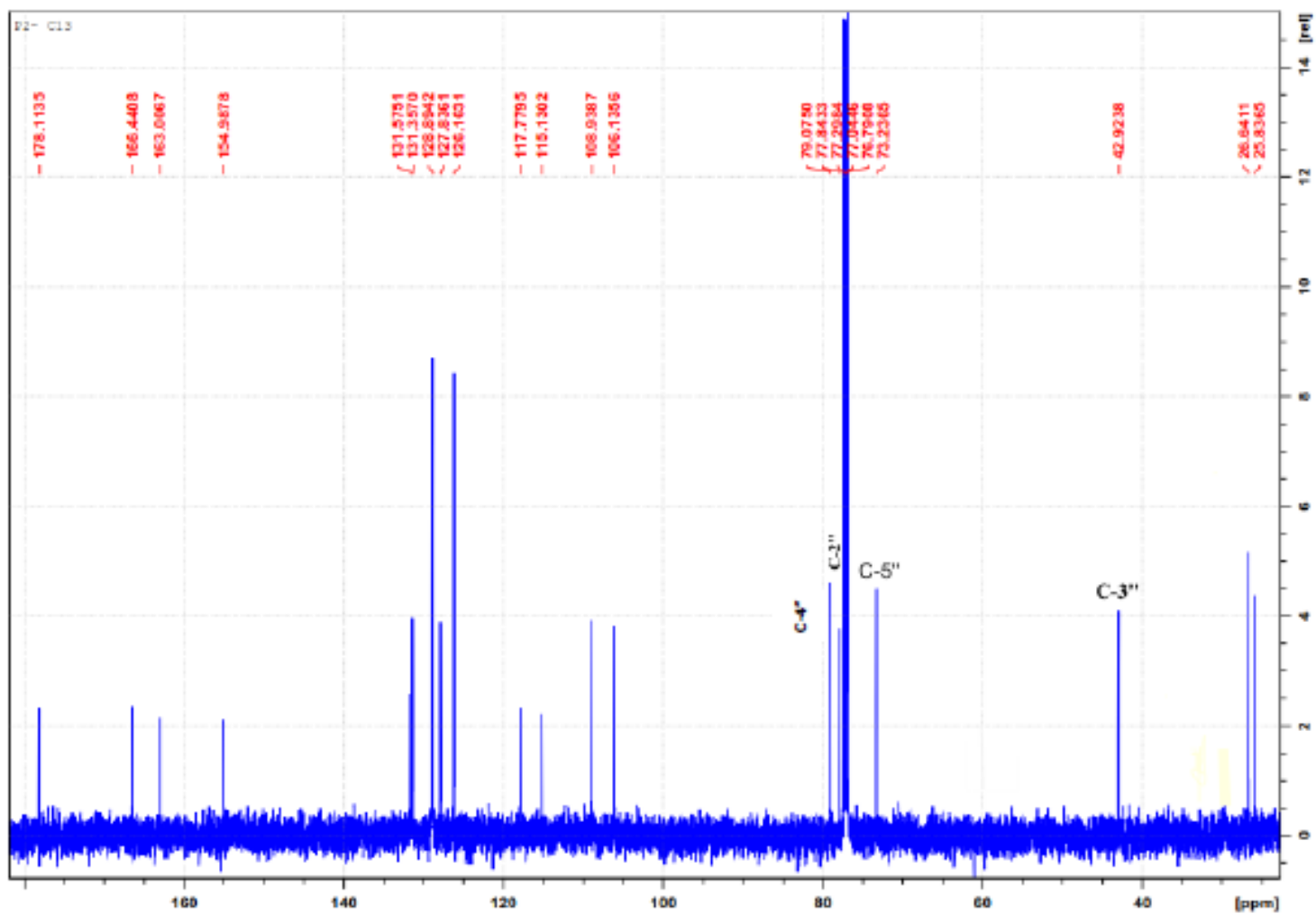


**Figure S50:**  $^1\text{H}$ NMR Spectrum of **5** in  $\text{CDCl}_3$  (expansion).

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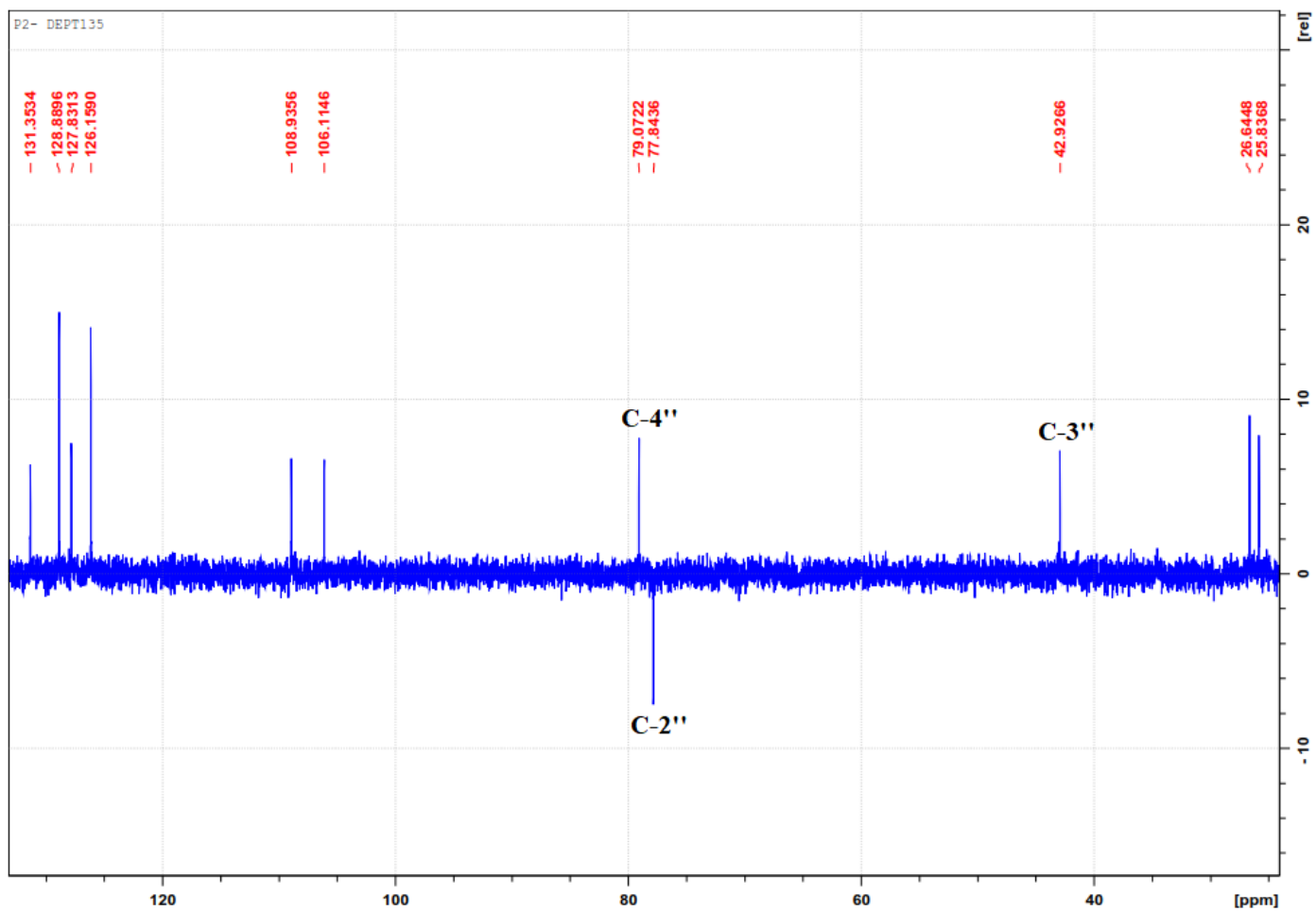


**Figure S51:**  $^1\text{H}$ NMR Spectrum of **5** in  $\text{CDCl}_3$  (expansion).



**Figure S52:** <sup>13</sup>CNMR Spectrum of **5** in CDCl<sub>3</sub>.

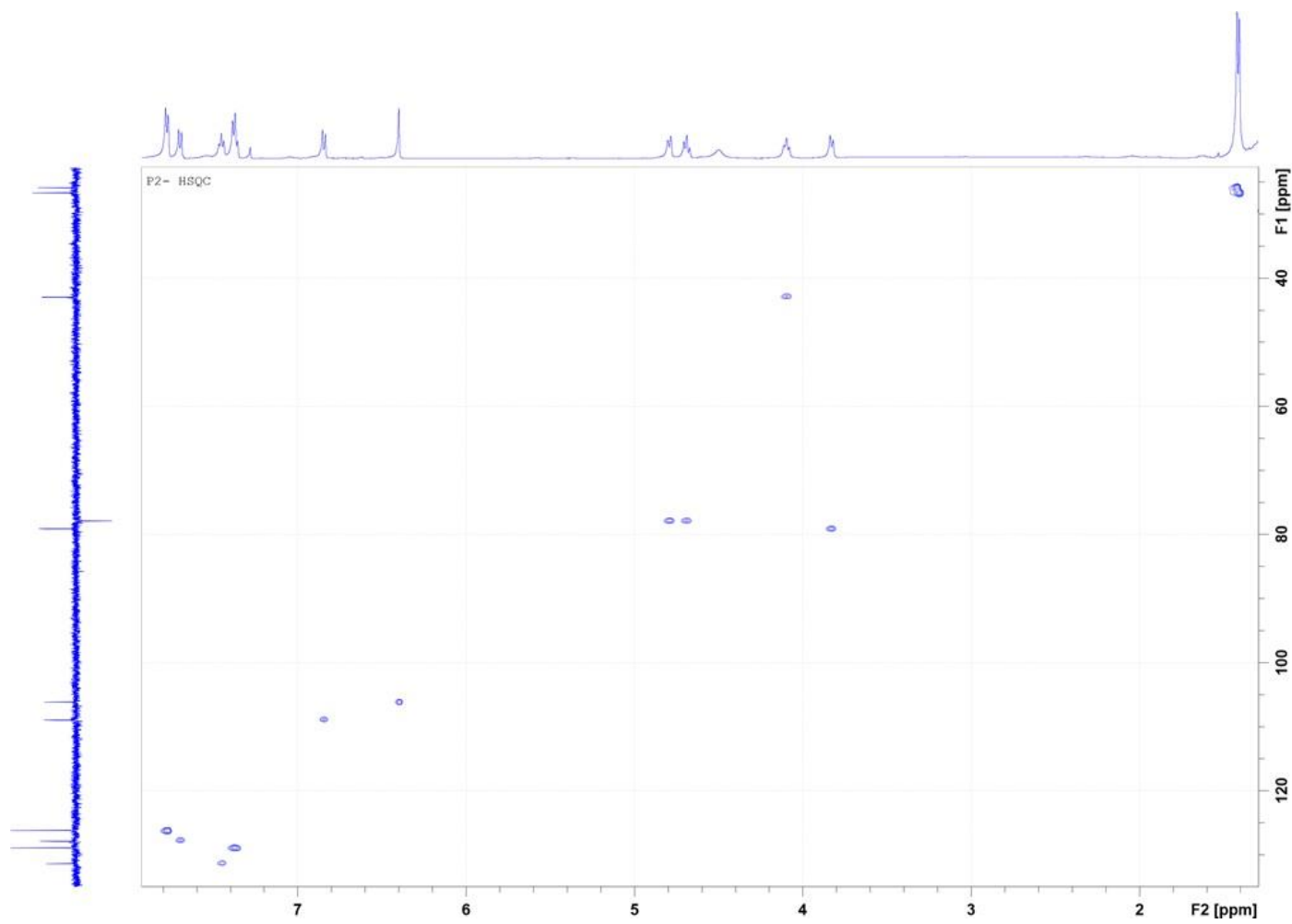
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**Figure S53:** DEPT135 Spectrum of **5** in  $\text{CDCl}_3$ .

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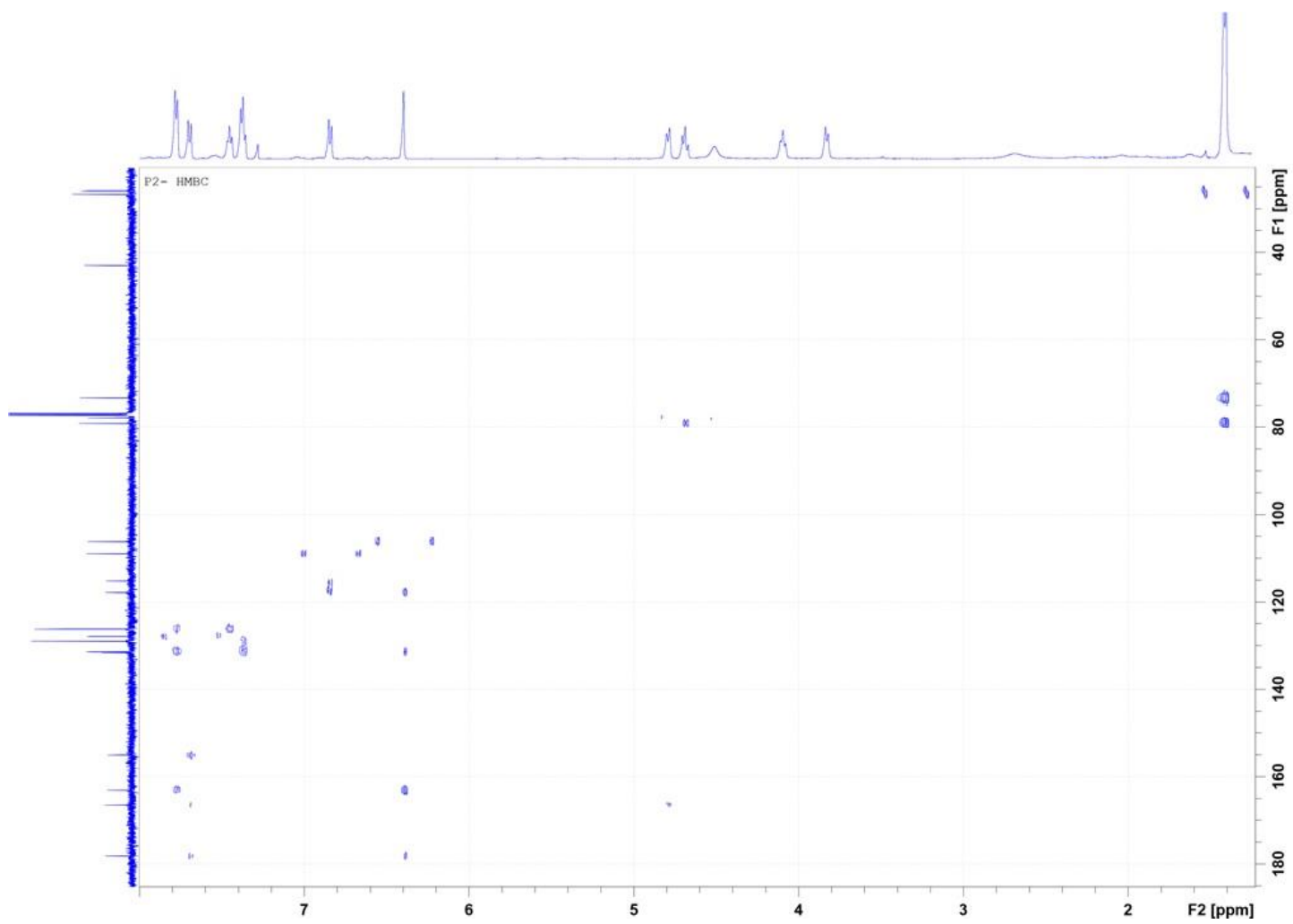




**Figure S55:** HSQC Spectrum of **5** in  $\text{CDCl}_3$ .

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**Figure S56:** HMBC Spectrum of **5** in  $\text{CDCl}_3$ .

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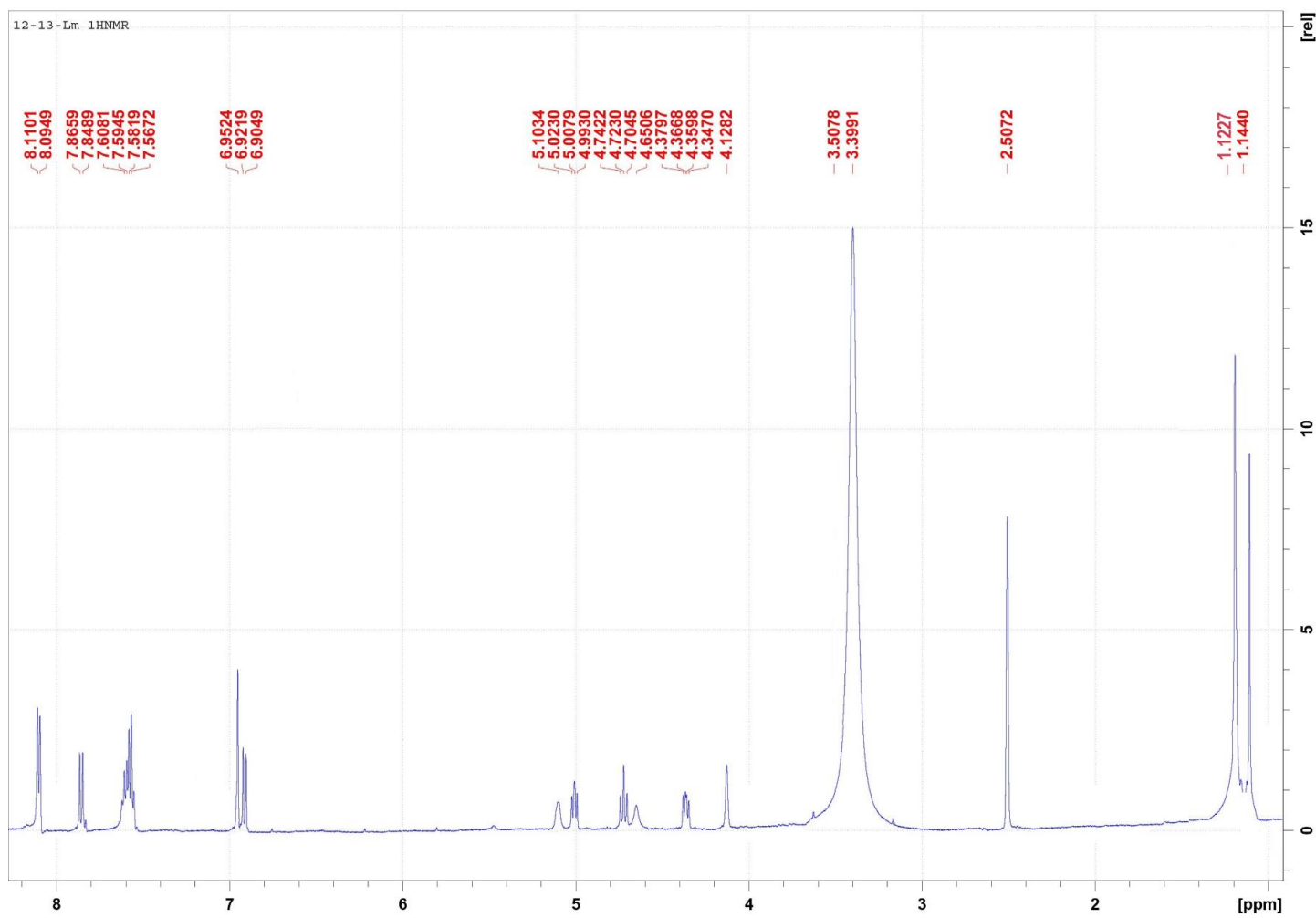
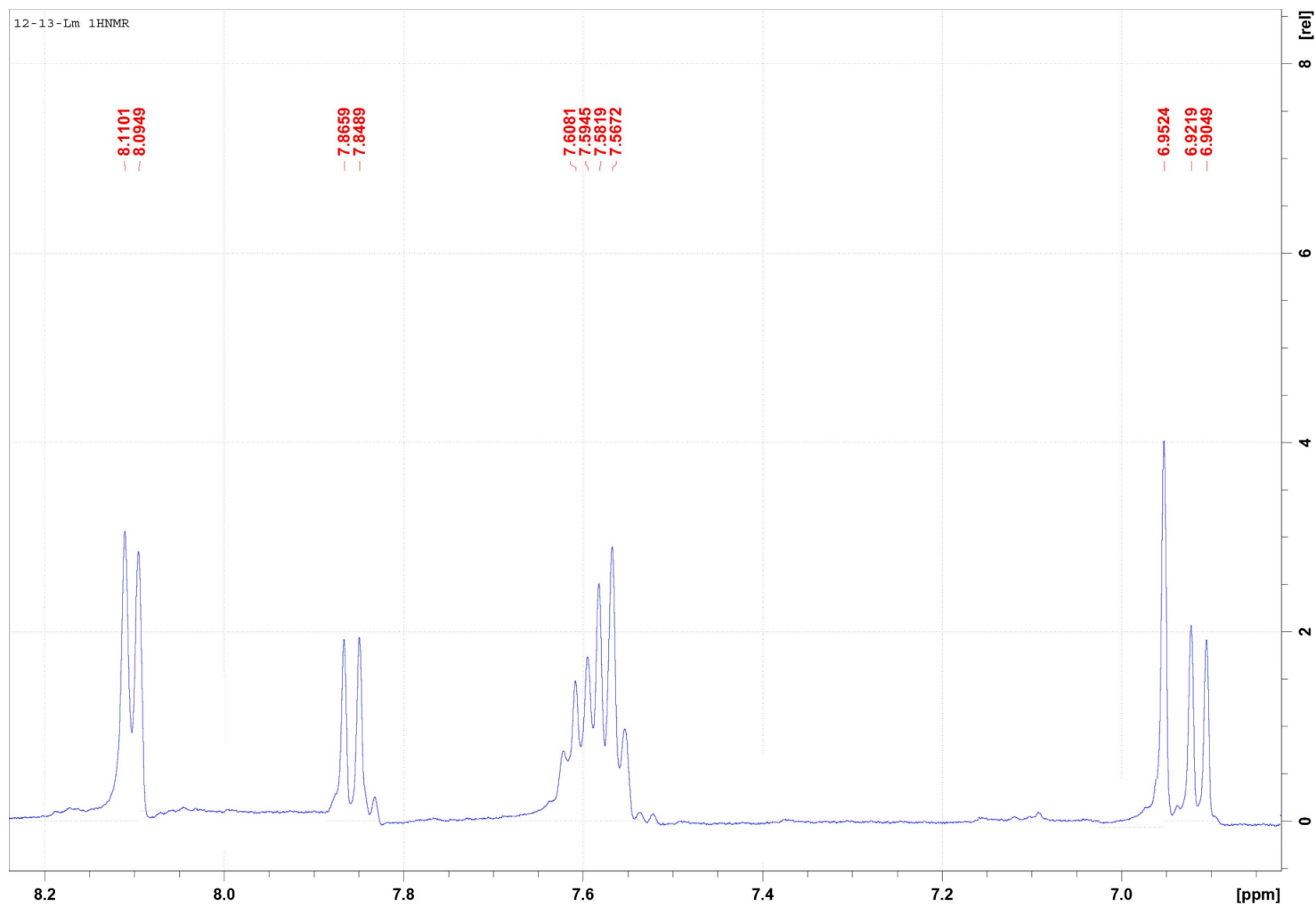


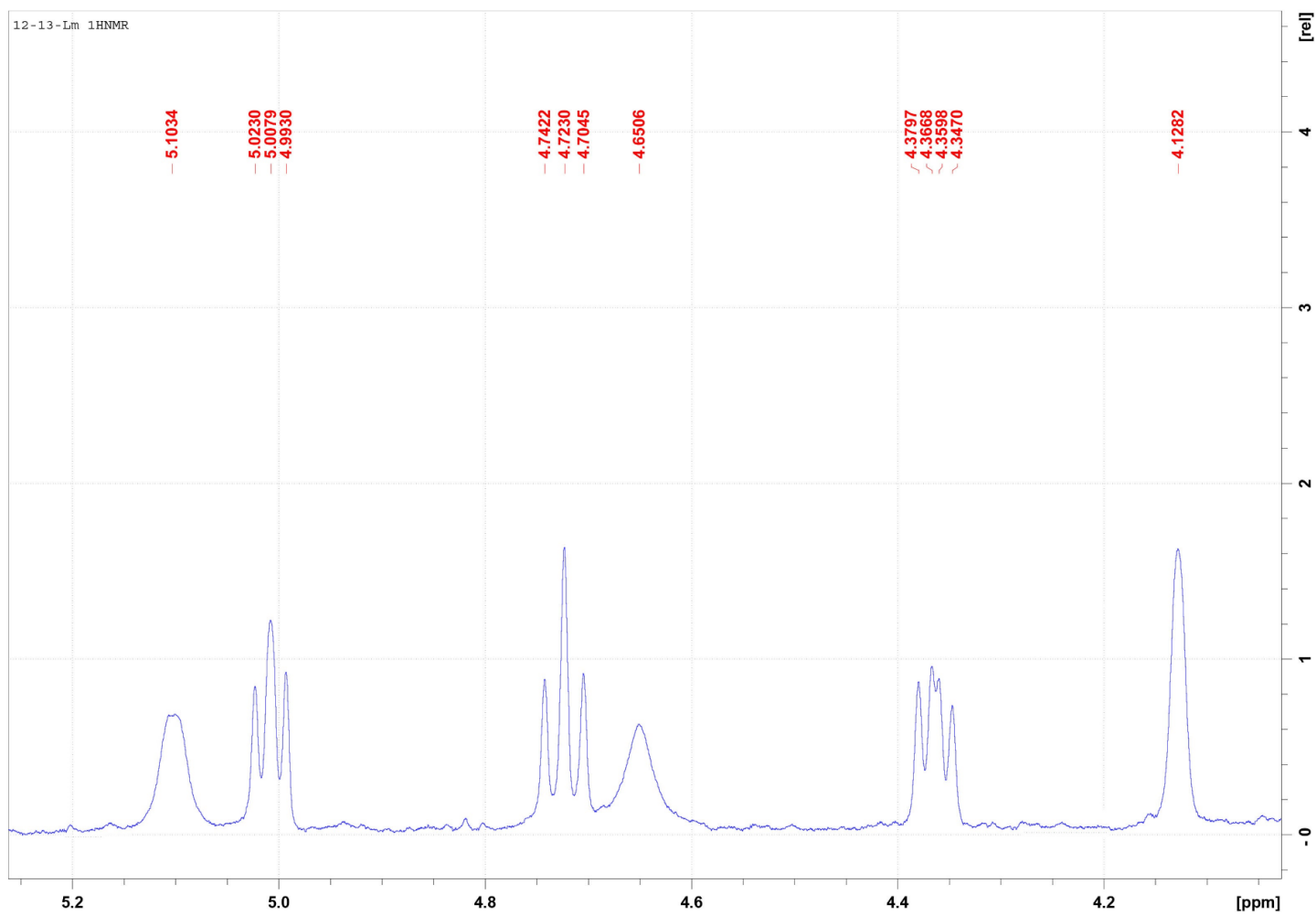
Figure S57:  $^1\text{H}$ NMR Spectrum of **6** in DMSO.

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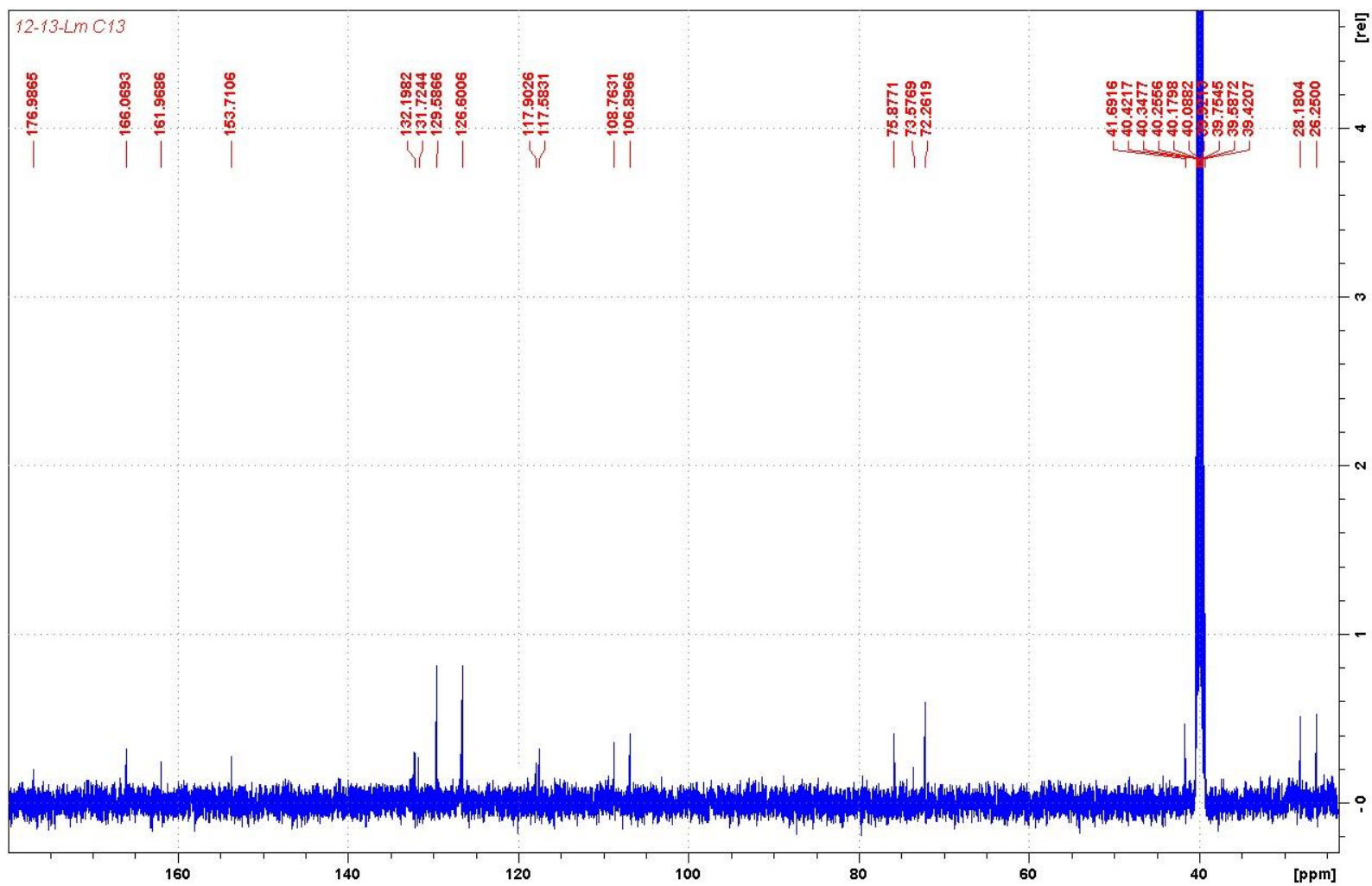
**Figure S58:**  $^1\text{H}$ NMR Spectrum of **6** in DMSO (expansion).

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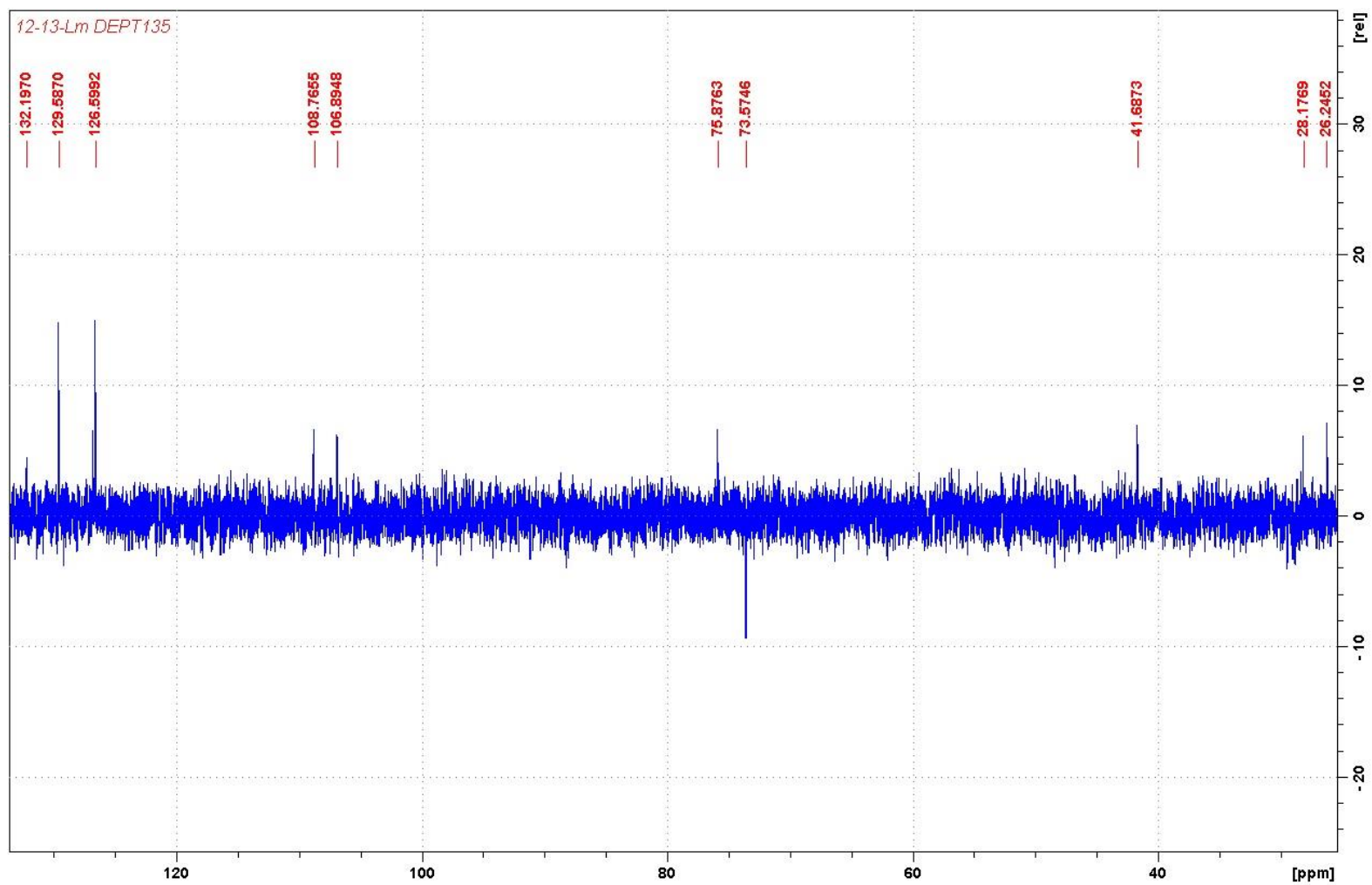
**Figure S59:**  $^1\text{H}$ NMR Spectrum of **6** in DMSO (expansion).

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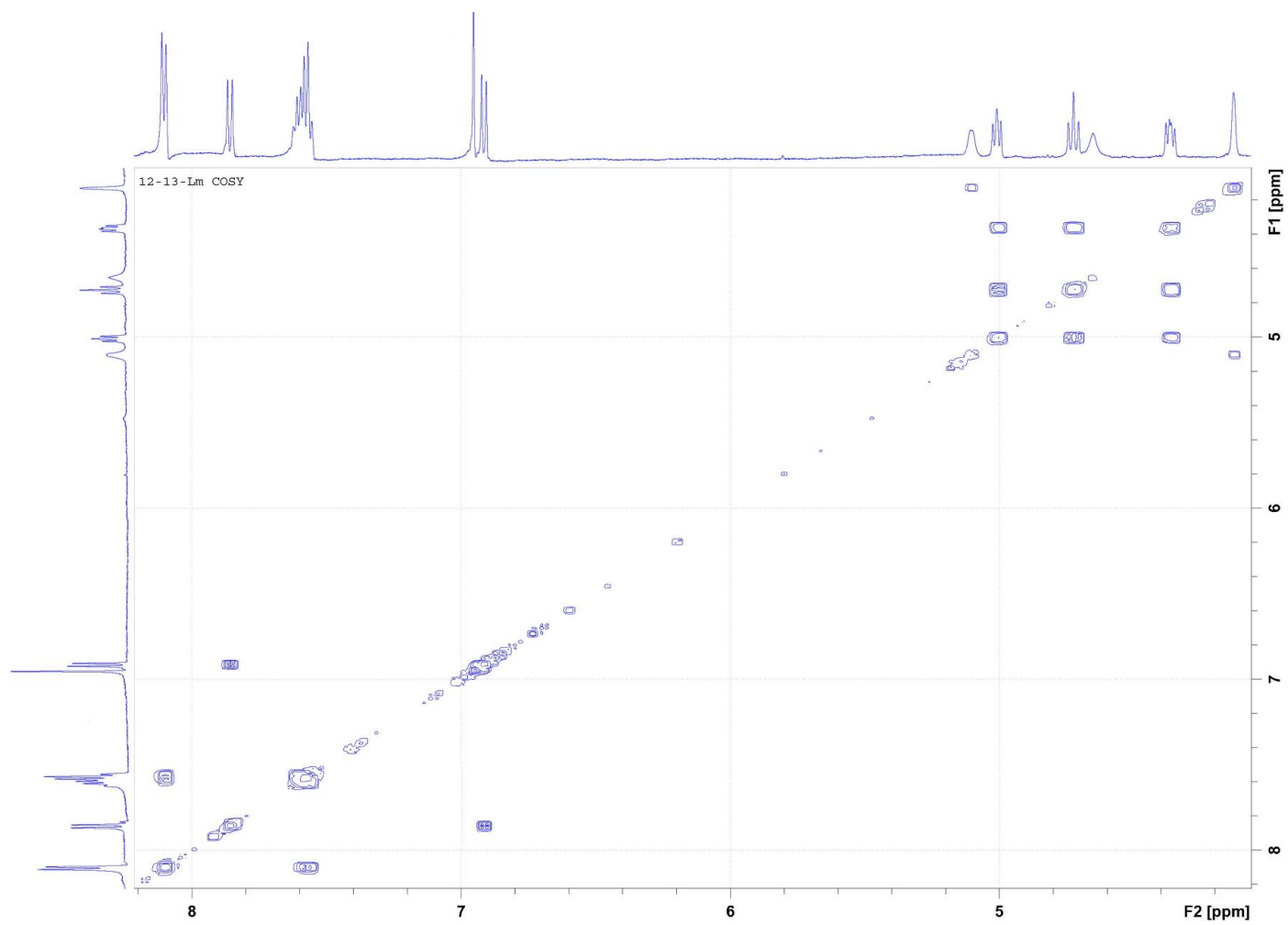
**Figure S60:**  $^{13}\text{C}$ NMR Spectrum of **6** in DMSO.

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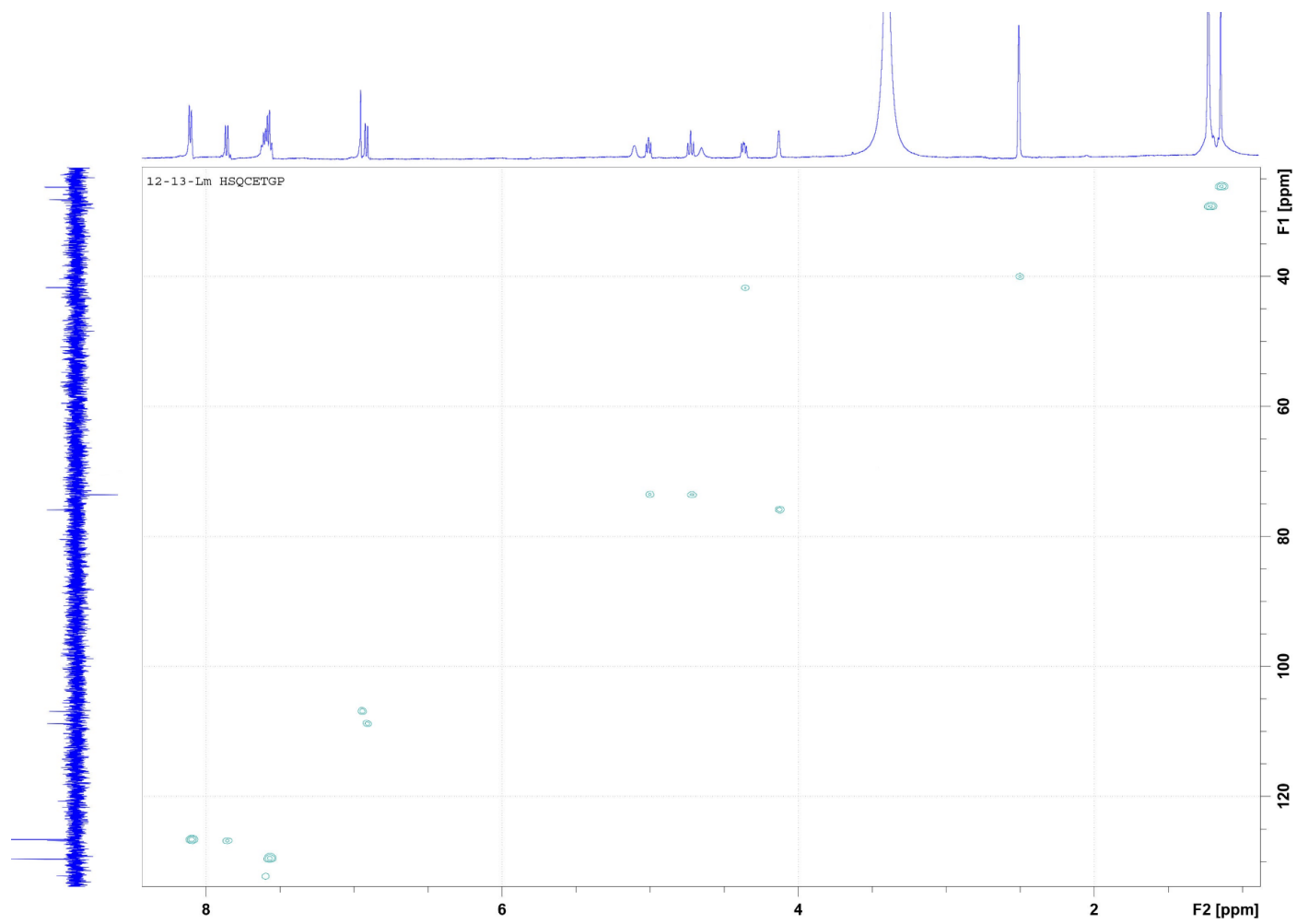
**Figure S61:** DEPT135 Spectrum of **6** in DMSO.

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**Figure S62:** COSY Spectrum of **6** in DMSO.

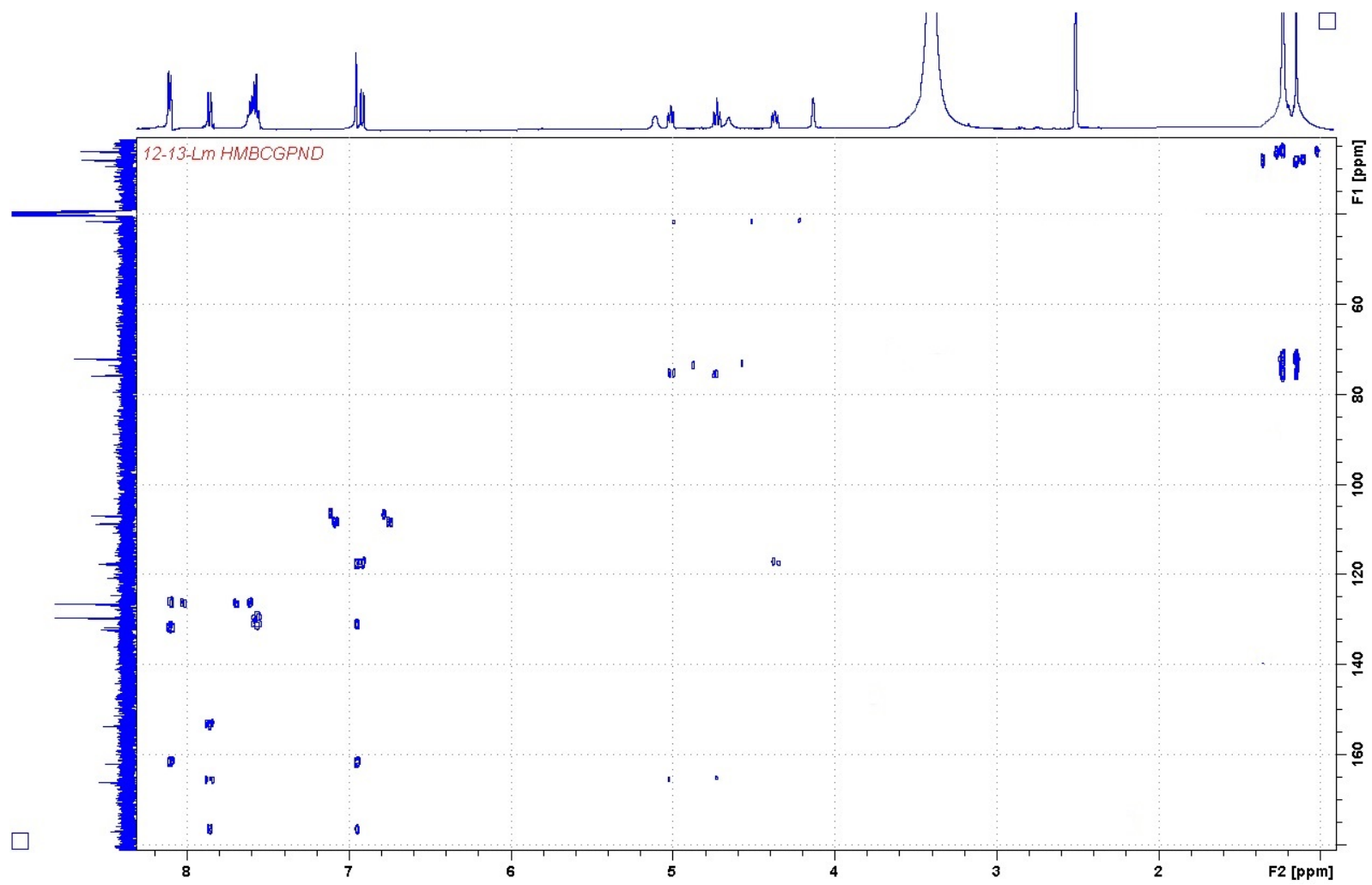
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**Figure S63:** HSQC Spectrum of **6** in DMSO.

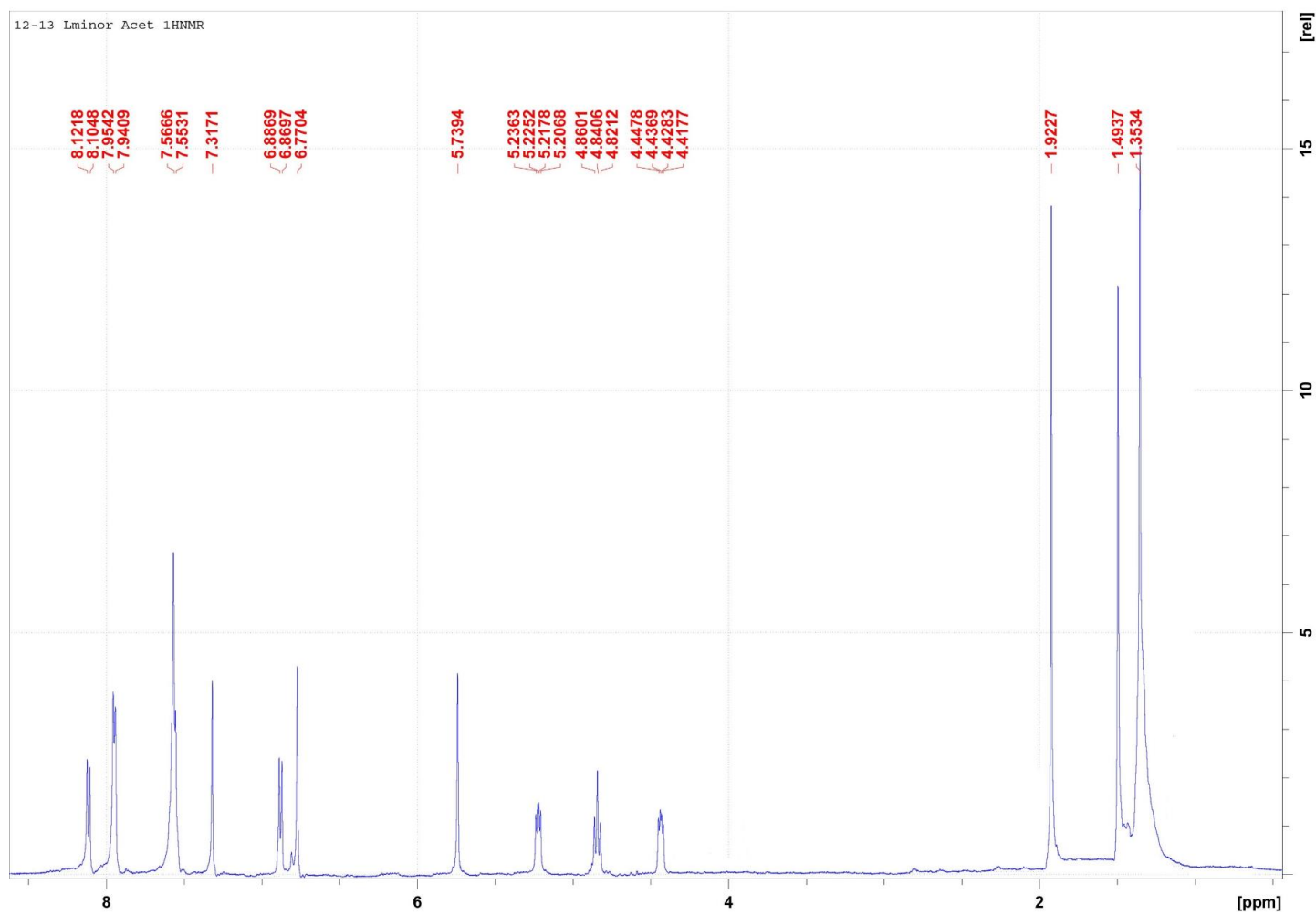
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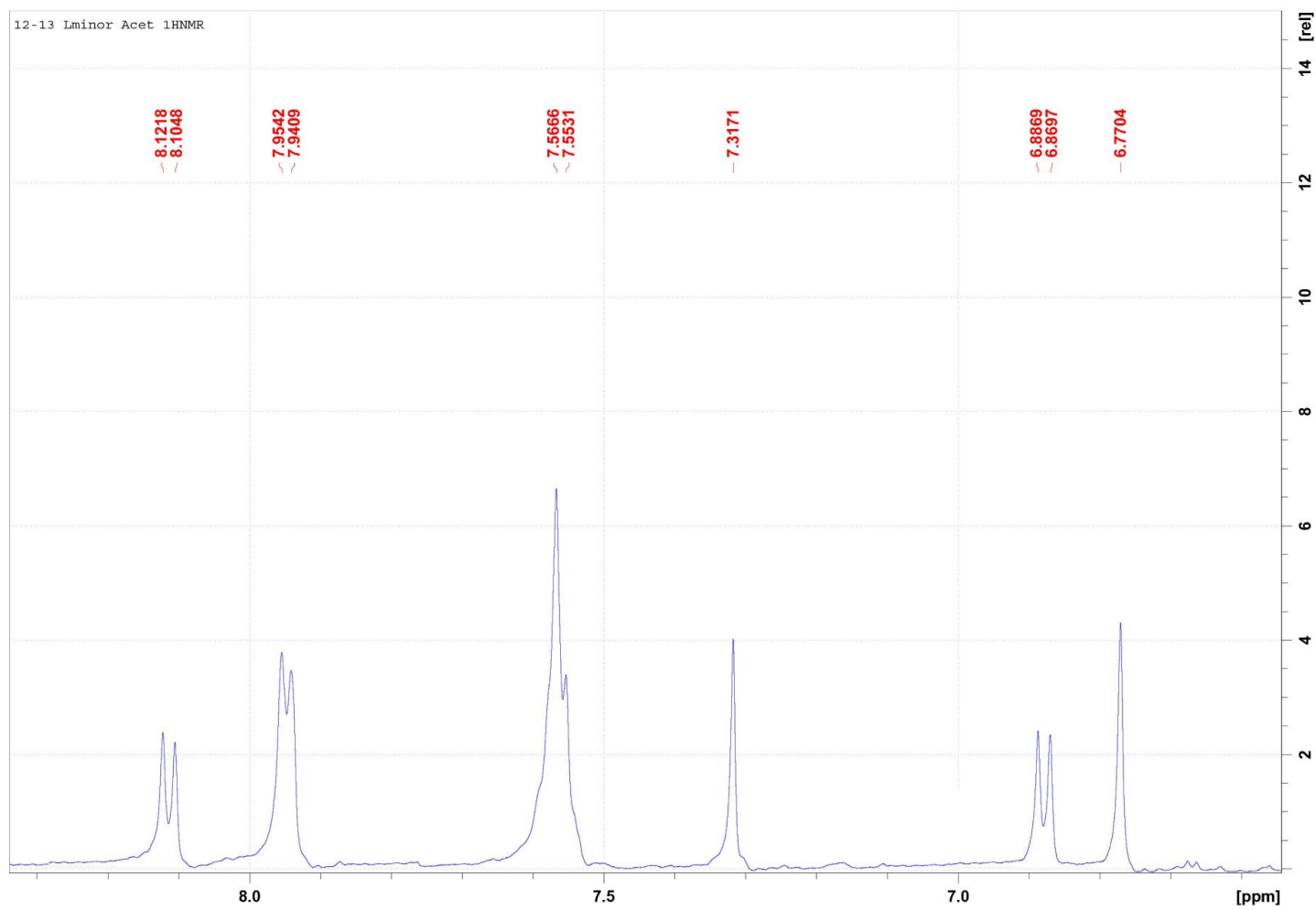
**Figure S64:** HMBC Spectrum of **6** in DMSO.

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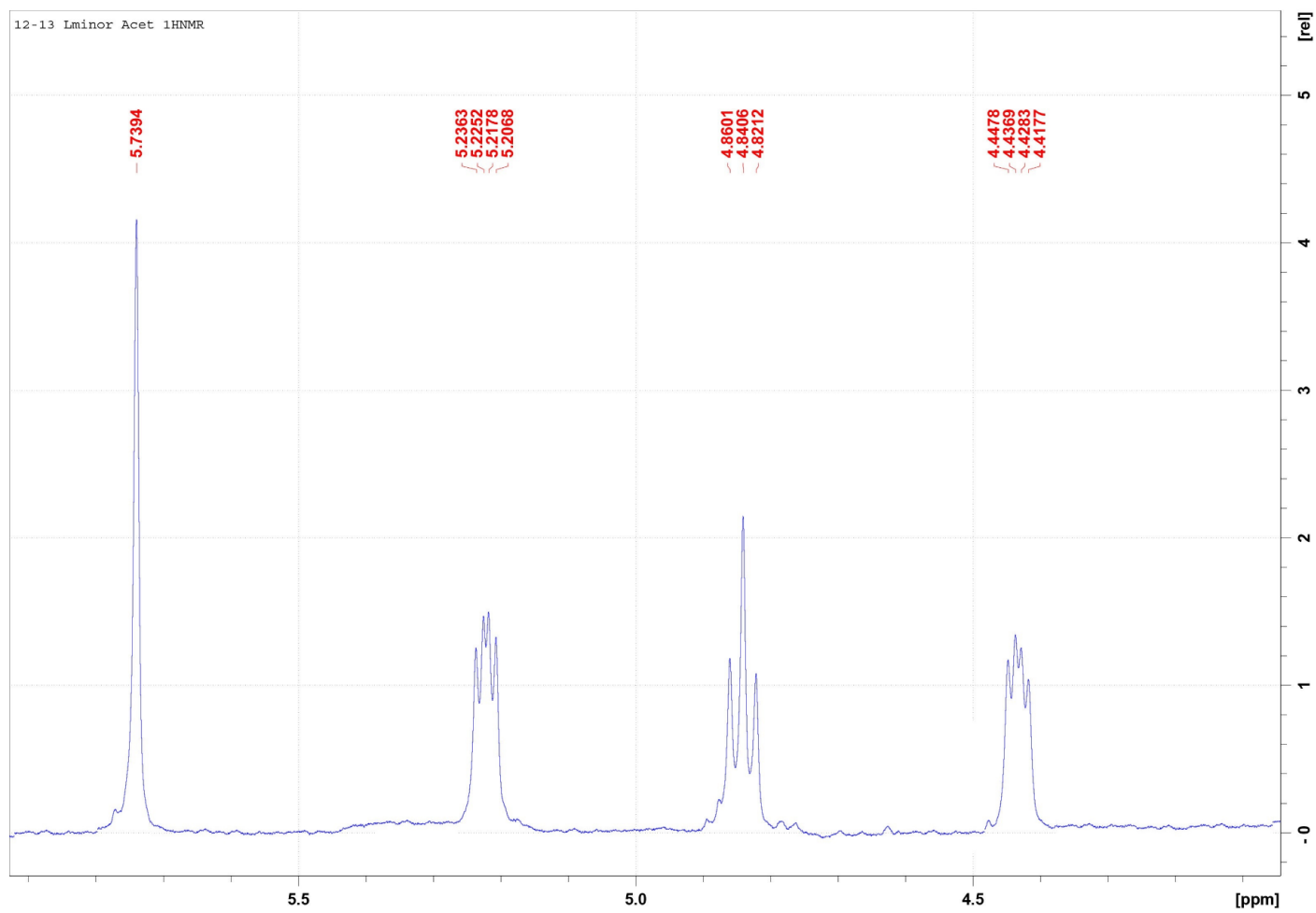


**Figure S65:**  $^1\text{H}$ NMR Spectrum of **6** acetate derivative in  $\text{CDCl}_3$ .

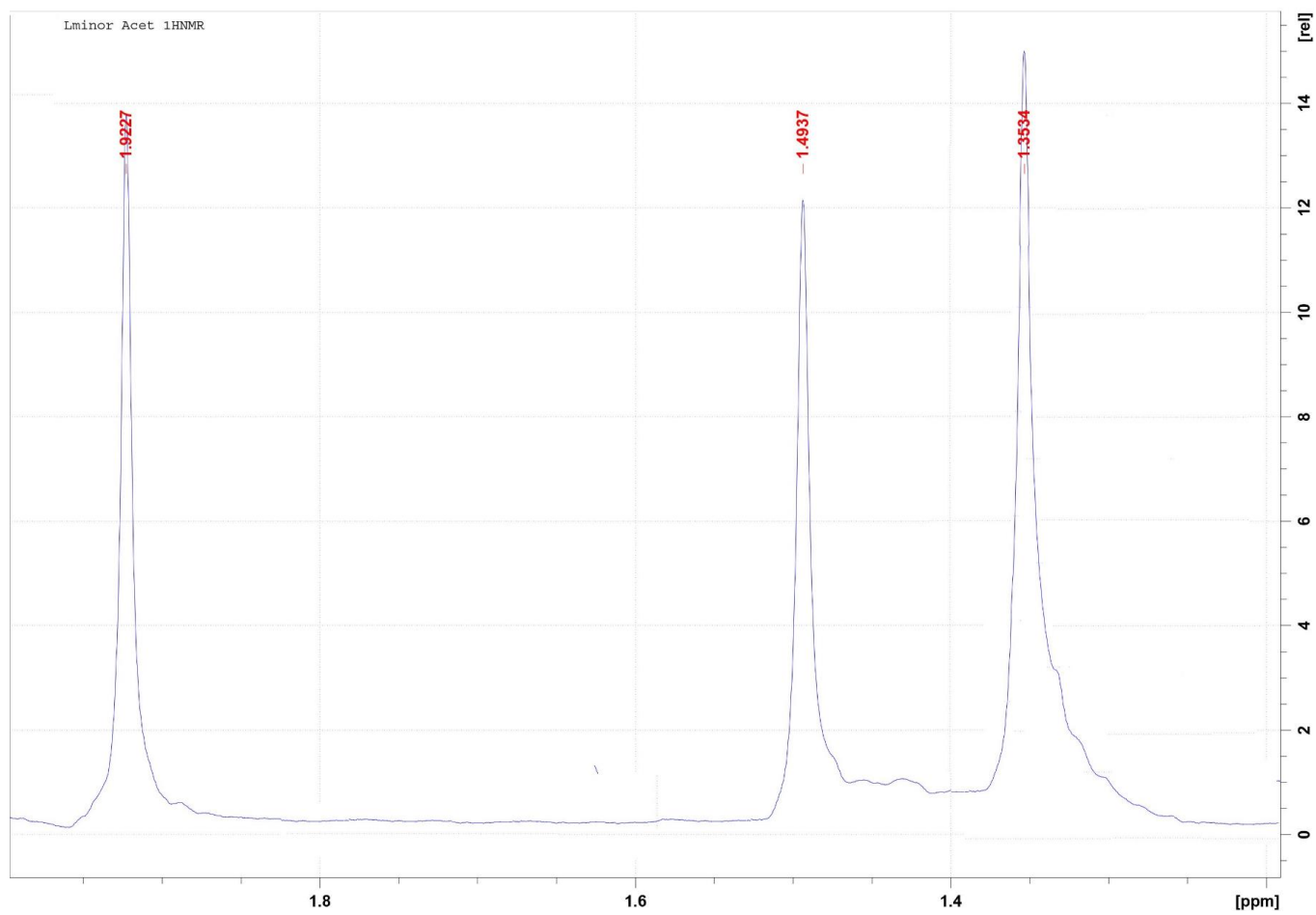
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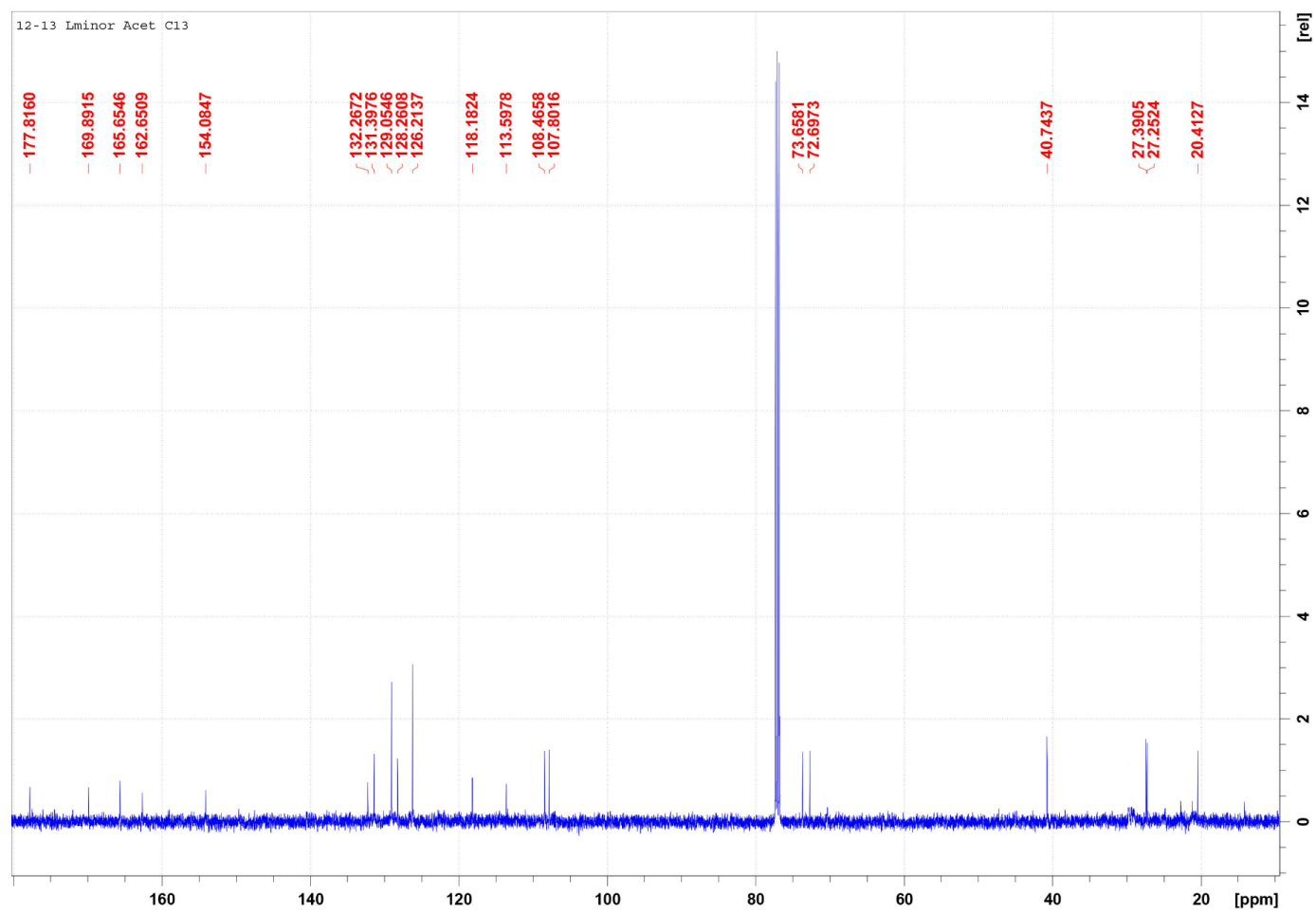
**Figure S66:**  $^1\text{H}$ NMR Spectrum of **6** acetate derivative in  $\text{CDCl}_3$  (expansion).



**Figure S67:**  $^1\text{H}$ NMR Spectrum of **6** acetate derivative in  $\text{CDCl}_3$  (expansion).



**Figure S68:**  $^1\text{H}$ NMR Spectrum of **6** acetate derivative in  $\text{CDCl}_3$  (expansion).



**Figure S69:**  $^{13}\text{C}$ NMR Spectrum of **6** acetate derivative in  $\text{CDCl}_3$ .

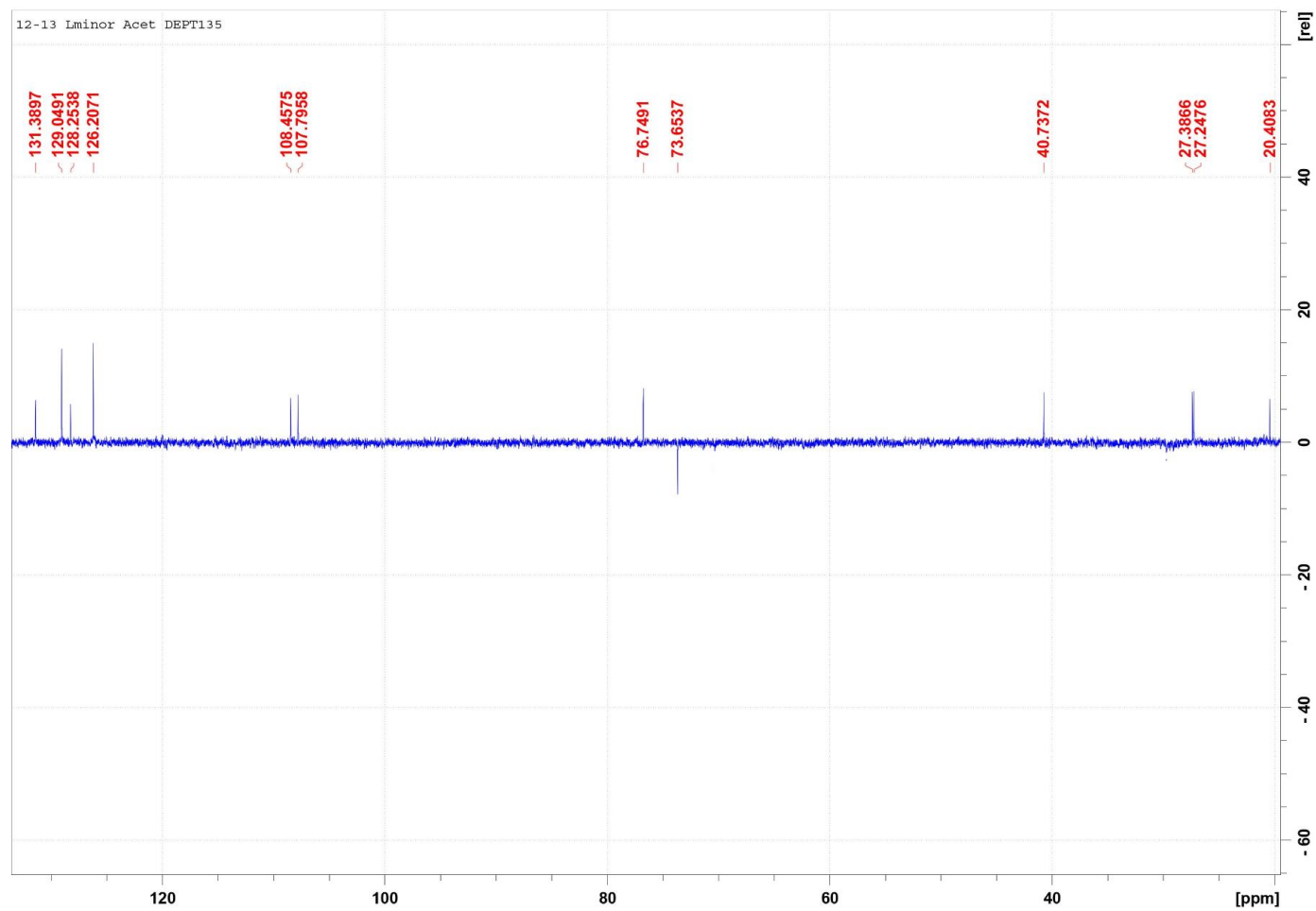
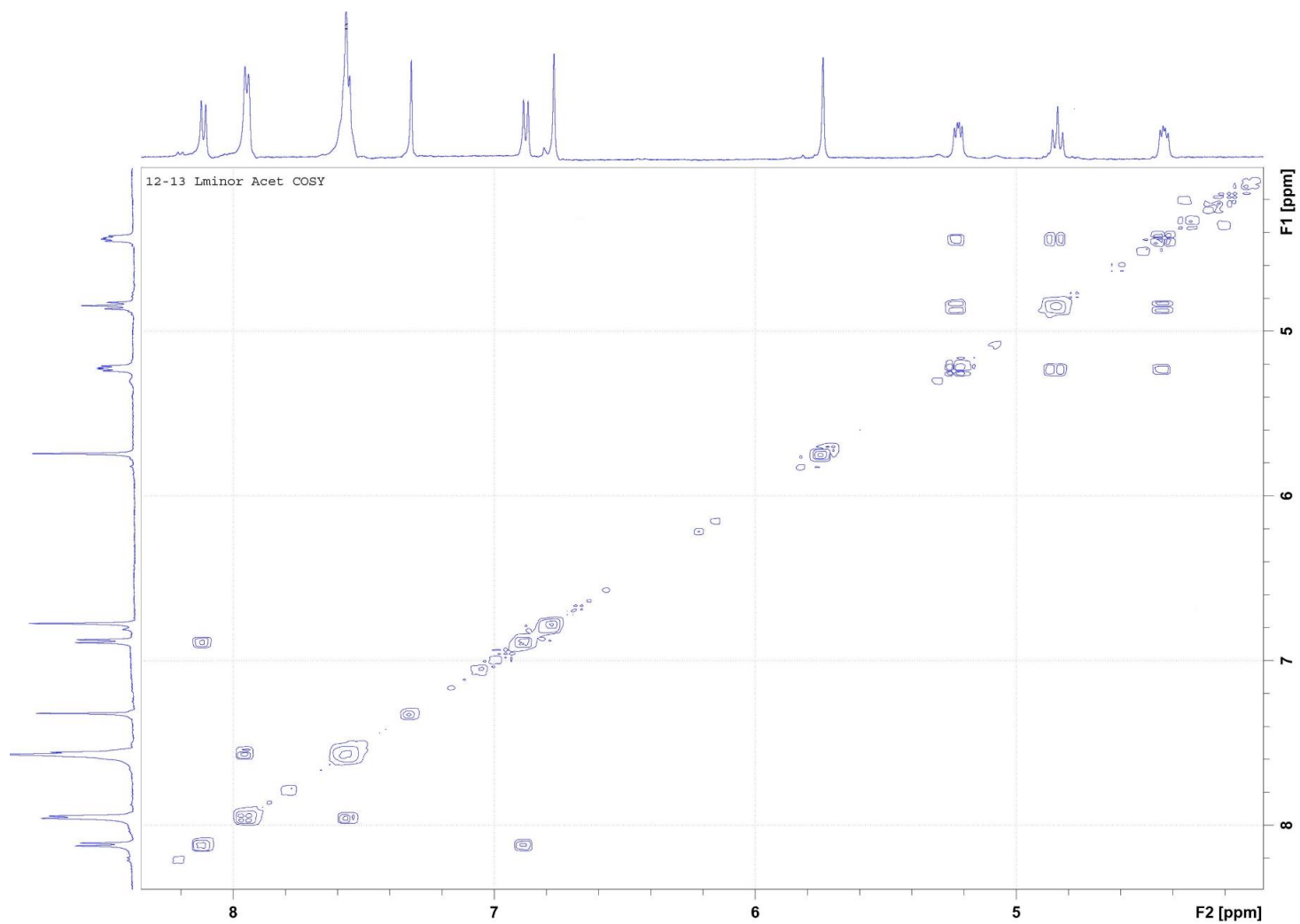


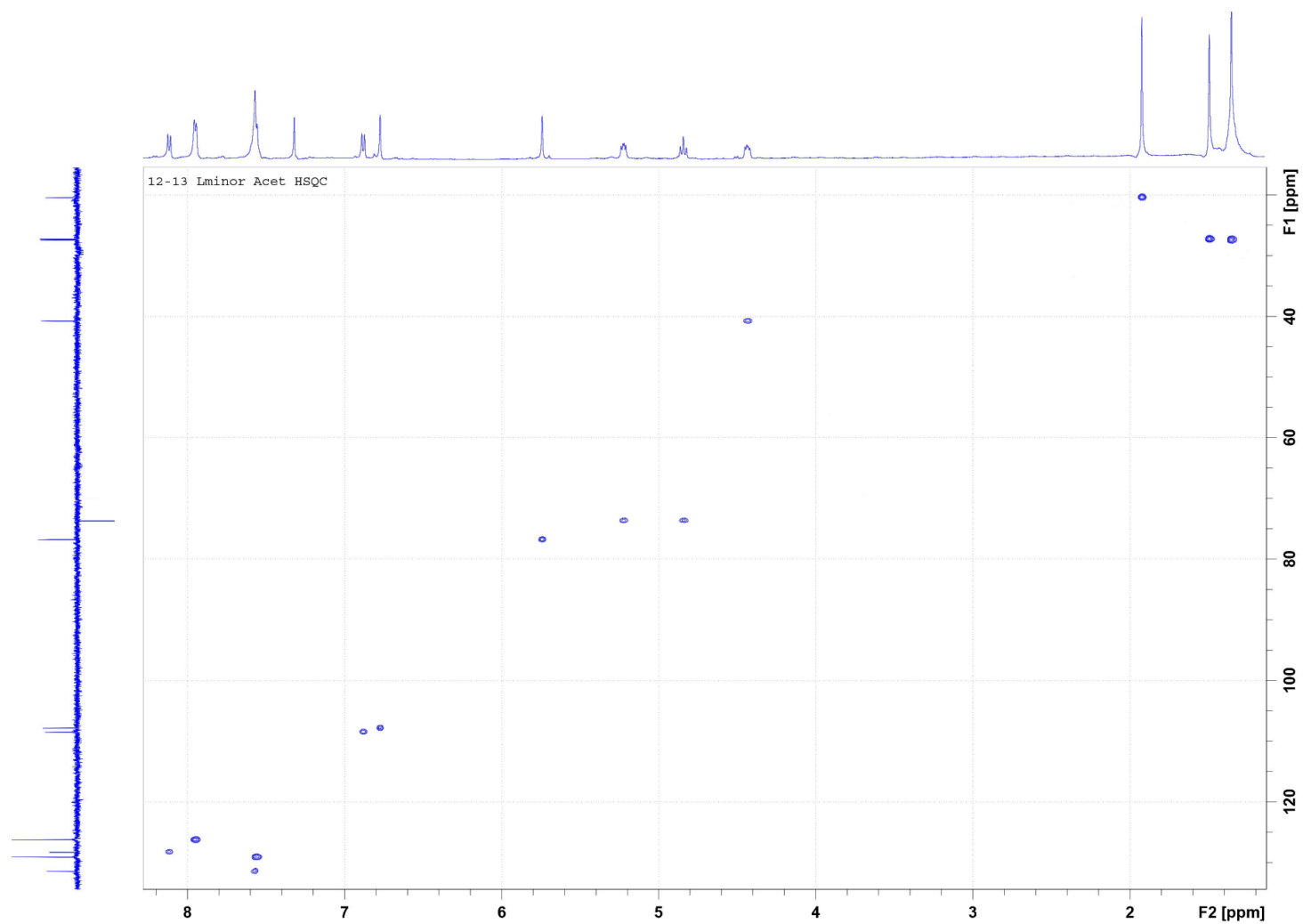
Figure S70: DEPT135 Spectrum of **6** acetate derivative in  $\text{CDCl}_3$ .



**Figure S71:** COSY Spectrum of **6** acetate derivative in  $\text{CDCl}_3$ .

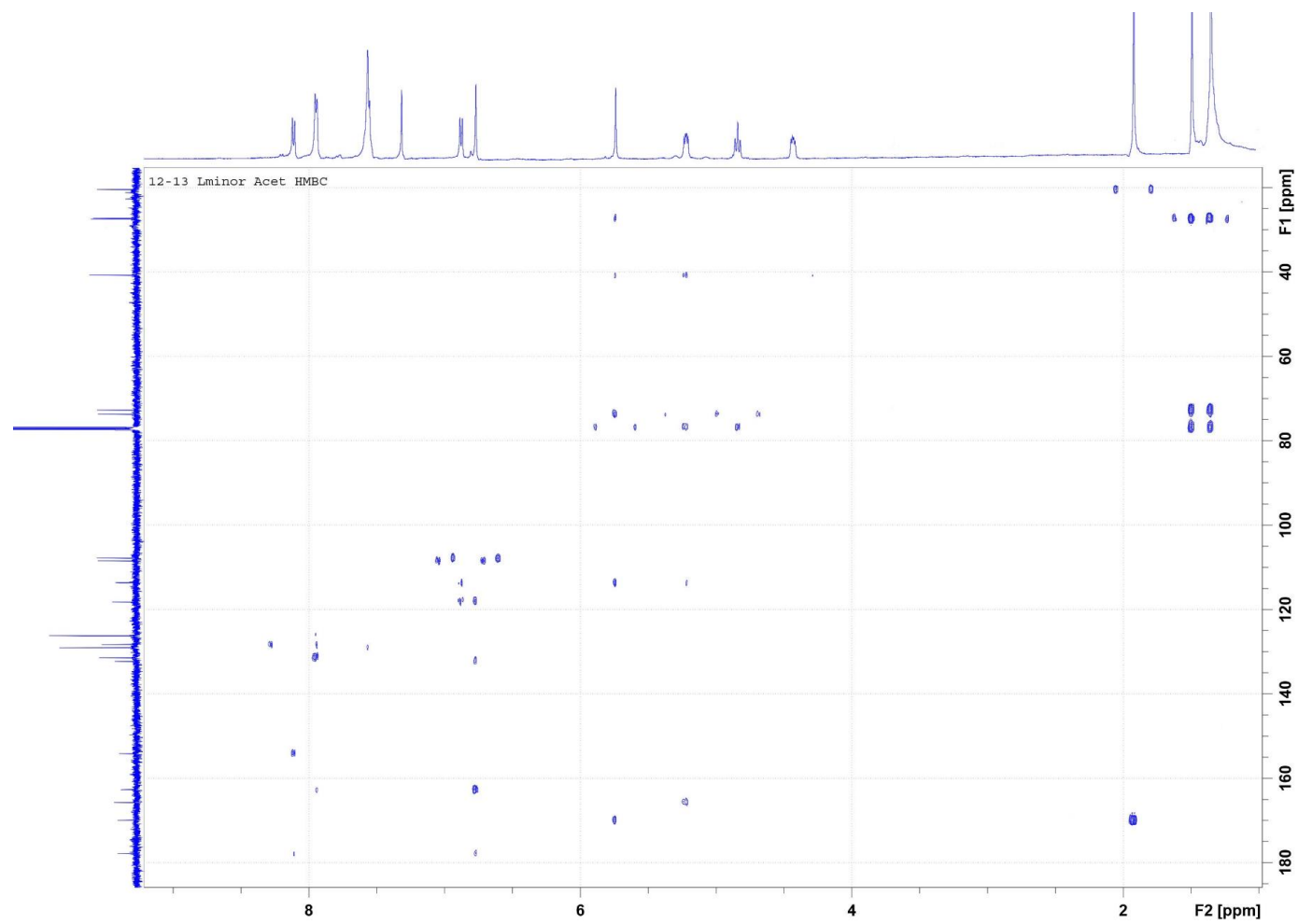
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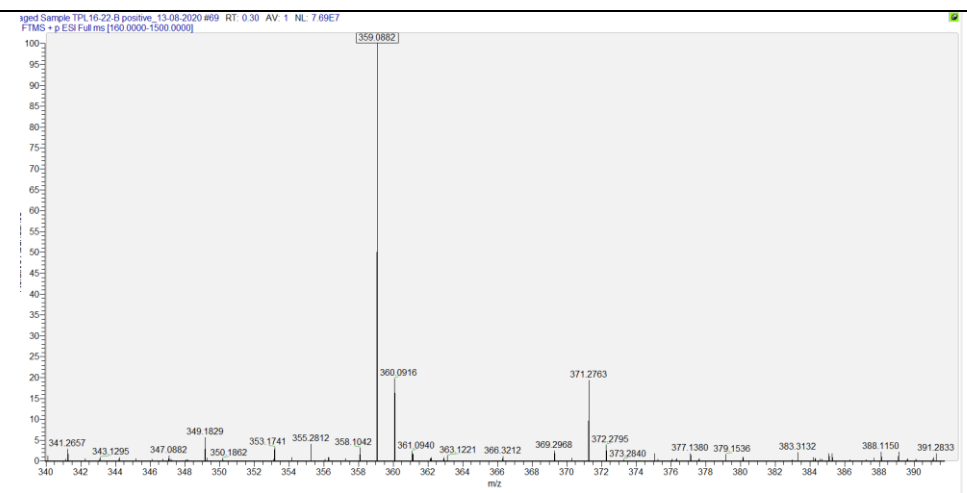
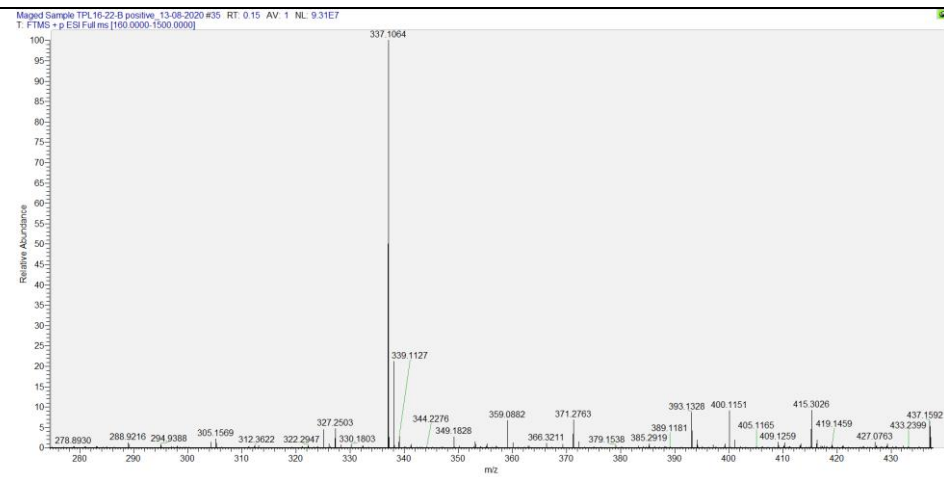


**Figure S72:** HSQC Spectrum of **6** acetate derivative in  $\text{CDCl}_3$ .

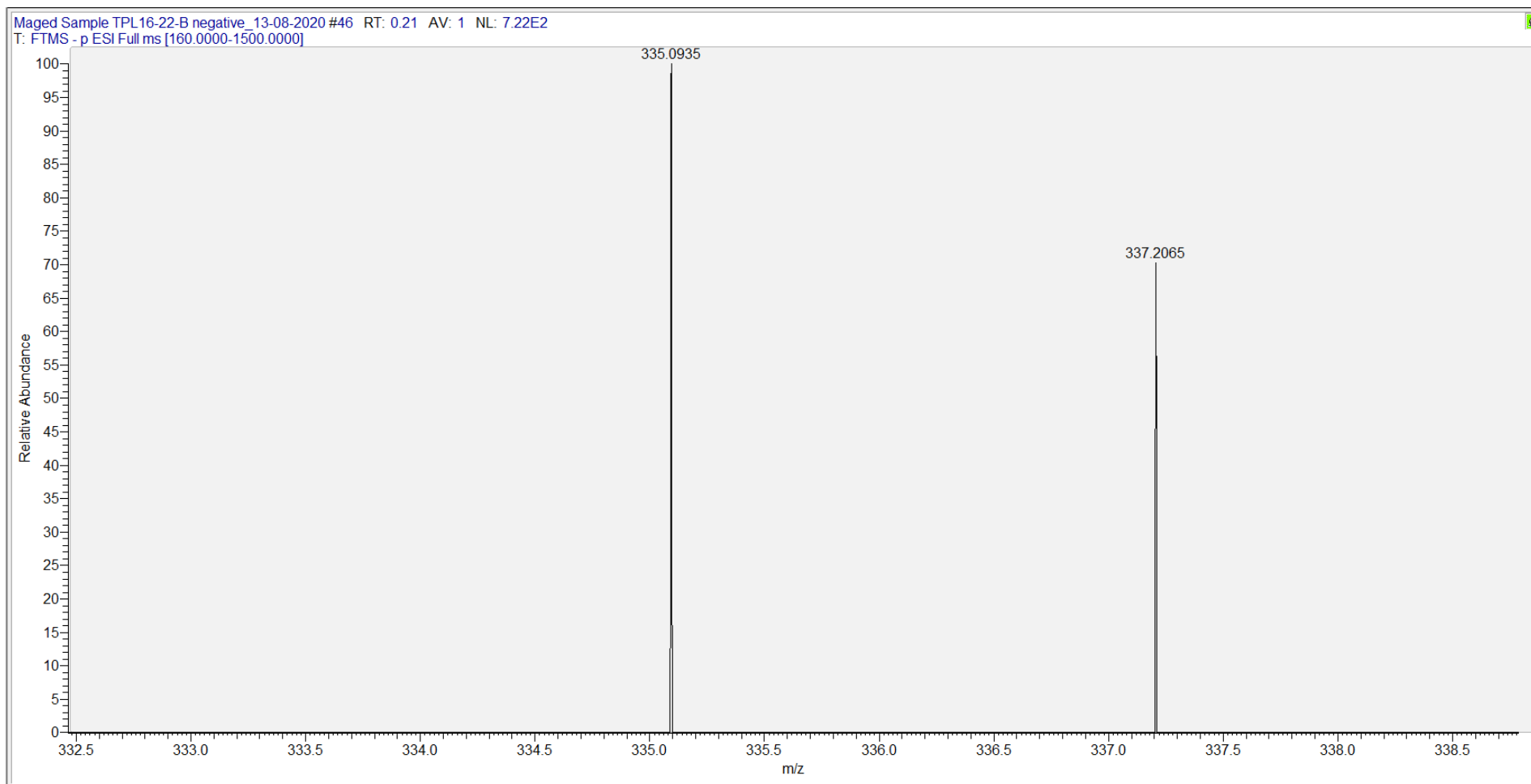
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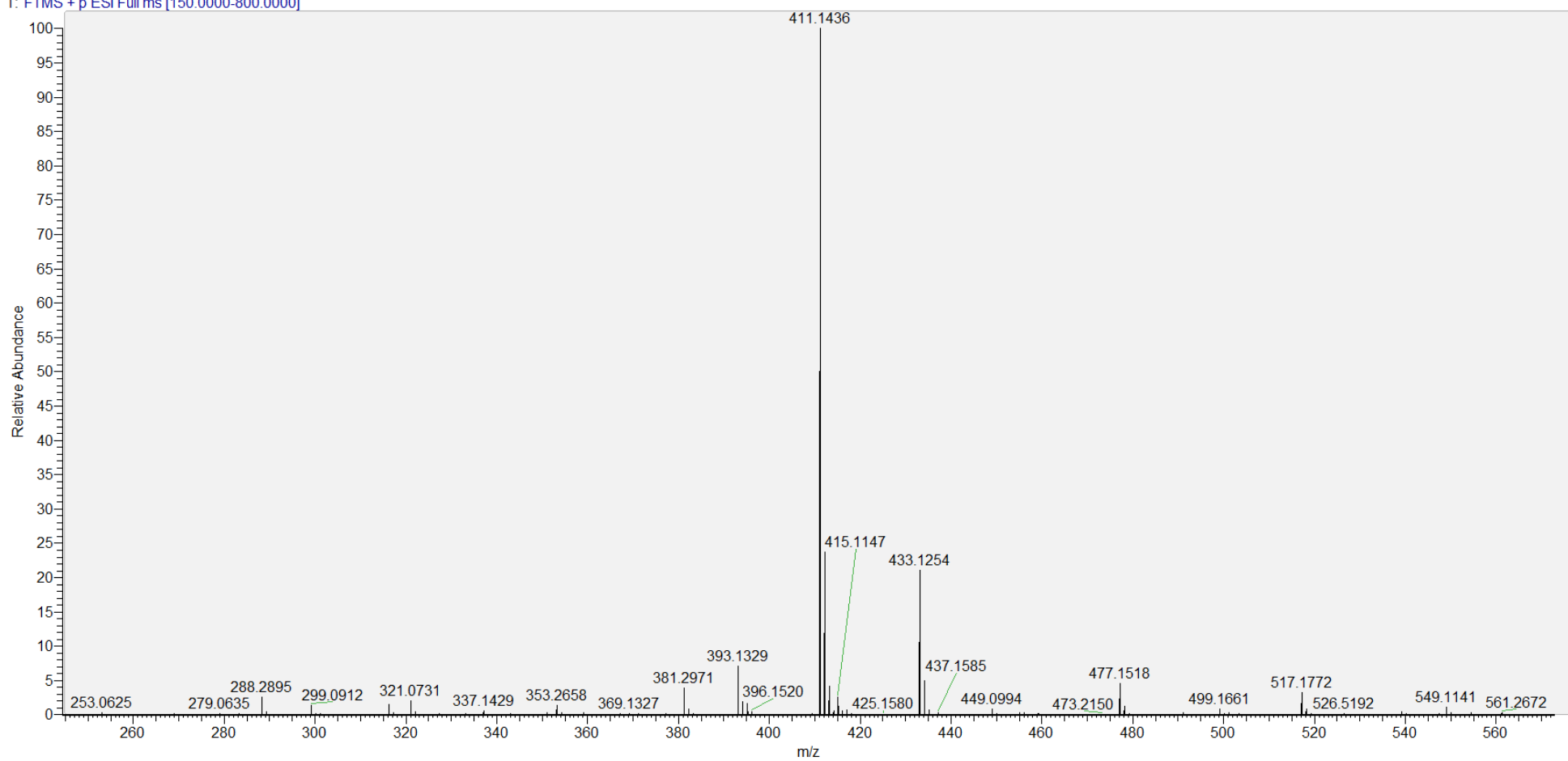
**Figure S73:** HMBC Spectrum of **6** acetate derivative in  $\text{CDCl}_3$ .



**Figure S74: HRESIMS Spectrum of 1 (Positive mode).**

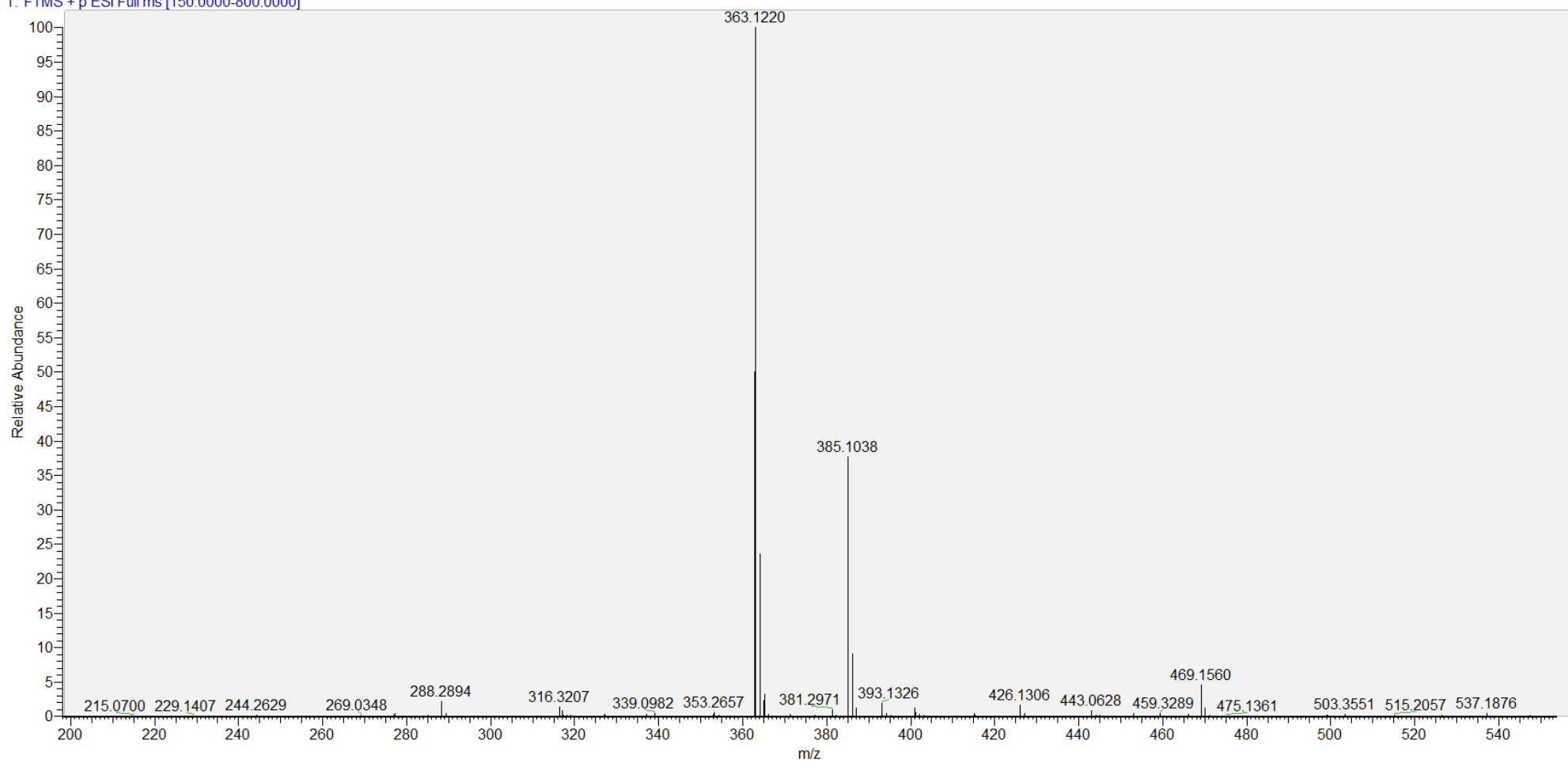


**Figure S75:** HRESIMS Spectrum of **1** (Negative mode).



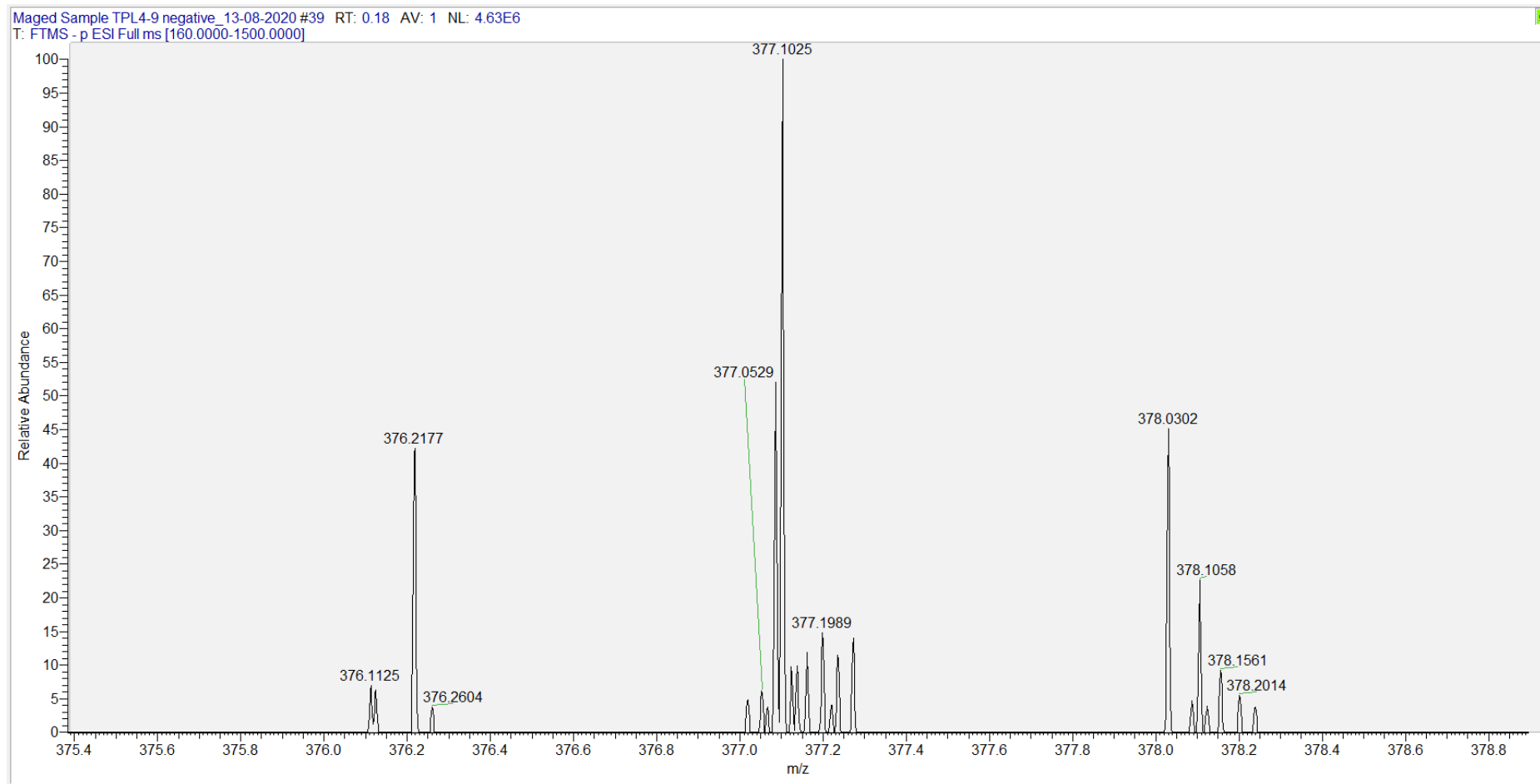
**Figure S76:** HRESIMS Spectrum of **2** (Positive mode).

Maged Sample N positive 15-04-2019 #49 RT: 0.21 AV: 1 NL: 2.88E9  
T: FTMS + p ESI Full ms [150.0000-800.0000]

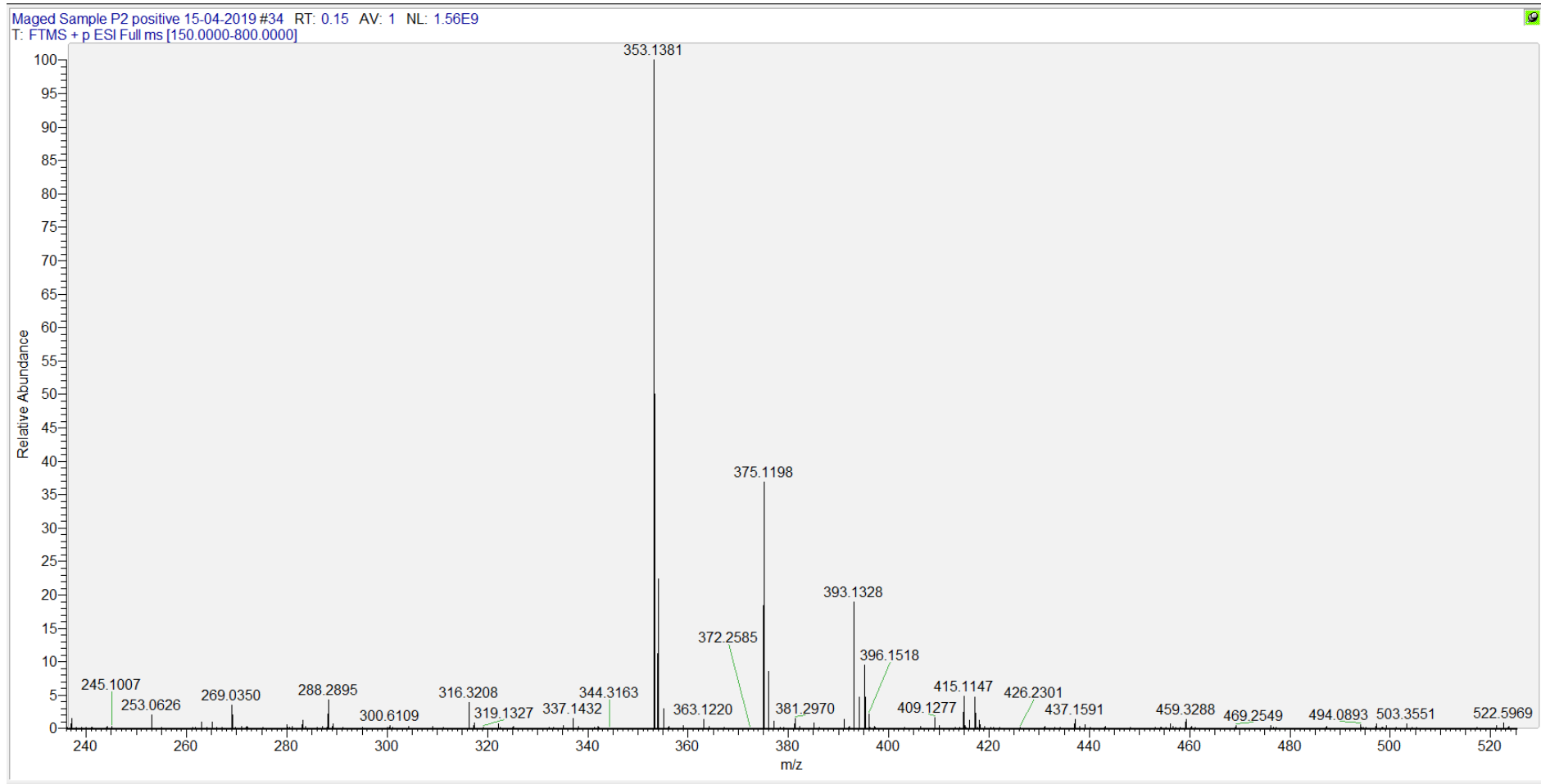


**Figure S77:** HRESIMS Spectrum of **4** (Positive mode).

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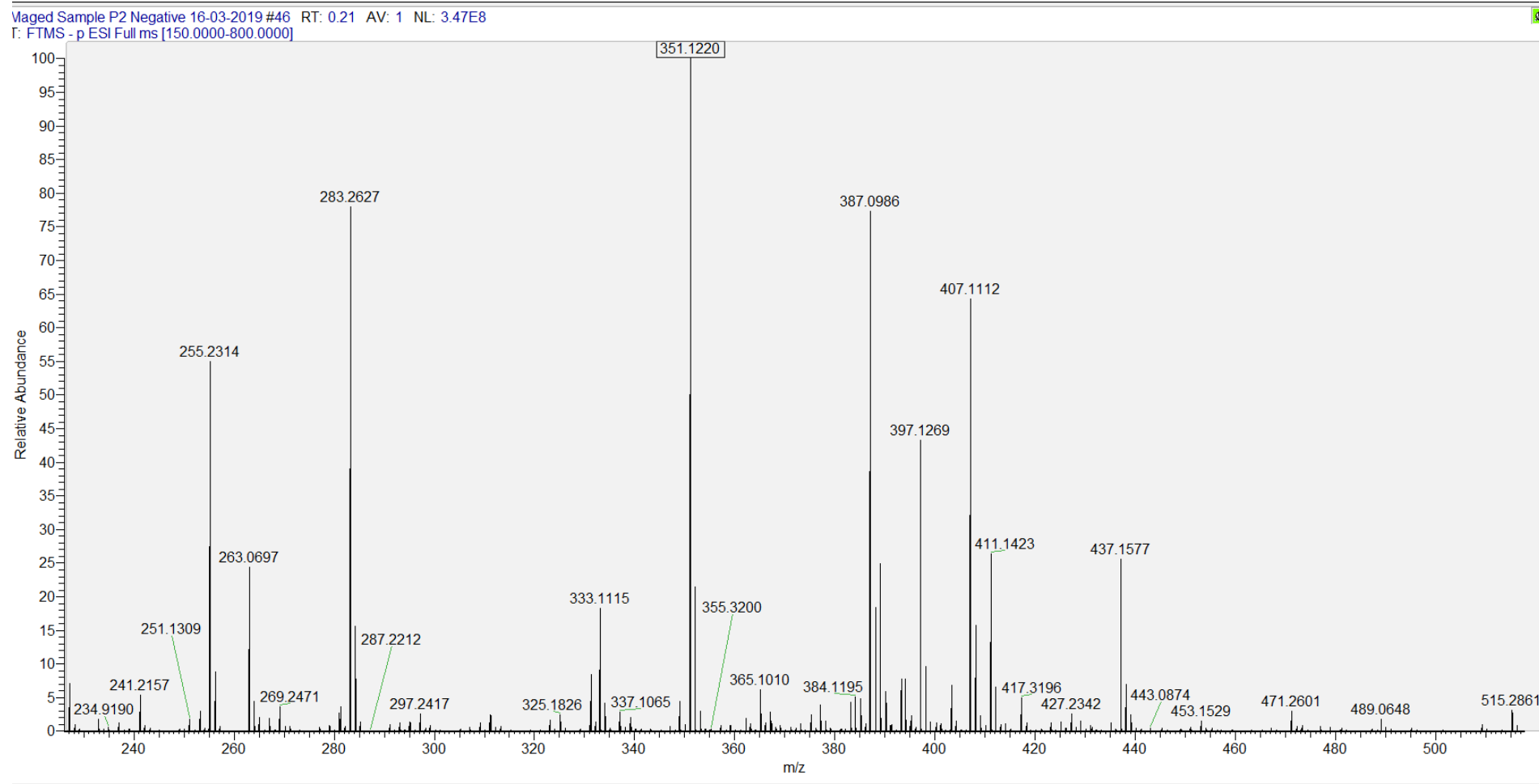


**Figure S78:** HRESIMS Spectrum of **4** (Negative mode).



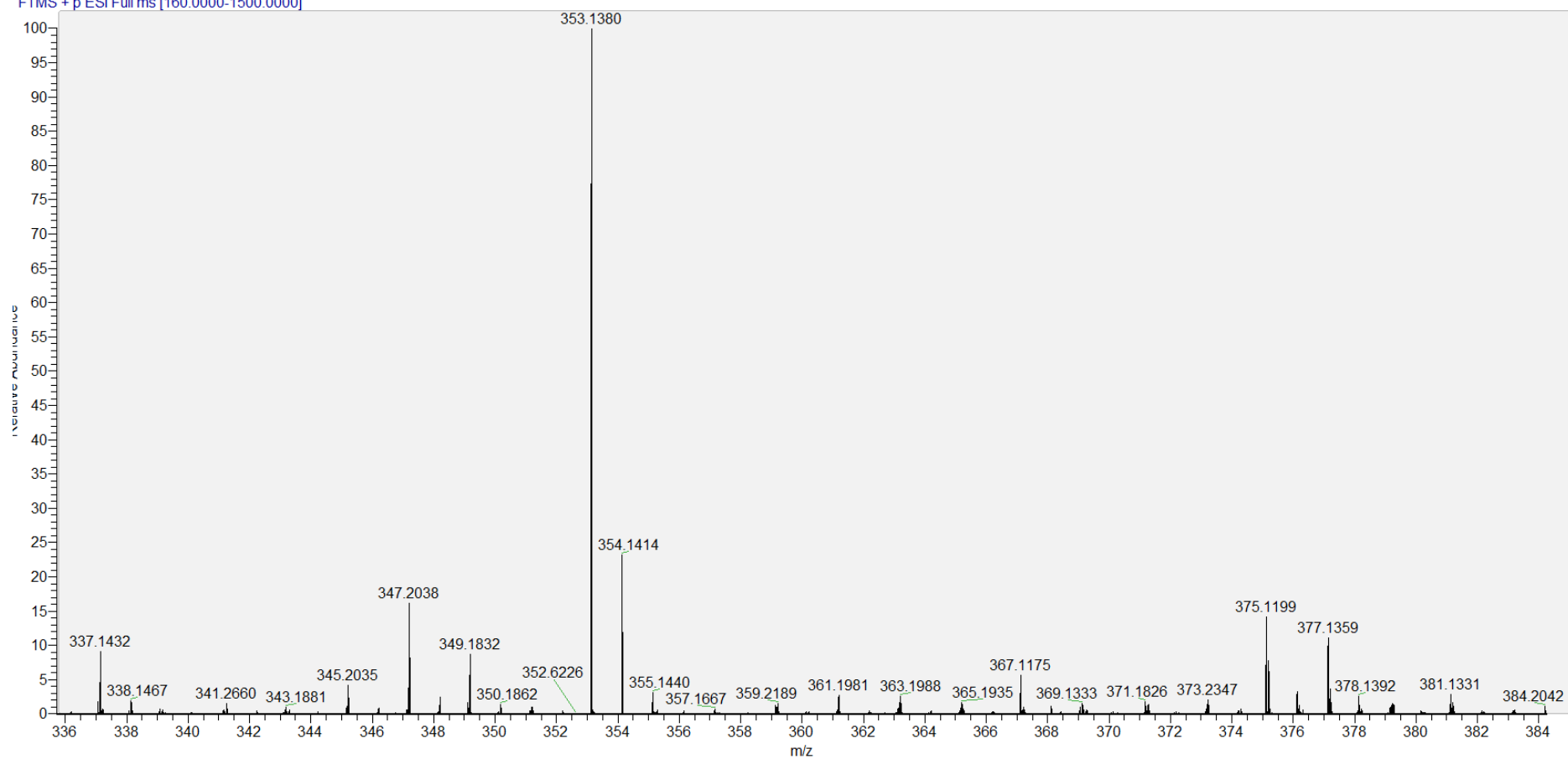
**Figure S79:** HRESIMS Spectrum of **5** (Positive mode).



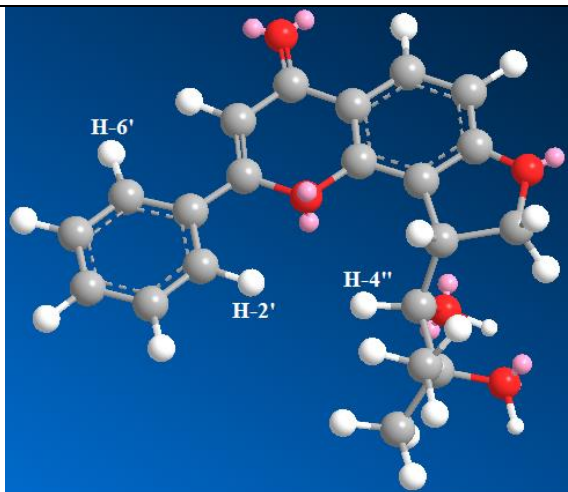


**Figure S80:** HRESIMS Spectrum of **5** (Negative mode).

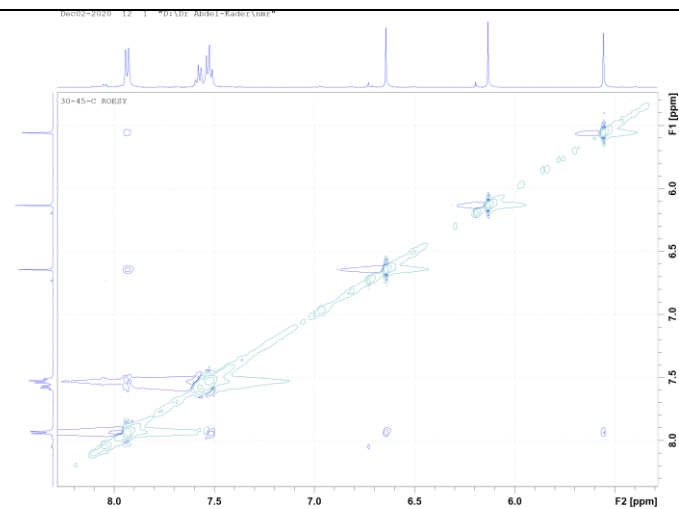
aged Sample TPL12-13-Lminor positive\_13-08-2020 #34 RT: 0.15 AV: 1 NL: 5.34E7  
FTMS + p ESI Full ms [160.0000-1500.0000]



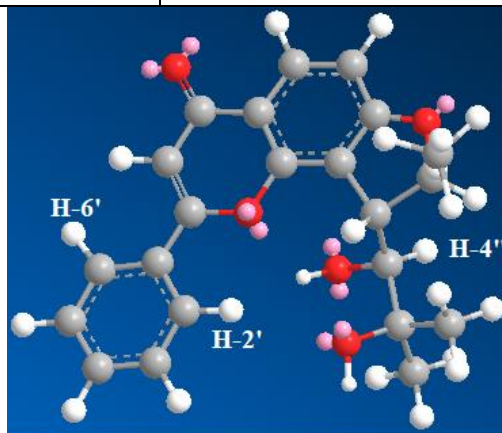
**Figure S81:** HRESIMS Spectrum of **6** (Positive mode).



Conformer A



ROESY experiment of 2



Conformer B

**Figure S82:** 3D Model of conformers A, B and ROESY Experiment of 2.

**Table S1.** <sup>1</sup>H-NMR data of compounds **2-6a** in comparison with published data for known epimers.

Pos	<b>2*</b>	<b>Tephropurpulin A*</b>	<b>4</b>	<b>Apollinin*</b>	<b>5</b>	<b>Tephroapoilin E*</b>	<b>6</b>	<b>6a</b>	<b>Tephroapoilin F*</b>
3	6.63 (s)	6.63 (s)	6.52 (s)	6.76 (s)	6.40 (s)	6.38 (s)	6.95 (s)	6.77 (s)	6.71 (s)
5	-	-	8.03 (d, 8.8)	8.26 (d, 9)	7.69 (d, 8.5)	7.67 (d, 8.5)	7.86 (d, 8.6)	8.11 (d, 8.5)	7.94 (d, 8.5)
6	6.26 (s)	6.26 (s)	6.86 (d, 8.8)	7.10	6.84 (d, 8.5)	6.74 (d, 8.5)	6.91 (d, 8.6)	6.87 (d, 8.5)	6.80 (d, 8.5)
2',6'	7.90 (d, 7.7, 2H)	7.88 (m)	7.54 (d, 6.9)	7.43-7.55 (m)	7.77 (d, 8.5)	7.65 (dd, 2.5, 8)	8.10 (d, 7.7)	7.95 (d, 6.7, 2H)	7.94 (dd, 2.5, 8)
3',5' 4'	7.54 (m, 3H)	7.55 (m)	7.27 (m)	7.73-7.86 (m) 7.43-7.55 (m)	7.37 (t, 7.4) 7.45 (t, 7.4)	7.44 (t, 8) 7.52 (t, 8)	7.58 (m)	7.55 m	7.45 (t, 8)
2''	4.75 (t, 12) 5.11 (dd, 6.2, 12.3)	4.72 (t, 19.0) 5.11 (dd, 19.0, 10.2)	-	-	4.69 (t, 8.4) 4.79 (d, 8.7)	4.76 (t, 9) 5.23 (dd, 2.8, 9)	4.72 (t, 9.6) 5.01 (t, 7.8)	4.84 (t, 9.7) 5.22 (q, 5.6)	4.69 (dd, 8.3, 9) 4.97 (dd, 2.8, 9)
3''	4.26 (dd, 6.2, 12.3)	4.25 (dd (10.2, 19.0)	-	-	4.10 (t, 7)	4.21 (dd, 7.5, 9)	4.36 (dd, 6.5, 10)	4.43 (q, 5.6)	4.21 (ddd, 2.8, 8.3, 9)
4''	5.62 (s)	5.61 (brs)	-	7.53 (s)	3.83 (d, 8.5)	4.41 (s)	4.13 (s)	5.74 (s)	5.08 (d, 9)
Gem	1.31 (s)	1.25 (s)	1.45 (s, 6H)	1.67 (s, 6H)	1.41 (s)	1.36 (s)	1.14 (s)	1.35 (s)	1.27 (s)
2 CH <sub>3</sub>	1.44 (s)	1.29 (s)	-	-	1.42 (s)	1.47 (s)	1.23 (s)	1.49 (s)	1.39 (s)
COCH <sub>3</sub>	1.93 (s)	1.92 (s)	-	-	-	-	-	1.92 (s)	1.97 (s)
OCH <sub>3</sub>	-	-	3.73 (s)	3.96 (s)	-	-	-	-	-

\*Spectra in CDCl<sub>3</sub>.

**Table S2.**  $^{13}\text{C}$ -NMR data of compounds **2-6a** in comparison with published data for known epimers.

Pos	<b>2</b> *	Tephropurpulin A*	<b>4</b>	Apollinin*	<b>5</b>	Tephroapoilin E*	<b>6</b>	<b>6a</b>	Tephroapoilin F*
2	163.42	163.4	161.70	161.6	163.01	162.6	162.00	162.65	162.0
3	106.13	106.3	107.28	107.2	106.14	106.9	106.90	107.80	106.7
4	182.25	182.2	177.73	177.5	178.11	177.6	177.03	177.82	177.8
5	163.53	163.6	128.08	128.0	127.83	127.7	126.77	128.26	128.1
6	94.21	94.2	109.36	109.3	108.94	109.1	108.76	108.47	109.1
7	167.12	166.9	163.17	163.0	166.44	166.4	166.07	165.65	166.6
8	103.68	103.5	107.65	114.2	115.13	115.0	117.58	118.18	117.8
9	153.23	153.2	154.84	158.0	154.99	153.8	153.71	154.08	154.2
10	105.36	105.4	117.98	117.8	117.78	117.5	117.90	113.60	114.4
1'	131.61	131.7	131.86	131.8	131.58	131.6	131.72	132.27	131.4
2',6'	126.23	126.2	126.19	126.1	126.16	125.9	126.60	126.21	126.2
3',5'	129.10	129.1	129.00	128.9	128.89	129.0	129.59	129.05	129.0
4'	131.78	131.7	131.55	131.4	131.36	131.6	132.20	131.40	131.7
2''	73.77	73.9	170.70	170.5	77.84	72.9	73.57	73.65	78.1
3''	40.04	40.1	124.16	124.0	42.92	42.5	41.69	40.74	40.7
4''	76.67	76.8	160.04	159.9	79.08	75.3	75.99	76.75	79.0
5''	72.55	72.6	85.02	84.9	73.24	72.9	72.26	70.97	72.2
Gem 2	27.15	27.1	25.83 (2X)	25.8 (2X)	25.84	25.6	26.25	27.25	25.2
CH <sub>3</sub>	27.36	27.5			26.64	27.7	28.18	27.39	27.5
COCH <sub>3</sub>	170.08	169.9	-		-			169.89	169.5
	20.48	20.5						20.41	20.4
OCH <sub>3</sub>			56.61		-			-	-

\*Spectra in CDCl<sub>3</sub>.