

## Supporting Information

*Rec. Nat. Prod.* 19:2 (2025) 157-168

### Investigation of Anti-oxidative Stress and Anti-inflammatory Constituents from *Sphaerocoryne affinis* Leaves

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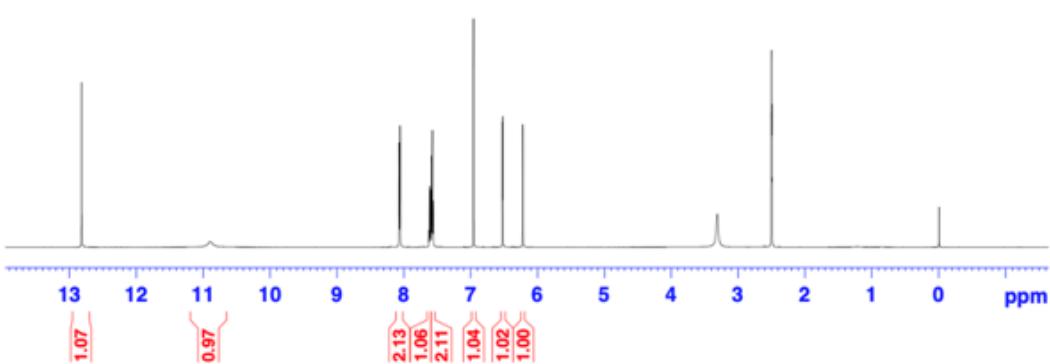
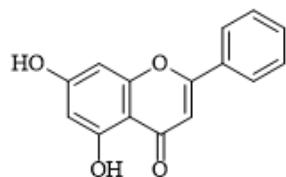
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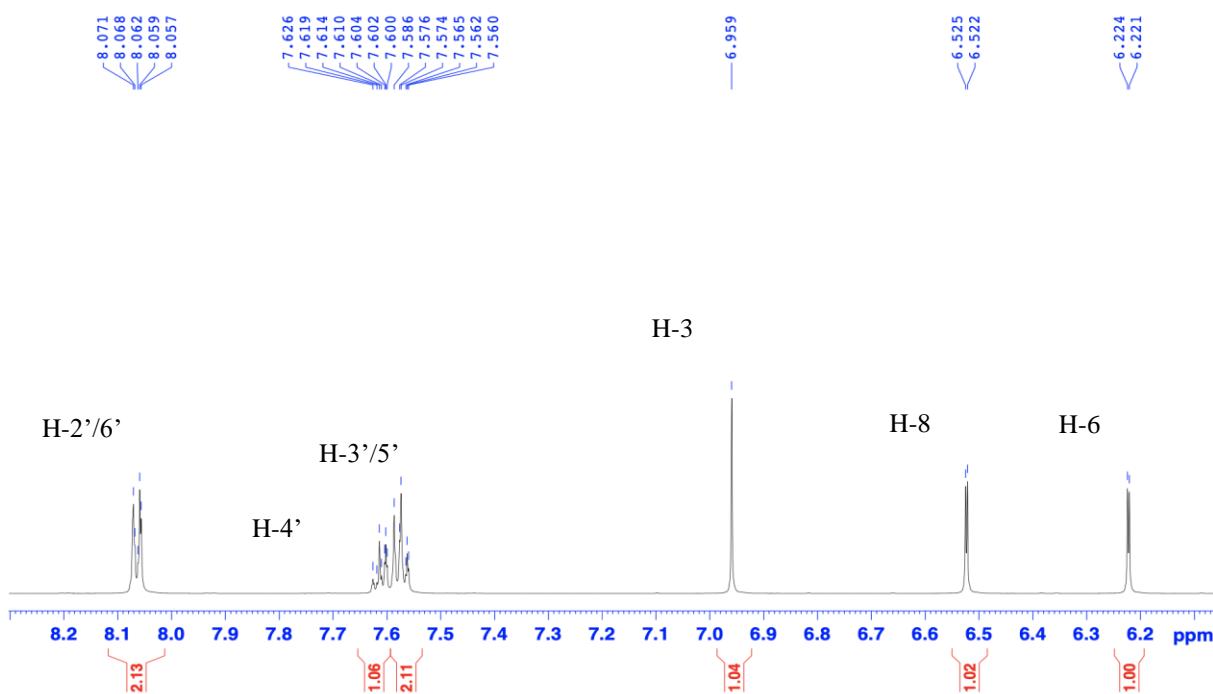
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**Table S1:** The comparison of NMR data of compound **1** with a similar compound (Chrysin)

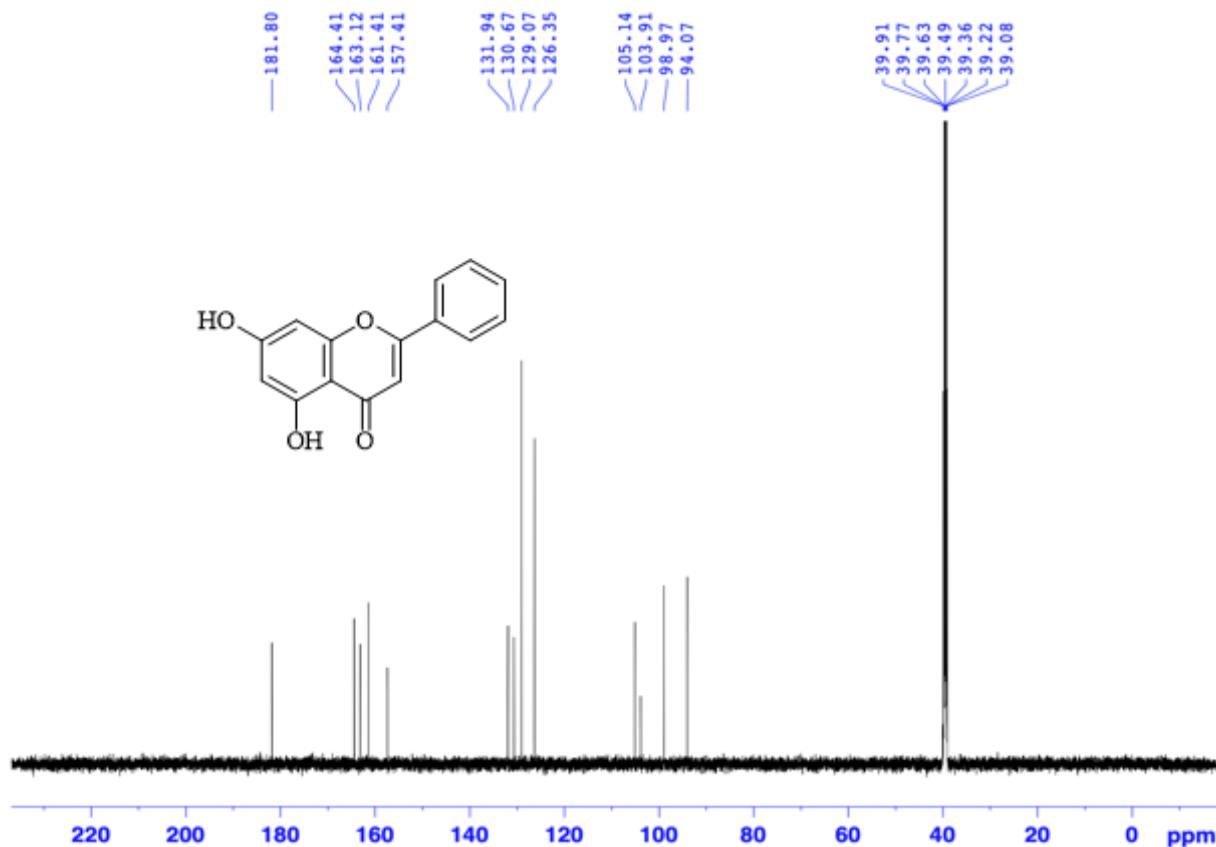
	Compound 1 (DMSO- <i>d</i> <sub>6</sub> )		Chrysins (DMSO- <i>d</i> <sub>6</sub> ) [28]	
Position	<sup>13</sup> C-NMR (150 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_{\text{H}}$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (500 MHz) $\delta_{\text{H}}$ ppm
2	161.4	-	161.95	-
3	105.1	6.95 (1H, <i>s</i> )	104.47	6.96 (1H, <i>s</i> )
4	181.8	-	182.34	-
5	163.1	-	163.69	-
6	98.9	6.22 (1H, <i>d</i> , 1.8 Hz)	99.51	6.20 (1H, <i>d</i> , 1.8 Hz)
7	164.4	-	164.91	-
8	94.0	6.52 (1H, <i>d</i> , 1.8 Hz)	94.61	6.51 (1H, <i>d</i> , 2.4 Hz)
9	157.4	-	157.96	-
10	103.9	-	105.68	-
1'	130.6	-	132.48	-
2',6'	126.3	8.07 (2H, <i>m</i> )	126.89	8.06 (2H, <i>m</i> )
3',5'	129.1	7.58 (2H, <i>m</i> )	129.61	7.58 (3H, <i>m</i> )
4'	131.9	7.62 (1H, <i>m</i> )	131.21	



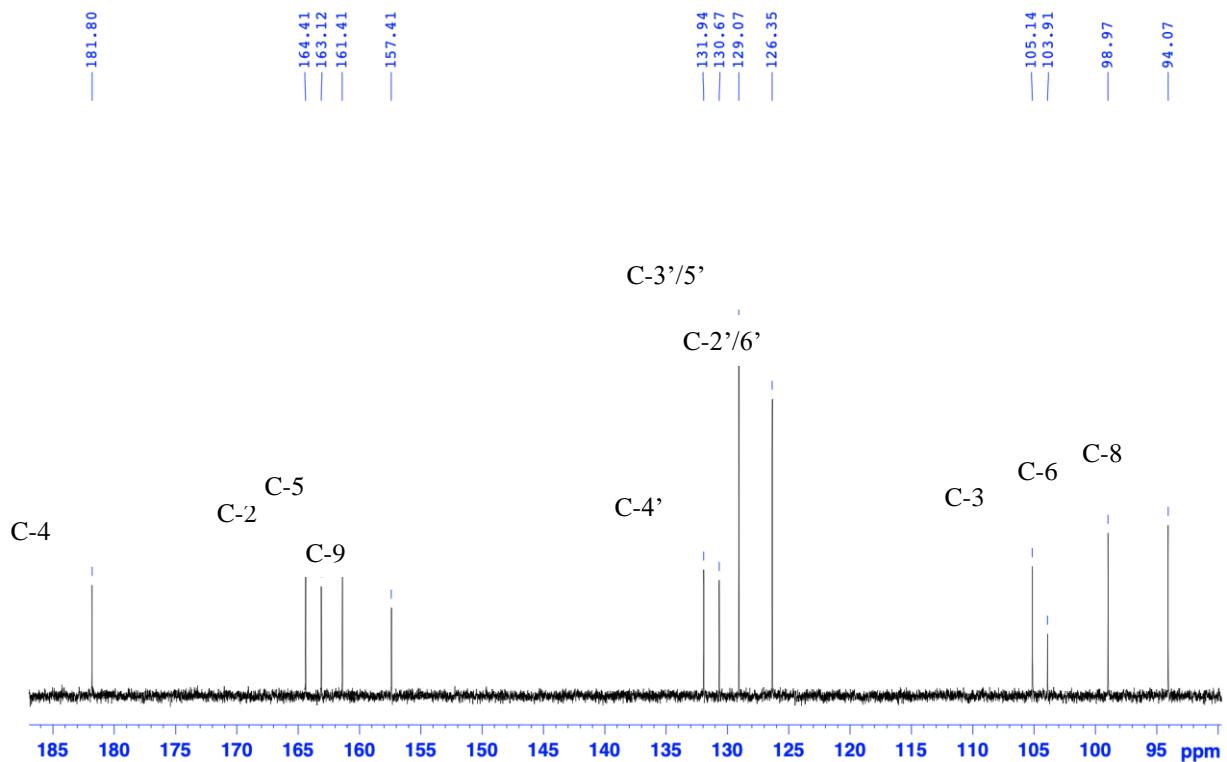
**Figure S1:**  $^1\text{H}$ -NMR (600 MHz, DMSO- $d_6$ ) spectrum of compound **1** (chrysin)



**Figure S2:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **1** (chrysin) (from  $\delta_{\text{H}}$  6 ppm to  $\delta_{\text{H}}$  9 ppm)



**Figure S3:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **1** (chrysin)

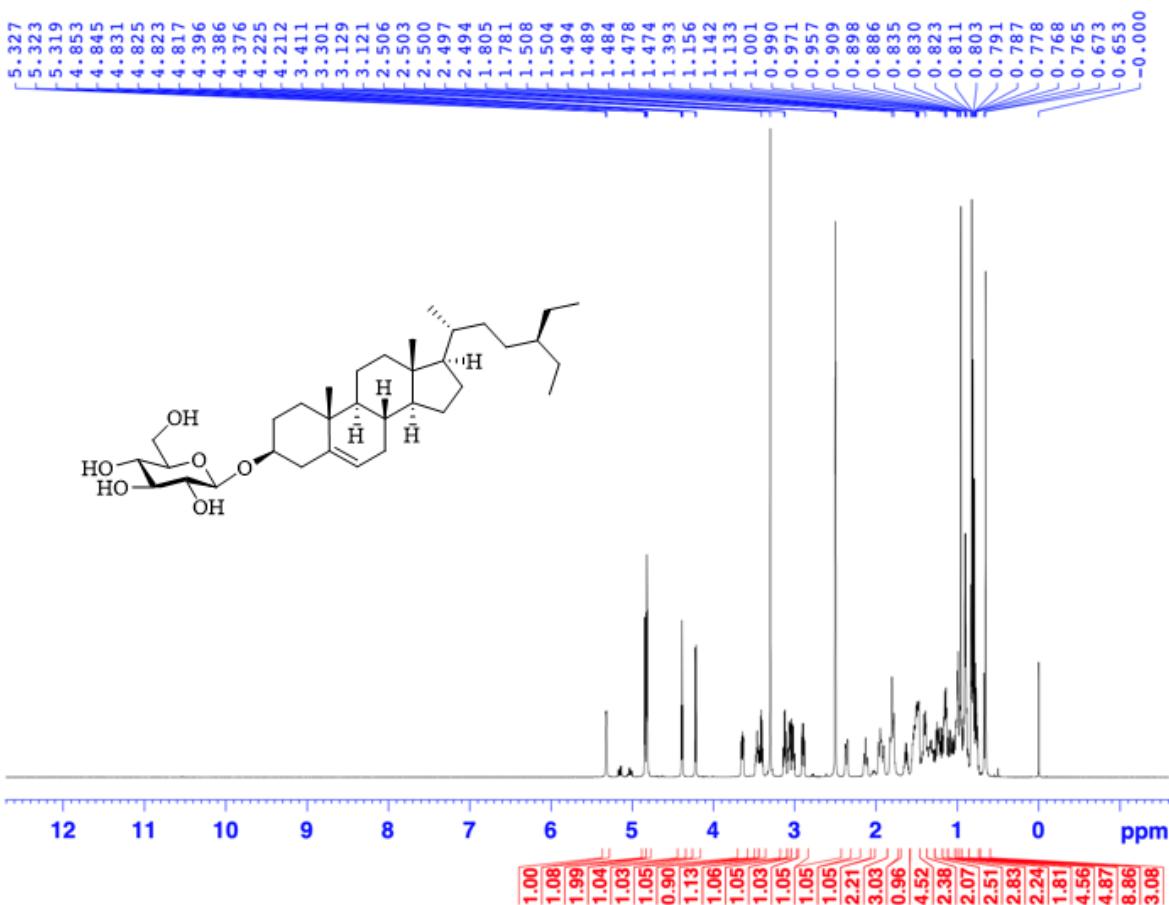


**Figure S4:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **1** (chrysanthemic acid) (from  $\delta_{\text{C}}$  95 ppm to  $\delta_{\text{C}}$  190 ppm)

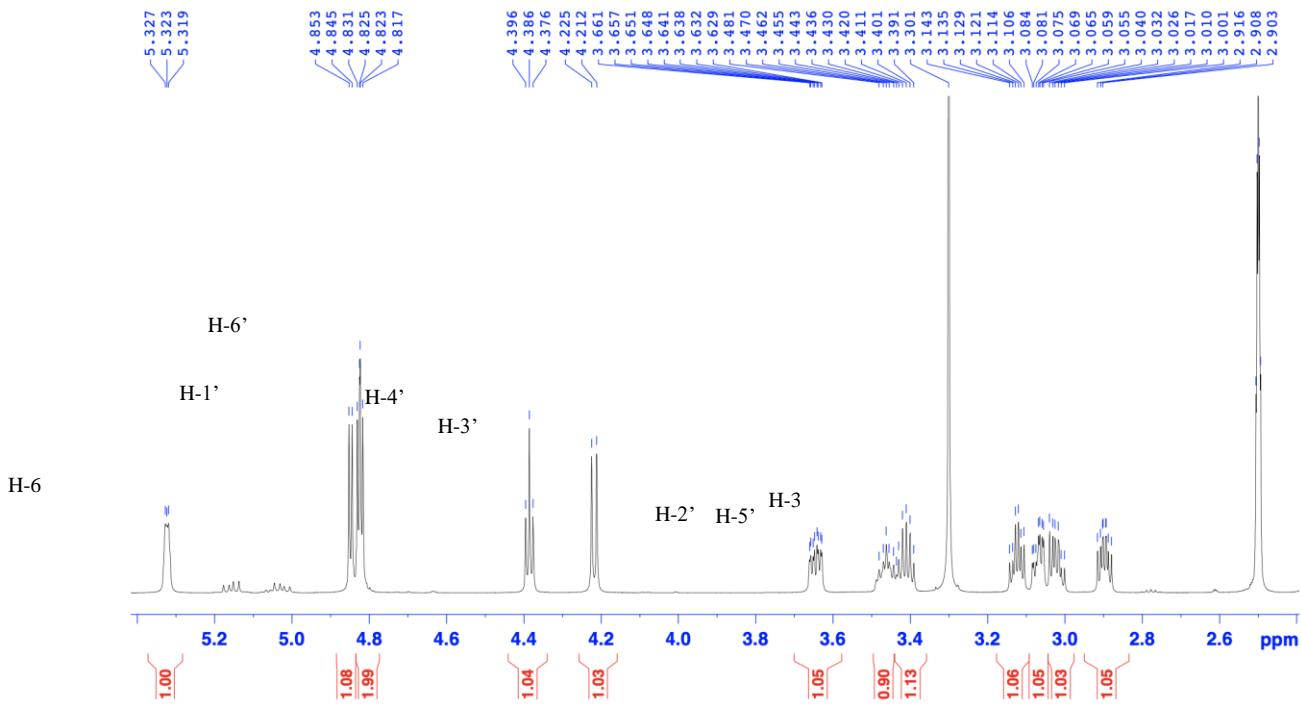
**Table S2 :** The comparison of NMR data of compound **2** with a similar compound (Daucosterol)

Position	Compound 2 (DMSO- <i>d</i> <sub>6</sub> )		Daucosterol (DMSO- <i>d</i> <sub>6</sub> ) [29]	
	<sup>13</sup> C-NMR (150 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (100 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (400 MHz) δ <sub>H</sub> ppm
1	36.2	-	36.1	-
2	31.3	-	31.3	-
3	76.7	3.66 (1H, <i>m</i> )	76.6	3.95 (1H, <i>m</i> )
4	38.3	2.50 (1H, <i>m</i> )	38.2	2.62 (1H, <i>m</i> ) 2.36 (1H, <i>m</i> )
5	140.4	-	140.3	-
6	121.1	-	121.0	-
7	31.4	-	31.3	-
8	31.3	-	31.2	-
9	49.6	-	49.5	-
10	35.4	-	35.5	-
11	20.6	-	20.5	-
12	39.2	-	39.2	-
13	41.8	-	41.8	-
14	56.1	-	56.1	-
15	23.8	-	23.4	-
16	27.7	-	27.7	-
17	55.4	-	55.3	-
18	11.6	0.70 (3H, <i>s</i> )	11.6	0.65 (3H, <i>s</i> )
19	19.6	0.71 (3H, <i>s</i> )	18.8	0.95 (3H, <i>s</i> )
20	36.8	-	36.7	-
21	20.6	0.89 (3H, <i>s</i> )	18.5	0.98 (3H, <i>d</i> , 6.5 Hz)
22	33.3	-	33.3	-
23	25.4	-	25.4	-
24	45.1	-	45.1	-
25	28.7	-	28.6	-
26	19.0	-	19.0	-
27	18.9	0.91 (3H, <i>s</i> )	19.6	0.87 (3H, <i>d</i> , 6.7 Hz)
28	22.6	0.90 (3H, <i>s</i> )	22.5	0.89 (3H, <i>d</i> , 6.5 Hz)
29	11.7	0.93 (3H, <i>s</i> )	11.7	0.88 (3H, <i>t</i> , 7.2 Hz)
1'	100.8	4.85 (1H, <i>m</i> )	100.7	4.87 (1H, <i>d</i> , 7.9 Hz)
2'	73.4	4.22 (1H, <i>m</i> )	73.4	4.05 (1H, <i>t</i> , 8.0 Hz)
3'	76.9	4.38 (1H, <i>m</i> )	76.9	4.25 (1H, <i>t</i> , 9.0 Hz)

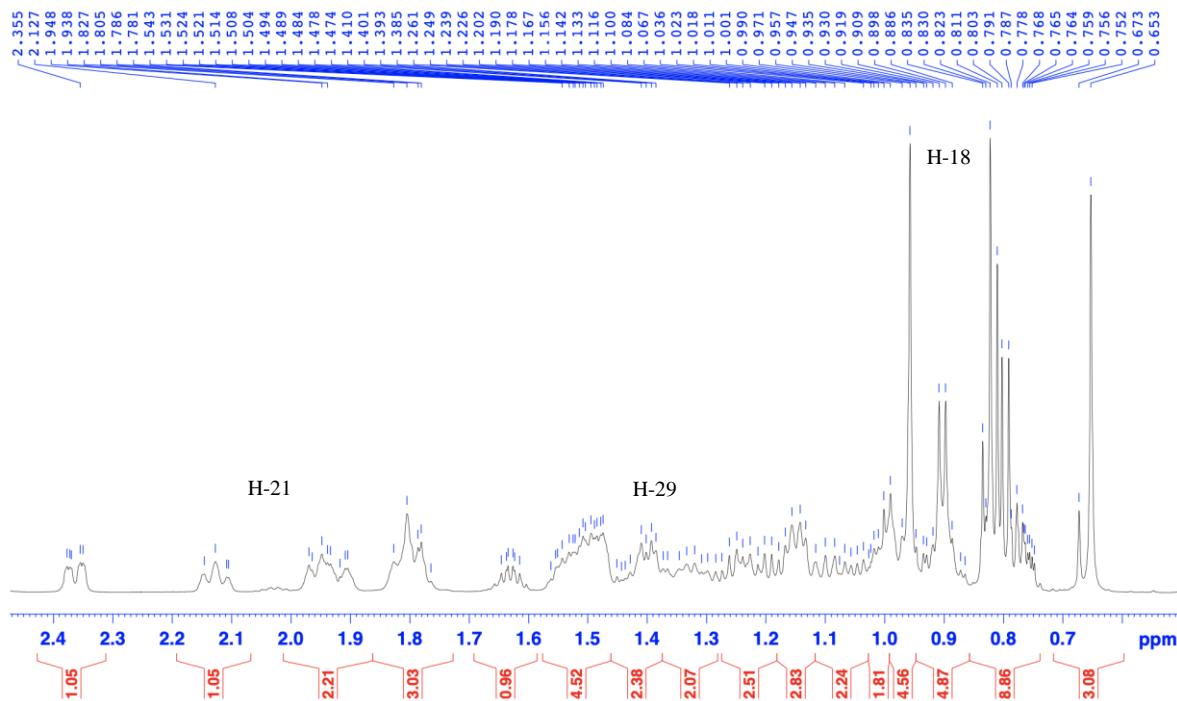
Position	Compound 2 (DMSO- <i>d</i> <sub>6</sub> )		Daucosterol (DMSO- <i>d</i> <sub>6</sub> ) [29]	
	<sup>13</sup> C-NMR (150 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_{\text{H}}$ ppm	<sup>13</sup> C-NMR (100 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (400 MHz) $\delta_{\text{H}}$ ppm
	4'	70.1	4.39 (1H, <i>m</i> )	70.0
5'	70.7	4.21(1H, <i>m</i> )	76.7	4.00 (1H, <i>m</i> )
6'	61.1	4.32 (2H, <i>m</i> )	61.0	4.55 (1H, <i>t</i> , 5.4 Hz) 4.39 (1H, <i>dd</i> , 12.0 Hz)



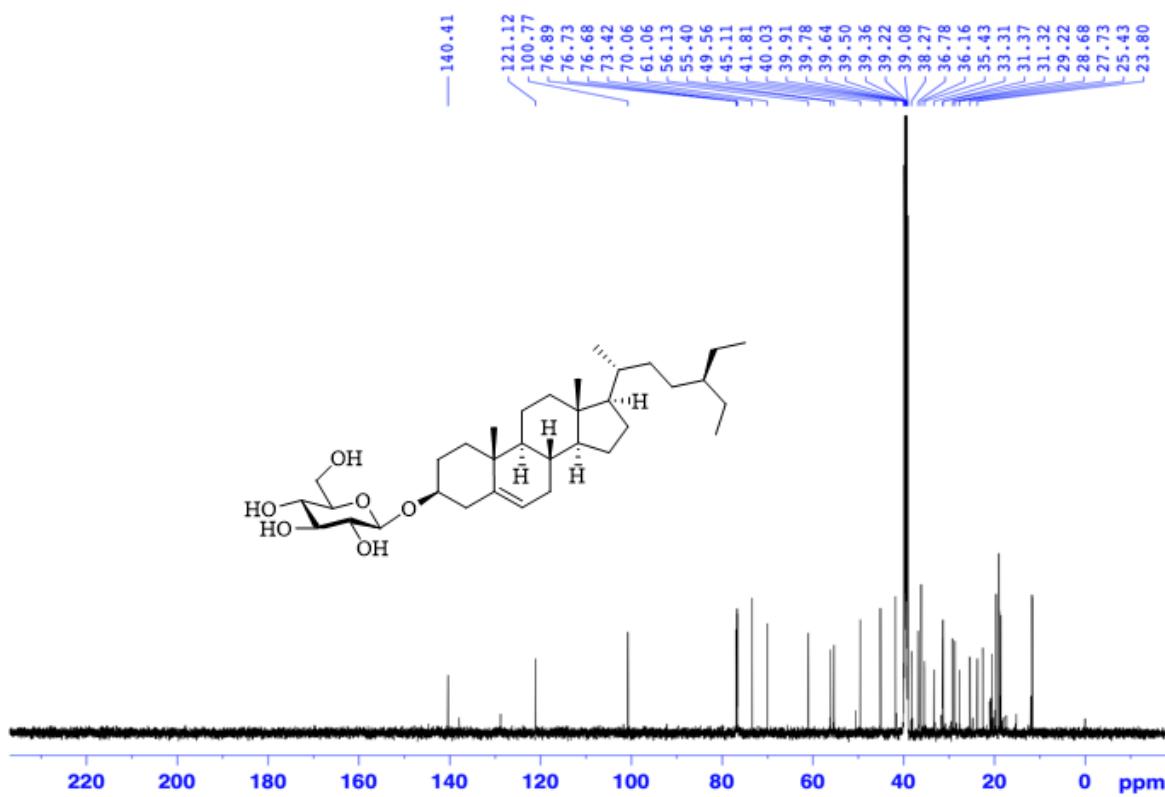
**Figure S5:**  $^1\text{H}$ -NMR (600 MHz, DMSO- $d_6$ ) spectrum of compound **2** (daucosterol)



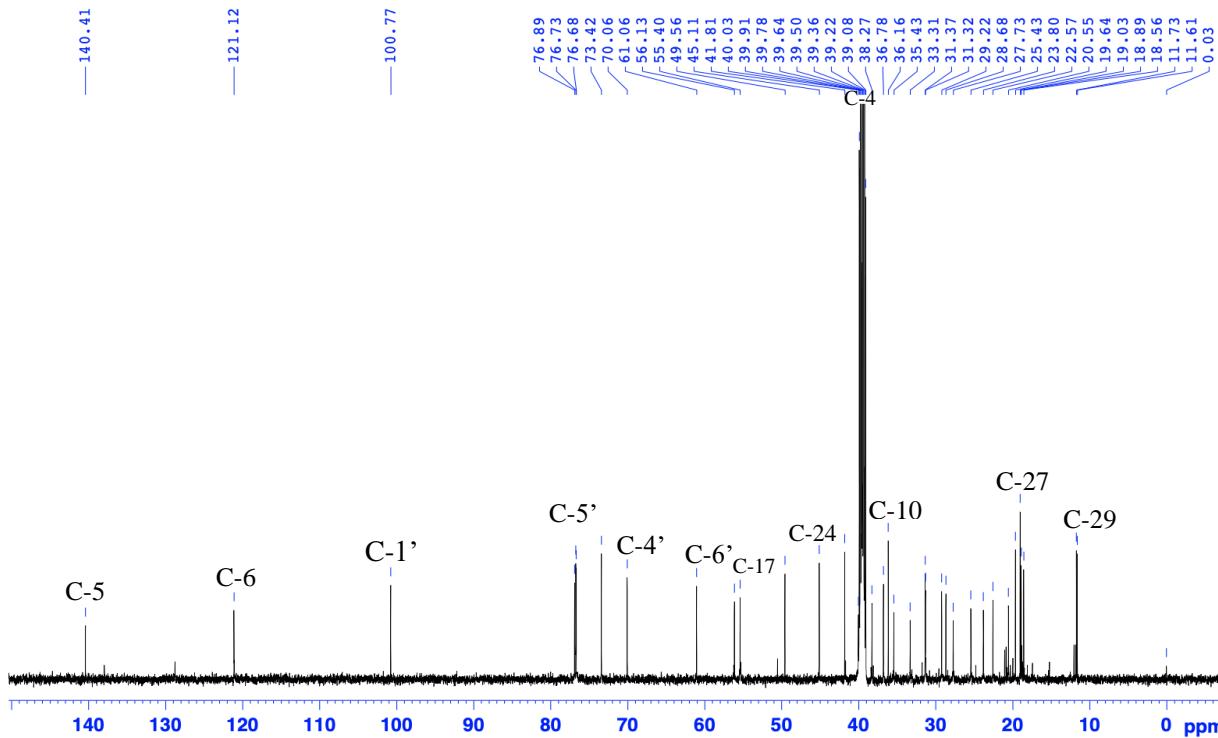
**Figure S6:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{H}}$  2.7 ppm to  $\delta_{\text{H}}$  5.3 ppm)



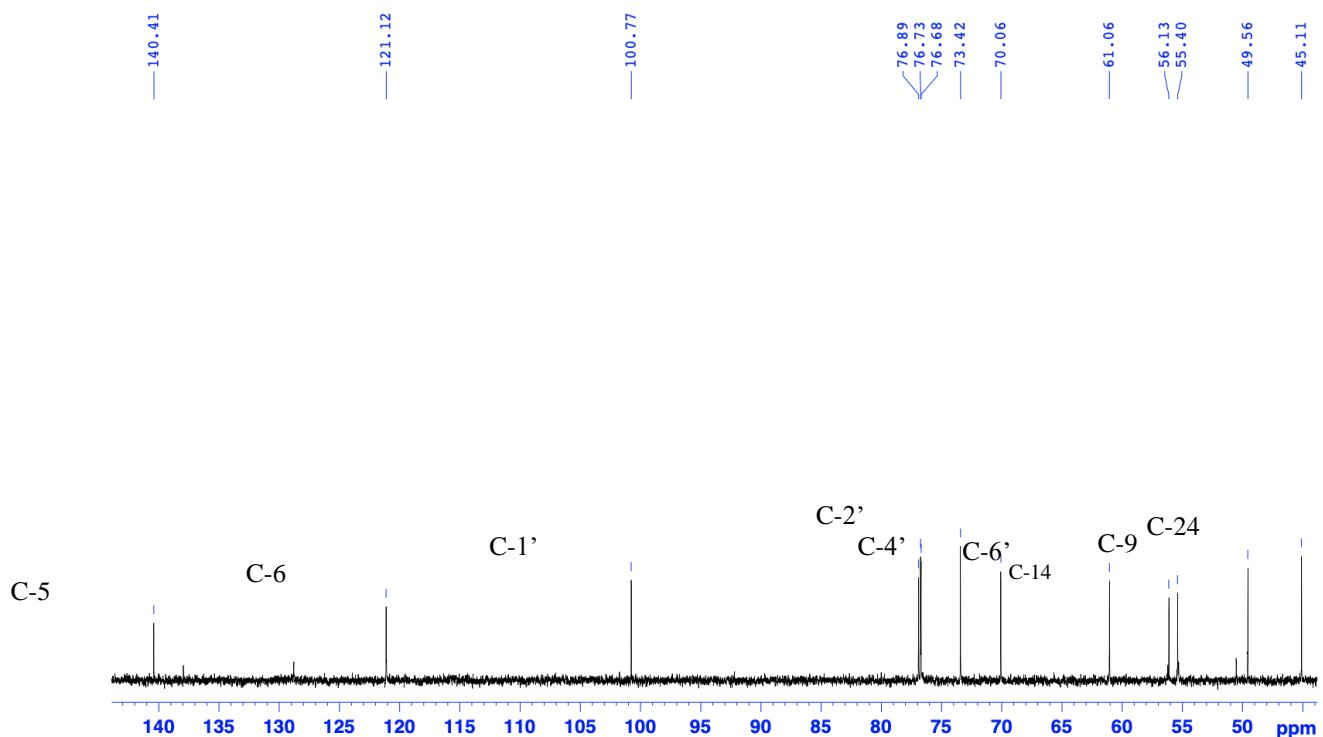
**Figure S7:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{H}}$  0.6 ppm to  $\delta_{\text{H}}$  2.4 ppm)



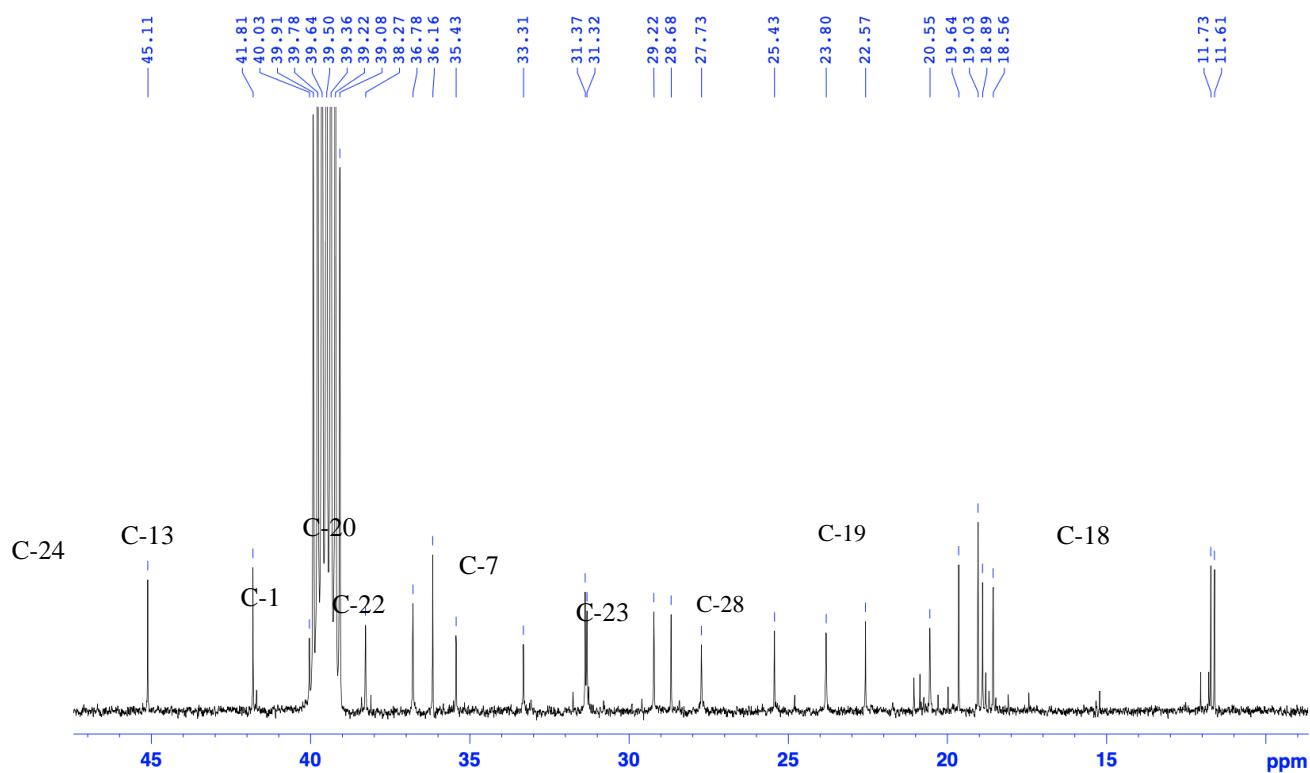
**Figure S8:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **2** (daucosterol)



**Figure S9:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{C}}$  0 ppm to  $\delta_{\text{C}}$  140 ppm)



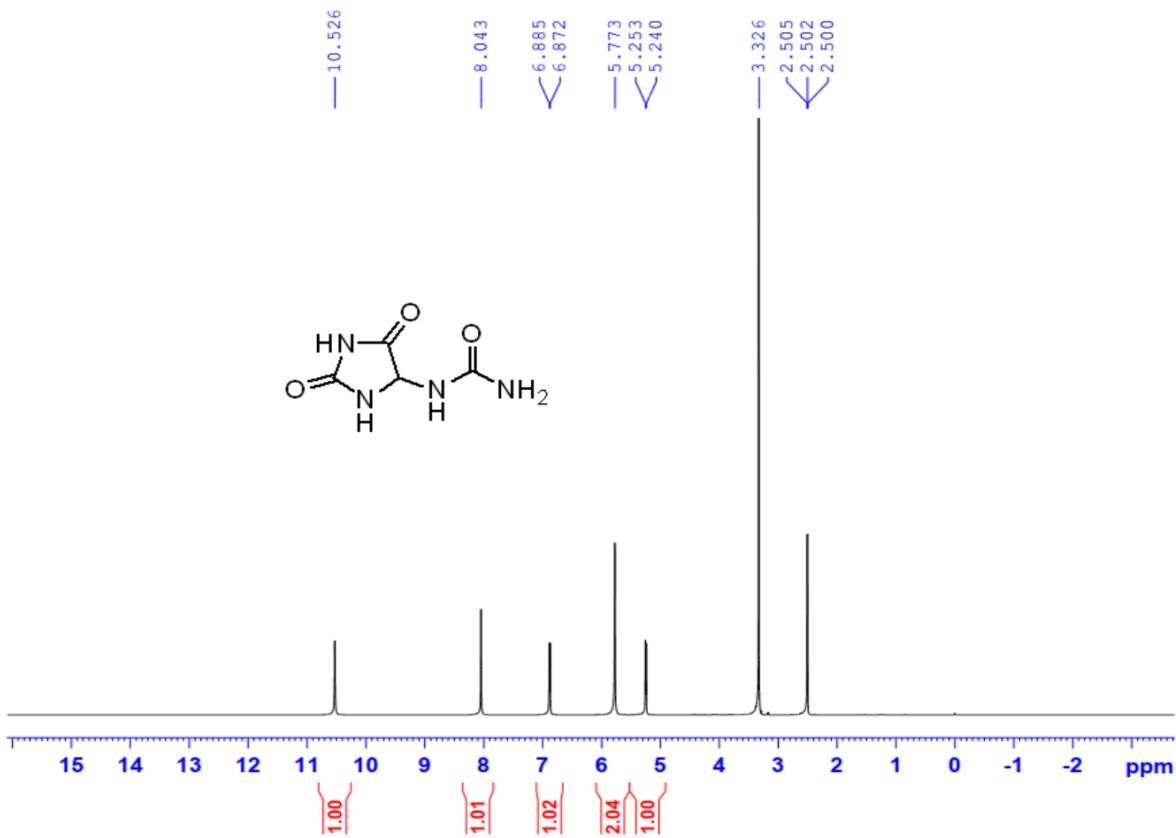
**Figure S10:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{C}}$  50 ppm to  $\delta_{\text{C}}$  140 ppm)



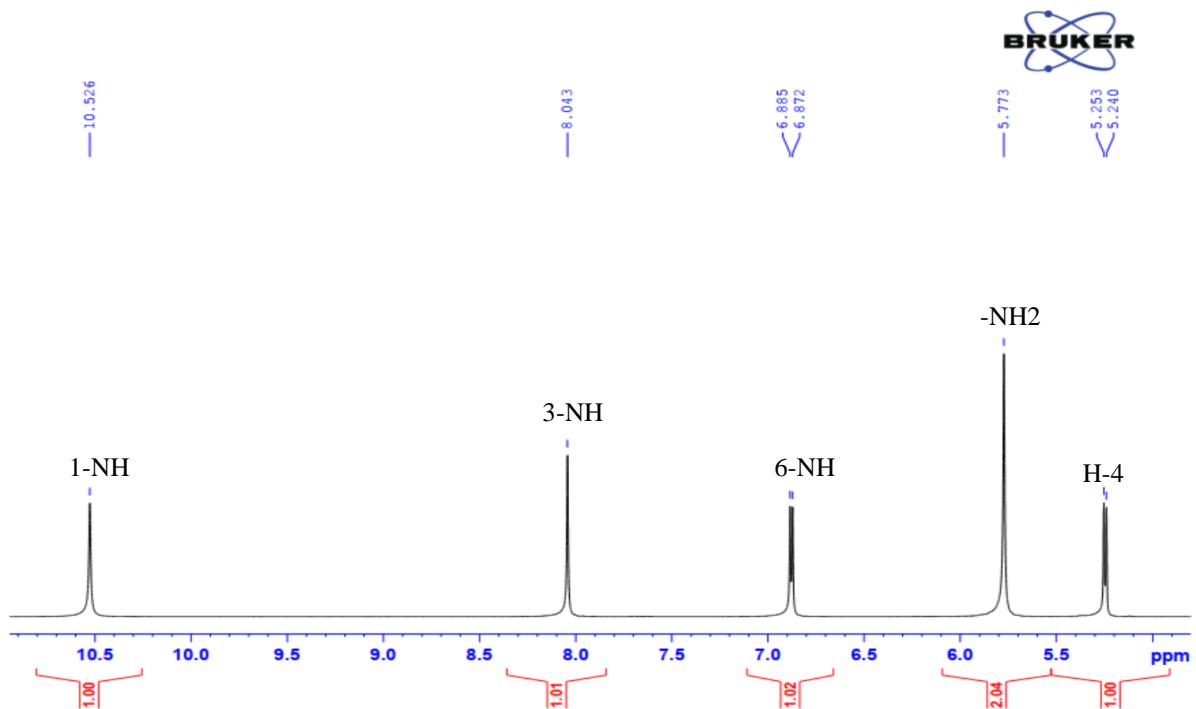
**Figure S11:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{C}}$  10 ppm to  $\delta_{\text{C}}$  47 ppm)

**Table S3 :** The comparison of NMR data of compound **3** with a similar compound (allatonin)

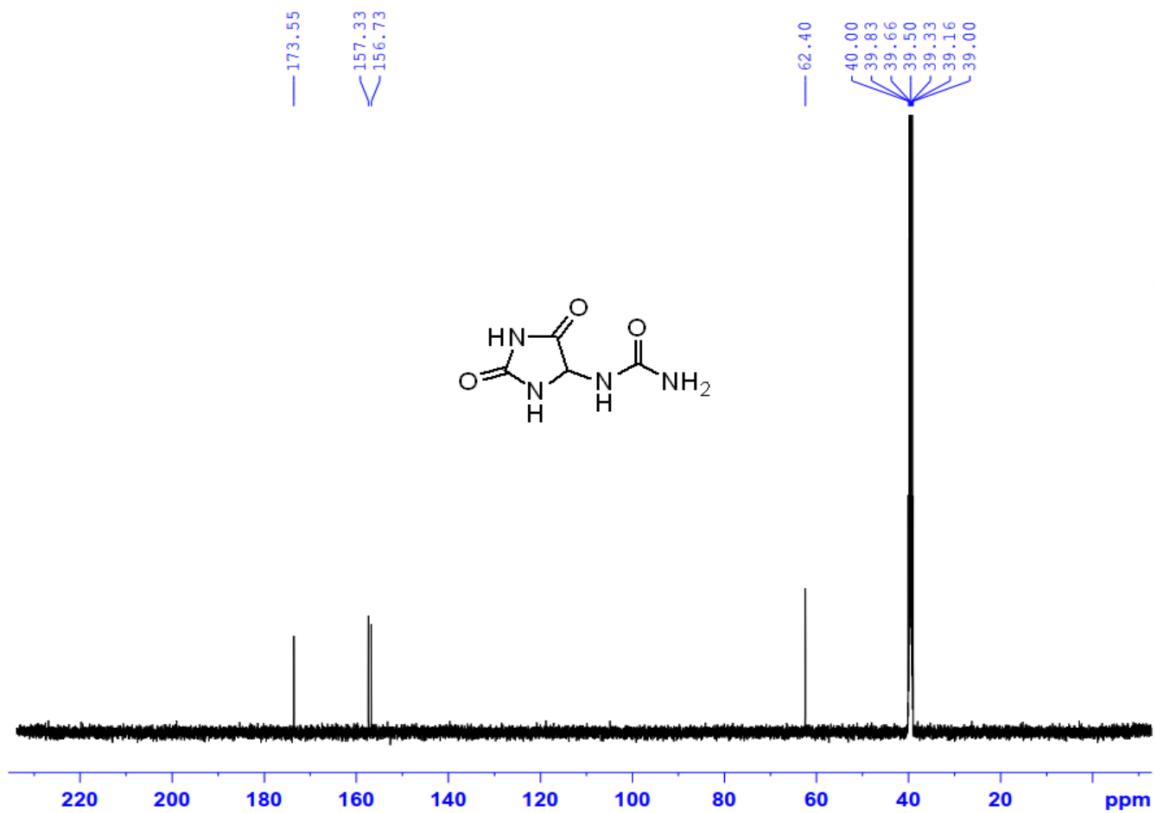
Position	Compound <b>3</b> (DMSO- <i>d</i> <sub>6</sub> )		Allatonin (DMSO- <i>d</i> <sub>6</sub> ) [30]	
	<sup>13</sup> C-NMR (125 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_{\text{H}}$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (500 MHz) $\delta_{\text{H}}$ ppm
1-NH		10.53 (1H, <i>s</i> )		10.50 (1H, <i>s</i> )
2	156.7		157.6	
3-NH		8.04 (1H, <i>s</i> )		8.10 (1H, <i>s</i> )
4	62.4	5.25 (1H, <i>d</i> , 7.8 Hz)	62.7	5.30 (1H, <i>d</i> , 8.1 Hz)
5	173.6		174.0	
6-NH		6.88 (1H, <i>d</i> , 7.8 Hz)		6.90 (1H, <i>d</i> , 8.1 Hz)
7	157.3		157.1	
-NH <sub>2</sub>		5.77 (2H, <i>s</i> )		5.80 (2H, <i>s</i> )



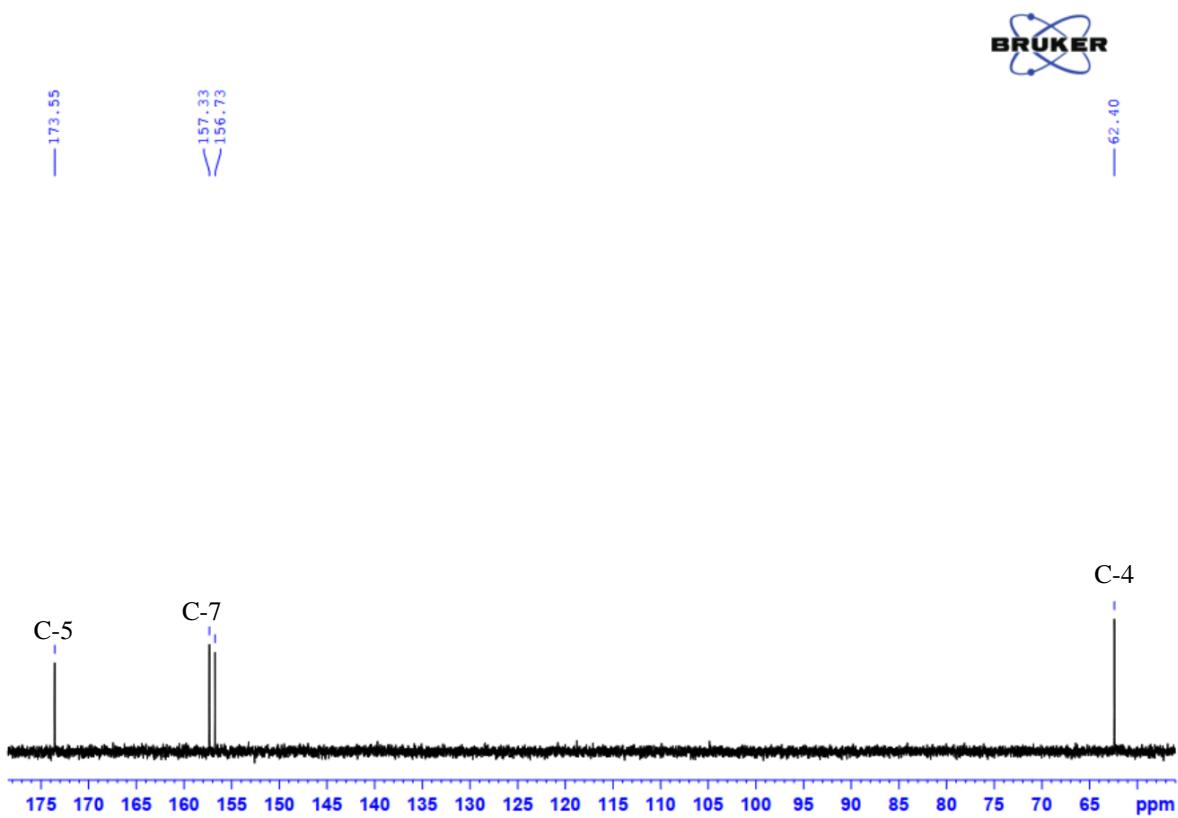
**Figure S12:** <sup>1</sup>H-NMR (600 MHz, DMSO-d<sub>6</sub>) spectrum of compound **3** (allatonin)



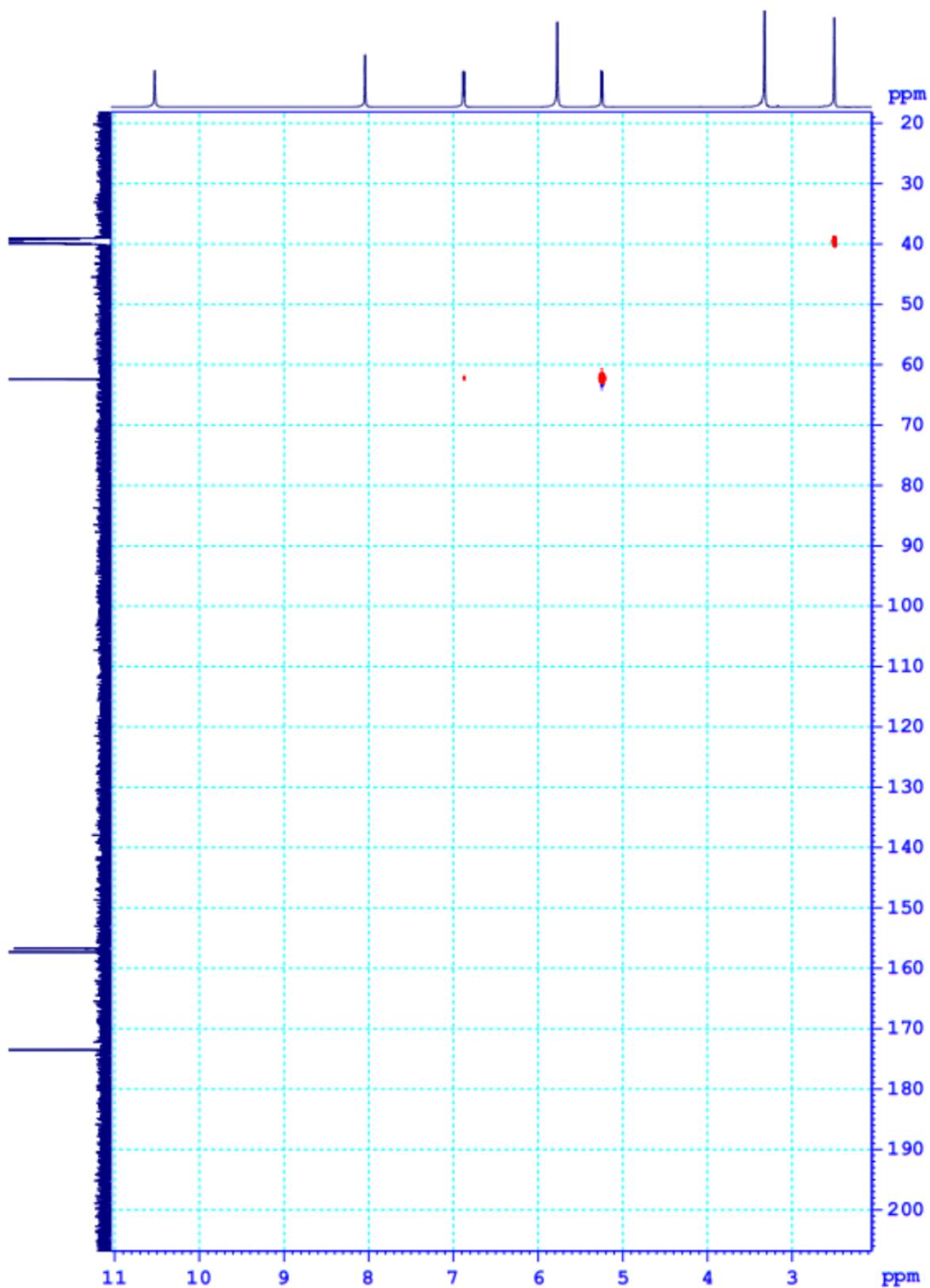
**Figure S13:**  $^1\text{H}$ -NMR (600 MHz, DMSO- $d_6$ ) spectrum of compound **3** (allatonin) (from  $\delta_{\text{H}}$  5 ppm to  $\delta_{\text{H}}$  11 ppm)



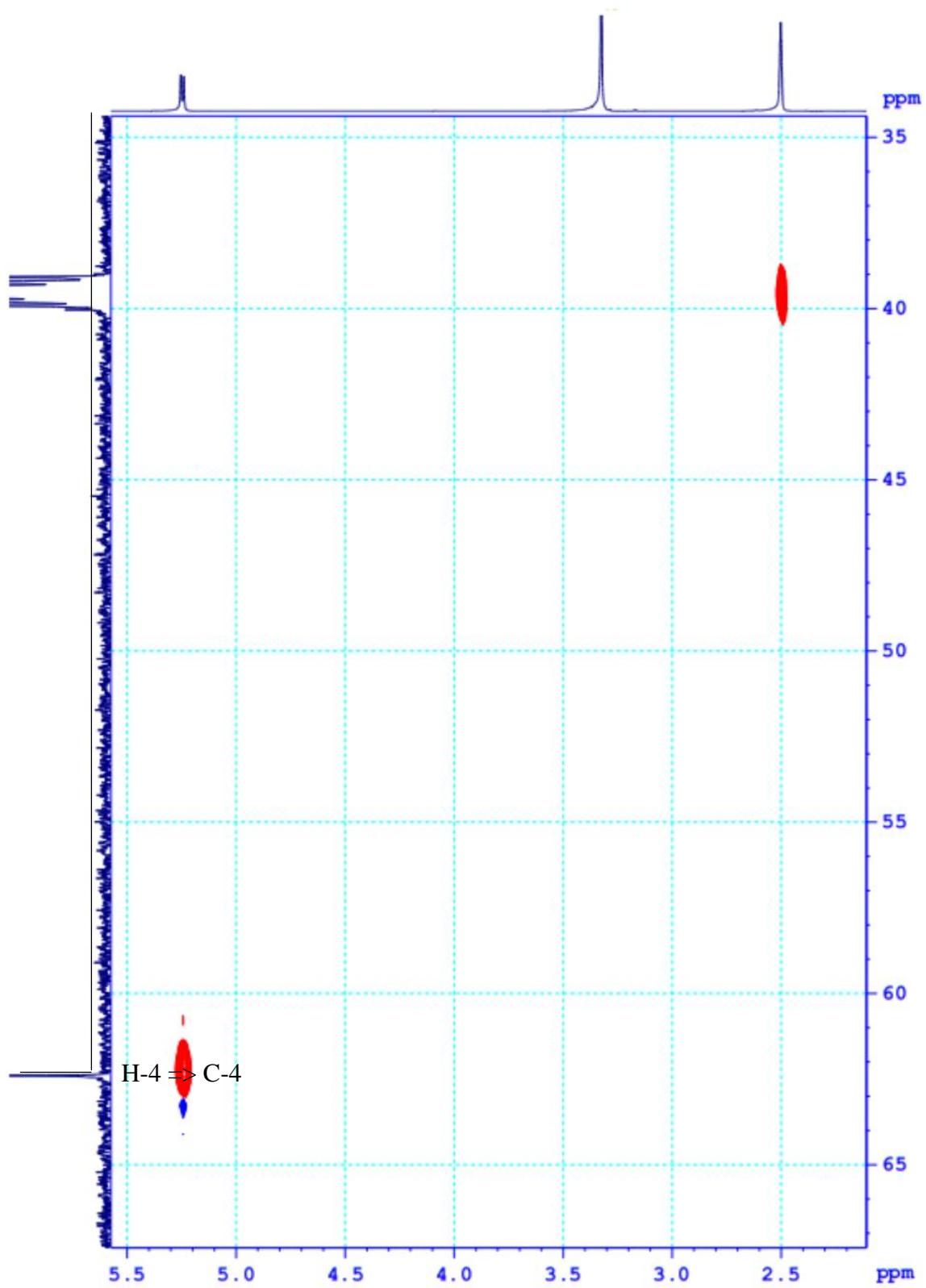
**Figure S14:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **3** (allatonin)



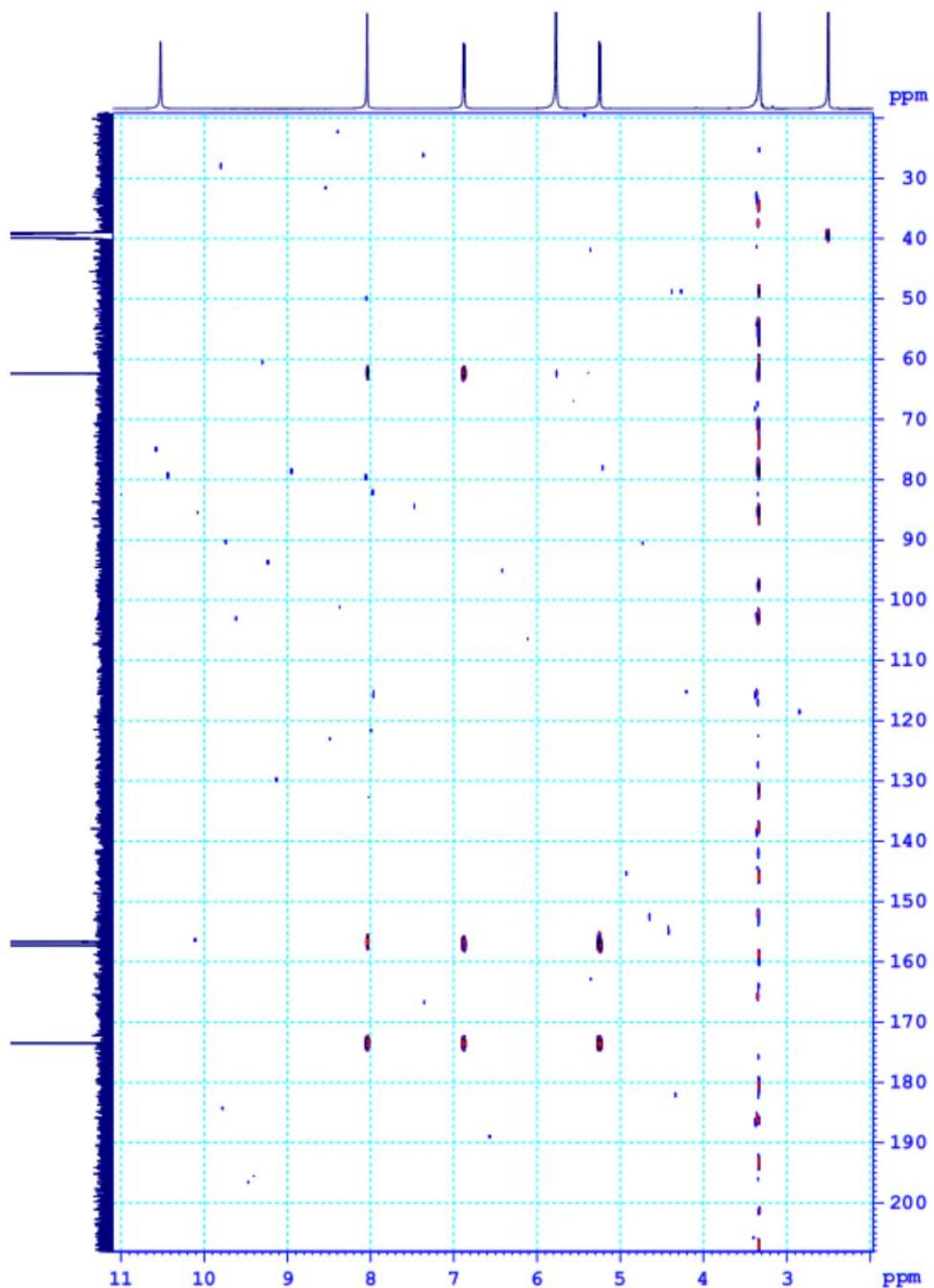
**Figure S15:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **3** (allatonin) (from  $\delta_{\text{C}}$  60 ppm to  $\delta_{\text{C}}$  175 ppm)



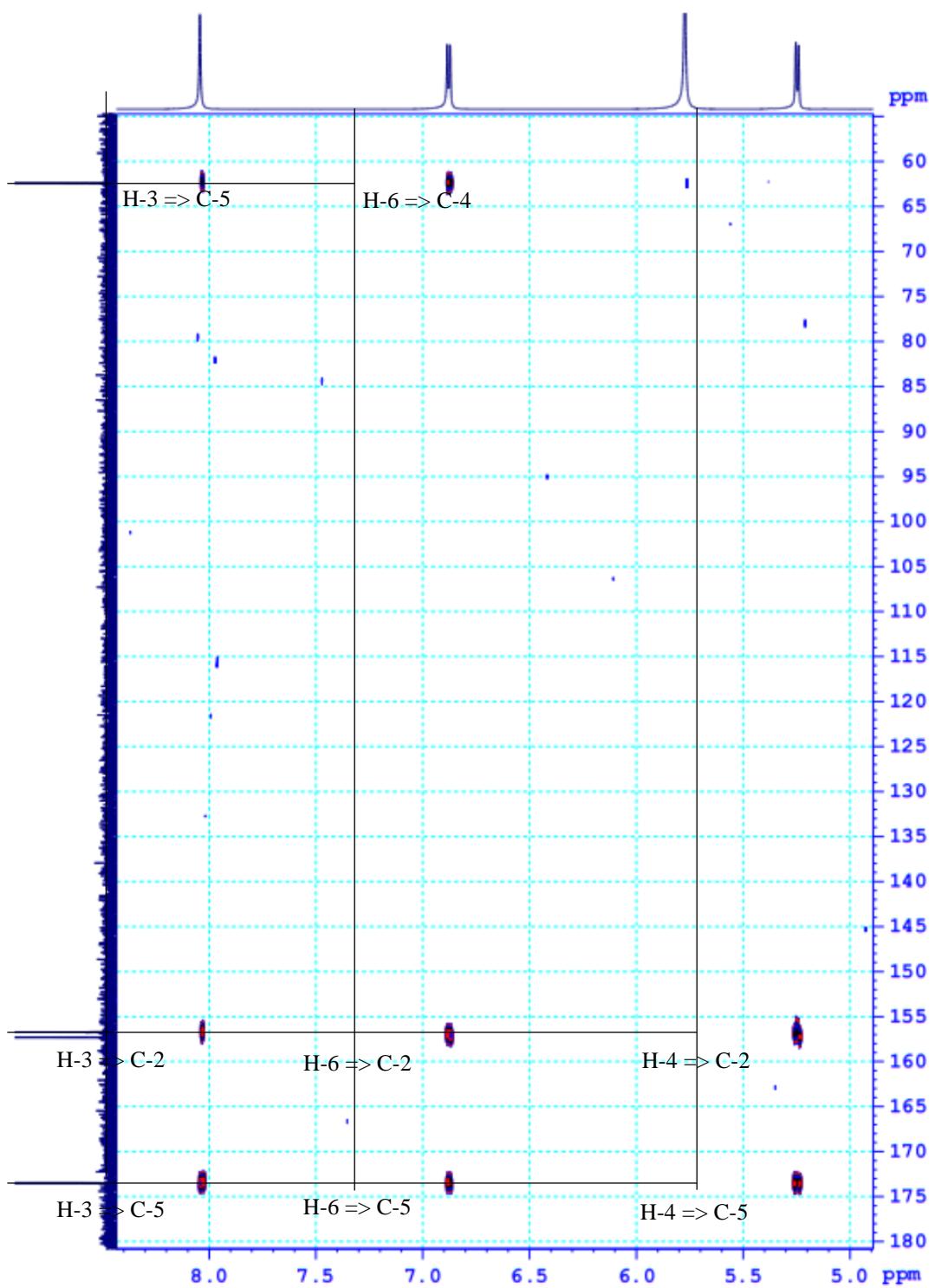
**Figure S16:** HSQC spectrum of compound **3** (allatonin)



**Figure S17:** HSQC spectrum of compound **3** (allatonin) (from  $\delta_{\text{C}}$  35 ppm to  $\delta_{\text{C}}$  65 ppm)



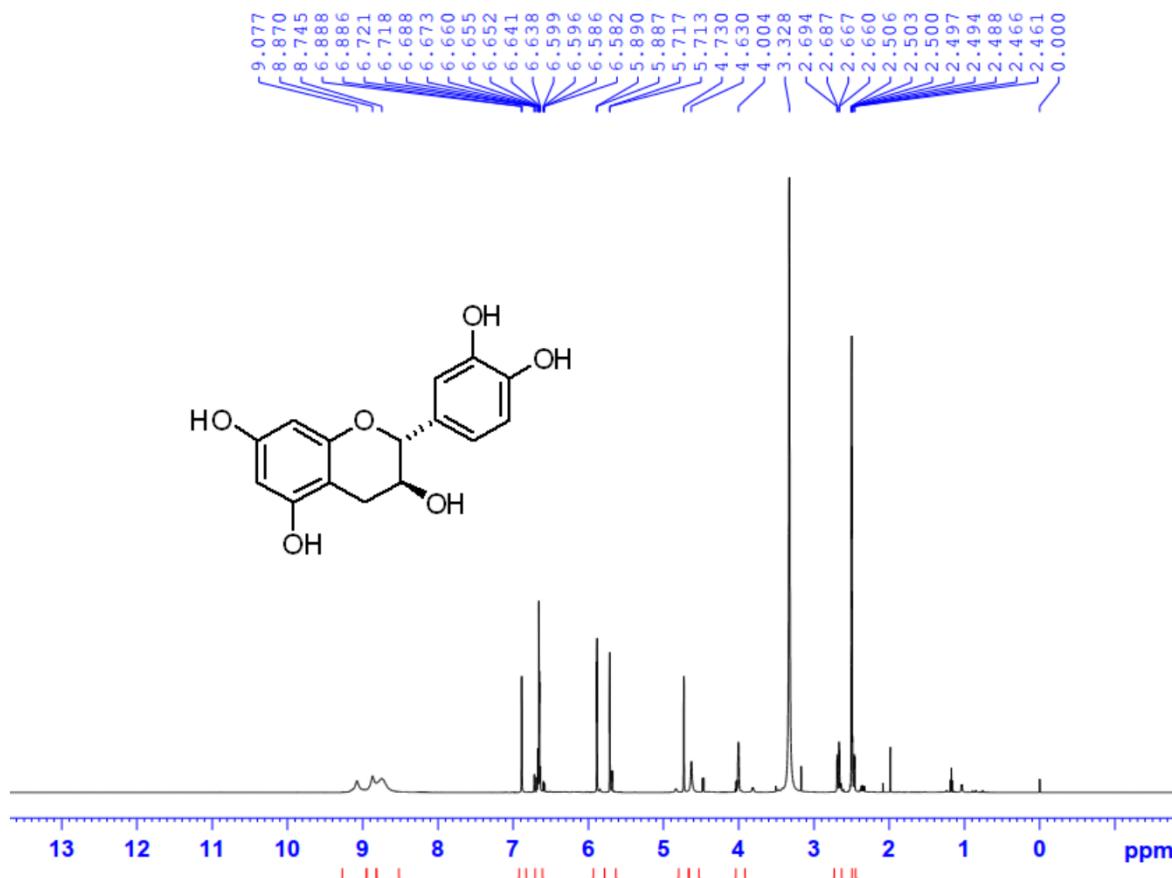
**Figure S18:** HMBC spectrum of compound **3** (allatonin)



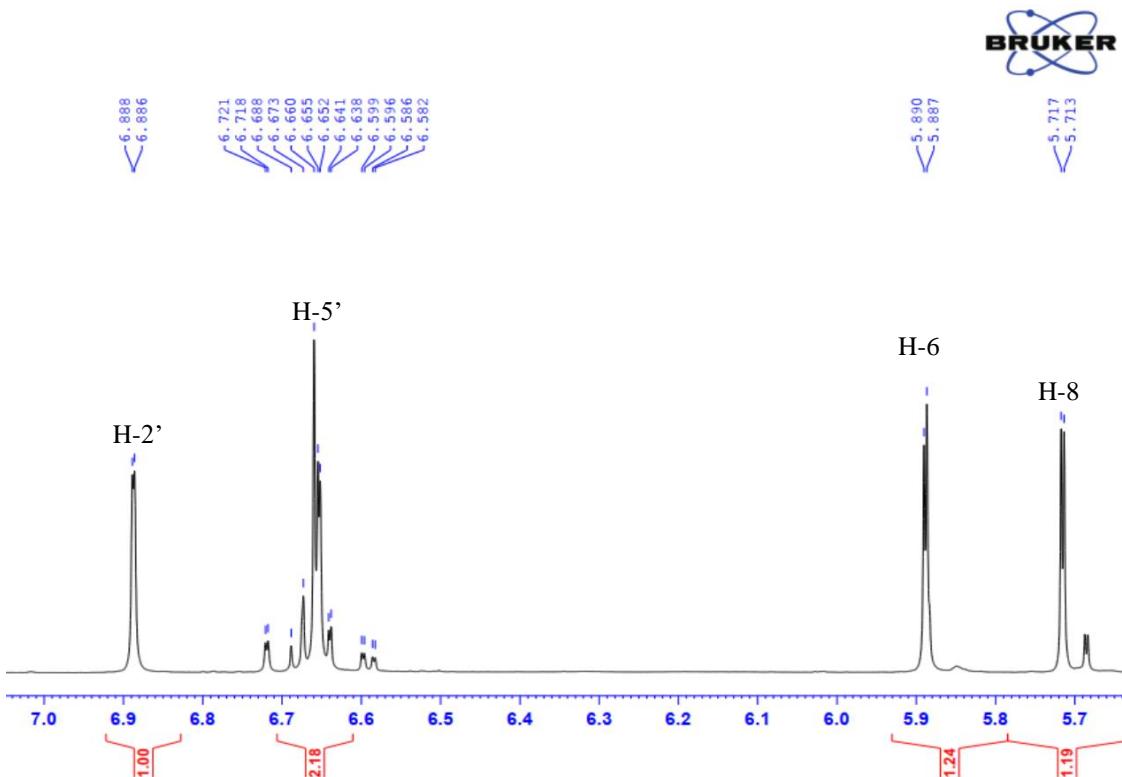
**Figure S19:** HMBC spectrum of compound **3** (allatonin) (from  $\delta_C$  60 ppm to  $\delta_C$  180 ppm)

**Table S4:** The comparison of NMR data of compound **4** with a similar compound ((+)-catechin)

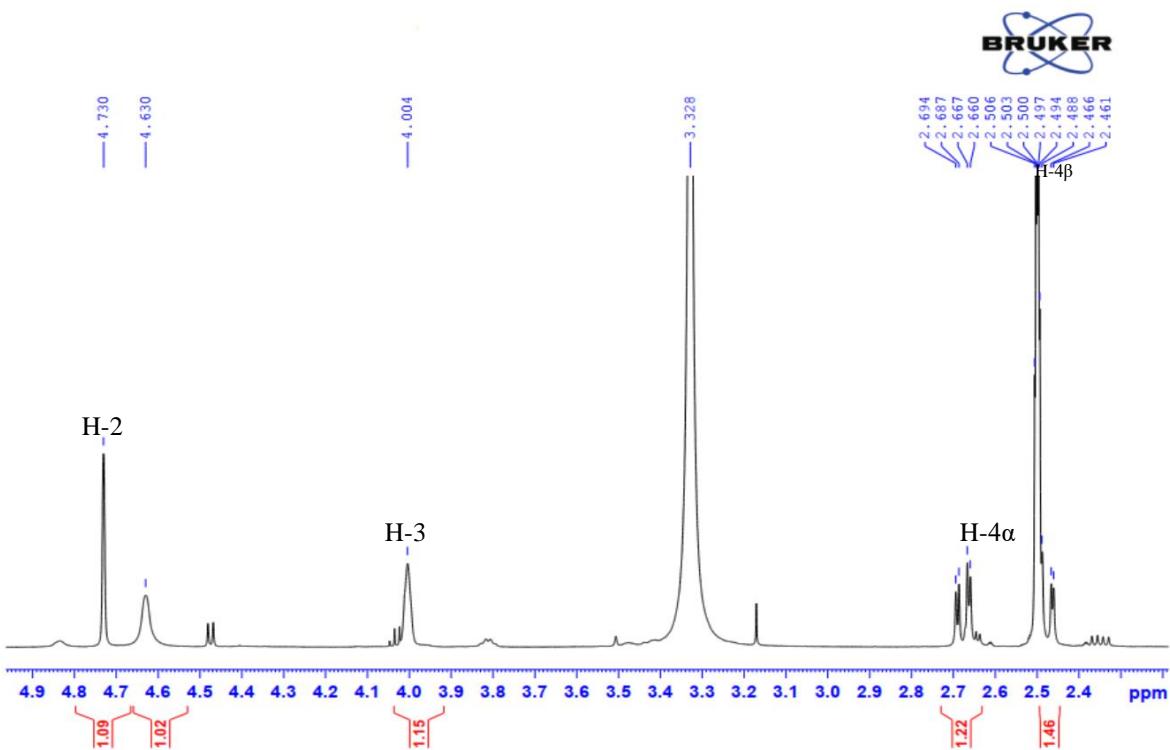
Position	Compound <b>4</b> ( $\text{DMSO}-d_6$ )		(+)-Catechin ( $\text{DMSO}-d_6$ ) [31]	
	$^{13}\text{C-NMR}$ (125 MHz) $\delta_{\text{C}}$ ppm	$^1\text{H-NMR}$ (600 MHz) $\delta_{\text{H}}$ ppm	$^{13}\text{C-NMR}$ (150 MHz) $\delta_{\text{C}}$ ppm	$^1\text{H-NMR}$ (600 MHz) $\delta_{\text{H}}$ ppm
2	78.0	4.73 (1H, <i>brs</i> )	82.9	4.55 (1H, <i>d</i> , 7.4 Hz)
3	64.9	4.00 (1H, <i>brs</i> )	68.8	3.96 (1H, <i>ddd</i> 5.5, 7.5, 8.1 Hz)
4	28.2	2.67 (1H, <i>dd</i> , 4.2, 16.2 Hz, H $\alpha$ ) 2.47 (1H, <i>dd</i> , 3.0, 16.2 Hz, H $\beta$ )	28.5	2.84 (1H, <i>dd</i> , 5.5, 15.9 Hz, H $\alpha$ ) 2.84 (1H, <i>dd</i> , 8.0, 15.9 Hz, H $\beta$ )
5	156.5	-	156.9	-
6	94.1	5.89 (1H, <i>d</i> , 2.4 Hz)	95.5	5.91 (1H, <i>d</i> , 2.2 Hz)
7	156.2	-	157.6	-
8	95.1	5.72 (1H, <i>d</i> , 2.4 Hz)	96.3	5.82 (1H, <i>d</i> , 2.2 Hz)
9	155.8	-	157.9	-
10	98.5	-	100.8	-
1'	130.5	-	132.4	-
2'	114.8	6.89 (1H, <i>d</i> , 1.2 Hz)	115.3	6.82 (1H, <i>d</i> , 1.9 Hz)
3'	144.4	-	146.2	-
4'	144.4	-	146.2	-
5'	144.7	6.66 (1H, <i>m</i> )	116.1	6.75 (1H, <i>d</i> , 8.2 Hz)
6'	117.9	6.65 (1H, <i>d</i> , 1.2 Hz)	120.0	6.70 (1H, <i>dd</i> , 1.9, 8.2 Hz)



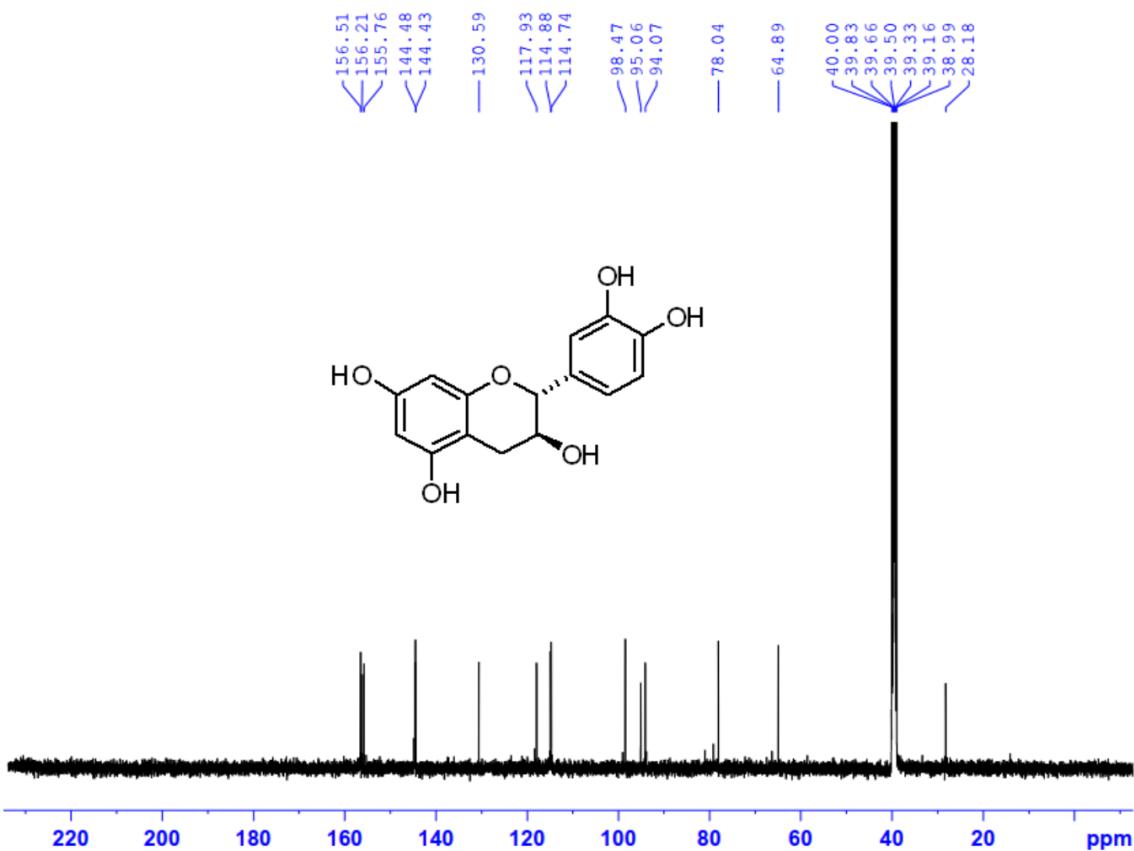
**Figure S20:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound 4 ((+)-catechin)



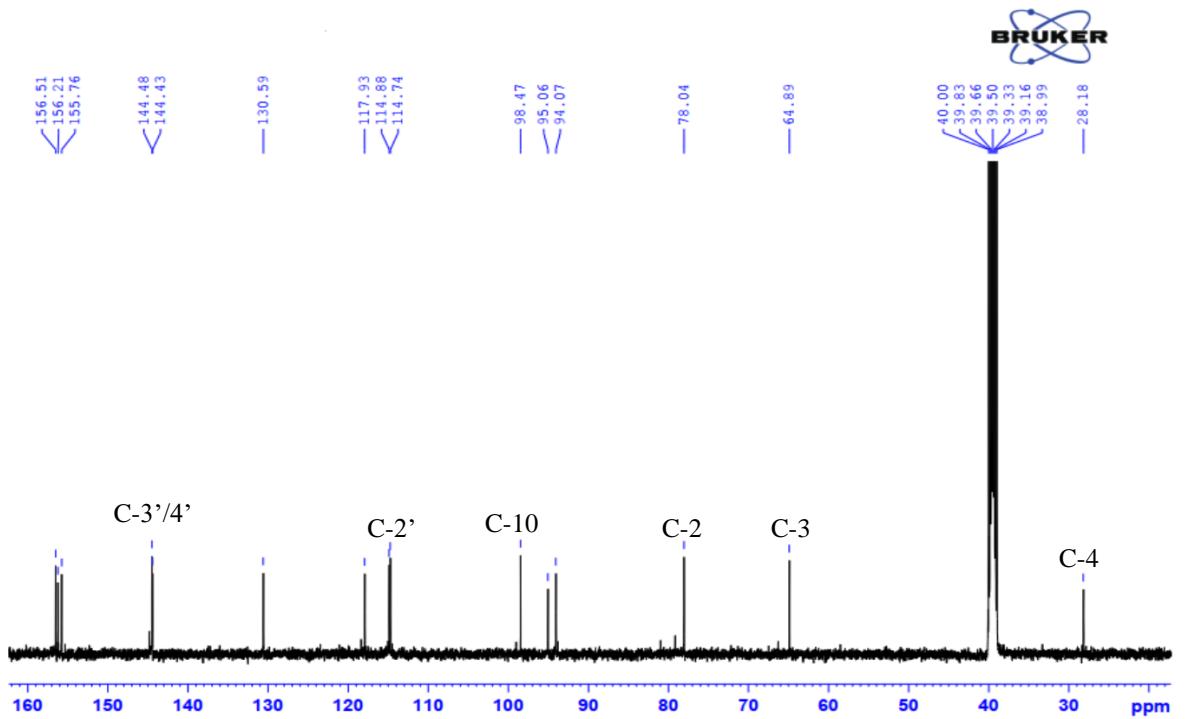
**Figure S21:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound 4 ((+)-catechin) (from  $\delta_{\text{H}}$  5.6 ppm to  $\delta_{\text{H}}$  7.0 ppm)



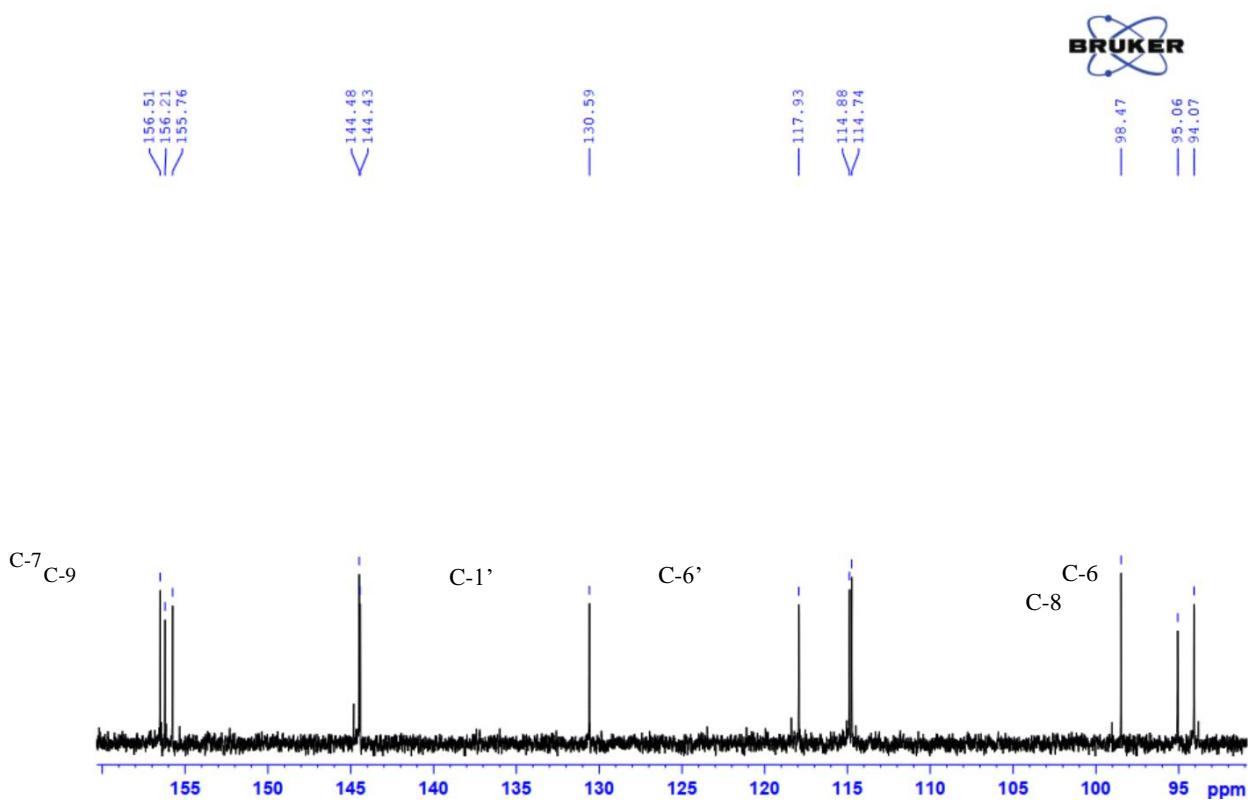
**Figure S22:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **4** ((+)-catechin) (from  $\delta_{\text{H}}$  2.3 ppm to  $\delta_{\text{H}}$  4.9 ppm)



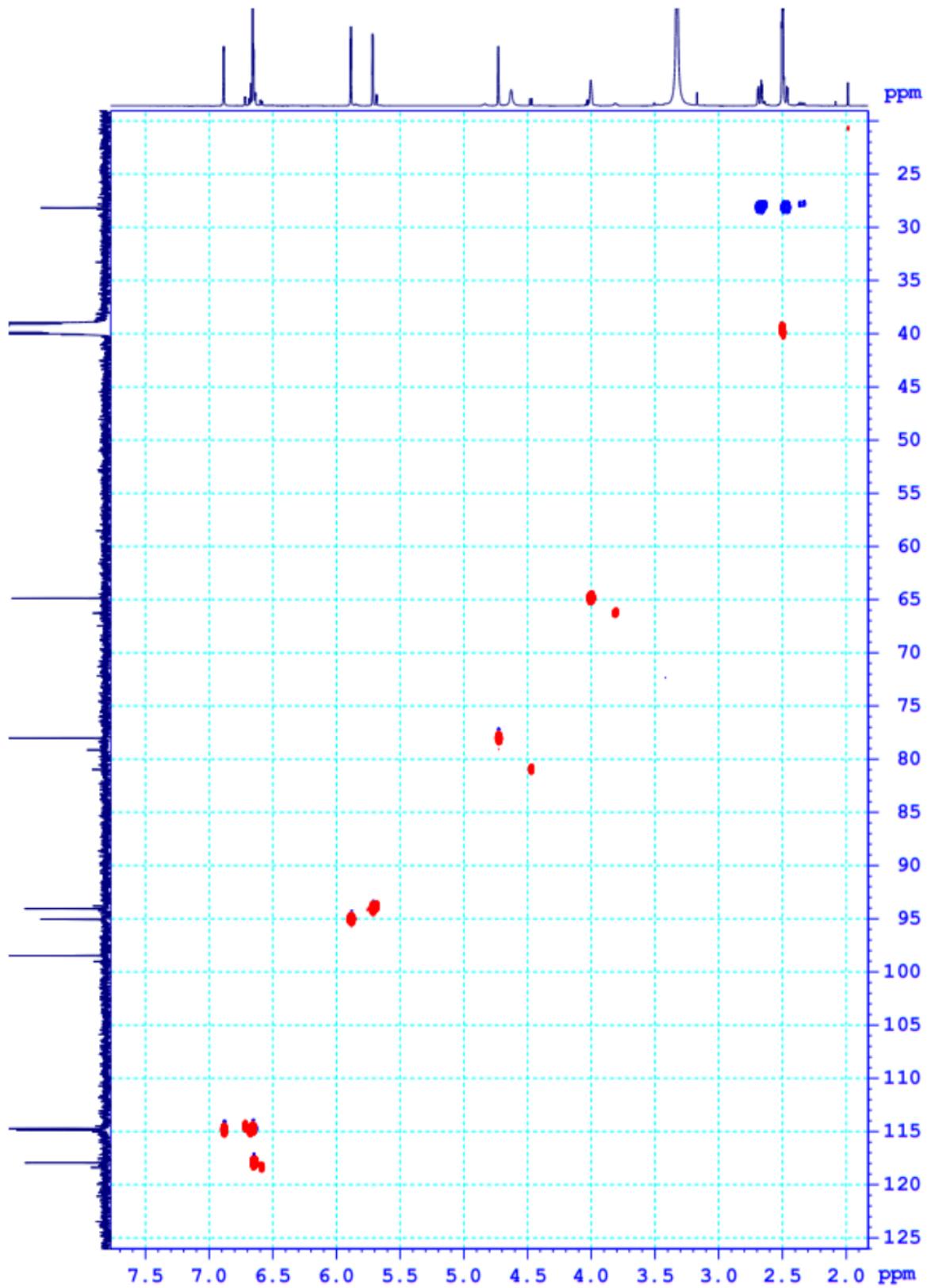
**Figure S23:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **4** ((+)-catechin)



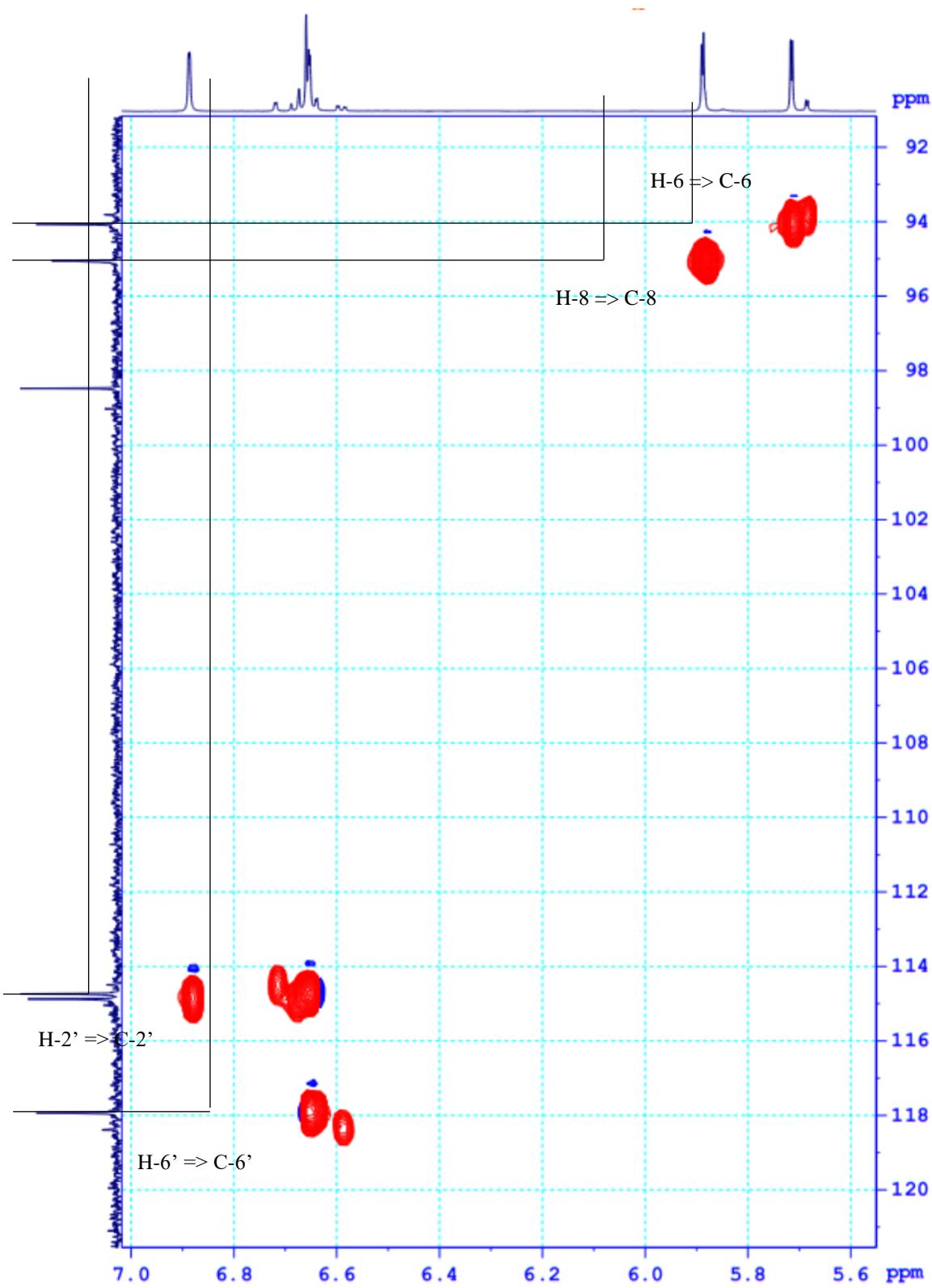
**Figure S24:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **4** ((+)-catechin) (from  $\delta_{\text{C}}$  20 ppm to  $\delta_{\text{C}}$  160 ppm)



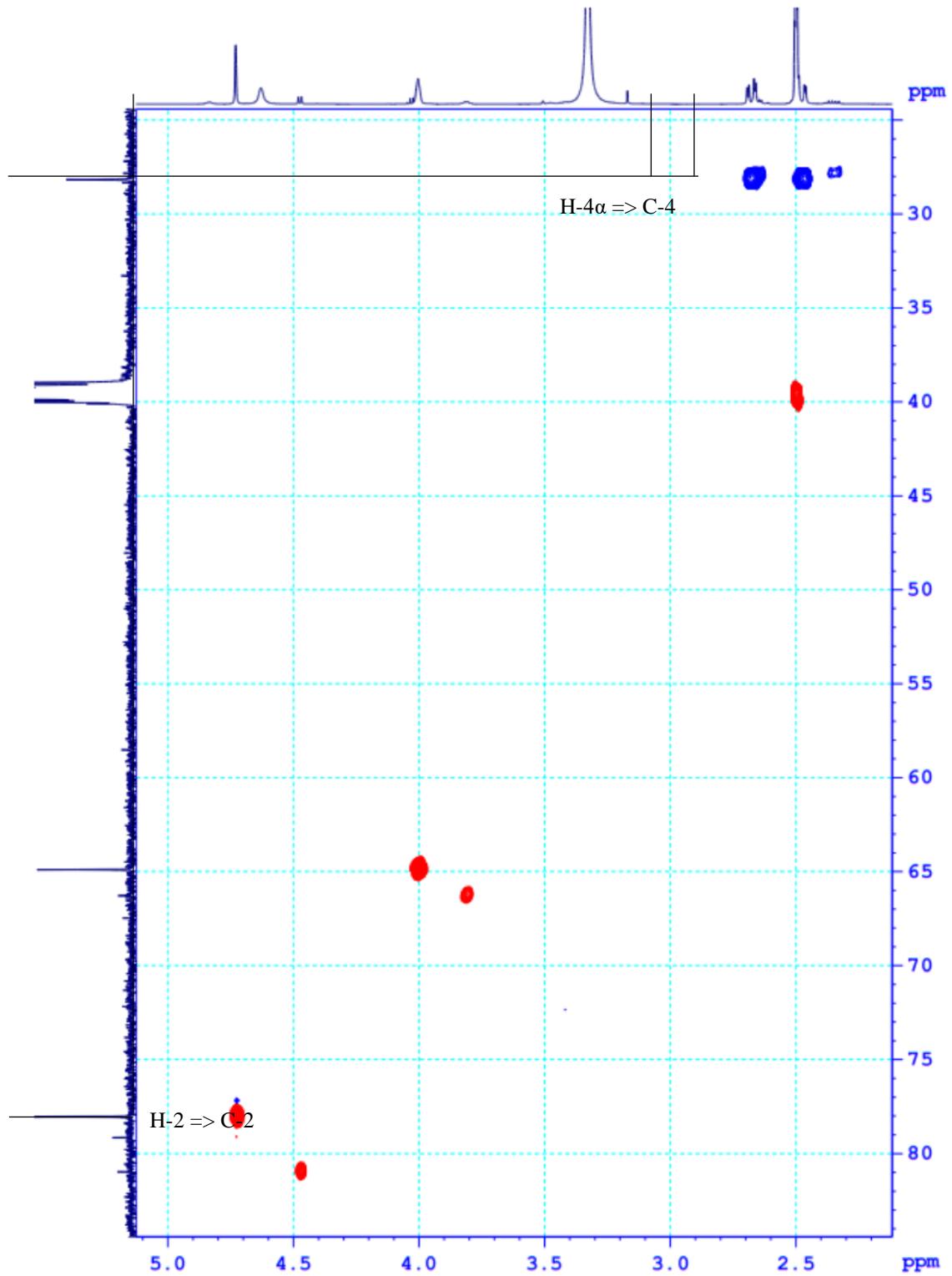
**Figure S25:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **4** ((+)-catechin) (from  $\delta_{\text{C}}$  90 ppm to  $\delta_{\text{C}}$  160 ppm)



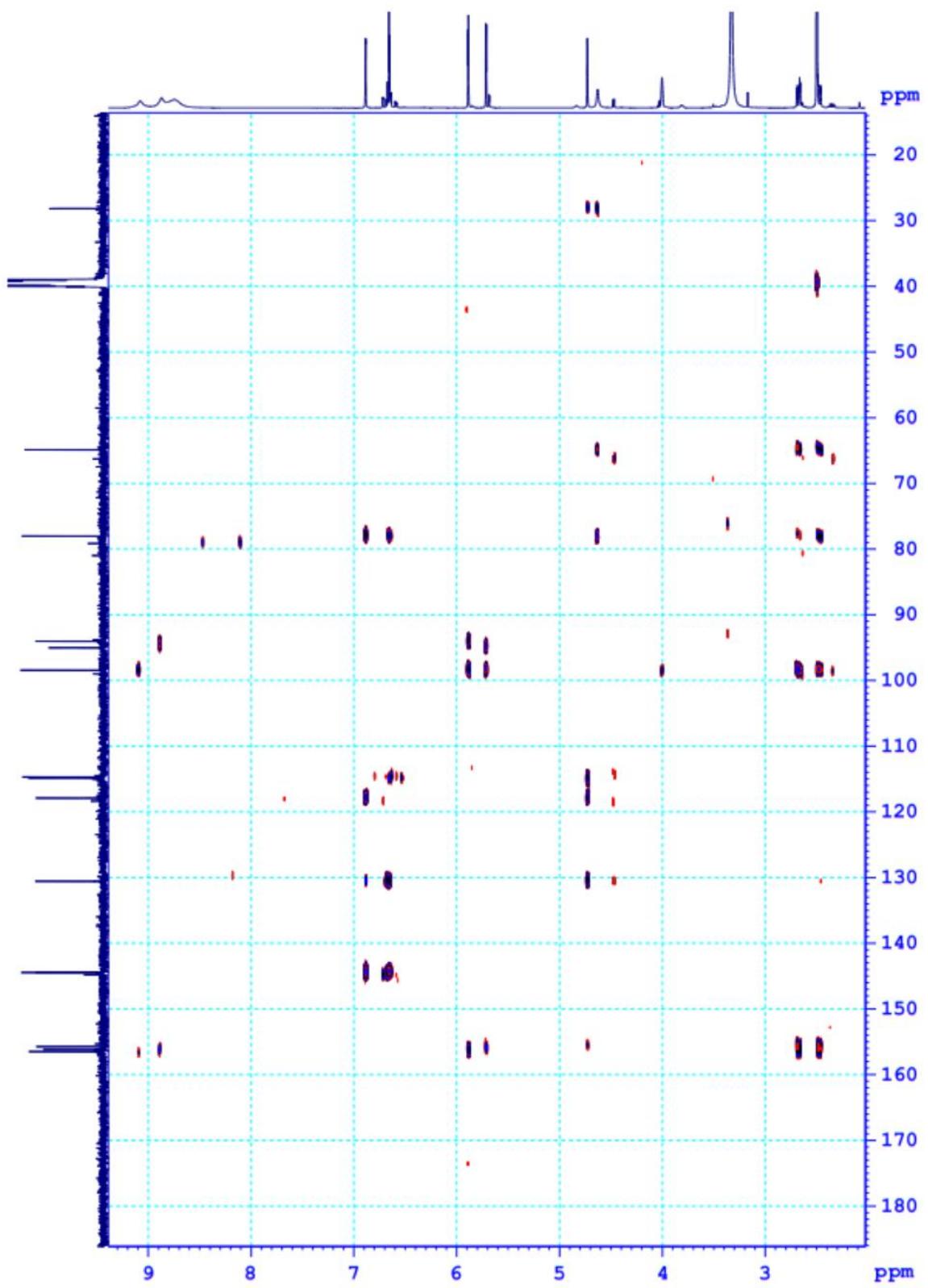
**Figure S26:** HSQC spectrum of compound 4 ((+)-catechin)



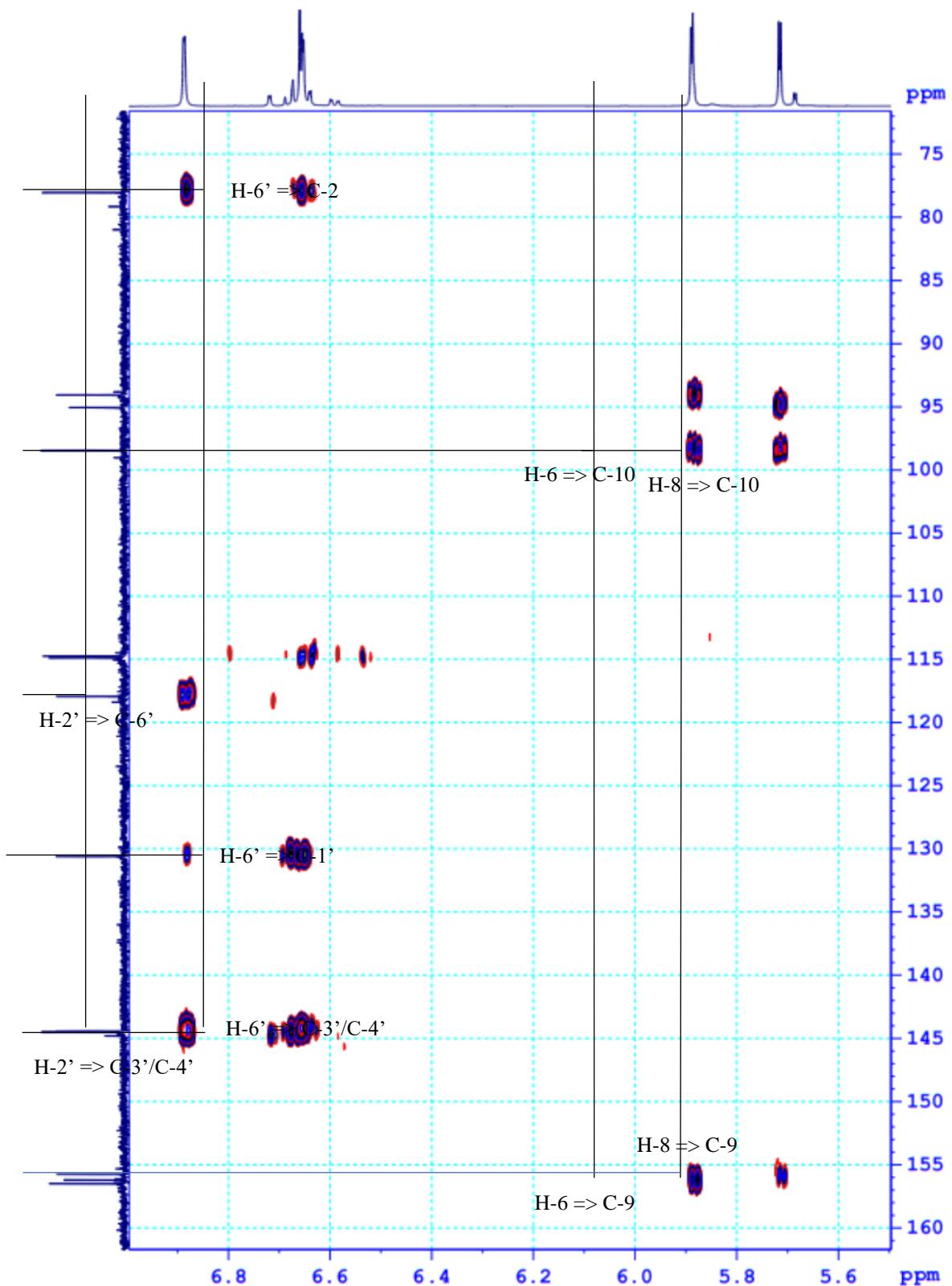
**Figure S27:** HSQC spectrum of compound 4 ((+)-catechin) (from  $\delta_{\text{C}}$  92 ppm to  $\delta_{\text{C}}$  120 ppm)



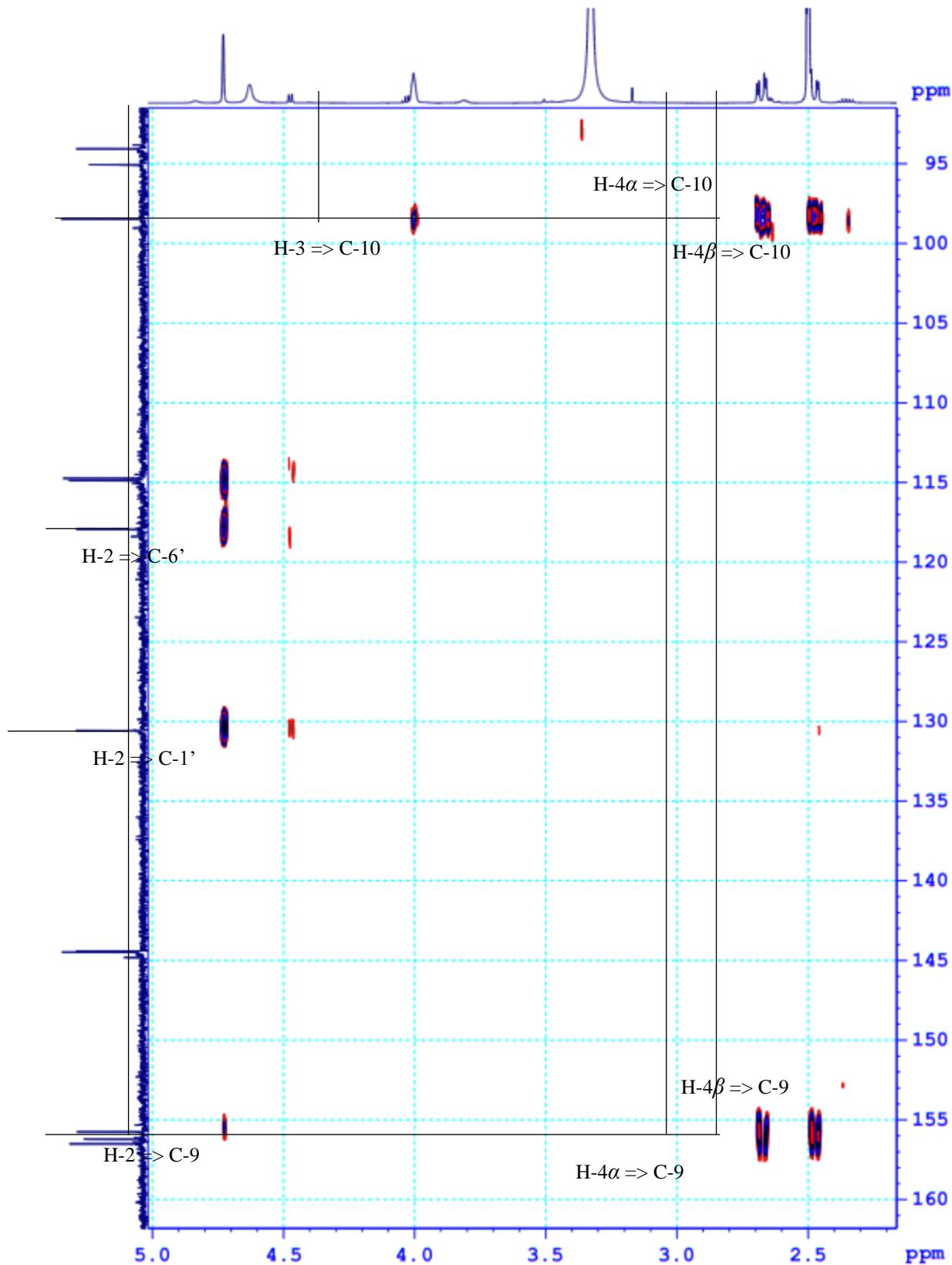
**Figure S28:** HSQC spectrum of compound **4** ((+)-catechin) (from  $\delta_{\text{C}}$  20 ppm to  $\delta_{\text{C}}$  90 ppm)



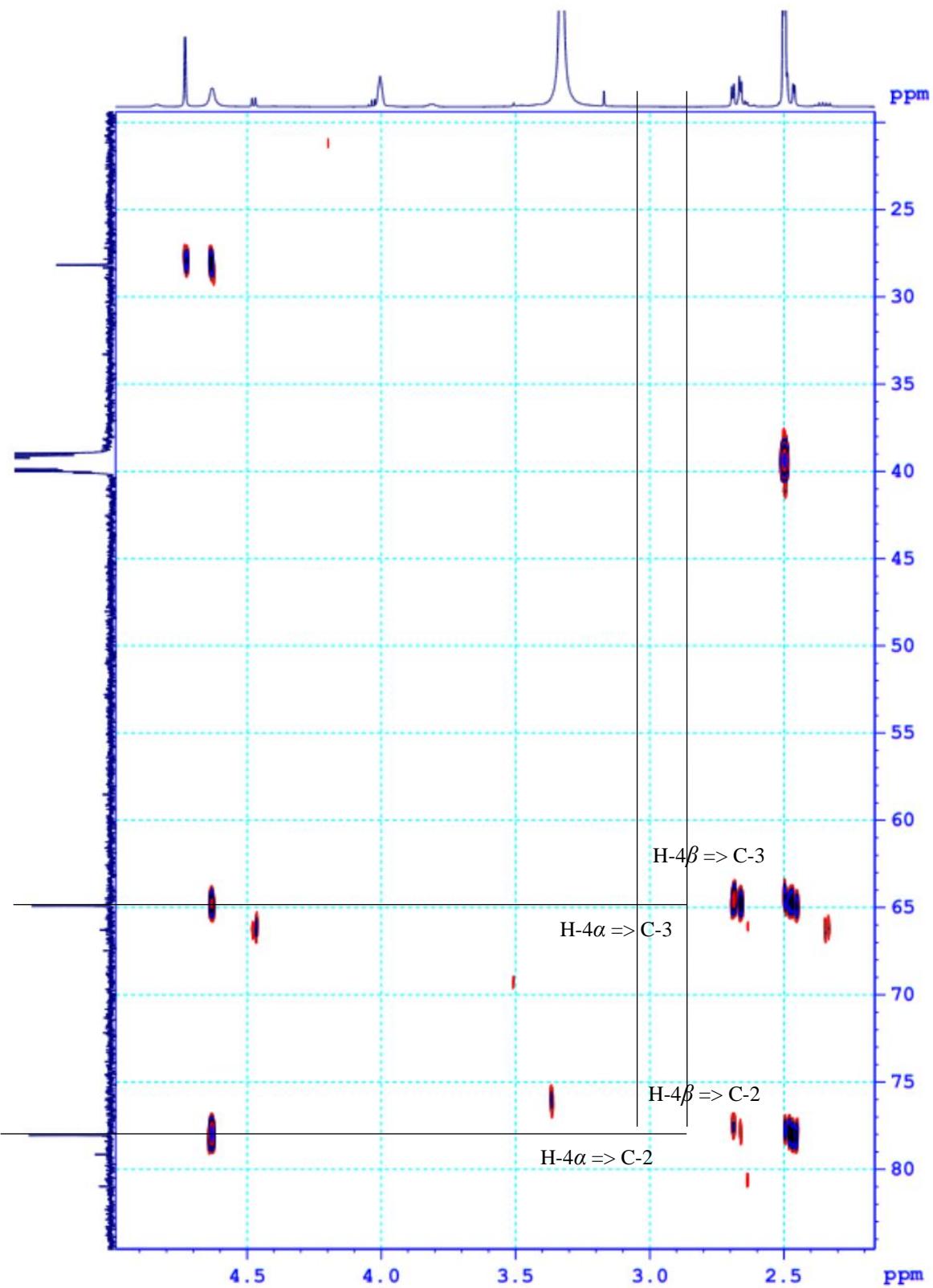
**Figure S29:** HMBC spectrum of compound **4** ((+)-catechin)



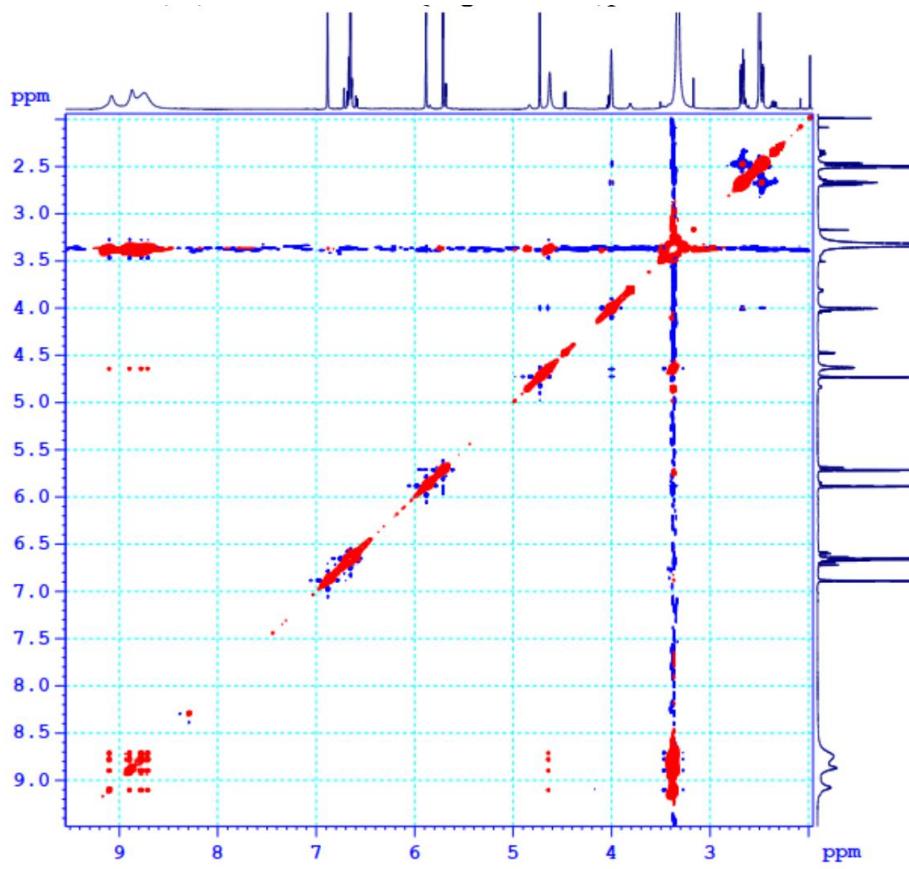
**Figure S30:** HMBC spectrum of compound 4 ((+)-catechin) (from  $\delta_{\text{C}}$  75 ppm to  $\delta_{\text{C}}$  160 ppm)



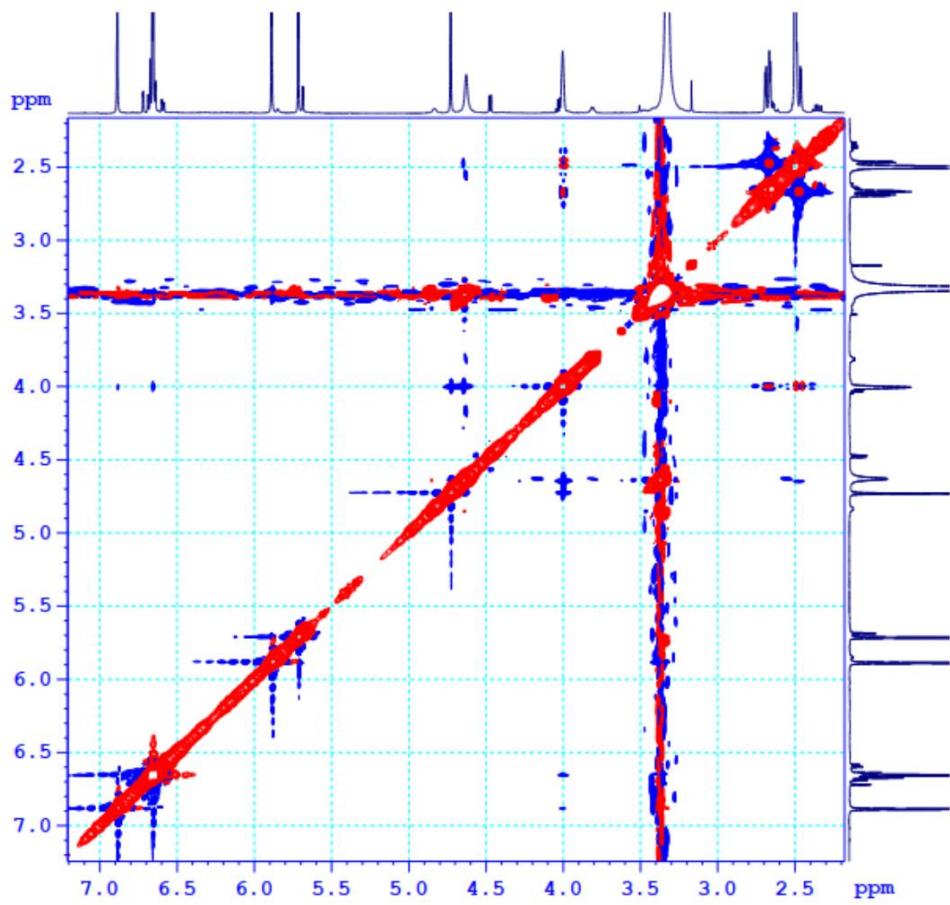
**Figure S31:** HMBC spectrum of compound 4 ((+)-catechin) (from  $\delta_c$  90 ppm to  $\delta_c$  160 ppm)



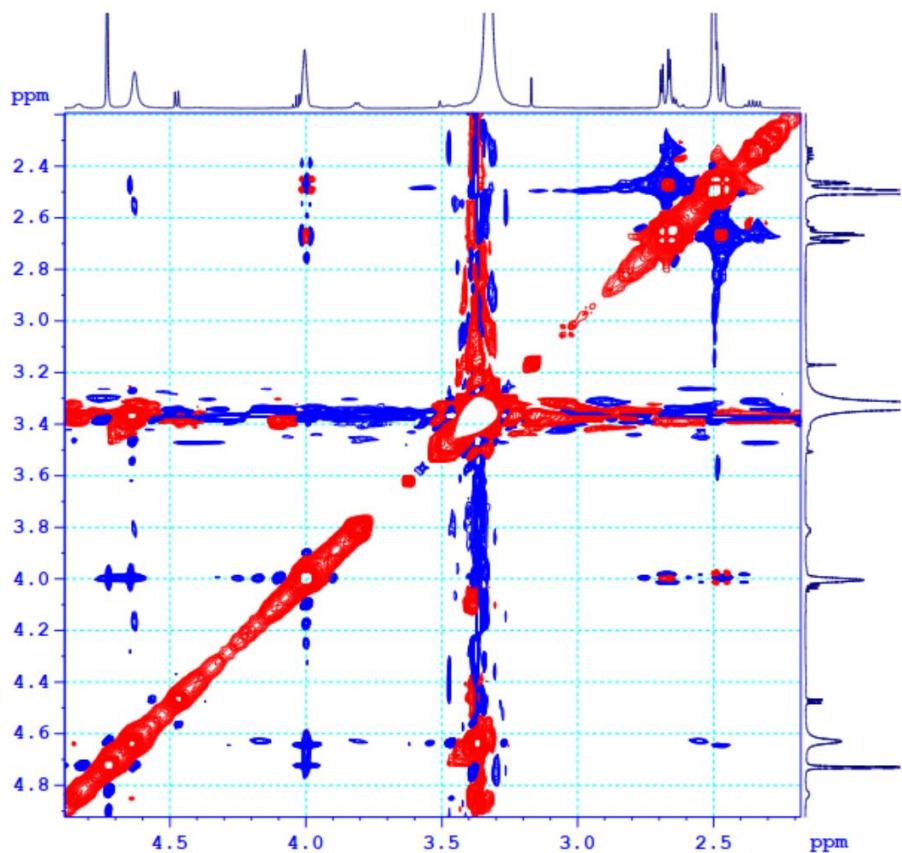
**Figure S32:** HMBC spectrum of compound 4 ((+)-catechin) (from  $\delta_C$  20 ppm to  $\delta_C$  90 ppm)



**Figure S33:** NOESY spectrum of compound 4 ((+)-catechin)



**Figure S34:** NOESY spectrum of compound 4 ((+)-catechin) (from  $\delta_H$  2.5 ppm to  $\delta_C$  7.0 ppm)



**Figure S35:** NOESY spectrum of compound 4 ((+)-catechin) (from  $\delta_H$  2.4 ppm to  $\delta_H$  4.8 ppm)

**Table S5:** The comparison of NMR data of compound **5** with a similar compound (Apigenin)

Position	Compound <b>5</b> (DMSO- <i>d</i> <sub>6</sub> )		Apigenin (DMSO- <i>d</i> <sub>6</sub> ) [32]	
	<sup>13</sup> C-NMR (150 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_{\text{H}}$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (500 MHz) $\delta_{\text{H}}$ ppm
2	163.7	-	163.7	-
3	102.8	6.76 (1H, <i>s</i> )	102.8	6.75 (1H, <i>s</i> )
4	181.7	-	181.7	-
5	161.2	-	161.2	-
6	98.9	6.18 (1H, <i>d</i> , 1.8 Hz)	98.9	6.15 (1H, <i>d</i> , 1.9 hz)
7	164.2	-	164.5	-
8	94.0	6.47 (1H, <i>d</i> , 1.8 Hz)	94.0	6.44 (1H, <i>d</i> , 1.9 Hz)
9	157.3	-	157.3	-
10	103.6	-	103.5	-
1'	121.1	-	121.1	-
2'	128.5	7.92 (2H, <i>d</i> , 9.0 Hz)	128.5	7.91 (2H, <i>d</i> , 9.0 Hz)
3'	115.9	6.92 (2H, <i>d</i> , 9.0 Hz)	116.0	6.90 (2H, <i>d</i> , 9.0 Hz)
4'	161.4	-	161.4	-
5'	115.9	6.92 (2H, <i>d</i> , 9.0 Hz)	116.0	6.90 (2H, <i>d</i> , 9.0 Hz)
6'	128.5	7.92 (2H, <i>d</i> , 9.0 Hz)	128.5	7.91 (2H, <i>d</i> , 9.0 Hz)

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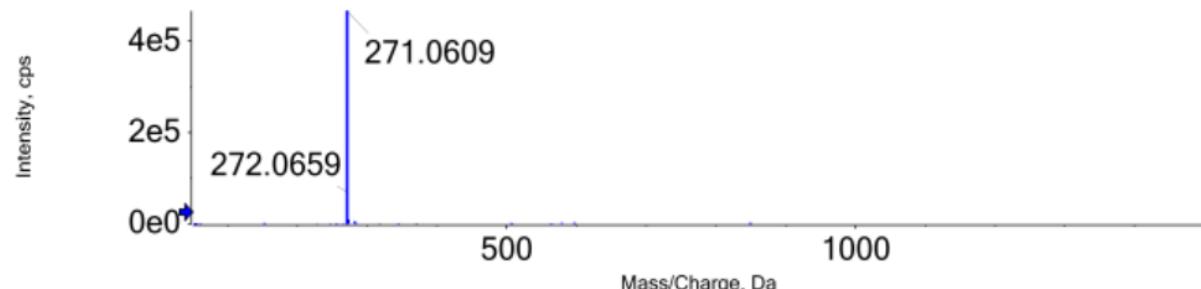
## ANALYSIS REPORT

### Injection details

<i>Sample name</i>	SAL	<i>Vial position</i>	38
<i>Sample file name</i>	SER.wiff2-YEN	<i>Inject volume</i>	5.00
<i>Acquisition date</i>	20/04/2023 10:47:59 AM	<i>Acquisition method</i>	<b>ESI_POS_SCAN</b>
<i>Operator</i>	CB21261708	<i>Instrument name</i>	X500 <sub>R</sub> QTOF

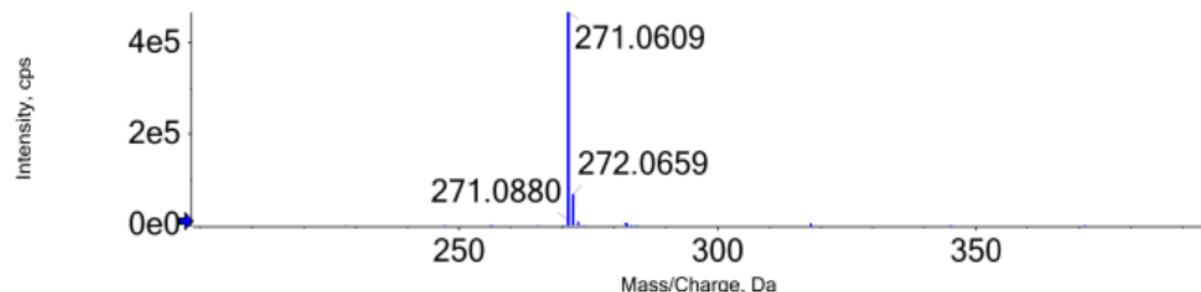
### Full mass spectrum

Spectrum from YEN\_SAL \_(+)-ESI 2023-04-20-10-47-59.wi...se multiplier = 1.5, Gaussian smoothed (0.5 points)

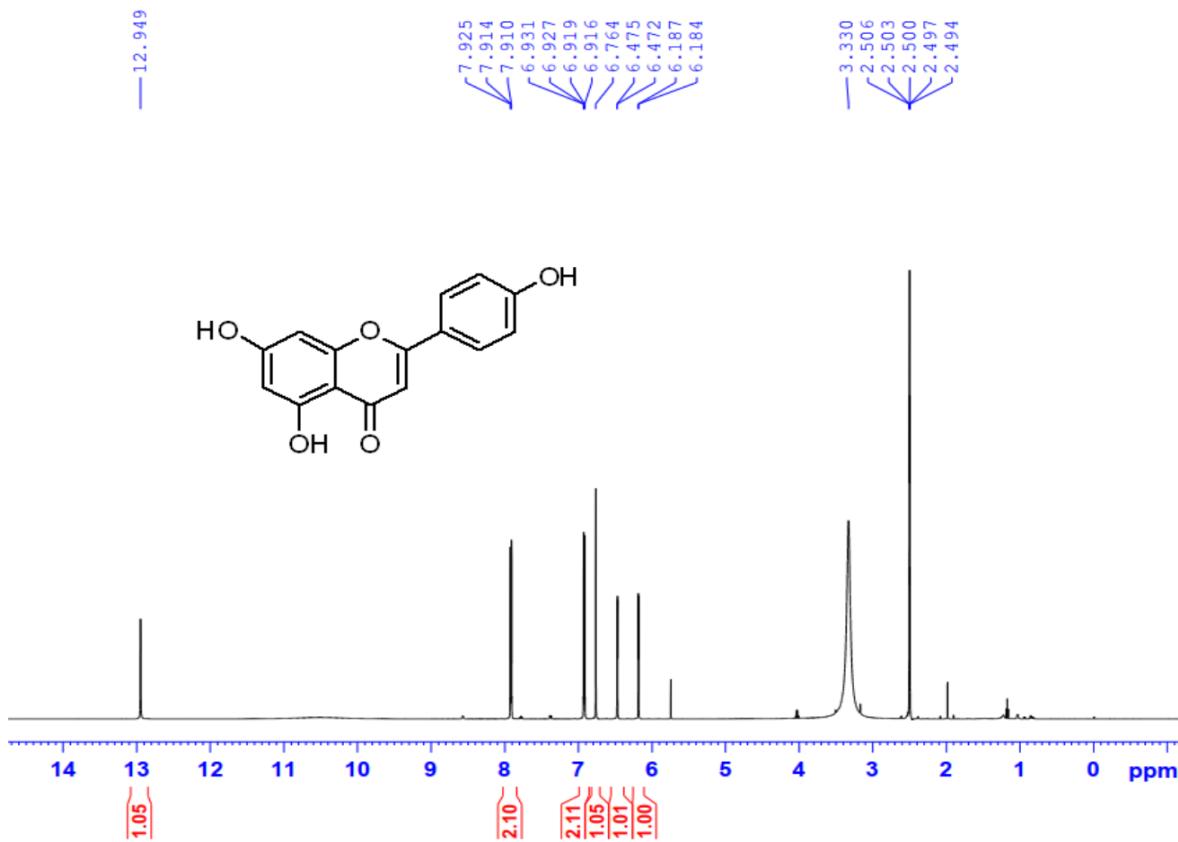


### Expanded spectrum

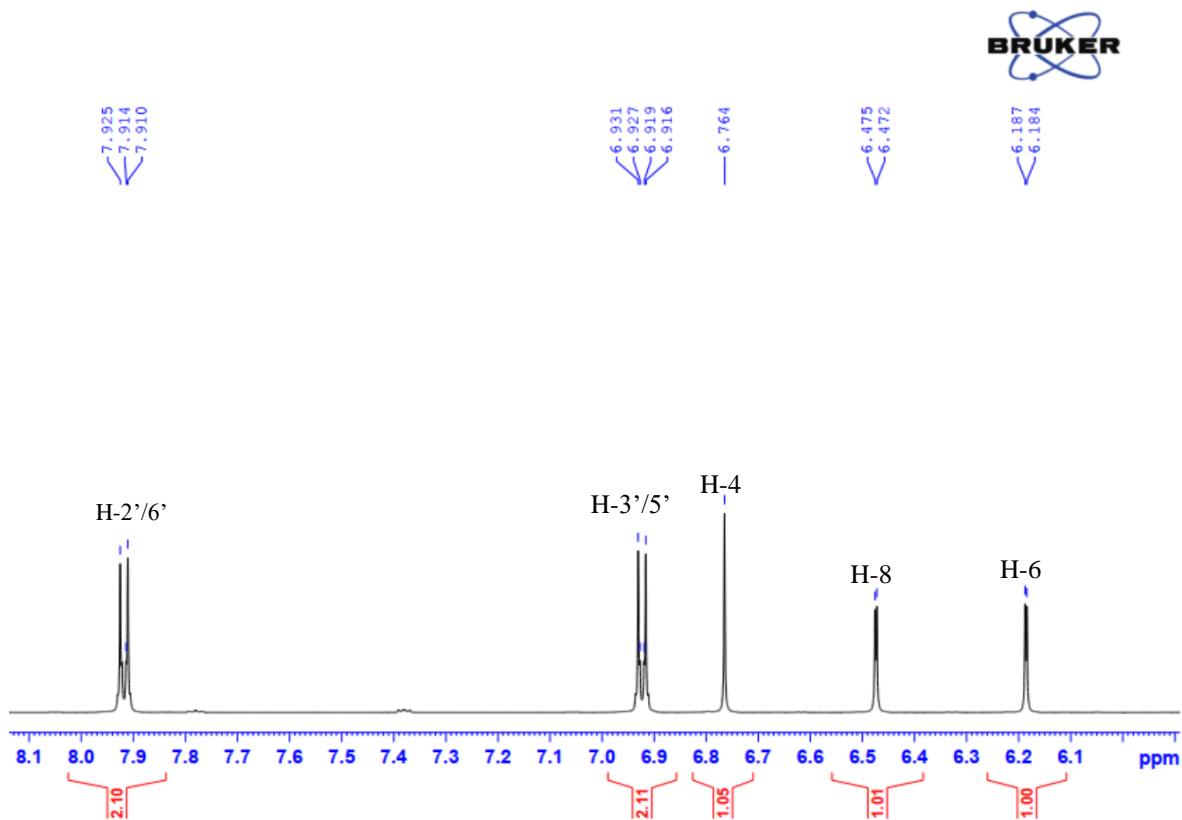
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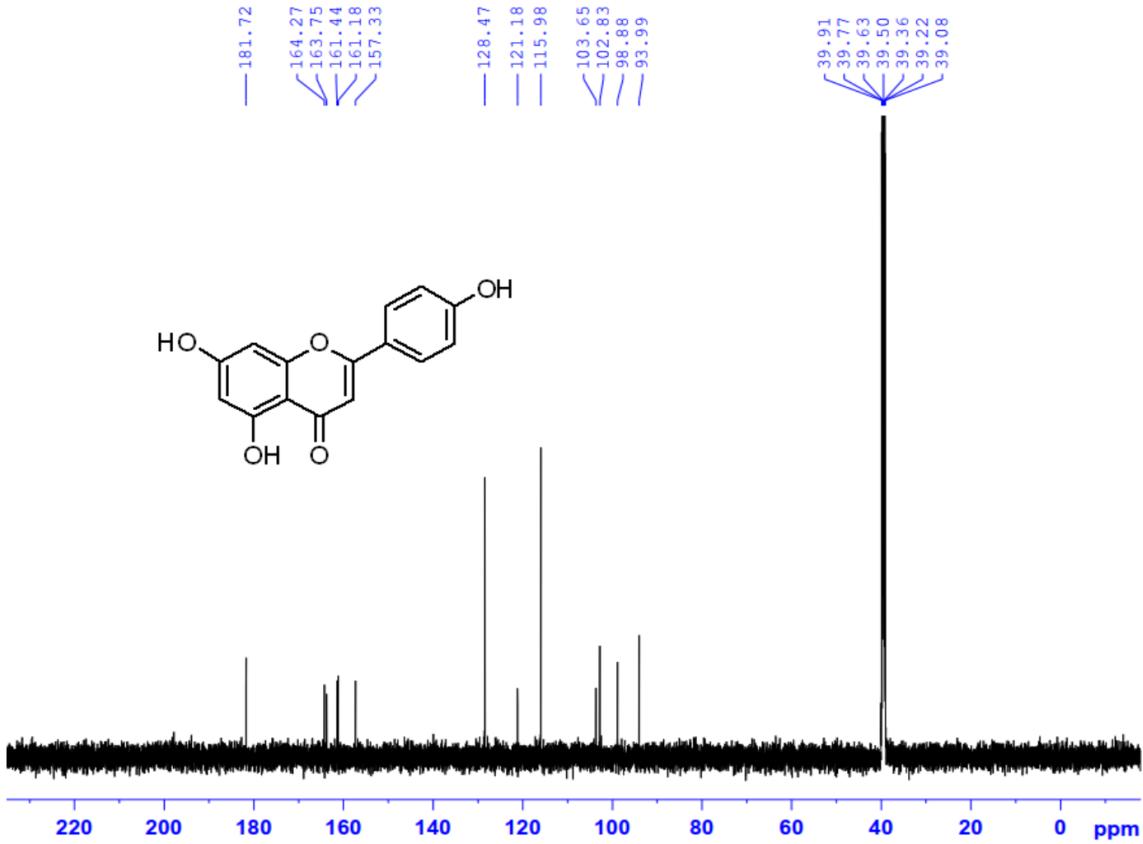
**Figure S36:** (+)-ESI-MS spectrum of compound **5** (apigenin)



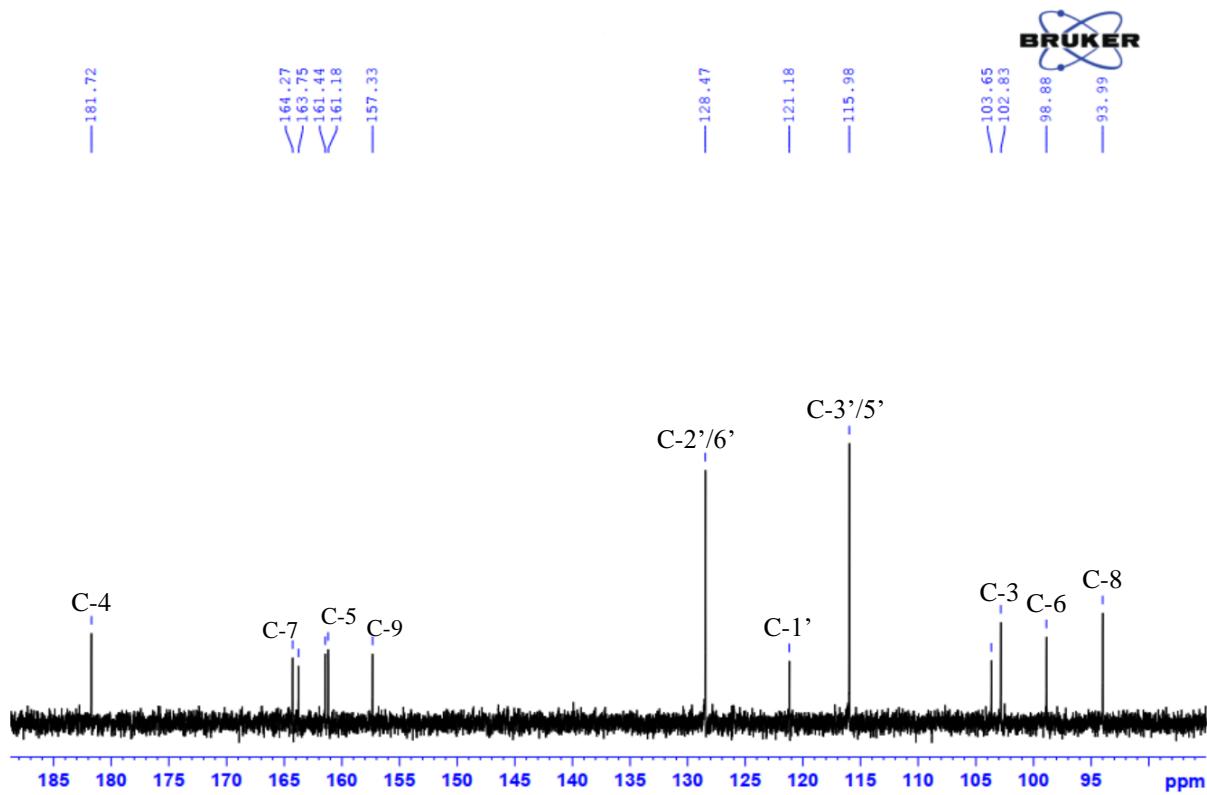
**Figure S37:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound 5 (apigenin)



**Figure S38:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound 5 (apigenin) (from  $\delta_{\text{H}}$  6.0 ppm to  $\delta_{\text{H}}$  8.1 ppm)



**Figure S39:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound 5 (apigenin)



**Figure S40:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound 5 (apigenin) (from  $\delta_C$  90 ppm to  $\delta_C$  185 ppm)

**Table S6:** The comparison of NMR data of compound **6** with a similar compound (Rutin)

Position	Compound <b>6</b> (DMSO- <i>d</i> <sub>6</sub> )		Rutin (DMSO- <i>d</i> <sub>6</sub> ) [33]	
	<sup>13</sup> C-NMR (150 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_{\text{H}}$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (500 MHz) $\delta_{\text{H}}$ ppm
2	156.4	-	158.4	-
3	133.3	-	135.6	-
4	177.3	-	179.3	-
5	161.2	-	162.5	-
6	98.8	6.17 (1H, <i>d</i> , 2.0 Hz)	99.9	6.20 (1H, <i>d</i> , 1.8 Hz)
7	164.6	-	165.9	-
8	93.6	6.36 (1H, <i>d</i> , 2.0 Hz)	94.8	6.39 (1H, <i>d</i> , 2.2 Hz)
9	156.5	-	159.3	-
10	103.7	-	105.6	-
1'	121.1	-	123.1	-
2'	116.2	7.55 (1H, <i>d</i> , 1.8 Hz)	117.6	7.66 (1H, <i>d</i> , 1.8 Hz)
3'	144.8	-	145.8	-
4'	148.5	-	149.7	-
5'	115.2	6.84 (1H, <i>d</i> , 8.4 Hz)	116.1	6.86 (1H, <i>d</i> , 8.0 Hz)
6'	121.6	7.53 (1H, <i>dd</i> , 8.4, 2.4 Hz)	123.5	7.60 (1H, <i>dd</i> , 8.0, 1.8 Hz)
1"	101.2	5.33 (1H, <i>d</i> , 7.2 Hz)	104.7	5.09 (1H, <i>d</i> , 7.8 Hz)
2"	74.1		75.7	
3"	75.9		77.2	
4"	70.0		71.4	
5"	76.4		78.1	
6"	67.0		68.6	
1'''	100.7	4.39 (1H, <i>s</i> )	102.4	4.51 (1H, <i>d</i> , 1.8 Hz)
2'''	70.3		72.0	
3'''	70.5		72.2	
4'''	71.8		73.9	
5'''	68.2		69.7	
6'''	17.7	0.99 (3H, <i>d</i> , 6.0 Hz)	17.9	1.11 (3H, <i>d</i> , 6.0 Hz)

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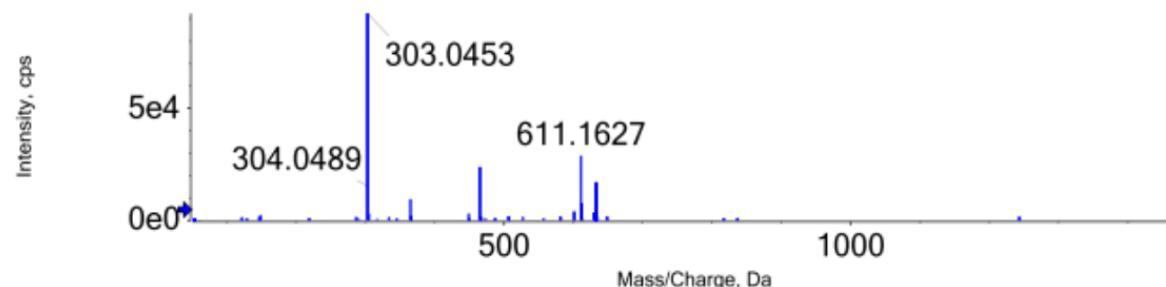
## ANALYSIS REPORT

**Injection details**

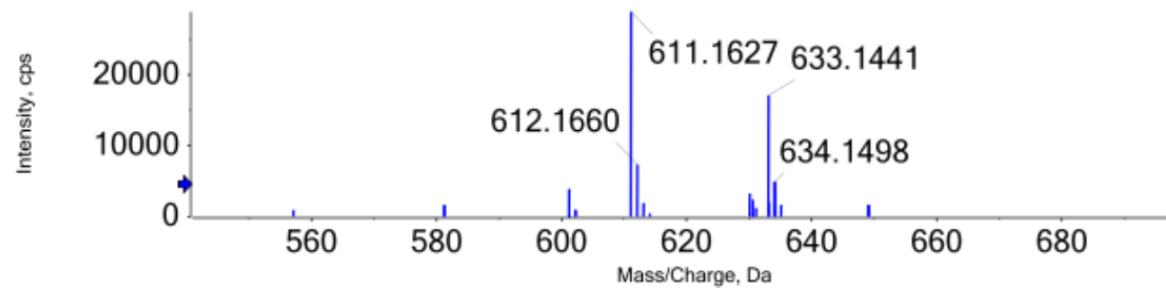
<i>Sample name</i>	SAL	<i>Vial position</i>	37
<i>Sample file name</i>	SER.wiff2-YEN	<i>Inject volume</i>	5.00
<i>Acquisition date</i>	20/04/2023 10:43:32 AM	<i>Acquisition method</i>	<b>ESI_POS_SCAN</b>
<i>Operator</i>	CB21261708	<i>Instrument name</i>	X500 <sub>R</sub> QTOF

**Full mass spectrum**

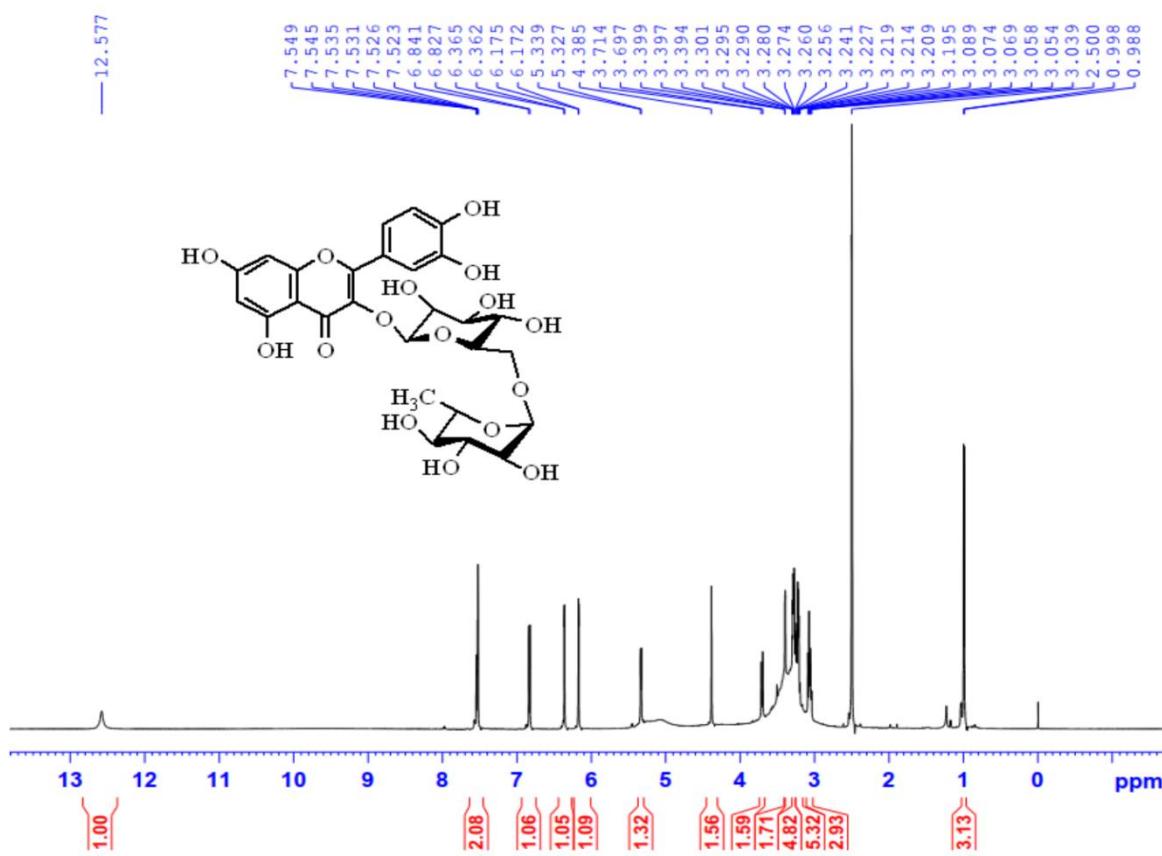
Spectrum from YEN\_SAL\_(\_+)\_ESI 2023-04-20-10-43-32.wiff2...se multiplier = 1.5), Gaussian smoothed (0.5 point)

**Expanded spectrum**

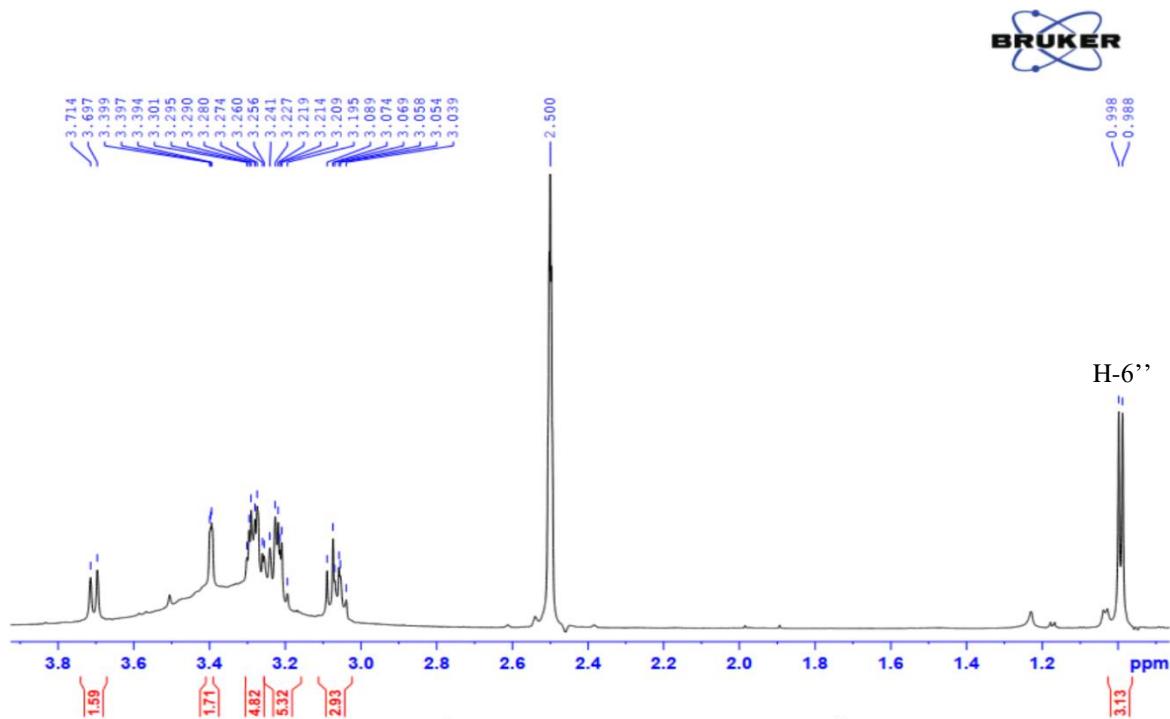
Spectrum from YEN\_SAL\_(\_+)\_ESI 2023-04-20-10-43-32.wiff2...se multiplier = 1.5), Gaussian smoothed (0.5 point)



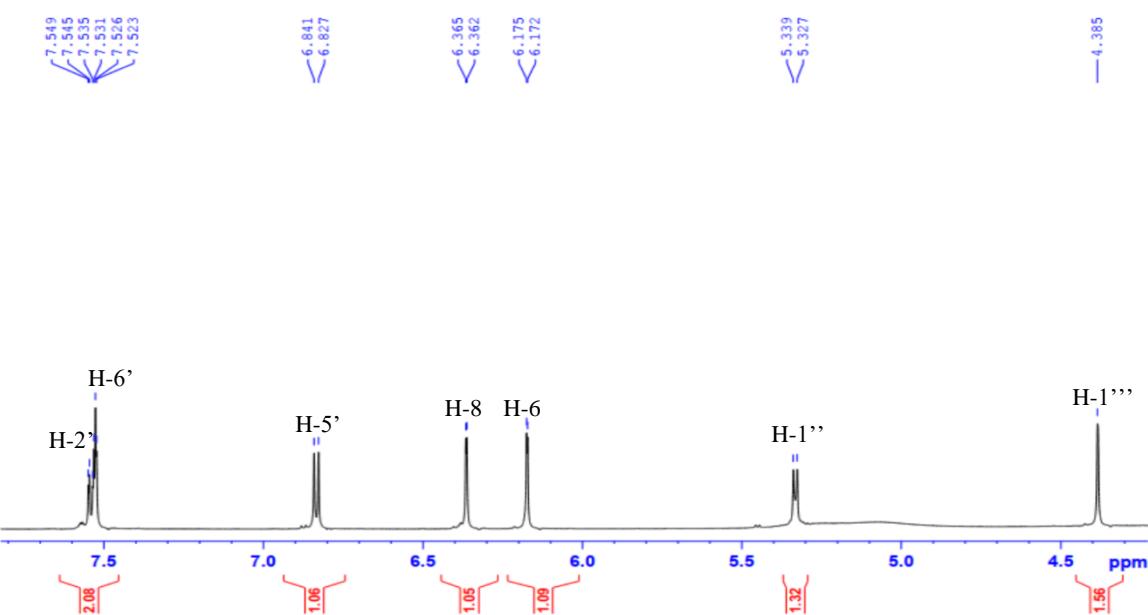
**Figure S41:** (+)ESI-MS spectrum of compound 6



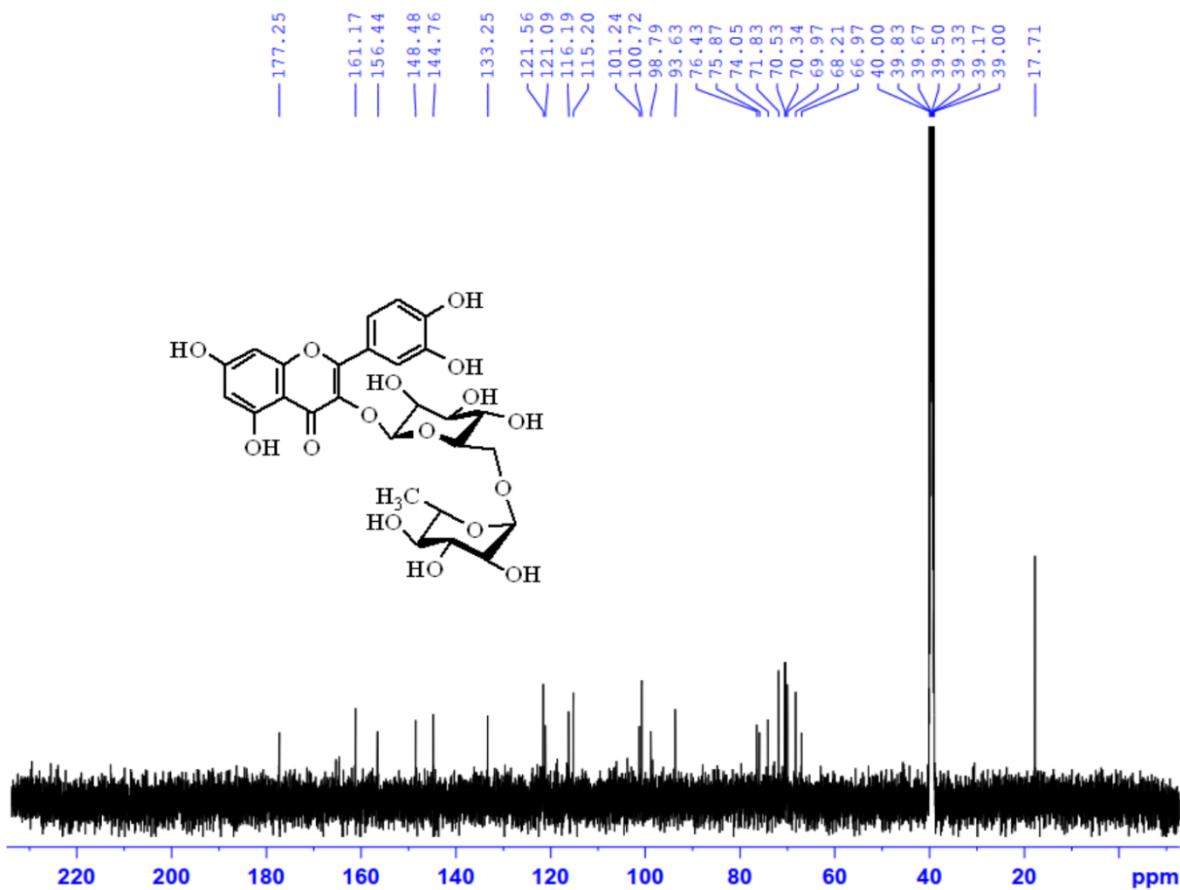
**Figure S42:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **6** (rutin)



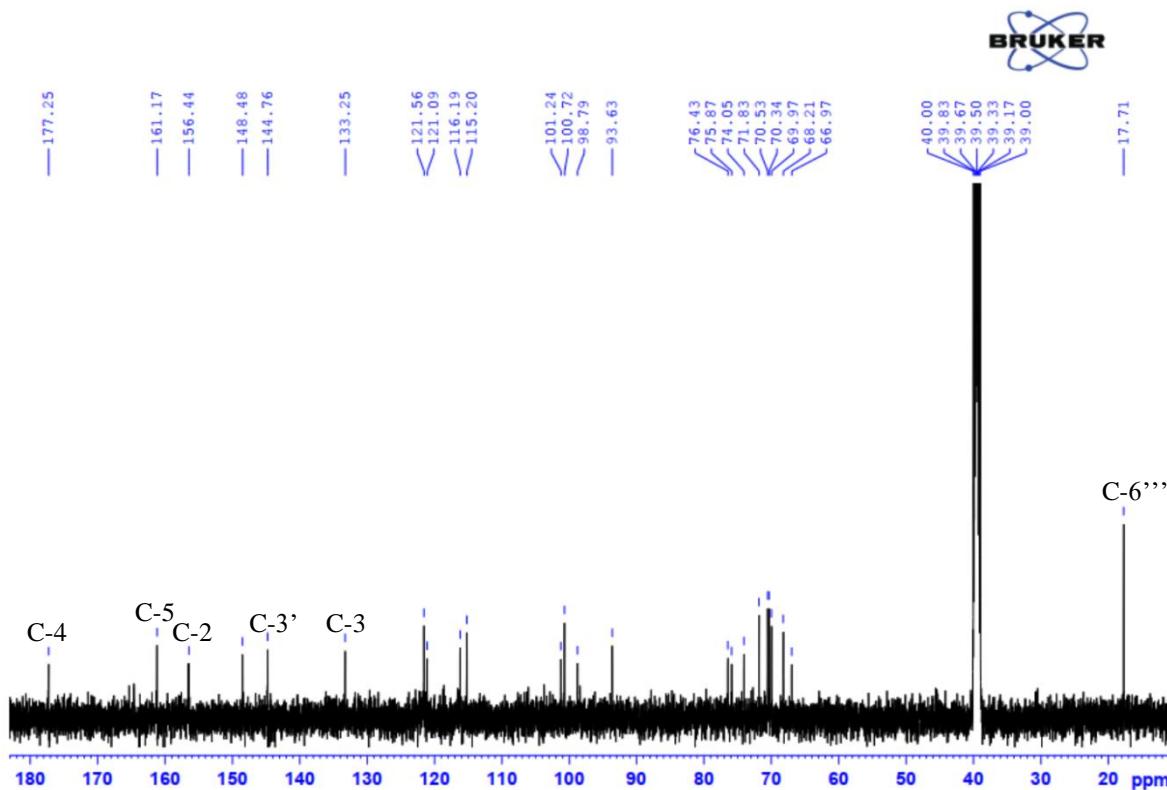
**Figure S43:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **6** (rutin) (from  $\delta_{\text{H}}$  1.0 ppm to  $\delta_{\text{H}}$  3.8 ppm)



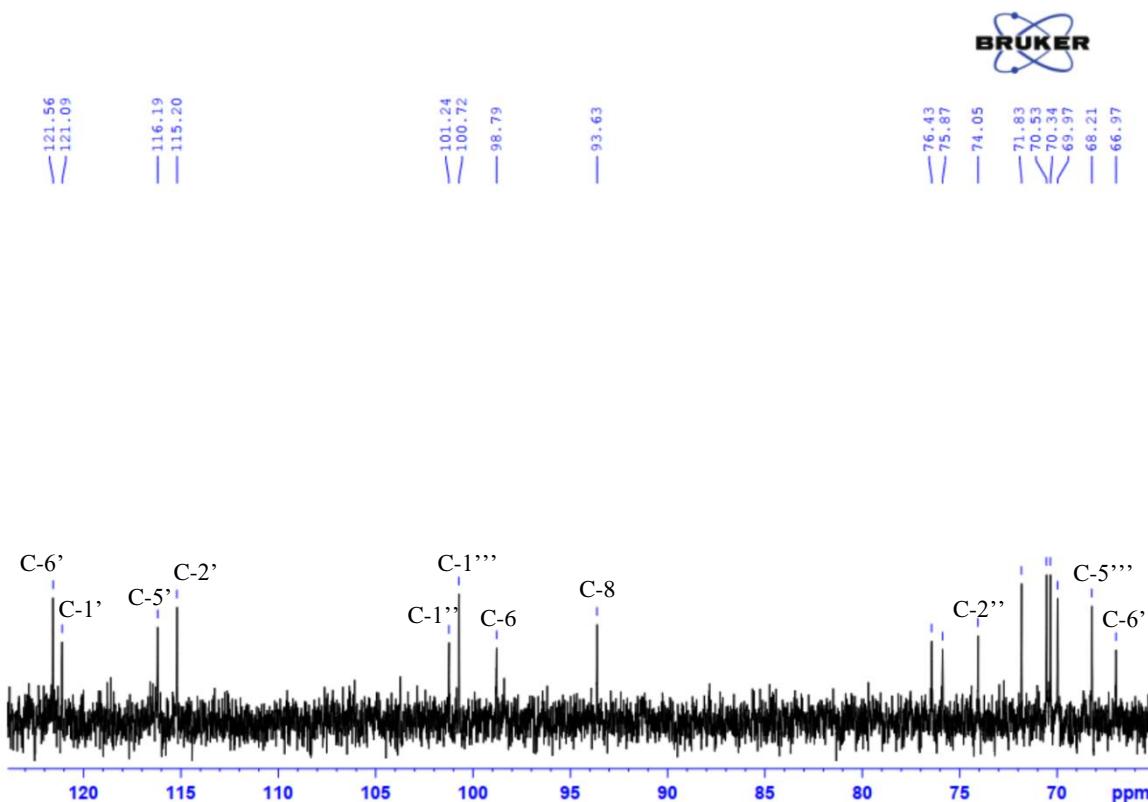
**Figure S44:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **6** (rutin) (from  $\delta_{\text{H}}$  4.3 ppm to  $\delta_{\text{H}}$  7.7 ppm)



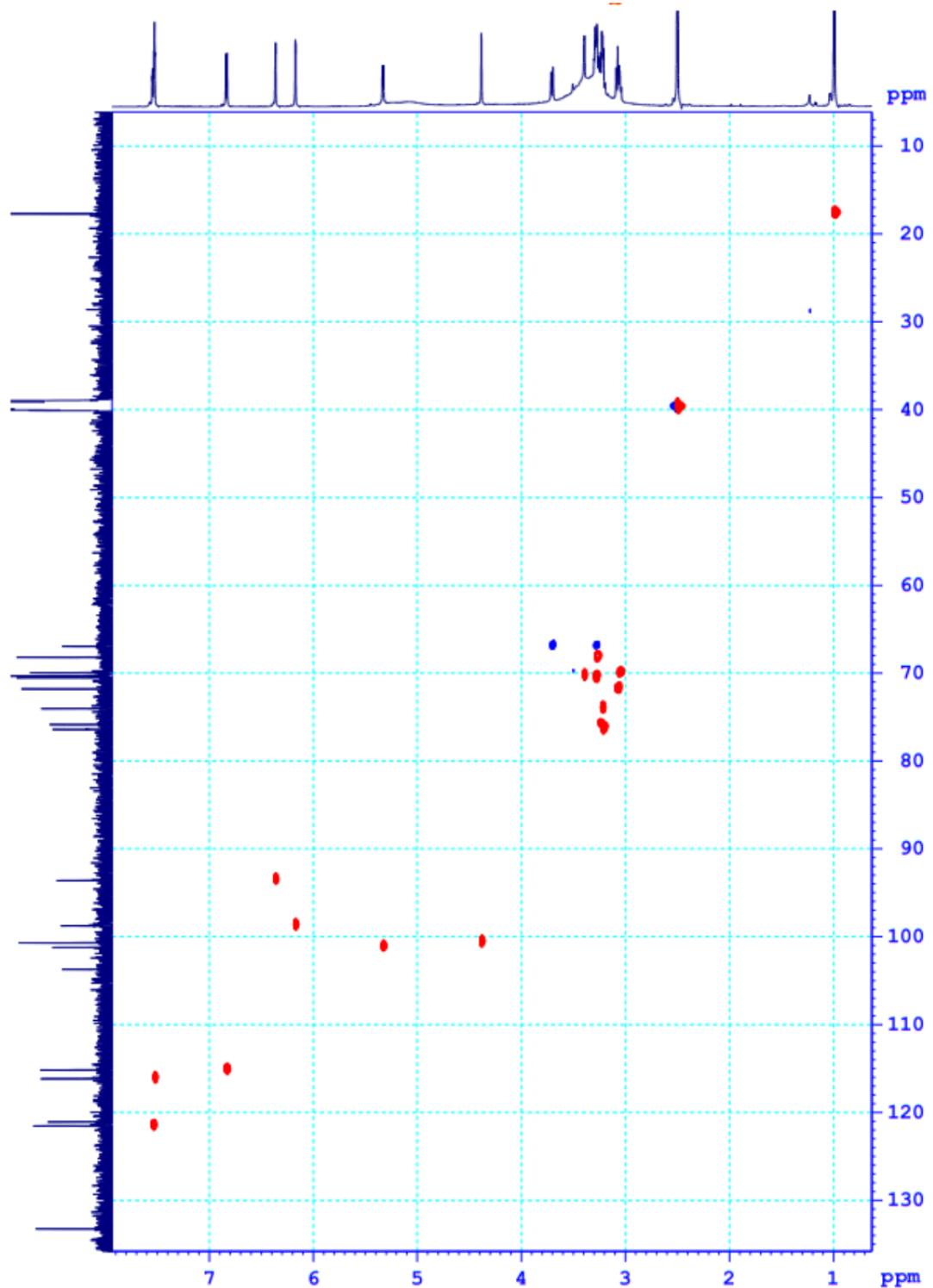
**Figure S45:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **6** (rutin)



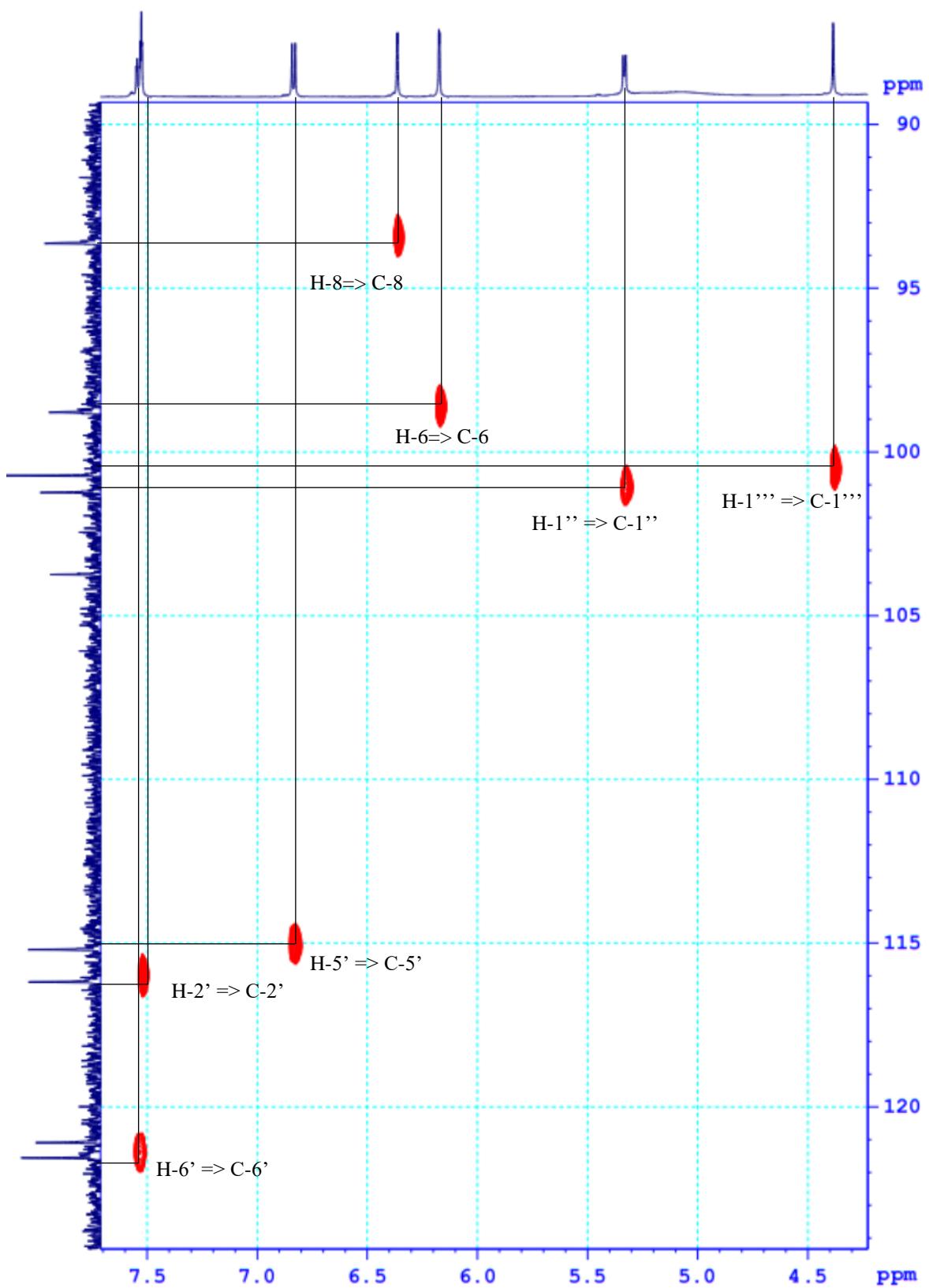
**Figure S46:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **6** (rutin) (from  $\delta_{\text{C}}$  15 ppm to  $\delta_{\text{C}}$  180 ppm)



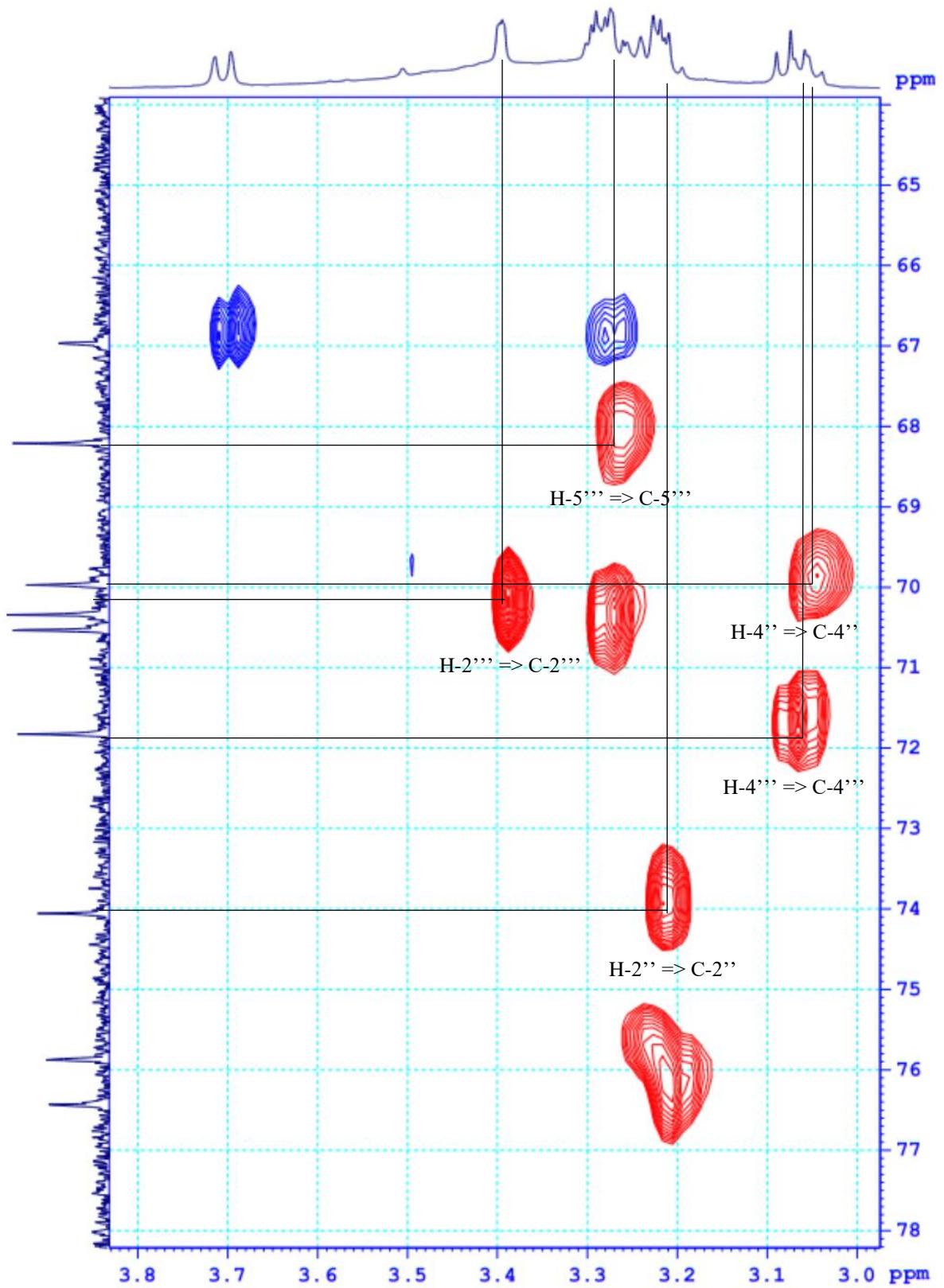
**Figure S47:**  $^{13}\text{C}$ -NMR (150 MHz, DMSO- $d_6$ ) spectrum of compound **6** (rutin) (from  $\delta_{\text{C}}$  60 ppm to  $\delta_{\text{C}}$  125 ppm)



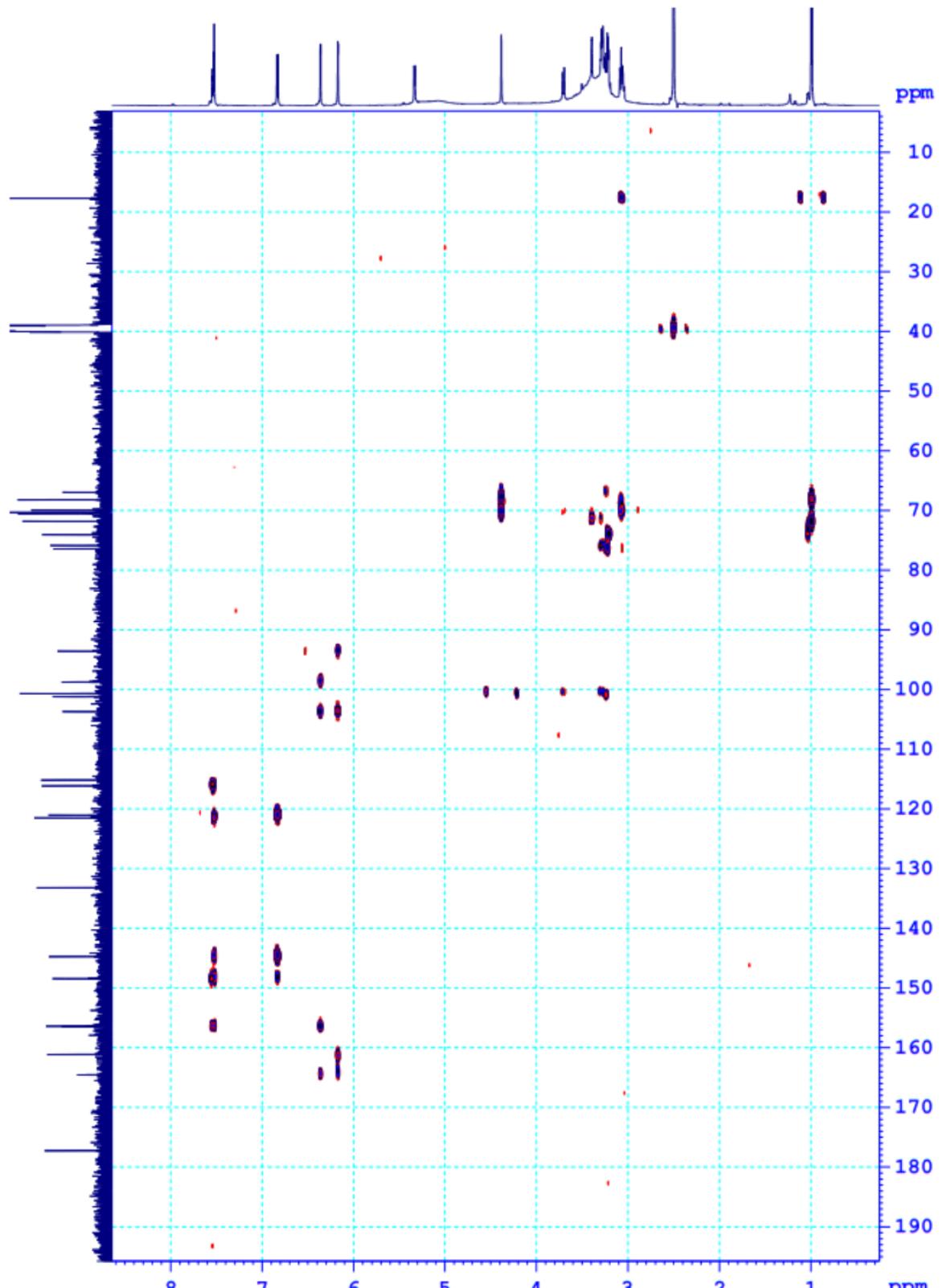
**Figure S48:** HSQC spectrum of compound **6** (rutin)



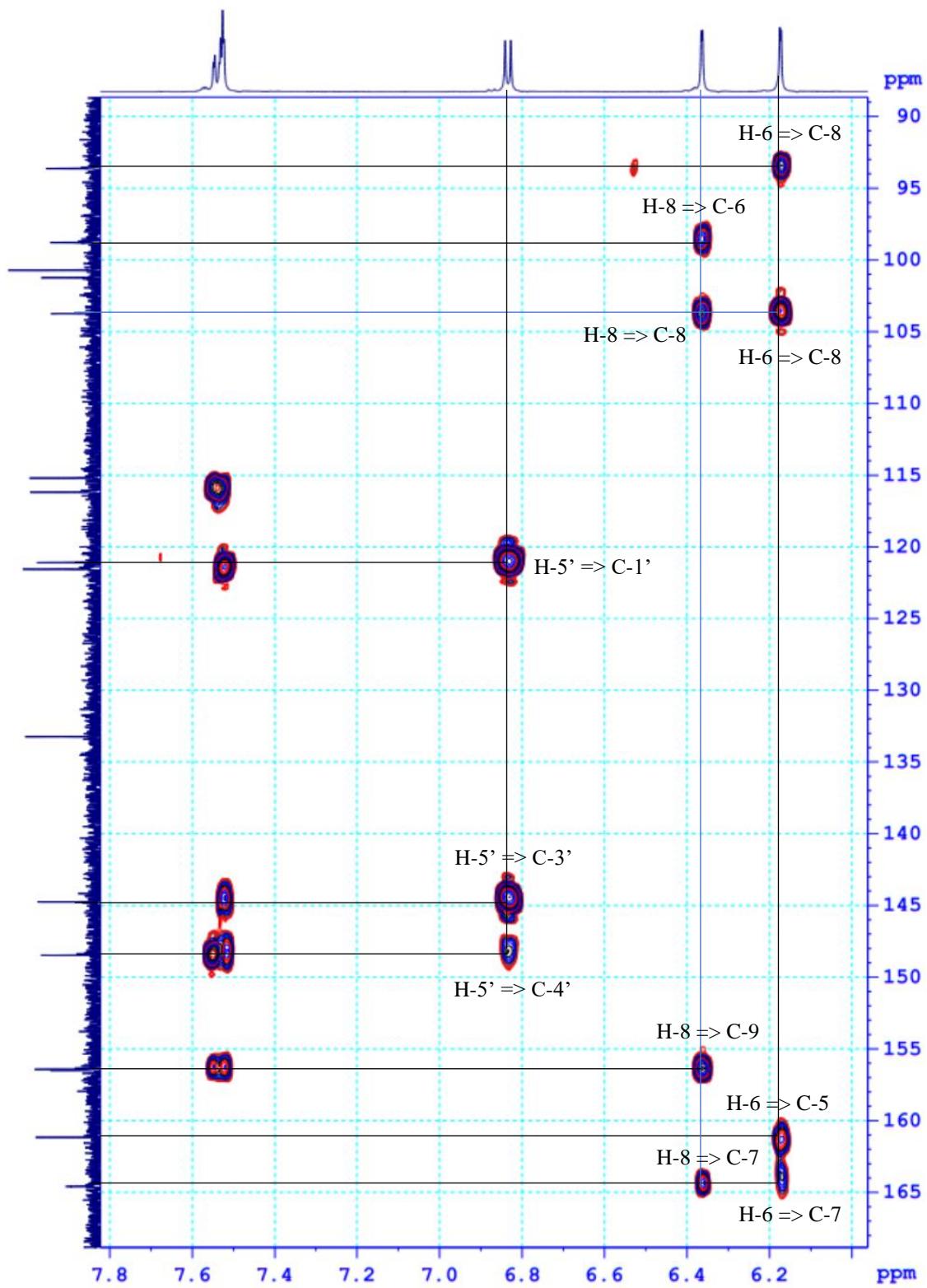
**Figure S49:** HSQC spectrum of compound **6** (rutin) (from  $\delta_{\text{C}}$  90 ppm to  $\delta_{\text{C}}$  125 ppm)



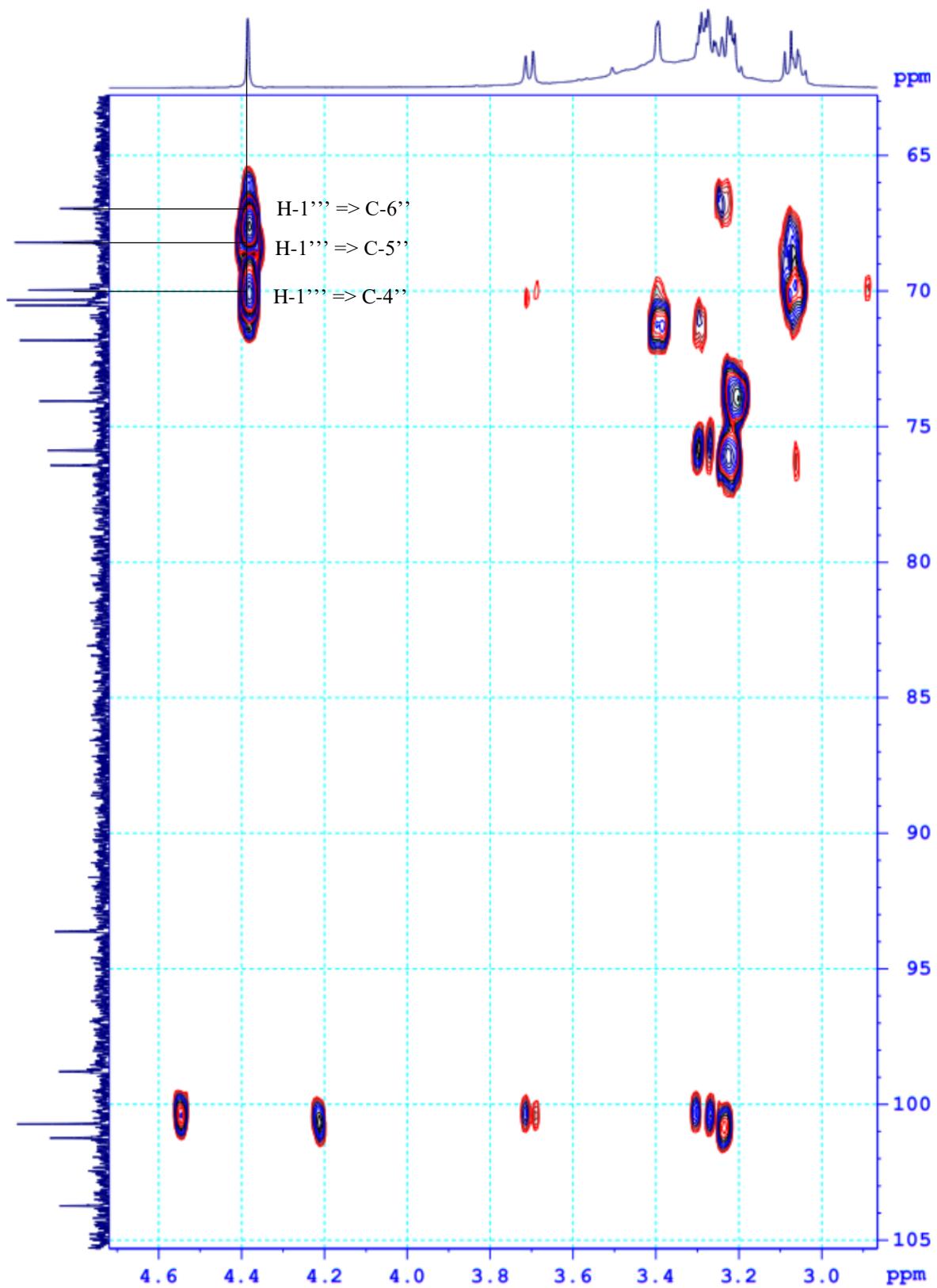
**Figure S50:** HSQC spectrum of compound **6** (rutin) (from  $\delta_{\text{C}}$  64 ppm to  $\delta_{\text{C}}$  78 ppm)



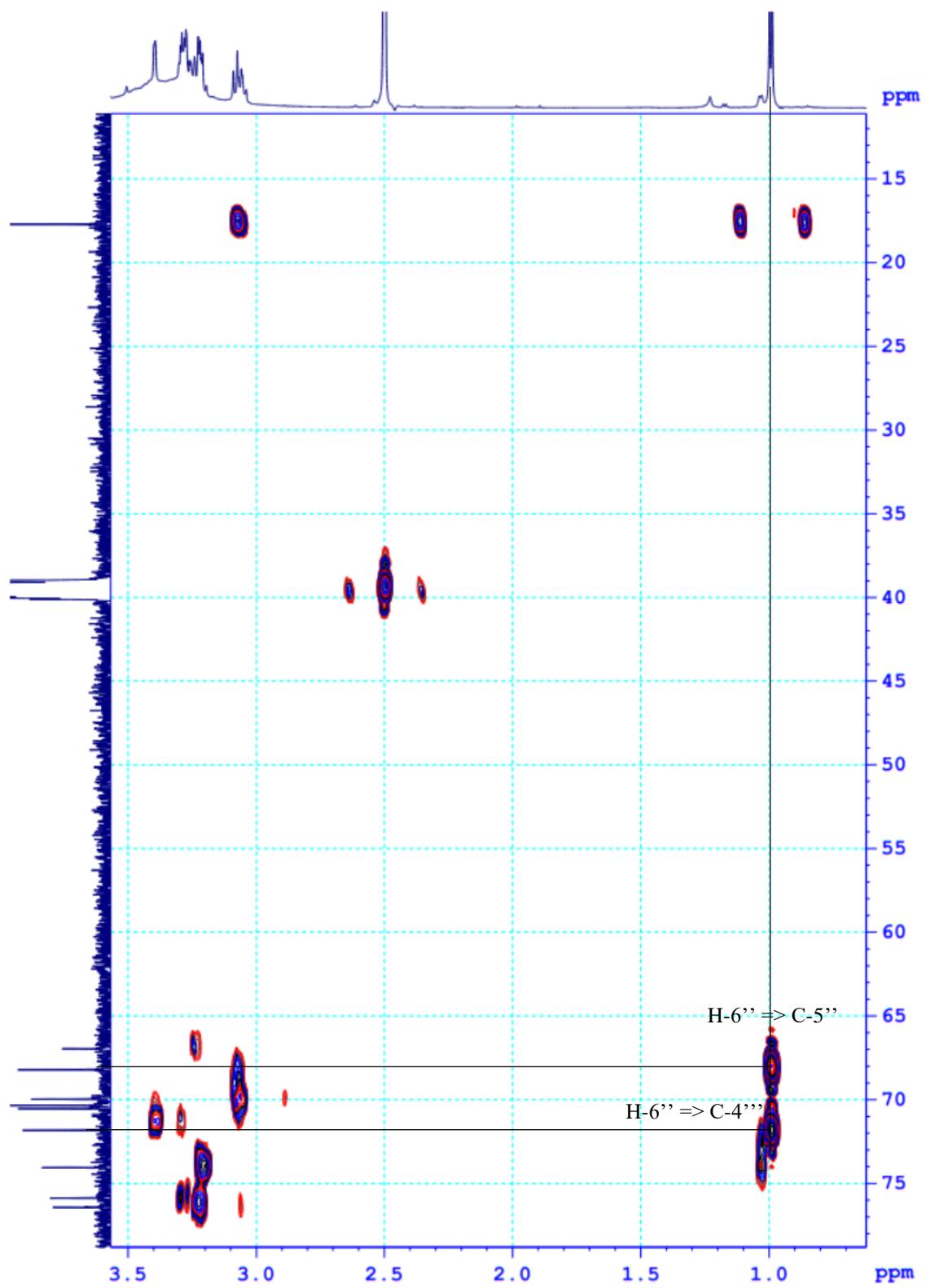
**Figure S51:** HMBC spectrum of compound 6 (rutin)



**Figure S52:** HMBC spectrum of compound **6** (rutin) (from  $\delta_C$  90 ppm to  $\delta_C$  165 ppm)



**Figure S53:** HMBC spectrum of compound **6** (rutin) (from  $\delta_C$  65 ppm to  $\delta_C$  105 ppm)



**Figure S54:** HMBC spectrum of compound **6** (rutin) (from  $\delta_{\text{C}}$  15 ppm to  $\delta_{\text{C}}$  75 ppm)

**Table S7:** The comparison of NMR data of compound **7** with a similar compound (Isatin)

<b>Position</b>	Compound <b>7</b> (MeOD)		Isatin ( $\text{CDCl}_3$ ) [34,35]	
	<b><math>^{13}\text{C-NMR}</math></b> (125 MHz) $\delta_{\text{C}}$ ppm	<b><math>^1\text{H-NMR}</math></b> (600 MHz) $\delta_{\text{H}}$ ppm	<b><math>^{13}\text{C-NMR}</math></b> (125 MHz) $\delta_{\text{C}}$ ppm	<b><math>^1\text{H-NMR}</math></b> (500 MHz) $\delta_{\text{H}}$ ppm
1-NH	-	-	-	8.01
2	161.4	-	159.5	-
3	185.4	-	184.6	-
3 $\alpha$	119.4	-	117.9	-
4	124.4	7.60 (1H, <i>td</i> , 7.8, 1.2 Hz)	122.9	7.63
5	126.0	7.12 (1H, <i>td</i> , 7.8, 0.6 Hz)	124.8	7.13
6	139.5	7.56 (1H, <i>dd</i> , 7.8, 0.6 Hz)	138.5	7.57
7	113.4	6.96 (1H, <i>d</i> , 8.4 Hz)	112.4	6.91
7 $\alpha$	152.0	-	150.9	-

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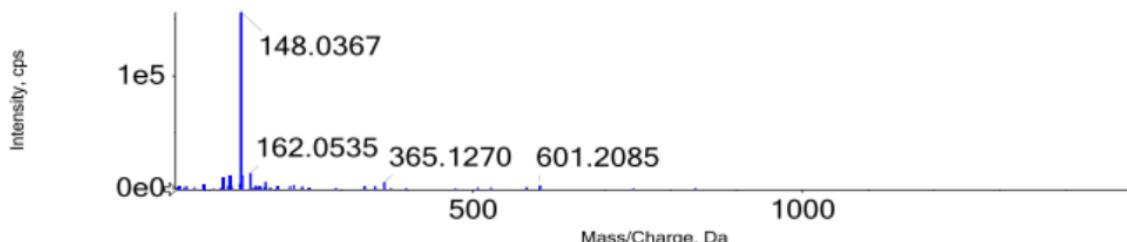
## ANALYSIS REPORT

### Injection details

Sample name	SAL	Vial position	39
Sample file name	SER.wiff2-YEN	Inject volume	5.00
Acquisition date	20/04/2023 10:51:32 AM	Acquisition method	<b>ESI_POS_SCAN</b>
Operator	CB21261708	Instrument name	X500R QTOF

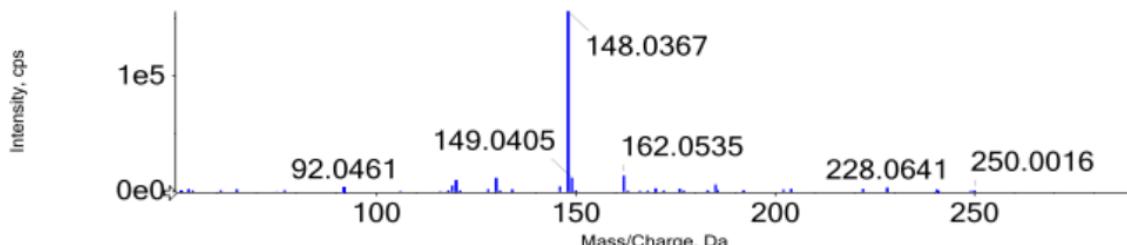
### Full mass spectrum

Spectrum from YEN\_SAL\_(\_+)\_ESI 2023-04-20-10-51-32.wiff2...se multiplier = 1.5, Gaussian smoothed (0.5 points)

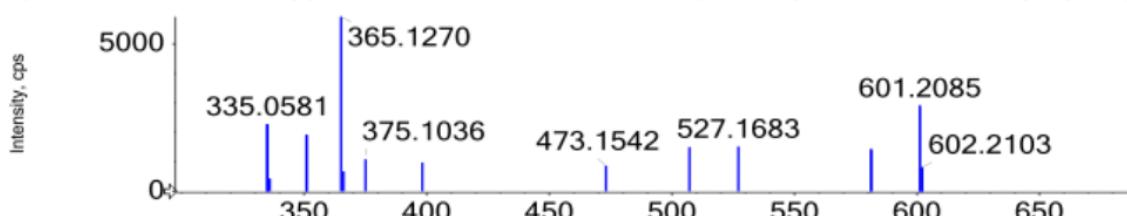


### Expanded spectrum

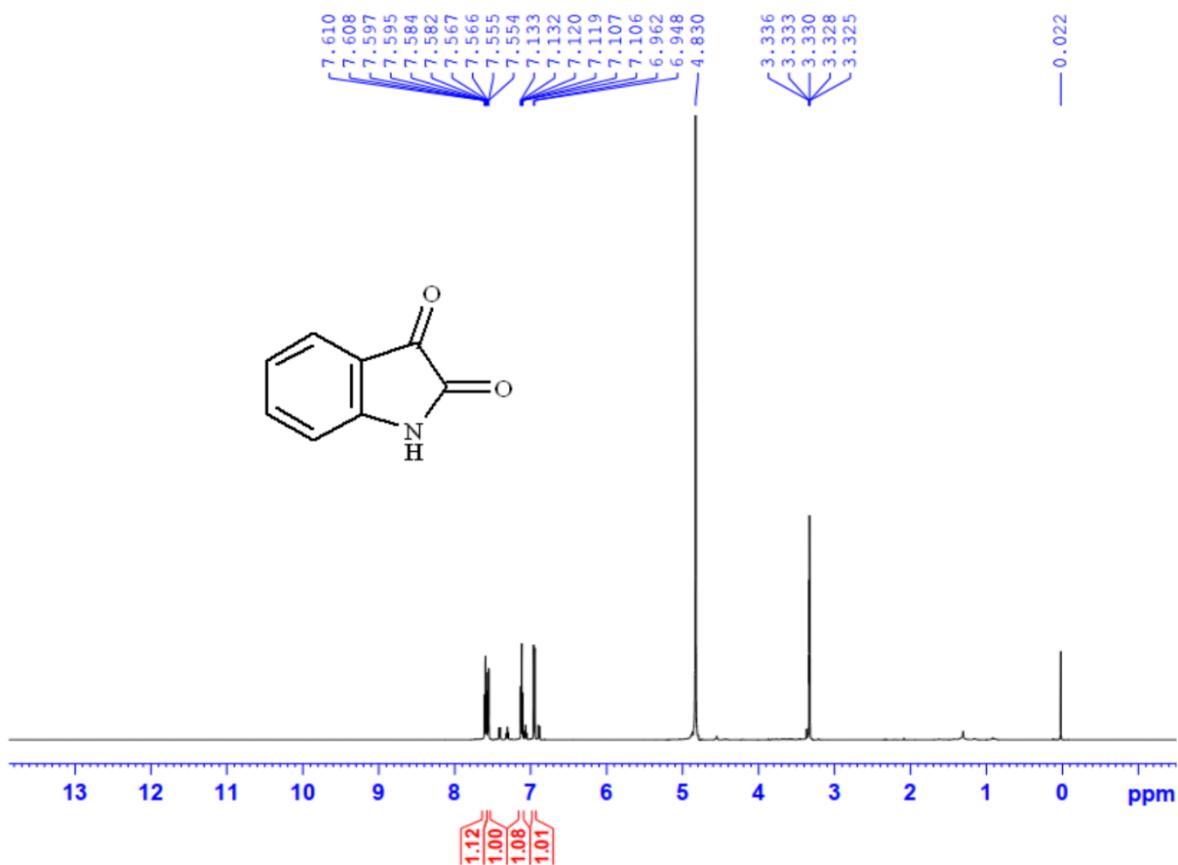
Spectrum from YEN\_SAL\_(\_+)\_ESI 2023-04-20-10-51-32.wiff2...se multiplier = 1.5, Gaussian smoothed (0.5 points)



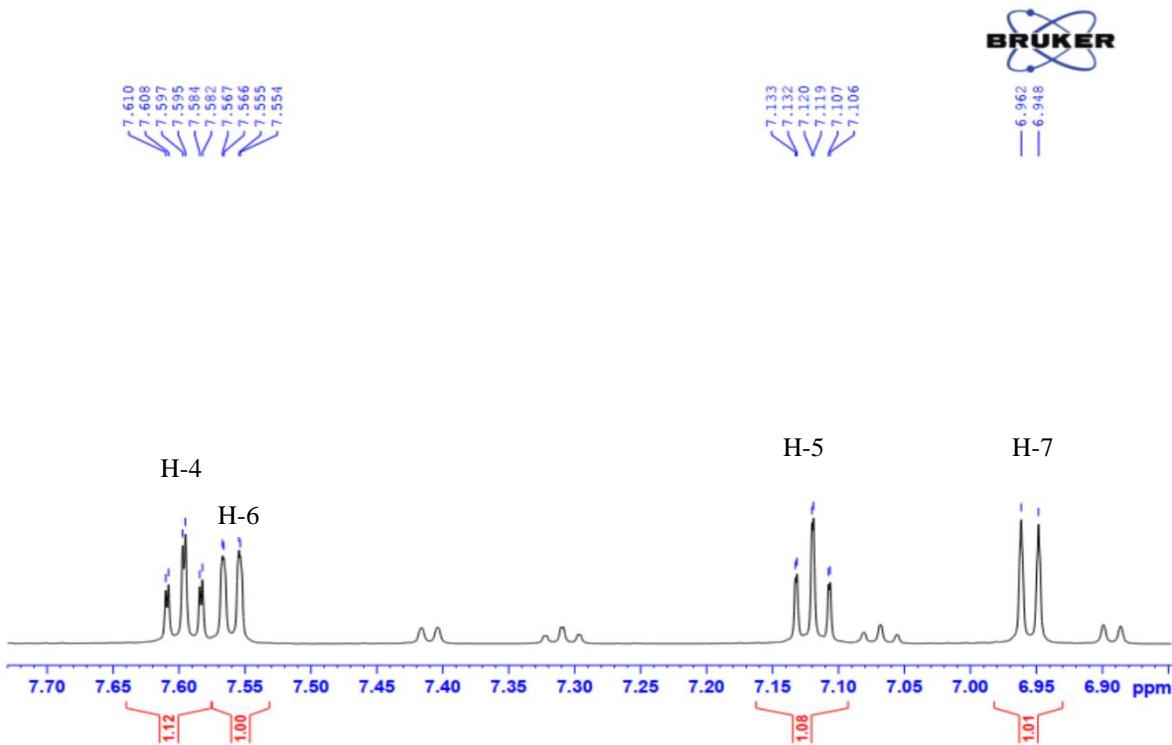
Spectrum from YEN\_SAL\_(\_+)\_ESI 2023-04-20-10-51-32.wiff2...se multiplier = 1.5, Gaussian smoothed (0.5 points)



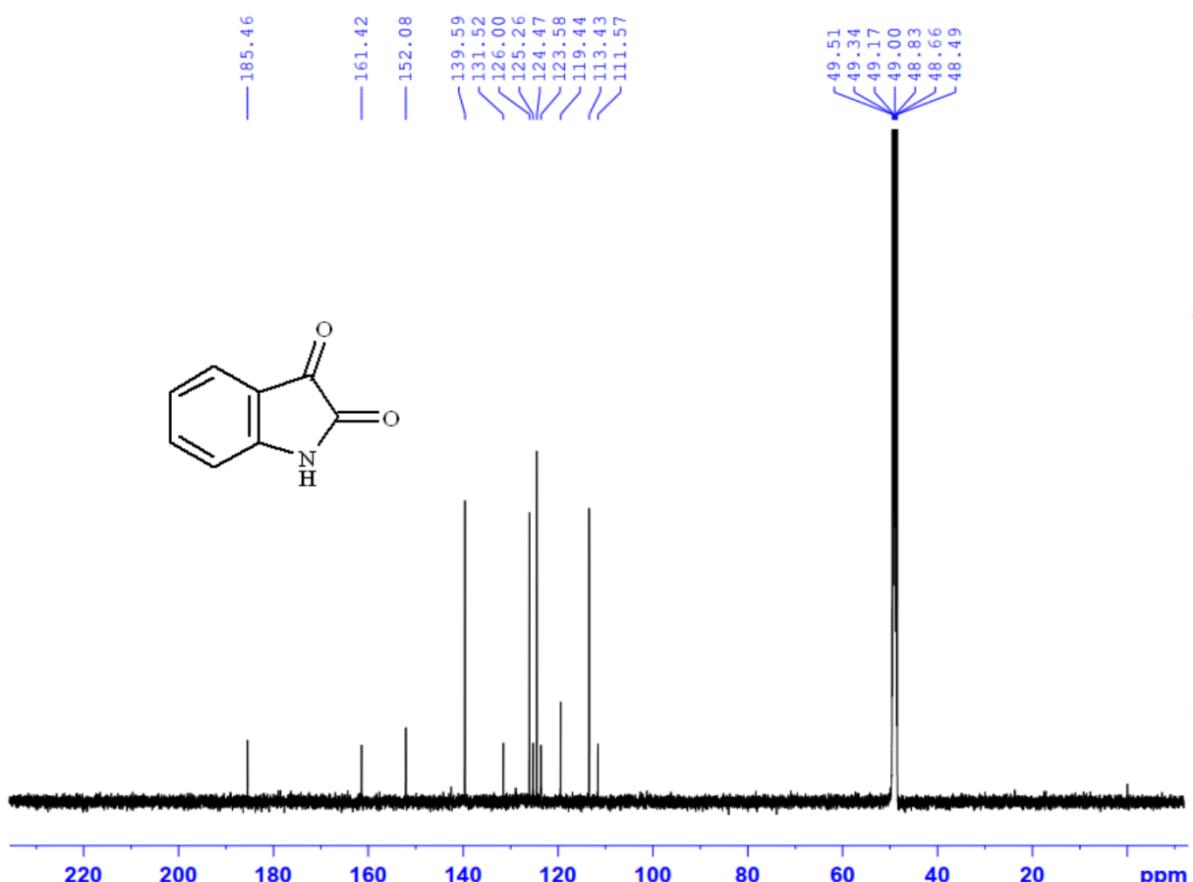
**Figure S55:** (+)ESI-MS spectrum of compound 7 (isatin)



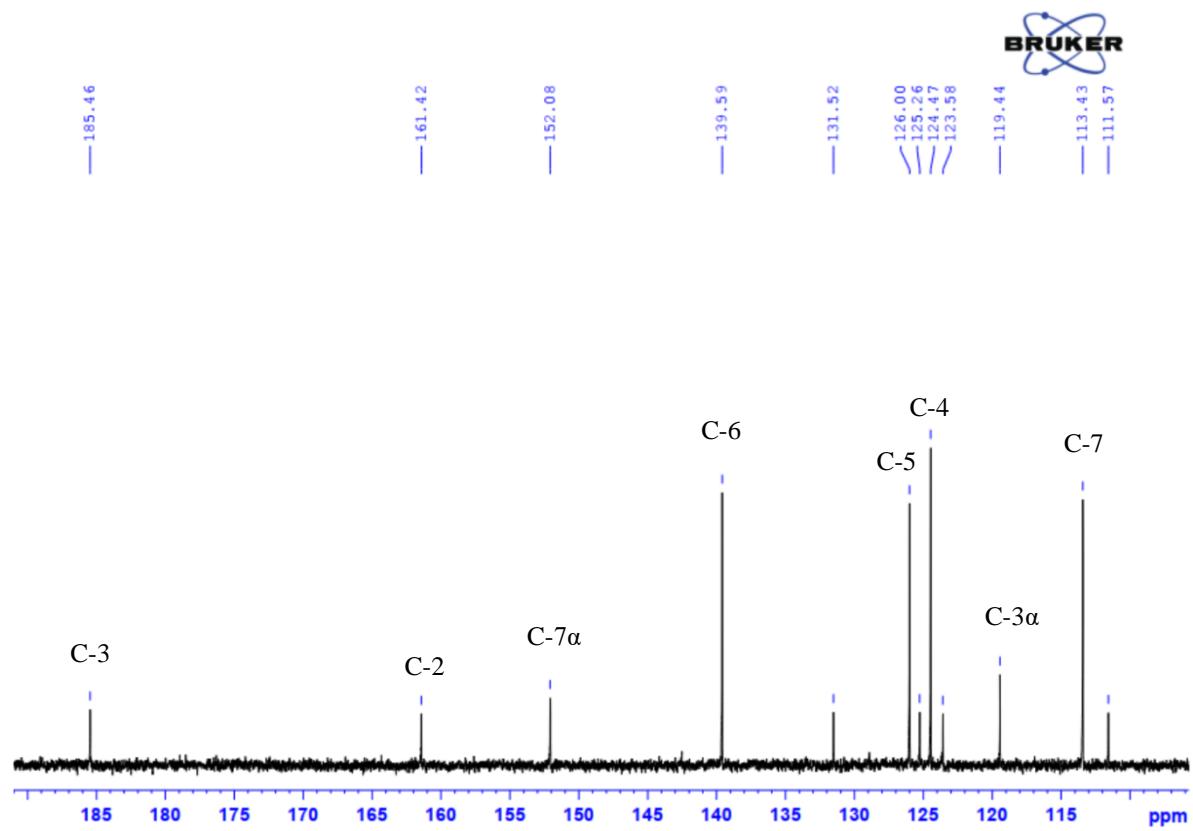
**Figure S56:**  $^1\text{H}$ -NMR (600 MHz,  $\text{MeOD}$ ) spectrum of compound 7 (isatin)



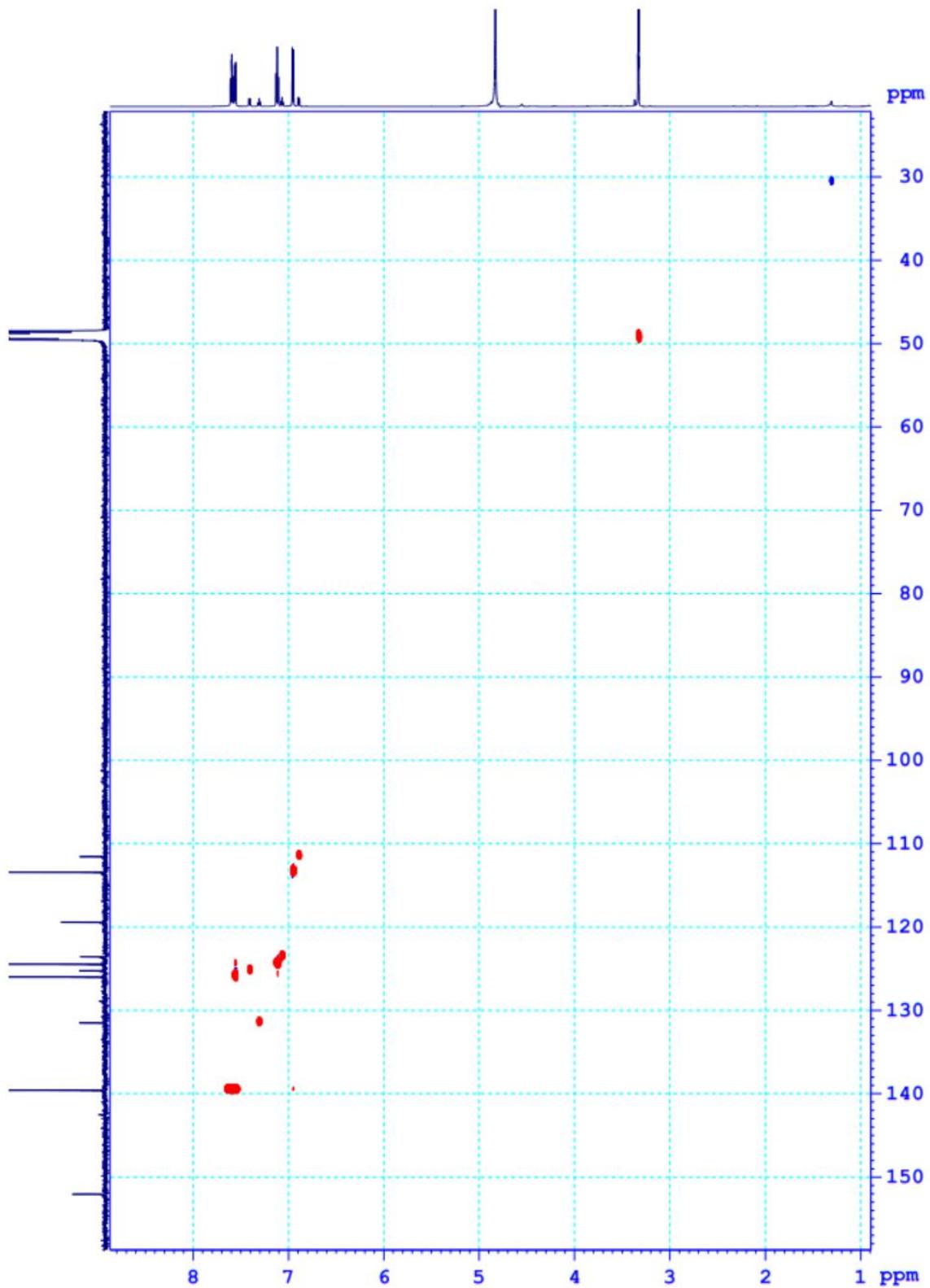
**Figure S57:**  $^1\text{H}$ -NMR spectrum of compound 7 (isatin) (from  $\delta_{\text{H}}$  6.9 ppm to  $\delta_{\text{H}}$  7.7 ppm)



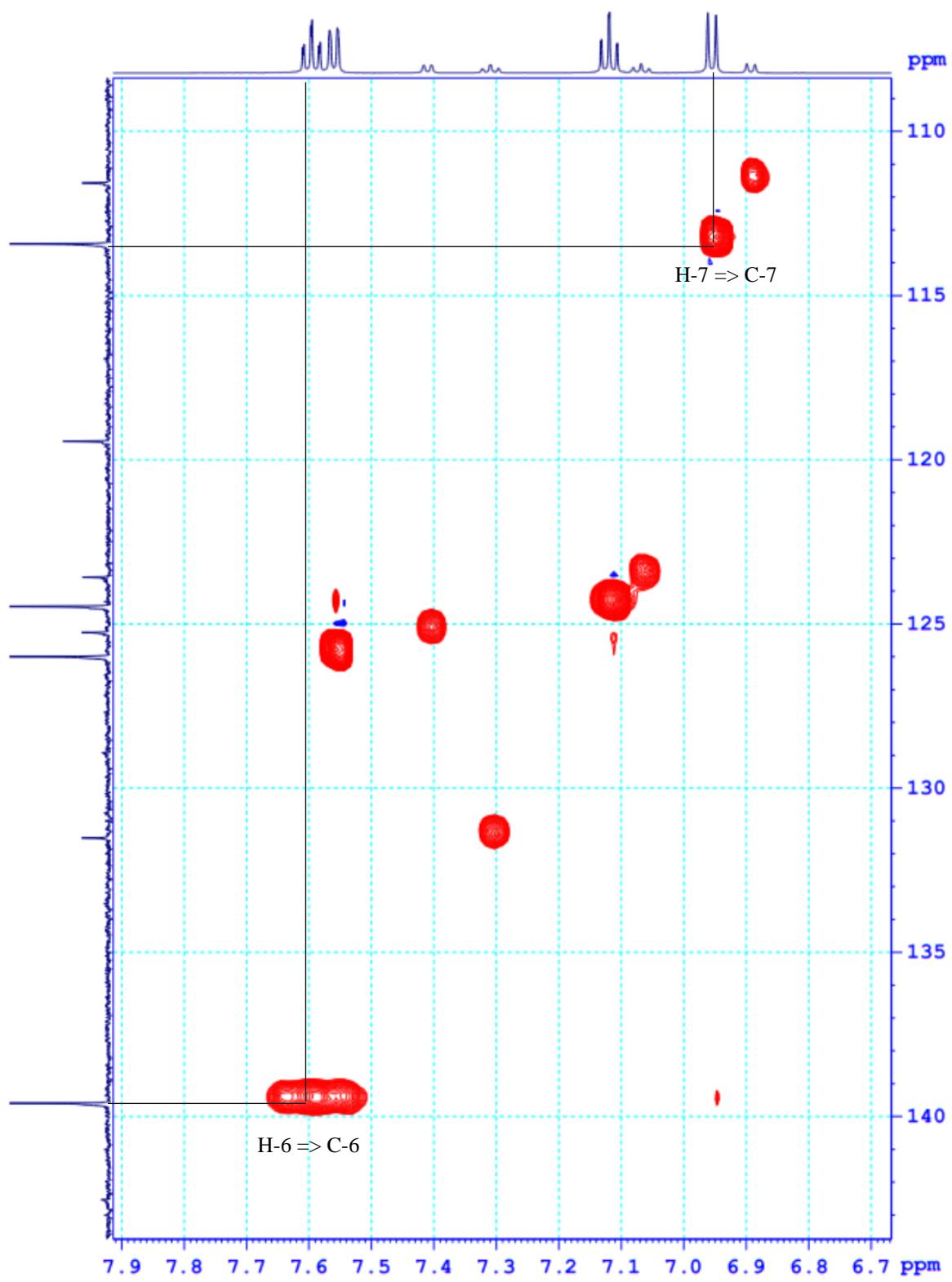
**Figure S58:**  $^{13}\text{C}$ -NMR (150MHz, MeOD) spectrum of compound 7 (isatin)



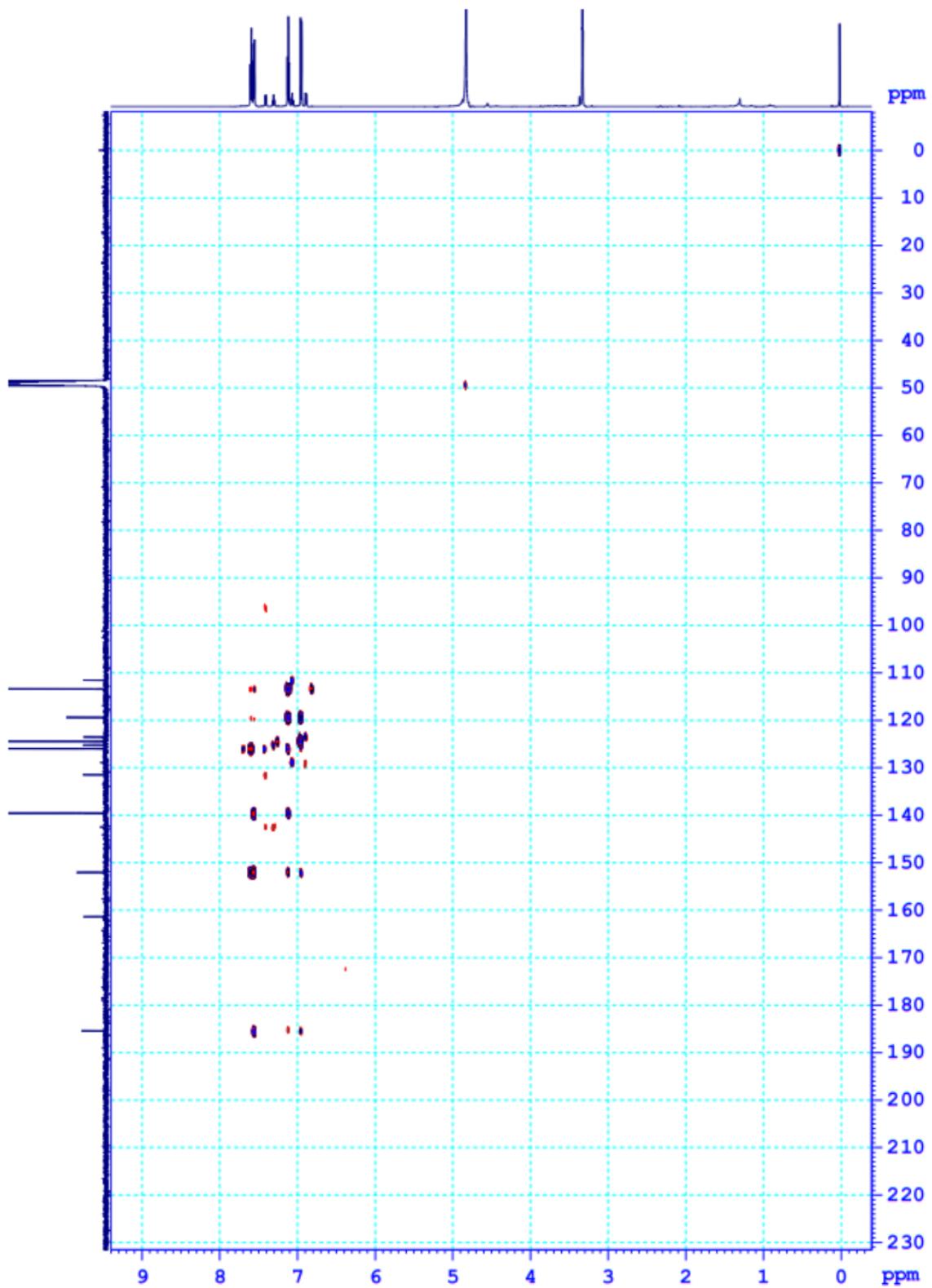
**Figure S59:**  $^{13}\text{C}$ -NMR spectrum of compound 7 (isatin) (from  $\delta_{\text{C}}$  110 ppm to  $\delta_{\text{C}}$  185 ppm)

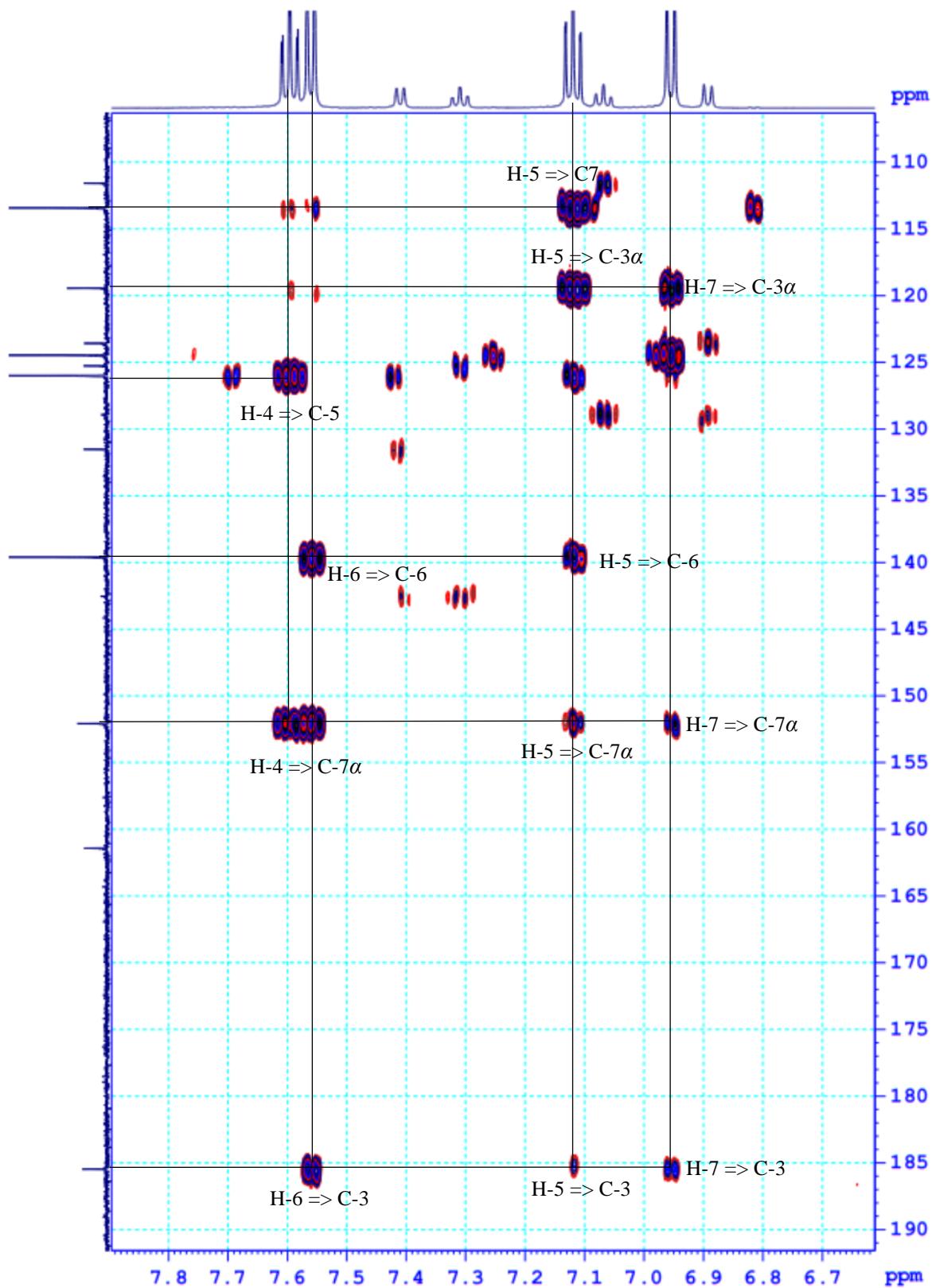


**Figure S60:** HSQC spectrum of compound 7 (isatin)



**Figure S61:** HSQC spectrum of compound 7 (isatin) (from  $\delta_{\text{C}}$  110 ppm to  $\delta_{\text{C}}$  140 ppm)

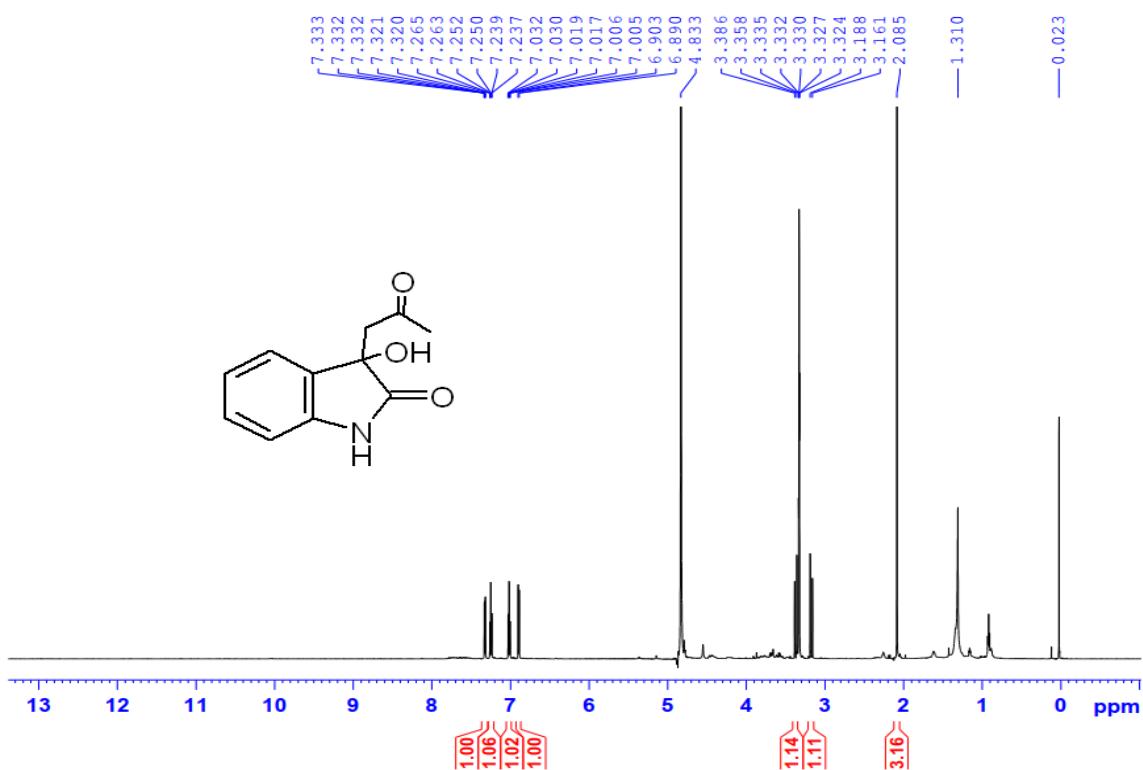




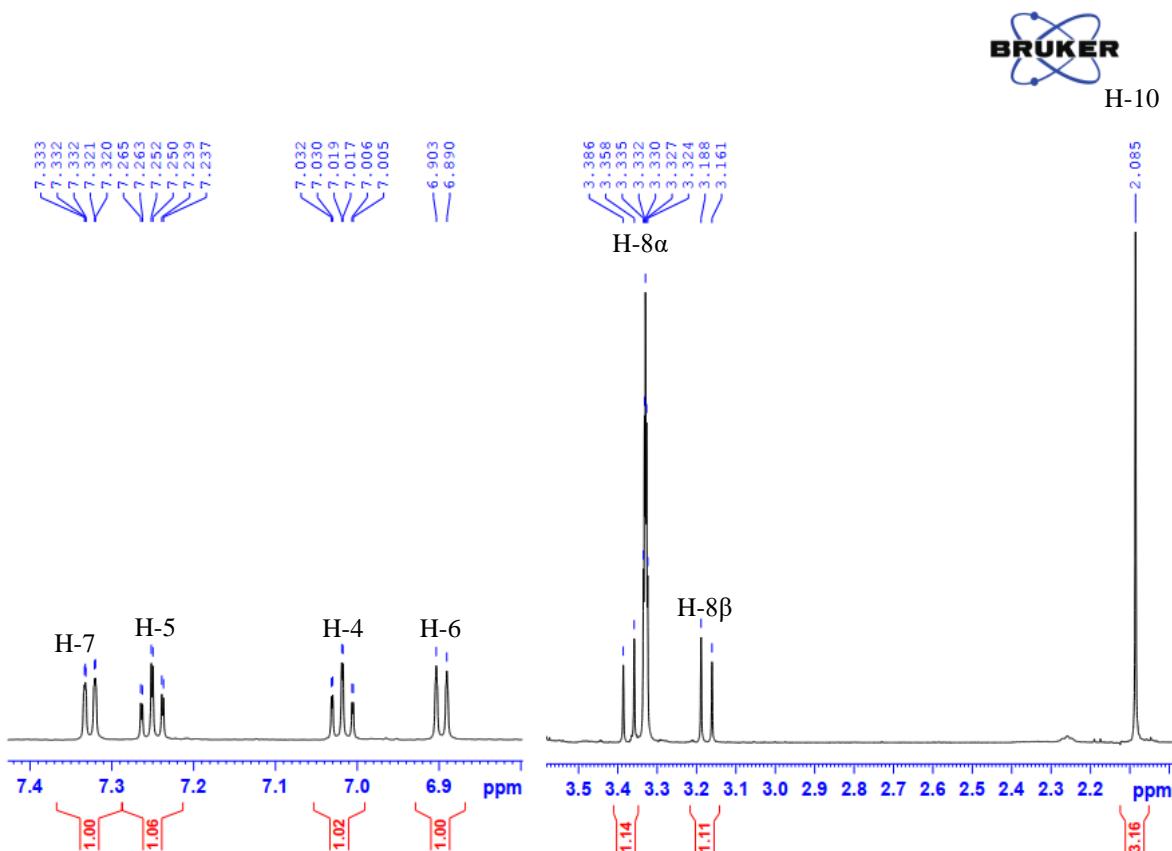
**Figure S63:** HMBC spectrum of compound 7 (isatin) (from  $\delta_C$  110 ppm to  $\delta_C$  190 ppm)

**Table S8:** The comparison of NMR data of compound **8** with a similar compound (3-hydroxy-3-(2-oxopropyl)indolin-2-one)

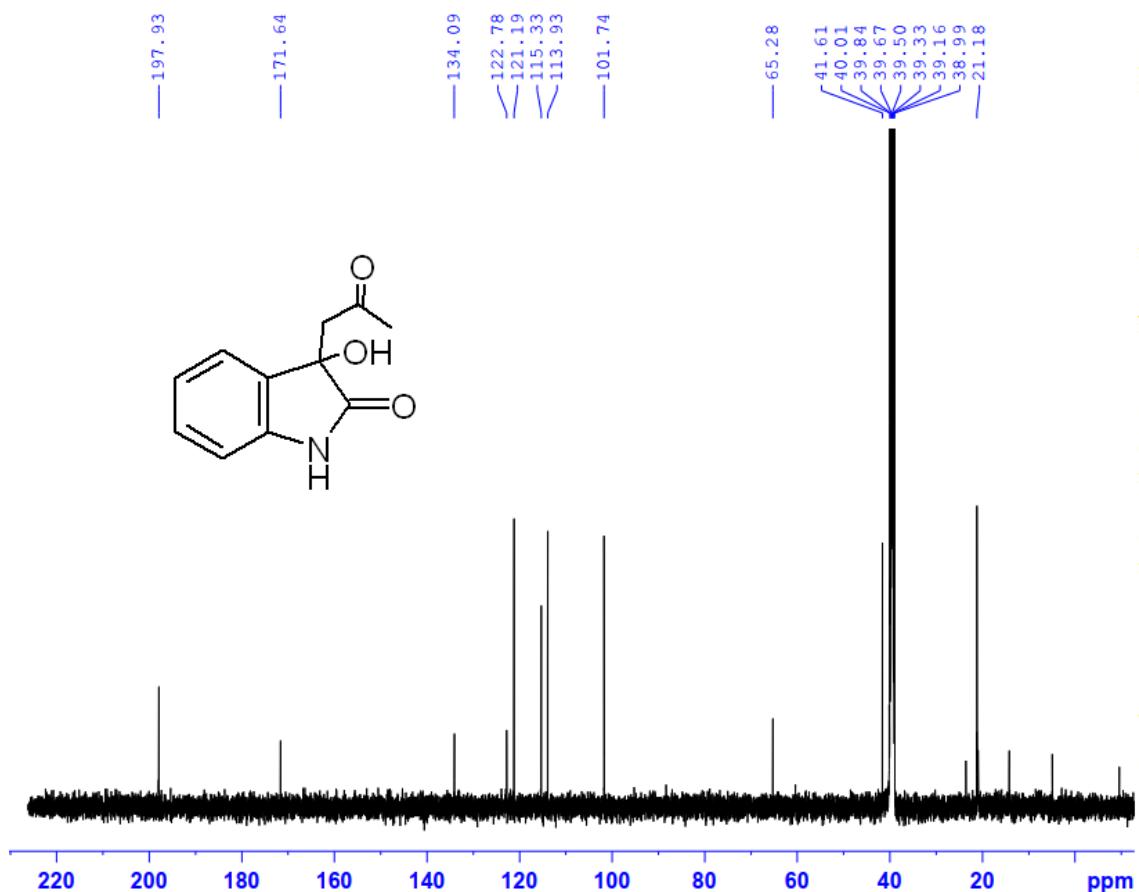
<b>Position</b>	Compound <b>8</b> (MeOD)		3-hydroxy-3-(2-oxopropyl)indolin-2-one (CDCl <sub>3</sub> ) [36]	
	<b><sup>13</sup>C-NMR</b> (125 MHz) $\delta_{\text{C}}$ ppm	<b><sup>1</sup>H-NMR</b> (600 MHz) $\delta_{\text{H}}$ ppm	<b><sup>13</sup>C-NMR</b> (100 MHz) $\delta_{\text{C}}$ ppm	<b><sup>1</sup>H-NMR</b> (400 MHz) $\delta_{\text{H}}$ ppm
1-NH	-		-	
2	181.1	-	179.8	-
3	74.8	-	76.2	-
3 $\alpha$	124.8	-	125.3	7.63 (1H, <i>d</i> , 7.8 Hz)
4	123.4	7.02 (1H, <i>td</i> , 1.2 Hz, 7.8 Hz)	123.0	7.07 (1H, <i>t</i> , 7.4 Hz)
5	130.7	7.25 (1H, <i>td</i> , 1.2 Hz, 7.8 Hz)	128.2	7.37 (1H, <i>d</i> , 7.6 Hz)
6	111.2	6.89 (1H, <i>d</i> , 7.8 Hz)	112.7	6.89 (1H, <i>d</i> , 7.6 Hz)
7	143.6	7.33 (1H, <i>dd</i> , 0.6 Hz, 7.2 Hz)	137.0	-
7 $\alpha$	132.3	-	132.3	-
8	51.1	3.36 (1H, <i>d</i> , 16.8 Hz) 3.19 (1H, <i>d</i> , 16.8 Hz)	49.5	3.20 (1H, <i>d</i> , 17.2 Hz) 2.98 (1H, <i>d</i> , 17.2 Hz)
9	207.4	-	207.4	-
10	30.7	2.09 (3H, <i>s</i> )	31.6	2.22 (3H, <i>s</i> )



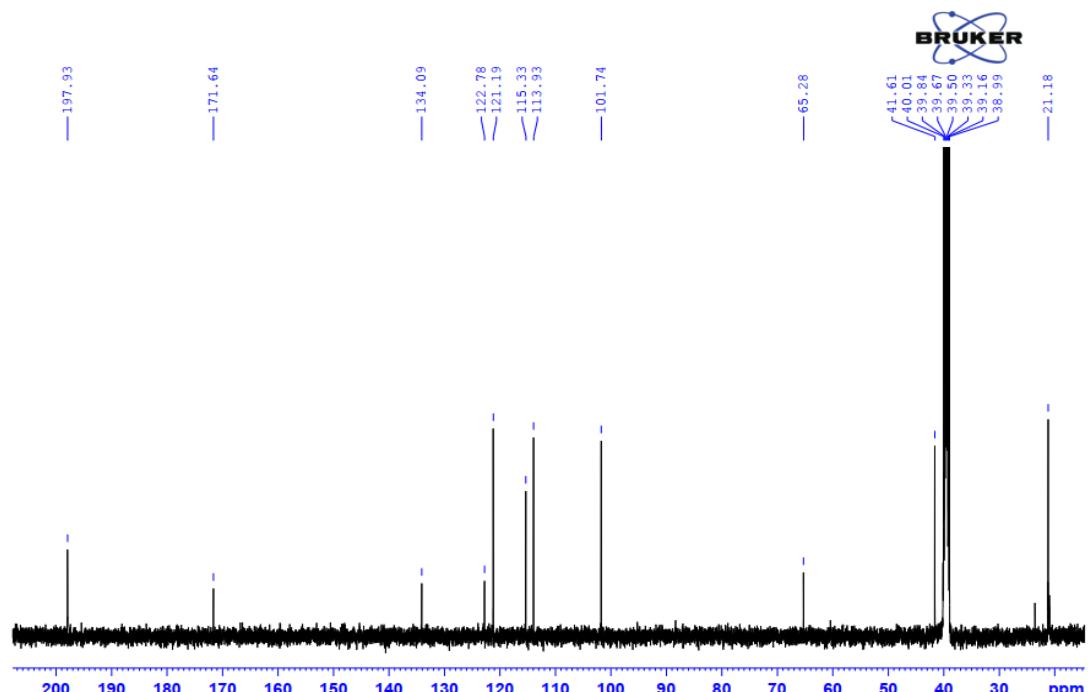
**Figure S64:**  $^1\text{H}$ -NMR (600 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one).



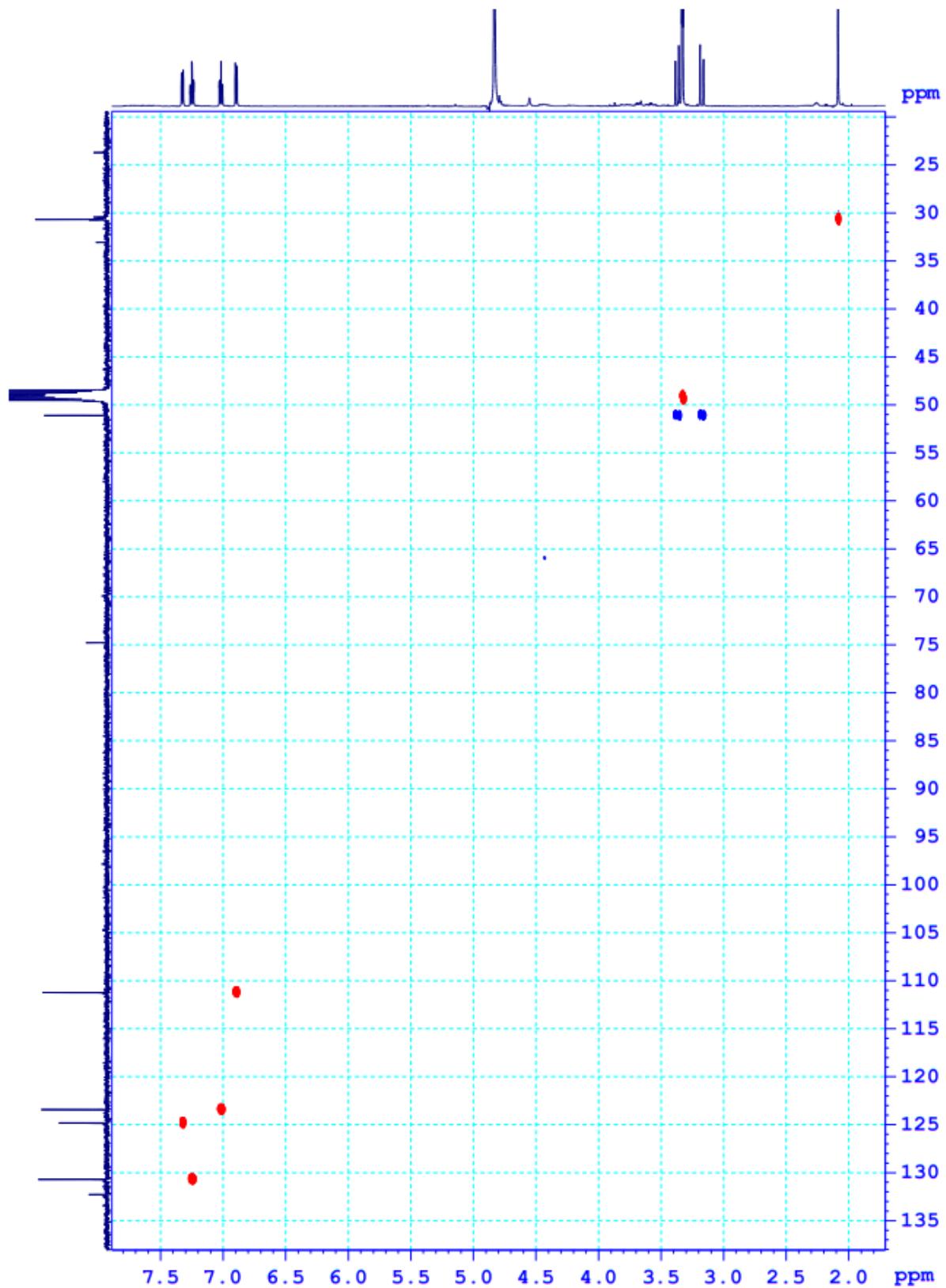
**Figure S65:**  $^1\text{H}$ -NMR (600 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{H}}$  2.0 ppm to  $\delta_{\text{H}}$  7.4 ppm)



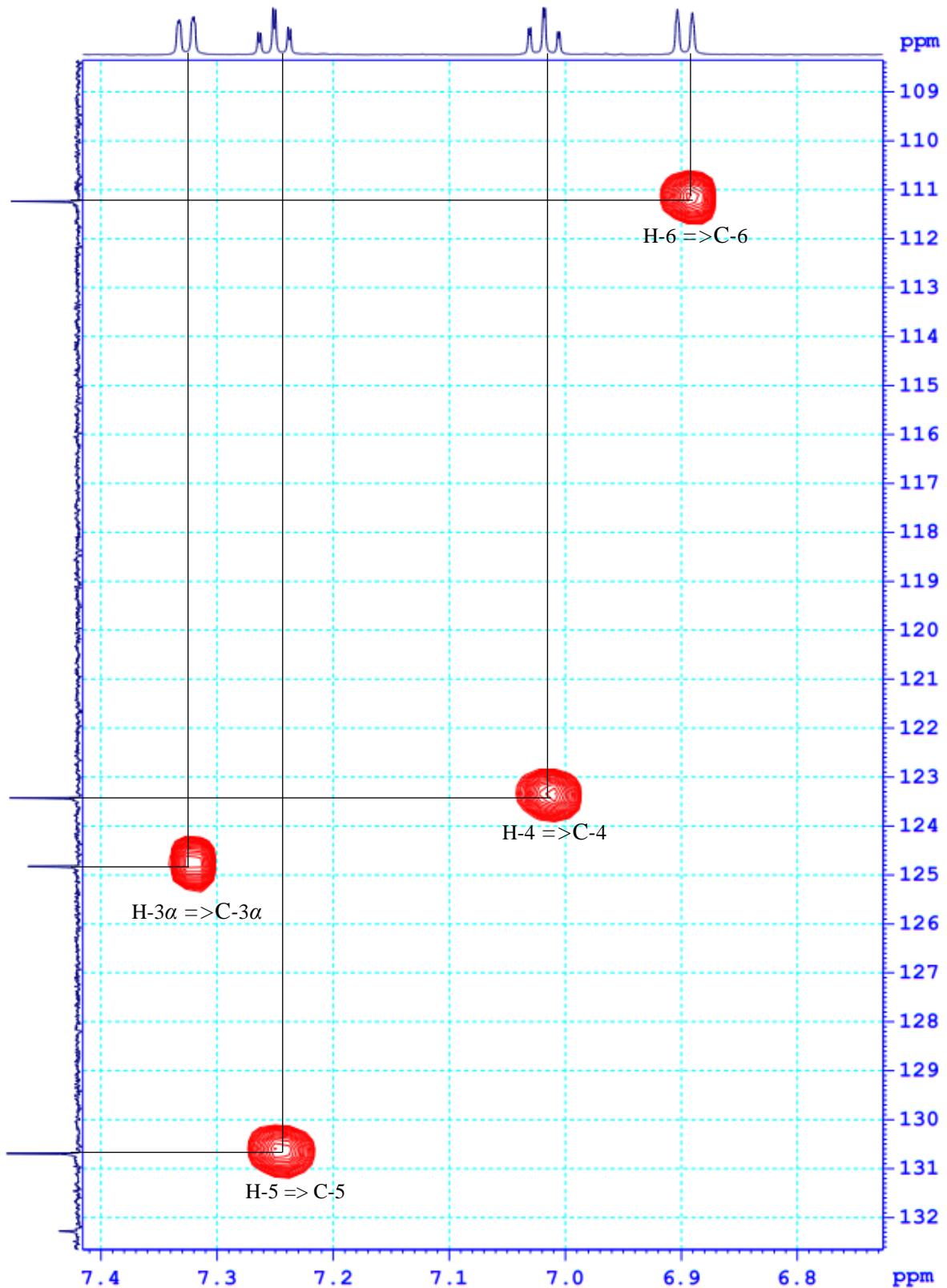
**Figure S66:**  $^{13}\text{C}$ -NMR (150 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)



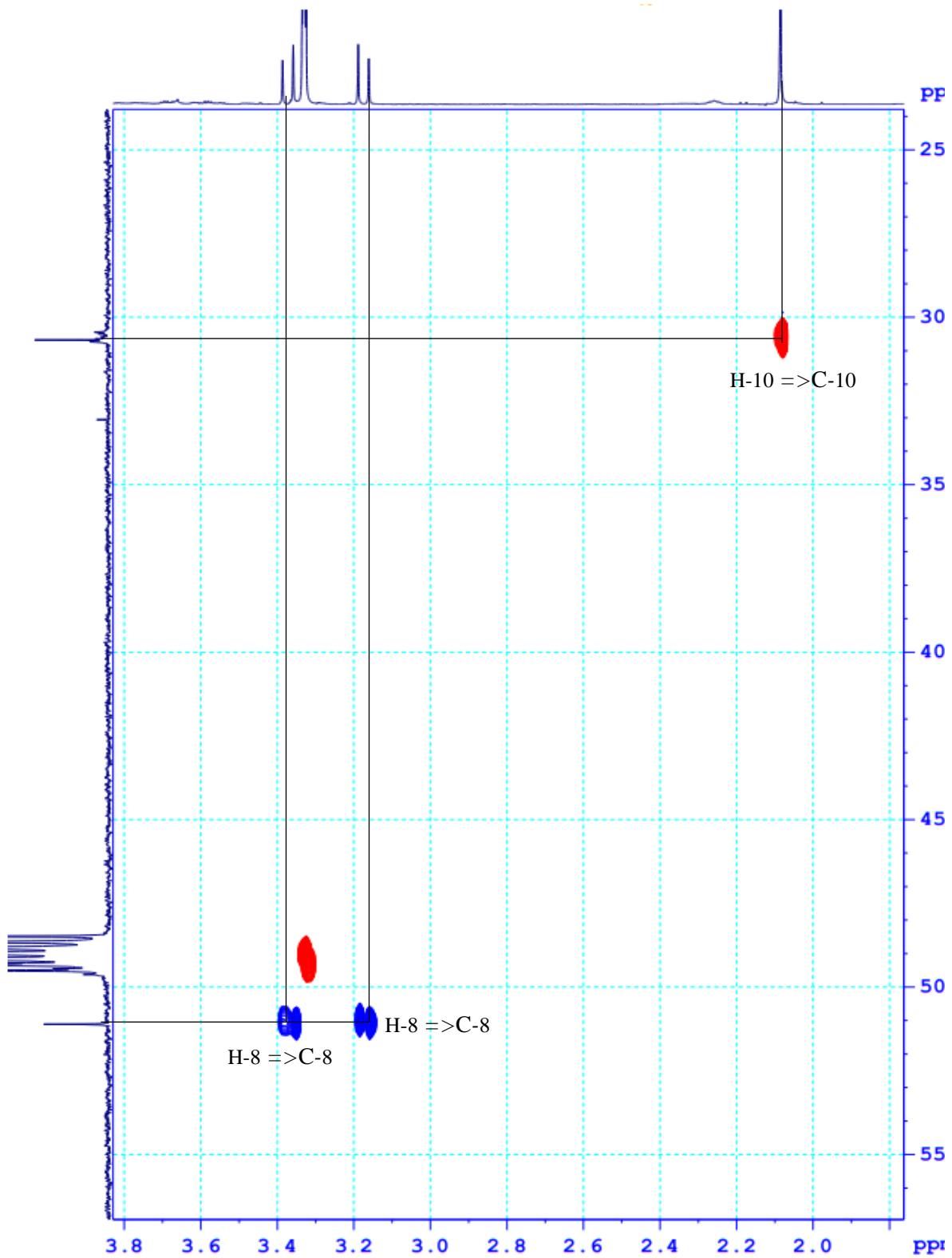
**Figure S67:**  $^{13}\text{C}$ -NMR spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{C}}$  20 ppm to  $\delta_{\text{C}}$  200 ppm)



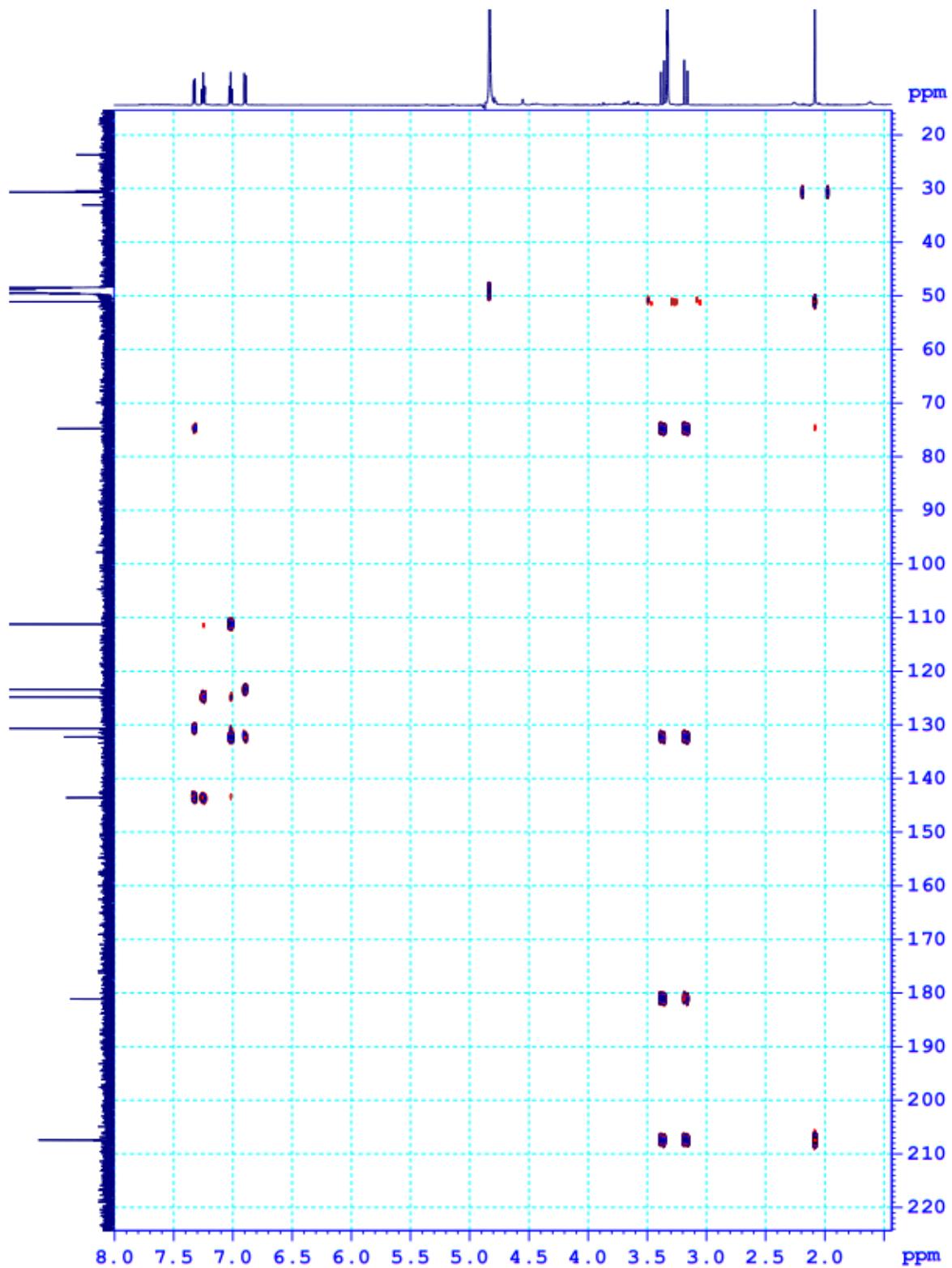
**Figure S68:** HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)



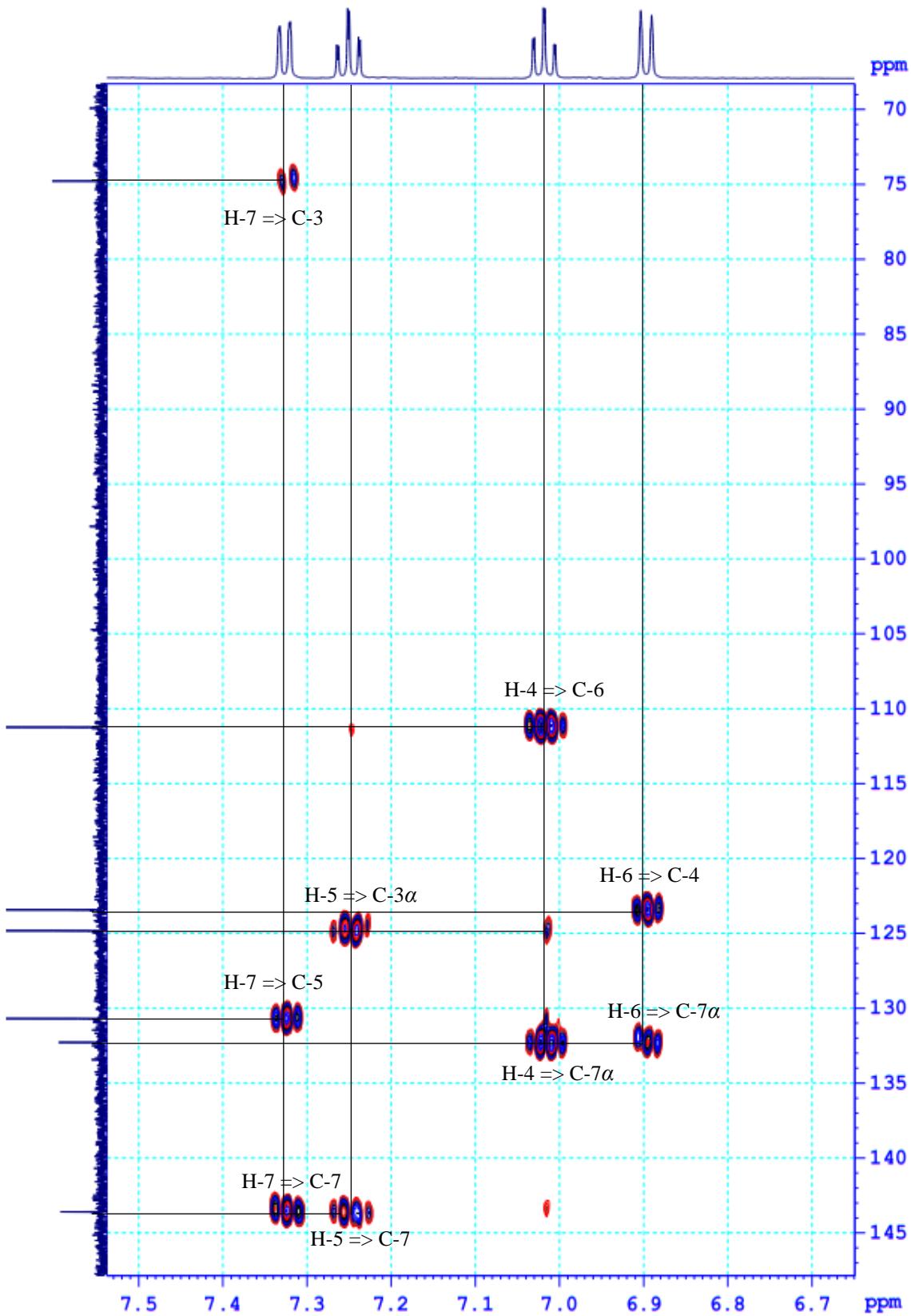
**Figure S69:** HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{C}} 109$  ppm to  $\delta_{\text{C}} 132$  ppm)



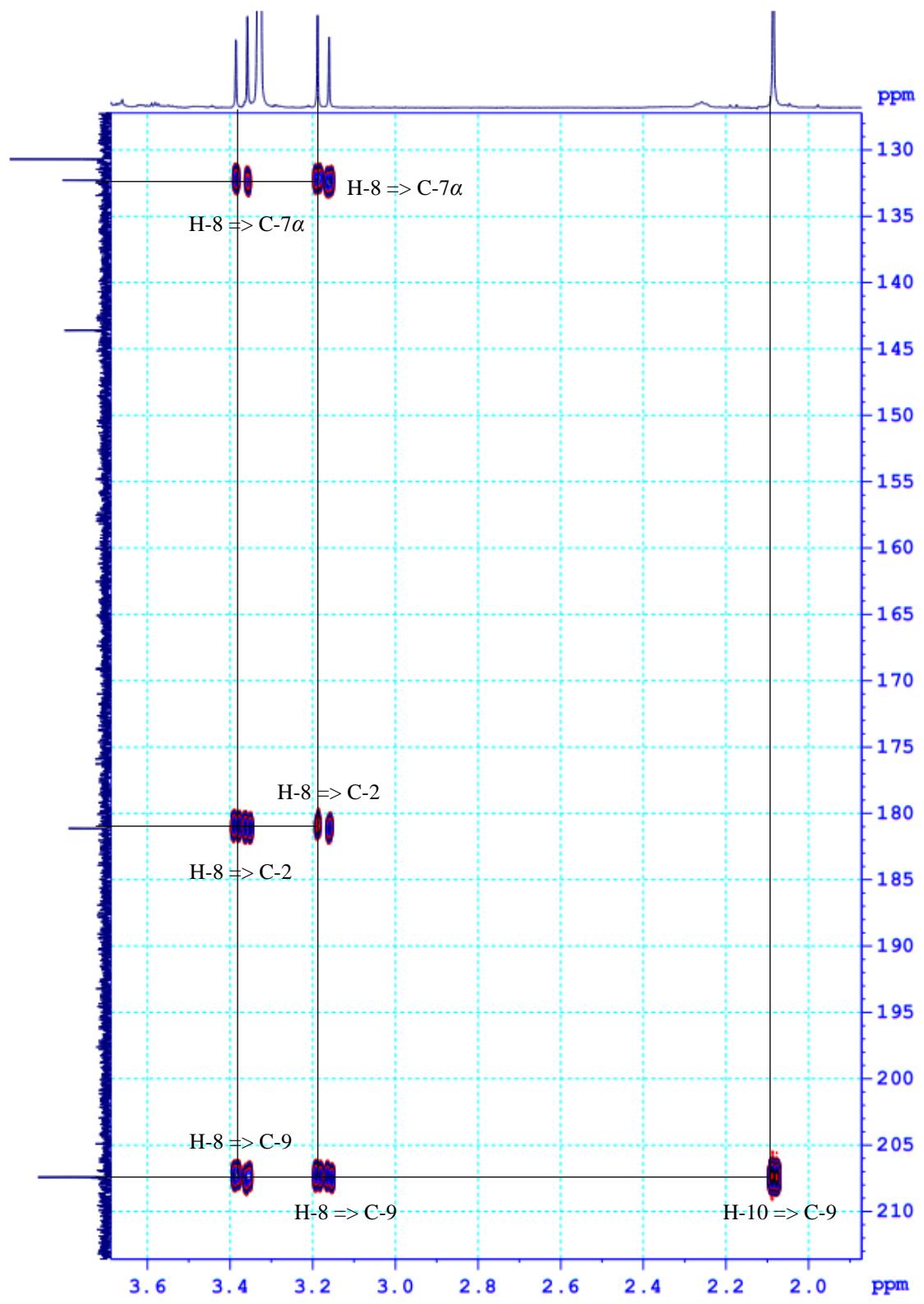
**Figure S70:** HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{C}}$  25 ppm to  $\delta_{\text{C}}$  55 ppm)



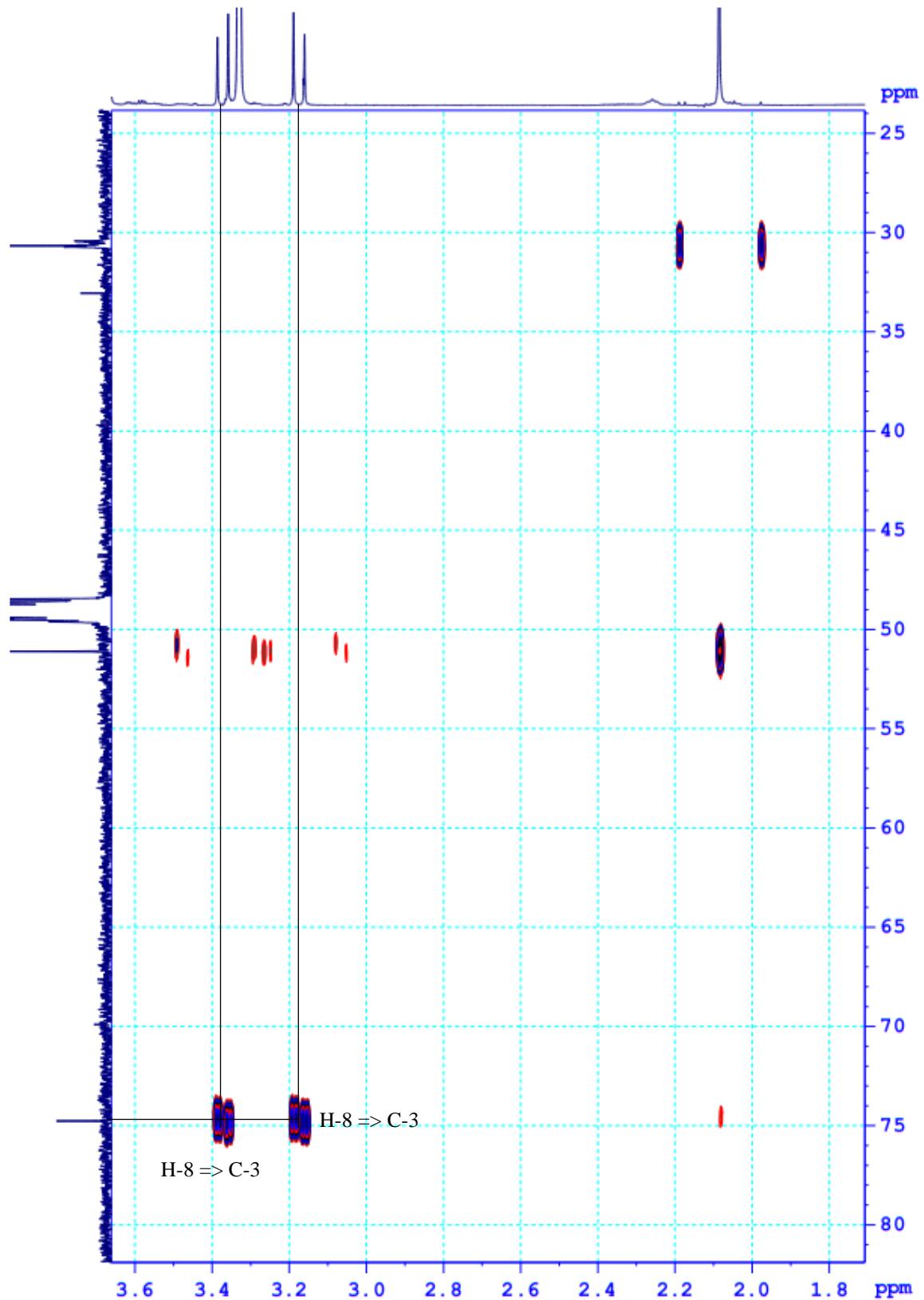
**Figure S71:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)



**Figure S72:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_c$  70 ppm to  $\delta_c$  145 ppm)



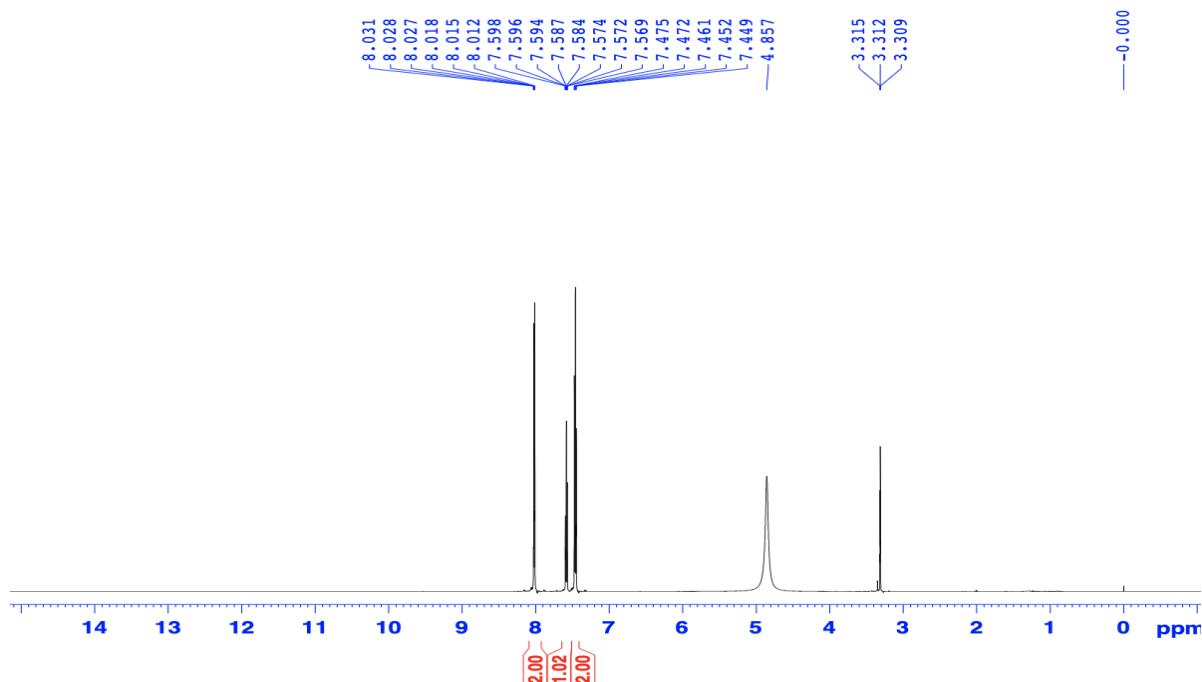
**Figure S73:** HMBC spectrum of compound 8 (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{C}}$  130 ppm to  $\delta_{\text{C}}$  210 ppm)



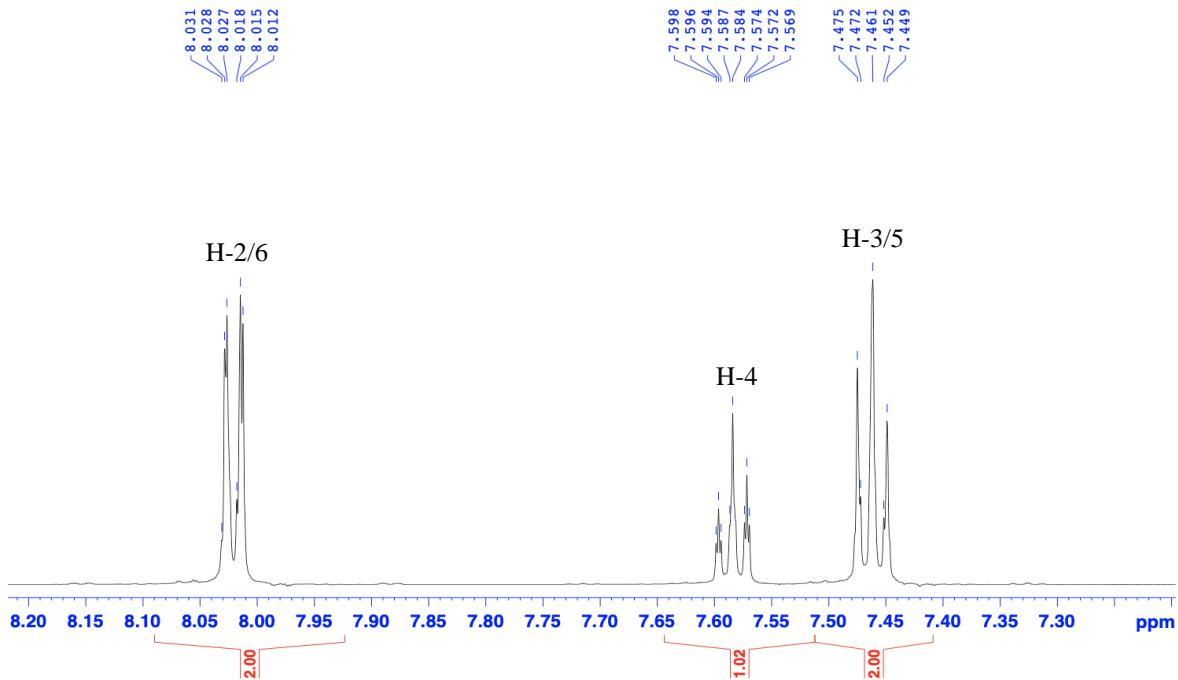
**Figure S74:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{C}}$  25 ppm to  $\delta_{\text{C}}$  80 ppm)

**Table S8:** The comparison of NMR data of compound **9** with a similar compound (benzoic acid)

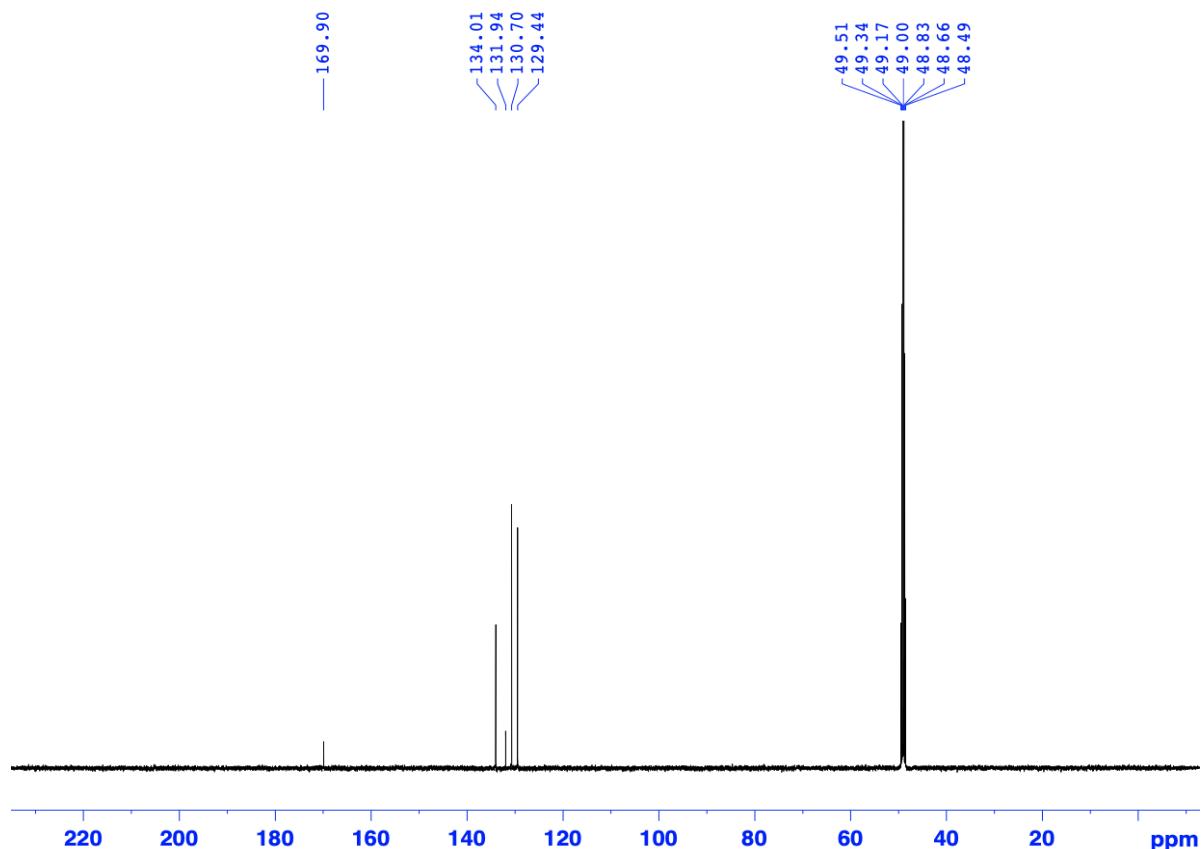
<b>Position</b>	Compound <b>9</b> (MeOD)		benzoic acid ( $\text{CDCl}_3$ ) [37]	
	$^{13}\text{C-NMR}$ (125 MHz) $\delta_{\text{C}}$ ppm	$^1\text{H-NMR}$ (600 MHz) $\delta_{\text{H}}$ ppm	$^{13}\text{C-NMR}$ (100 MHz) $\delta_{\text{C}}$ ppm	$^1\text{H-NMR}$ (400 MHz) $\delta_{\text{H}}$ ppm
1	131.9	-	129.3	-
2 & 6	130.7	8.02 (2H, <i>dd</i> )	130.2	8.13 (2H, <i>d</i> , 7.4 Hz)
3 & 5	129.4	7.46 (2H, <i>m</i> )	128.5	7.47 (2H, <i>t</i> , 7.4 Hz)
4	134.0	7.58 (1H, <i>m</i> )	133.8	7.61 (1H, <i>t</i> , 7.4 Hz)
1'	169.9	-	172.4	-



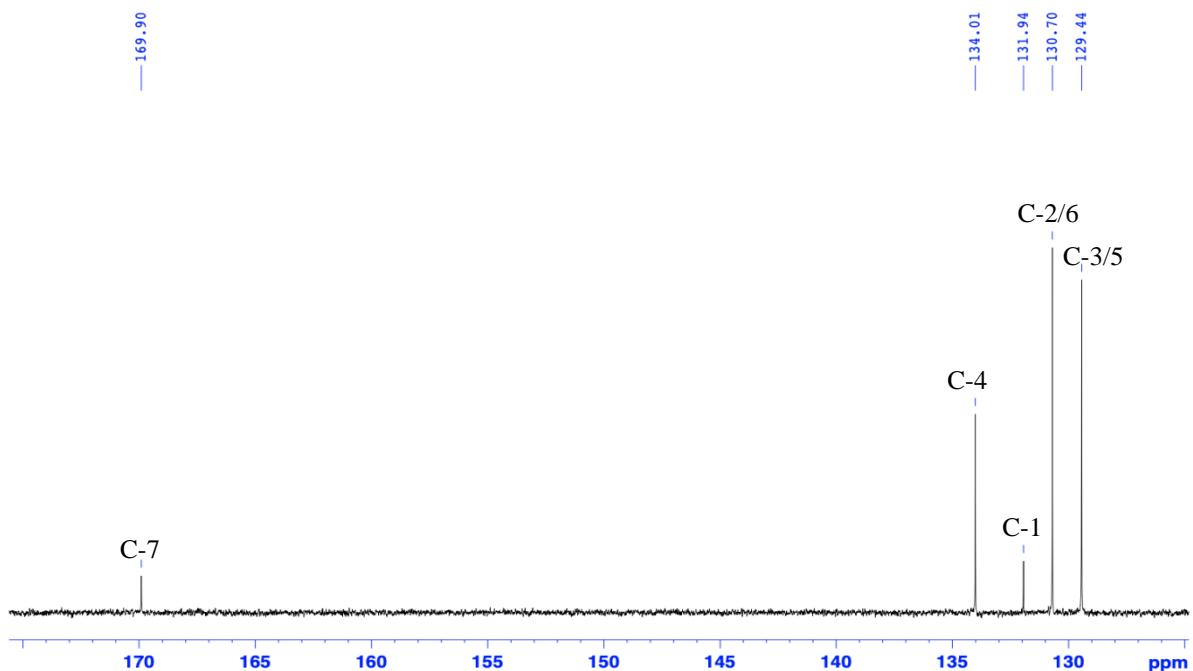
**Figure S75:**  $^1\text{H-NMR}$  (600 MHz, MeOD) spectrum of compound **9** (benzoic acid)



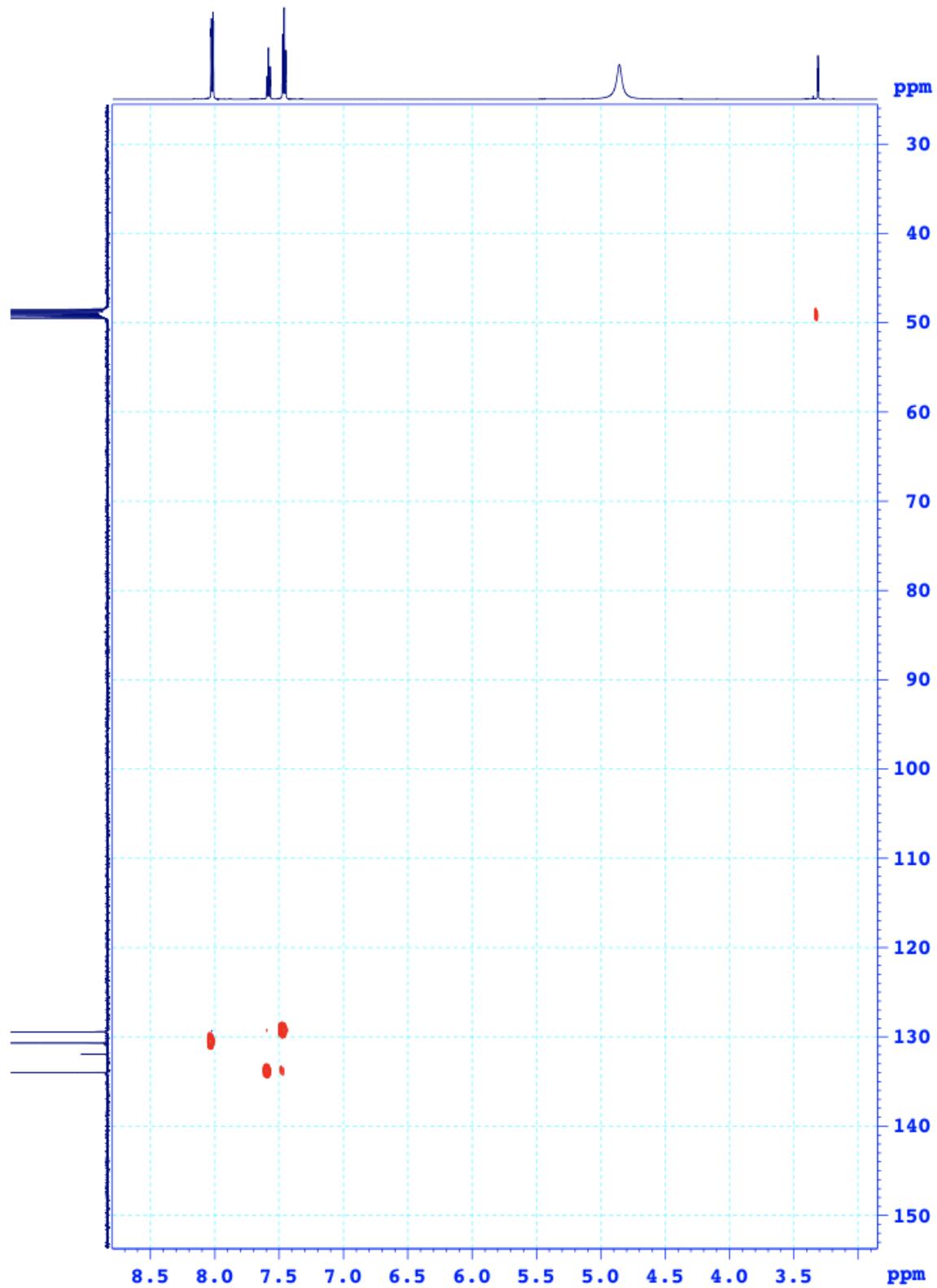
**Figure S76:**  $^1\text{H}$ -NMR spectrum of compound **9** (benzoic acid) (from  $\delta_{\text{H}}$  7.3 ppm to  $\delta_{\text{H}}$  8.2 ppm)



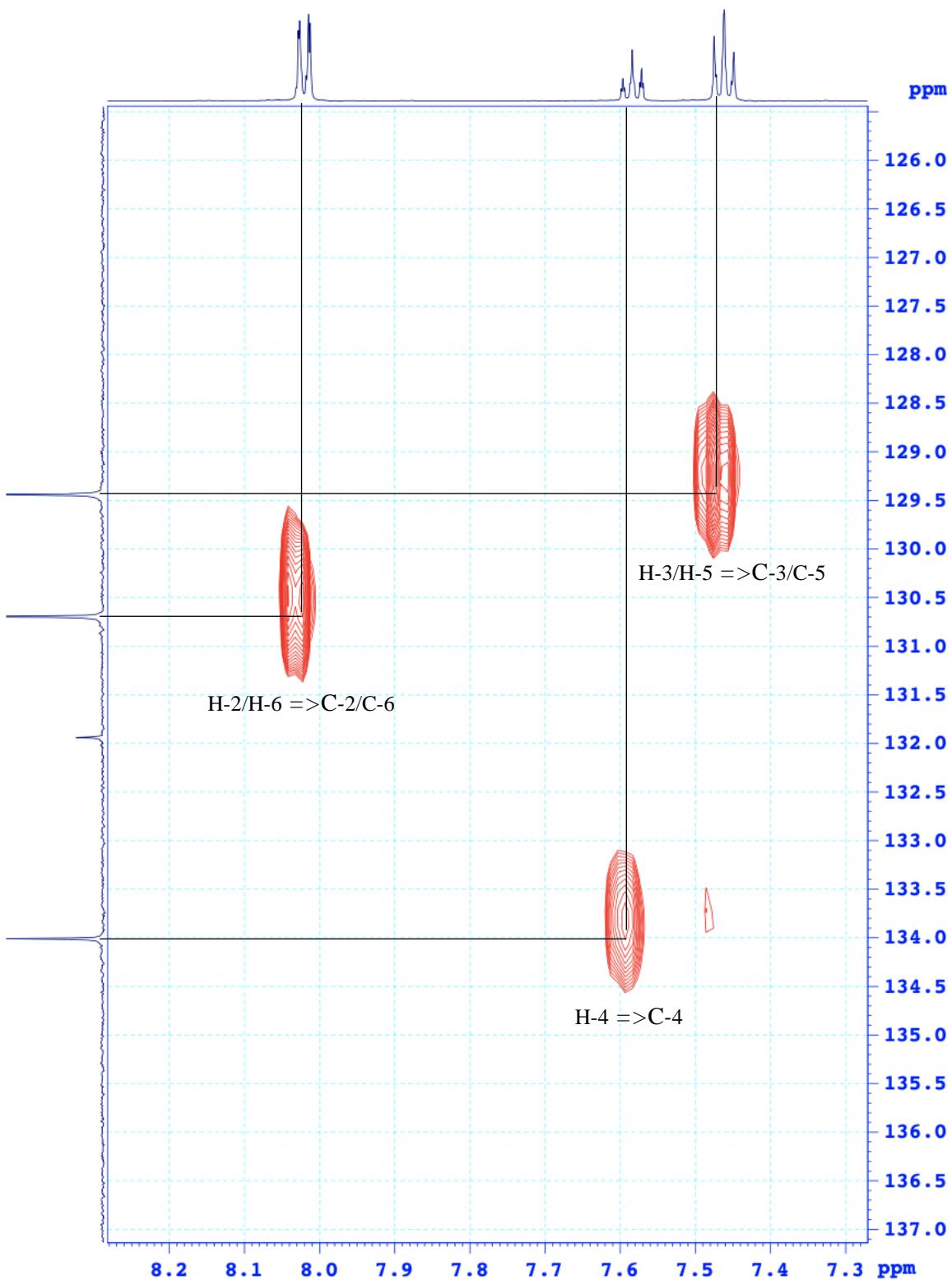
**Figure S77:**  $^{13}\text{C}$ -NMR (150 MHz, MeOD) spectrum of compound **9** (benzoic acid)



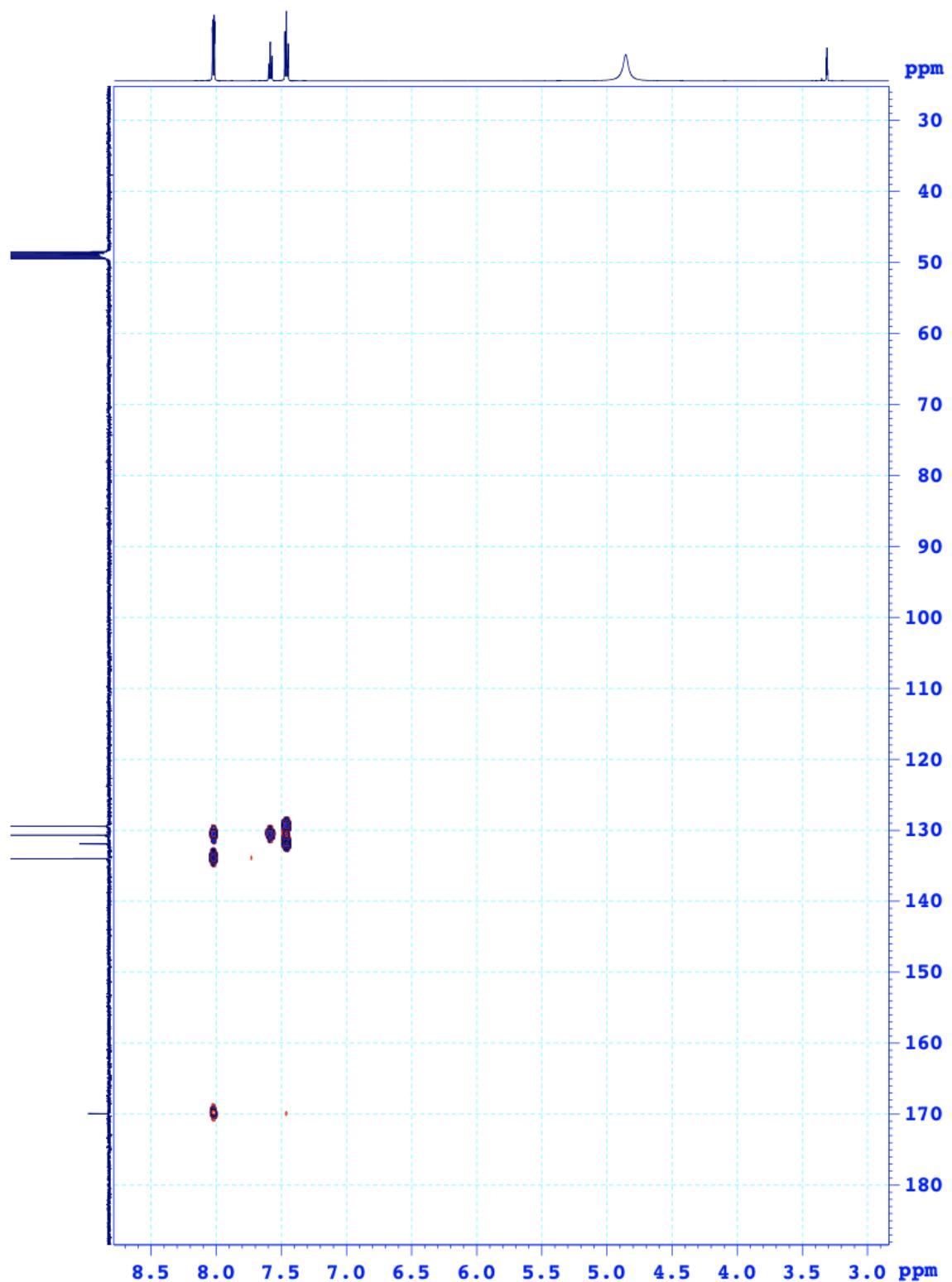
**Figure S78:**  $^{13}\text{C}$ -NMR spectrum of compound 9 (benzoic acid) (from  $\delta_{\text{C}}$  130 ppm to  $\delta_{\text{C}}$  170 ppm)



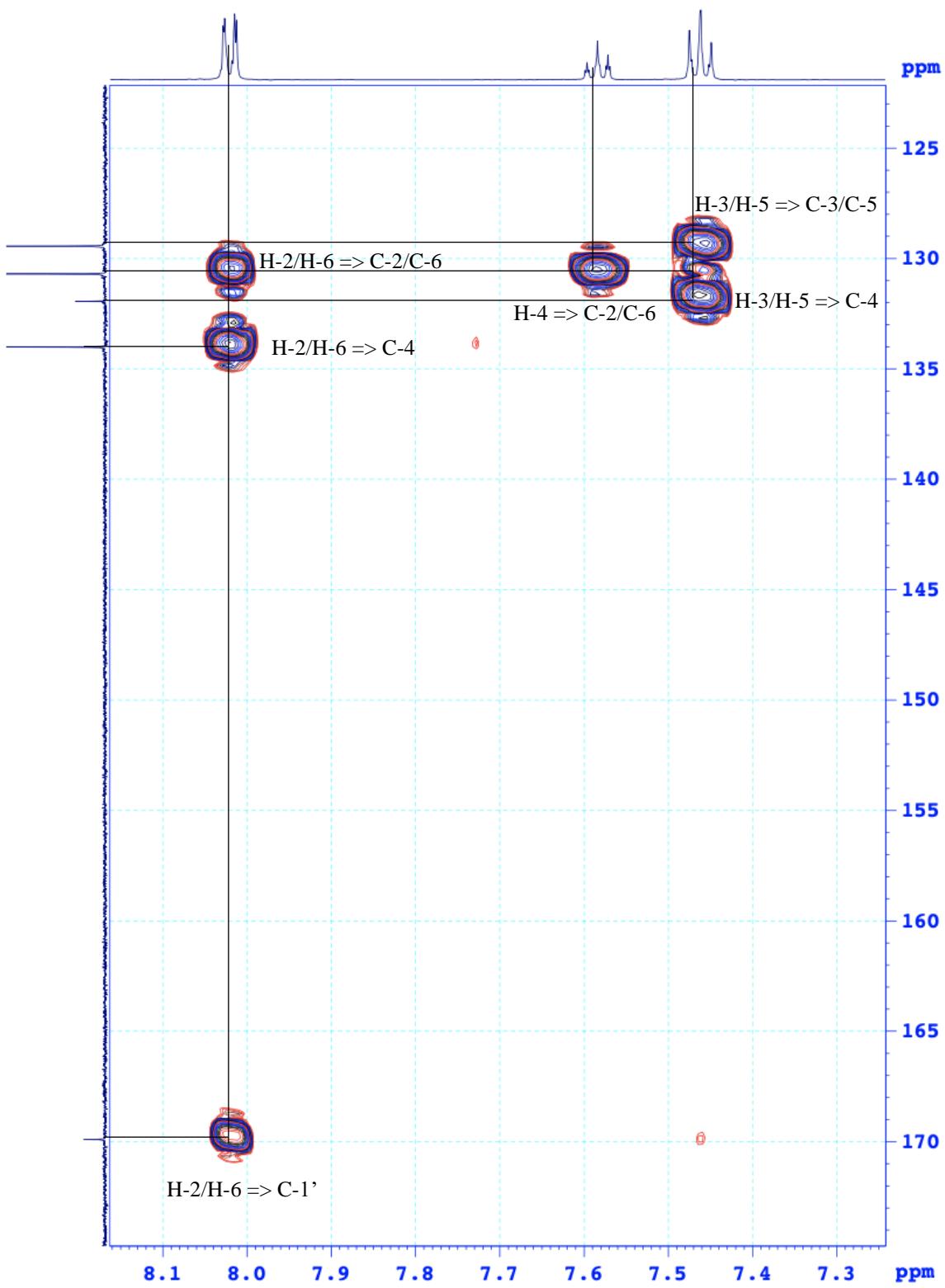
**Figure S79:** HSQC spectrum of compound 9 (benzoic acid)



**Figure S80:** HSQC spectrum of compound 9 (benzoic acid) (from  $\delta_{\text{C}}$  126 ppm to  $\delta_{\text{C}}$  137 ppm)



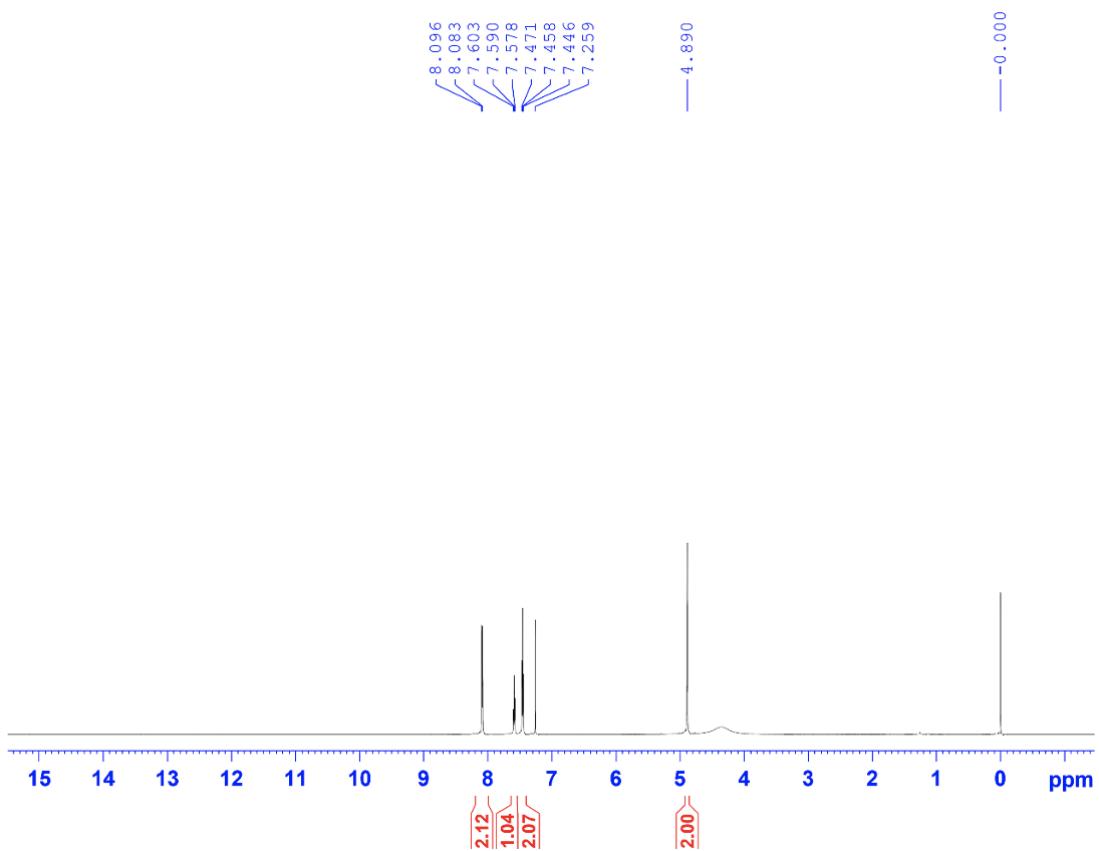
**Figure S81:** HMBC spectrum of compound 9 (benzoic acid)



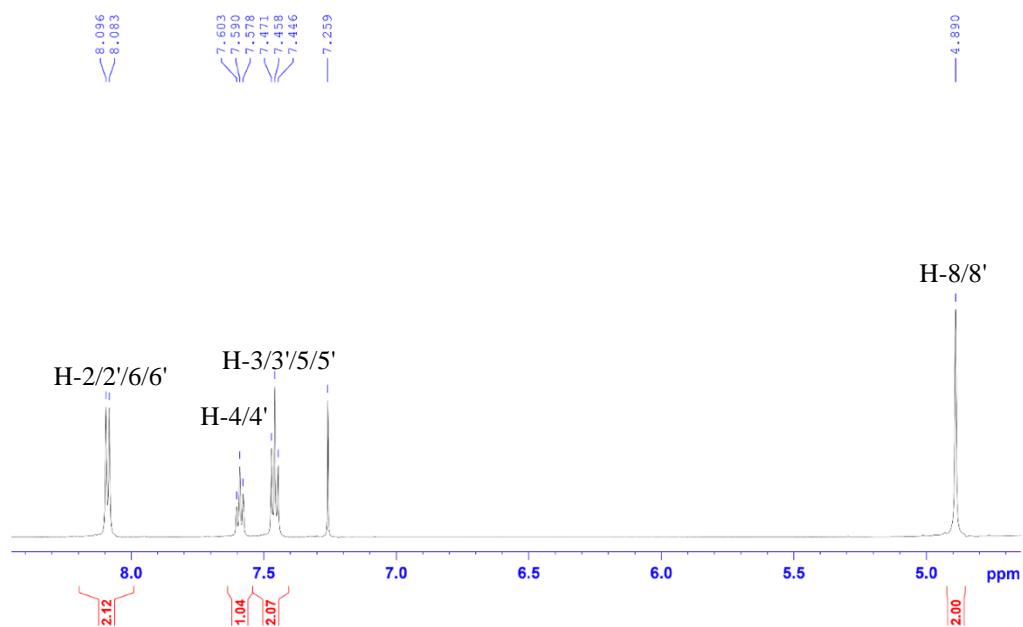
**Figure S82:** HMBC spectrum of compound **9** (benzoic acid) (from  $\delta_c$  125 ppm to  $\delta_c$  170 ppm)

**Table S10:** The comparison of NMR data of compound **10** with a similar compound (ethylene glycol dibenzoate)

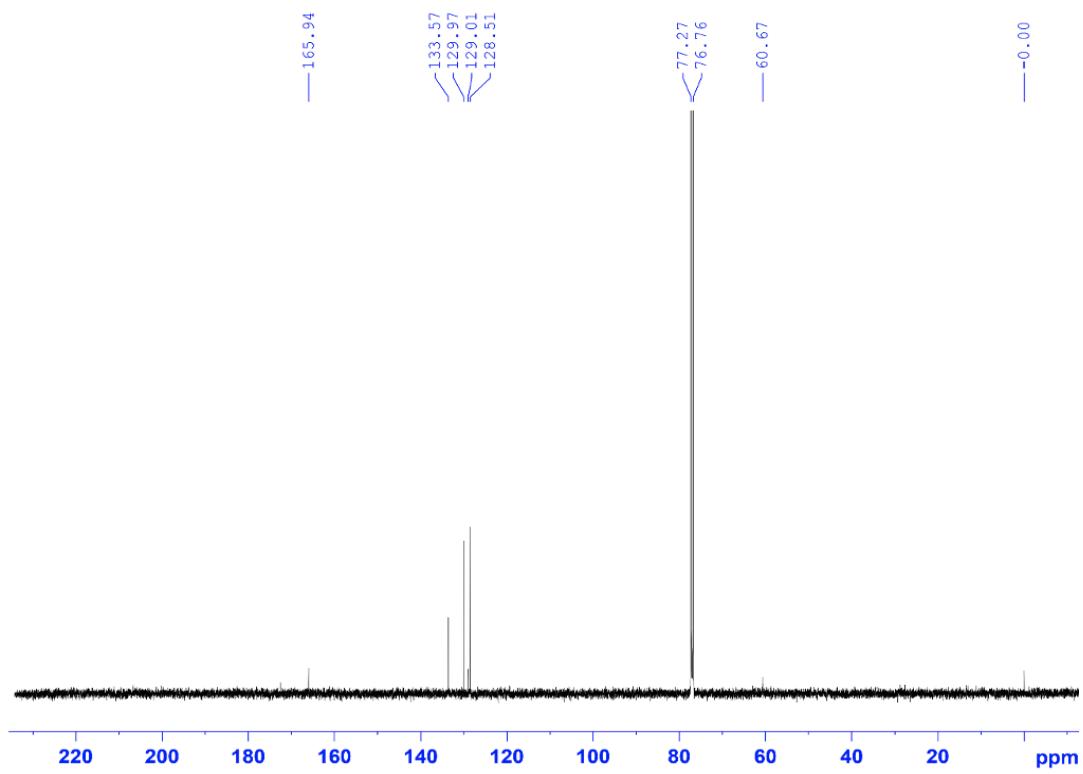
Position	Compound <b>10</b> (DMSO- <i>d</i> <sub>6</sub> )		Ethylene glycol dibenzoate (CDCl <sub>3</sub> ) [38]	
	<sup>13</sup> C-NMR (150 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_{\text{H}}$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_{\text{C}}$ ppm	<sup>1</sup> H-NMR (500 MHz) $\delta_{\text{H}}$ ppm
2	156.4	-	158.4	-
3	133.3	-	135.6	-
4	177.3	-	179.3	-
5	161.2	-	162.5	-
6	98.8	6.17 (1H, <i>d</i> , 2.0 Hz)	99.9	6.20 (1H, <i>d</i> , 1.8 Hz)
7	164.6	-	165.9	-
8	93.6	6.36 (1H, <i>d</i> , 2.0 Hz)	94.8	6.39 (1H, <i>d</i> , 2.2 Hz)
9	156.5	-	159.3	-
10	103.7	-	105.6	-
1'	121.1	-	123.1	-
2'	115.2	7.55 (1H, <i>d</i> , 1.8 Hz)	117.6	7.66 (1H, <i>d</i> , 1.8 Hz)
3'	144.8	-	145.8	-
4'	148.5	-	149.7	-
5'	116.2	6.84 (1H, <i>d</i> , 8.4 Hz)	116.1	6.86 (1H, <i>d</i> , 8.0 Hz)
6'	121.6	7.53 (1H, <i>dd</i> , 8.4, 2.4 Hz)	123.5	7.60 (1H, <i>dd</i> , 8.0, 1.8 Hz)
1"	101.2	5.33 (1H, <i>d</i> , 7.2 Hz)	104.7	5.09 (1H, <i>d</i> , 7.8 Hz)
2"	74.1		75.7	
3"	75.9		77.2	
4"	70.0		71.4	
5"	76.4		78.1	
6"	67.0		68.6	
1'''	100.7	4.39 (1H, <i>s</i> )	102.4	4.51 (1H, <i>d</i> , 1.8 Hz)
2'''	70.3		72.0	
3'''	70.5		72.2	
4'''	71.8		73.9	
5'''	68.2		69.7	
6'''	17.7	0.99 (3H, <i>d</i> , 6.0 Hz)	17.9	1.11 (3H, <i>d</i> , 6.0 Hz)



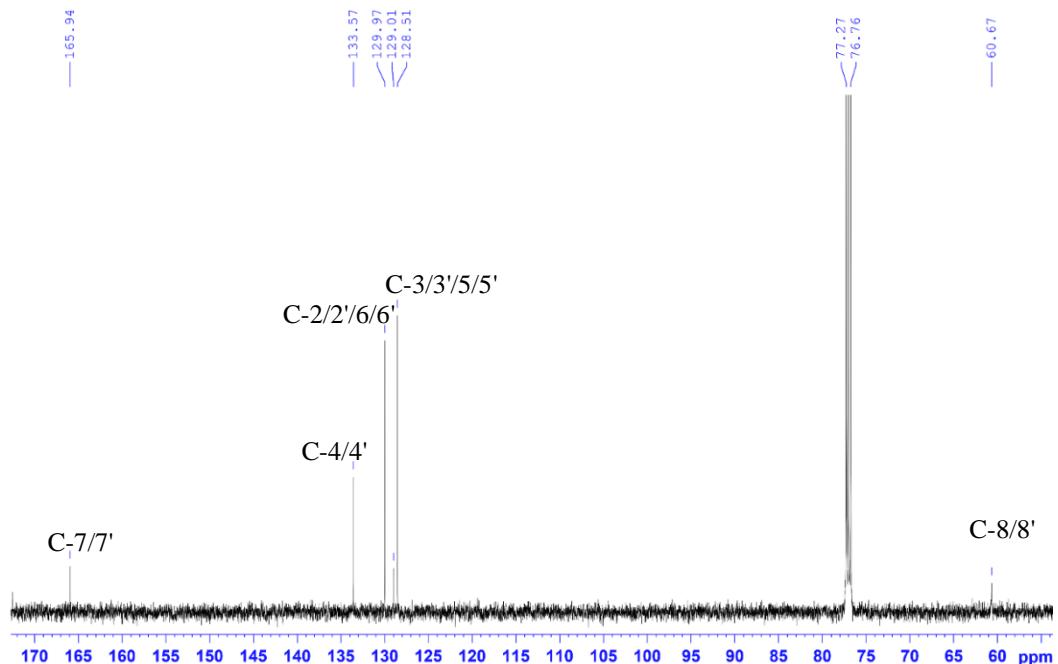
**Figure S83:**  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **10** (ethylene glycol dibenzoate)



**Figure S84:**  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **10** (ethylene glycol dibenzoate)  
(from  $\delta_{\text{H}}$  4.7 ppm to  $\delta_{\text{H}}$  8.5 ppm)



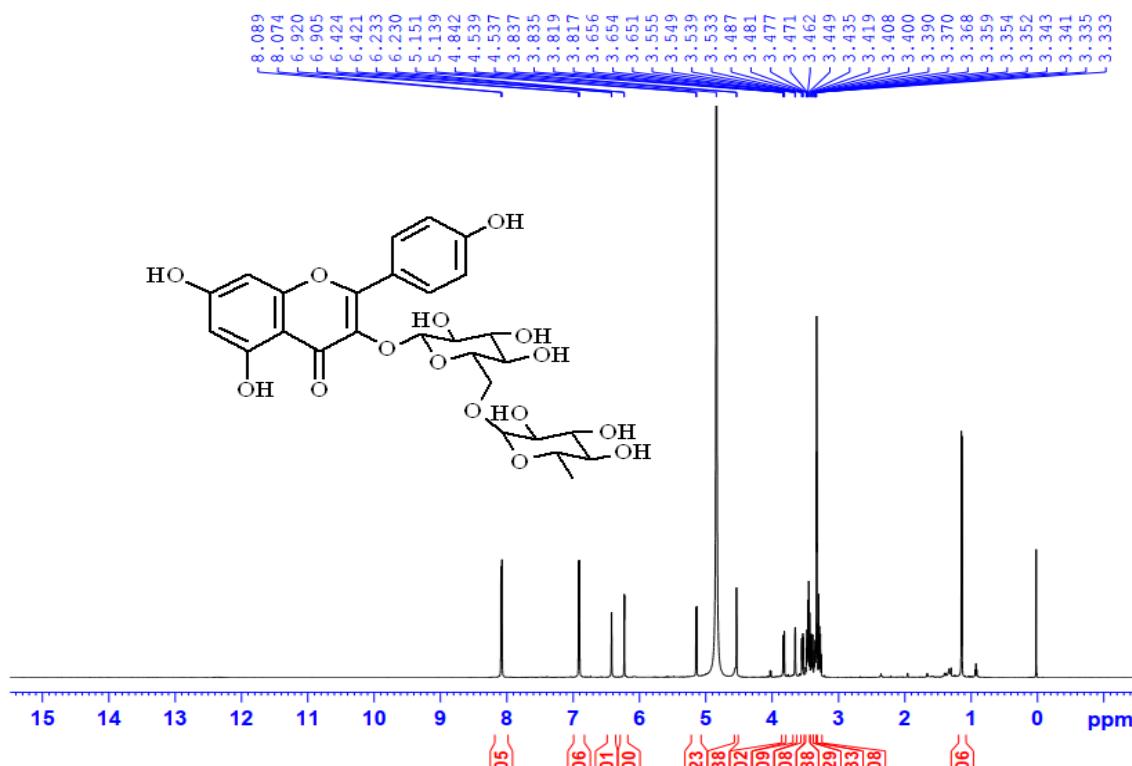
**Figure S85:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **10** (ethylene glycol dibenzoate)



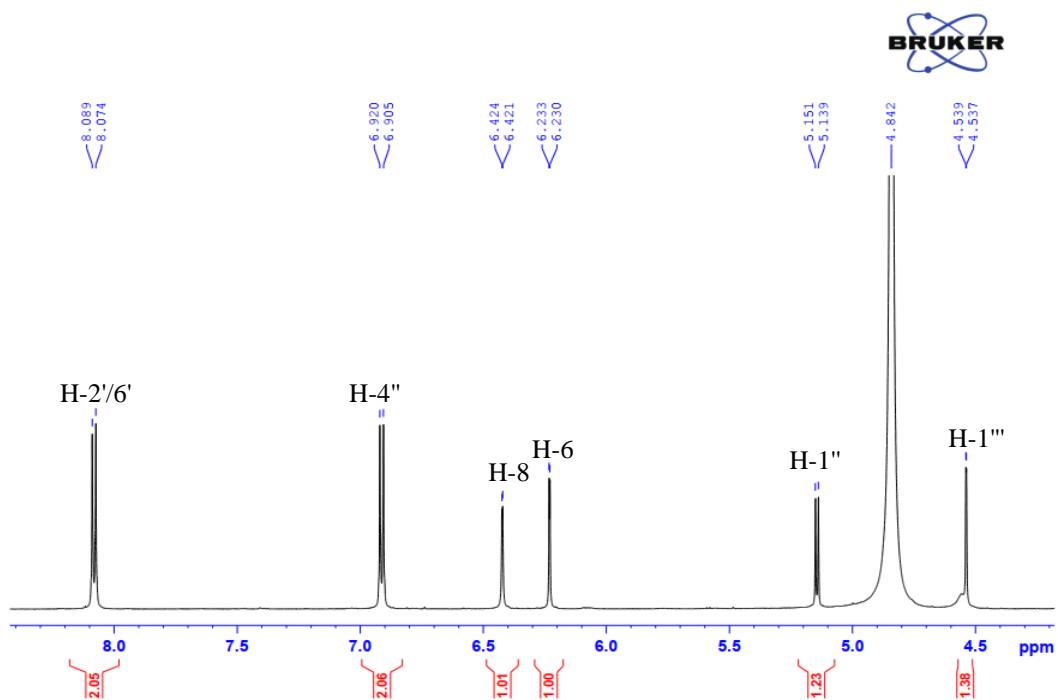
**Figure S86:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound **10** (ethylene glycol dibenzoate)  
(from  $\delta_{\text{C}}$  60 ppm to  $\delta_{\text{C}}$  170 ppm)

**Table S11:** The comparison of NMR data of compound **11** with a similar compound (Nicotiflorin)

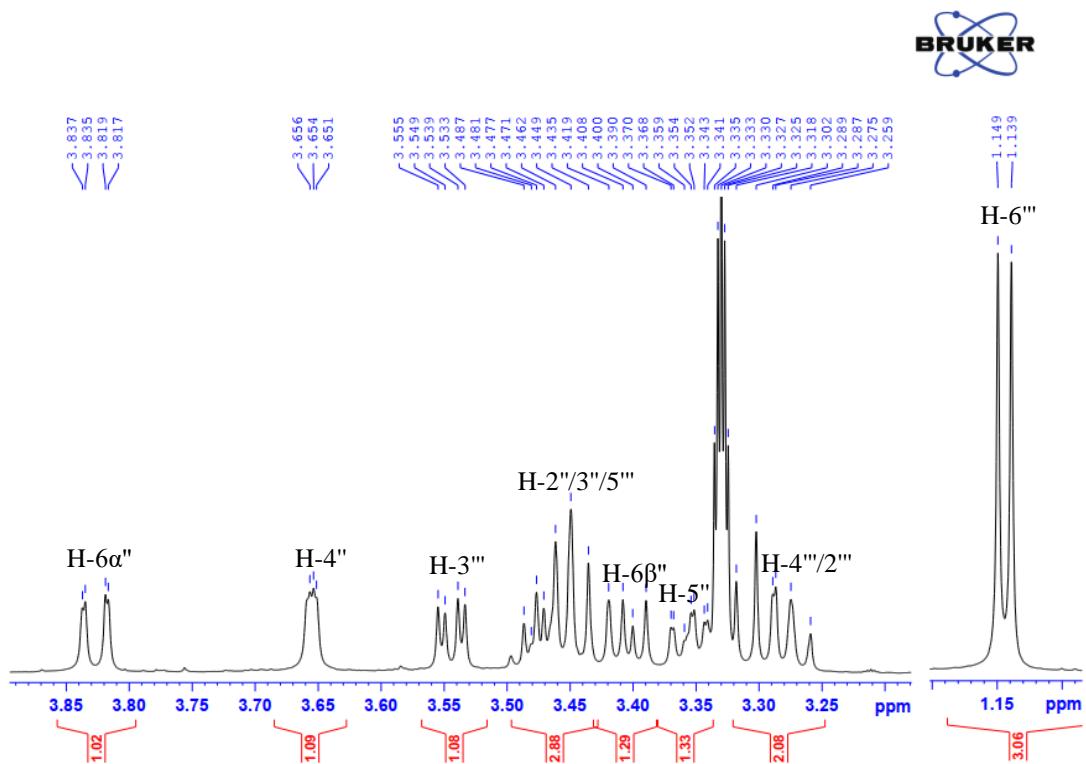
Position	Compound <b>11</b> (MeOD)		Nicotiflorin (MeOD) [39]	
	<sup>13</sup> C-NMR (150 MHz) $\delta_c$ ppm	<sup>1</sup> H-NMR (600 MHz) $\delta_h$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_c$ ppm	<sup>1</sup> H-NMR (500 MHz) $\delta_h$ ppm
2	159.4	-	159.4	-
3	135.5	-	135.5	-
4	179.4	-	179.4	-
5	163.0	-	163.0	-
6	100.0	6.23 (1H, <i>d</i> , 1.8 Hz)	100.1	6.23 (1H, <i>d</i> , 2.1 Hz)
7	166.2	-	166.4	-
8	95.0	6.42 (1H, <i>d</i> , 1.8 Hz)	95.0	6.43 (1H, <i>d</i> , 2.1 Hz)
9	158.9	-	158.6	-
10	105.6	-	105.6	-
1'	122.8	-	122.7	-
2' & 6'	132.4	8.07 (2H, <i>d</i> , 9.0 Hz)	132.4	8.10 (2H, <i>d</i> , 8.9 Hz)
3' & 5'	116.1	6.92 (2H, <i>d</i> , 9.0 Hz)	116.1	6.93 (2H, <i>d</i> , 8.9 Hz)
4'	161.5	-	161.5	-
1"	104.6	5.15 (1H, <i>d</i> , 7.2 Hz)	104.6	5.00 (1H, <i>d</i> , 7.4 Hz)
2"	75.8	3.47 (3H, <i>m</i> )	75.8	3.41-3.49 ( <i>m</i> )
3"	78.2	3.47 (3H, <i>m</i> )	78.1	3.41-3.49 ( <i>m</i> )
4"	72.1	3.65 (1H, <i>brs</i> )	72.1	3.28-3.33 ( <i>m</i> )
5"	77.2	3.36 (1H, <i>ddd</i> , 1.2 Hz, 6.6 Hz, 10.8 Hz)	77.2	3.41-3.49 ( <i>m</i> )
6"	68.6	3.84 (1H, <i>dd</i> , 1.2 Hz, 10.8 Hz) 3.40 (1H, <i>dd</i> , 6.0 Hz, 10.8 Hz)	68.6	3.83 (1H, <i>d</i> , 9.6 Hz) 3.41-3.49 ( <i>m</i> )
1'''	102.4	4.54 (1H, <i>d</i> , 1.2 Hz)	102.4	4.53 (1H, <i>d</i> , 1.3 Hz)
2'''	71.5	3.29 (2H, <i>m</i> )	71.4	3.67 (1H, <i>dd</i> , 1.6 Hz, 3.4 Hz)
3'''	72.3	3.54 (1H, <i>dd</i> , 3.6 Hz, 9.6 Hz)	72.3	3.56 (1H, <i>dd</i> , 3.5 Hz, 9.5 Hz)
4'''	73.9	3.29 (2H, <i>m</i> )	73.9	3.29-3.36 ( <i>m</i> )
5'''	69.7	3.47 (3H, <i>m</i> )	69.7	3.46-3.50 ( <i>m</i> )
6'''	17.9	1.14 (3H, <i>d</i> , 6.0 Hz)	17.9	1.16 (3H, <i>d</i> , 6.2 Hz)



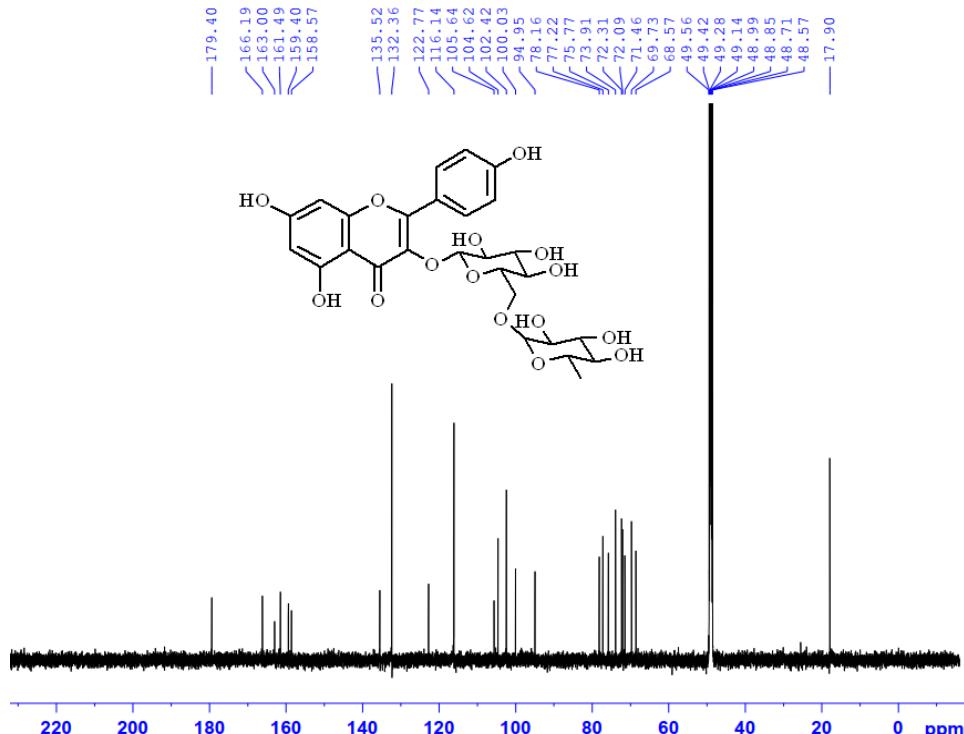
**Figure S87:**  $^1\text{H}$ -NMR (600 MHz,  $\text{MeOD}$ ) spectrum of compound **11** (nicotiflorin)



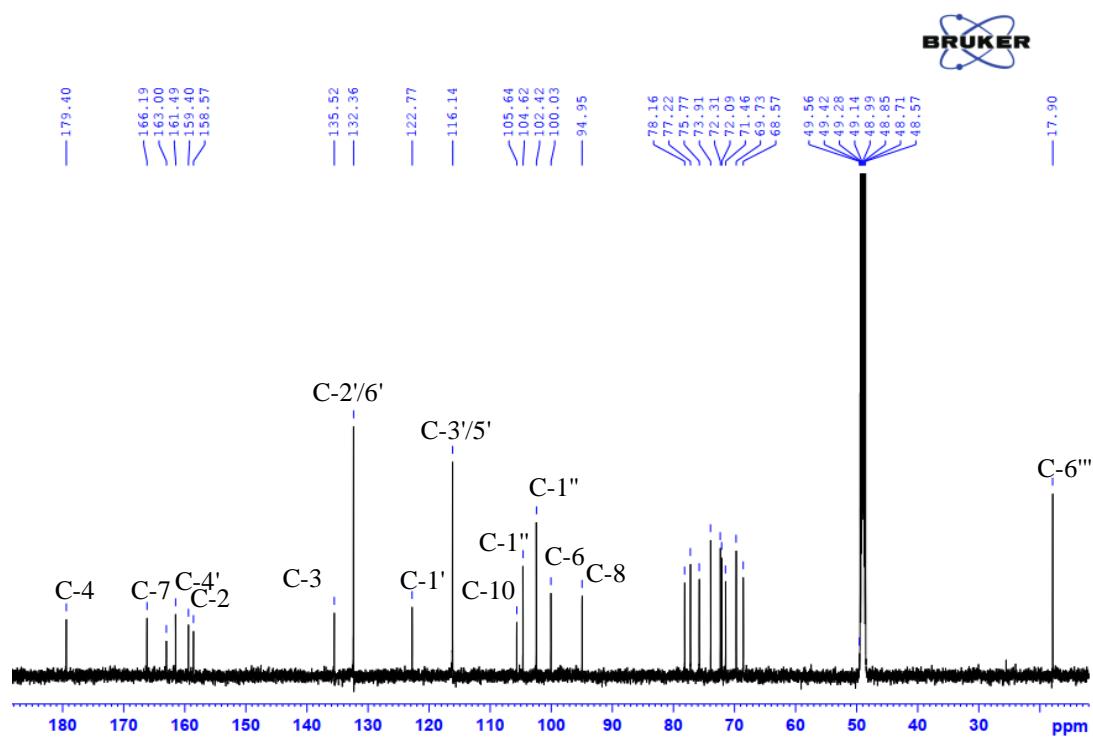
**Figure S88:**  $^1\text{H}$ -NMR (600 MHz,  $\text{MeOD}$ ) spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{H}}$  4.5 ppm to  $\delta_{\text{H}}$  8.0 ppm)



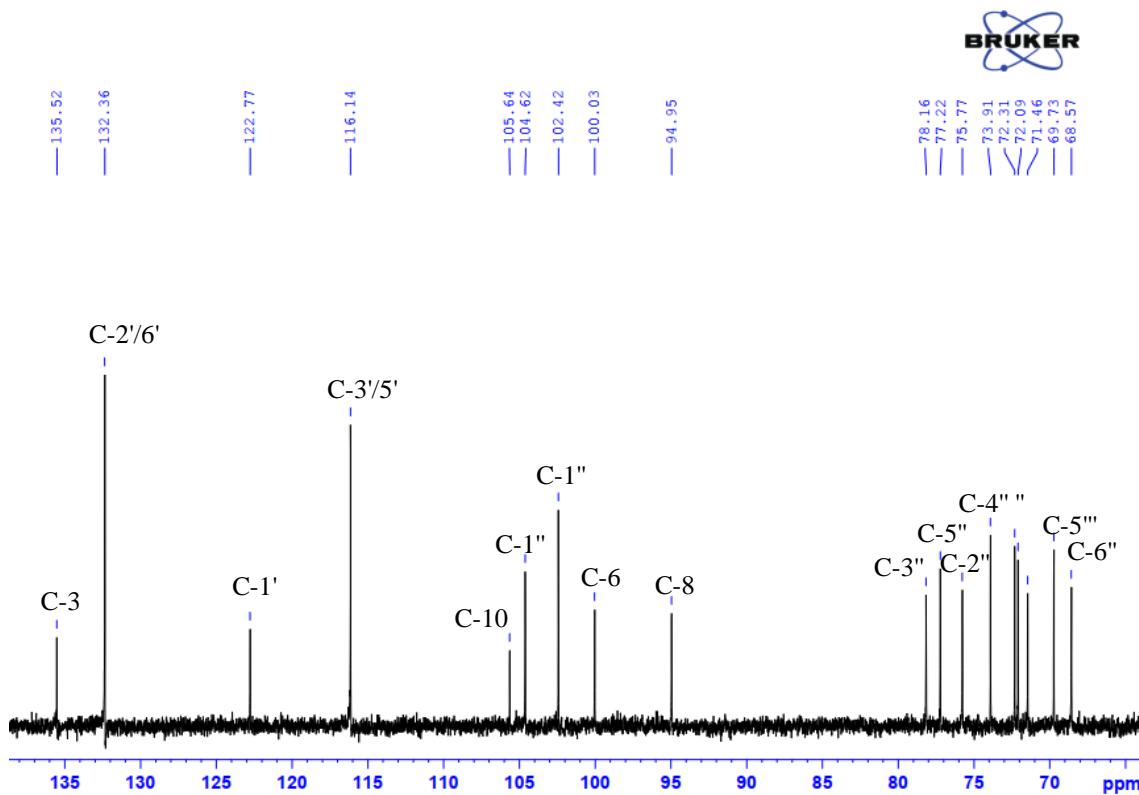
**Figure S89:**  $^1\text{H}$ -NMR (600 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{H}}$  1.10 ppm



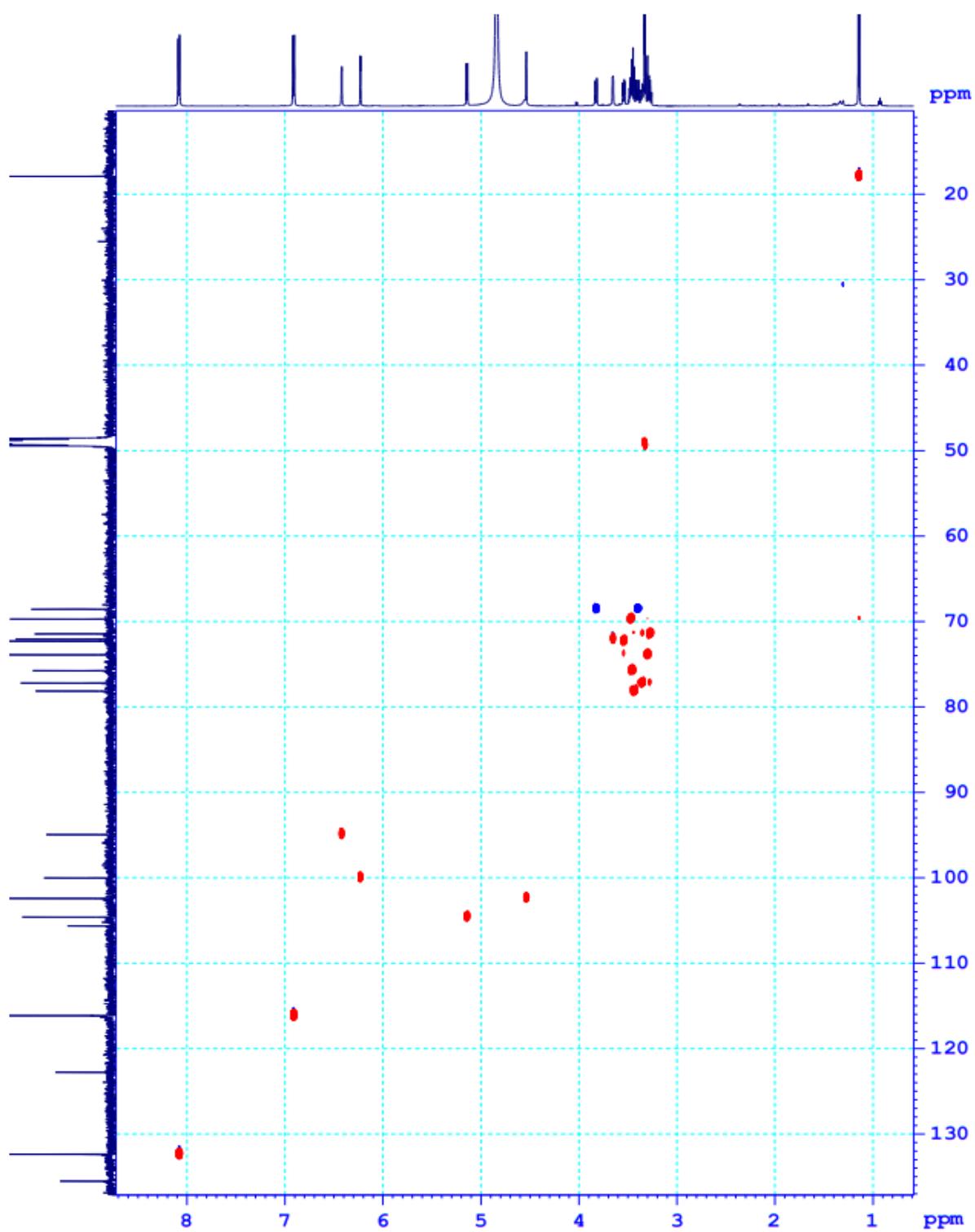
**Figure S90:**  $^{13}\text{C}$ -NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin)



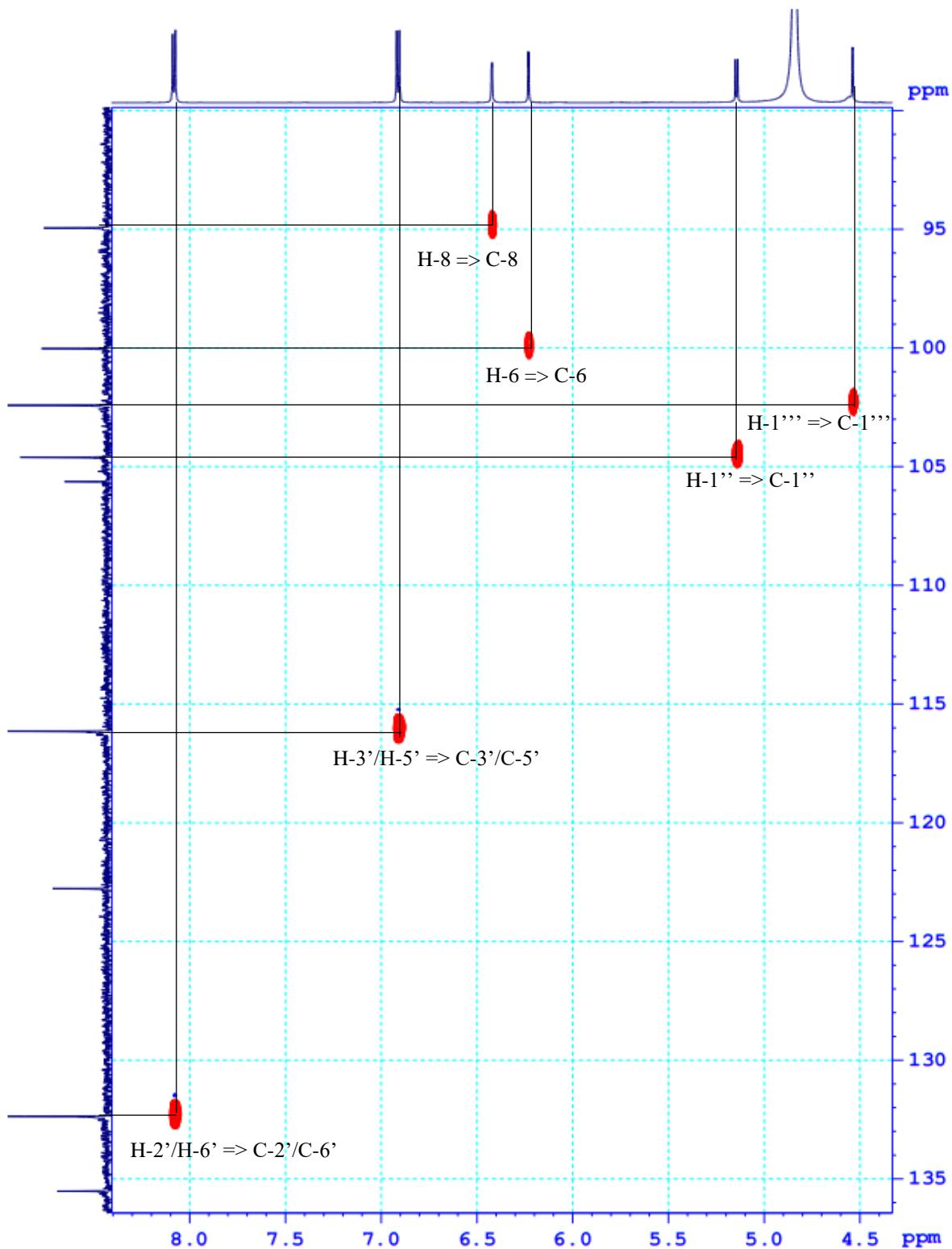
**Figure S91:**  $^{13}\text{C}$ -NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{C}}$  20 ppm to  $\delta_{\text{C}}$  180 ppm)



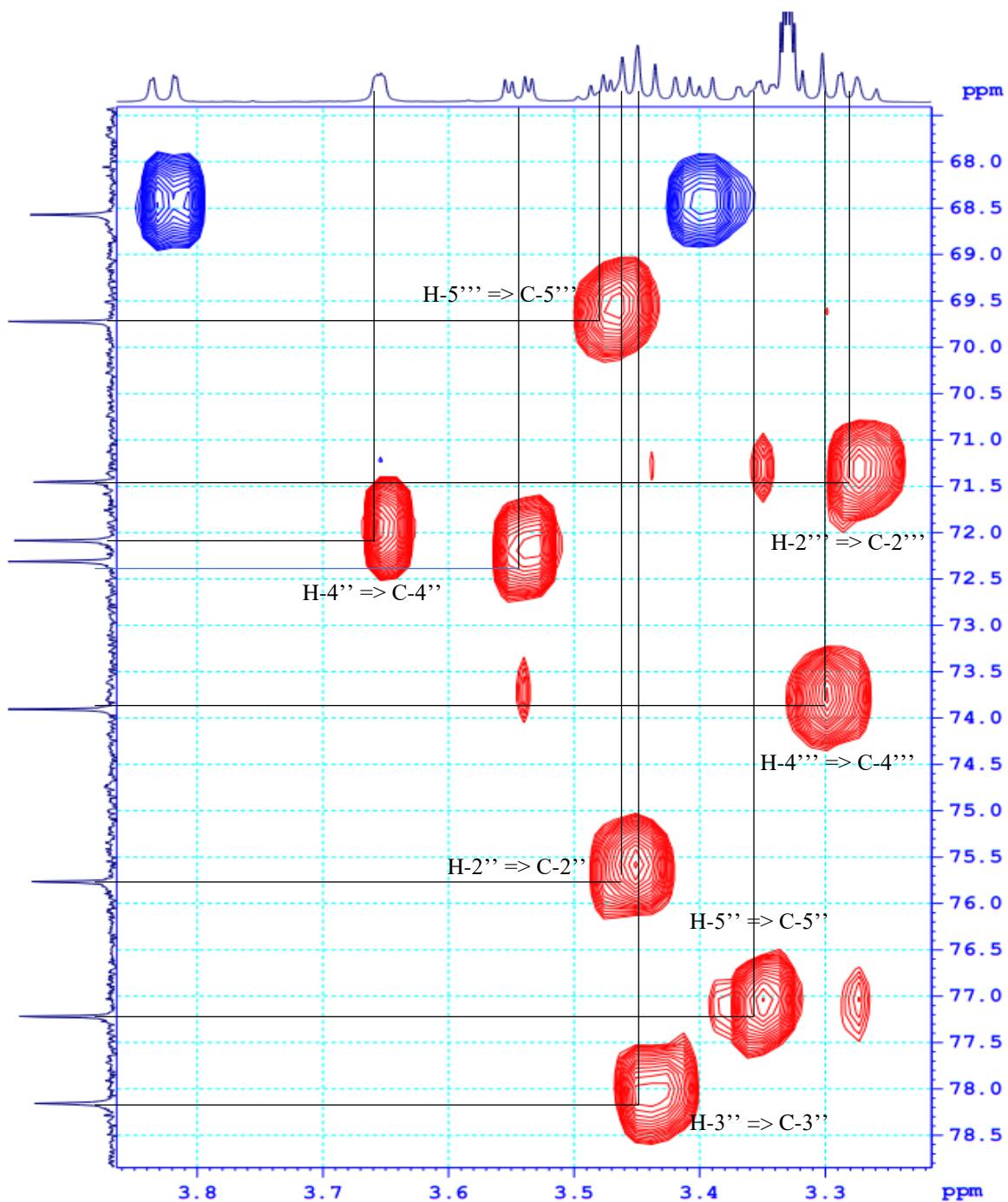
**Figure S92:**  $^{13}\text{C}$ -NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{C}}$  65 ppm to  $\delta_{\text{C}}$  135 ppm)



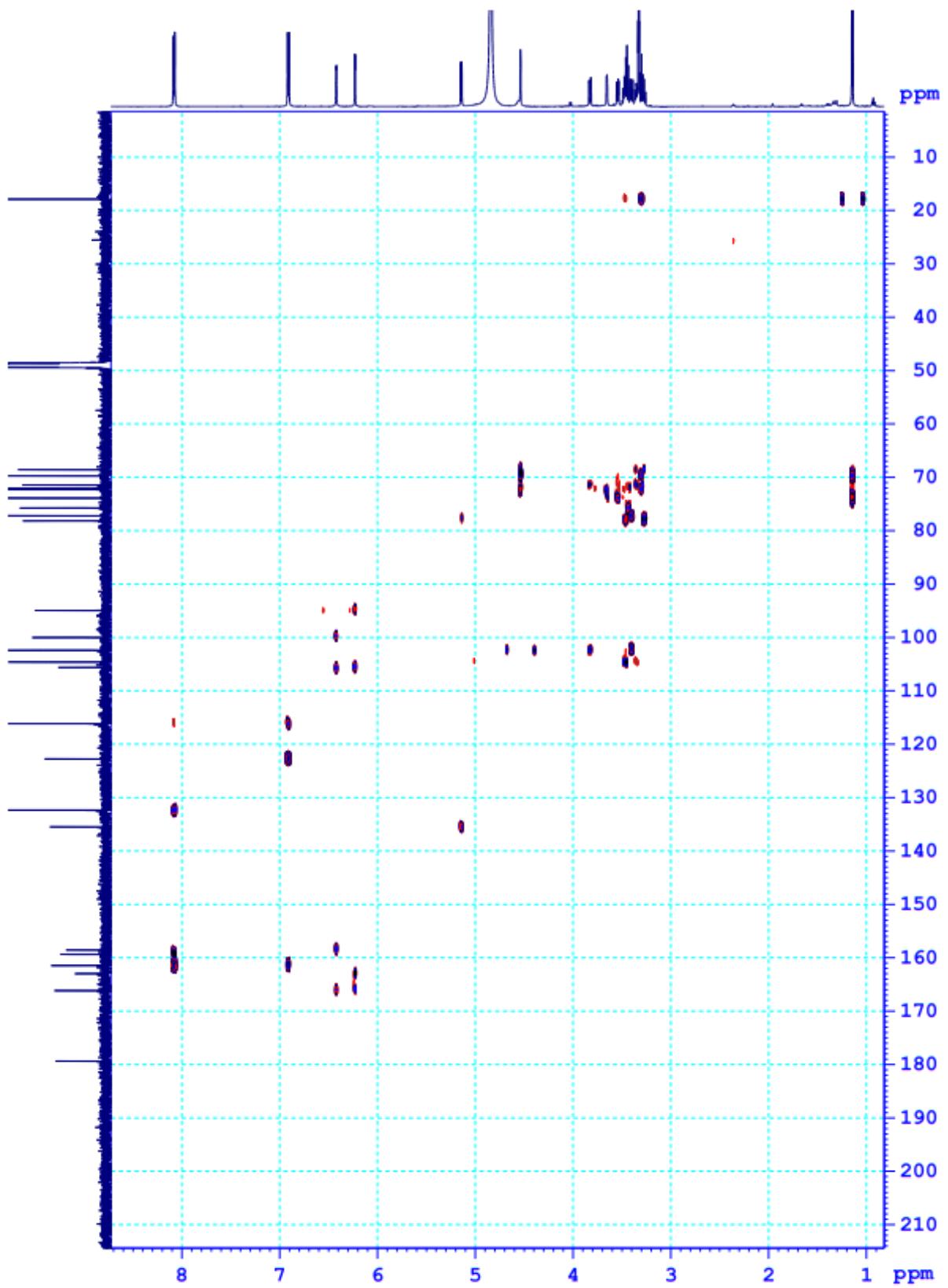
**Figure S93:** HSQC spectrum of compound **11** (nicotiflorin)



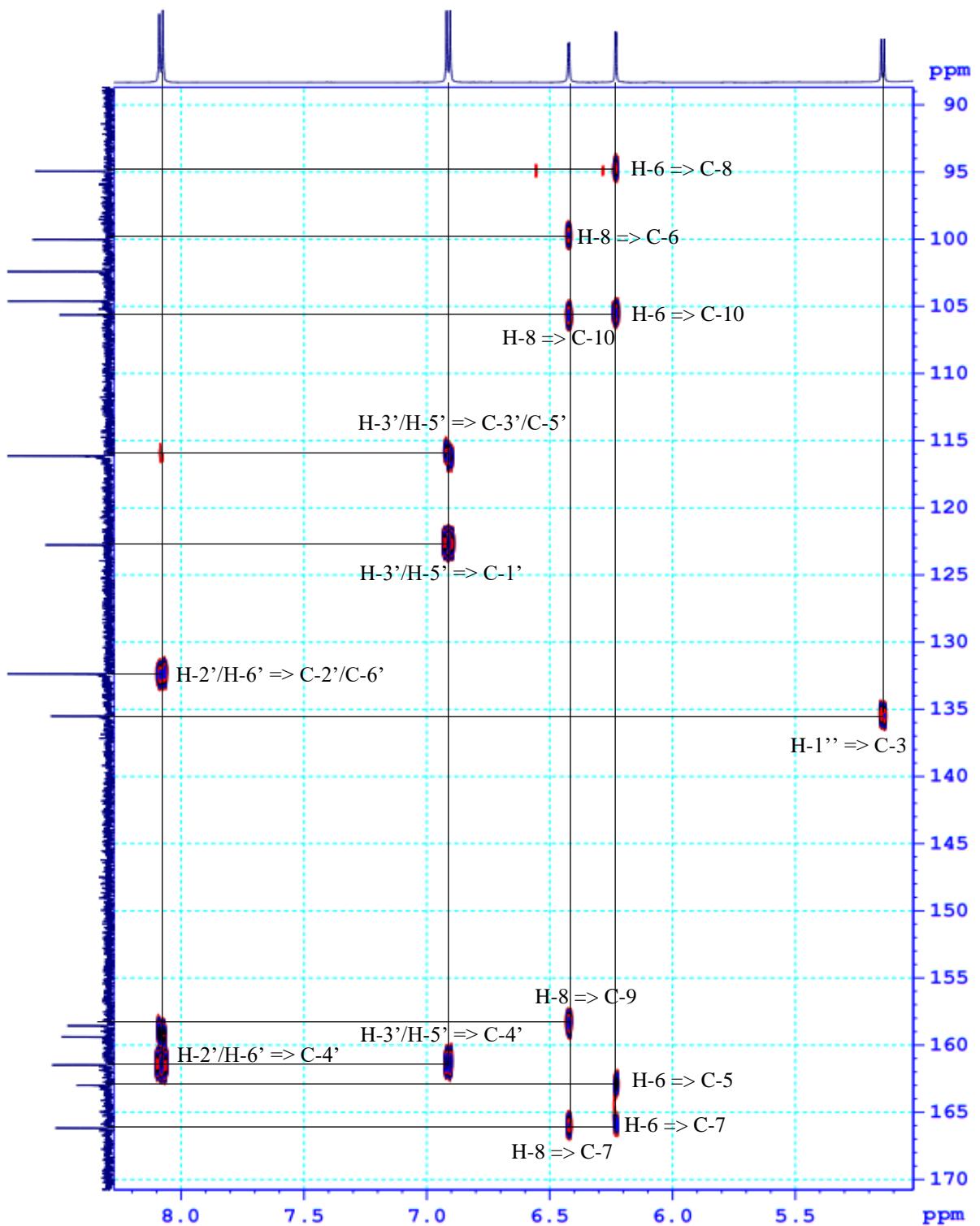
**Figure S94:** HSQC spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{C}}$  90 ppm to  $\delta_{\text{C}}$  135 ppm)



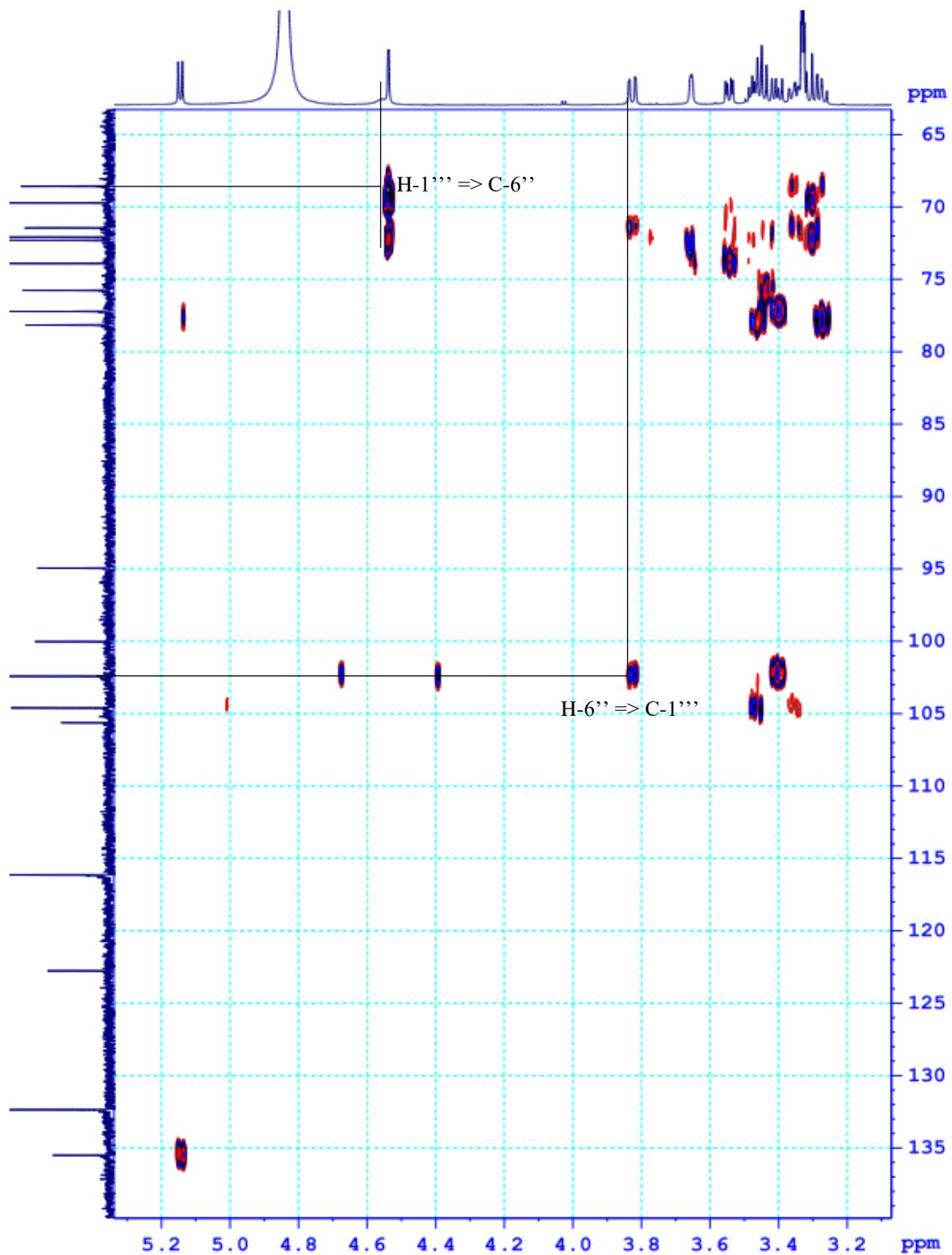
**Figure S95:** HSQC spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{C}}$  67.5 ppm to  $\delta_{\text{C}}$  78.5 ppm)



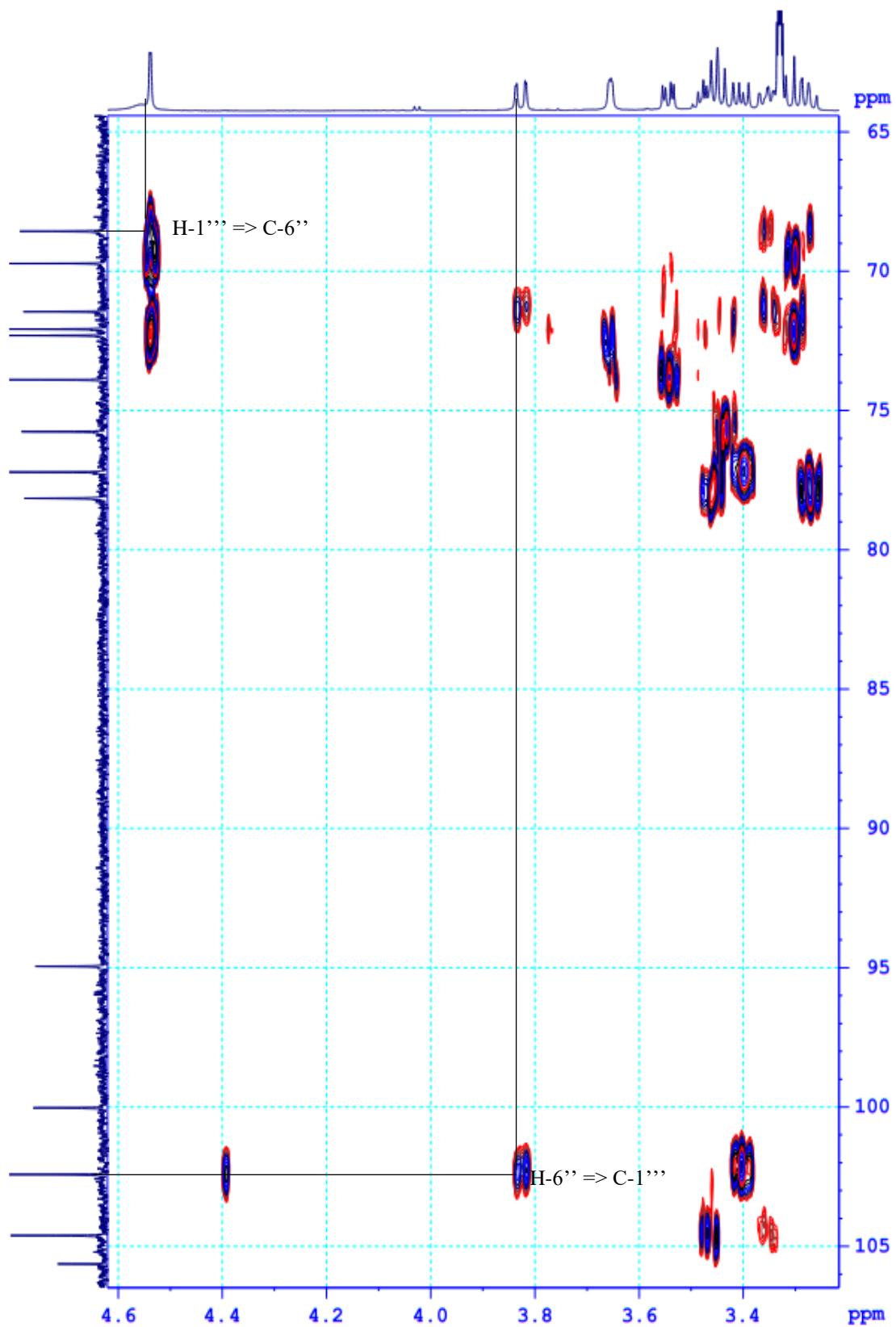
**Figure S96:** HMBC spectrum of compound **11** (nicotiflorin)



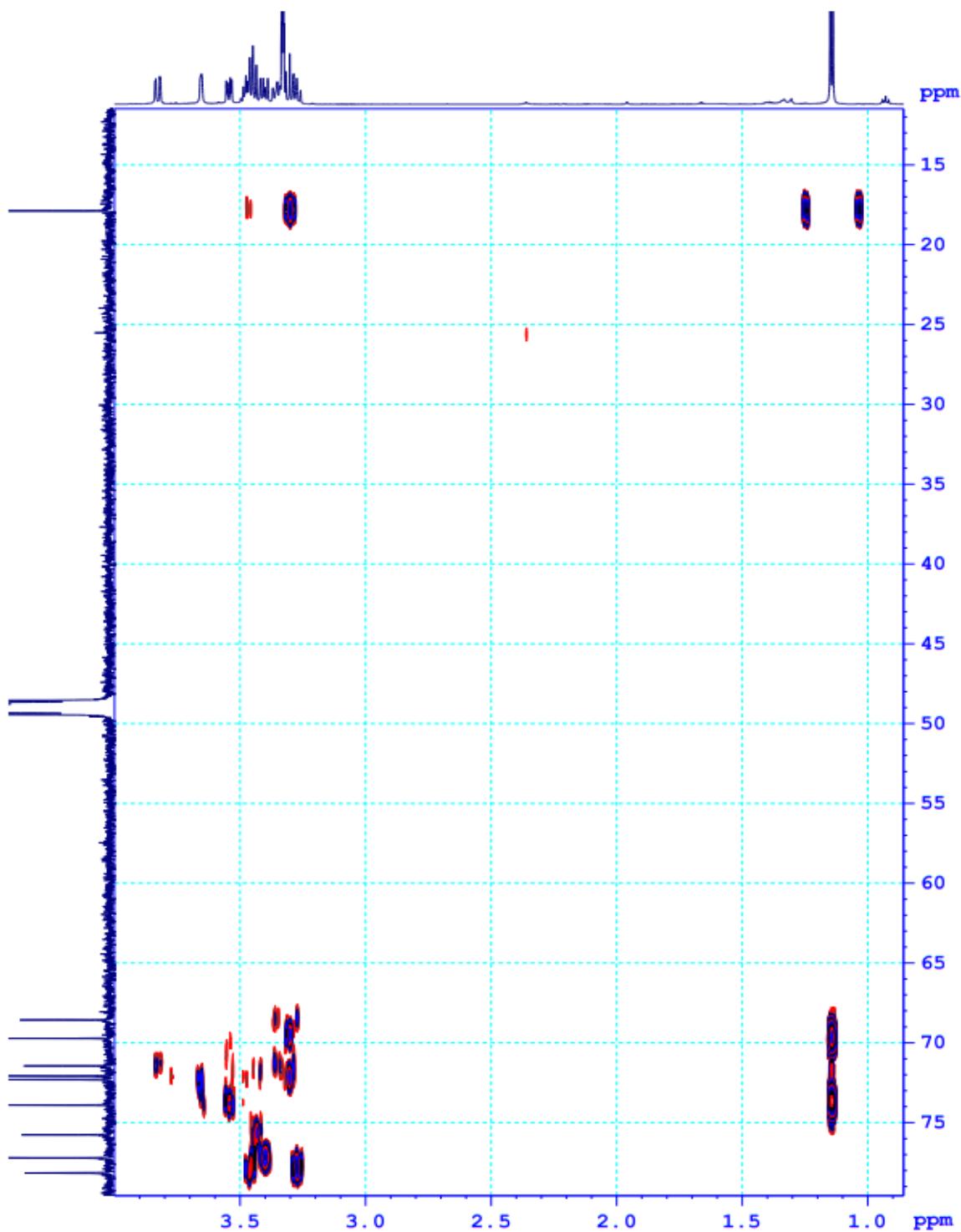
**Figure S97:** HMBC spectrum of compound **11** (nicotiflorin) (from  $\delta_C$  90 ppm to  $\delta_C$  170 ppm)



**Figure S98:** HMBC spectrum of compound **11** (nicotiflorin) (from  $\delta_C$  65 ppm to  $\delta_C$  140 ppm)



**Figure S99:** HMBC spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{C}}$  65 ppm to  $\delta_{\text{C}}$  105 ppm)

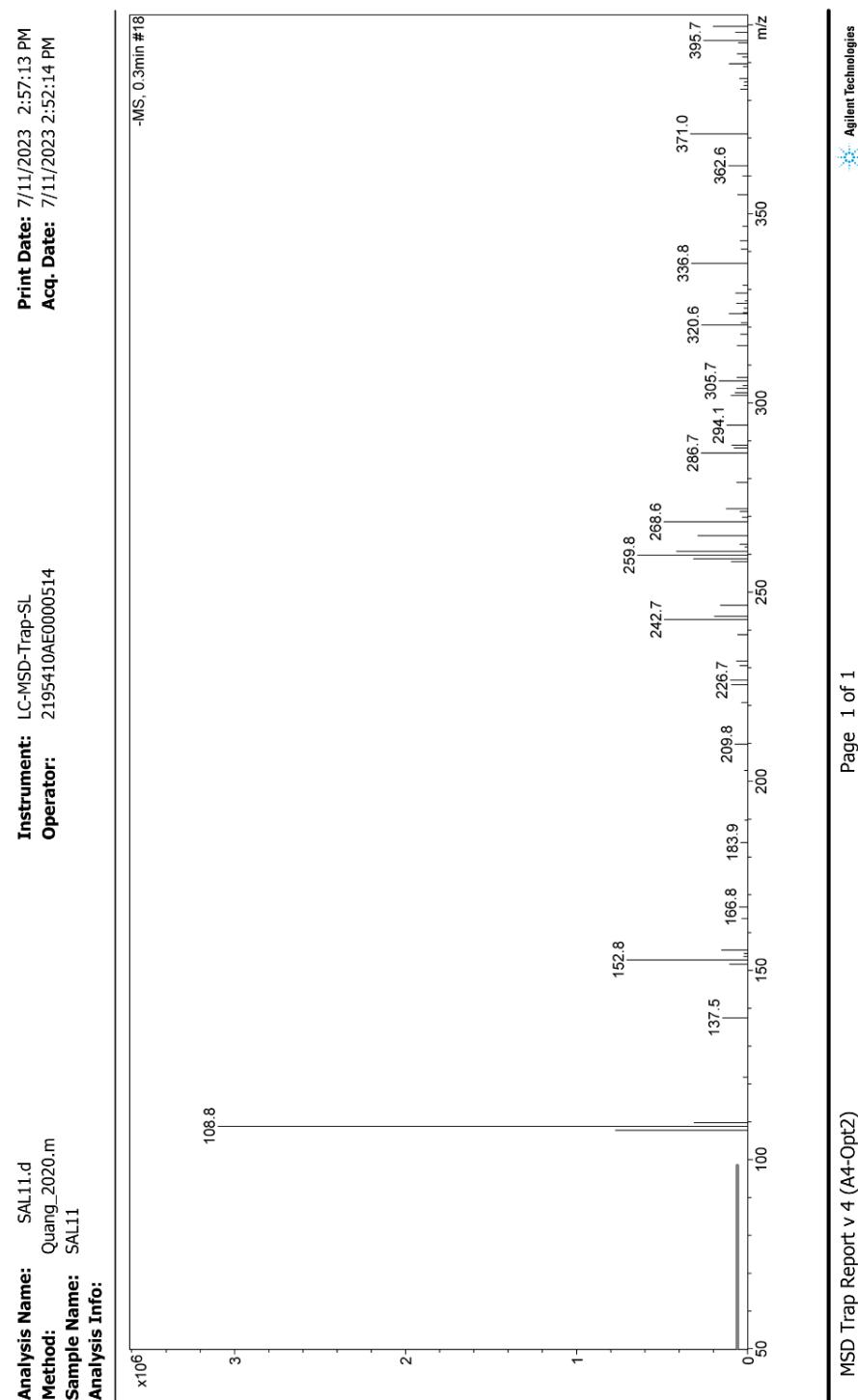


**Figure S100:** HMBC spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{C}}$  15 ppm to  $\delta_{\text{C}}$  80 ppm)

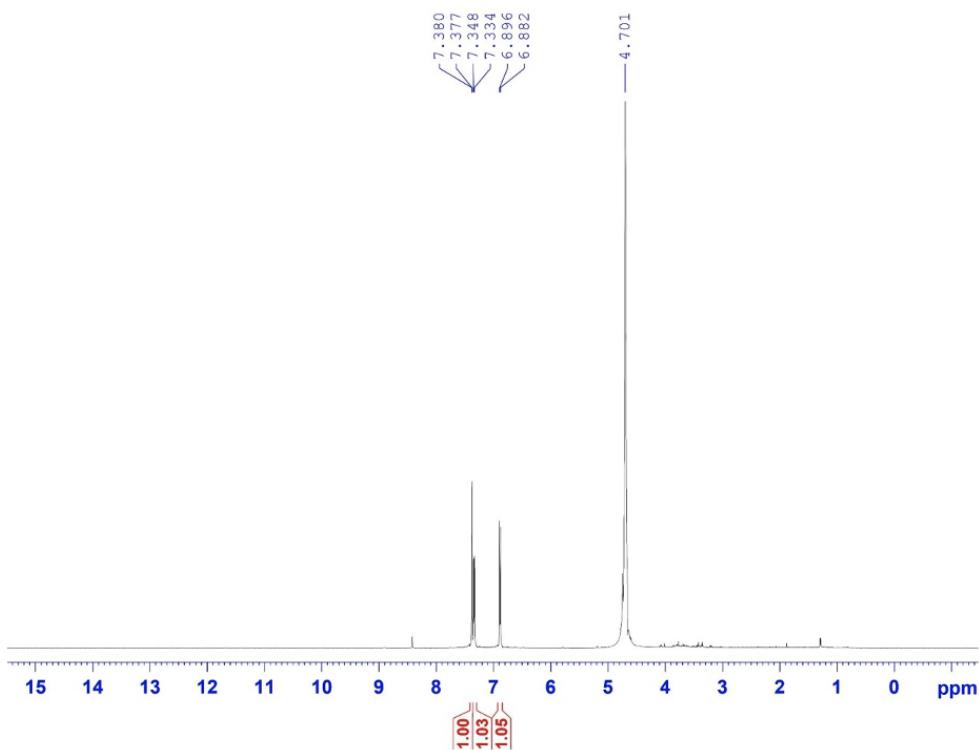
**Table S12:** The comparison of NMR data of compound **12** with a similar compound (3,3',4,4'-tetrahydroxybiphenyl)

Position	Compound <b>12</b> ( $D_2O$ )		3,3',4,4'-tetrahydroxybiphenyl ( $CDCl_3$ ) [40]		
	<sup>13</sup> C-NMR (150 MHz) $\delta_C$ ppm		<sup>1</sup> H-NMR (600 MHz) $\delta_H$ ppm	<sup>13</sup> C-NMR (125 MHz) $\delta_C$ ppm	
	$\delta_C$ ppm		$\delta_H$ ppm	$\delta_H$ ppm	
1 & 1'	128.8	-		134.8	-
2 & 2'	117.0	7.33 (1H, <i>brd</i> , 8.4 Hz)		116.5	6.97 (1H, <i>d</i> , 2.0 Hz)
3 & 3'	143.3	-		145.2	
4 & 4'	147.1	-		146.3	
5 & 5'	115.4	6.88 (1H, <i>d</i> , 8.4 Hz)		114.6	6.77 (2H, <i>d</i> , 8.0 Hz)
6 & 6'	122.5	7.38 (1H, <i>d</i> , 1.8 Hz)		118.9	6.85 (2H, <i>dd</i> , 8.0 Hz, 2.0 Hz)

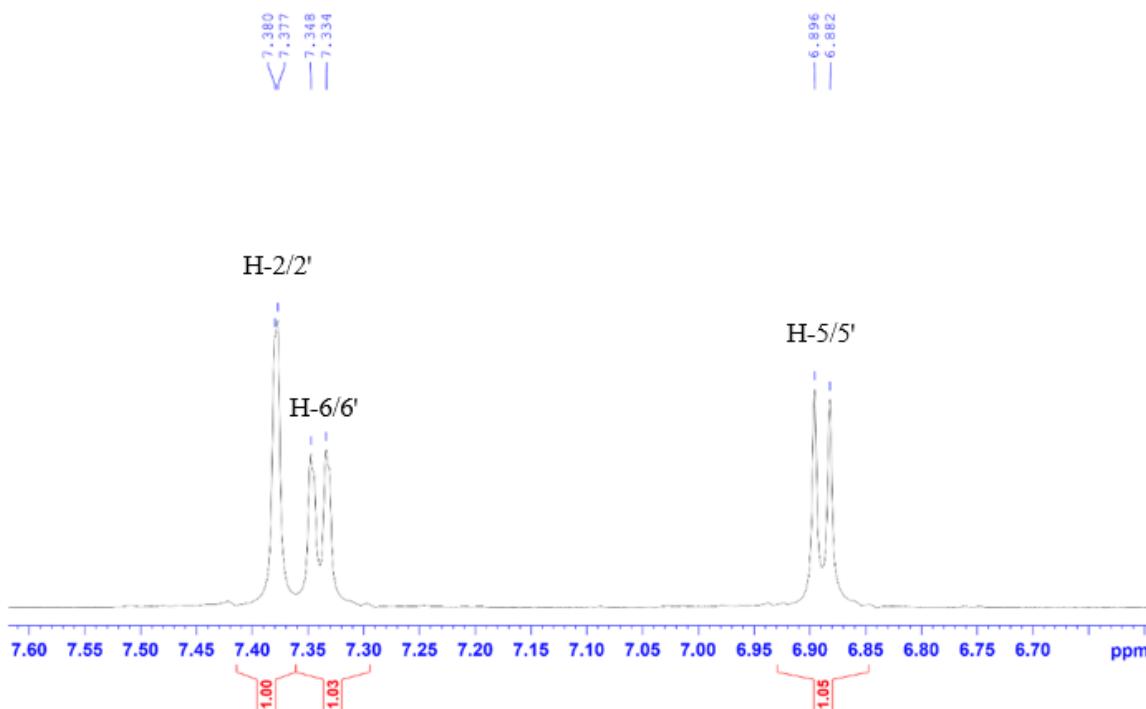
## Display Report - Selected Window Selected Analysis



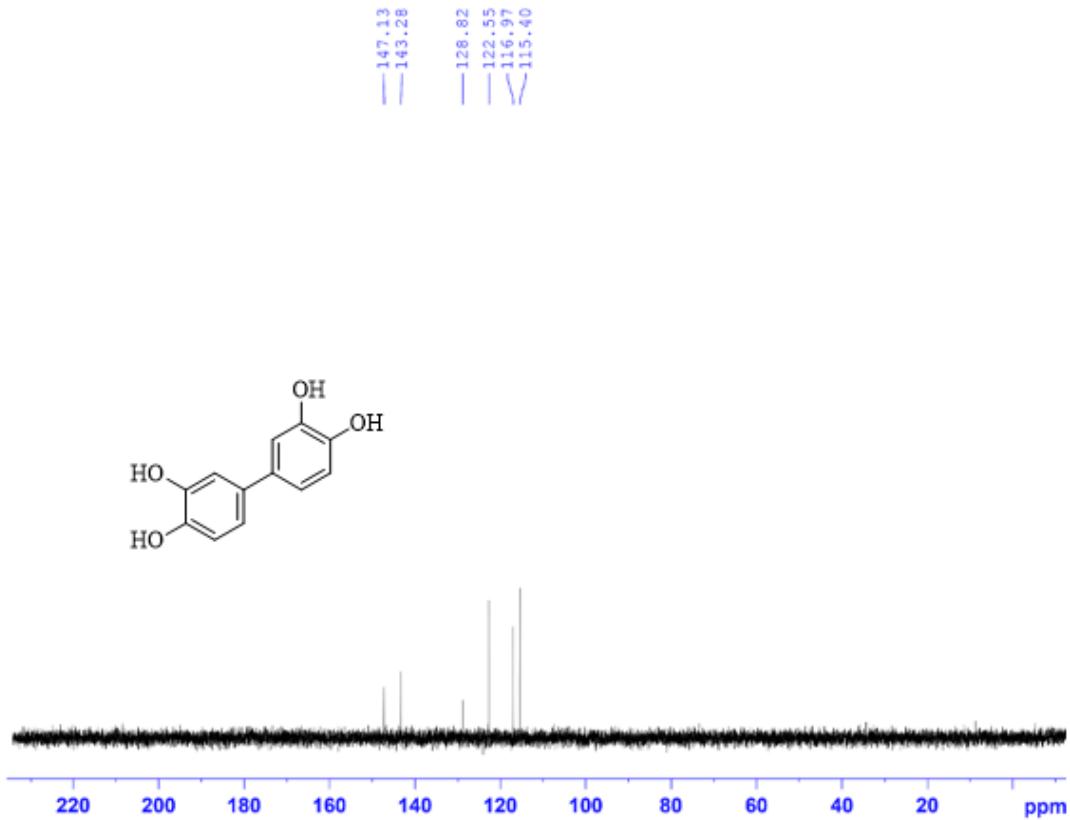
**Figure S101:** (-)-ESI-MS spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)



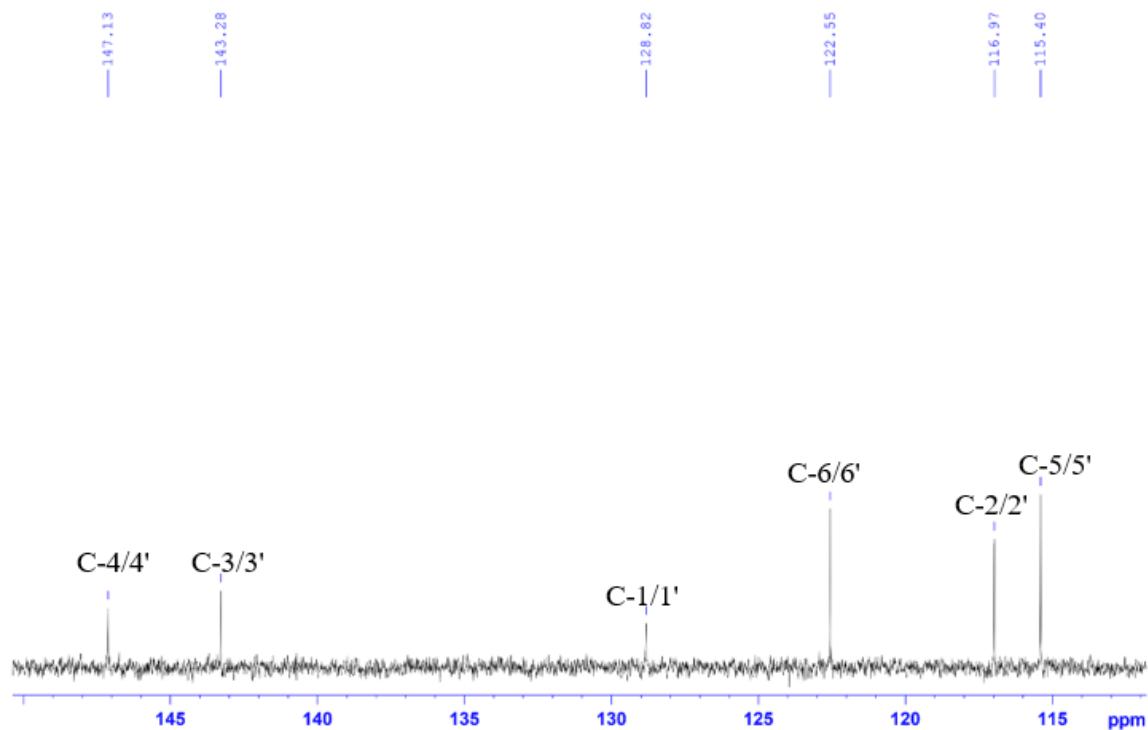
**Figure S102:**  $^1\text{H}$ -NMR (600 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound **12** ( $3,3',4,4'$ -tetrahydroxybiphenyl)



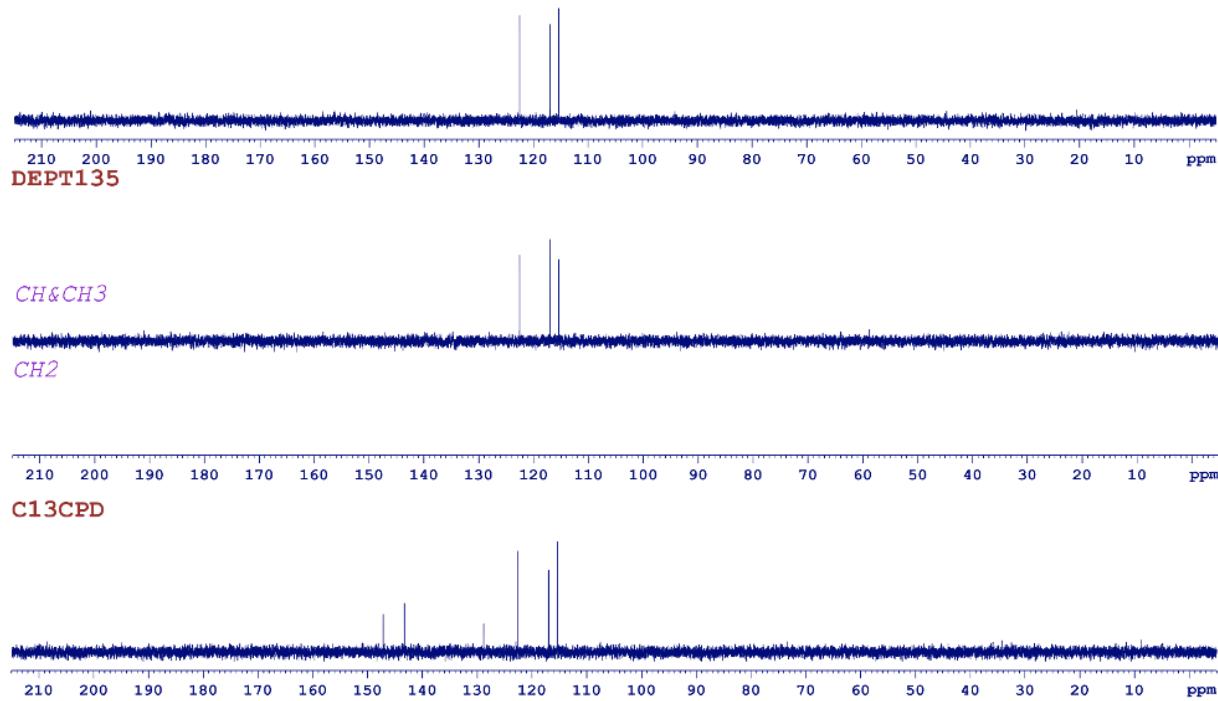
**Figure S103:**  $^1\text{H}$ -NMR (600 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound 12 ( $3,3',4,4'$ -tetrahydroxybiphenyl) (from  $\delta_{\text{H}}$  6.6 ppm to  $\delta_{\text{H}}$  7.6 ppm)



**Figure S104:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)



**Figure S105:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl) (from  $\delta_{\text{C}}$  115 ppm to  $\delta_{\text{C}}$  150 ppm)



**Figure S106:** DEPT-90 spectrum of compound **12** ( $3,3',4,4'$ -tetrahydroxybiphenyl)



**Figure S107:** Fresh leaves of *Sphaerocoryne affinis* from Phu Quoc Island, Vietnam