

# Supporting Information

*Rec. Nat. Prod.* X:X (202X) XX-XX.

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

Huynh Kim Yen<sup>1</sup>, Nguyen Trong Tuan<sup>2</sup>, Tran Thanh Men<sup>3</sup>, Chong Kim Thien Duc<sup>2</sup>, Ma Huu Dat<sup>2</sup>, Truong Thi Tu Tran<sup>1</sup>, Vu Thi Yen<sup>1</sup>, Nguyen Thi Thu Hau<sup>1</sup>, Nguyen Huu Khiem<sup>4</sup>, Vo Thanh Khang<sup>4</sup>  
and Thanh Q. C. Nguyen<sup>5\*</sup>

<sup>1</sup>Department of Food, College of Food Science and Health, Kien Giang University, Kien Giang, Vietnam

<sup>2</sup>Department of Health Sciences, College of Natural Sciences, Can Tho University, Can Tho, Vietnam

<sup>3</sup>Department of Biology, College of Natural Sciences, Can Tho University, Can Tho, Vietnam

<sup>4</sup>Bioassay Laboratory, CTU Hi-tech Building, Can Tho University, Can Tho, Vietnam

<sup>5</sup>Department of Chemistry, College of Natural Sciences, Can Tho University, Can Tho, Vietnam

Table of Contents	Page
<b>Table S1:</b> The comparison of NMR data of compound 1 with a similar compound (chrysin)	6
<b>Figure S1:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound 1	6
<b>Figure S2:</b> Expanded <sup>1</sup> H-NMR spectrum of compound 1	7
<b>Figure S3:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound 1	7
<b>Figure S4:</b> Expanded <sup>13</sup> C-NMR spectrum of compound 1	8
<b>Table S2:</b> The comparison of NMR data of compound 2 with a similar compound (daucosterol)	9
<b>Figure S5:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound 2	10
<b>Figure S6:</b> Expanded <sup>1</sup> H-NMR spectrum of compound 2	11
<b>Figure S7:</b> Expanded <sup>1</sup> H-NMR spectrum of compound 2	11
<b>Figure S8:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound 2	12
<b>Figure S9:</b> Expanded <sup>13</sup> C-NMR spectrum of compound 2	12
<b>Figure S10:</b> Expanded <sup>13</sup> C-NMR spectrum of compound 2	13

\* Corresponding author: E-Mail: [nqcthanh@ctu.edu.vn](mailto:nqcthanh@ctu.edu.vn) (Thanh Q. C. Nguyen); Phone: 084-909-747-547

---

<b>Figure S11:</b> Expanded $^{13}\text{C}$ -NMR spectrum of compound <b>2</b>	13
<b>Table S3:</b> The comparison of NMR data of compound <b>3</b> with a similar compound (allatonin)	14
<b>Figure S12:</b> Complete assignment $^1\text{H}$ -NMR spectrum of compound <b>3</b>	14
<b>Figure S13:</b> Expanded $^1\text{H}$ -NMR spectrum of compound <b>3</b>	15
<b>Figure S14:</b> Complete assignment $^{13}\text{C}$ -NMR spectrum of compound <b>3</b>	15
<b>Figure S15:</b> Expanded $^{13}\text{C}$ -NMR spectrum of compound <b>3</b>	16
<b>Figure S16:</b> Complete assignment HSQC spectrum of compound <b>3</b>	17
<b>Figure S17:</b> Expanded HSQC spectrum of compound <b>3</b>	18
<b>Figure S18:</b> Complete assignment HMBC spectrum of compound <b>3</b>	19
<b>Figure S19:</b> Expanded HMBC spectrum of compound <b>3</b>	20
<b>Table S4:</b> The comparison of NMR data of compound <b>4</b> with a similar compound ((+)-catechin)	21
<b>Figure S20:</b> Complete assignment $^1\text{H}$ -NMR spectrum of compound <b>4</b>	22
<b>Figure S21:</b> Expanded $^1\text{H}$ -NMR spectrum of compound <b>4</b>	22
<b>Figure S22:</b> Expanded $^1\text{H}$ -NMR spectrum of compound <b>4</b>	23
<b>Figure S23:</b> Complete assignment $^{13}\text{C}$ -NMR spectrum of compound <b>4</b>	23
<b>Figure S24:</b> Expanded $^{13}\text{C}$ -NMR spectrum of compound <b>4</b>	24
<b>Figure S25:</b> Expanded $^{13}\text{C}$ -NMR spectrum of compound <b>4</b>	24
<b>Figure S26:</b> Complete assignment HSQC spectrum of compound <b>4</b>	25
<b>Figure S27:</b> Expanded HSQC spectrum of compound <b>4</b>	26
<b>Figure S28:</b> Expanded HSQC spectrum of compound <b>4</b>	27
<b>Figure S29:</b> Complete assignment HMBC spectrum of compound <b>4</b>	28
<b>Figure S30:</b> Expanded HMBC spectrum of compound <b>4</b>	29
<b>Figure S31:</b> Expanded HMBC spectrum of compound <b>4</b>	30
<b>Figure S32:</b> Expanded HMBC spectrum of compound <b>4</b>	31
<b>Figure S33:</b> Complete assignment NOESY spectrum of compound <b>4</b>	32
<b>Figure S34:</b> Expanded NOESY spectrum of compound <b>4</b>	33
<b>Figure S35:</b> Expanded NOESY spectrum of compound <b>4</b>	33
<b>Table 5:</b> The comparison of NMR data of compound <b>5</b> with a similar compound (Apigenin).	34
<b>Figure S36:</b> Complete assignment (+)ESI-MS spectrum of compound <b>5</b>	35
<b>Figure S37:</b> Complete assignment $^1\text{H}$ -NMR spectrum of compound <b>5</b>	36
<b>Figure S38:</b> Expanded $^1\text{H}$ -NMR spectrum of compound <b>5</b>	36
<b>Figure S39:</b> Complete assignment $^{13}\text{C}$ -NMR spectrum of compound <b>5</b>	37

---

---

<b>Figure S40:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>5</b>	37
<b>Table S6:</b> The comparison of NMR data of compound <b>6</b> with a similar compound (rutin)	38
<b>Figure S41:</b> Complete assignment (+)ESI-MS spectrum of compound <b>6</b>	39
<b>Figure S42:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>6</b>	40
<b>Figure S43:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>6</b>	40
<b>Figure S44:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>6</b>	41
<b>Figure S45:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>6</b>	41
<b>Figure S46:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>6</b>	42
<b>Figure S47:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>6</b>	42
<b>Figure S48:</b> Complete assignment HSQC spectrum of compound <b>6</b>	43
<b>Figure S49:</b> Expanded HSQC spectrum of compound <b>6</b>	44
<b>Figure S50:</b> Expanded HSQC spectrum of compound <b>6</b>	45
<b>Figure S51:</b> Complete assignment HMBC spectrum of compound <b>6</b>	46
<b>Figure S52:</b> Expanded HMBC spectrum of compound <b>6</b>	47
<b>Figure S53:</b> Expanded HMBC spectrum of compound <b>6</b>	48
<b>Figure S54:</b> Expanded HMBC spectrum of compound <b>6</b>	49
<b>Table S7:</b> The comparison of NMR data of compound <b>7</b> with a similar compound (isatin)	50
<b>Figure S55:</b> Complete assignment (+)ESI-MS spectrum of compound <b>7</b>	51
<b>Figure S56:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>7</b>	52
<b>Figure S57:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>7</b>	52
<b>Figure S58:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>7</b>	53
<b>Figure S59:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>7</b>	53
<b>Figure S60:</b> Complete assignment HSQC spectrum of compound <b>7</b>	54
<b>Figure S61:</b> Expanded HSQC spectrum of compound <b>7</b>	55
<b>Figure S62:</b> Complete assignment HMBC spectrum of compound <b>7</b>	56
<b>Figure S63:</b> Expanded HMBC spectrum of compound <b>7</b>	57
<b>Table S8:</b> The comparison of NMR data of compound <b>8</b> with a similar compound (3-hydroxy-3-(2-oxopropyl)indolin-2-one).	58
<b>Figure S64:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>8</b>	59
<b>Figure S65:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>8</b>	59
<b>Figure S66:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>8</b>	60
<b>Figure S67:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>8</b>	60

---

---

<b>Figure S68:</b> Complete assignment HSQC spectrum of compound <b>8</b>	61
<b>Figure S69:</b> Expanded HSQC spectrum of compound <b>8</b>	62
<b>Figure S70:</b> Expanded HSQC spectrum of compound <b>8</b>	63
<b>Figure S71:</b> Complete assignment HMBC spectrum of compound <b>8</b>	64
<b>Figure S72:</b> Expanded HMBC spectrum of compound <b>8</b>	65
<b>Figure S73:</b> Expanded HMBC spectrum of compound <b>8</b>	66
<b>Figure S74:</b> Expanded HMBC spectrum of compound <b>8</b>	67
<b>Table S9:</b> The comparison of NMR data of compound <b>9</b> with a similar compound (benzoic acid)	68
<b>Figure S75:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>9</b>	68
<b>Figure S76:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>9</b>	69
<b>Figure S77:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>9</b>	69
<b>Figure S78:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>9</b>	70
<b>Figure S79:</b> Complete assignment HSQC spectrum of compound <b>9</b>	71
<b>Figure S80:</b> Expanded HSQC spectrum of compound <b>9</b>	72
<b>Figure S81:</b> Complete assignment HMBC spectrum of compound <b>9</b>	73
<b>Figure S82:</b> Expanded HMBC spectrum of compound <b>8</b>	74
<b>Table S10:</b> The comparison of NMR data of compound <b>10</b> with a similar compound (ethylene glycol dibenzoate)	75
<b>Figure S83:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>10</b>	76
<b>Figure S84:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>10</b>	76
<b>Figure S85:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>10</b>	77
<b>Figure S86:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>10</b>	77
<b>Table S11:</b> The comparison of NMR data of compound <b>11</b> with a similar compound (nicotiflorin)	78
<b>Figure S87:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>11</b>	79
<b>Figure S88:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>11</b>	80
<b>Figure S89:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>11</b>	80
<b>Figure S90:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>11</b>	80
<b>Figure S91:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>11</b>	81
<b>Figure S92:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>11</b>	82
<b>Figure S93:</b> Complete assignment HSQC spectrum of compound <b>11</b>	82
<b>Figure S94:</b> Expanded HSQC spectrum of compound <b>11</b>	83
<b>Figure S95:</b> Expanded HSQC spectrum of compound <b>11</b>	84

---

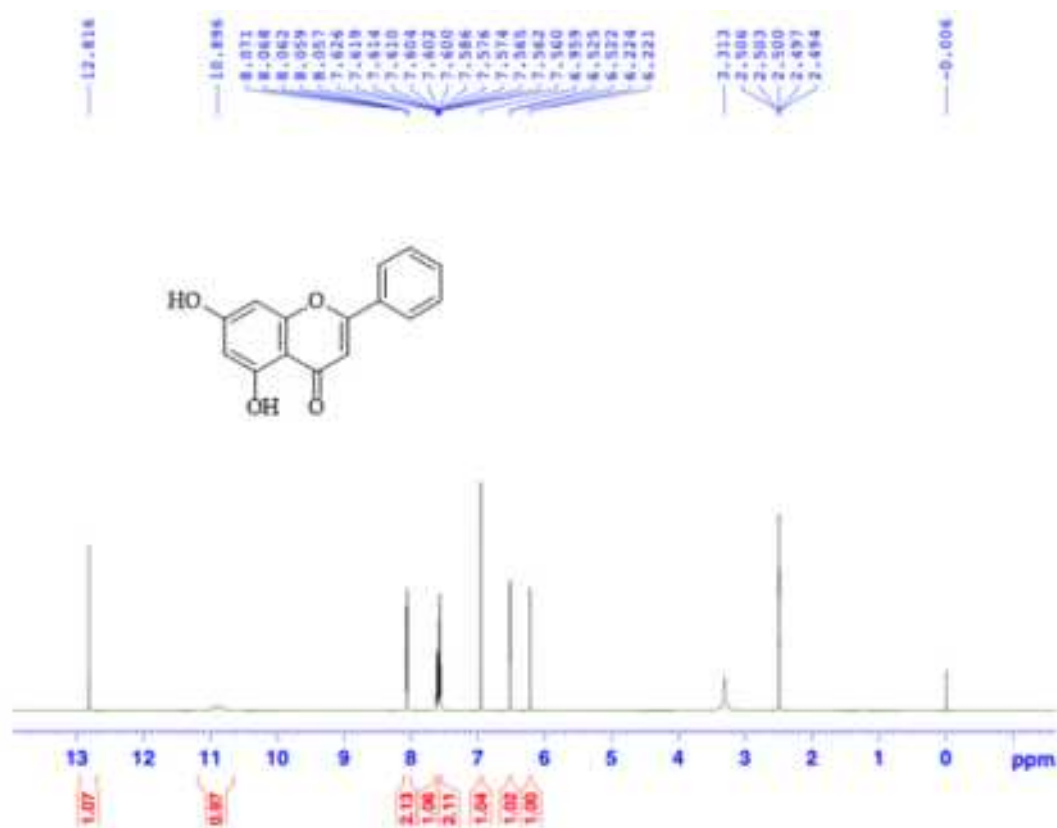
---

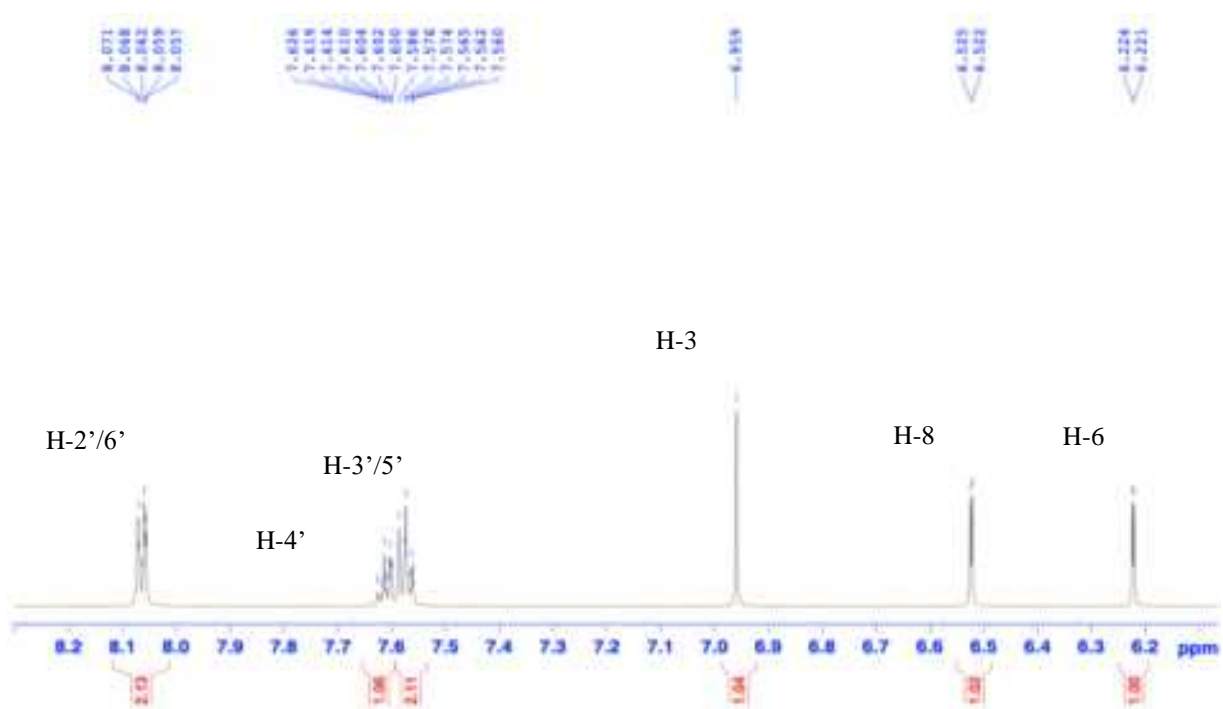
<b>Figure S96:</b> Complete assignment HMBC spectrum of compound <b>11</b>	85
<b>Figure S97:</b> Expanded HMBC spectrum of compound <b>11</b>	86
<b>Figure S98:</b> Expanded HMBC spectrum of compound <b>11</b>	87
<b>Figure S99:</b> Expanded HMBC spectrum of compound <b>11</b>	88
<b>Figure S100:</b> Expanded HMBC spectrum of compound <b>11</b>	89
<b>Table S12:</b> The comparison of NMR data of compound <b>12</b> with a similar compound (3,3',4,4'-tetrahydroxybiphenyl)	90
<b>Figure S101:</b> Complete assignment (+)ESI-MS spectrum of compound <b>12</b>	91
<b>Figure S102:</b> Complete assignment <sup>1</sup> H-NMR spectrum of compound <b>12</b>	92
<b>Figure S103:</b> Expanded <sup>1</sup> H-NMR spectrum of compound <b>12</b>	92
<b>Figure S104:</b> Complete assignment <sup>13</sup> C-NMR spectrum of compound <b>12</b>	93
<b>Figure S105:</b> Expanded <sup>13</sup> C-NMR spectrum of compound <b>12</b>	93
<b>Figure S106:</b> Complete assignment DEPT spectrum of compound <b>12</b>	94
<b>Figure S107:</b> Fresh leaves of <i>Sphaerocoryne affinis</i> from Phu Quoc Island, Vietnam	94

---

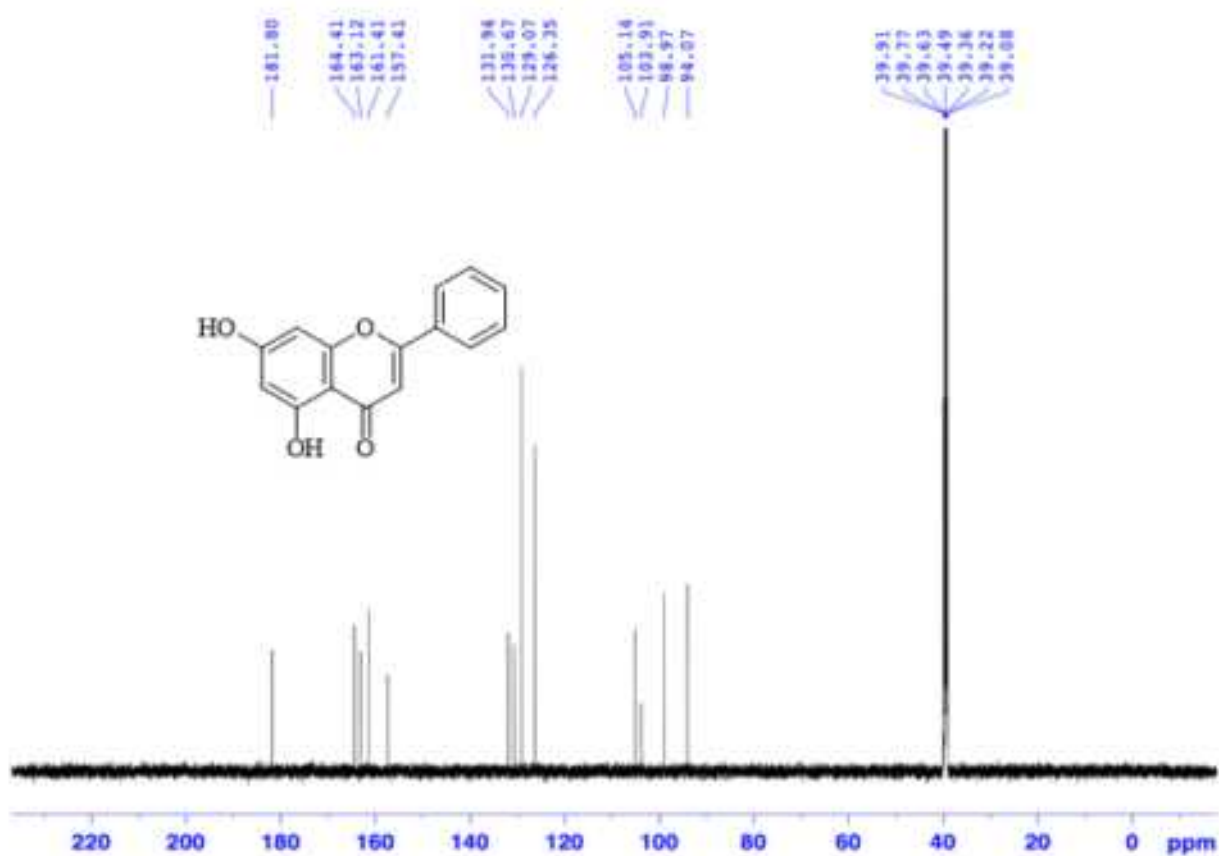
**Table S1:** The comparison of NMR data of compound **1** with a similar compound (Chrysin)

Position	Compound 1 (DMSO- <i>d</i> <sub>6</sub> )		Chrysin (DMSO- <i>d</i> <sub>6</sub> ) [28]	
	<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 (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> 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	-

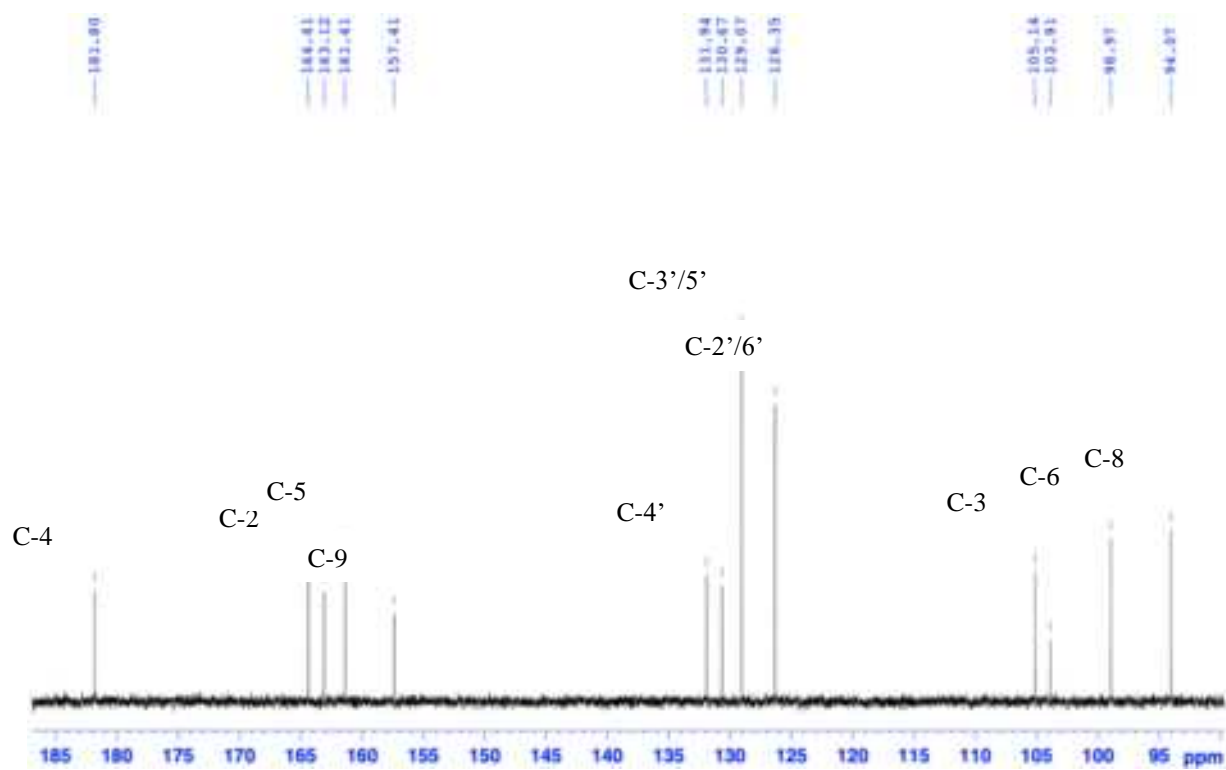
**Figure S1:** <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **1** (chrysin)



**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)



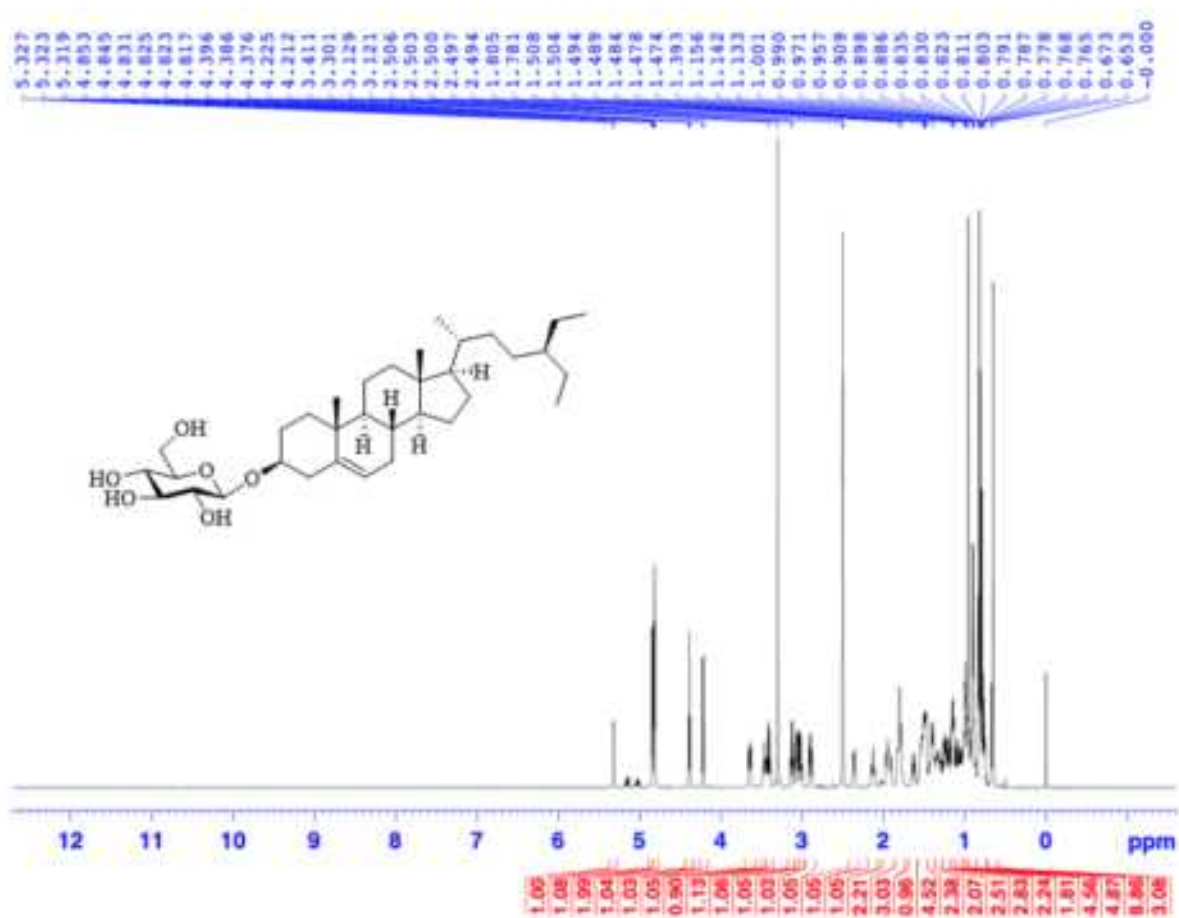
**Figure S4:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **1** (chrysin) (from  $\delta_{\text{C}}$  95 ppm to  $\delta_{\text{C}}$  190 ppm)



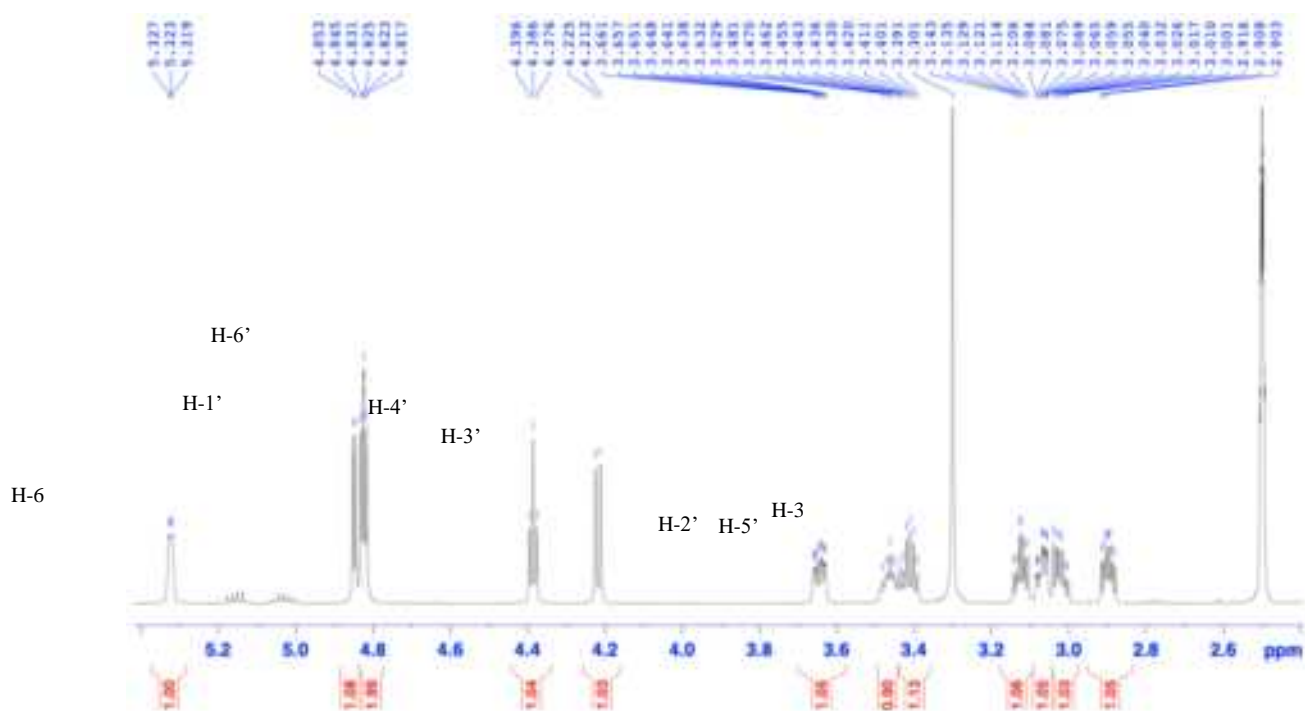
**Table S2** : The comparison of NMR data of compound **2** with a similar compound (Daucosterol)

Position	Compound <b>2</b> (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)

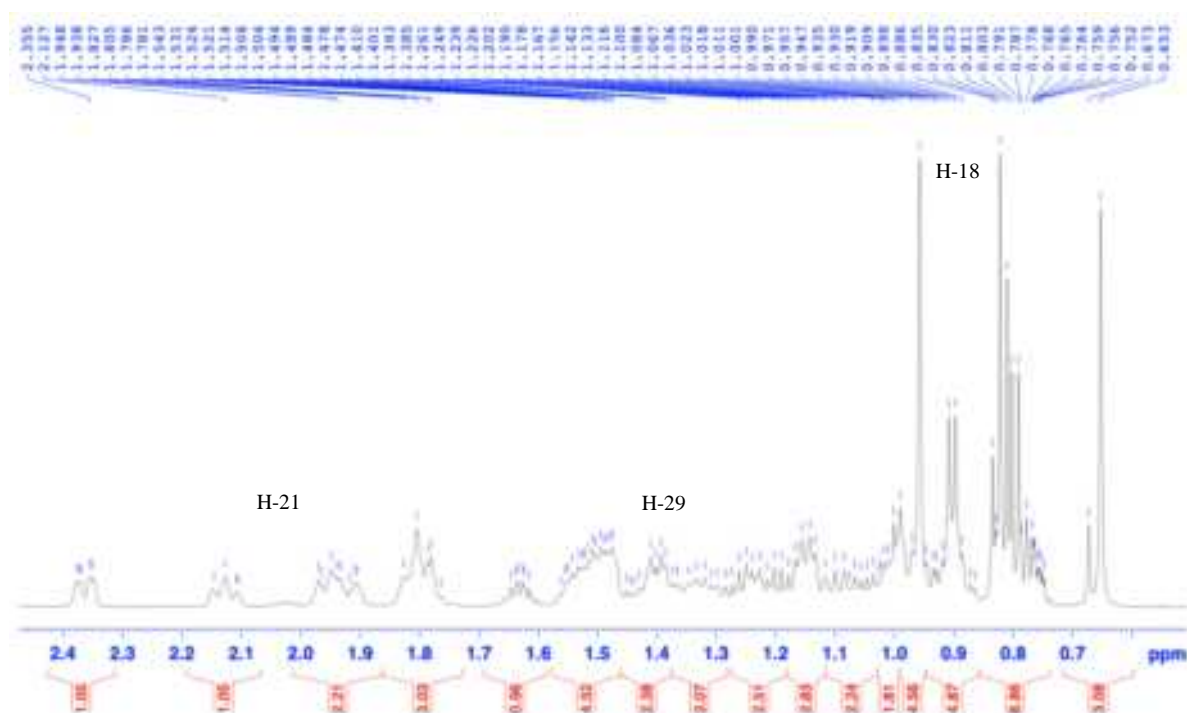
Position	Compound 2 (DMSO- <i>d</i> <sub>6</sub> )		Daucosterol (DMSO- <i>d</i> <sub>6</sub> ) [29]	
	<sup>13</sup> C-NMR (150 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (100 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (400 MHz) δ <sub>H</sub> ppm
4'	70.1	4.39 (1H, <i>m</i> )	70.0	4.28 (1H, <i>t</i> , 8,0 Hz)
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)



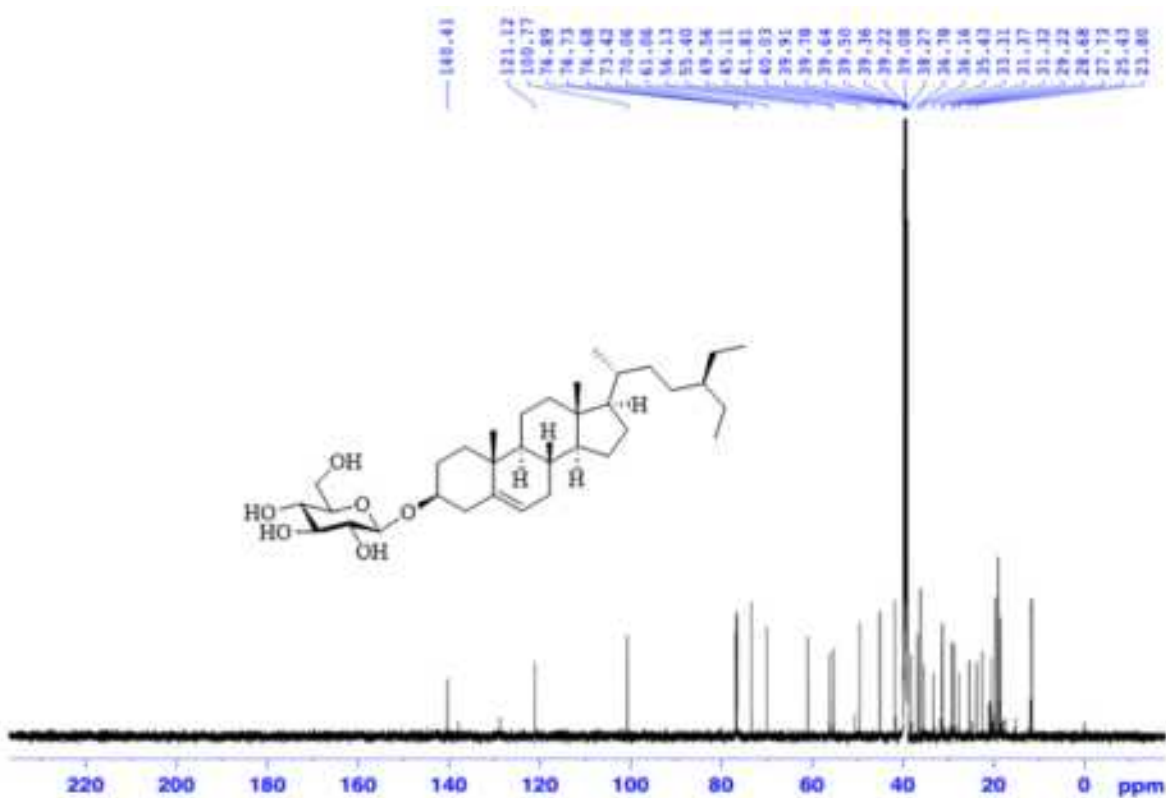
**Figure S5:** <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 2 (daucosterol)



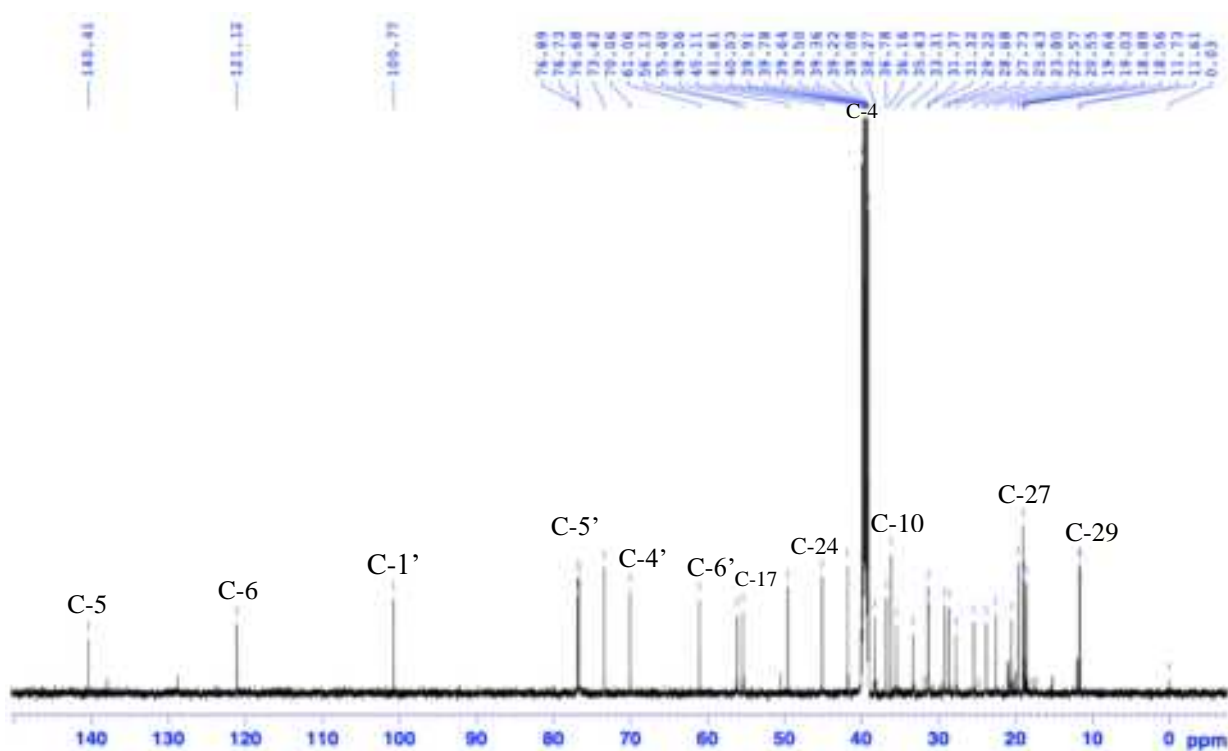
**Figure S6:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{H}}$  2.7 ppm to  $\delta_{\text{H}}$  5.3 ppm)



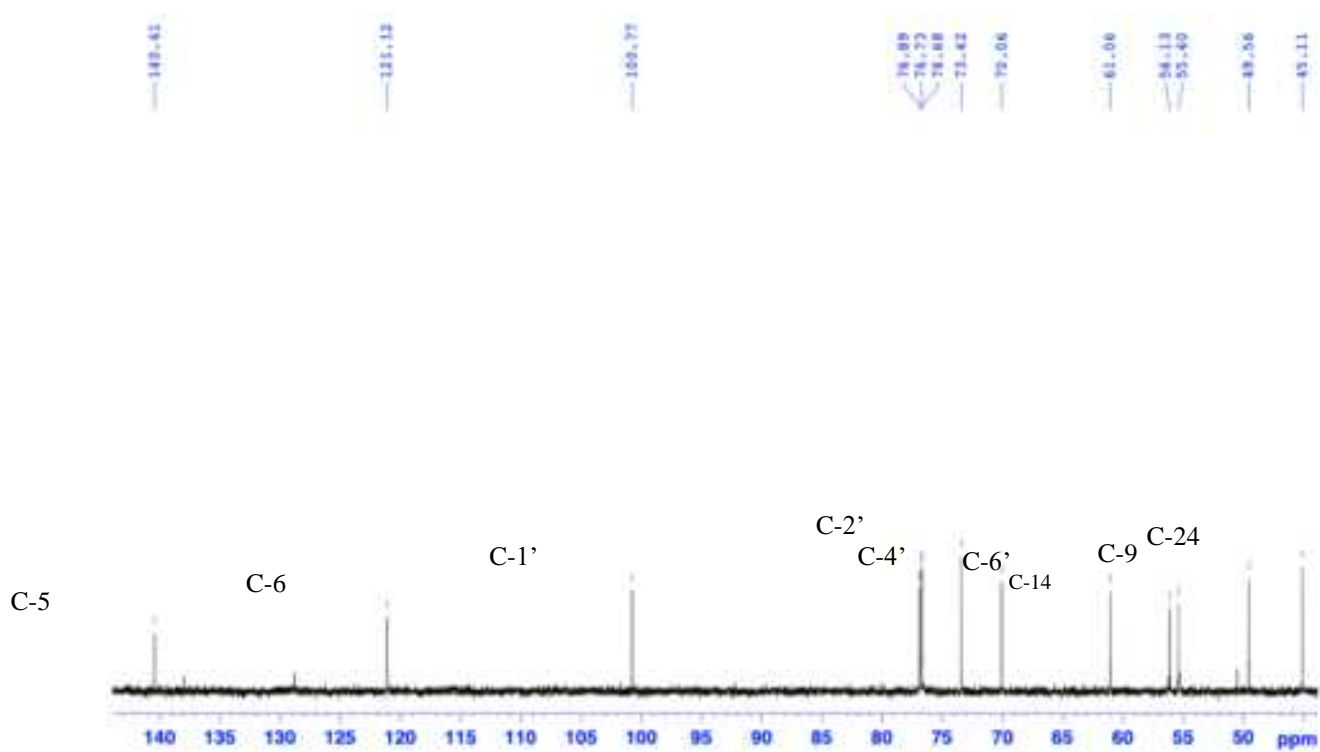
**Figure S7:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{H}}$  0.6 ppm to  $\delta_{\text{H}}$  2.4 ppm)



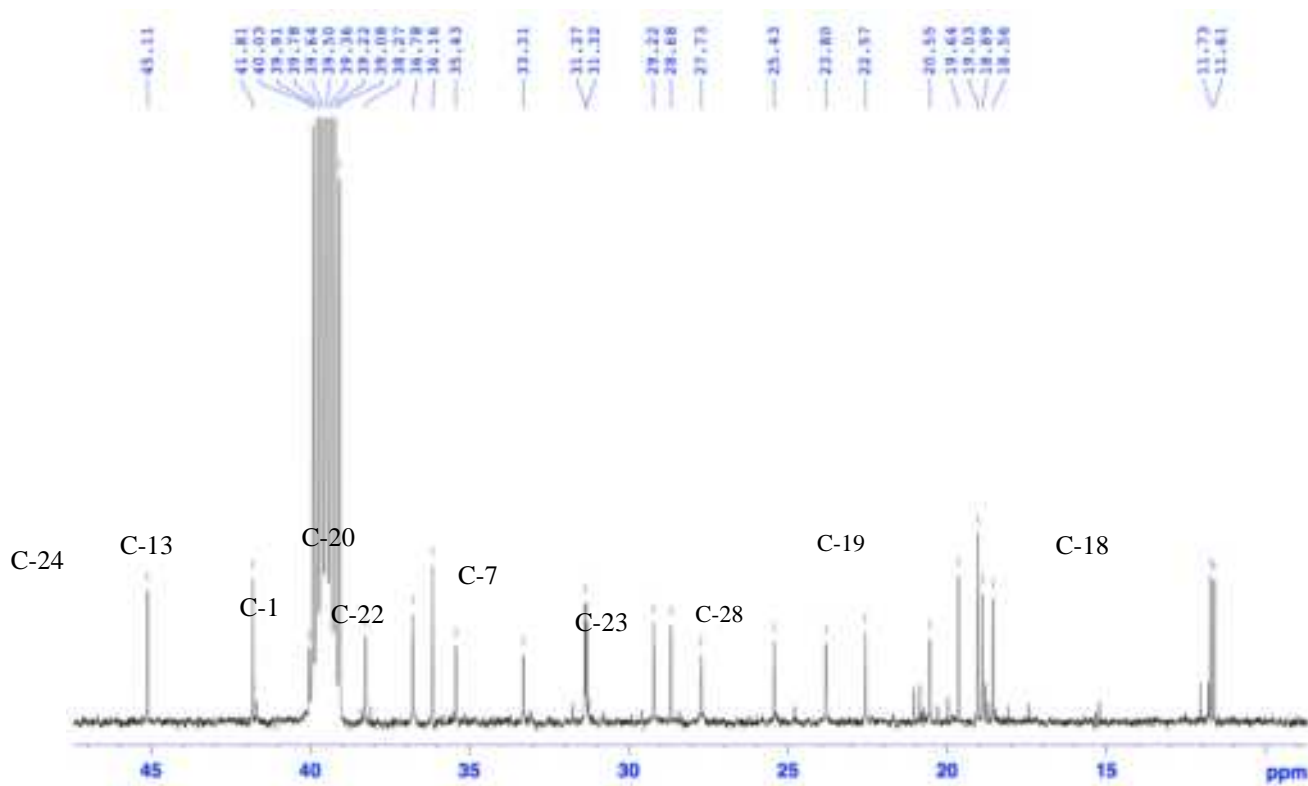
**Figure S8:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2** (daucosterol)



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



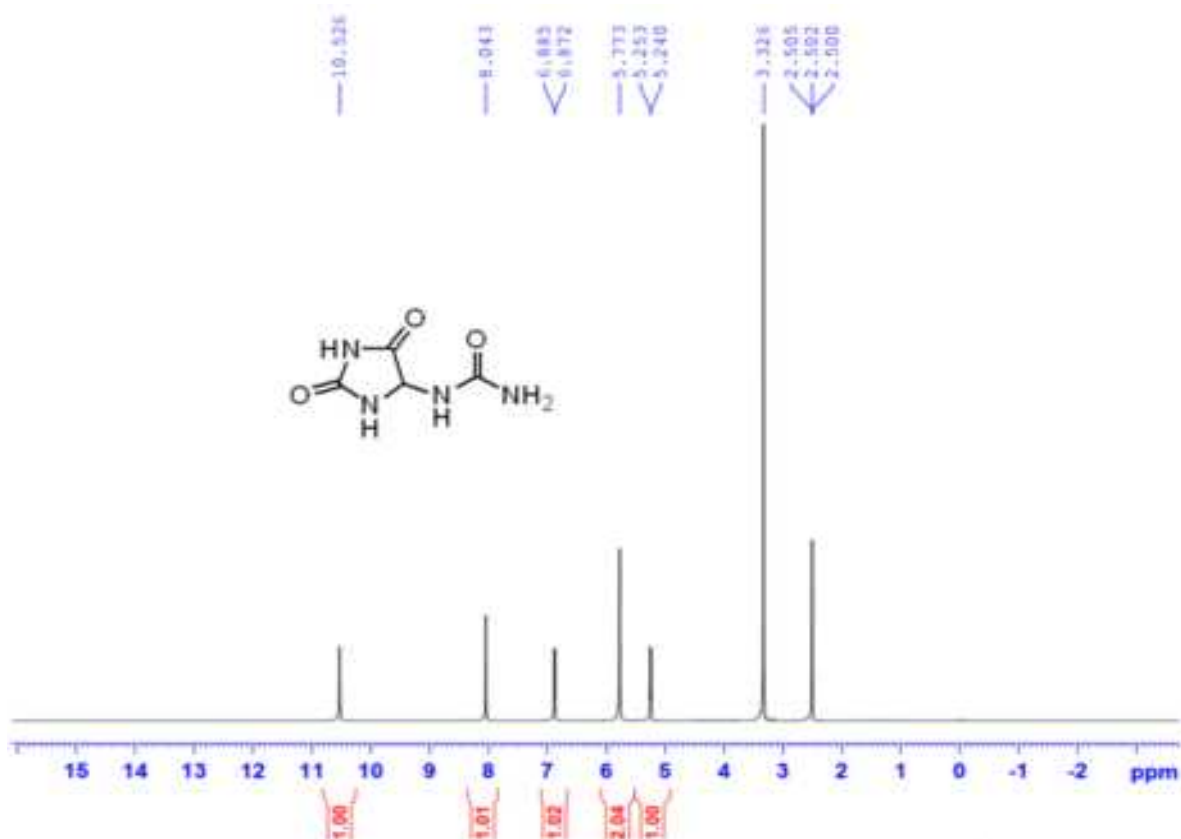
**Figure S10:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{C}}$  50 ppm to  $\delta_{\text{C}}$  140 ppm)



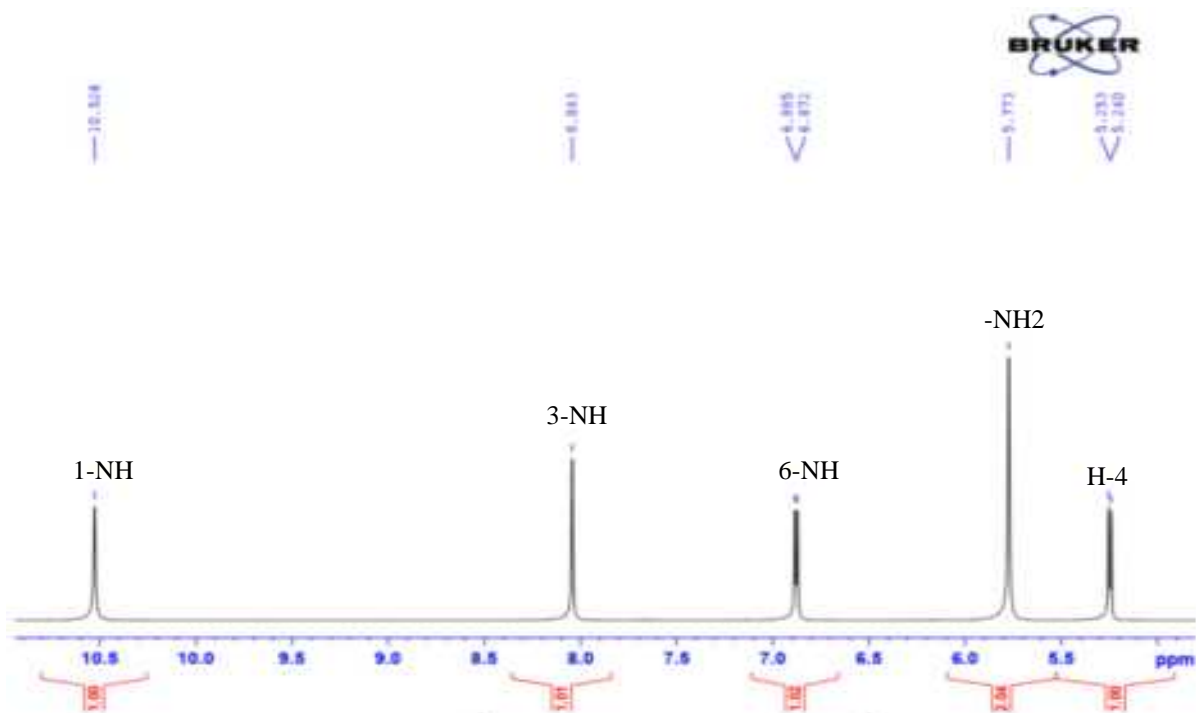
**Figure S11:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2** (daucosterol) (from  $\delta_{\text{C}}$  10 ppm to  $\delta_{\text{C}}$  47 ppm)

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

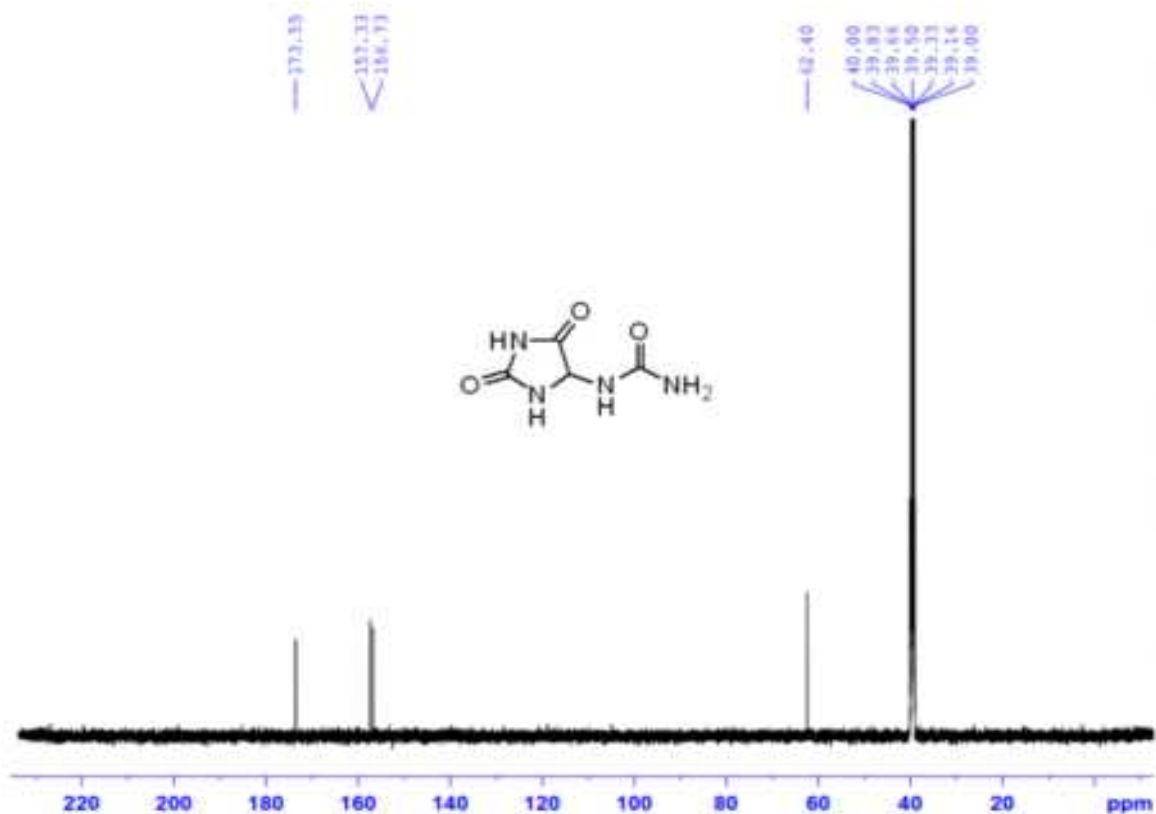
Position	Compound <b>3</b> (DMSO- <i>d</i> <sub>6</sub> )		Allatonin (DMSO- <i>d</i> <sub>6</sub> ) [30]	
	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> ppm
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> )



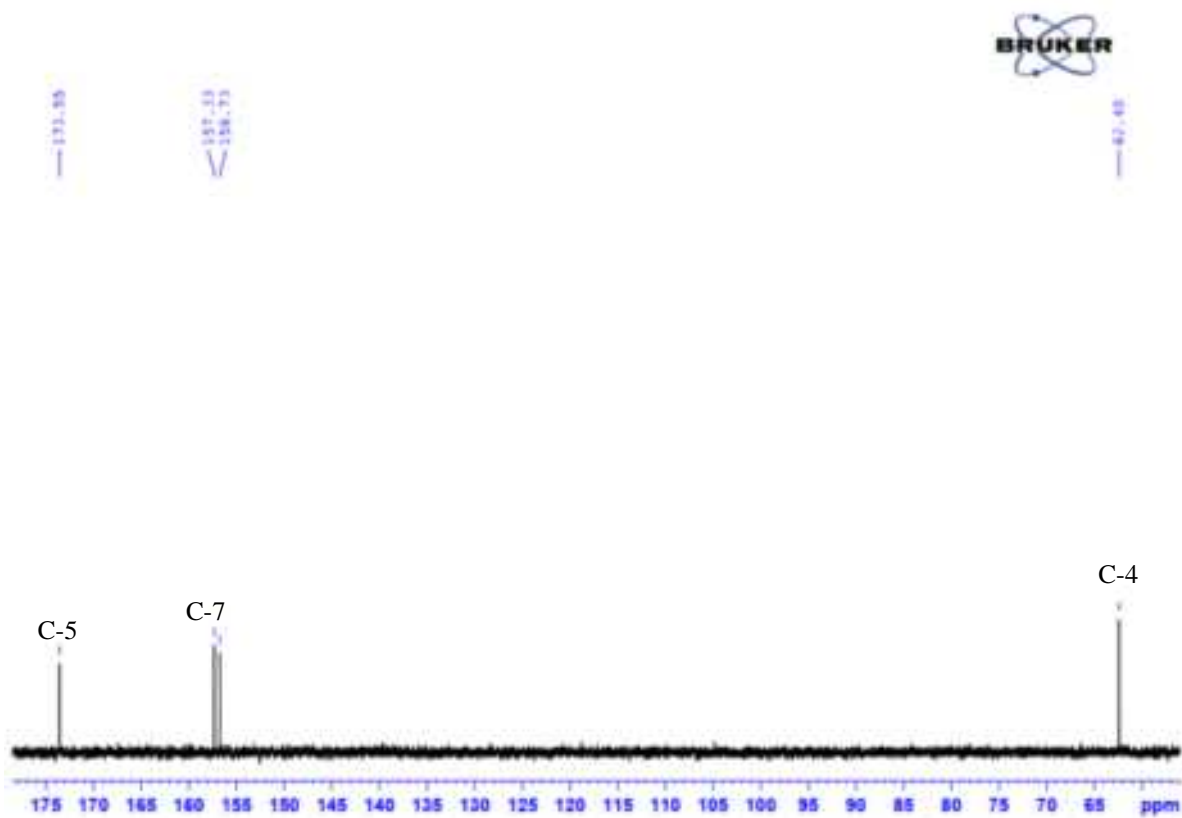
**Figure S12:** <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **3** (allatonin)



**Figure S13:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-d}_6$ ) spectrum of compound 3 (allatonin) (from  $\delta_{\text{H}}$  5 ppm to  $\delta_{\text{H}}$  11 ppm)

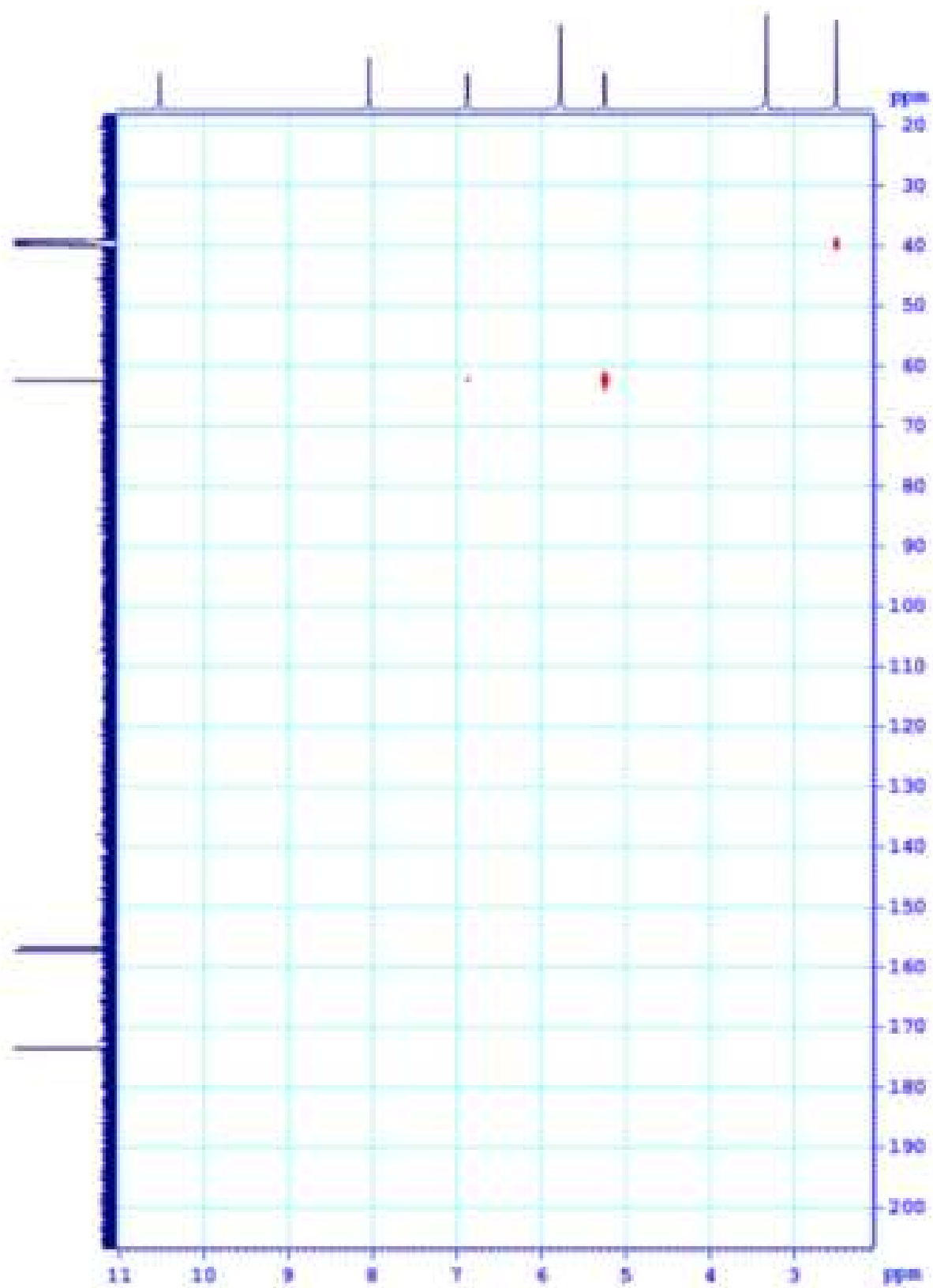


**Figure S14:**  $^{13}\text{C-NMR}$  (150 MHz,  $\text{DMSO-d}_6$ ) spectrum of compound 3 (allatonin)

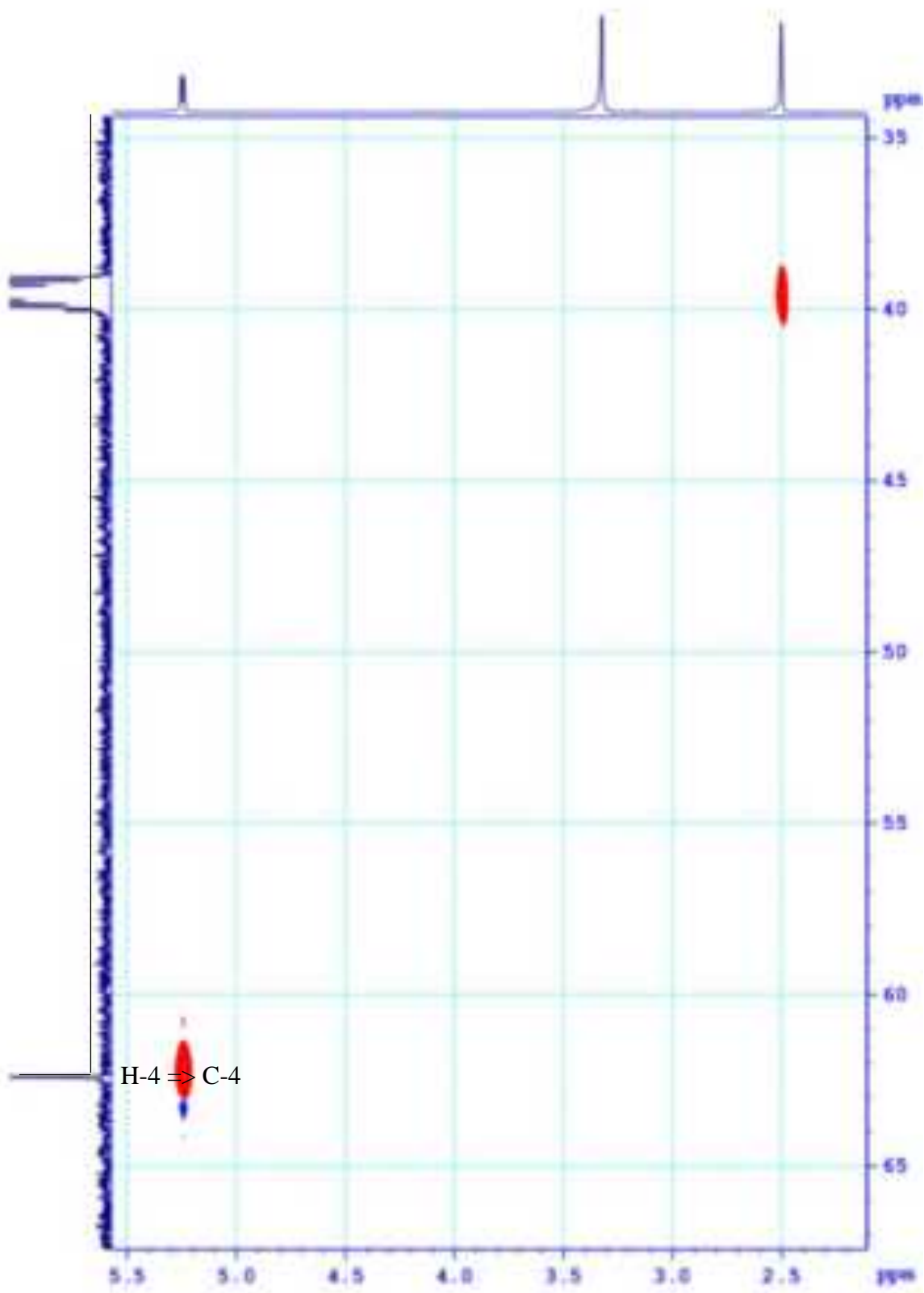


**Figure S15:** <sup>13</sup>C-NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **3** (allatonin) (from  $\delta_c$  60 ppm to  $\delta_c$  175 ppm)

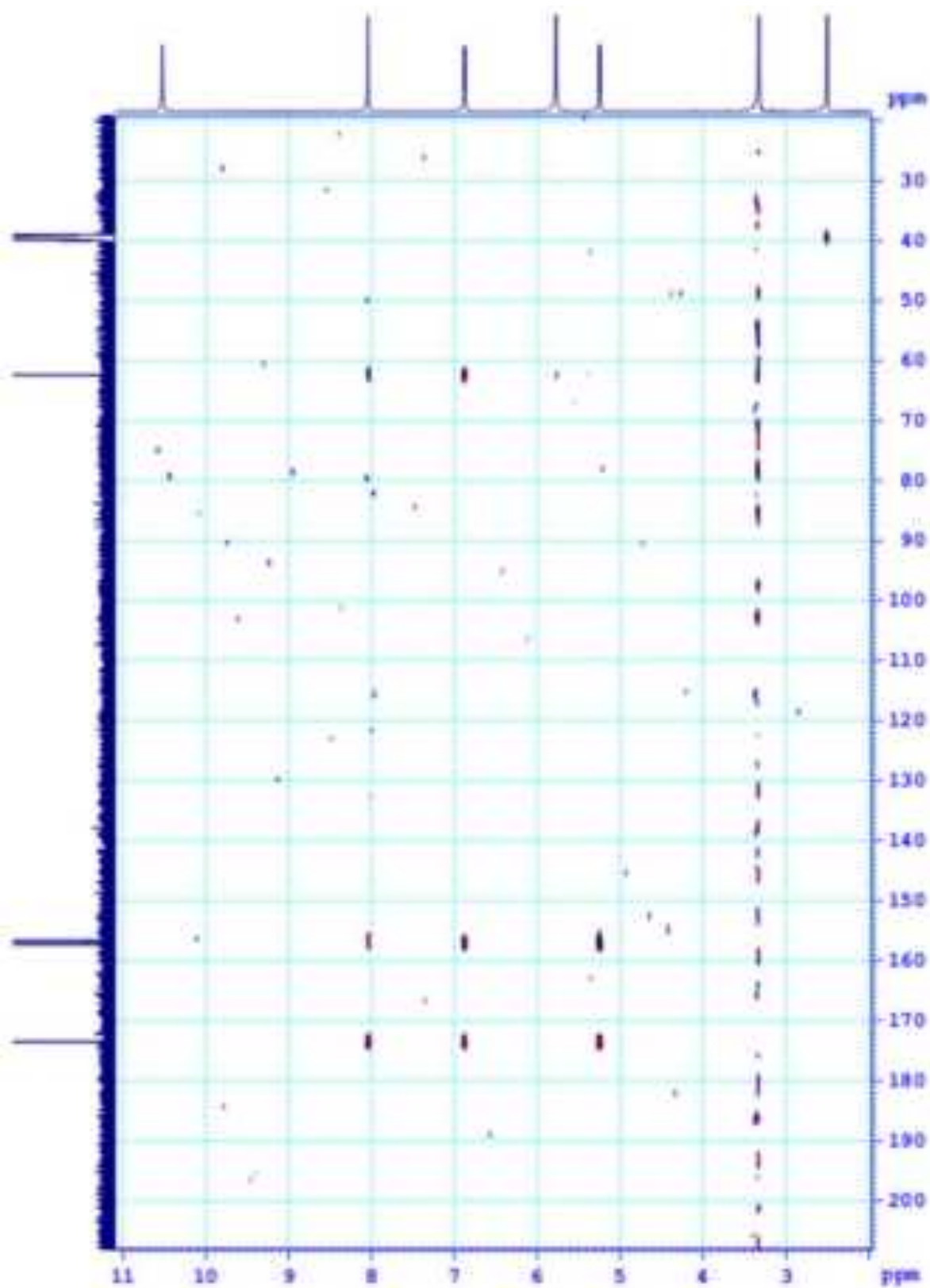




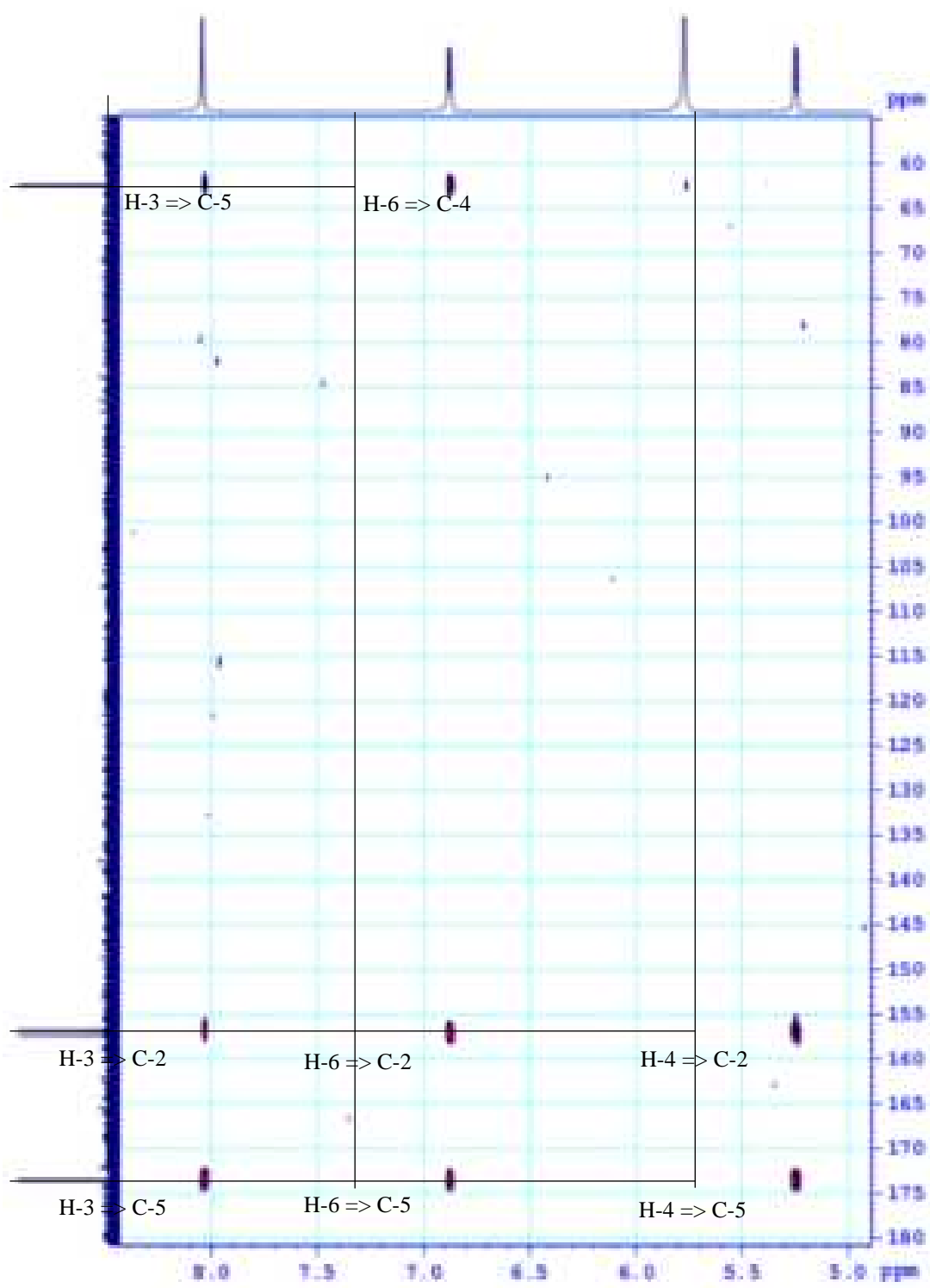
**Figure S16:** HSQC spectrum of compound **3** (allatonin)



**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> (DMSO- <i>d</i> <sub>6</sub> )		(+)-Catechin (DMSO- <i>d</i> <sub>6</sub> ) [31]	
	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (150 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> 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)

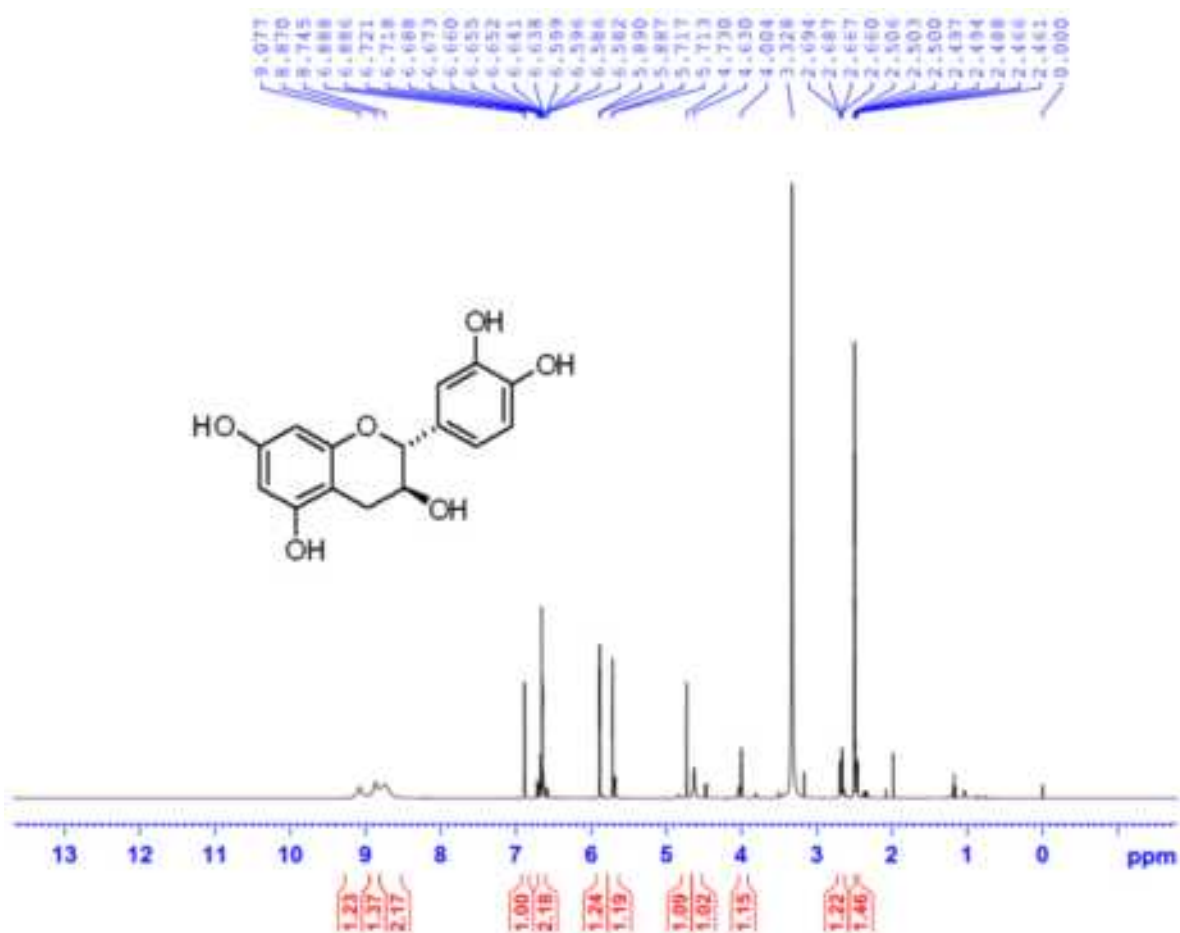


Figure S20:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 4 ((+)-catechin)

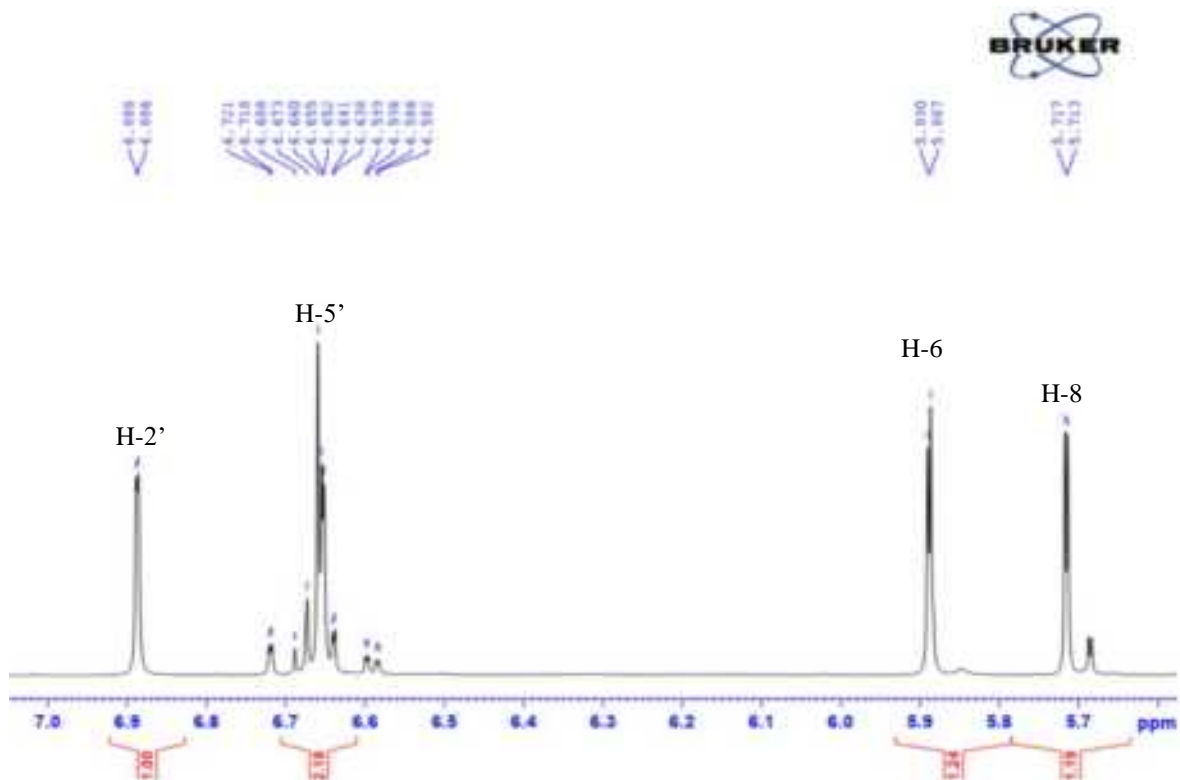
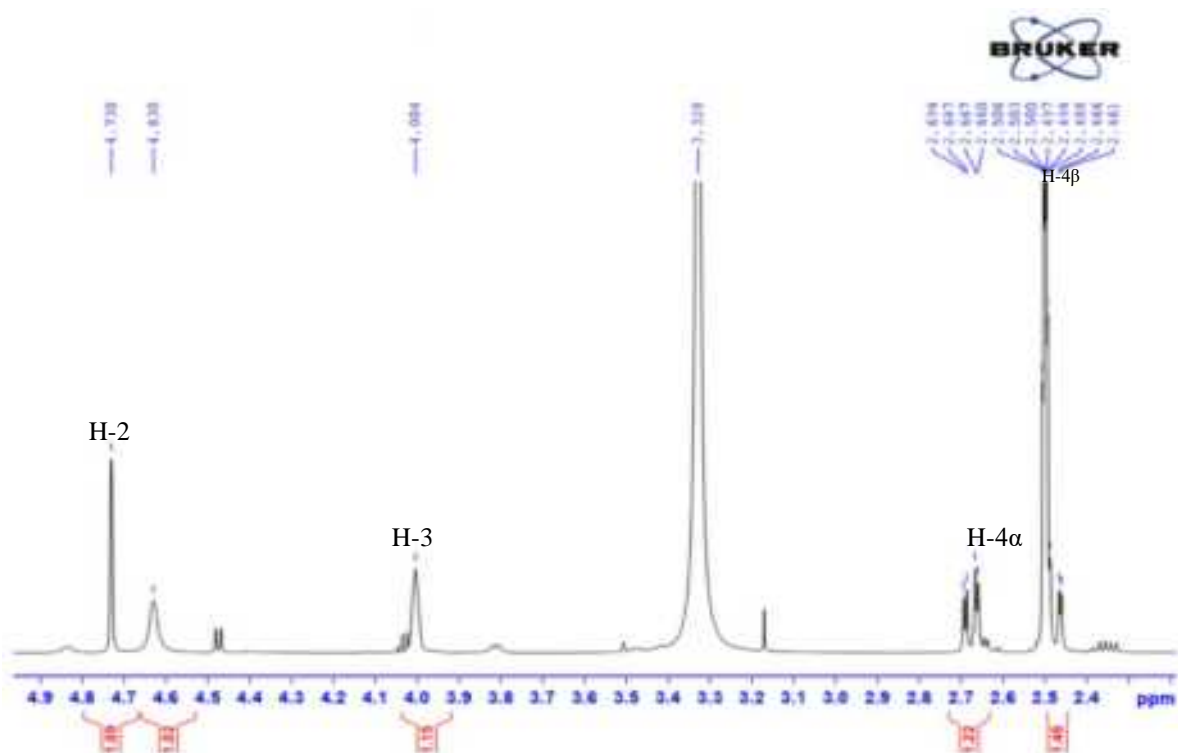
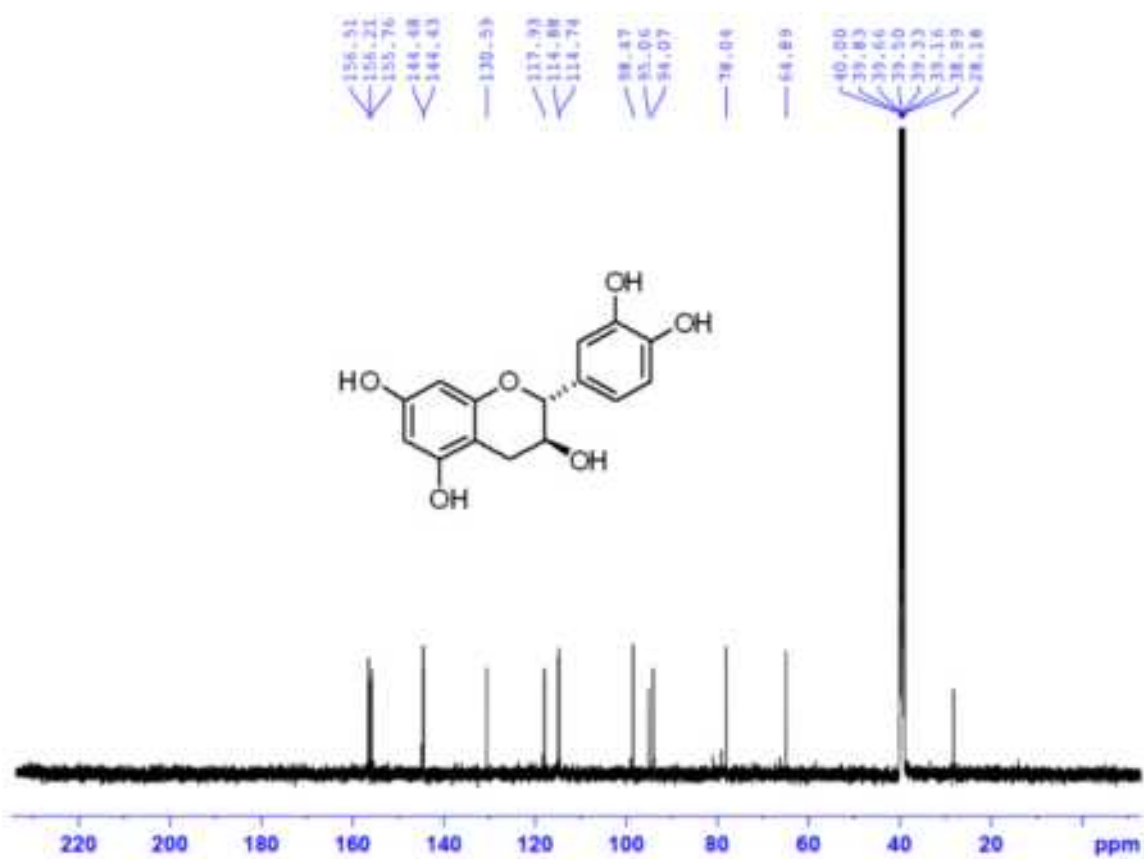


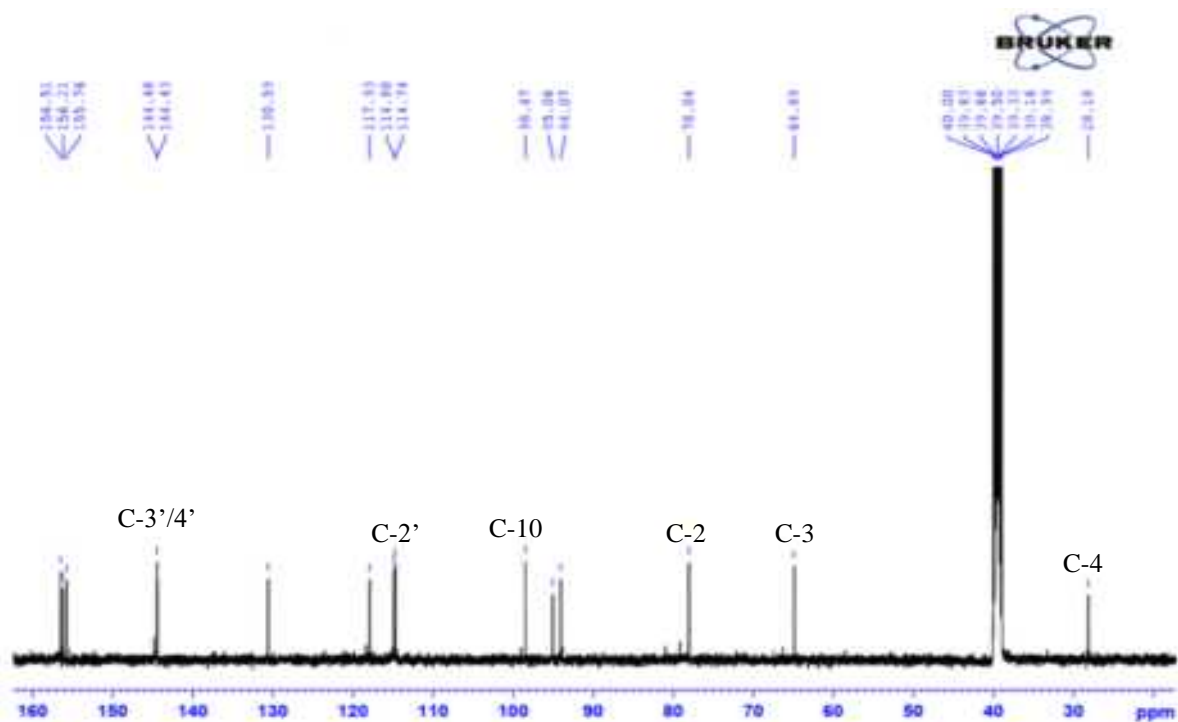
Figure S21:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 4 ((+)-catechin) (from  $\delta_{\text{H}}$  5.6 ppm to  $\delta_{\text{H}}$  7.0 ppm)



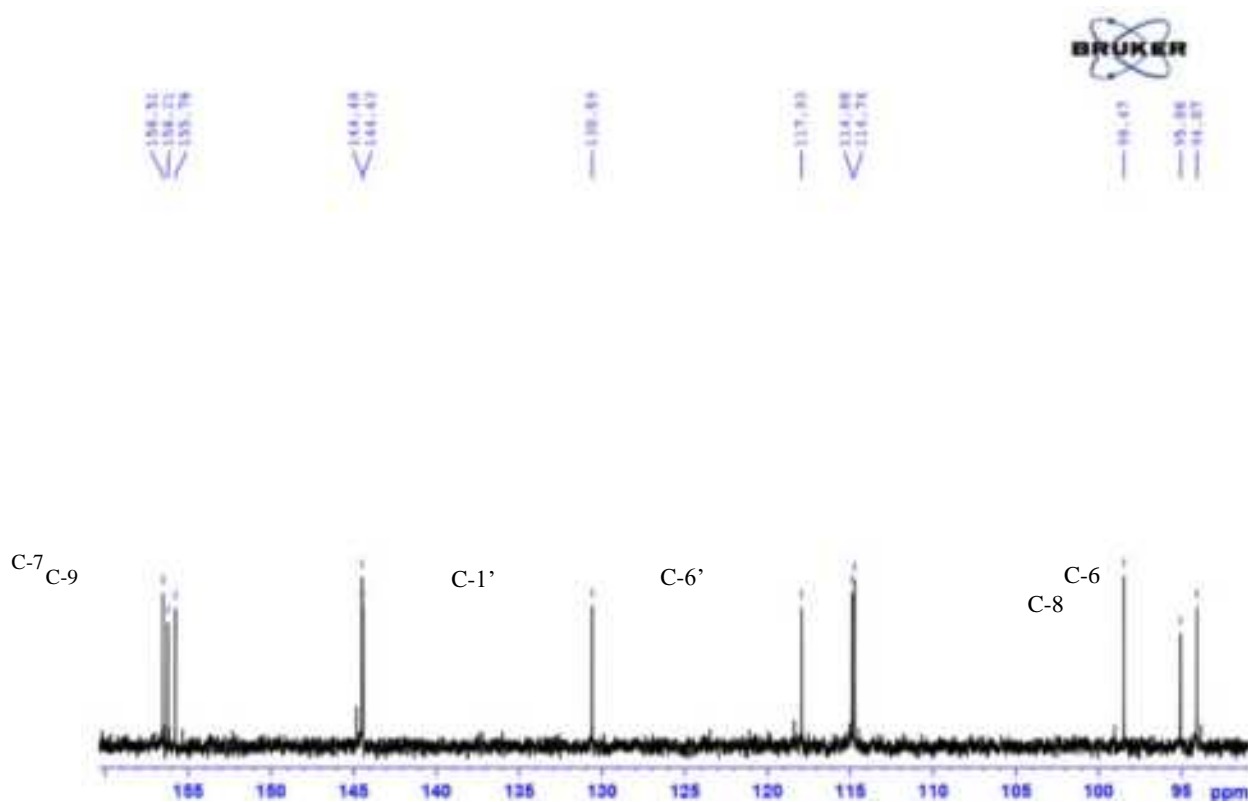
**Figure S22:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **4** ((+)-catechin) (from  $\delta_{\text{H}}$  2.3 ppm to  $\delta_{\text{H}}$  4.9 ppm)



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

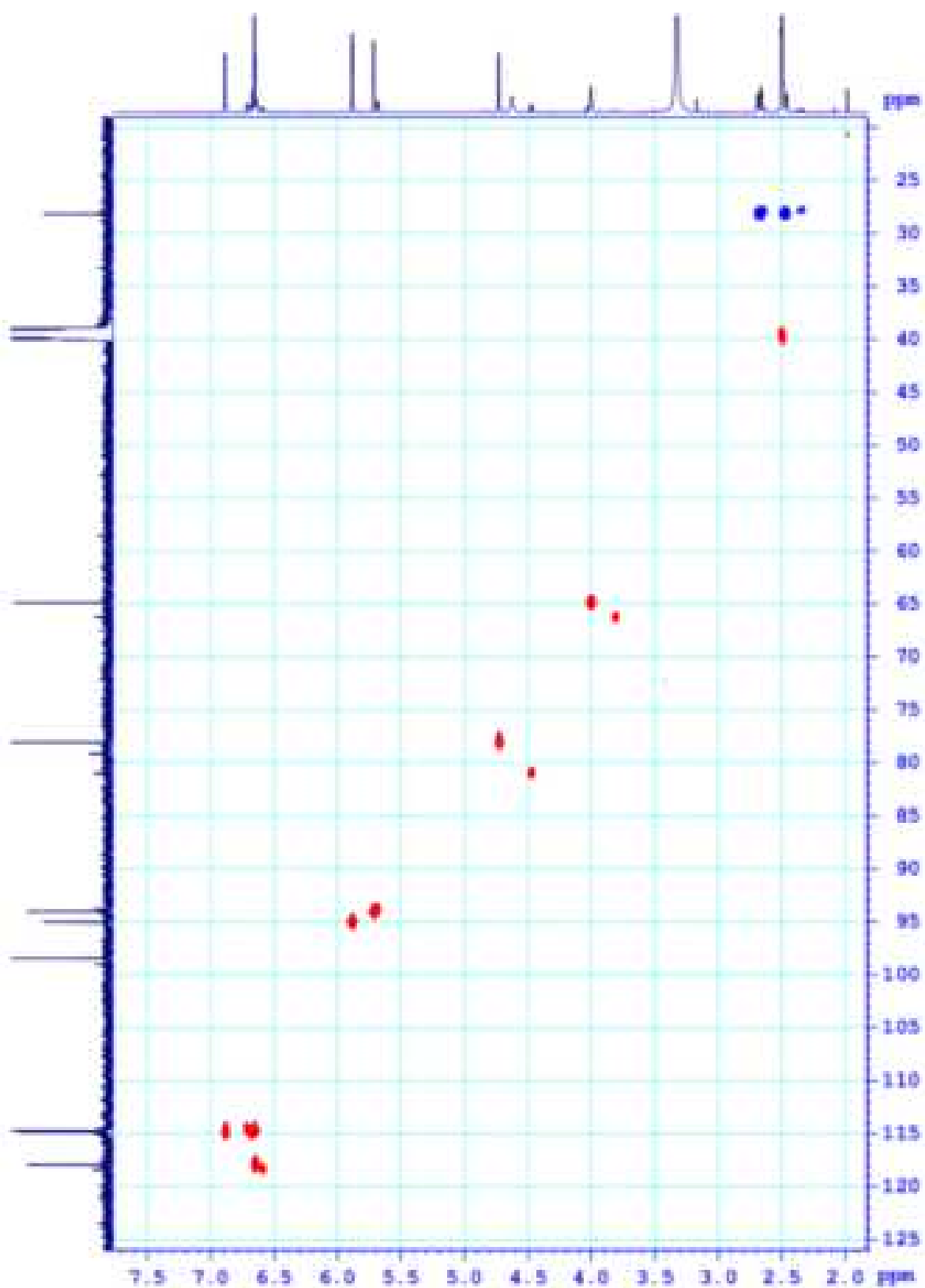


**Figure S24:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **4** ((+)-catechin) (from  $\delta_c$  20 ppm to  $\delta_c$  160 ppm)

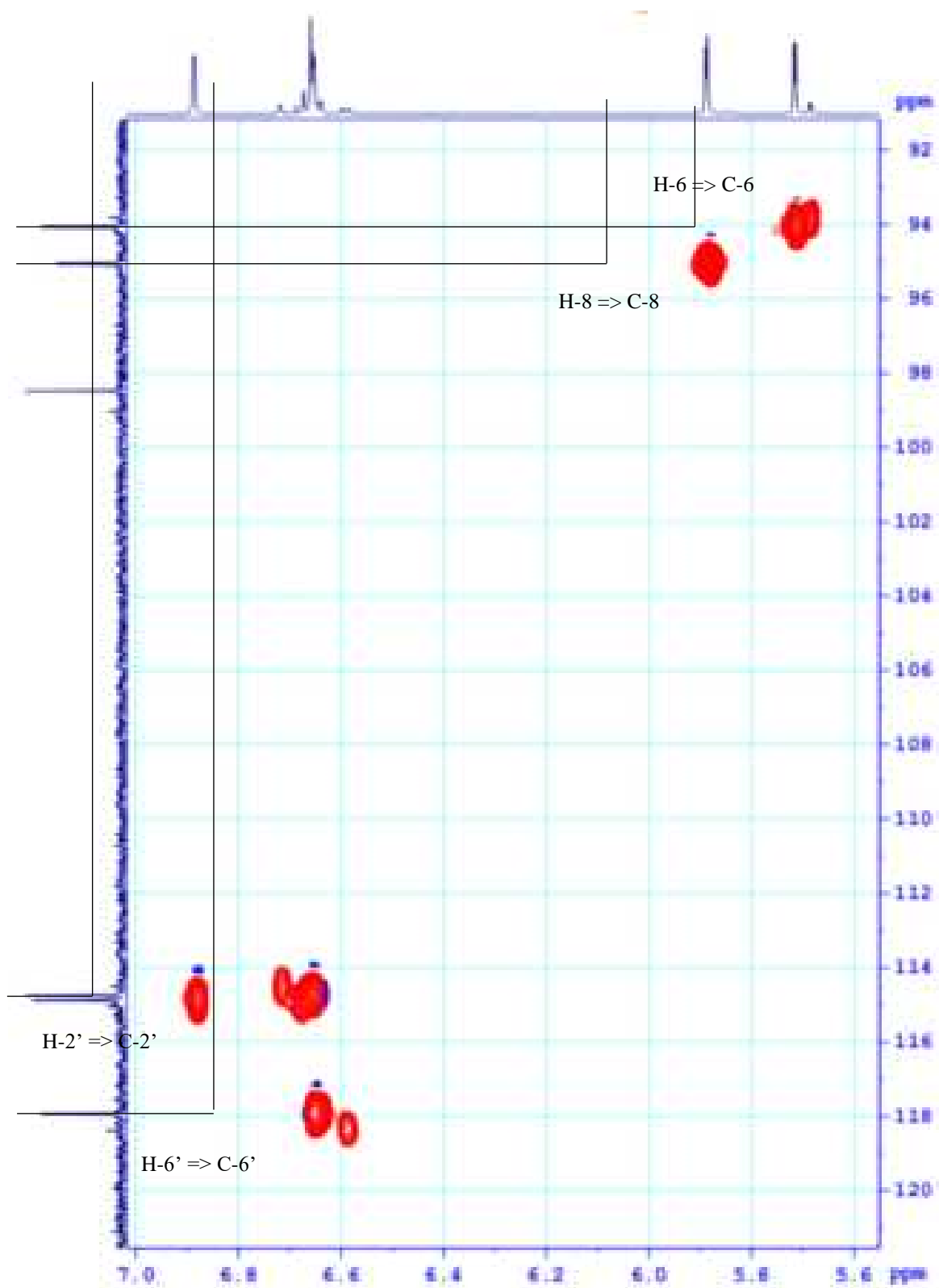


**Figure S25:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **4** ((+)-catechin) (from  $\delta_c$  90 ppm to  $\delta_c$  160 ppm)

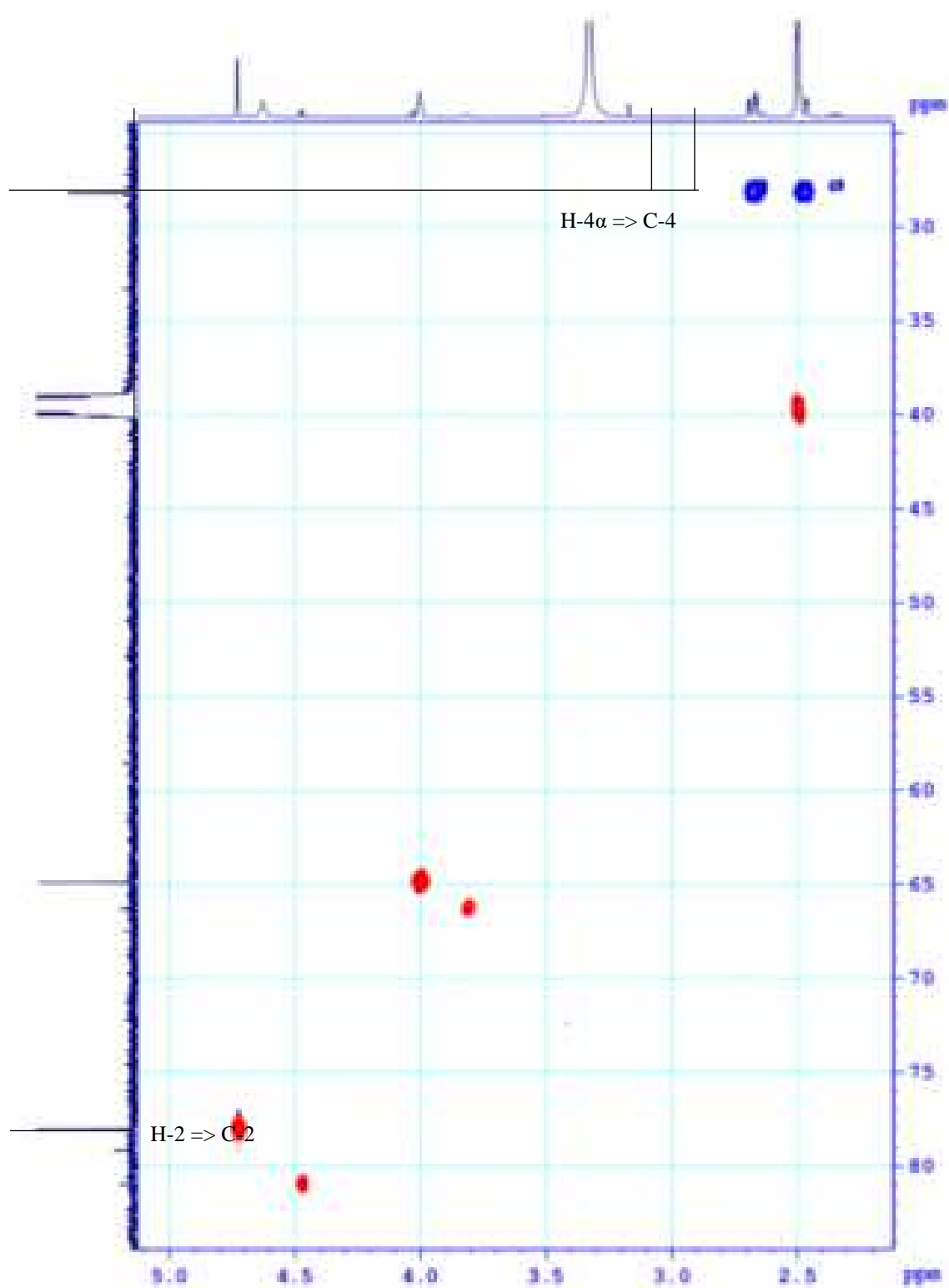




**Figure S26:** HSQC spectrum of compound **4** ((+)-catechin)

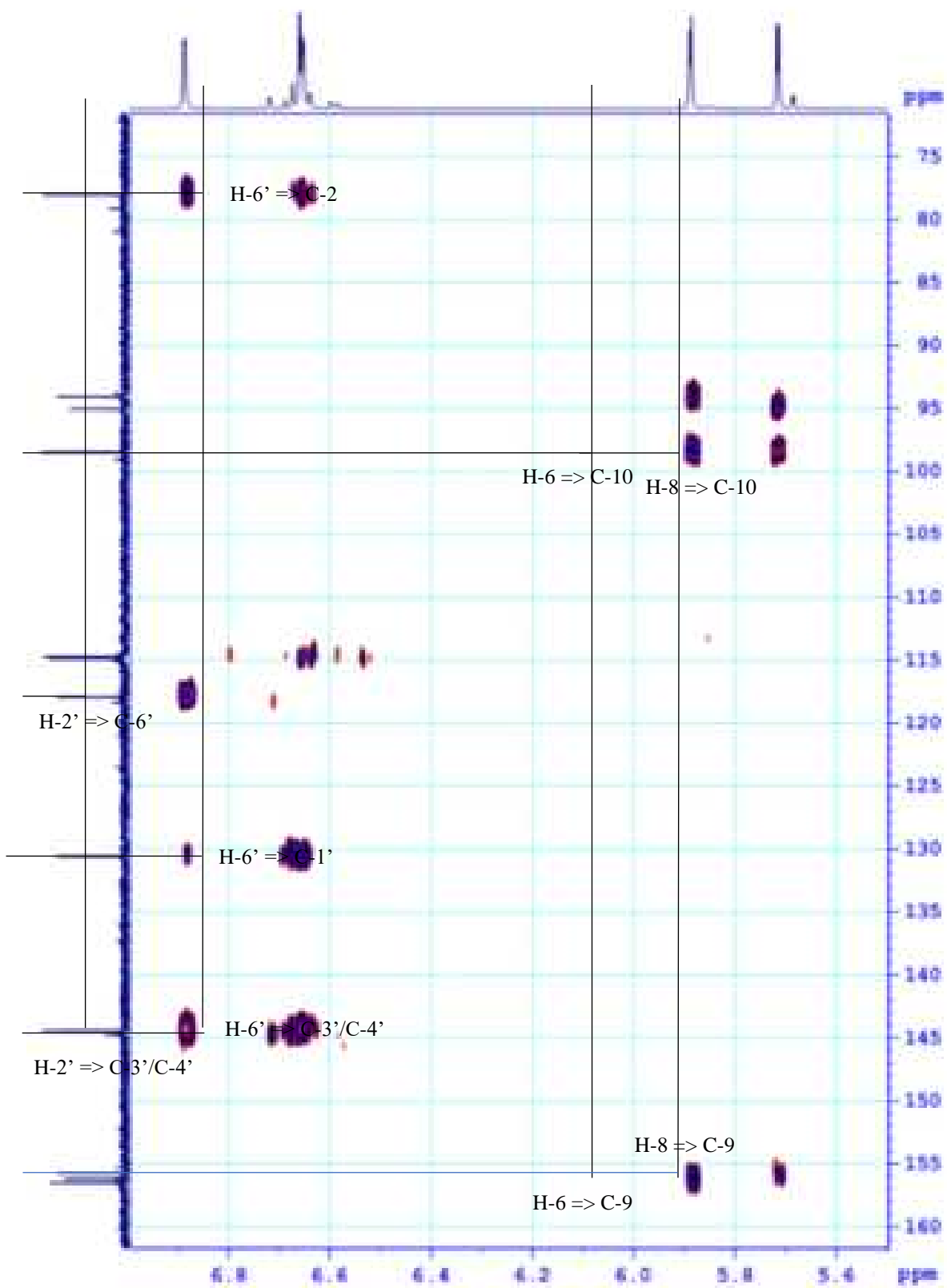


**Figure S27:** HSQC spectrum of compound 4 ((+)-catechin) (from  $\delta_{\text{C}}$  92 ppm to  $\delta_{\text{C}}$  120 ppm)

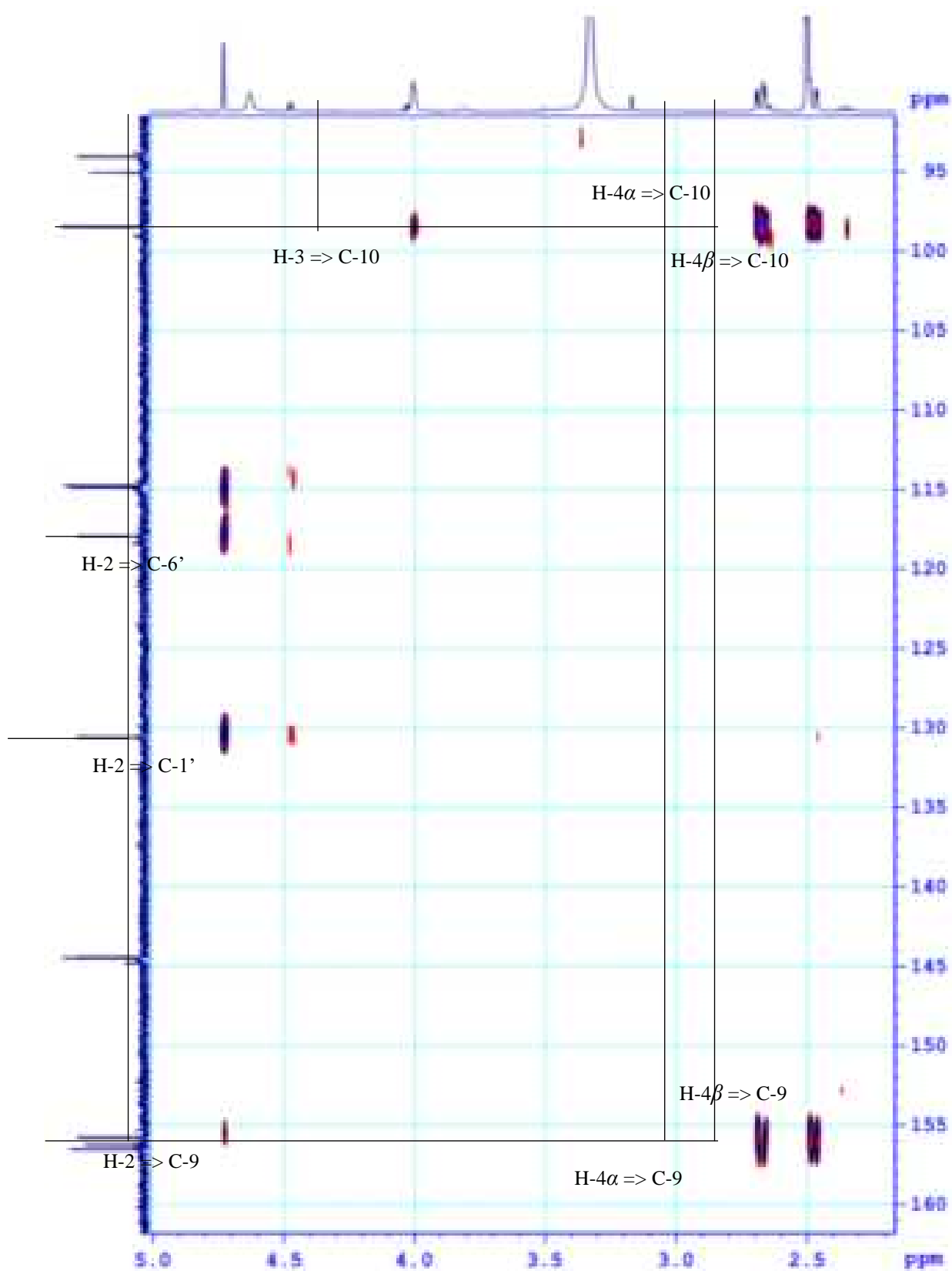


**Figure S28:** HSQC spectrum of compound **4** ((+)-catechin) (from  $\delta_{\text{C}}$  20 ppm to  $\delta_{\text{C}}$  90 ppm)

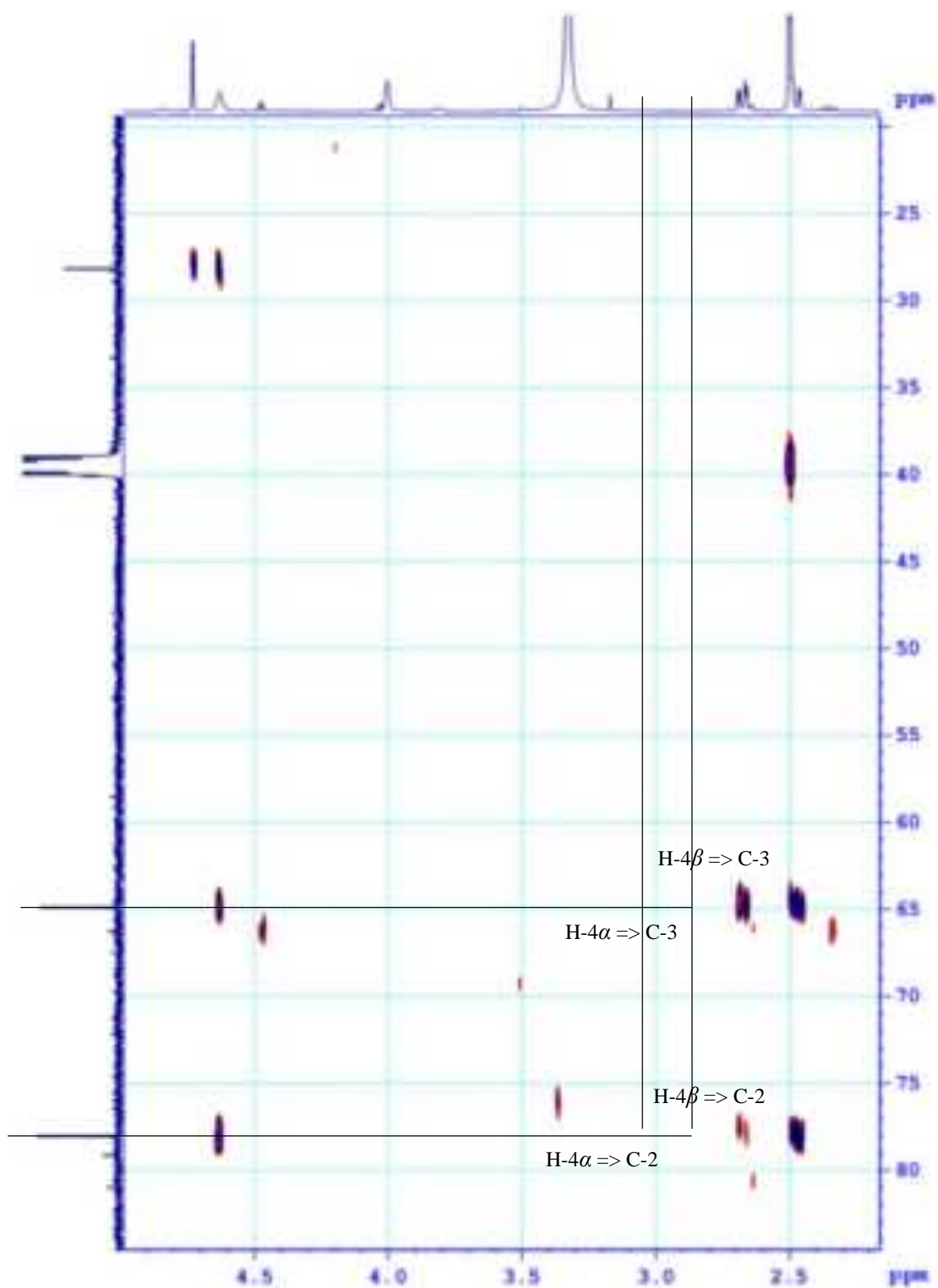




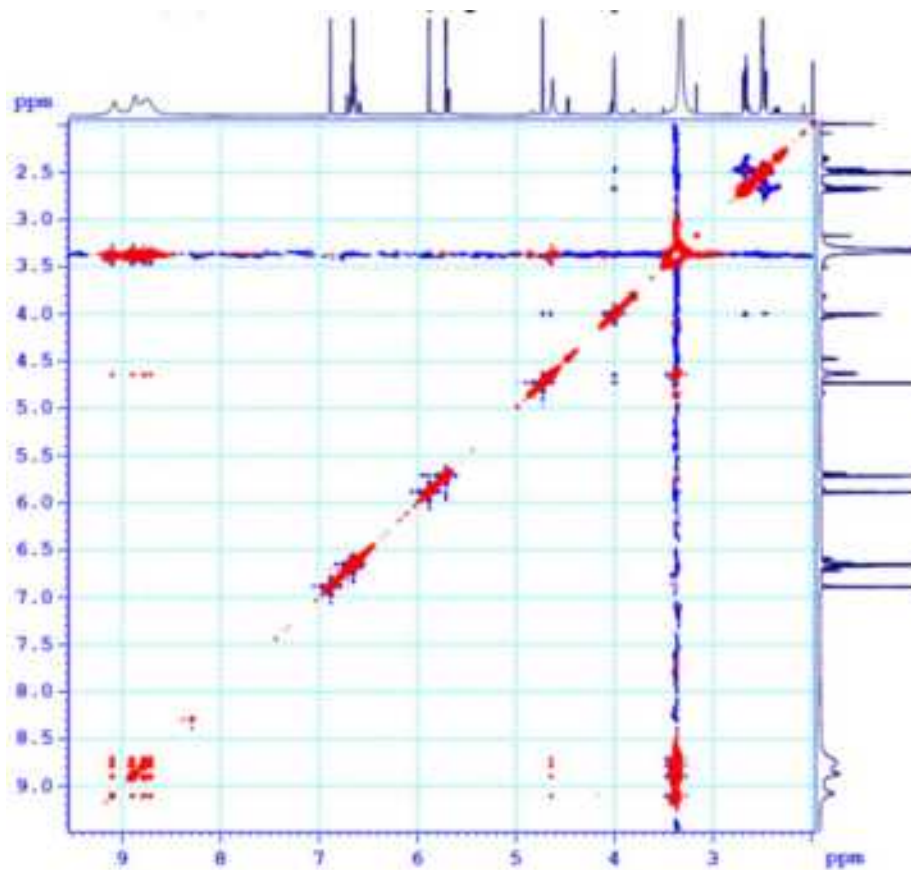
**Figure S30:** HMBC spectrum of compound **4** ((+)-catechin) (from  $\delta_C$  75 ppm to  $\delta_C$  160 ppm)



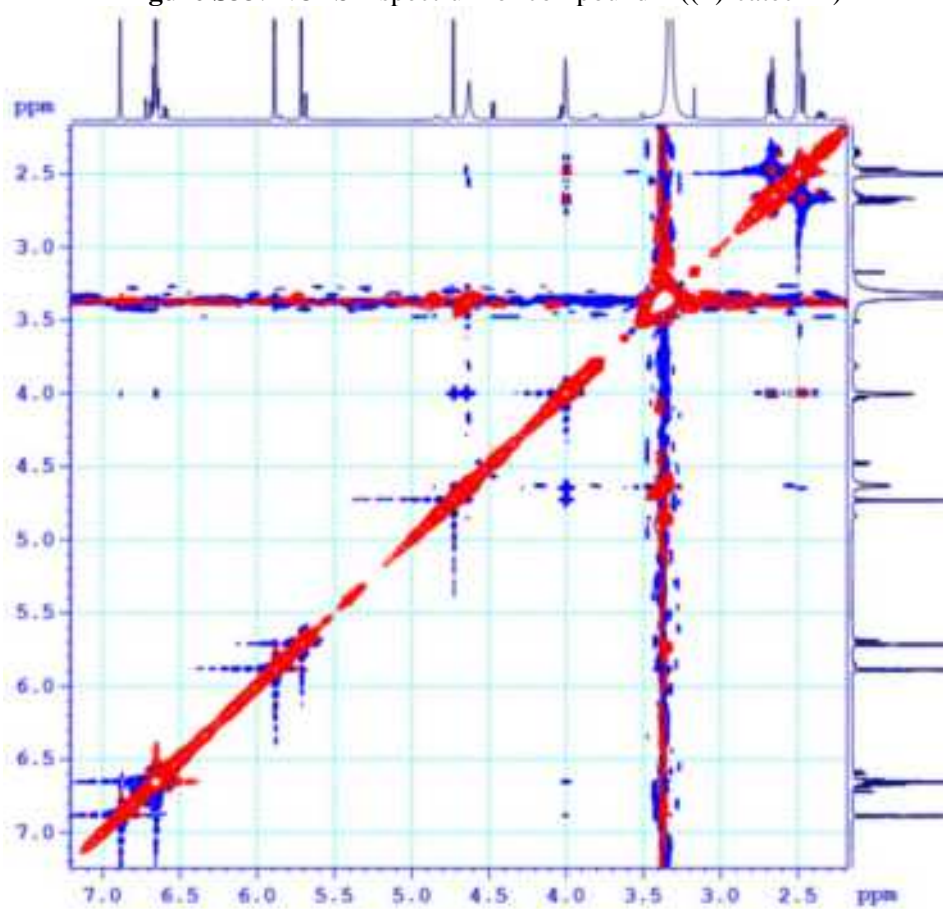
**Figure S31:** HMBC spectrum of compound **4** ((+)-catechin) (from  $\delta_C$  90 ppm to  $\delta_C$  160 ppm)



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

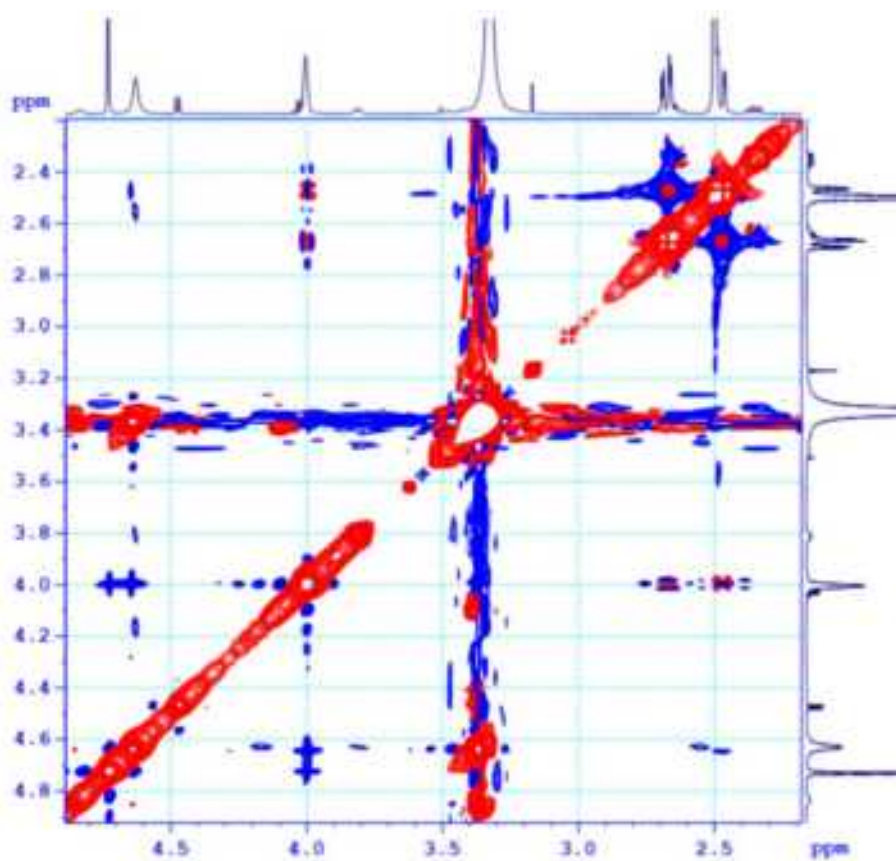


**Figure S33:** NOESY spectrum of compound **4** ((+)-catechin)



**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  $\delta_{\text{H}}$  2.4 ppm to  $\delta_{\text{H}}$  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) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> 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)

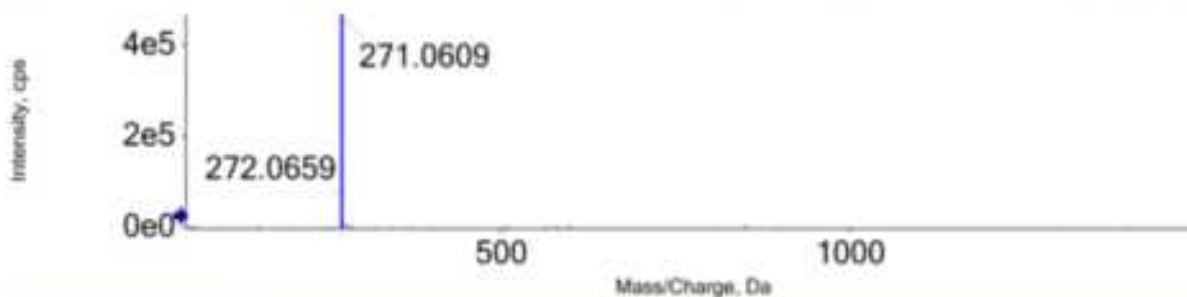
## ANALYSIS REPORT

### 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>g</sub> QTOF

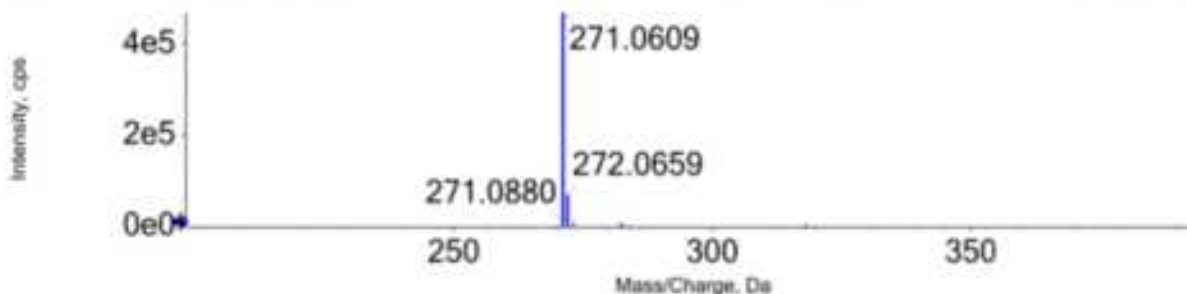
### Full mass spectrum

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



### Expanded spectrum

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



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

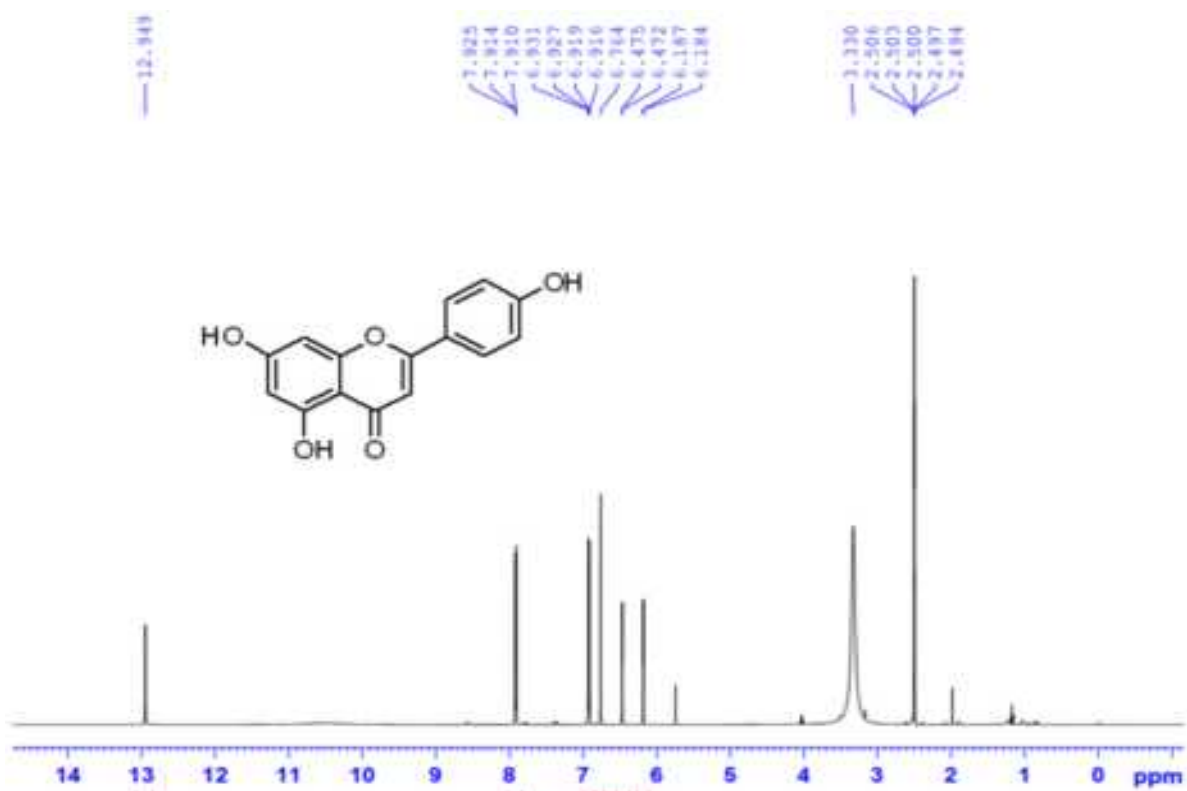


Figure S37:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **5** (apigenin)

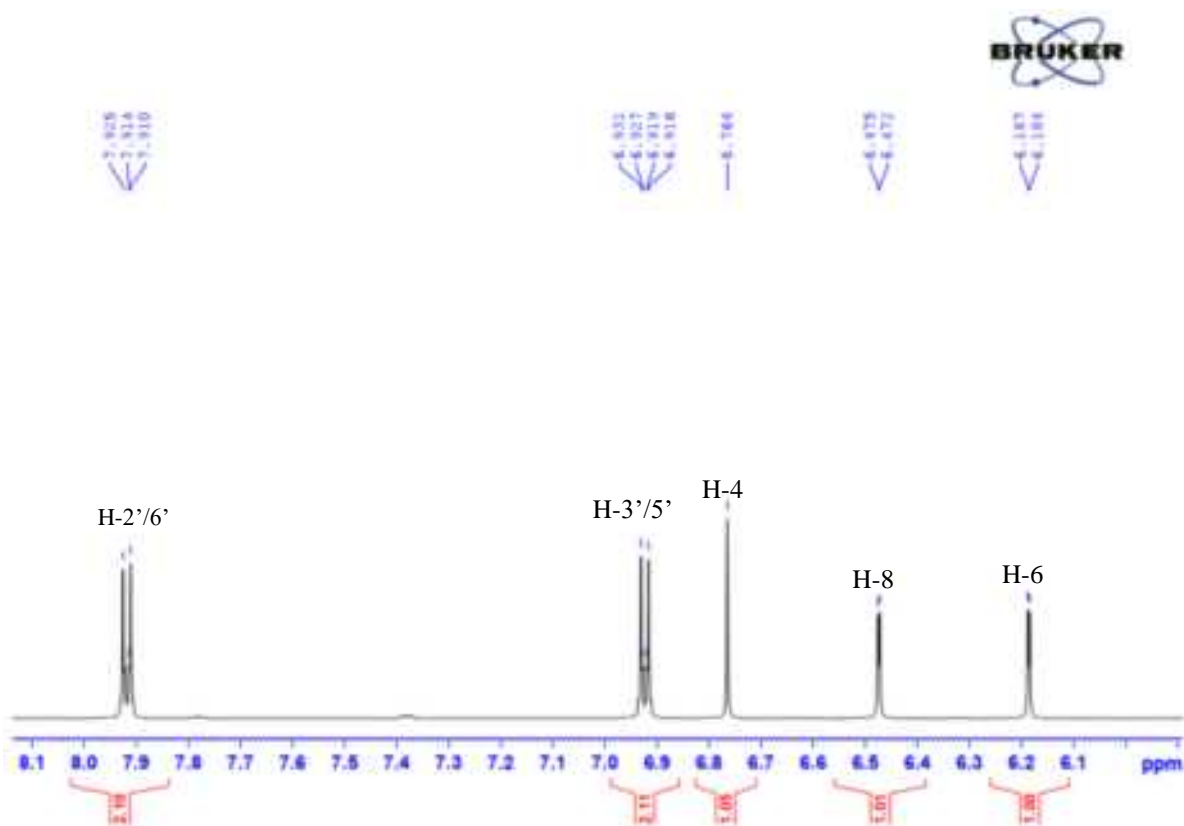


Figure S38:  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **5** (apigenin) (from  $\delta_{\text{H}}$  6.0 ppm to  $\delta_{\text{H}}$  8.1 ppm)

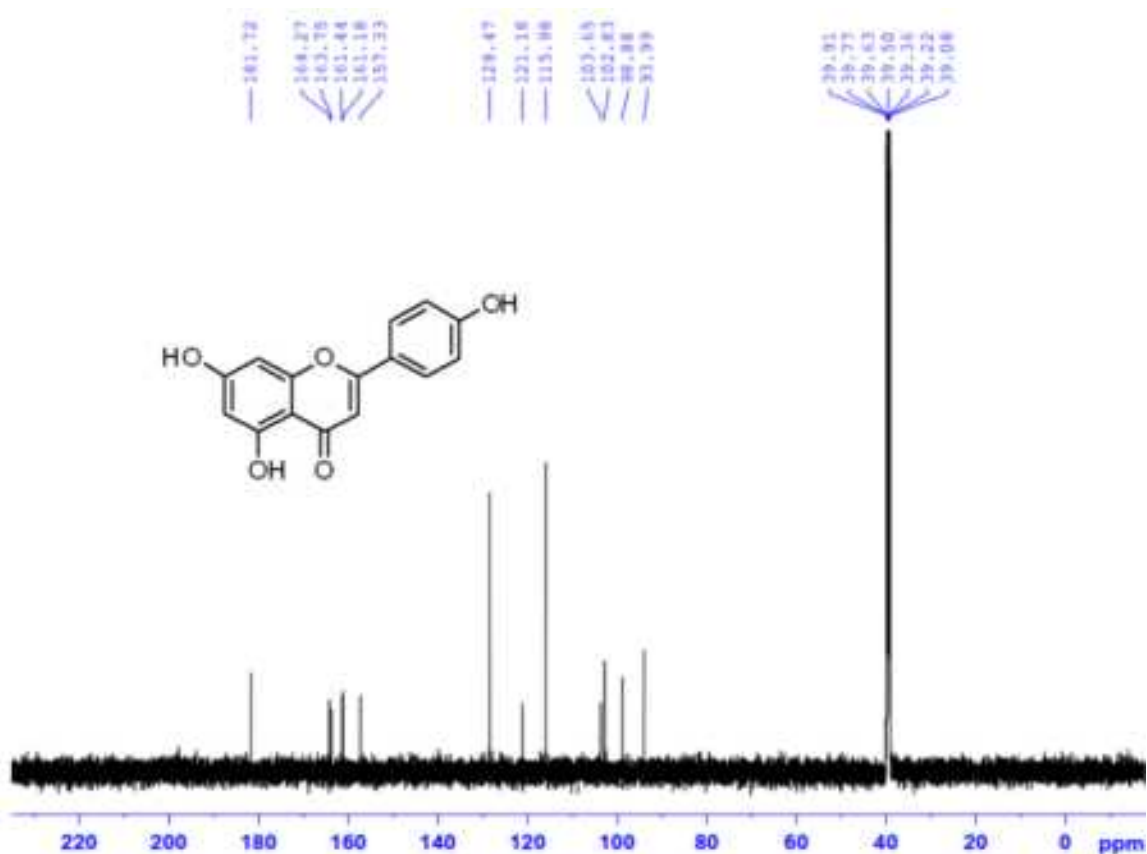


Figure S39:  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 5 (apigenin)

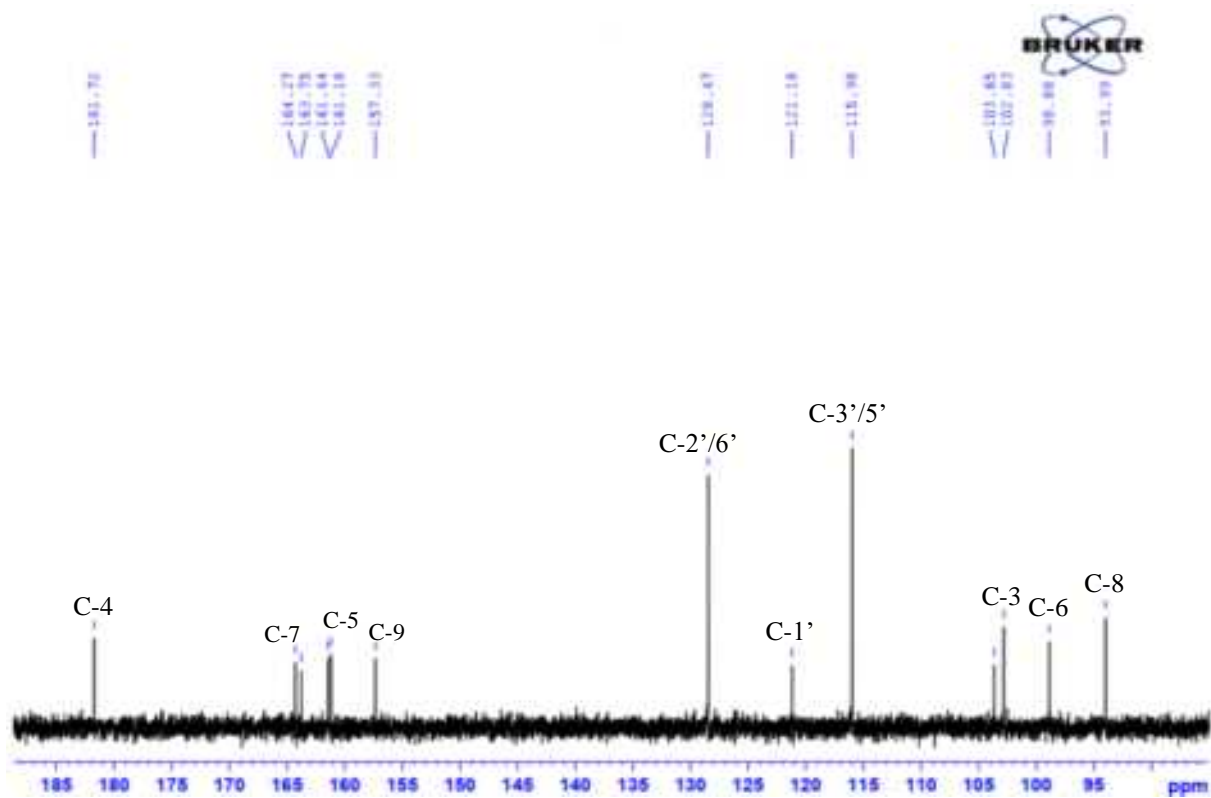


Figure S40:  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 5 (apigenin) (from  $\delta_{\text{C}}$  90 ppm to  $\delta_{\text{C}}$  185 ppm)

**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) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> 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)

## 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>	X500R_QTOF

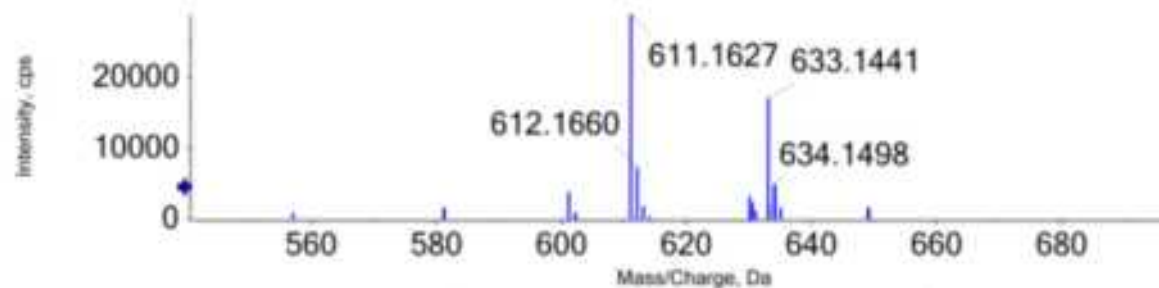
### Full mass spectrum

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



### Expanded spectrum

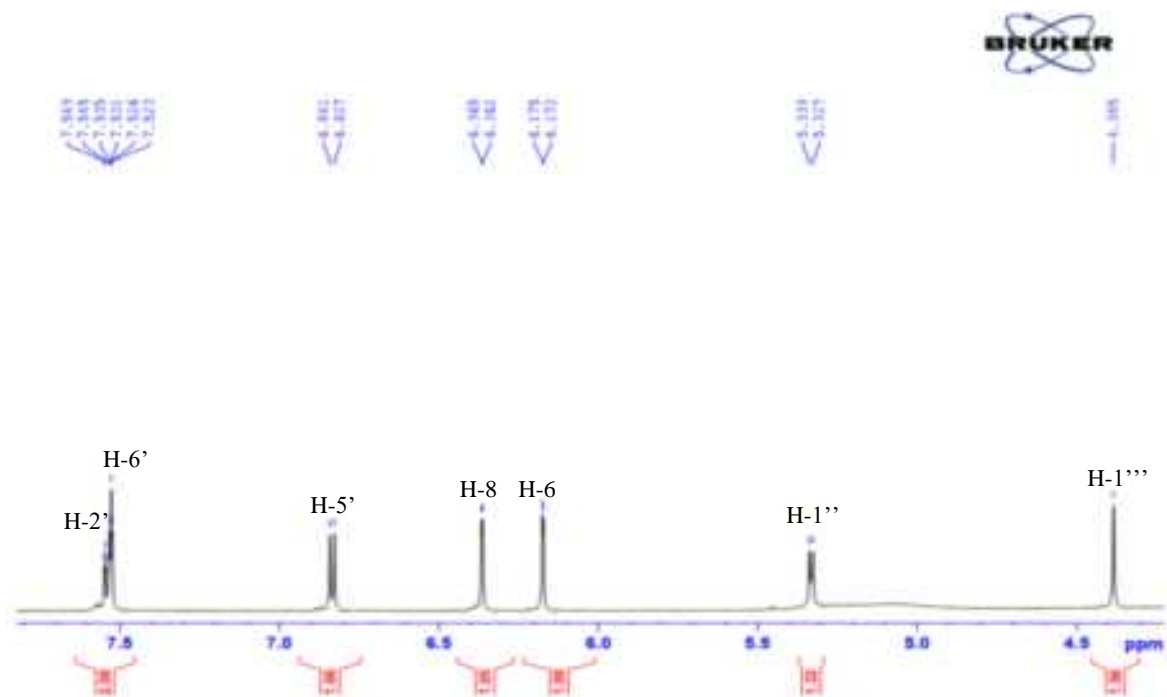
Spectrum from YEN\_SAL\_(+)ESI 2023-04-20-10-43-32.wi...se multiplier = 1.5), Gaussian smoothed (0.5 poin



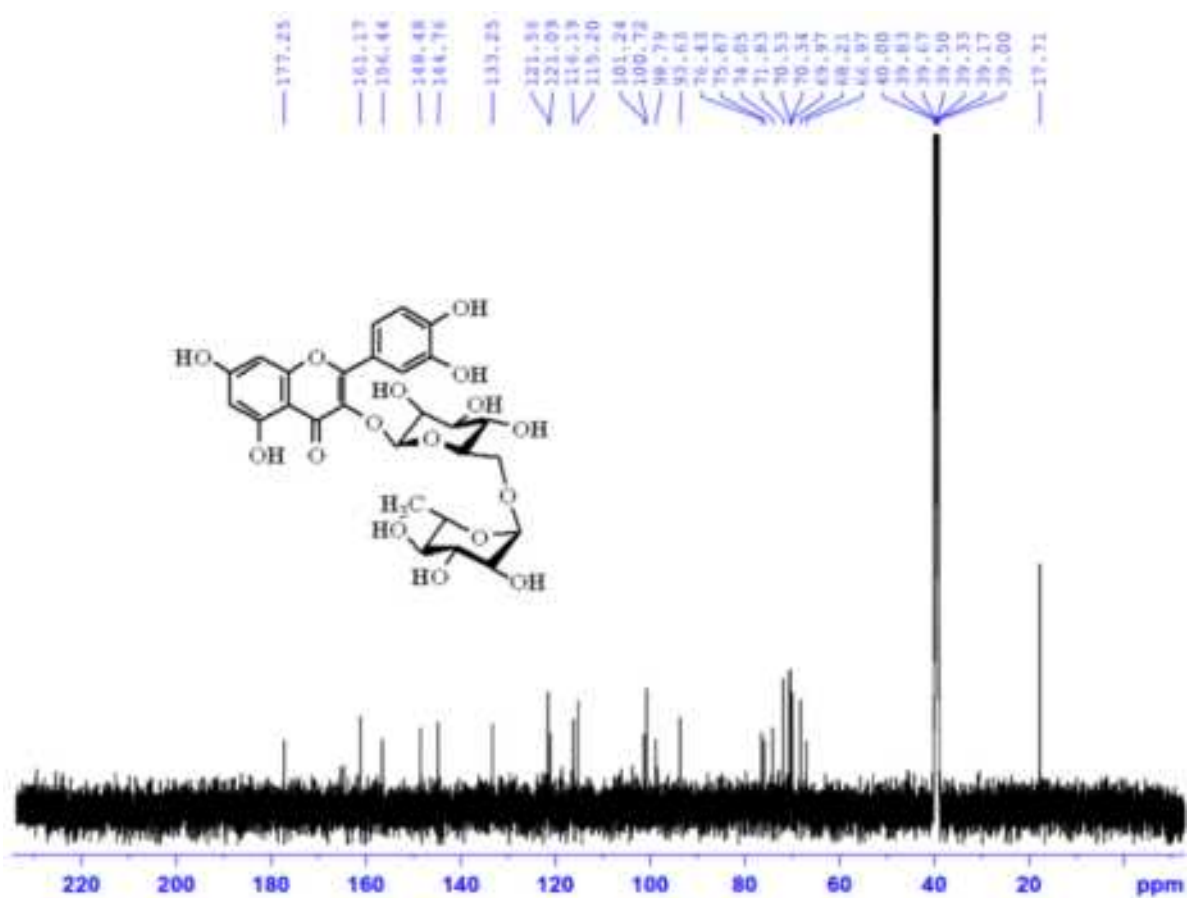
**Figure S41:** (+)ESI-MS spectrum of compound **6**



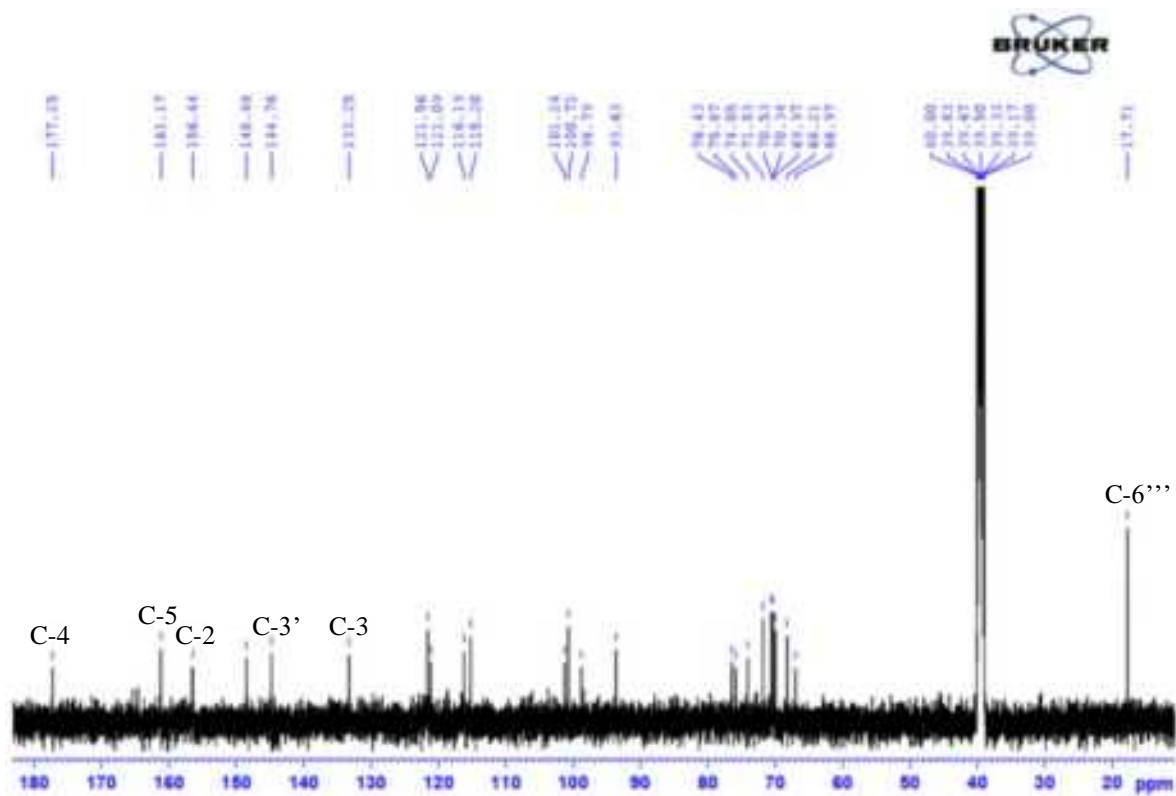




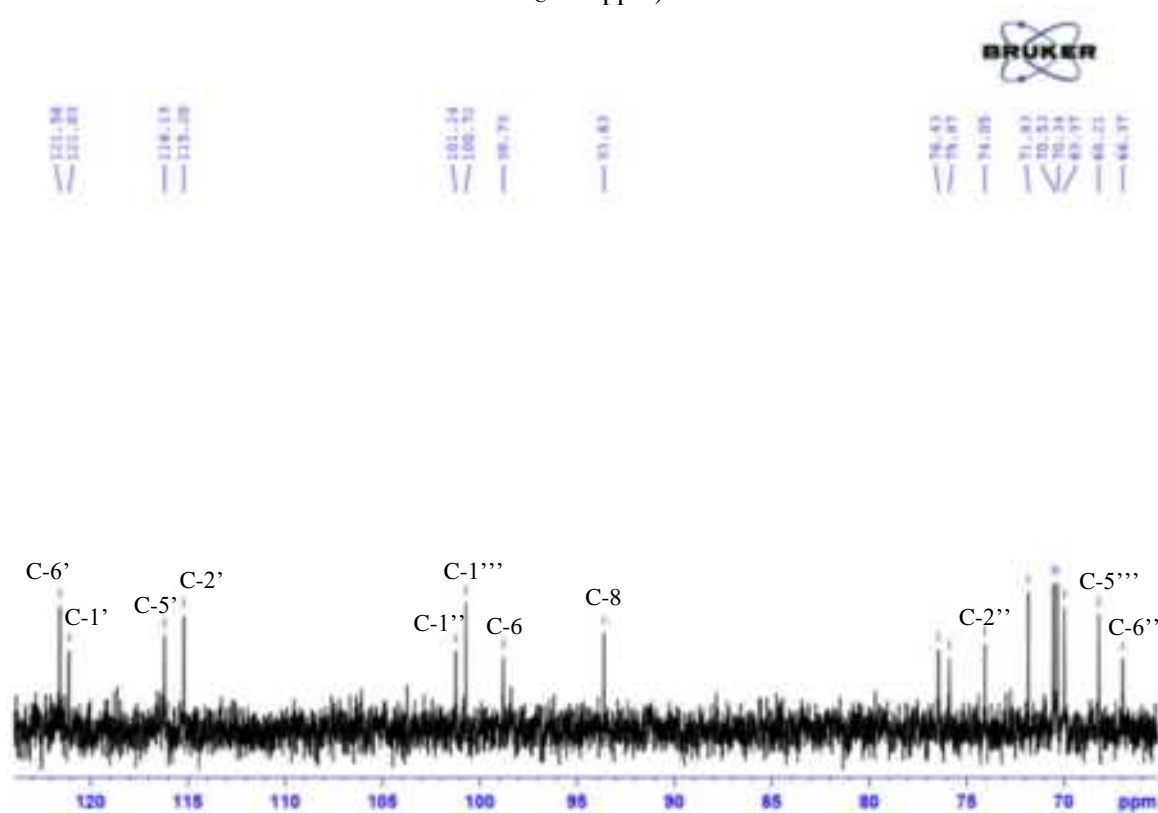
**Figure S44:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6** (rutin) (from  $\delta_{\text{H}}$  4.3 ppm to  $\delta_{\text{H}}$  7.7 ppm)



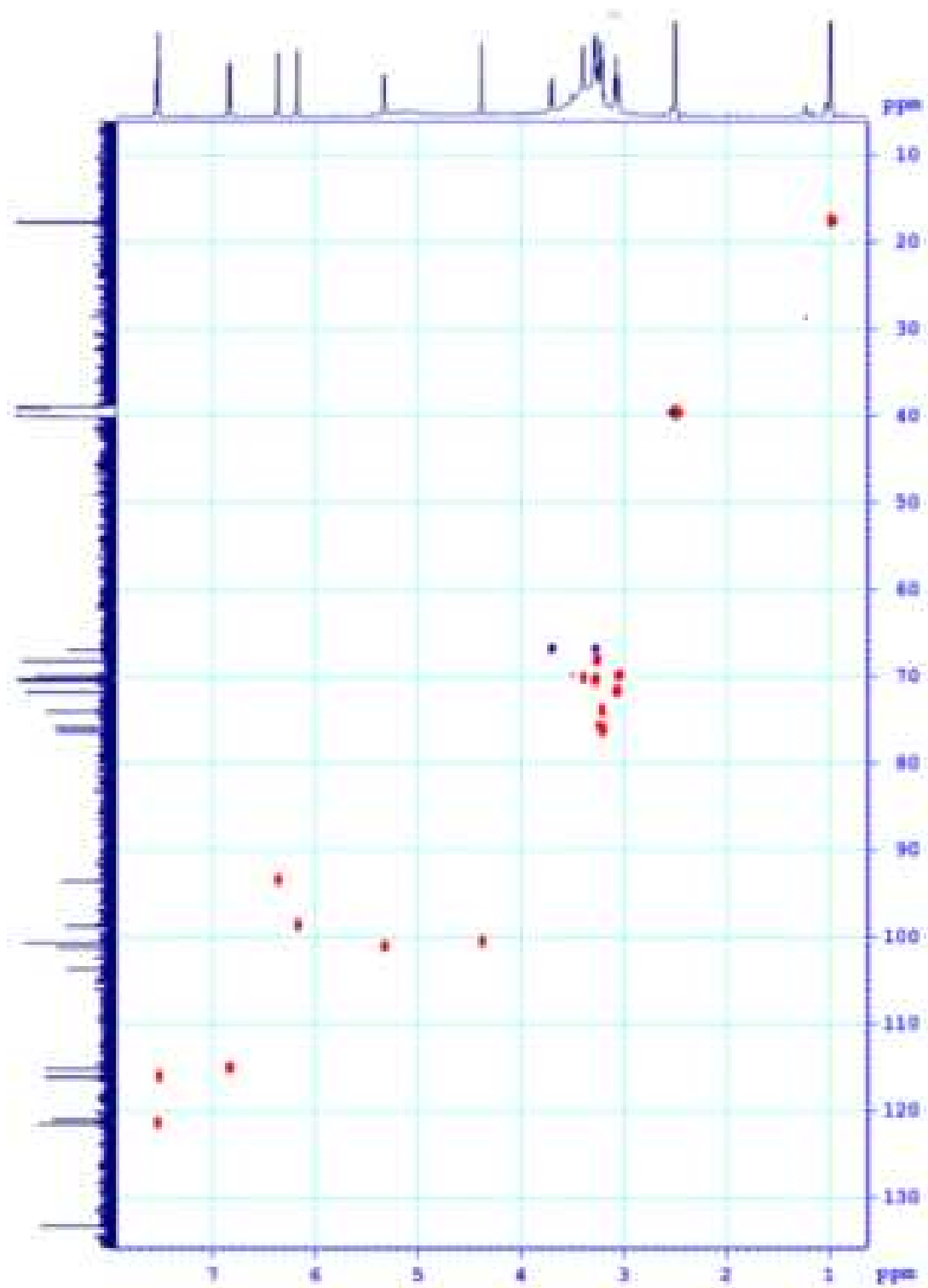
**Figure S45:**  $^{13}\text{C-NMR}$  (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6** (rutin)



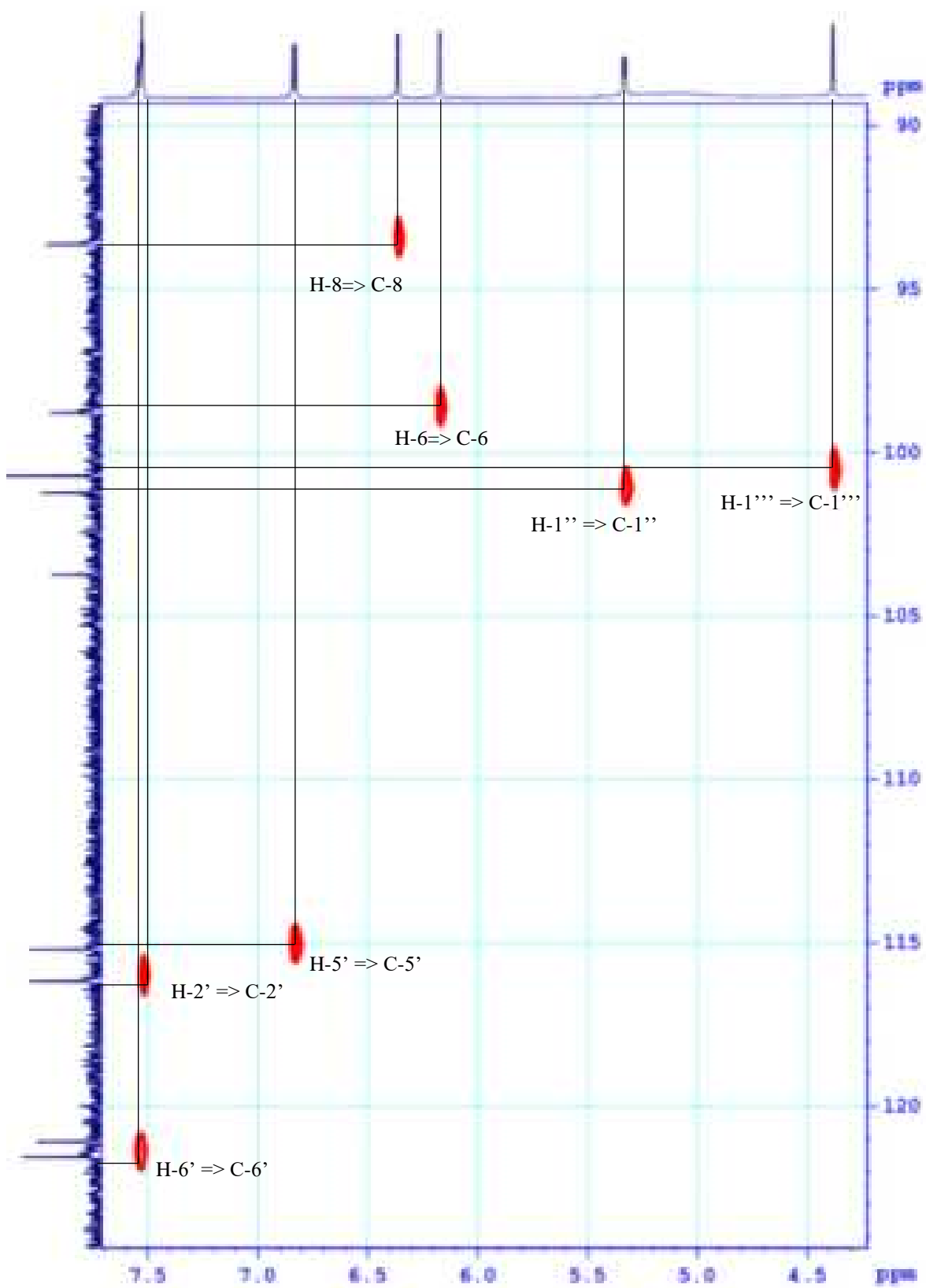
**Figure S46:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6** (rutin) (from  $\delta_{\text{C}}$  15 ppm to  $\delta_{\text{C}}$  180 ppm)



**Figure S47:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) 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)

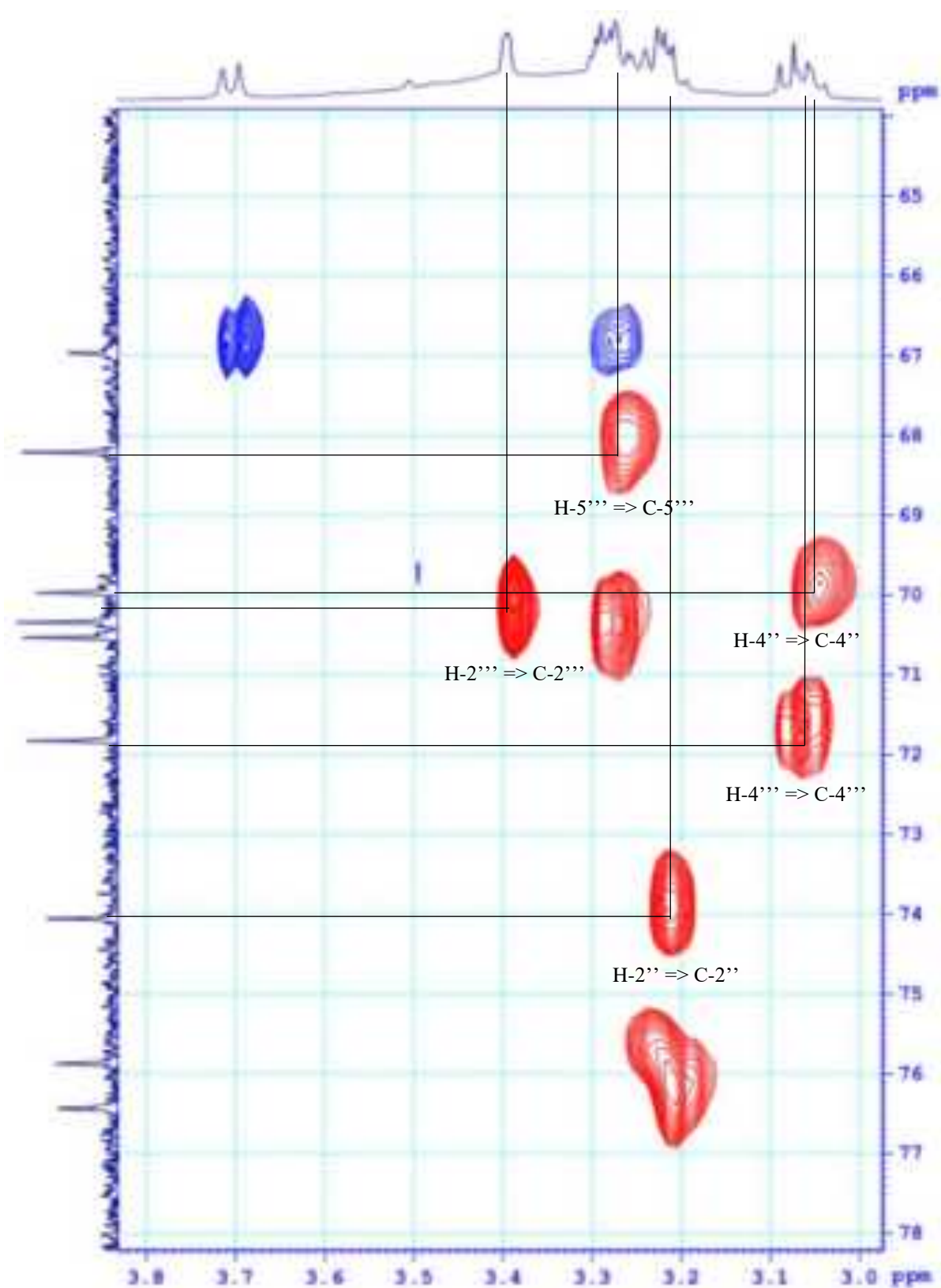


Figure S50: HSQC spectrum of compound 6 (rutin) (from  $\delta_{\text{C}}$  64 ppm to  $\delta_{\text{C}}$  78 ppm)

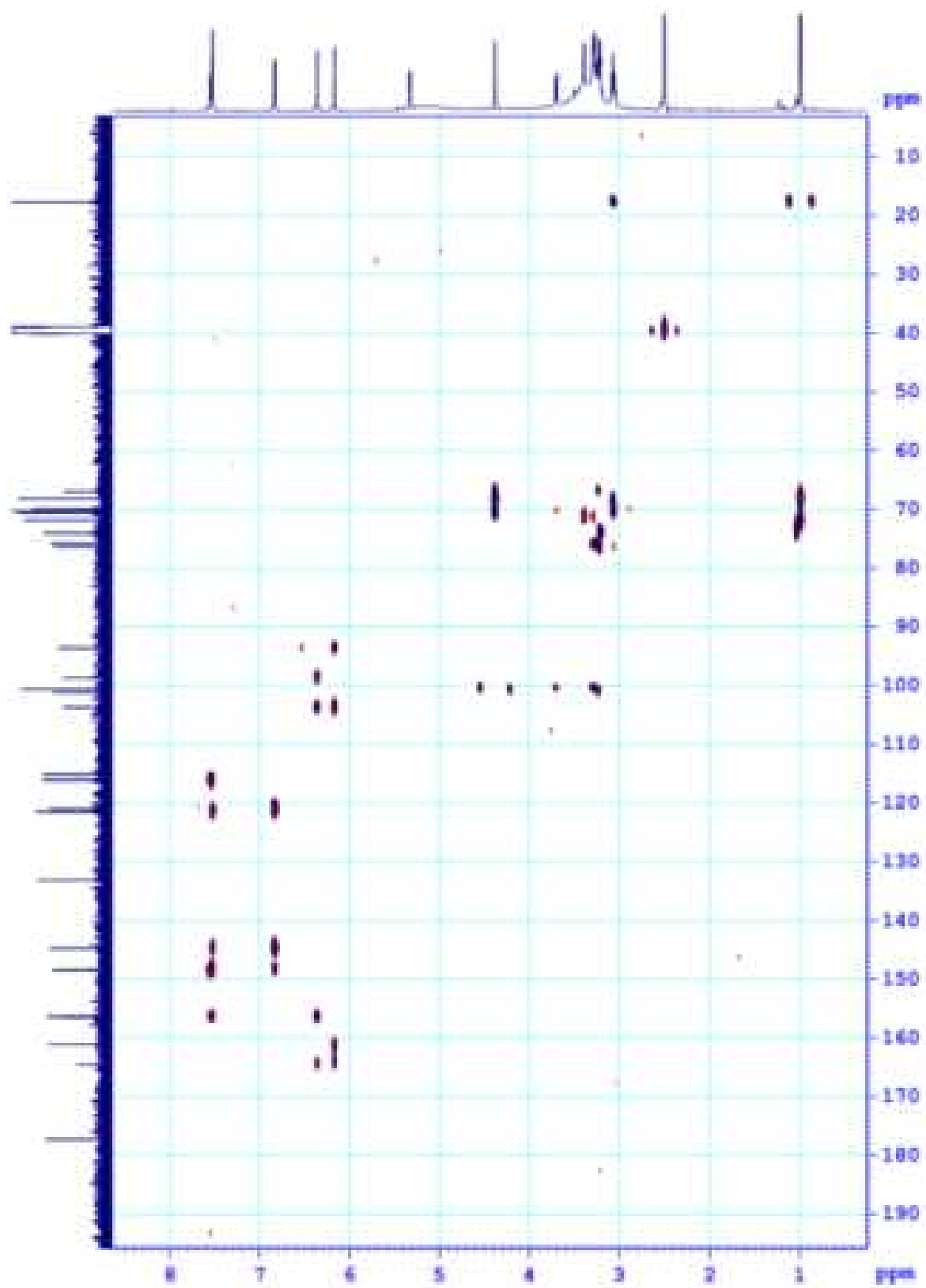


Figure S51: HMBC spectrum of compound 6 (rutin)

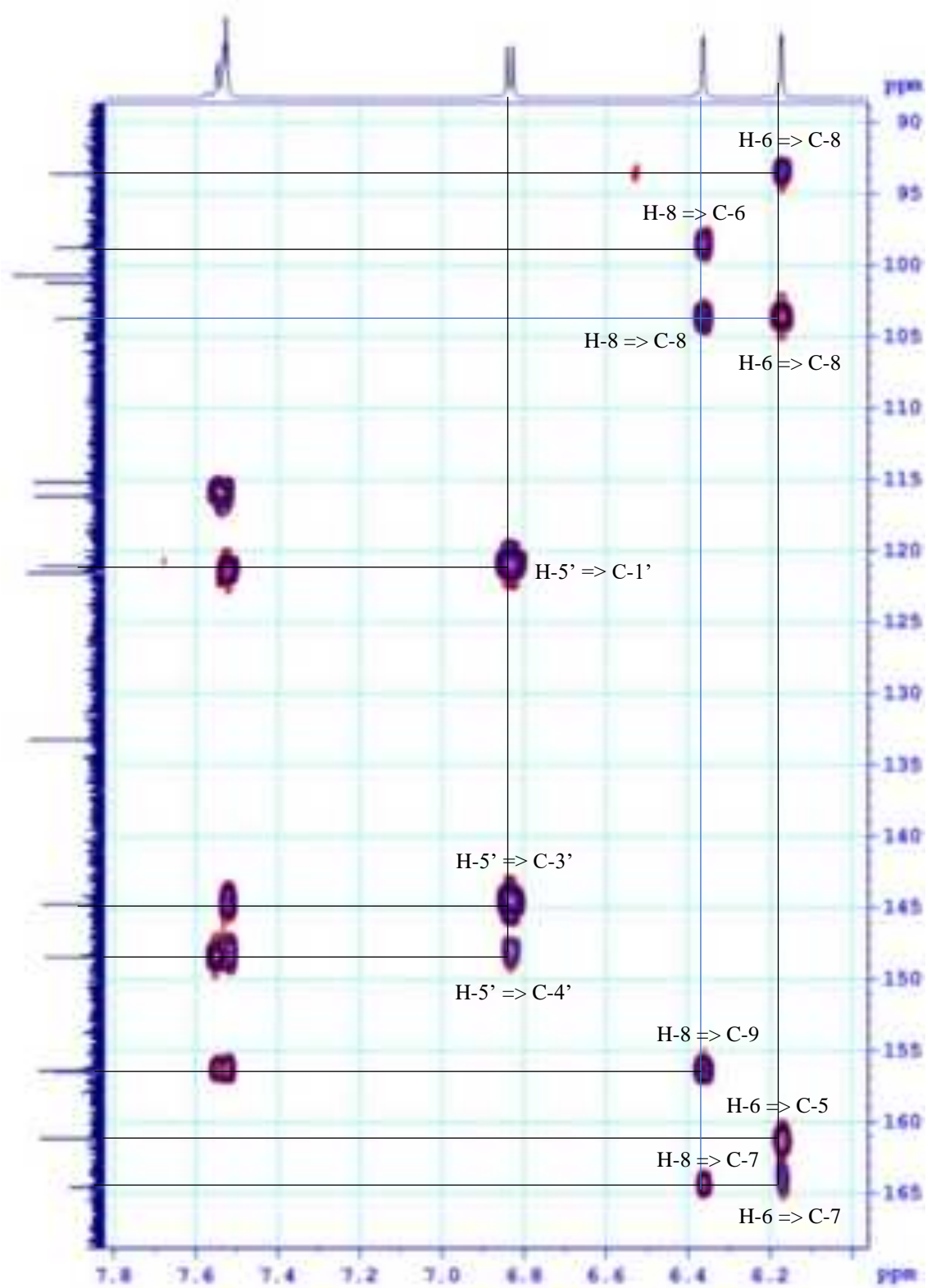


Figure S52: HMBC spectrum of compound 6 (rutin) (from  $\delta_c$  90 ppm to  $\delta_c$  165 ppm)

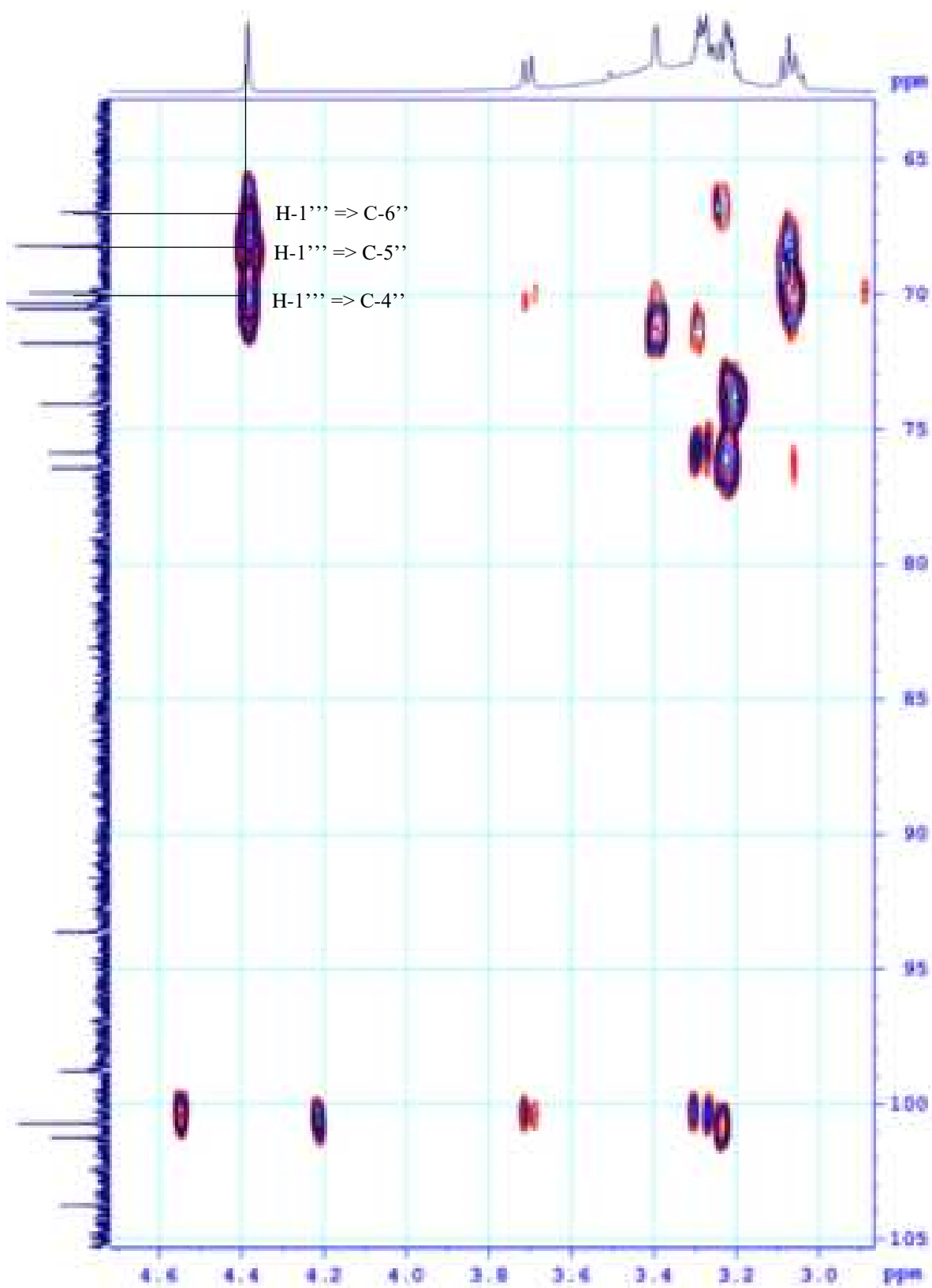


Figure S53: HMBC spectrum of compound **6** (rutin) (from  $\delta_c$  65 ppm to  $\delta_c$  105 ppm)



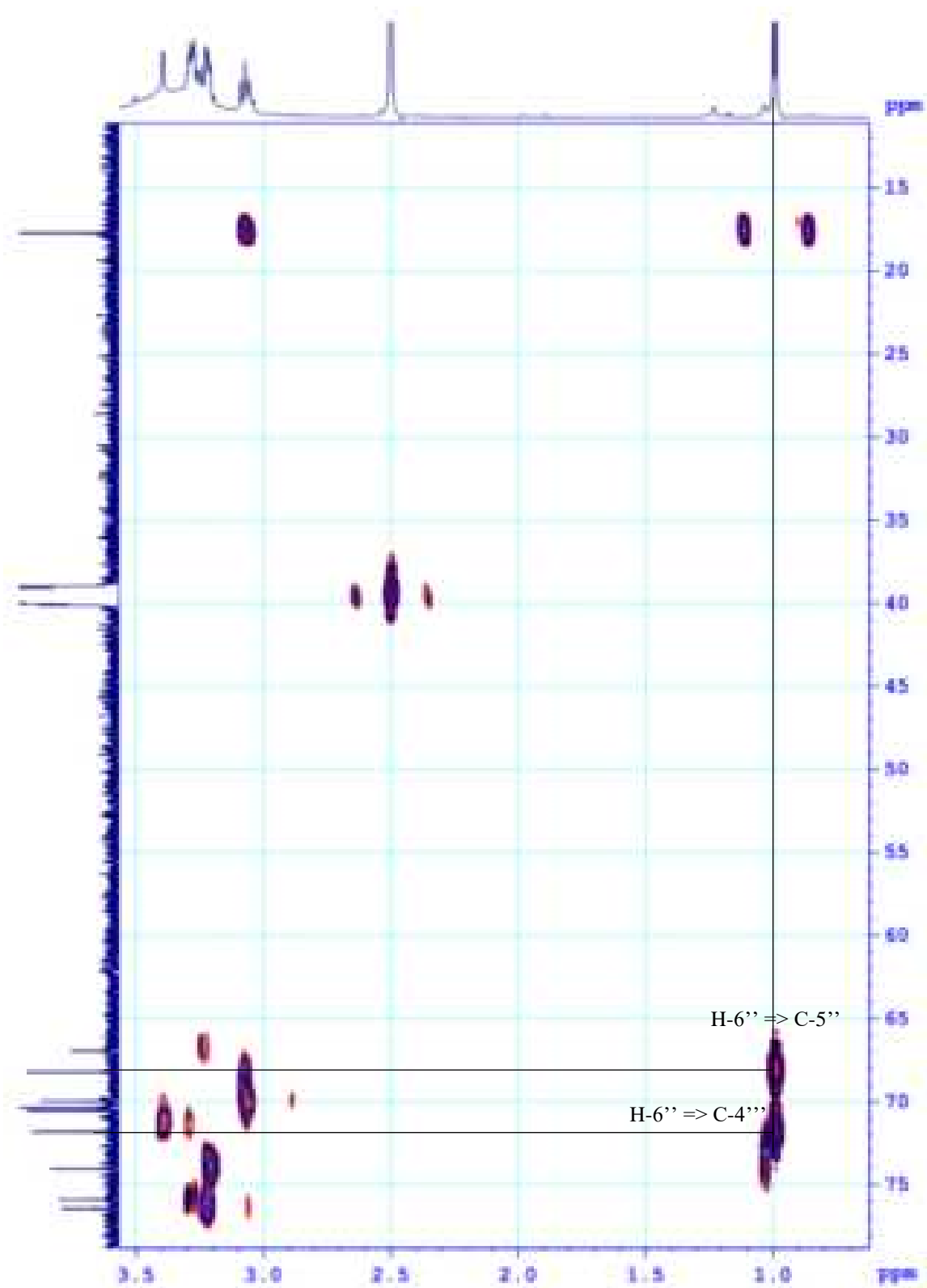


Figure S54: HMBC spectrum of compound 6 (rutin) (from  $\delta_c$  15 ppm to  $\delta_c$  75 ppm)

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

Position	Compound <b>7</b> (MeOD)		Isatin (CDCl <sub>3</sub> ) [34,35]	
	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> ppm
1-NH	-	-	-	8.01
2	161.4	-	159.5	-
3	185.4	-	184.6	-
3α	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
7α	152.0	-	150.9	-

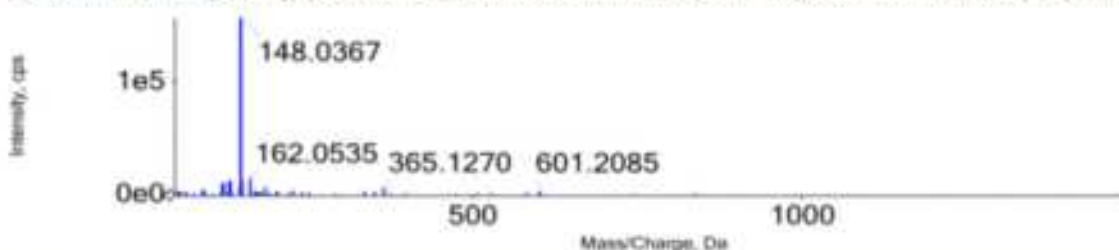
## ANALYSIS REPORT

### Injection details

<i>Sample name</i>	SAL	<i>Vial position</i>	39
<i>Sample file name</i>	SER. wif2-YEN	<i>Inject volume</i>	5.00
<i>Acquisition date</i>	20/04/2023 10:51:32 AM	<i>Acquisition method</i>	<b>ESI_POS_SCAN</b>
<i>Operator</i>	CB21261708	<i>Instrument name</i>	X500 <sub>k</sub> QTOF

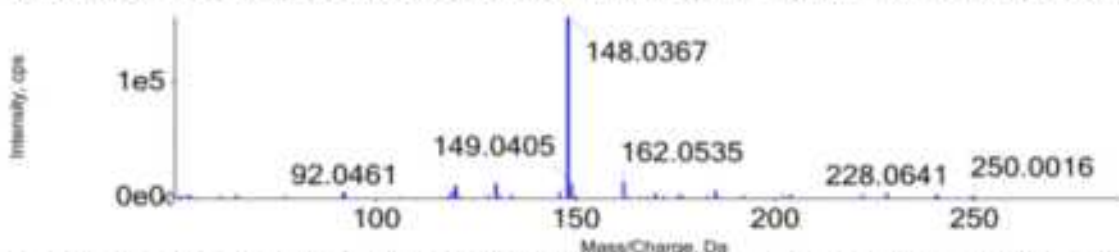
### Full mass spectrum

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

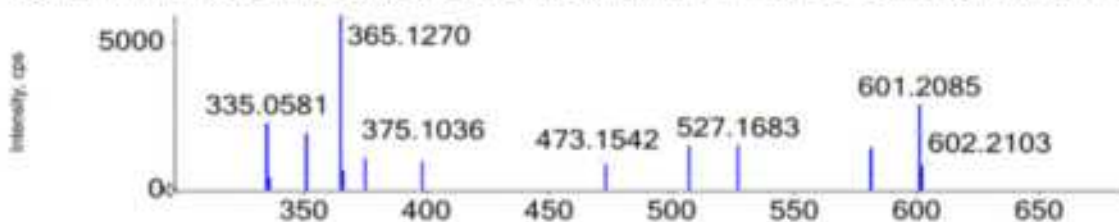


### Expanded spectrum

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



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



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



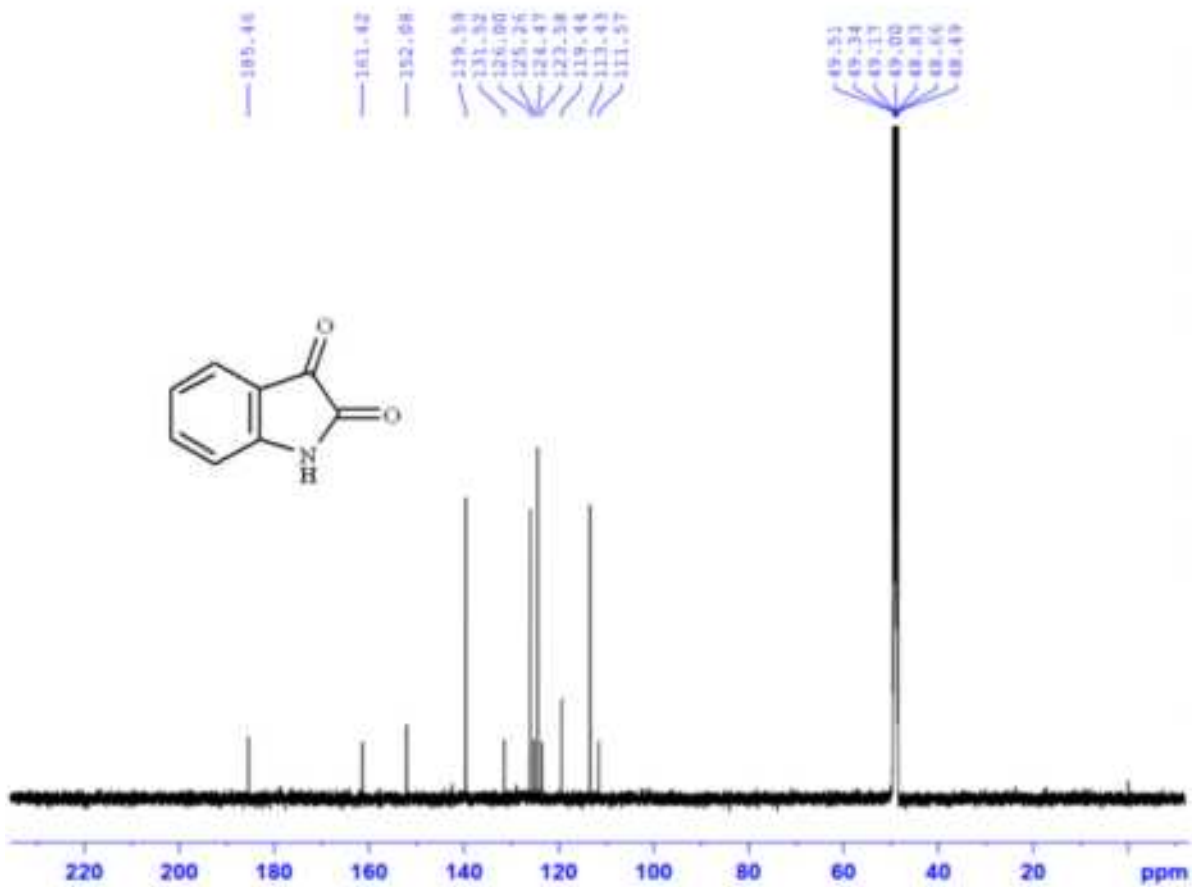


Figure S58:  $^{13}\text{C}$ -NMR (150MHz, MeOD) spectrum of compound 7 (isatin)

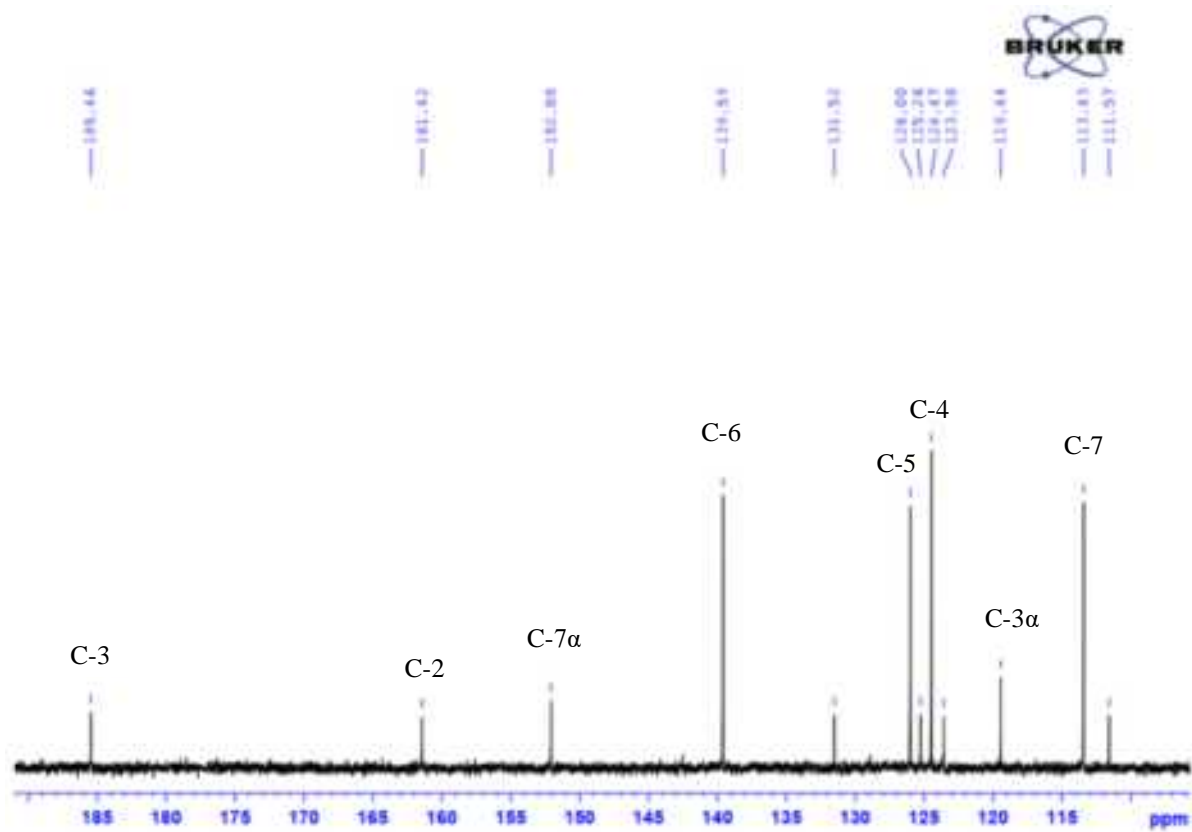
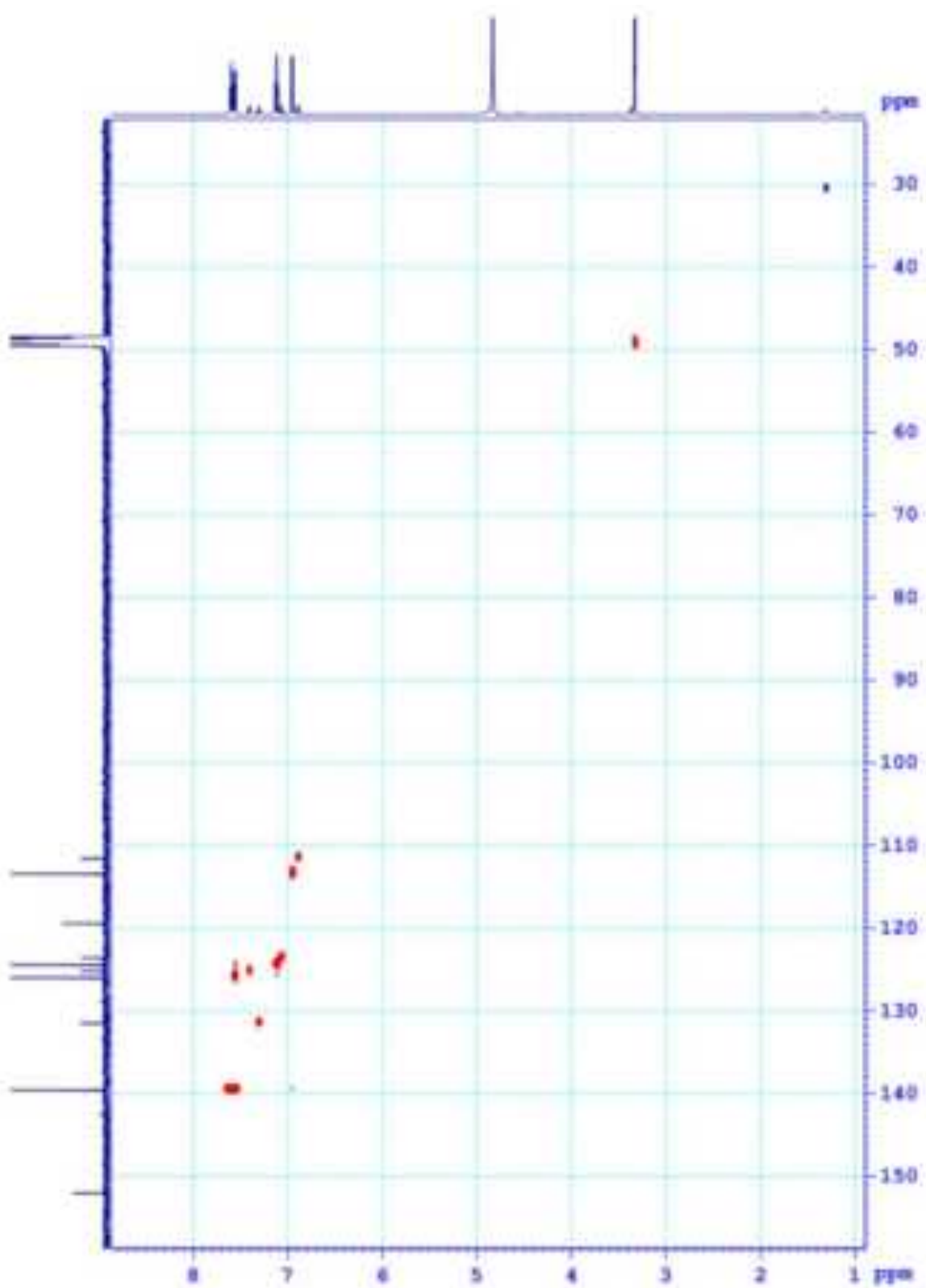
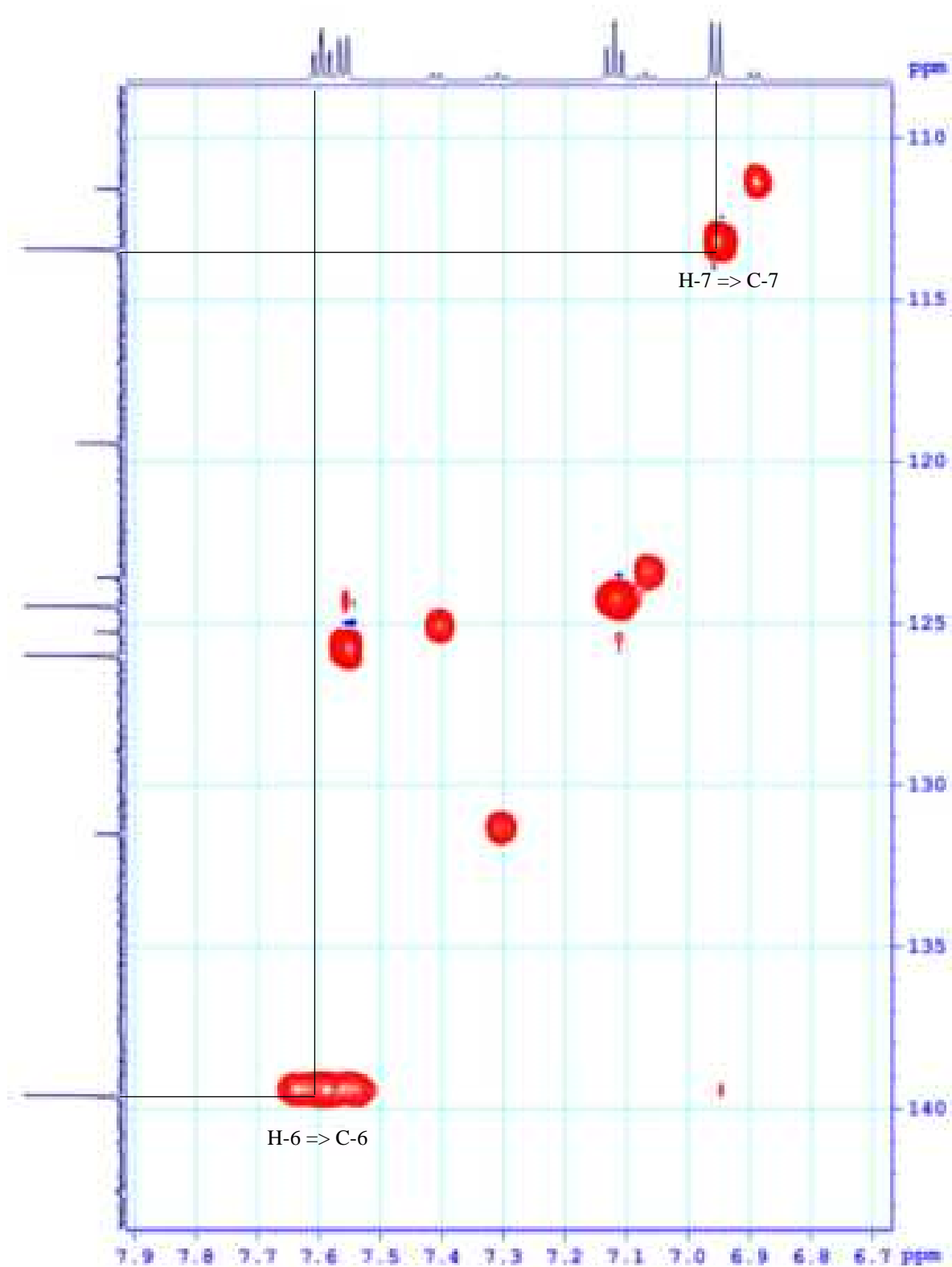


Figure S59:  $^{13}\text{C}$ -NMR spectrum of compound 7 (isatin) (from  $\delta_{\text{C}}$  110 ppm to  $\delta_{\text{C}}$  185 ppm)



**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)

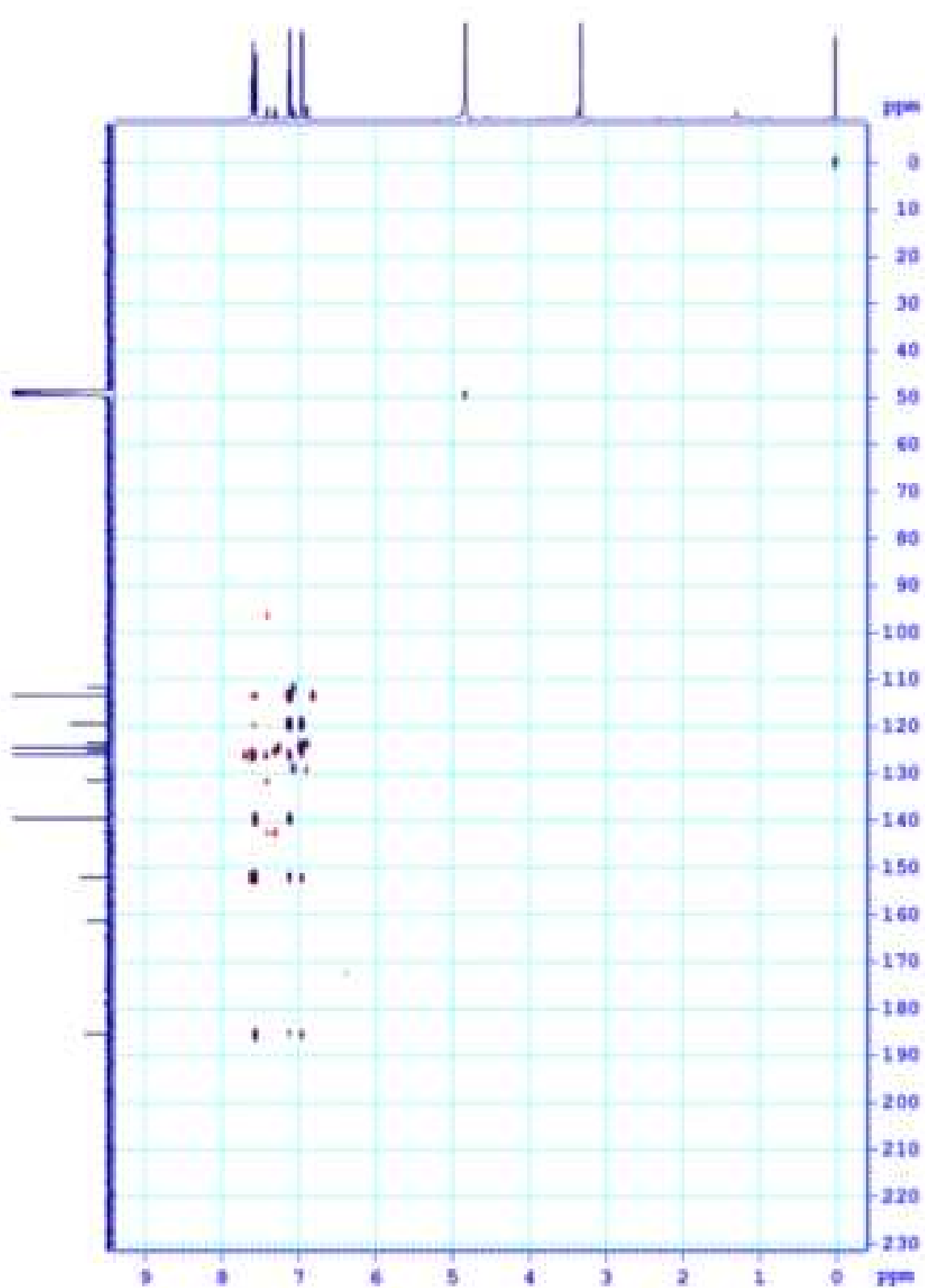
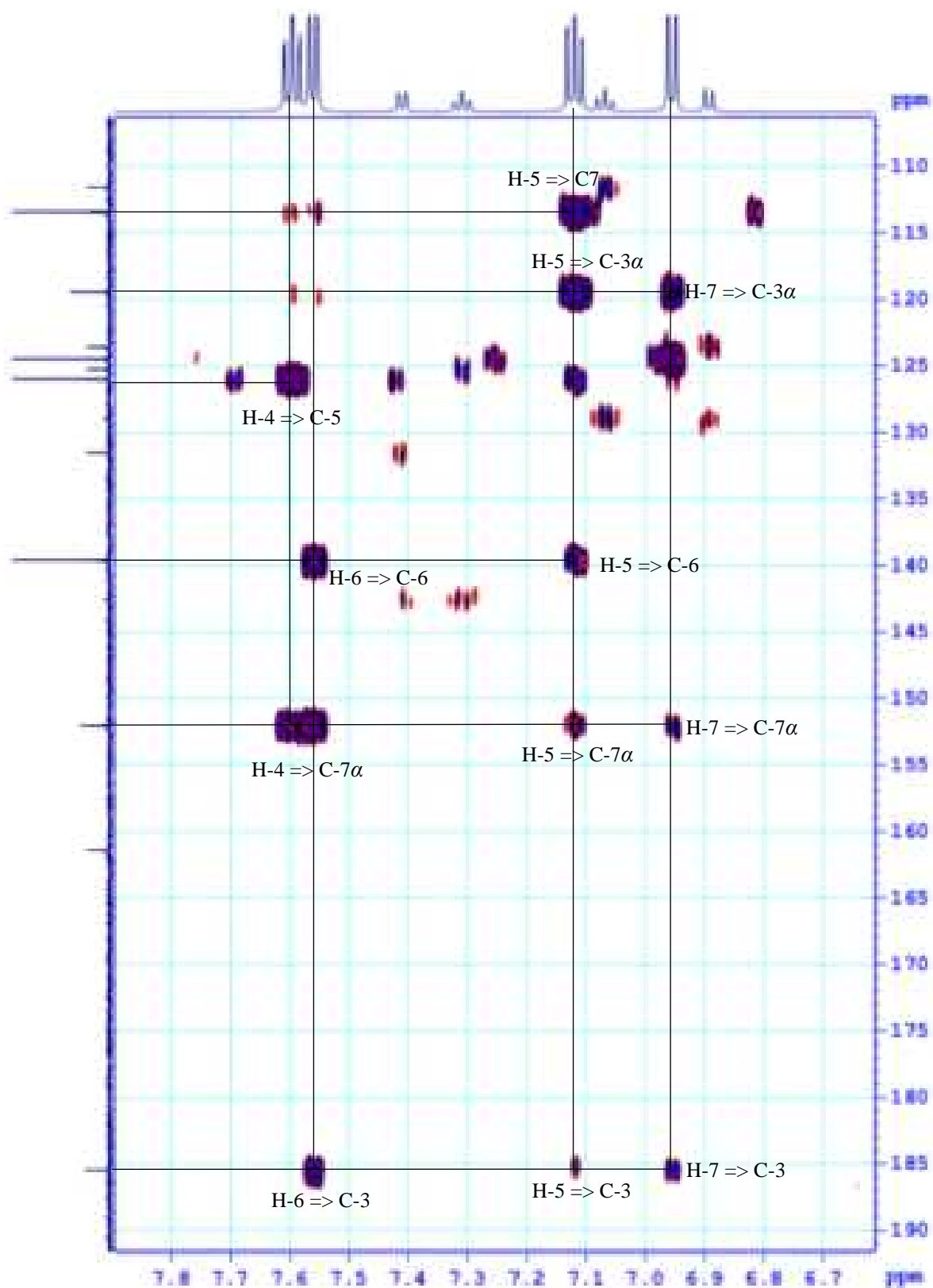


Figure S62: HMBC spectrum of compound 7 (isatin)

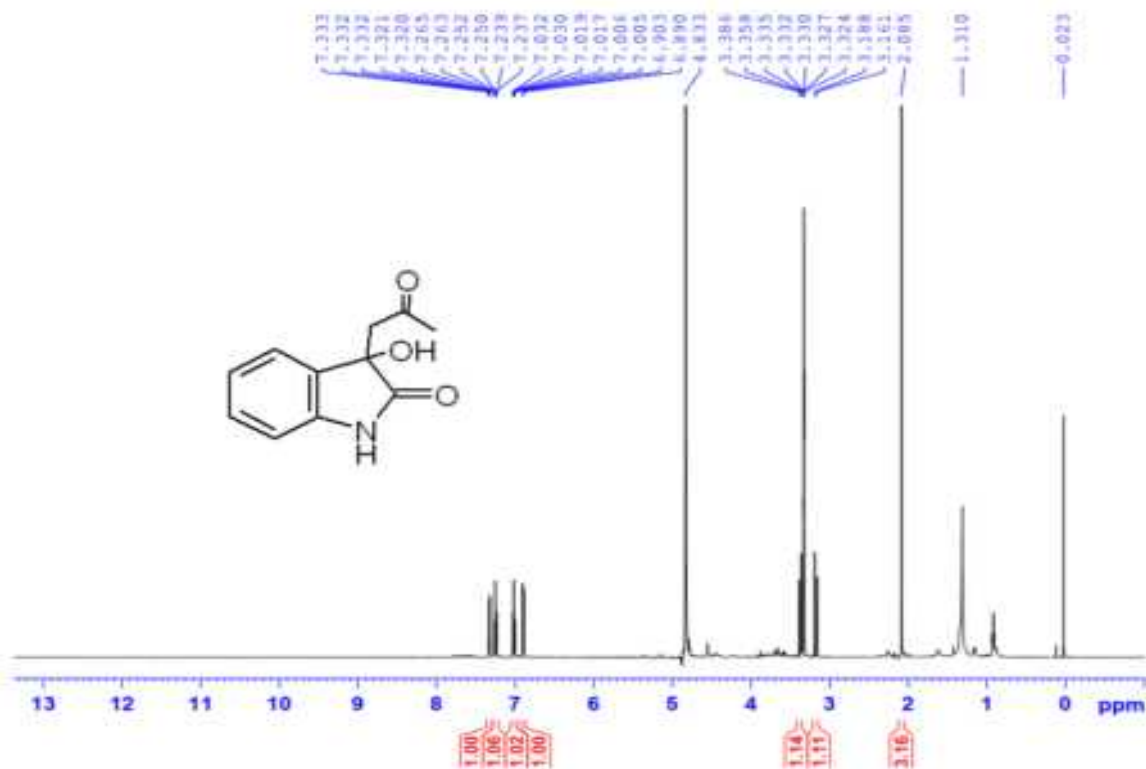




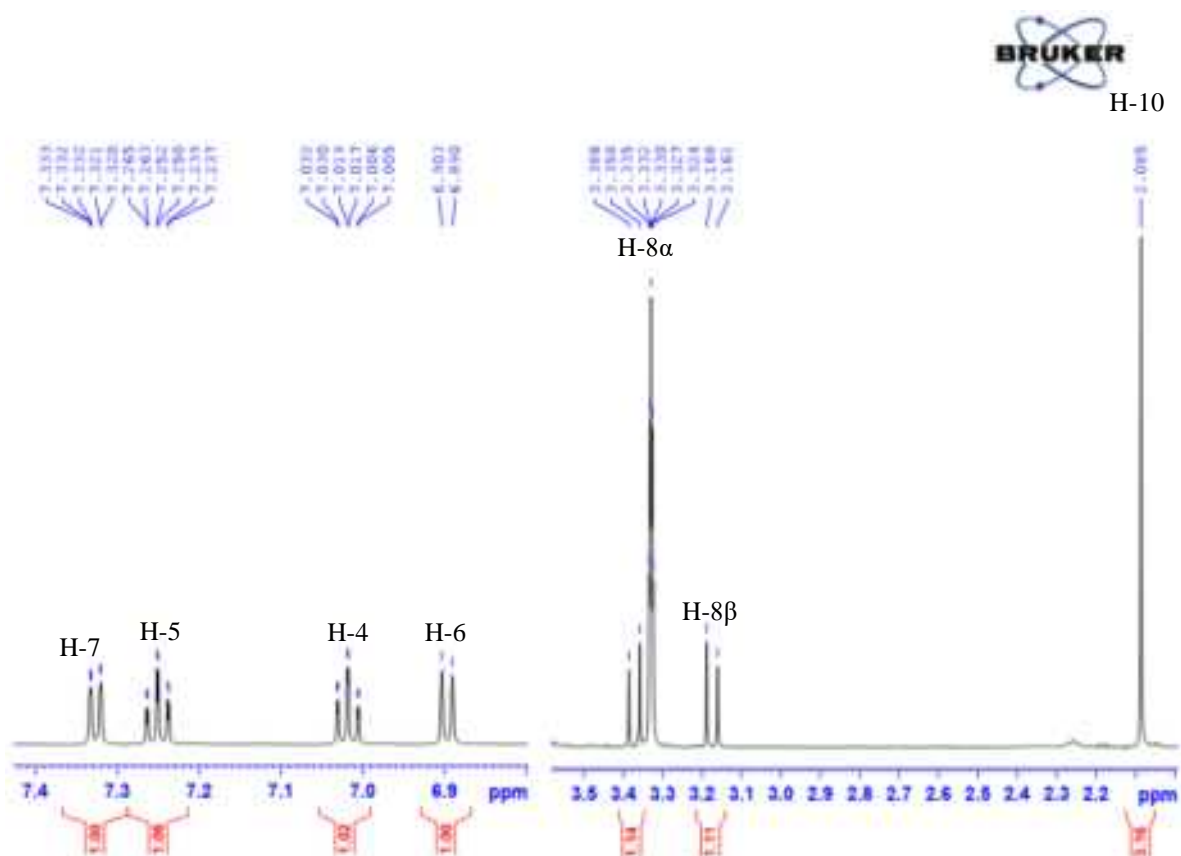
**Figure S63:** HMBC spectrum of compound 7 (isatin) (from  $\delta_c$  110 ppm to  $\delta_c$  190 ppm)

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

Position	Compound <b>8</b> (MeOD)		3-hydroxy-3-(2-oxopropyl)indolin-2-one (CDCl <sub>3</sub> ) [36]	
	<sup>13</sup> C-NMR (125 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-NH	-		-	
2	181.1	-	179.8	-
3	74.8	-	76.2	-
3α	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	-
7α	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> )

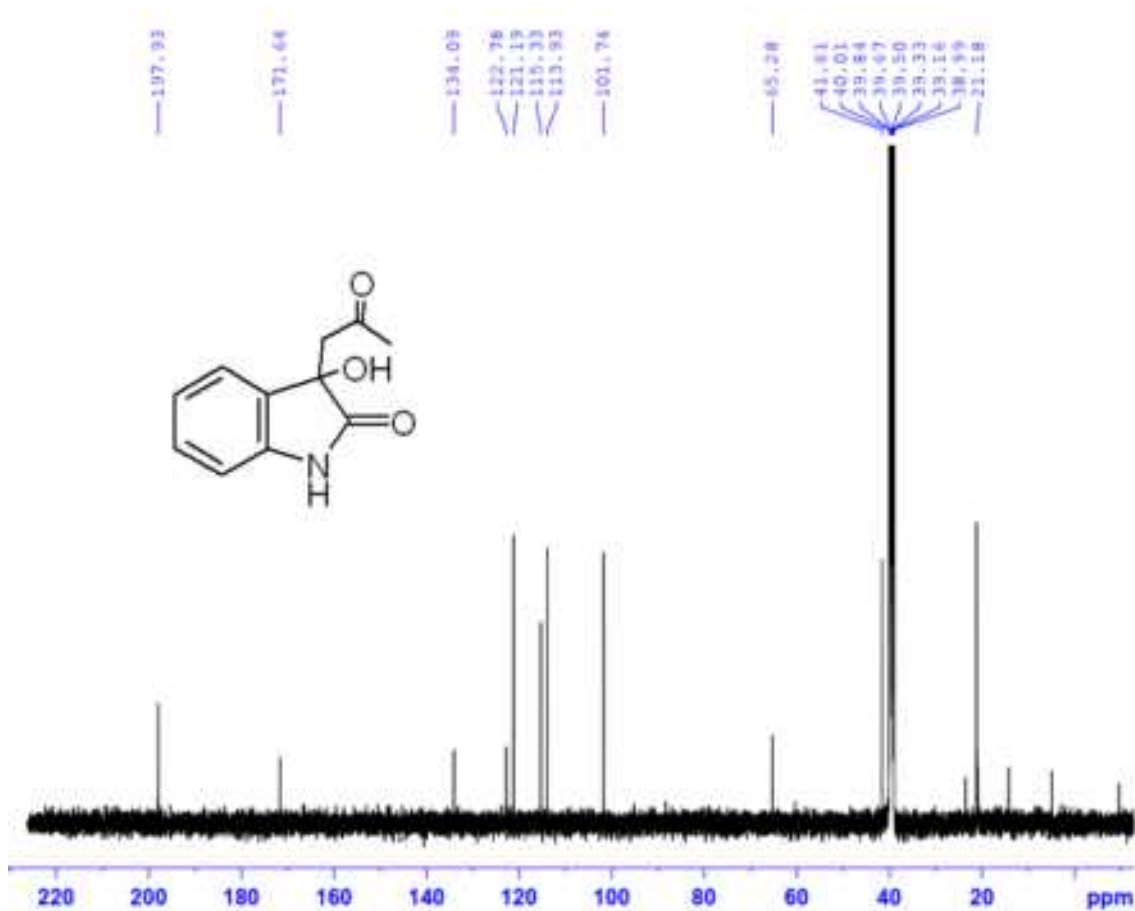


**Figure S64:** <sup>1</sup>H-NMR (600 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one).

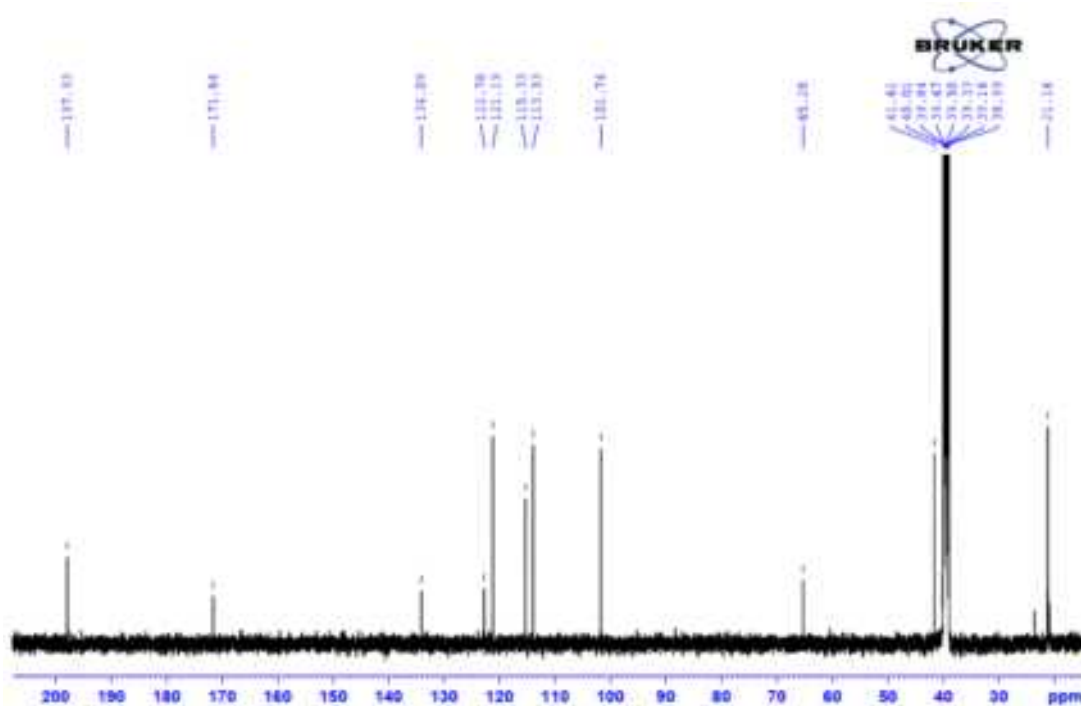


**Figure S65:** <sup>1</sup>H-NMR (600 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_H$  2.0 ppm to  $\delta_H$  7.4 ppm)

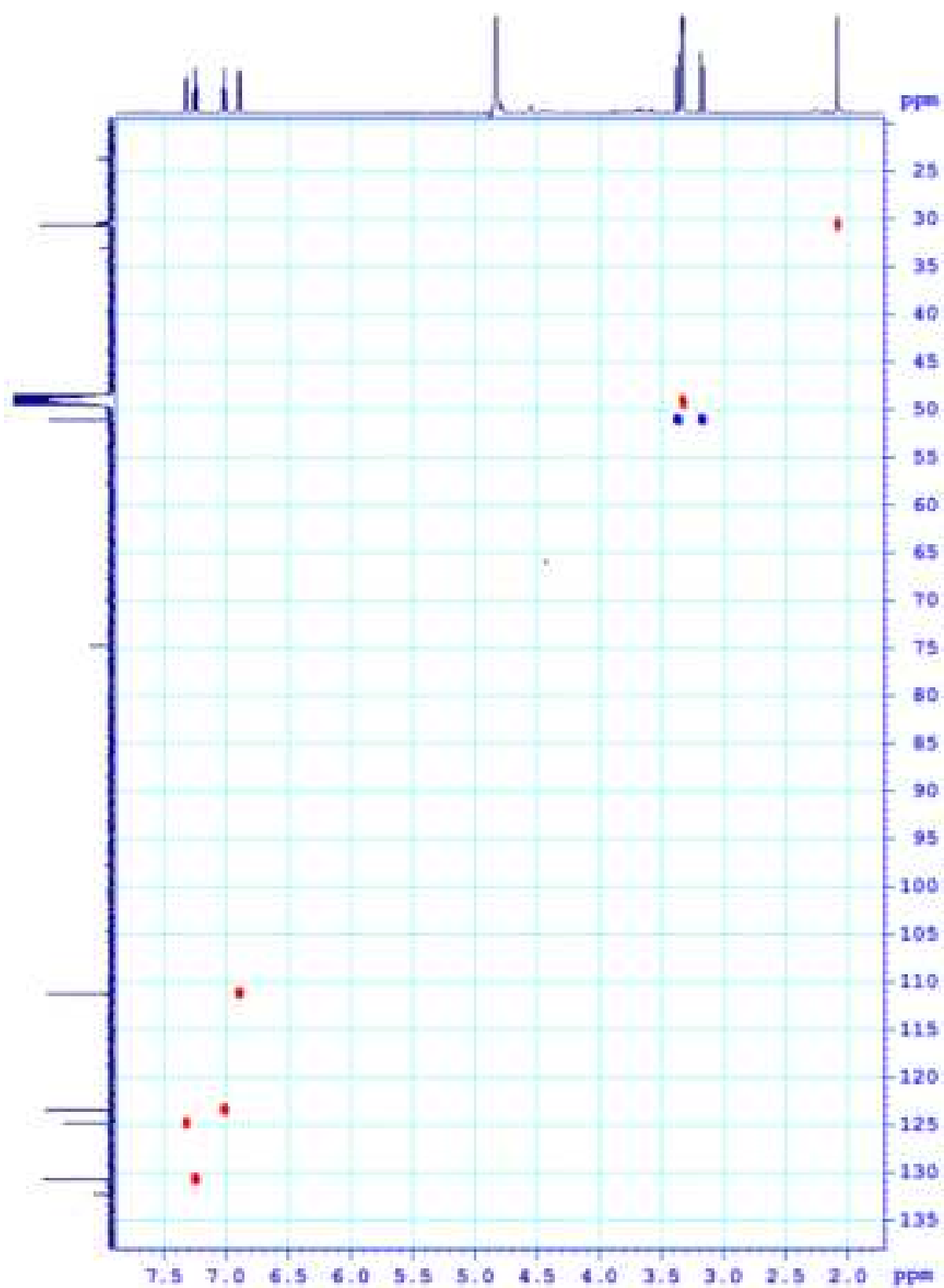
© 2025 ACG Publications. All rights reserved.



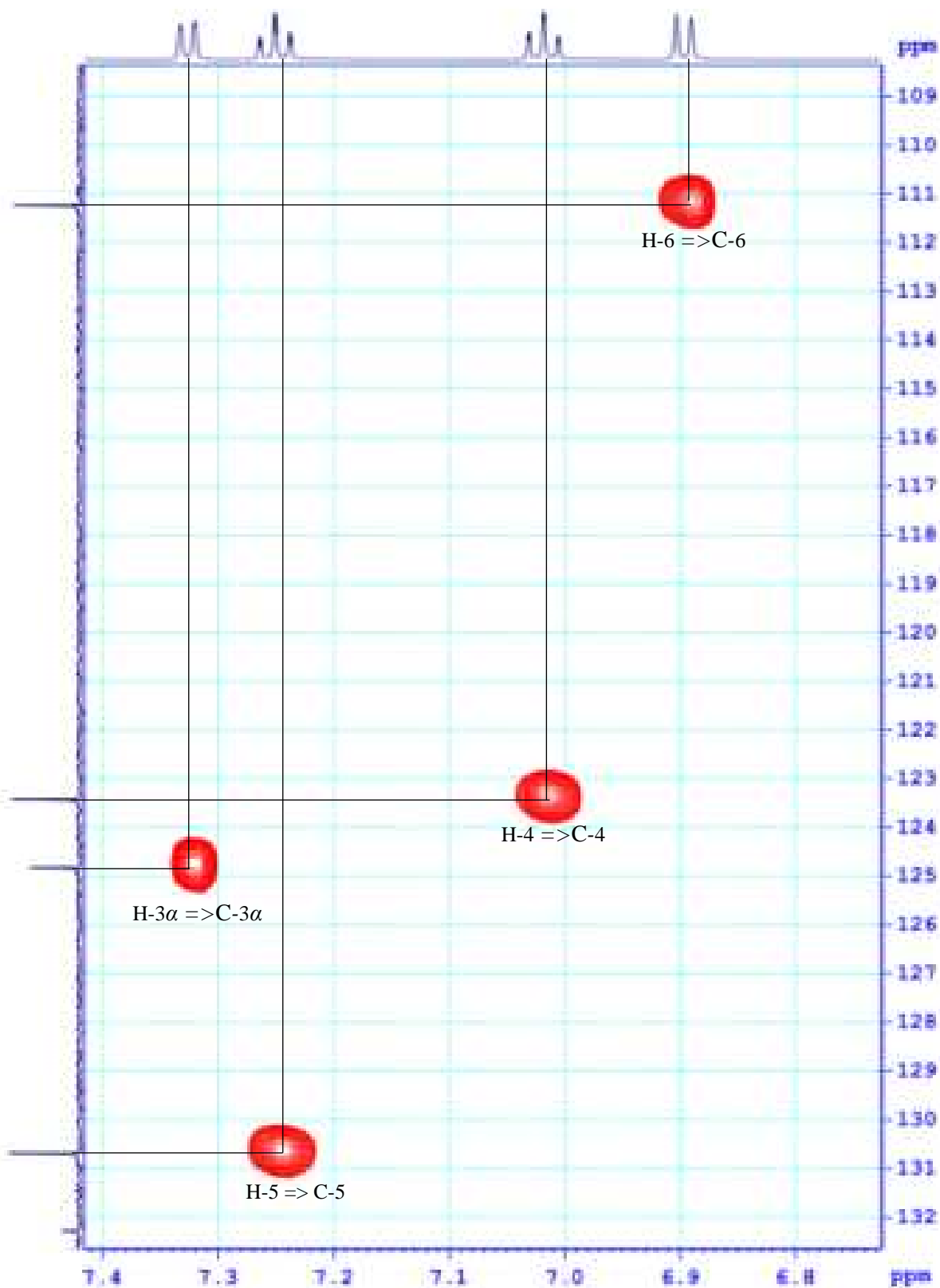
**Figure S66:** <sup>13</sup>C-NMR (150 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)



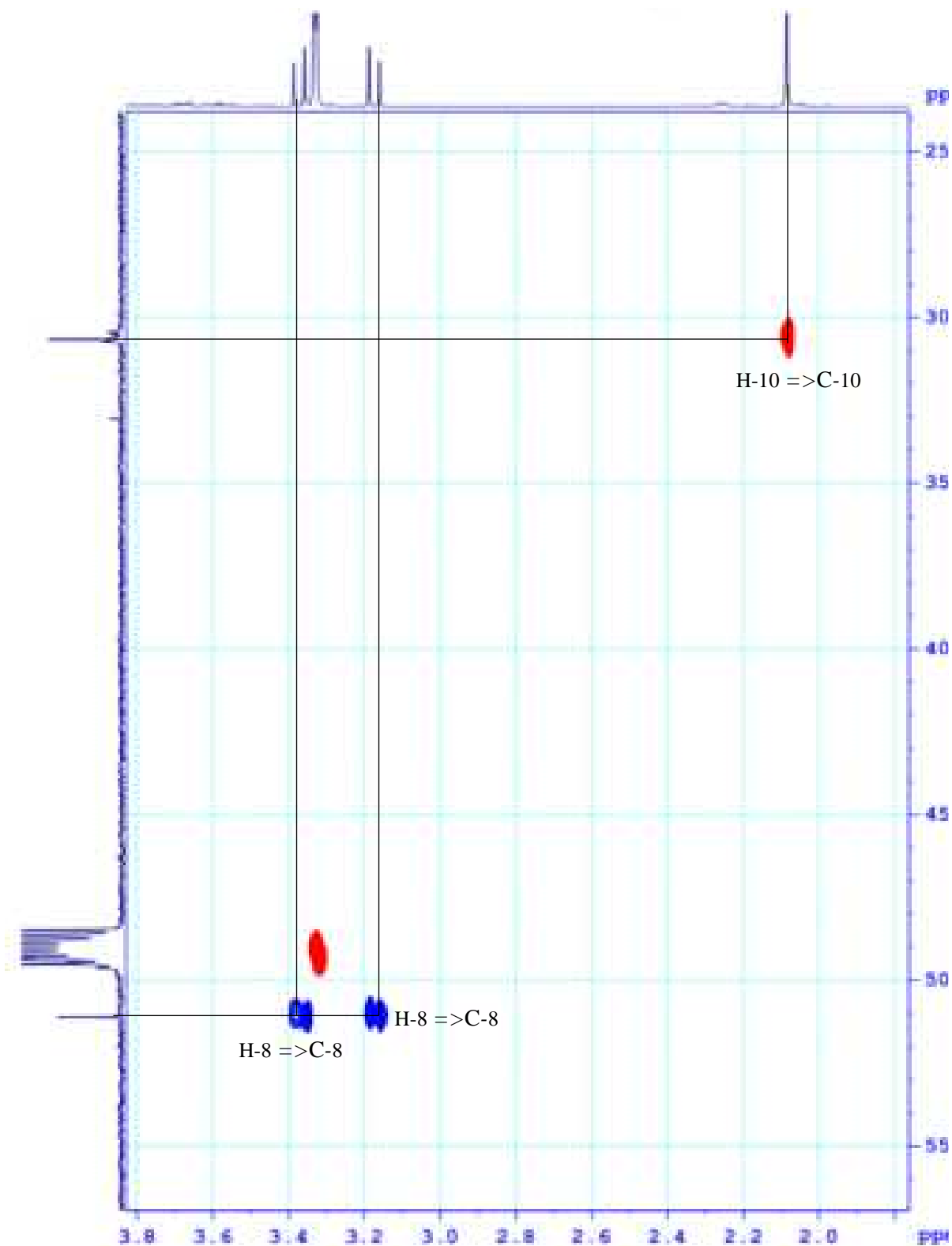
**Figure S67:** <sup>13</sup>C-NMR spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_c$  20 ppm to  $\delta_c$  200 ppm)



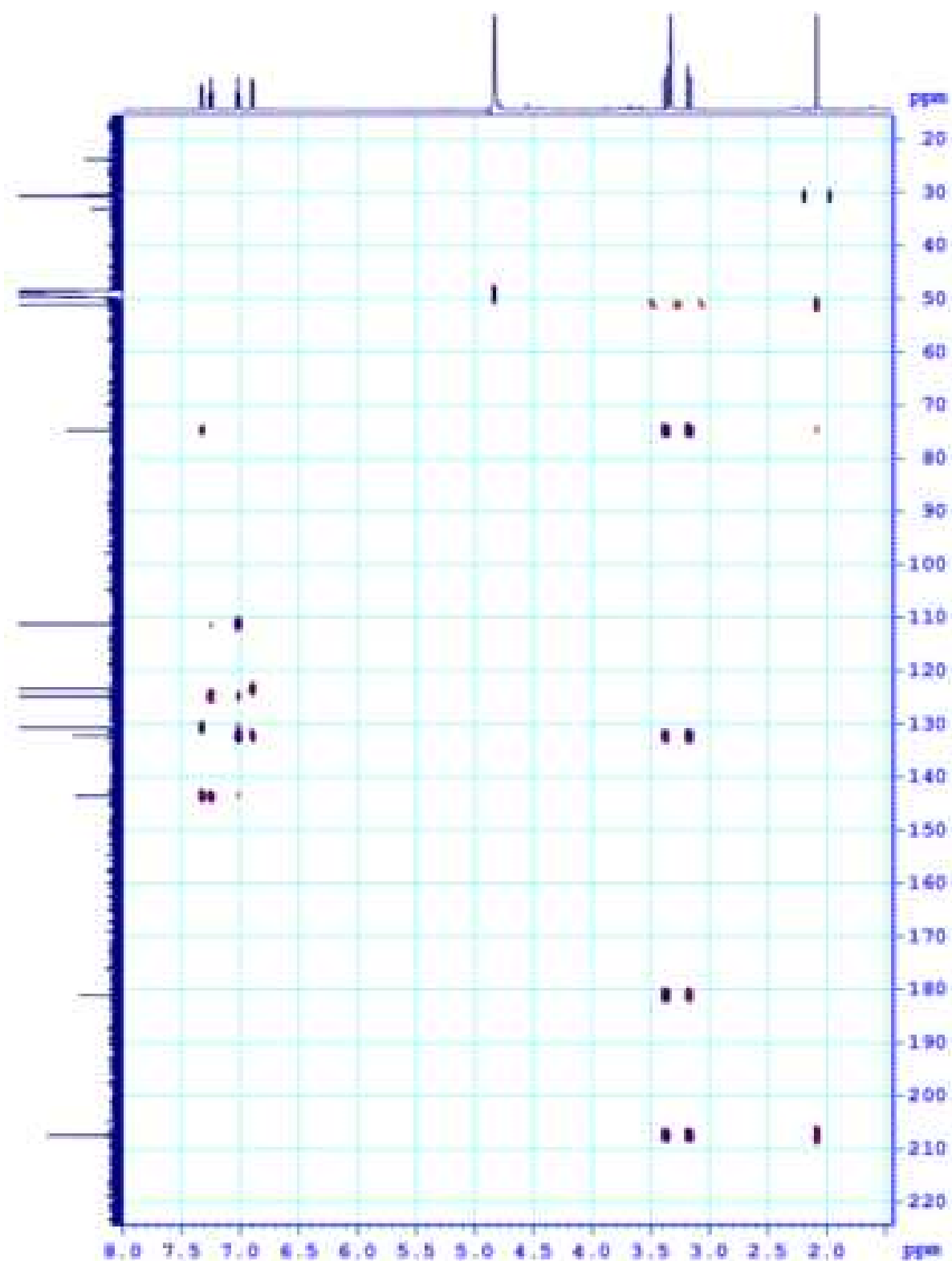
**Figure S68:** HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)



**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)

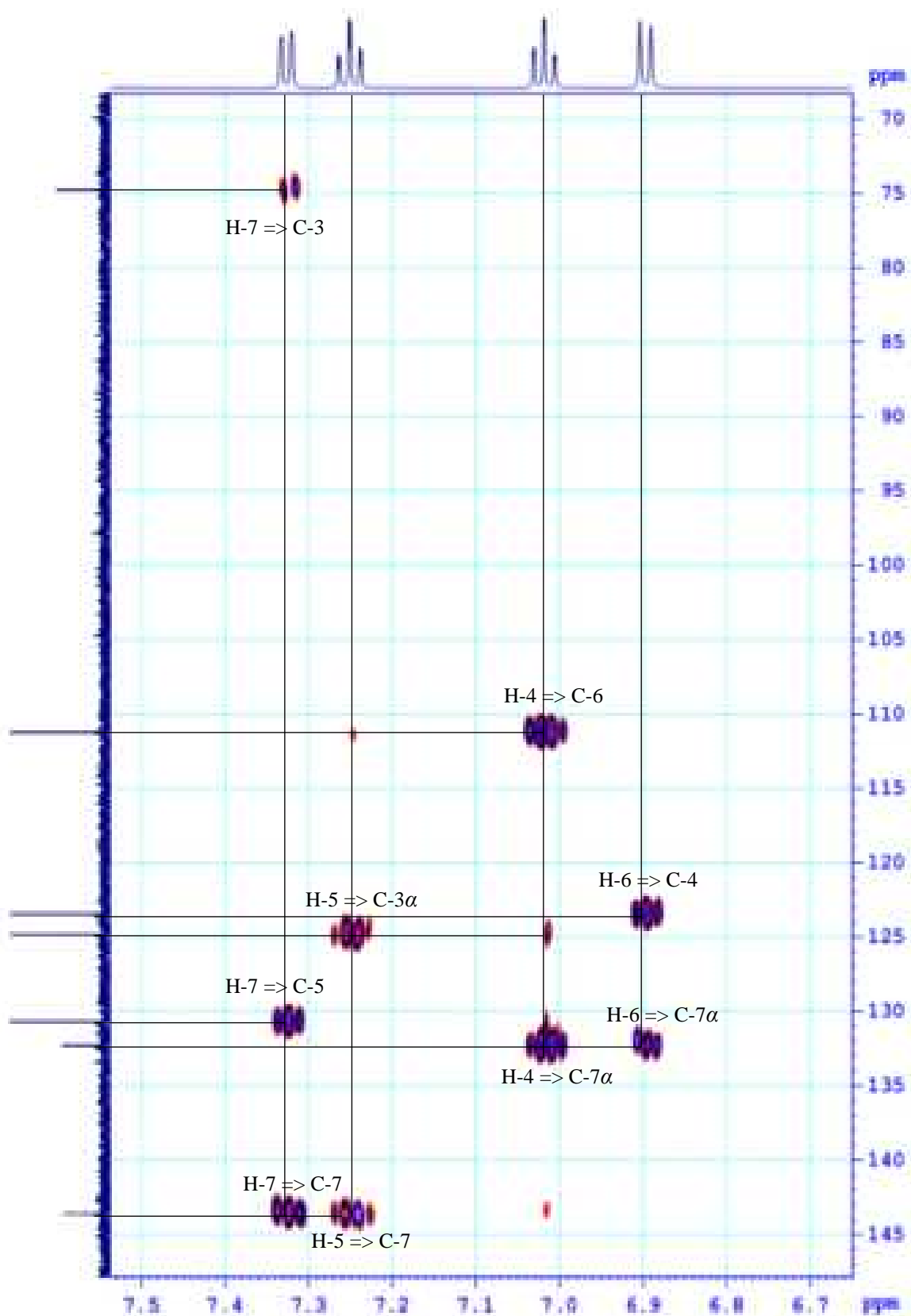


**Figure S70:** HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_{\text{C}}$  25 ppm to  $\delta_{\text{C}}$  55 ppm)

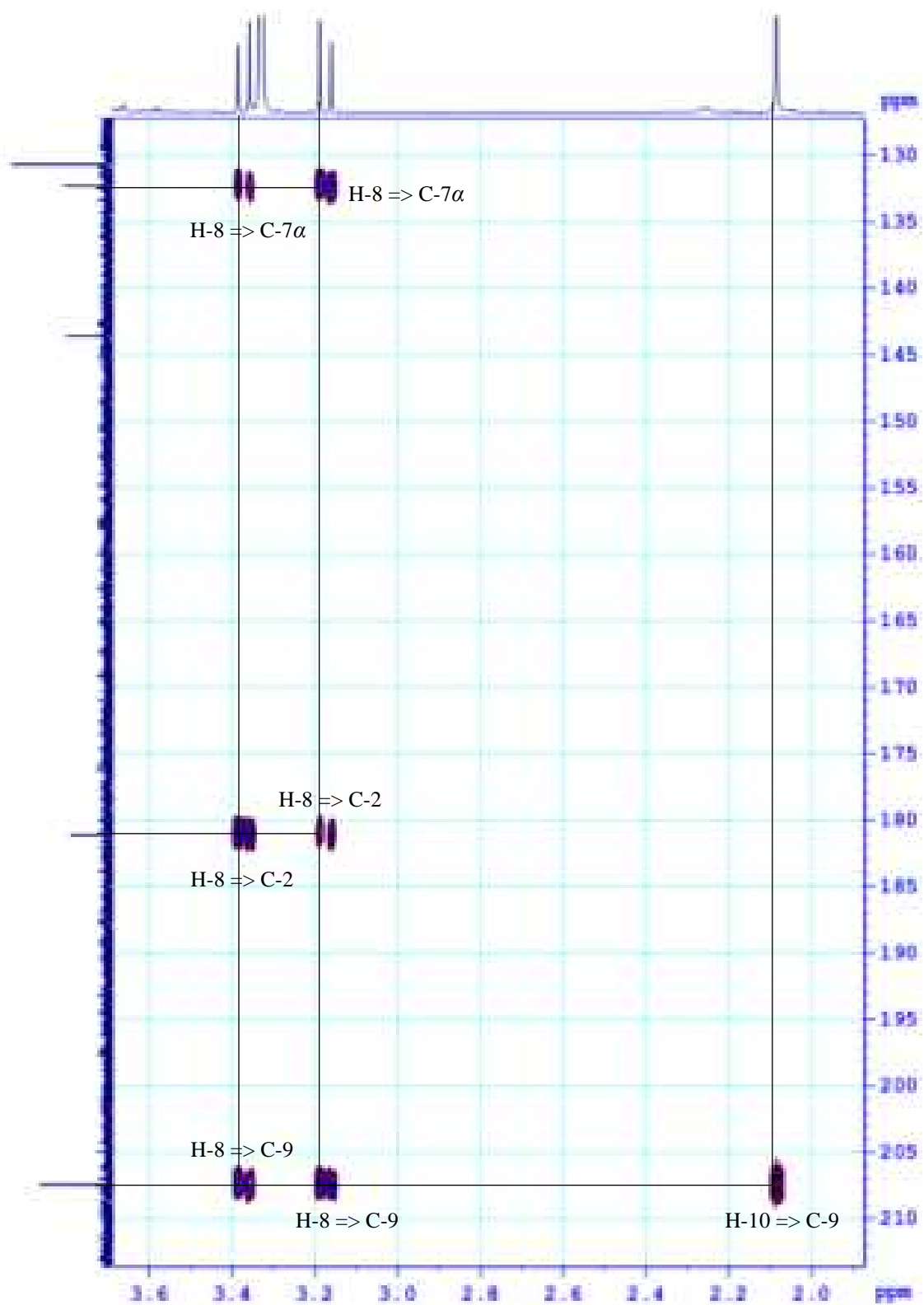


**Figure S71:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)

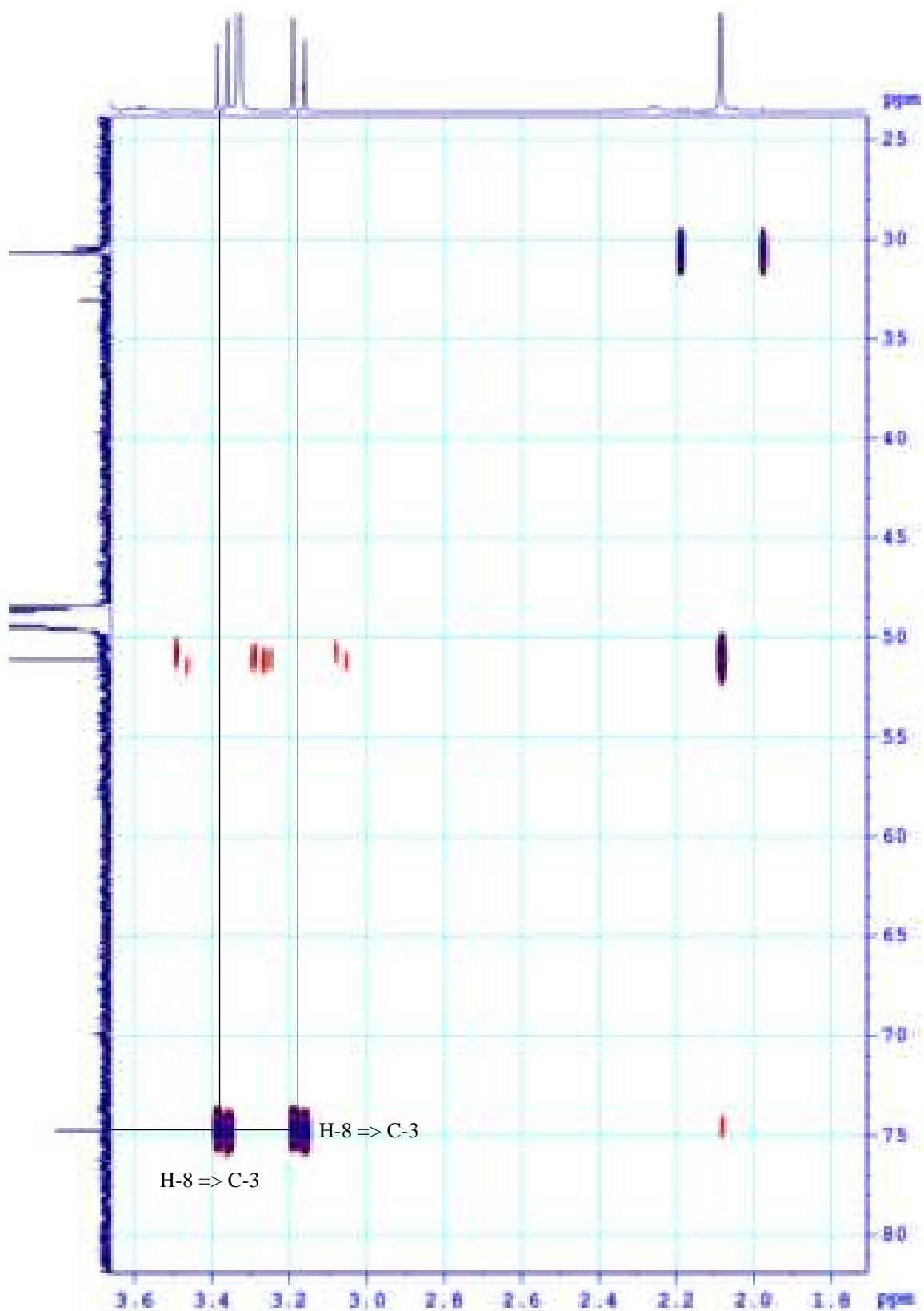




**Figure S72:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_c$  70 ppm to  $\delta_c$  145 ppm)



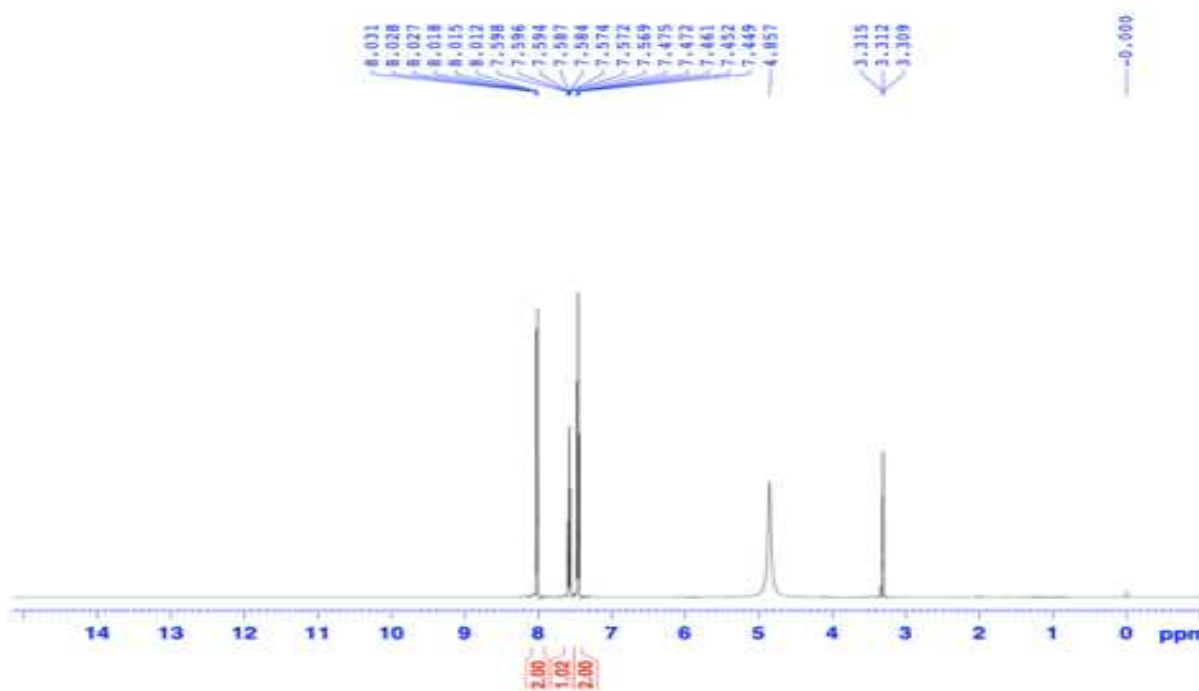
**Figure S73:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_C$  130 ppm to  $\delta_C$  210 ppm)



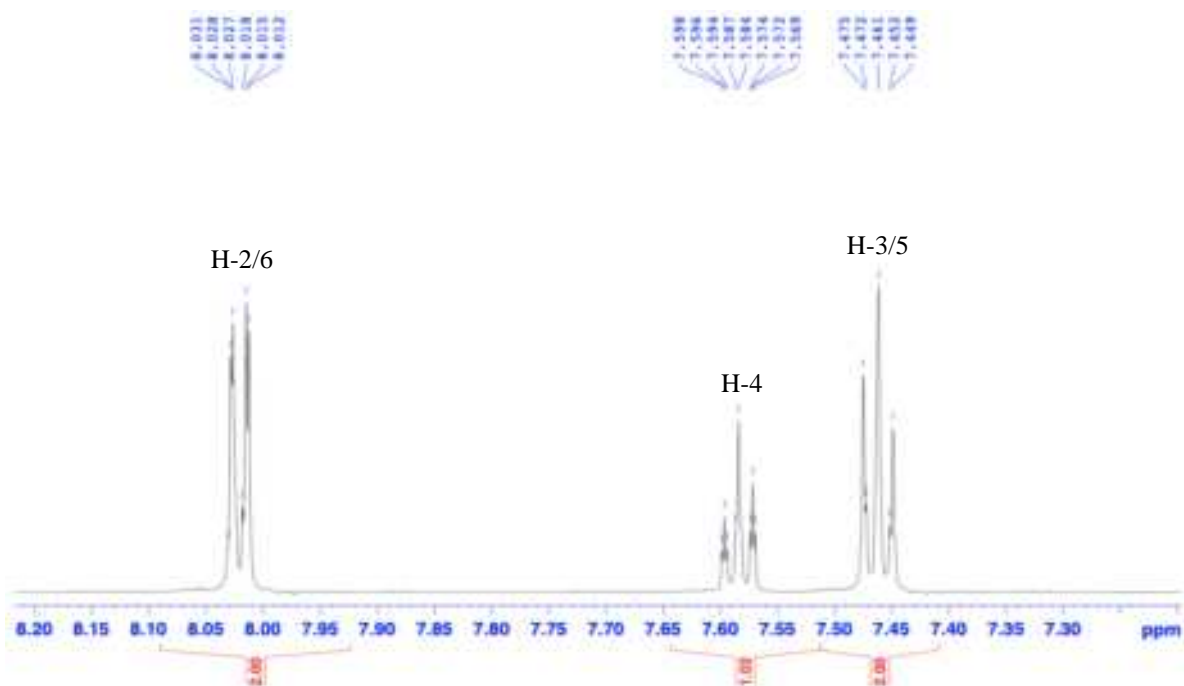
**Figure S74:** HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from  $\delta_C$  25 ppm to  $\delta_C$  80 ppm)

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

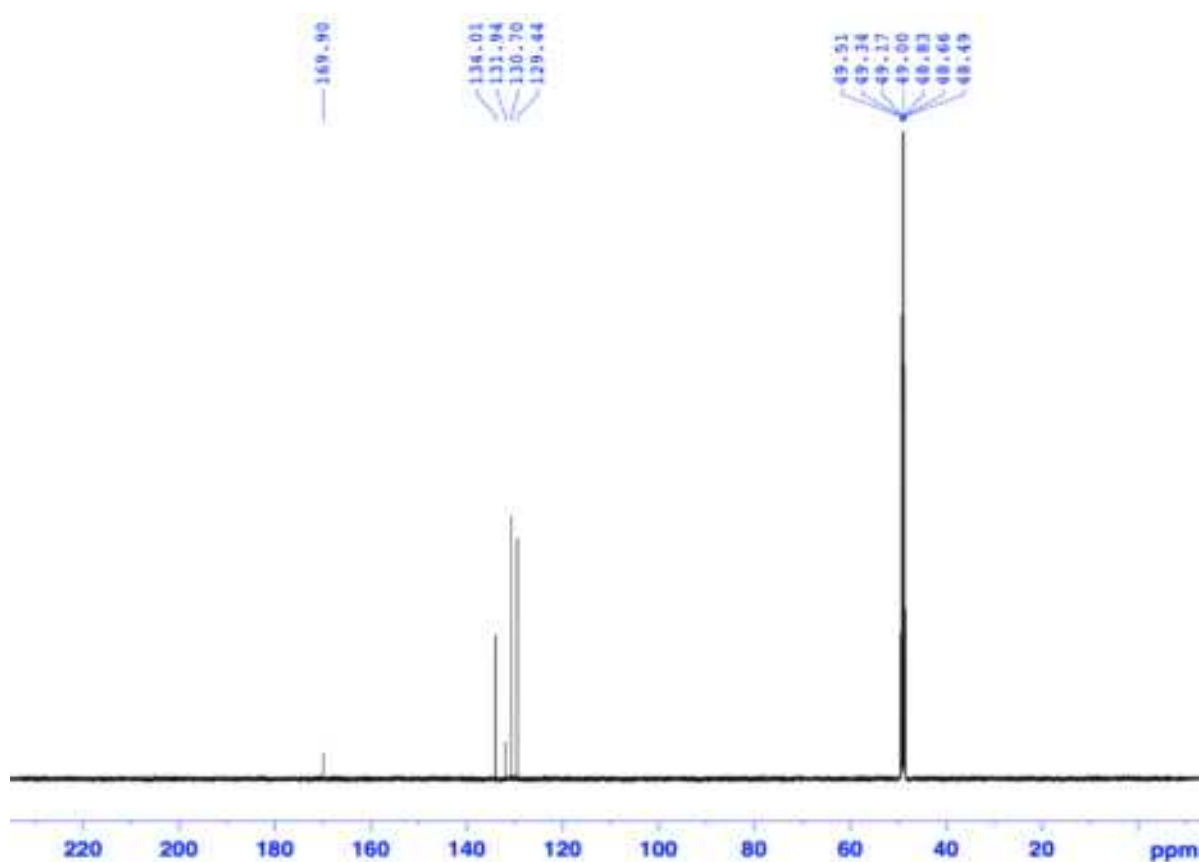
Position	Compound <b>9</b> (MeOD)		benzoic acid (CDCl <sub>3</sub> ) [37]	
	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (100 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (400 MHz) δ <sub>H</sub> ppm
1	131.9	-	129.3	-
2 & 6	130.7	8.02 (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:** <sup>1</sup>H-NMR (600 MHz, MeOD) spectrum of compound **9** (benzoic acid)

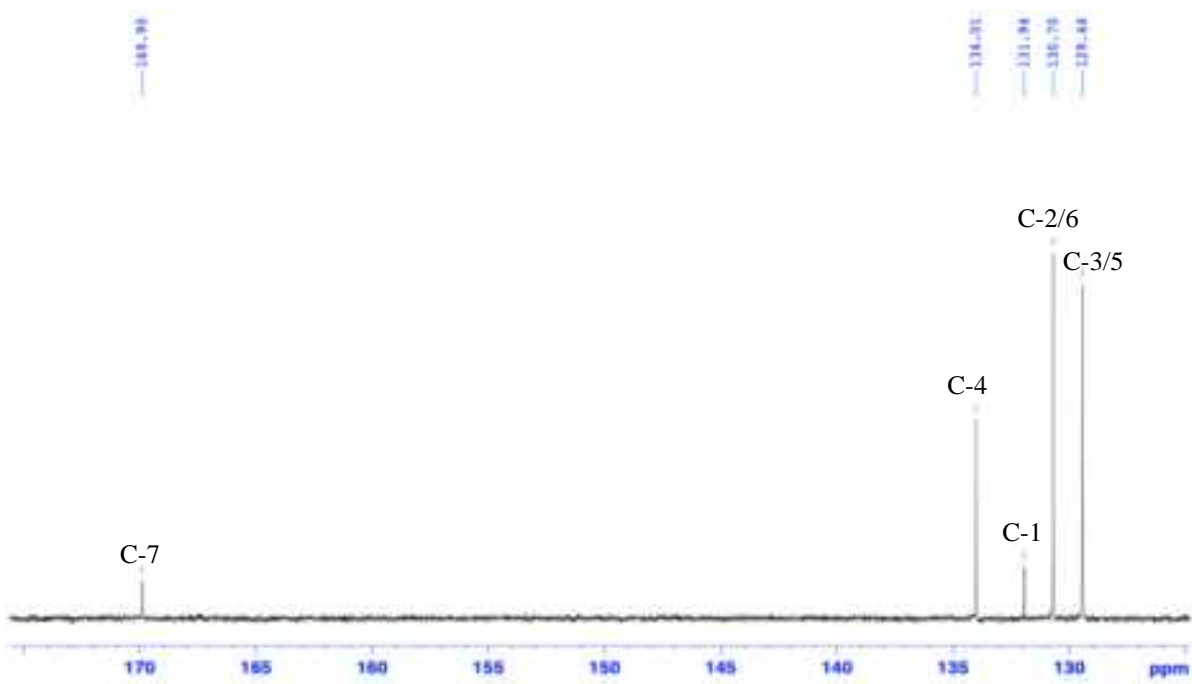


**Figure S76:** <sup>1</sup>H-NMR spectrum of compound **9** (benzoic acid) (from  $\delta_H$  7.3 ppm to  $\delta_H$  8.2 ppm)



**Figure S77:** <sup>13</sup>C-NMR (150 MHz, MeOD) spectrum of compound **9** (benzoic acid)

© 2025 ACG Publications. All rights reserved.



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

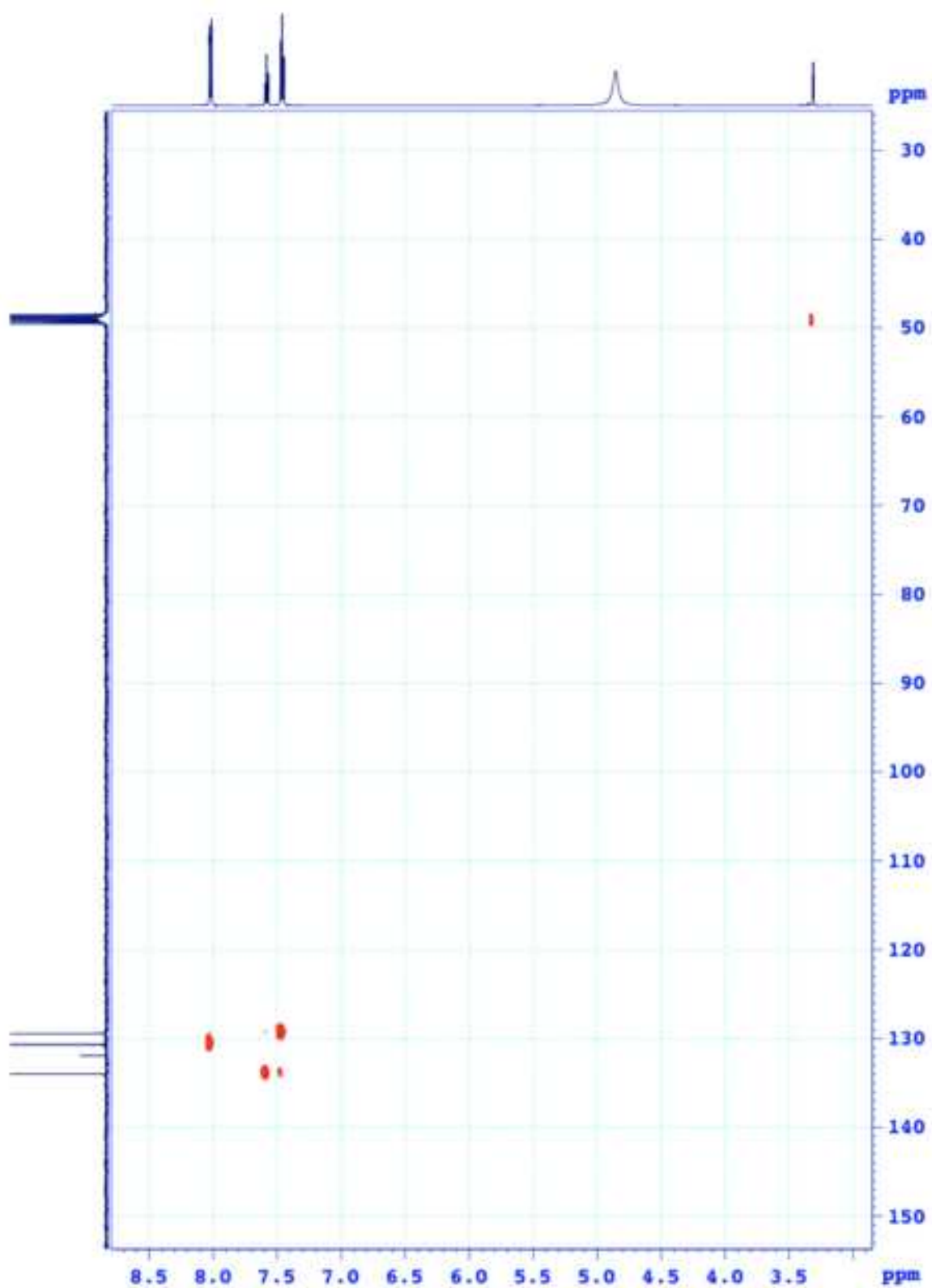
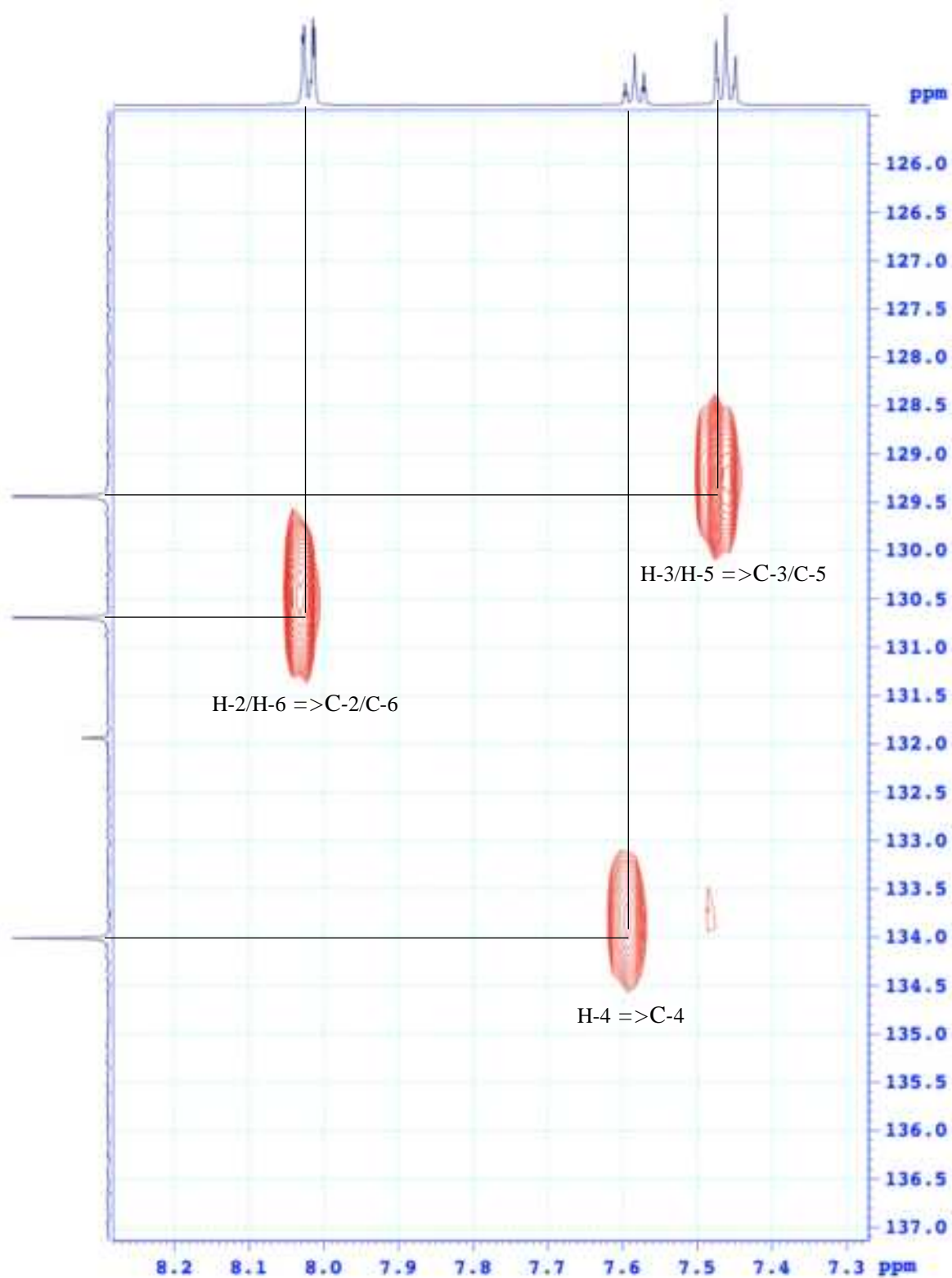
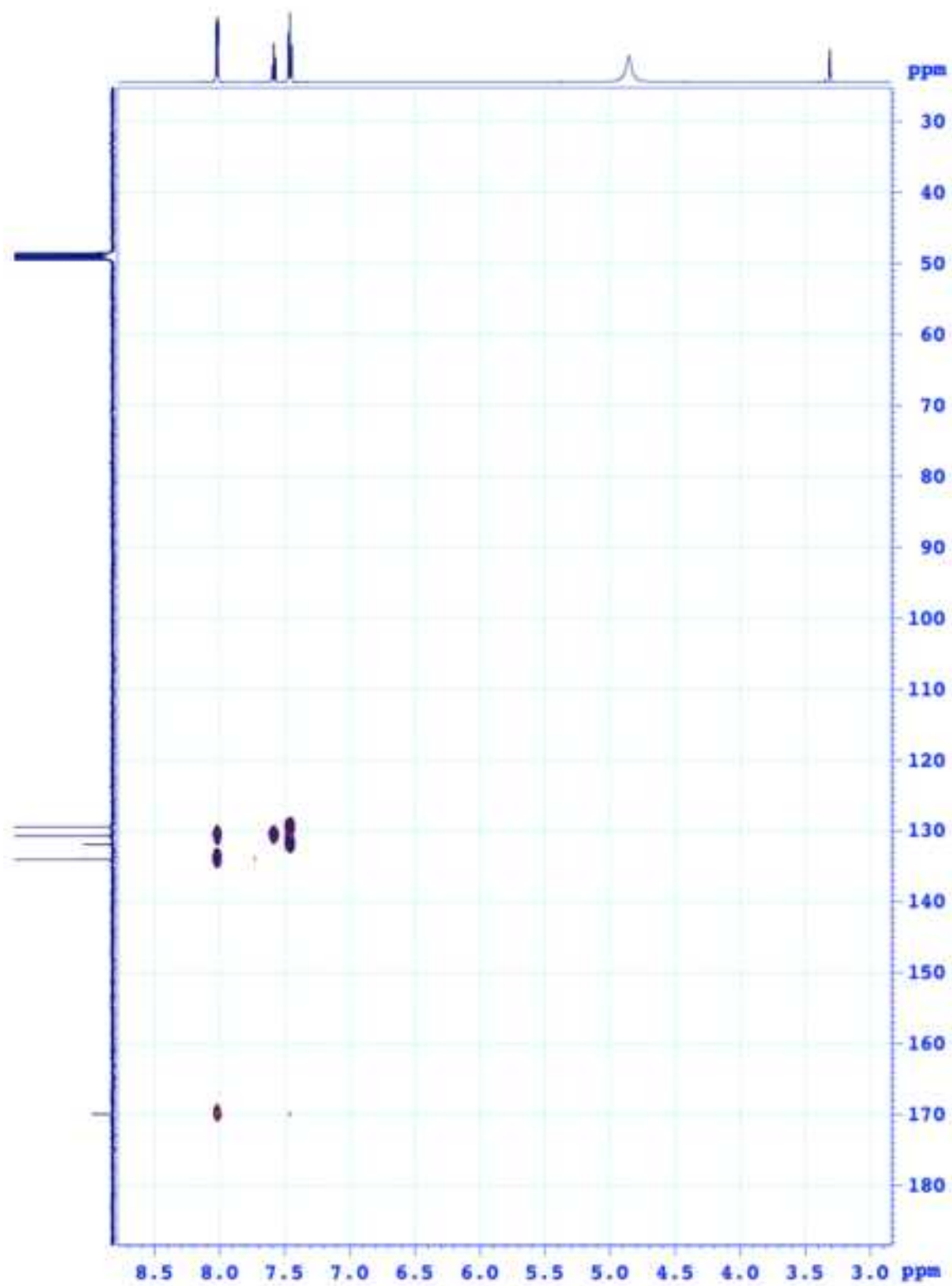


Figure S79: HSQC spectrum of compound 9 (benzoic acid)

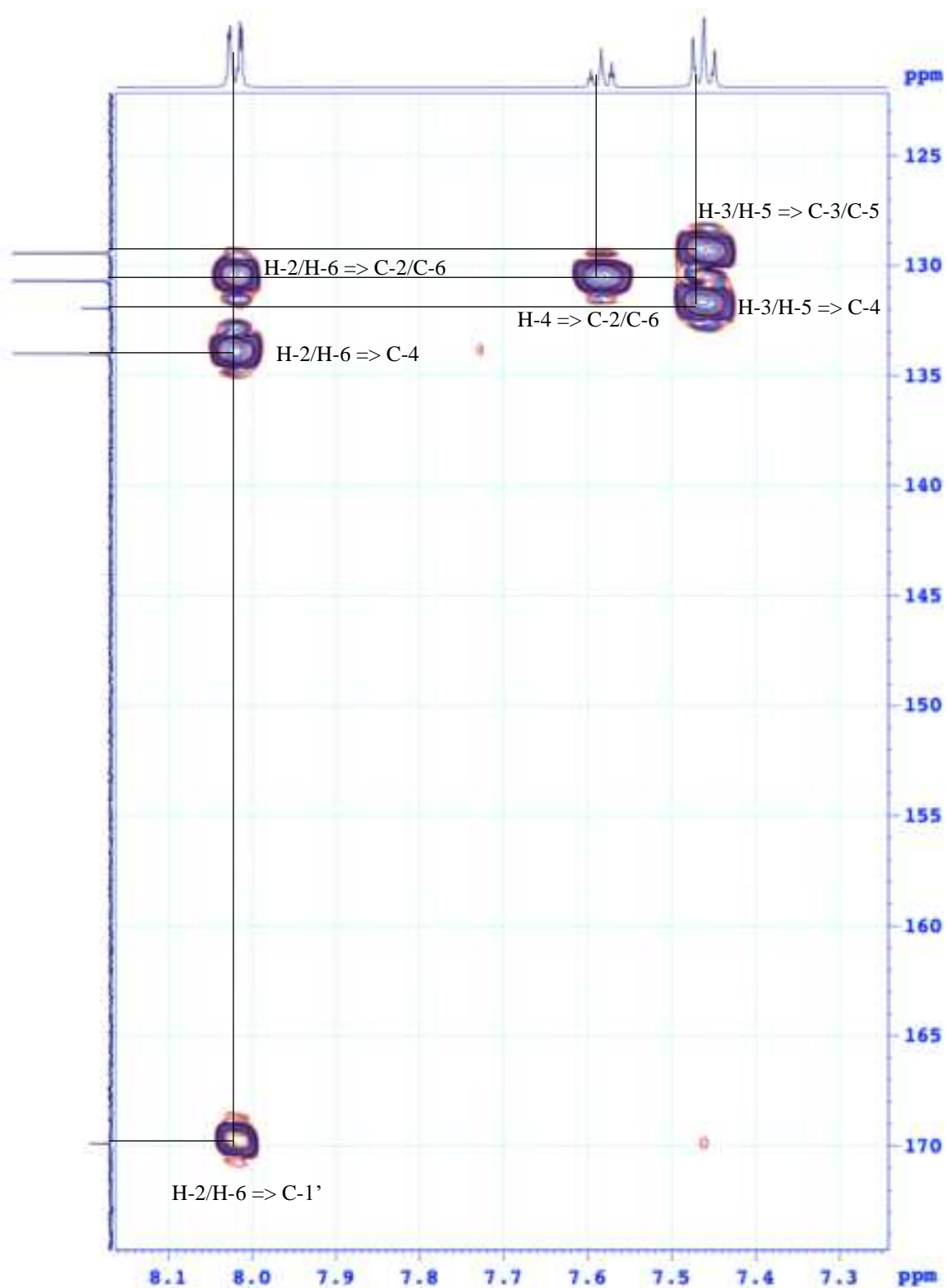


**Figure S80:** HSQC spectrum of compound **9** (benzoic acid) (from  $\delta_{\text{C}}$  126 ppm to  $\delta_{\text{C}}$  137 ppm)





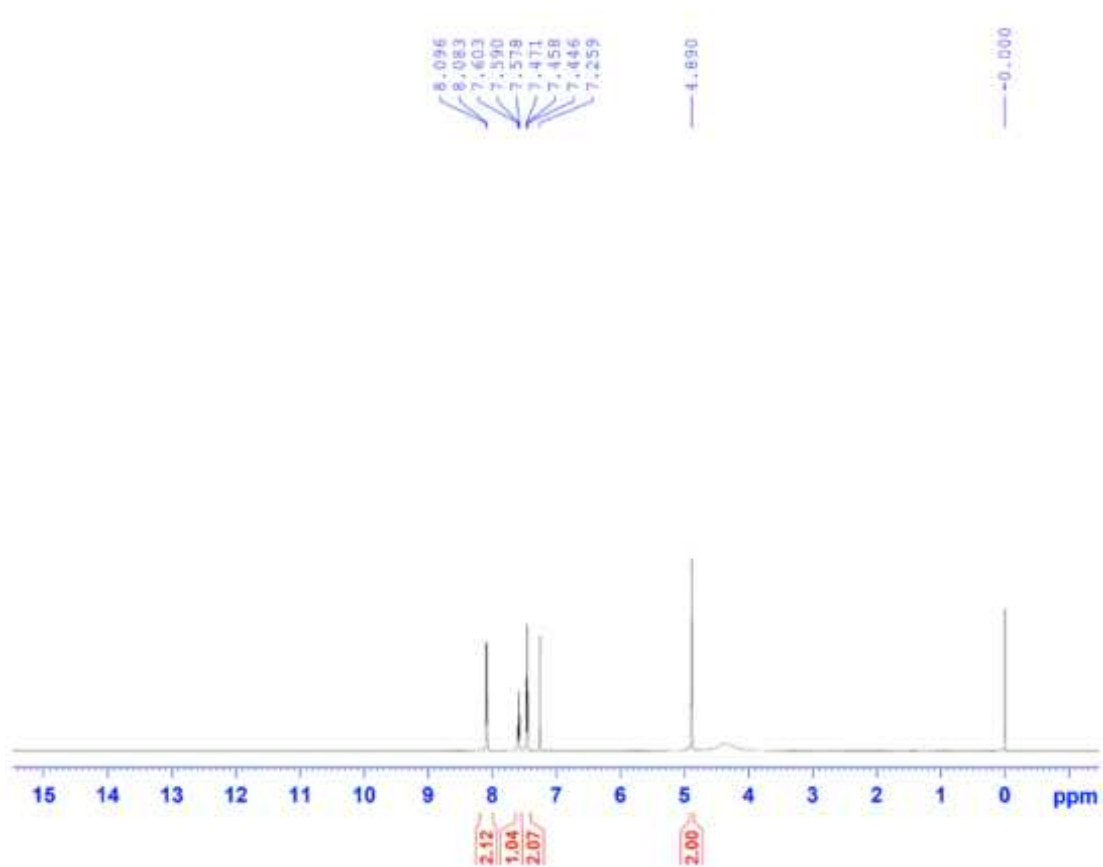
**Figure S81:** HMBC spectrum of compound 9 (benzoic acid)



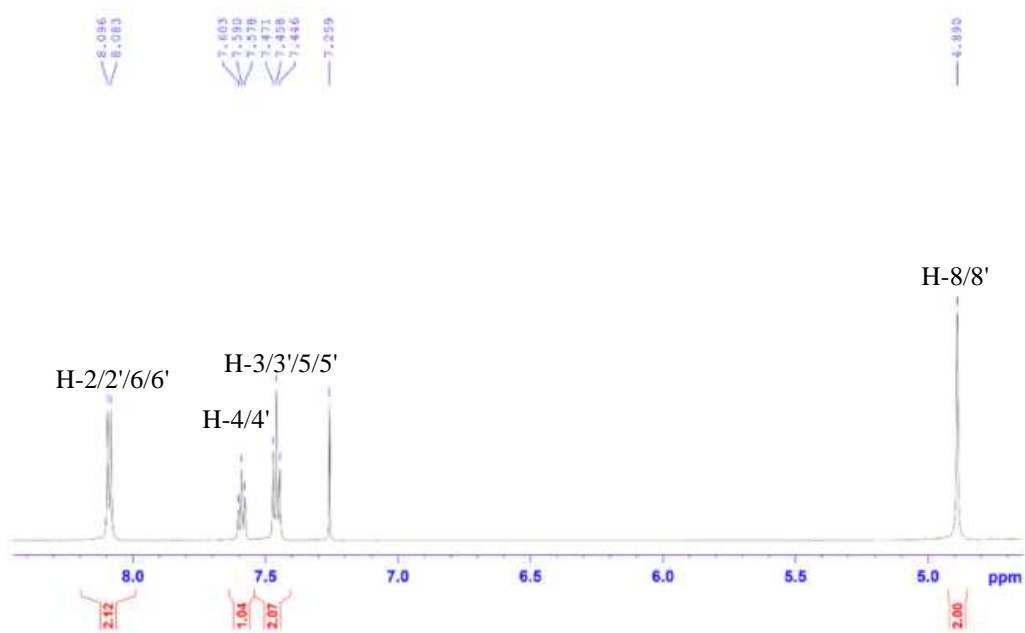
**Figure S82:** HMBC spectrum of compound **9** (benzoic acid) (from  $\delta_c$  125 ppm to  $\delta_c$  170 ppm)

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

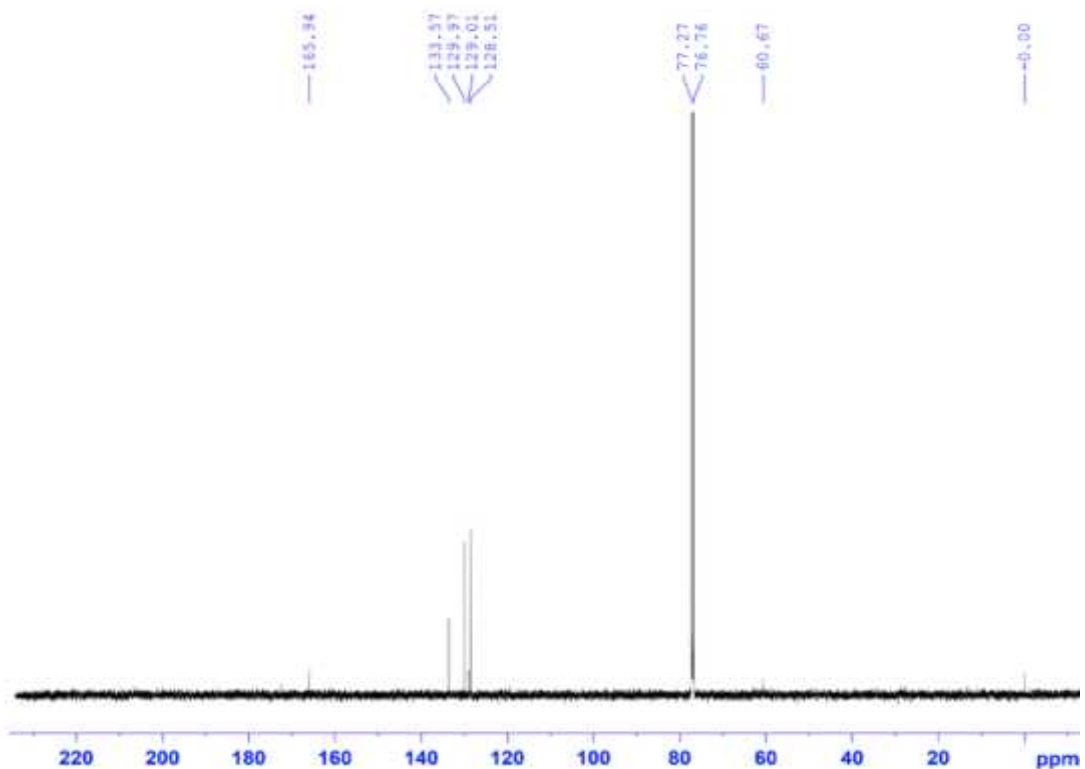
Position	Compound <b>10</b> (DMSO- <i>d</i> <sub>6</sub> )		Ethylene glycol dibenzoate (CDCl <sub>3</sub> ) [38]	
	<sup>13</sup> C-NMR (150 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> 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)



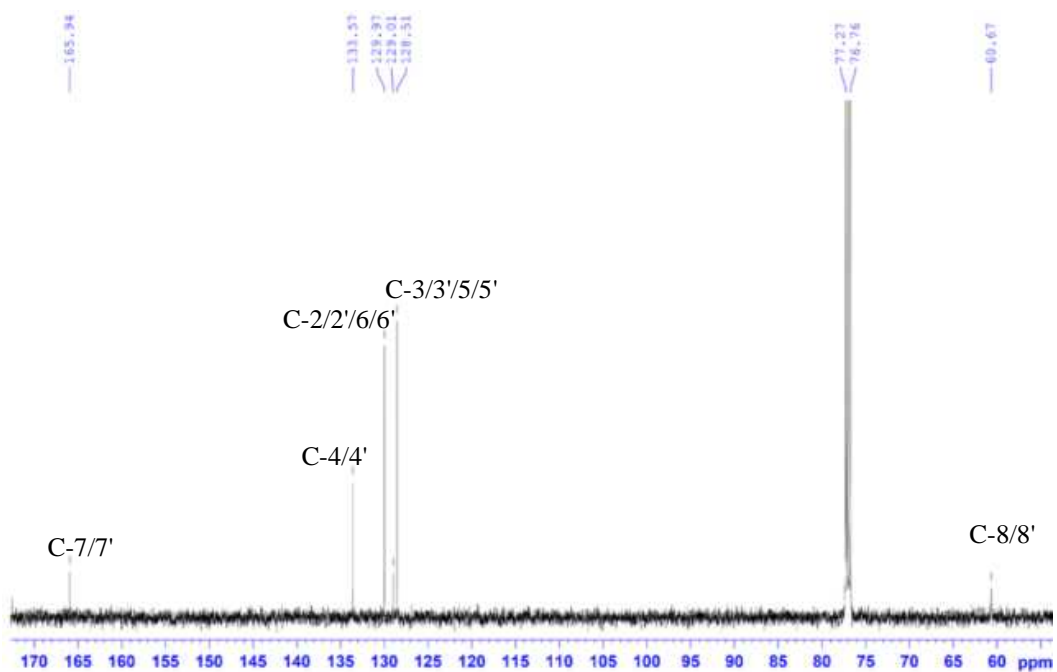
**Figure S83:**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **10** (ethylene glycol dibenzoate)



**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) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (600 MHz) δ <sub>H</sub> ppm	<sup>13</sup> C-NMR (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> 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)

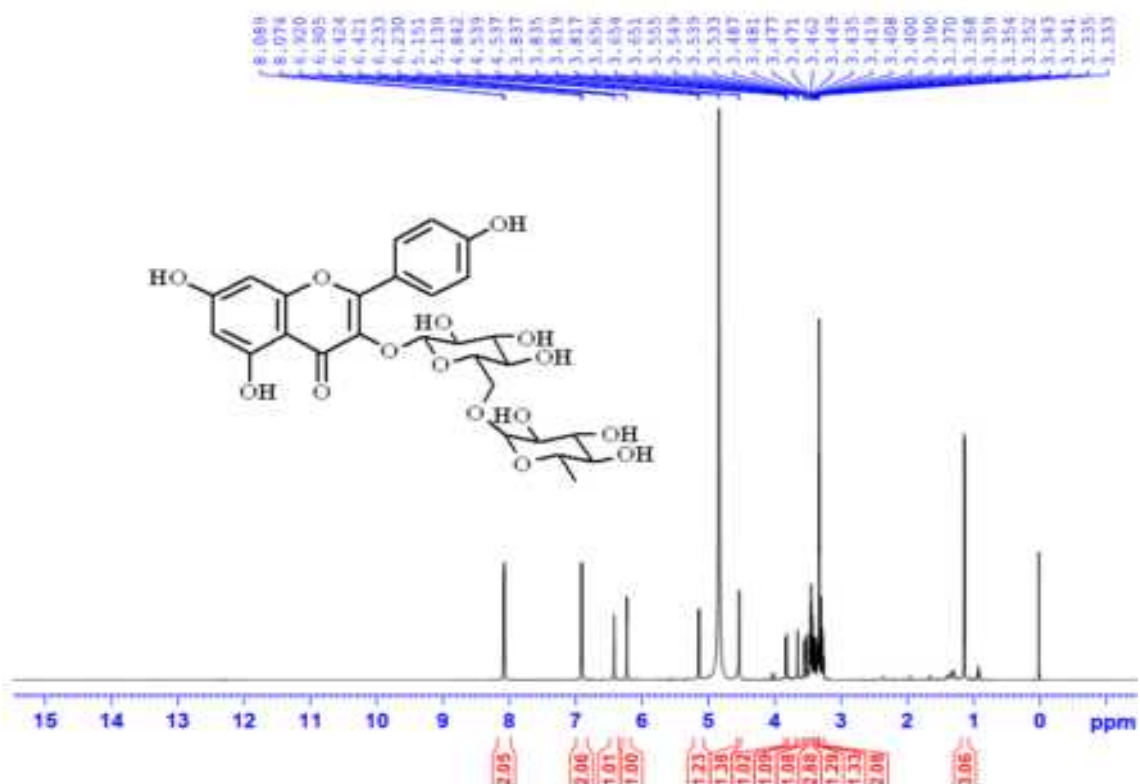


Figure S87:  $^1\text{H-NMR}$  (600 MHz, MeOD) spectrum of compound **11** (nicotiflorin)

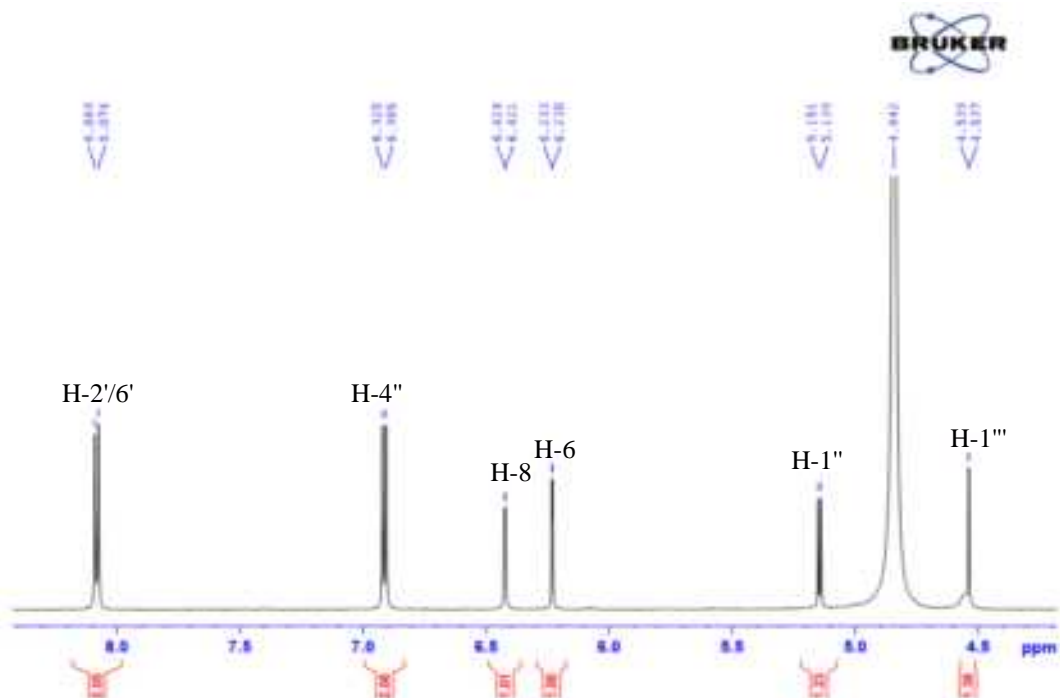
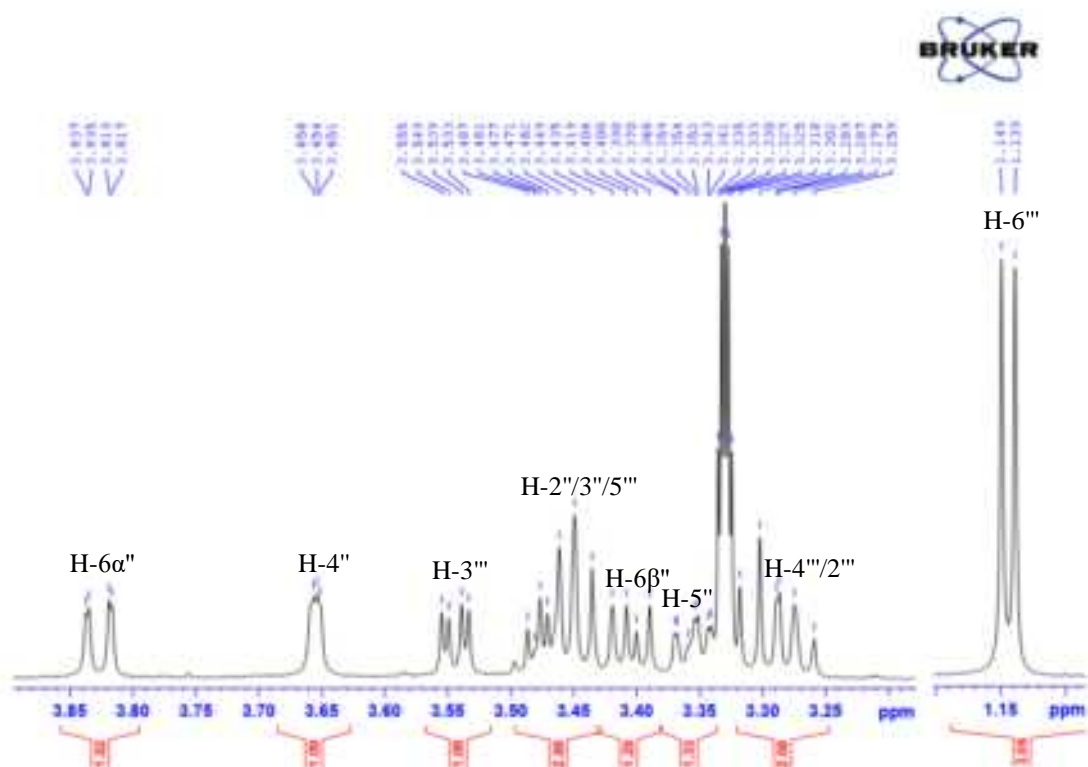
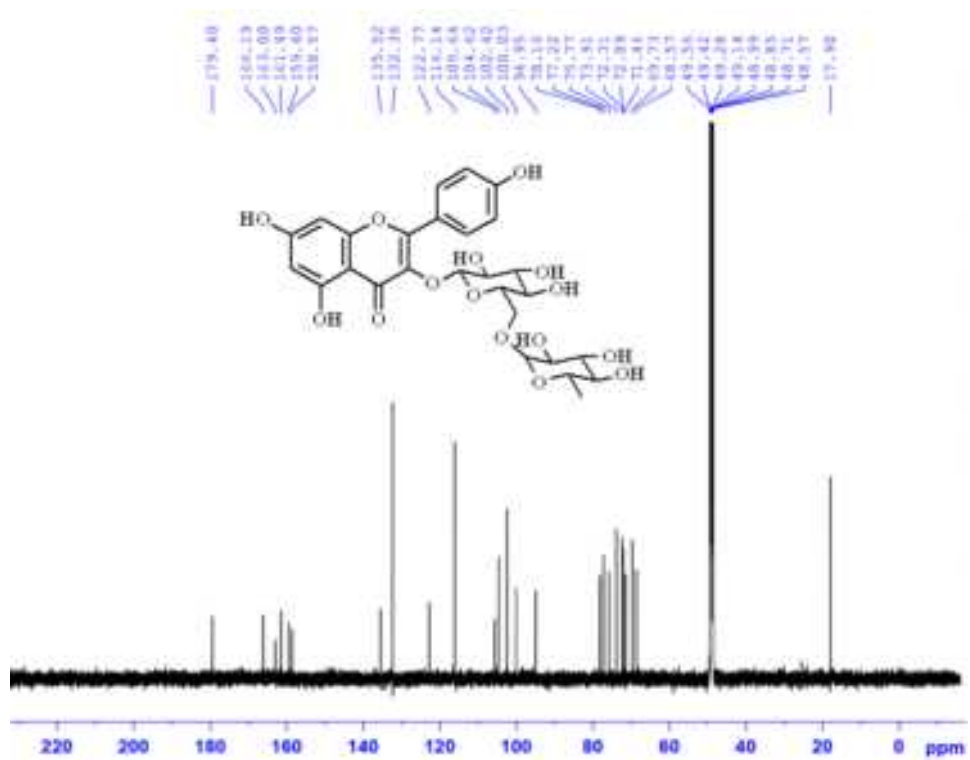


Figure S88:  $^1\text{H-NMR}$  (600 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{H}}$  4.5 ppm to  $\delta_{\text{H}}$  8.0 ppm)

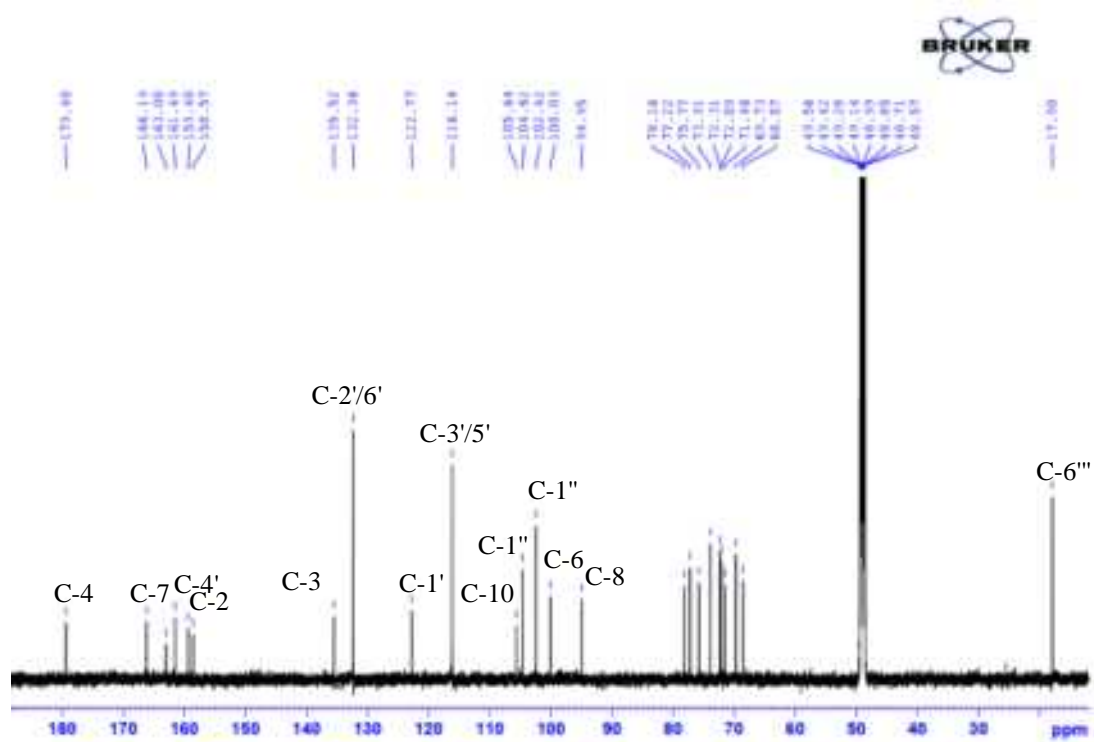


**Figure S89:**  $^1\text{H-NMR}$  (600 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_{\text{H}}$  1.10 ppm)

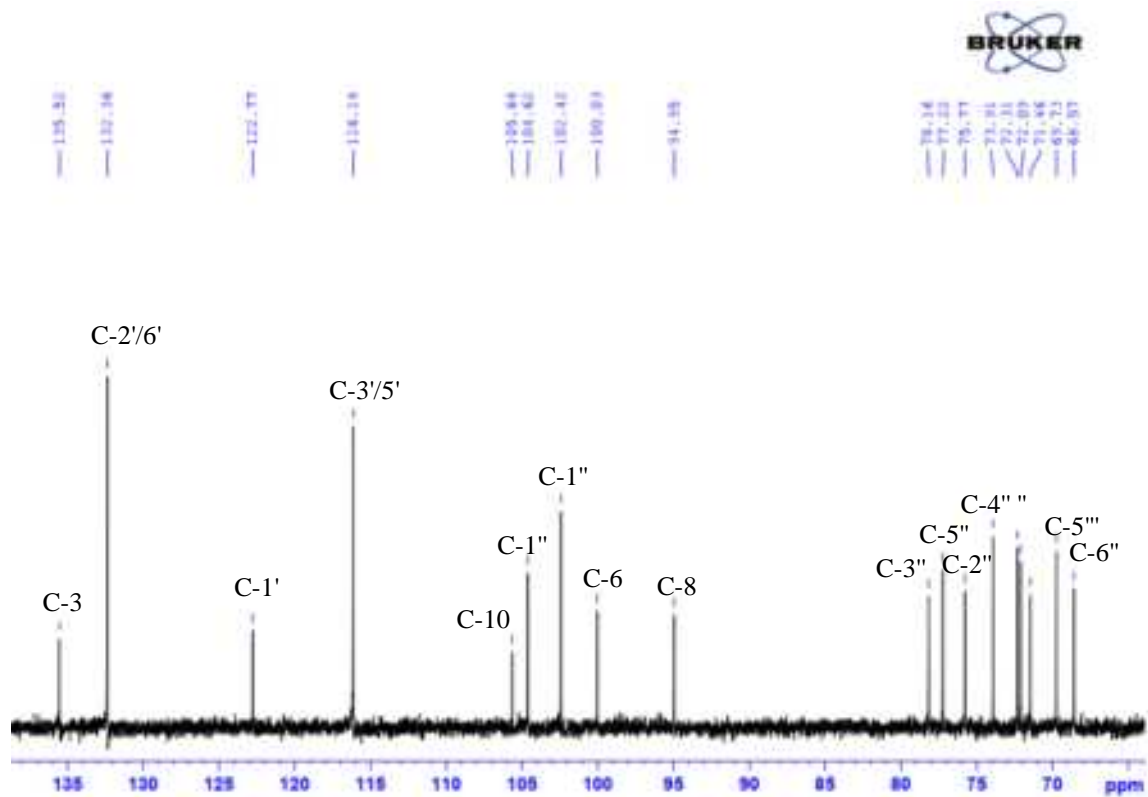


**Figure S90:**  $^{13}\text{C-NMR}$  (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin)

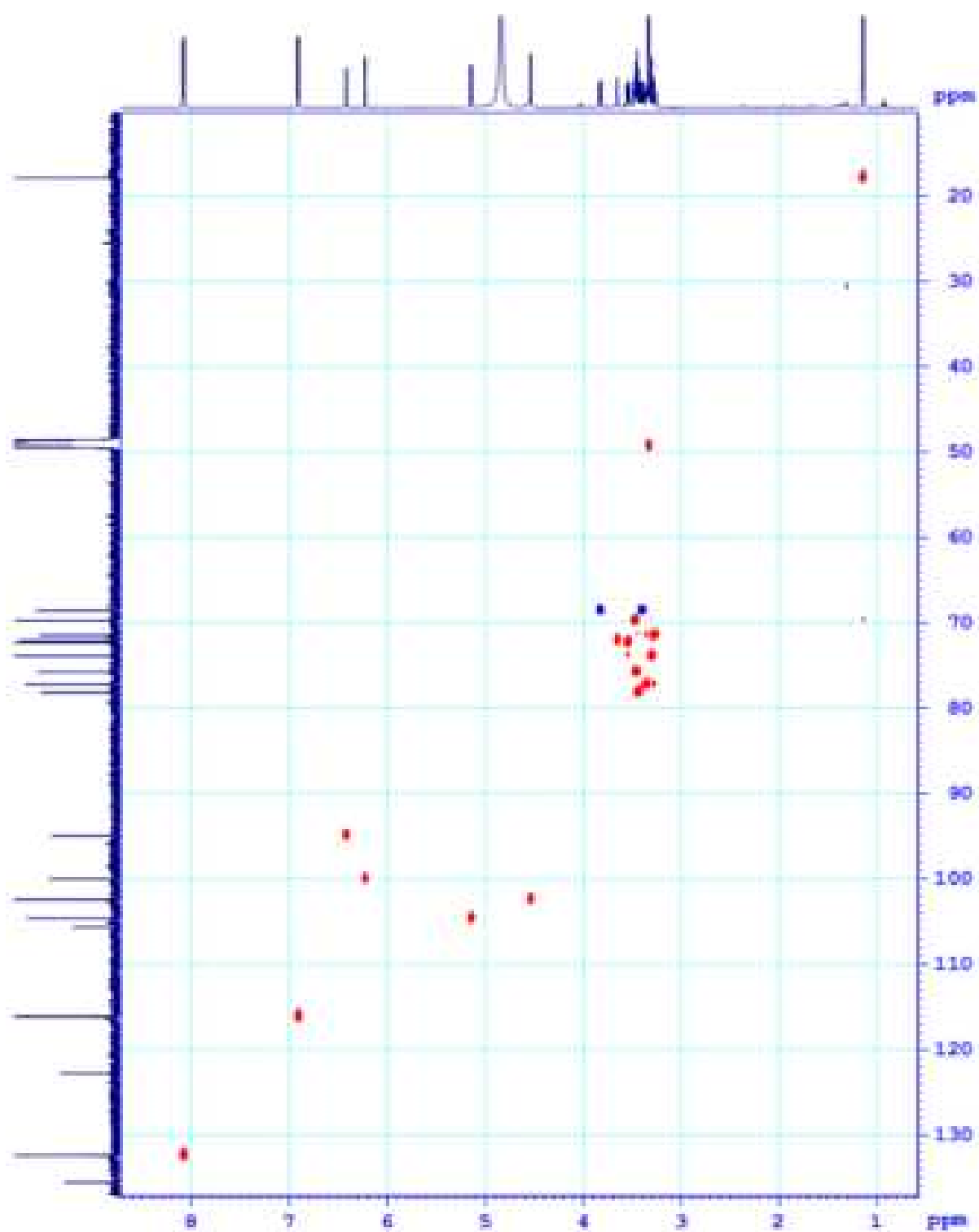




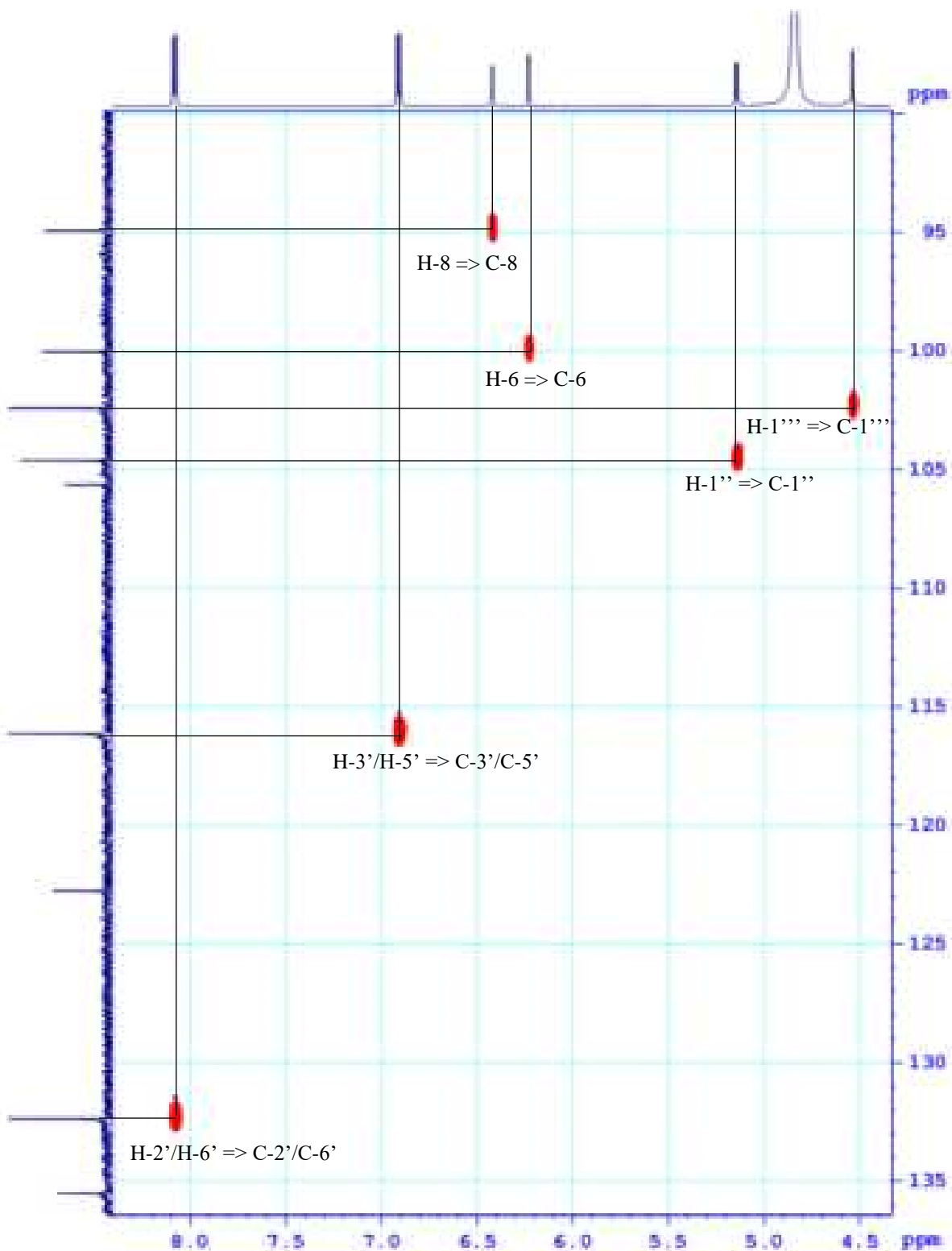
**Figure S91:** <sup>13</sup>C-NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_C$  20 ppm to  $\delta_C$  180 ppm)



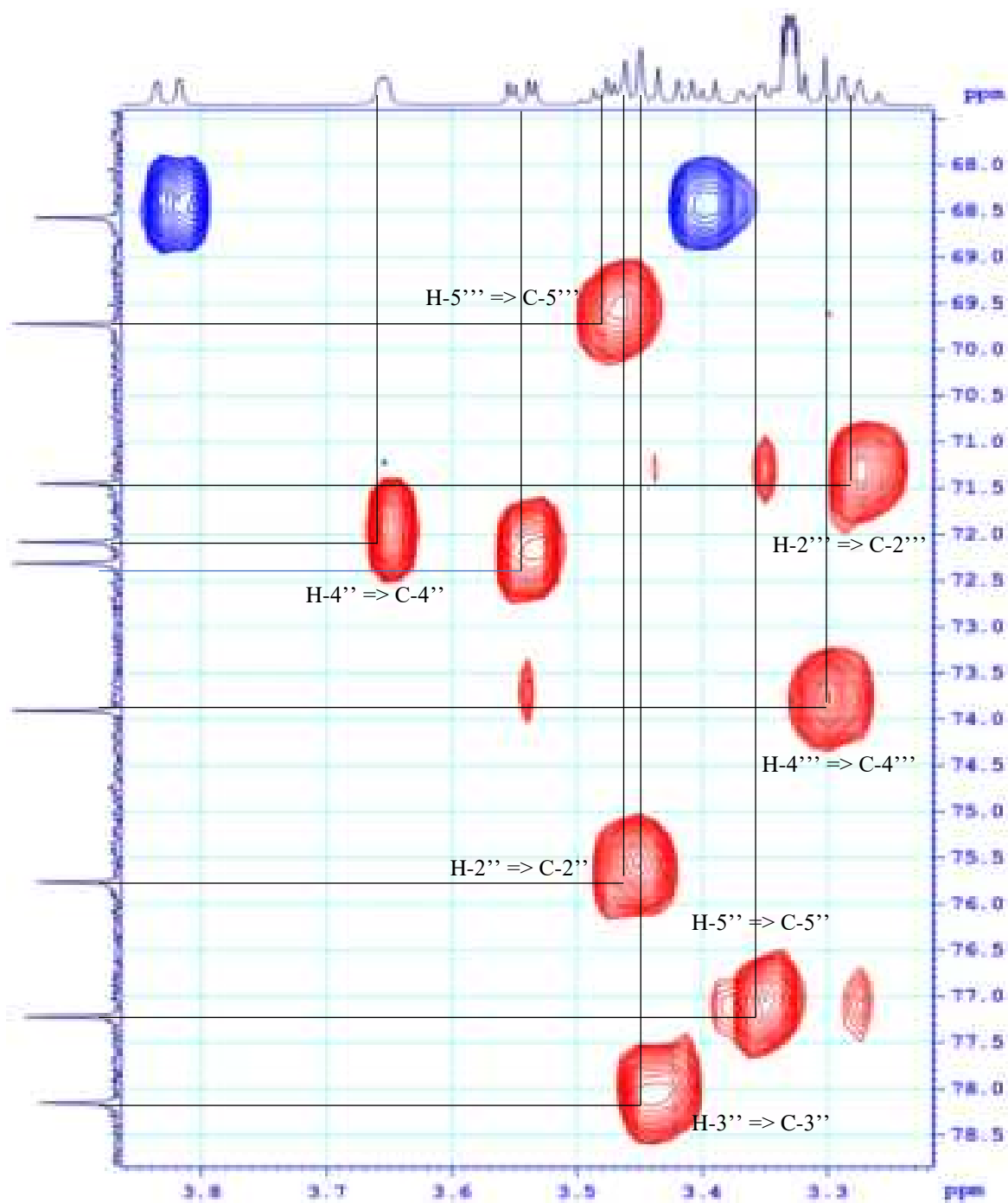
**Figure S92:** <sup>13</sup>C-NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from  $\delta_C$  65 ppm to  $\delta_C$  135 ppm)



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



**Figure S94:** HSQC spectrum of compound **11** (nicotiflorin) (from  $\delta_c$  90 ppm to  $\delta_c$  135 ppm)



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

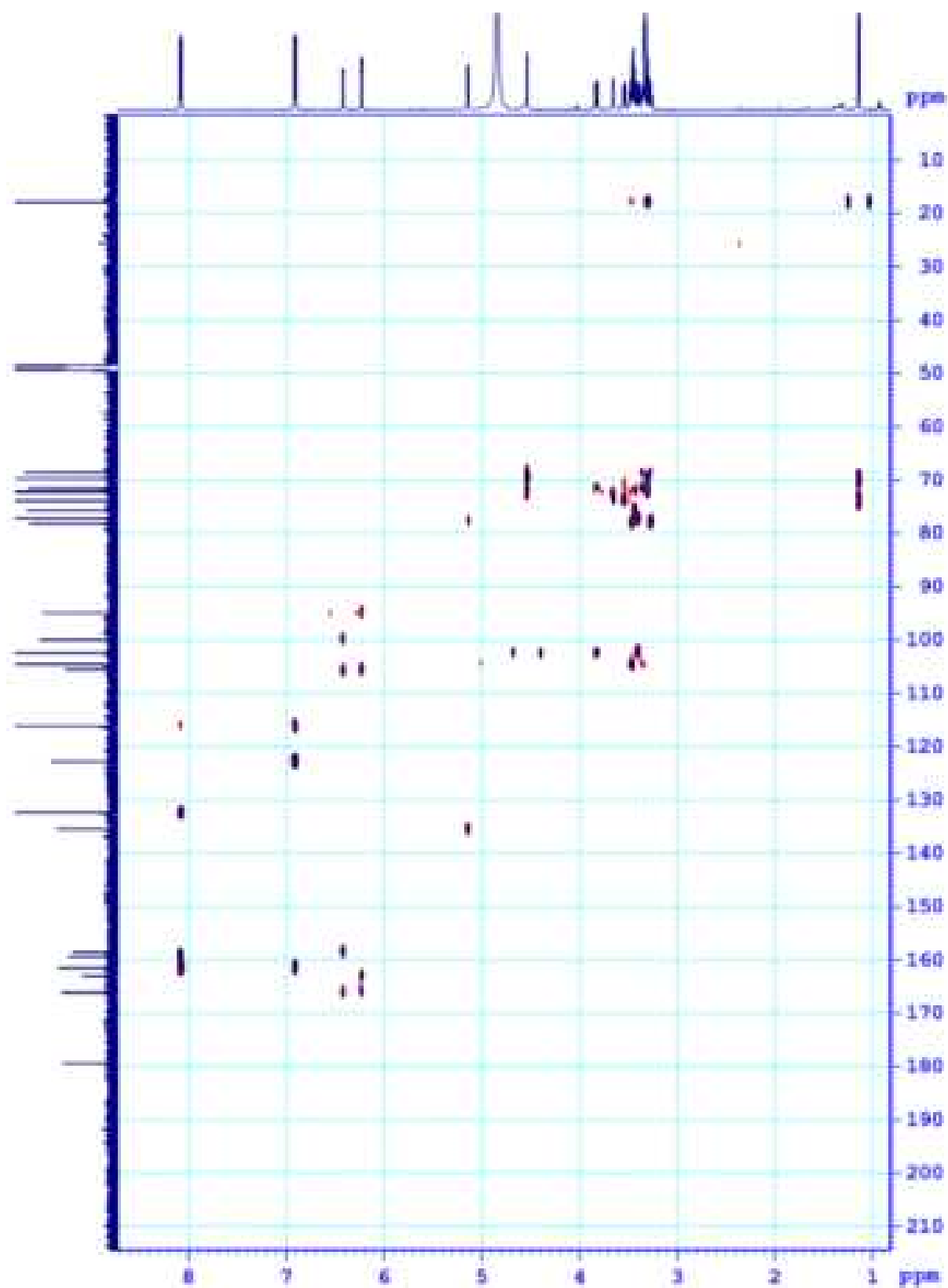
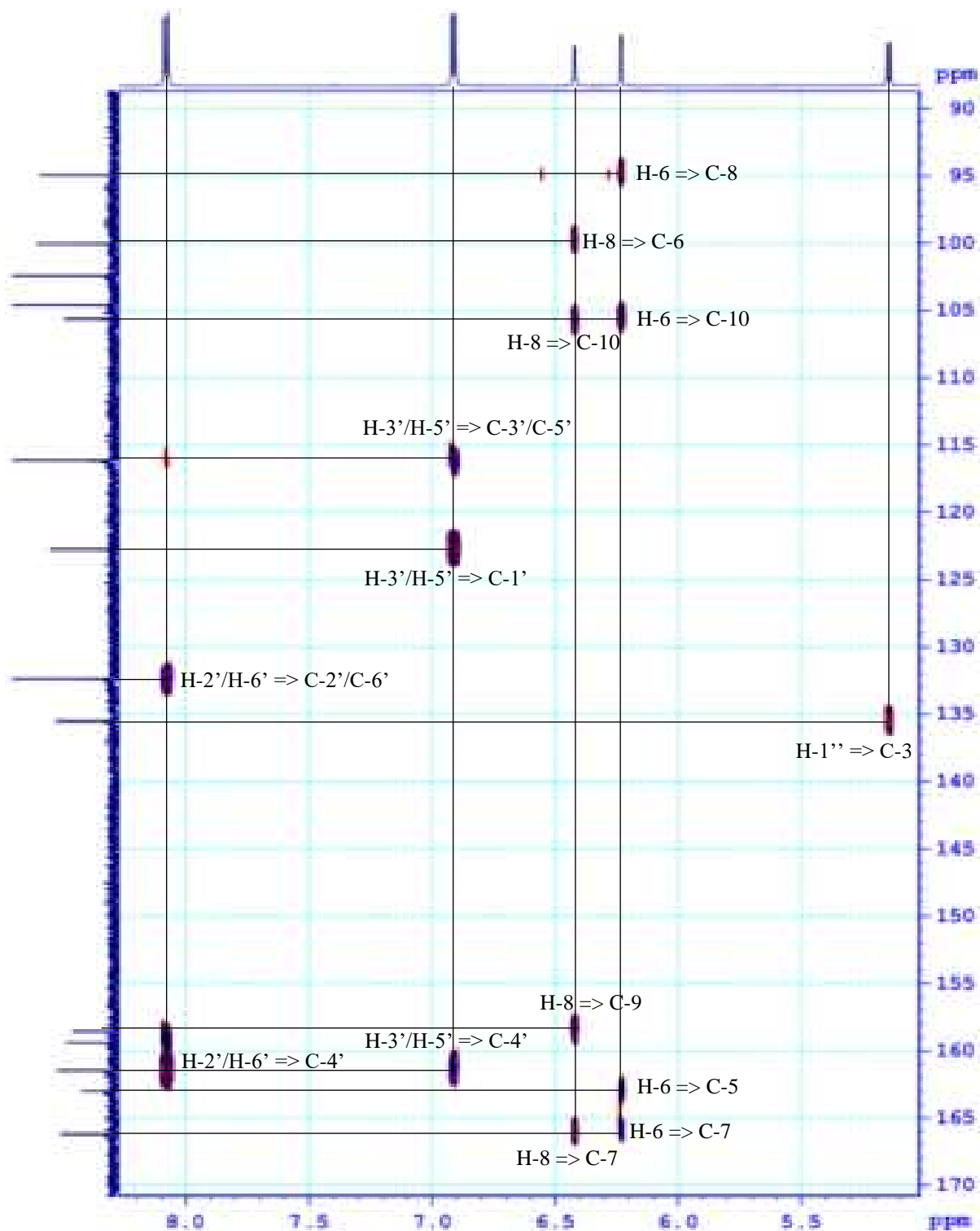


Figure S96: HMBC spectrum of compound **11** (nicotiflorin)



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

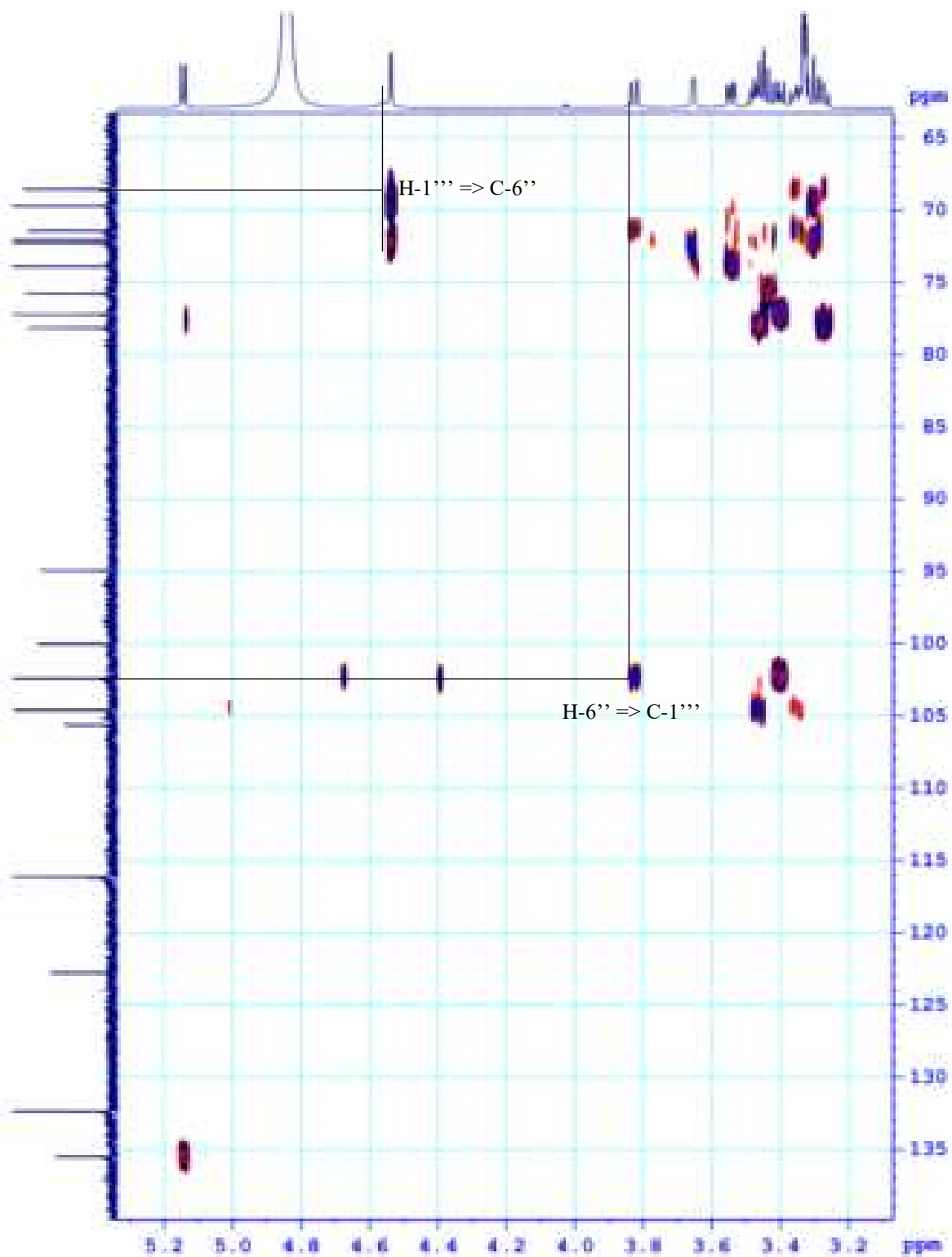
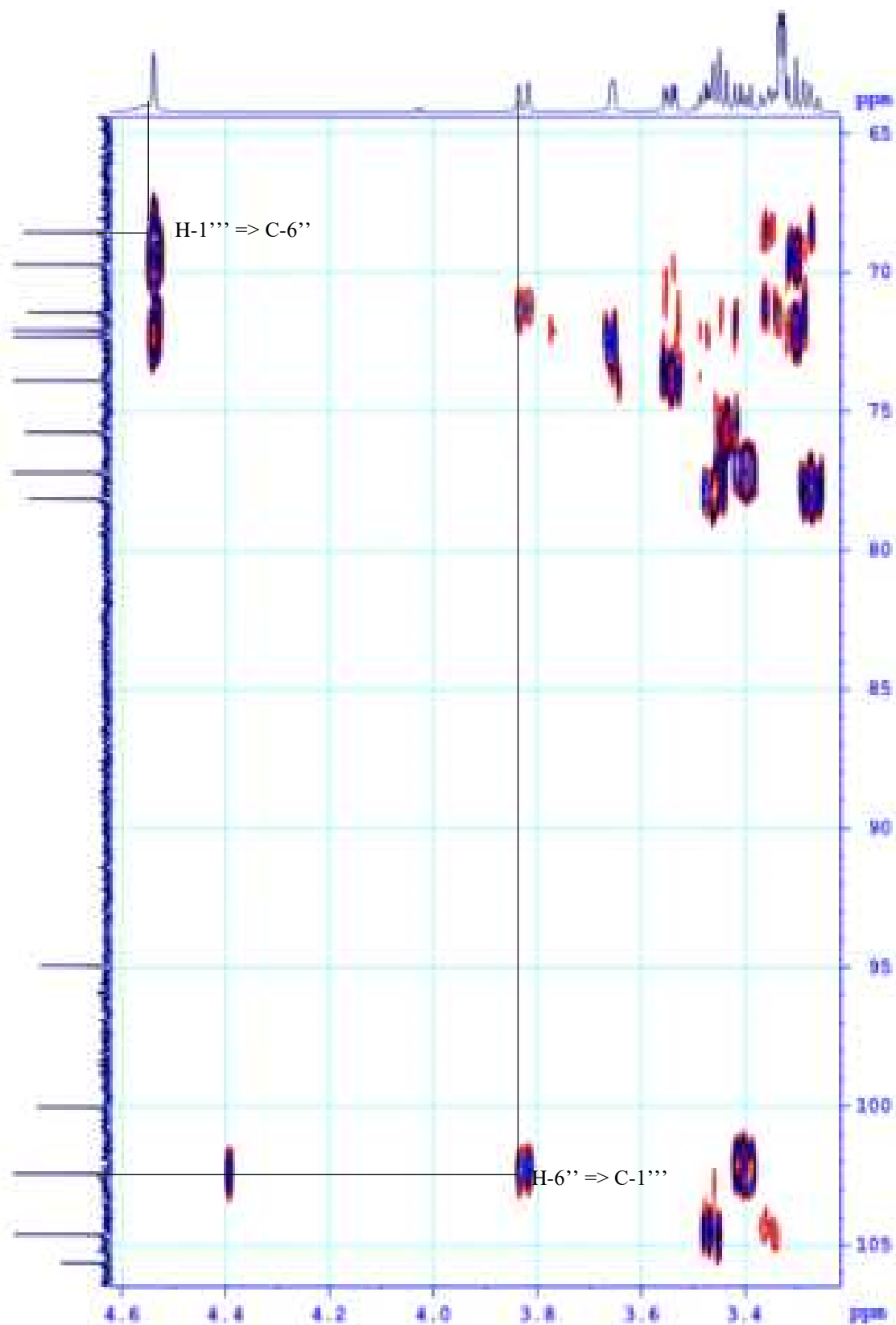
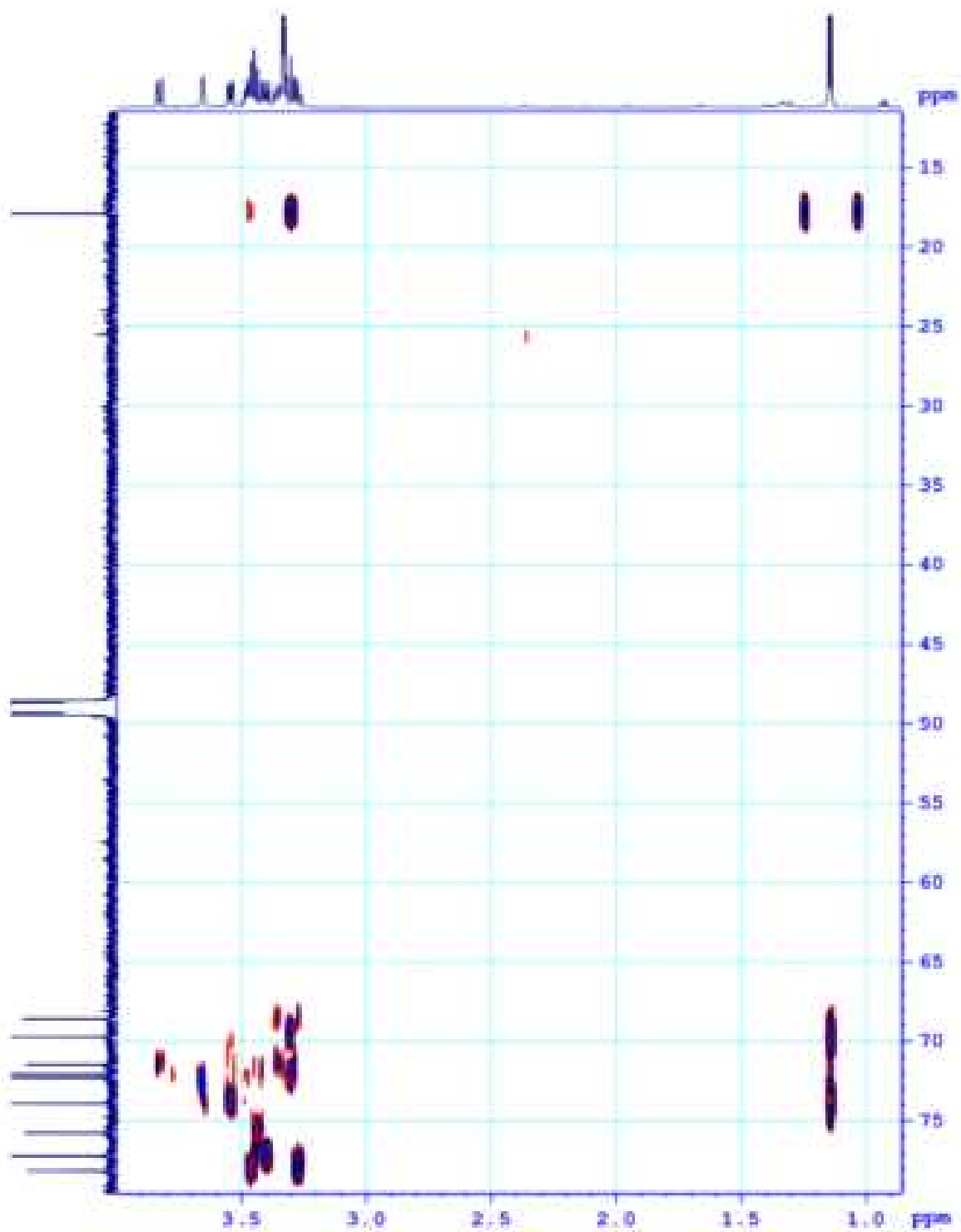


Figure S98: HMBC spectrum of compound 11 (nicotiflorin) (from  $\delta_C$  65 ppm to  $\delta_C$  140 ppm)



**Figure S99:** HMBC spectrum of compound **11** (nicotiflorin) (from  $\delta_c$  65 ppm to  $\delta_c$  105 ppm)





**Figure S100:** HMBC spectrum of compound **11** (nicotiflorin) (from  $\delta_c$  15 ppm to  $\delta_c$  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 <sub>2</sub> O)		3,3',4,4'-tetrahydroxybiphenyl (CDCl <sub>3</sub> ) [40]	
	<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 (125 MHz) δ <sub>C</sub> ppm	<sup>1</sup> H-NMR (500 MHz) δ <sub>H</sub> 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

Print Date: 7/11/2023 2:57:13 PM  
Acq. Date: 7/11/2023 2:52:14 PM

Instrument: LC-MSD-Trip-SL  
Operator: 21954104E0000514

Analysis Name: SALL1.d  
Method: Quag\_2020.m  
Sample Name: SALL1  
Analysis Info:

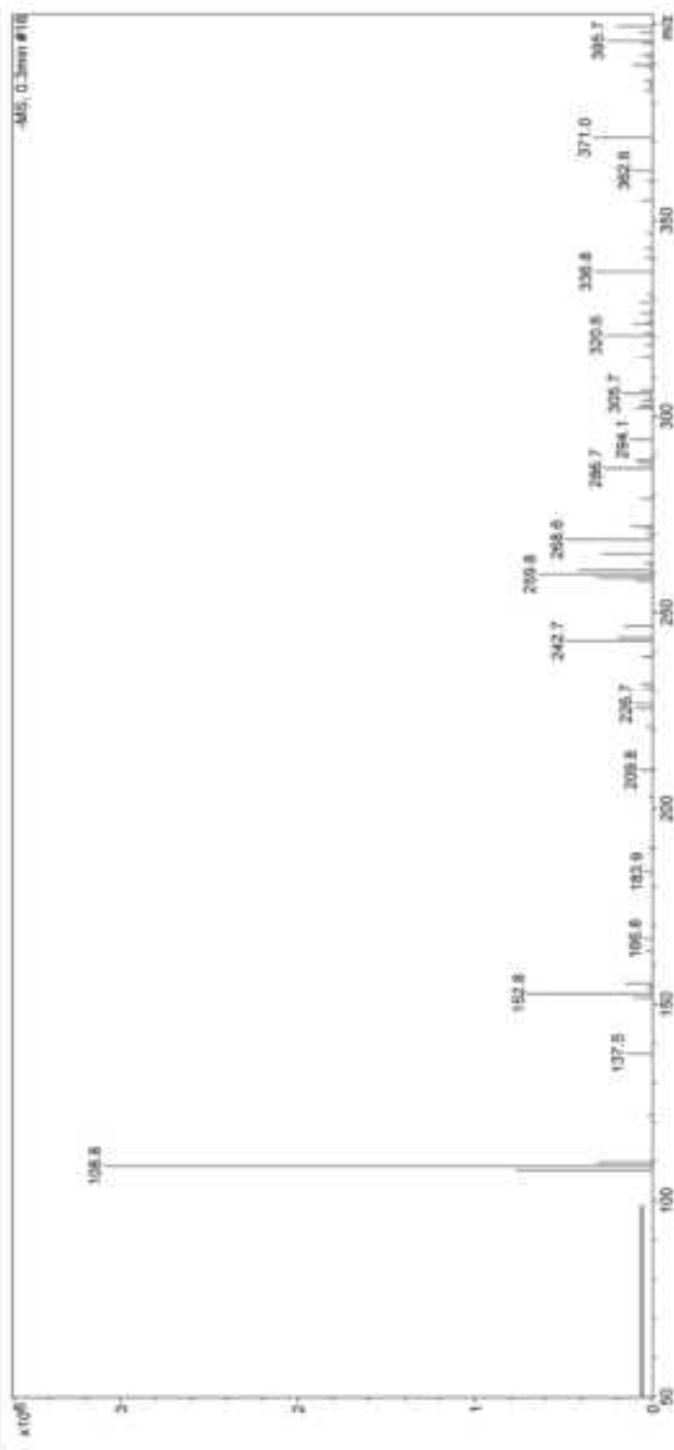
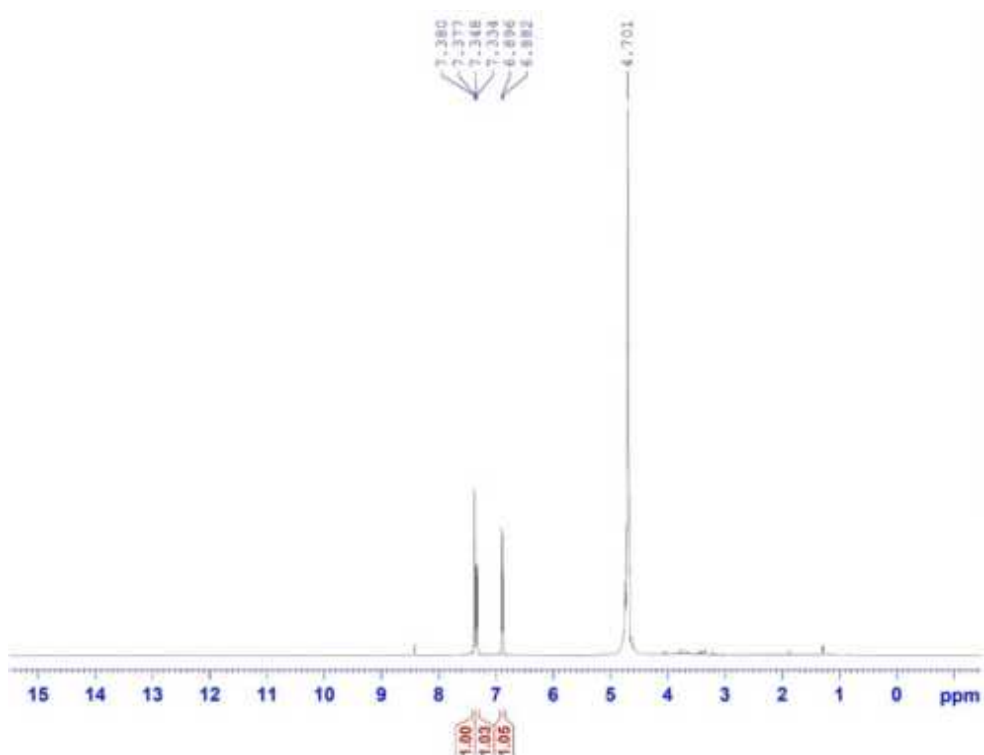
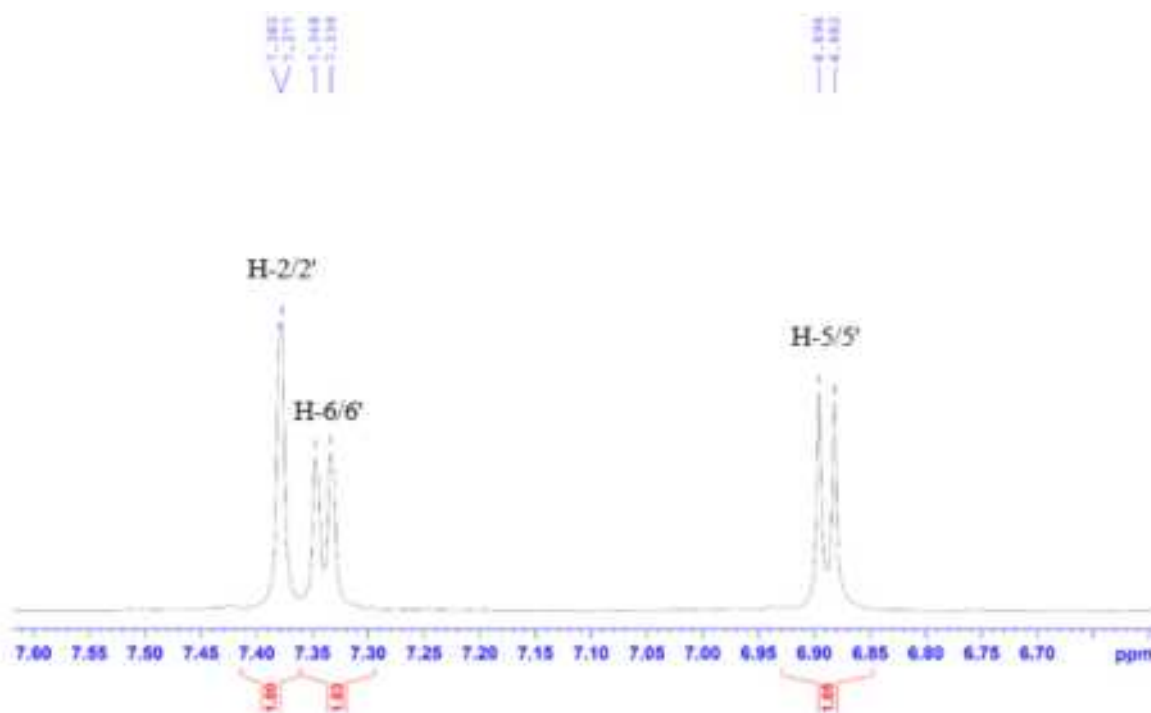


Figure S101: (-)-ESI-MS spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)



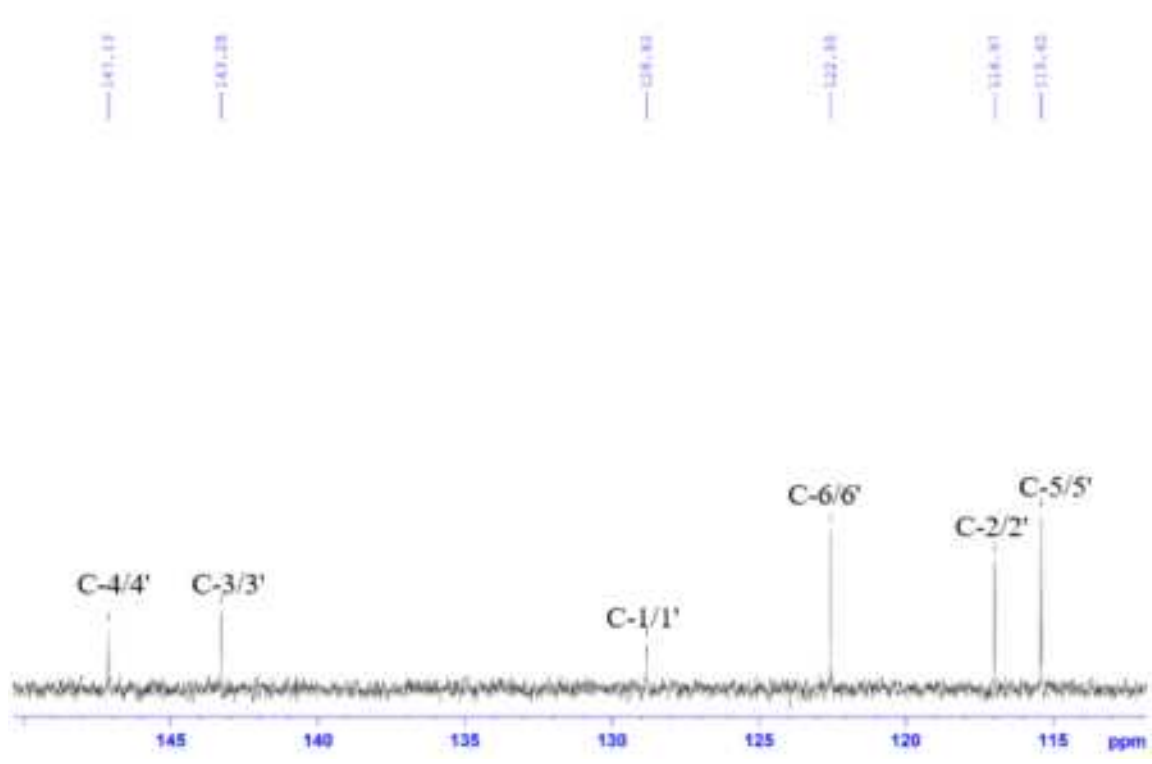
**Figure S102:**  $^1\text{H-NMR}$  (600 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)



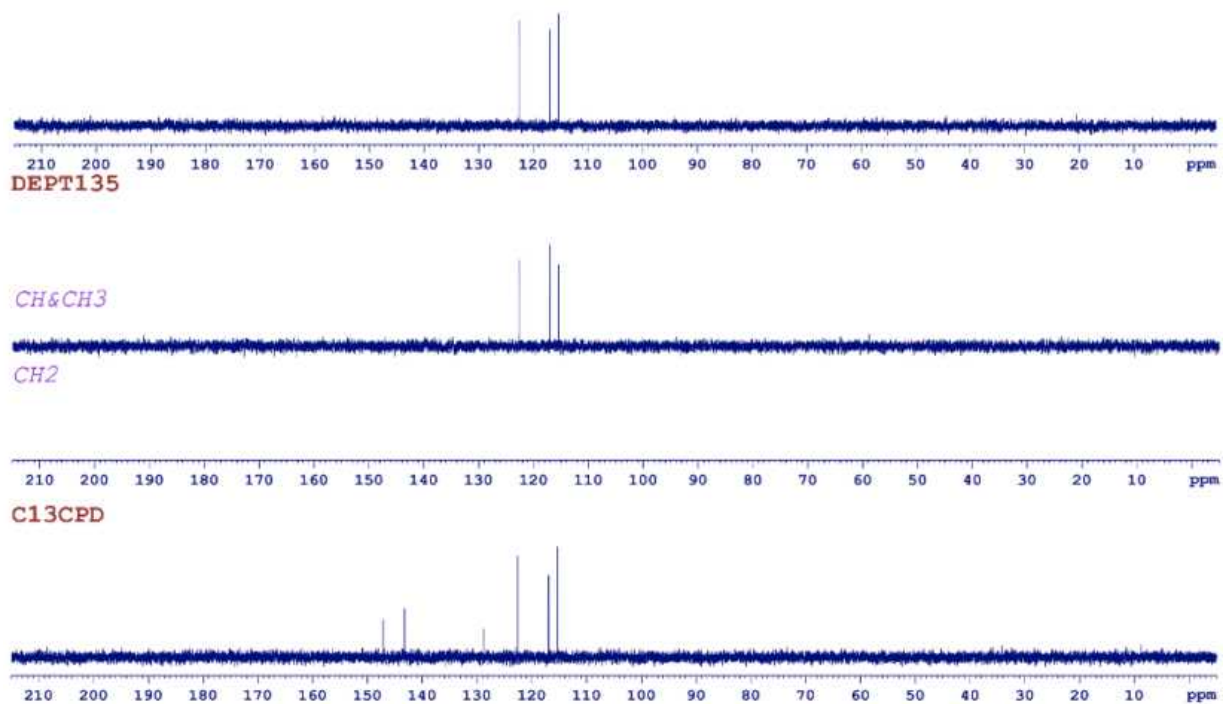
**Figure S103:**  $^1\text{H-NMR}$  (600 MHz,  $\text{D}_2\text{O}$ ) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl) (from  $\delta_{\text{H}}$  6.6 ppm to  $\delta_{\text{H}}$  7.6 ppm)



**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