Supporting Information

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

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

Position	Compound 1 (DMSO-d_6)		Chrysin (DMSO-d_6) [28]	
	^{13}C-NMR (150 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_H ppm
2	161.4	-	161.95	-
3	105.1	6.95 (1H, *s*)	104.47	6.96 (1H, *s*)
4	181.8	-	182.34	-
5	163.1	-	163.69	-
6	98.9	6.22 (1H, *d*, 1.8 Hz)	99.51	6.20 (1H, *d*, 1.8 Hz)
7	164.4	-	164.91	-
8	94.0	6.52 (1H, *d*, 1.8 Hz)	94.61	6.51 (1H, *d*, 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, *m*)	126.89	8.06 (2H, *m*)
3', 5'	129.1	7.58 (2H, *m*)	129.61	7.58 (3H, *m*)
4'	131.9	7.62 (1H, *m*)	131.21	

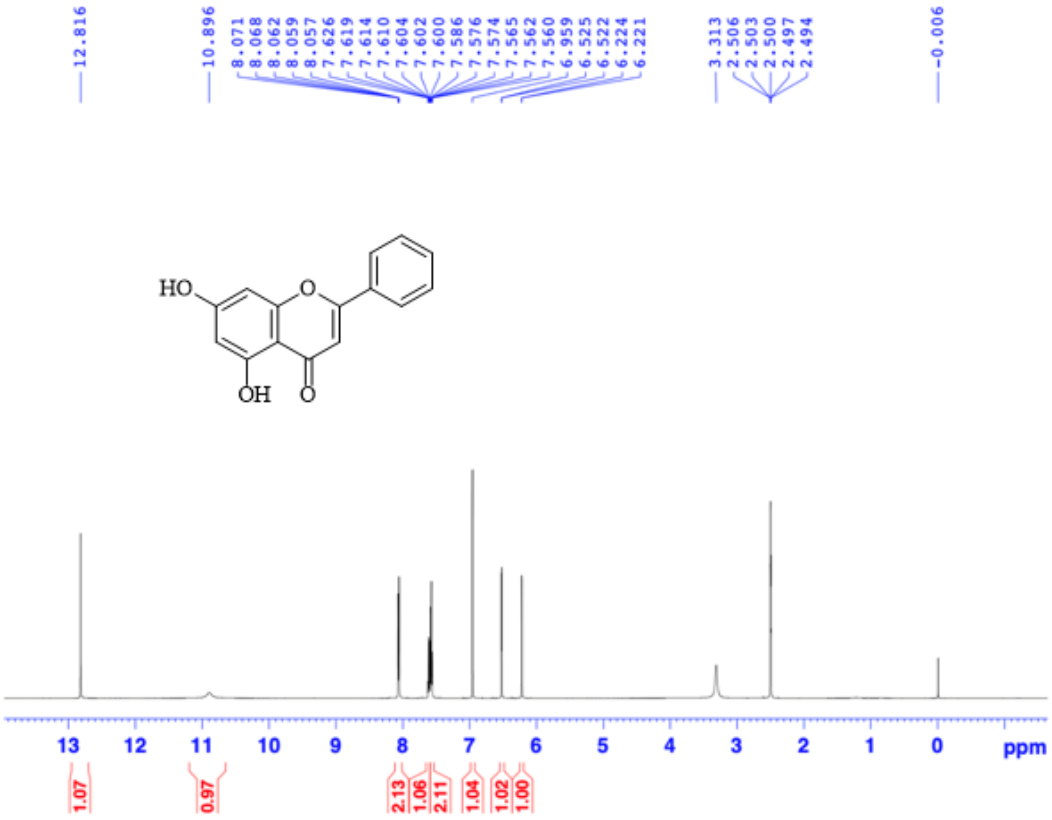

Figure S1: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **1** (chrysin)

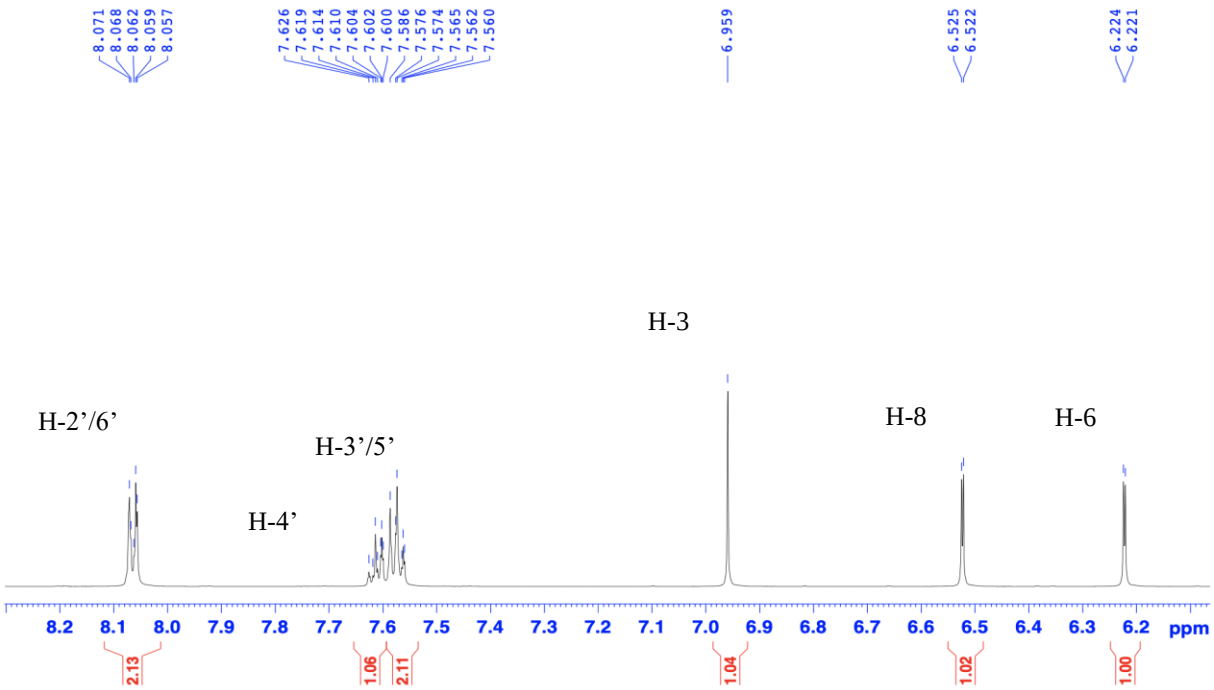

Figure S2: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **1** (chrysin) (from δ_H 6 ppm to δ_H 9 ppm)

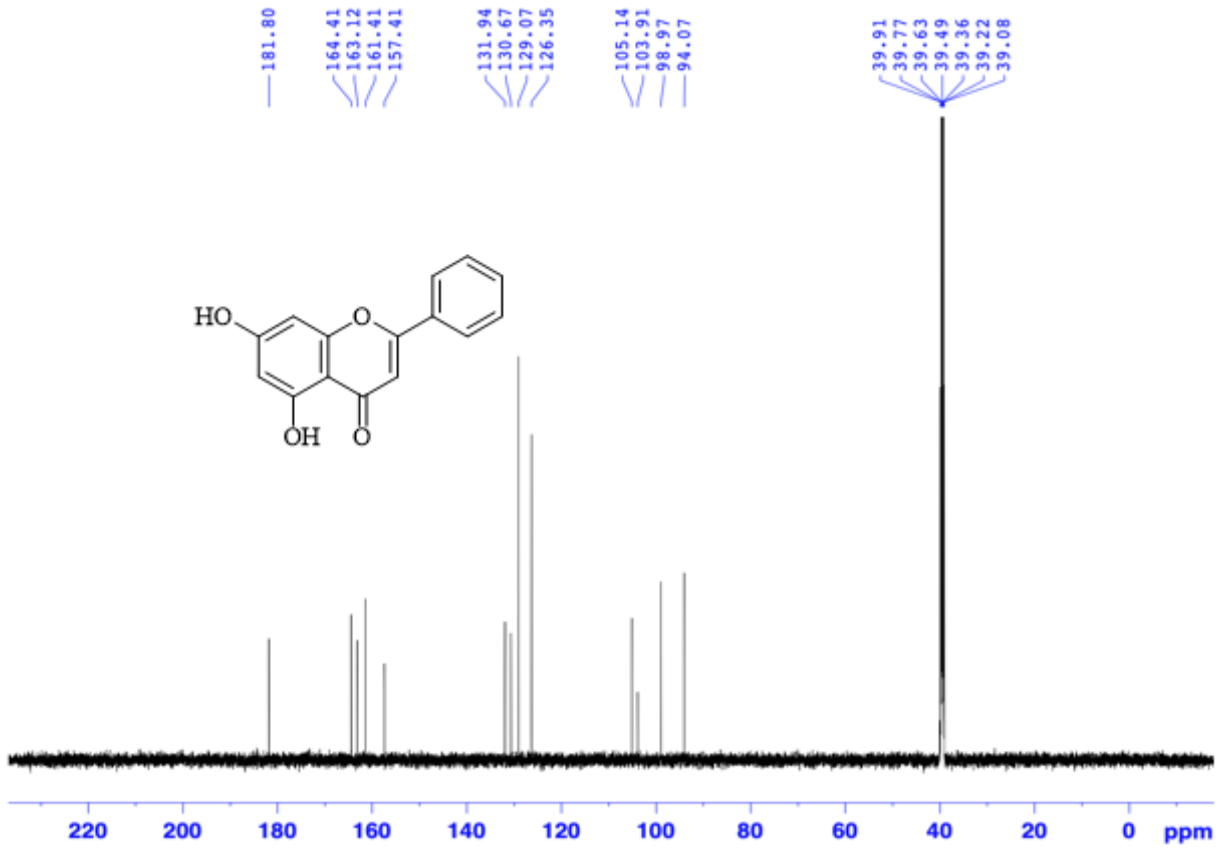

Figure S3: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **1** (chrysin)

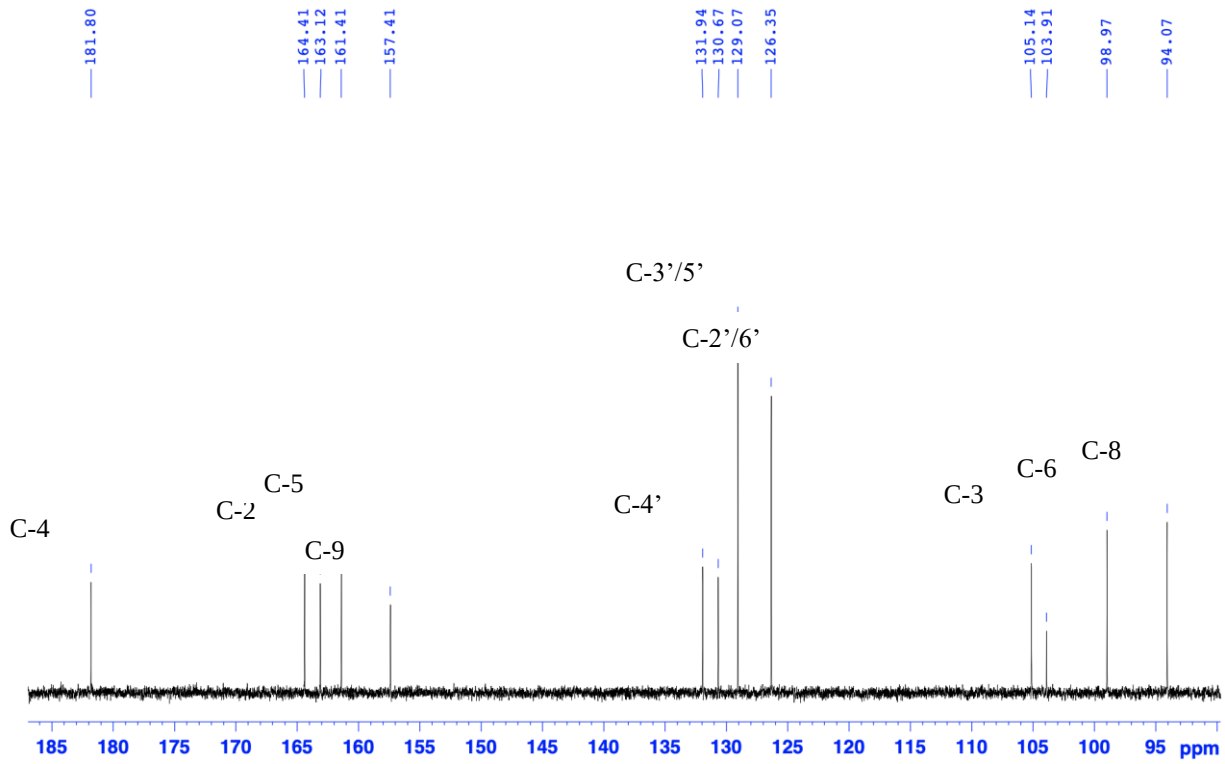

Figure S4: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **1** (chrysin) (from δ_C 95 ppm to δ_C 190 ppm)

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

Position	Compound 2 (DMSO-d_6)		Daucosterol (DMSO-d_6) [29]	
	^{13}C-NMR (150 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (100 MHz) δ_C ppm	**^{1}H-NMR** (400 MHz) δ_H ppm
1	36.2	-	36.1	-
2	31.3	-	31.3	-
3	76.7	3.66 (1H, *m*)	76.6	3.95 (1H, *m*)
4	38.3	2.50 (1H, *m*)	38.2	2.62 (1H, *m*) 2.36 (1H, *m*)
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, *s*)	11.6	0.65 (3H, *s*)
19	19.6	0.71 (3H, *s*)	18.8	0.95 (3H, *s*)
20	36.8	-	36.7	-
21	20.6	0.89 (3H, *s*)	18.5	0.98 (3H, *d*, 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, *s*)	19.6	0.87 (3H, *d*, 6.7 Hz)
28	22.6	0.90 (3H, *s*)	22.5	0.89 (3H, *d*, 6.5 Hz)
29	11.7	0.93 (3H, *s*)	11.7	0.88 (3H, *t*, 7.2 Hz)
1'	100.8	4.85 (1H, *m*)	100.7	4.87 (1H, *d*, 7.9 Hz)
2'	73.4	4.22 (1H, *m*)	73.4	4.05 (1H, *t*, 8,0 Hz)
3'	76.9	4.38 (1H, *m*)	76.9	4.25(1H, *t*, 9,0 Hz)

Position	Compound 2 (DMSO-d_6)		Daucosterol (DMSO-d_6) [29]	
	^{13}C-NMR (150 MHz) δ_C ppm	^{1}H-NMR (600 MHz) δ_H ppm	^{13}C-NMR (100 MHz) δ_C ppm	^{1}H-NMR (400 MHz) δ_H ppm
4'	70.1	4.39 (1H, *m*)	70.0	4.28 (1H, *t*, 8,0 Hz)
5'	70.7	4.21(1H, *m*)	76.7	4.00 (1H, *m*)
6'	61.1	4.32 (2H, *m*)	61.0	4.55 (1H, *t*, 5.4 Hz) 4.39 (1H, *dd*, 12.0 Hz)

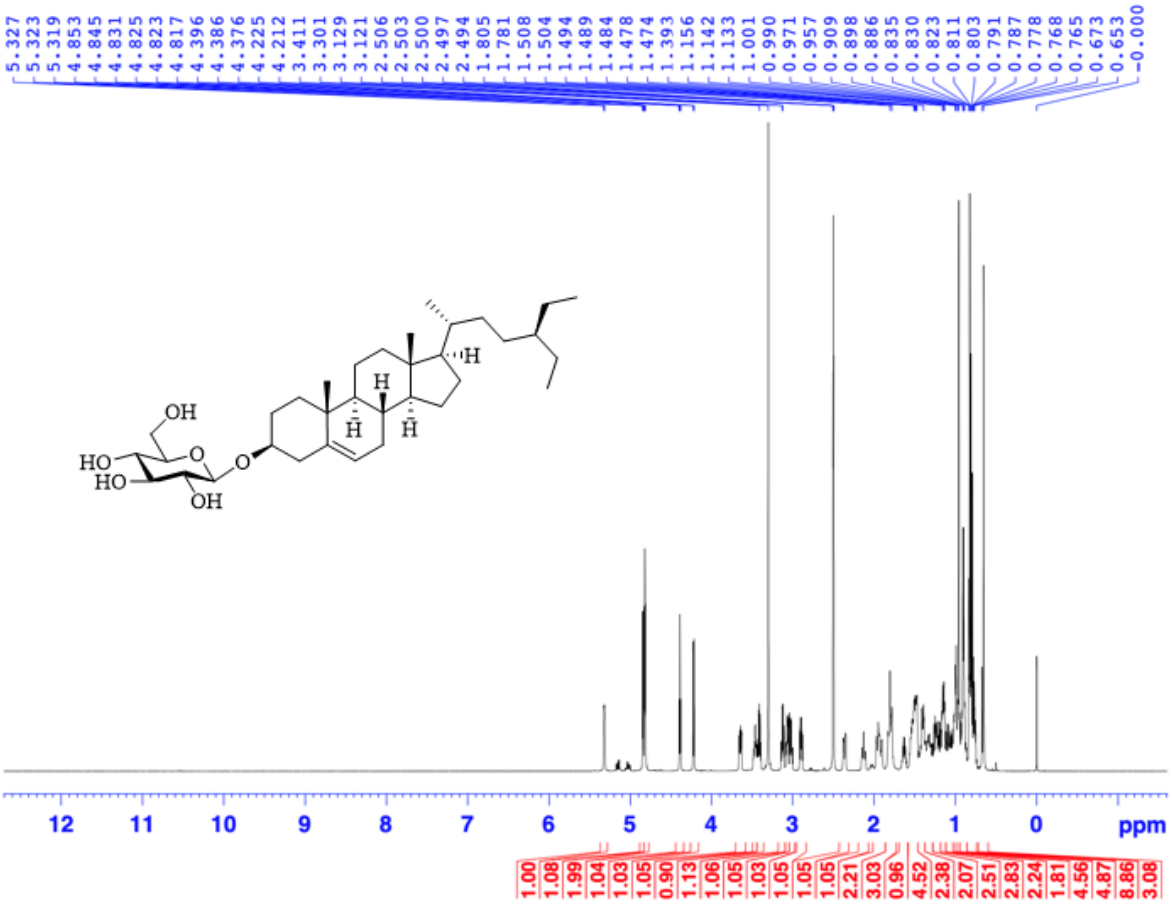

Figure S5: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol)

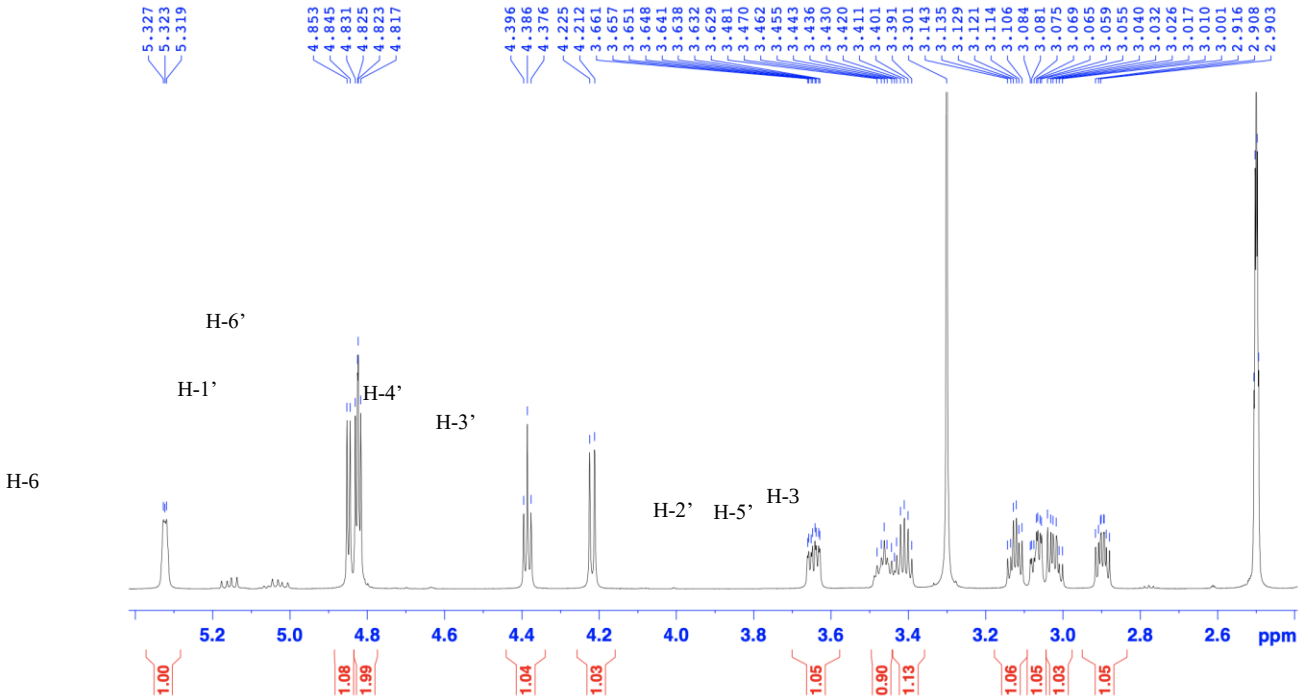

Figure S6: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol) (from δ_H 2.7 ppm to δ_H 5.3 ppm)

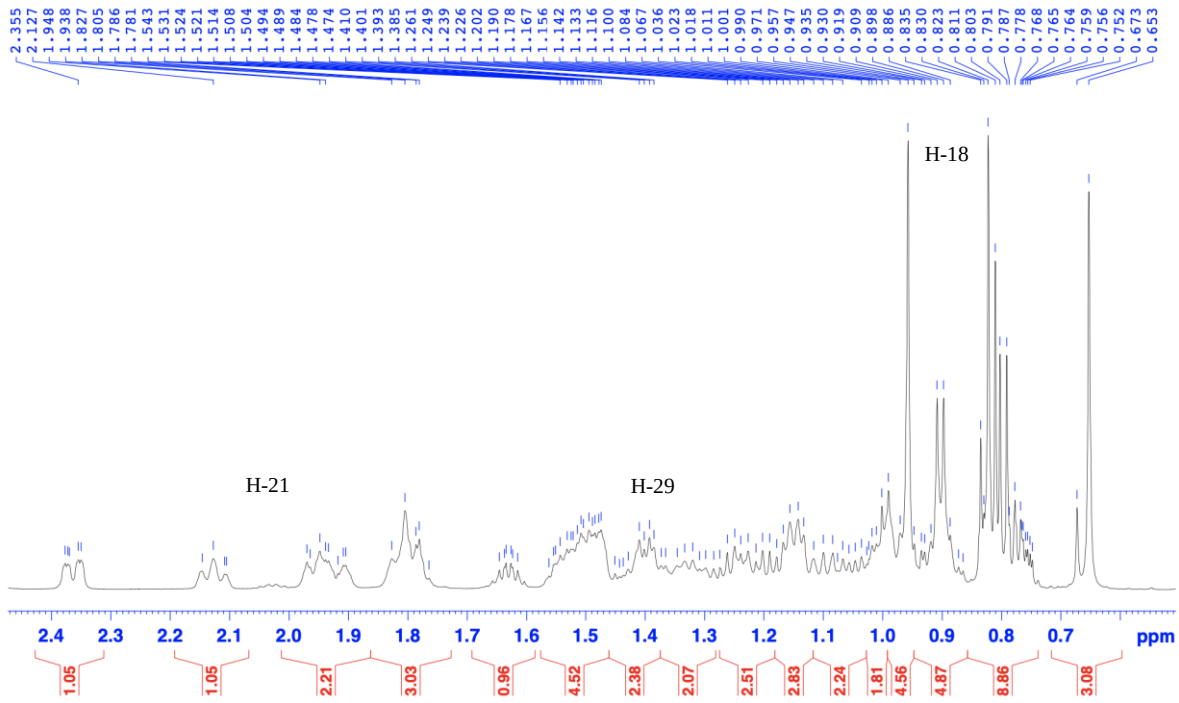

Figure S7: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol) (from δ_H 0.6 ppm to δ_H 2.4 ppm)

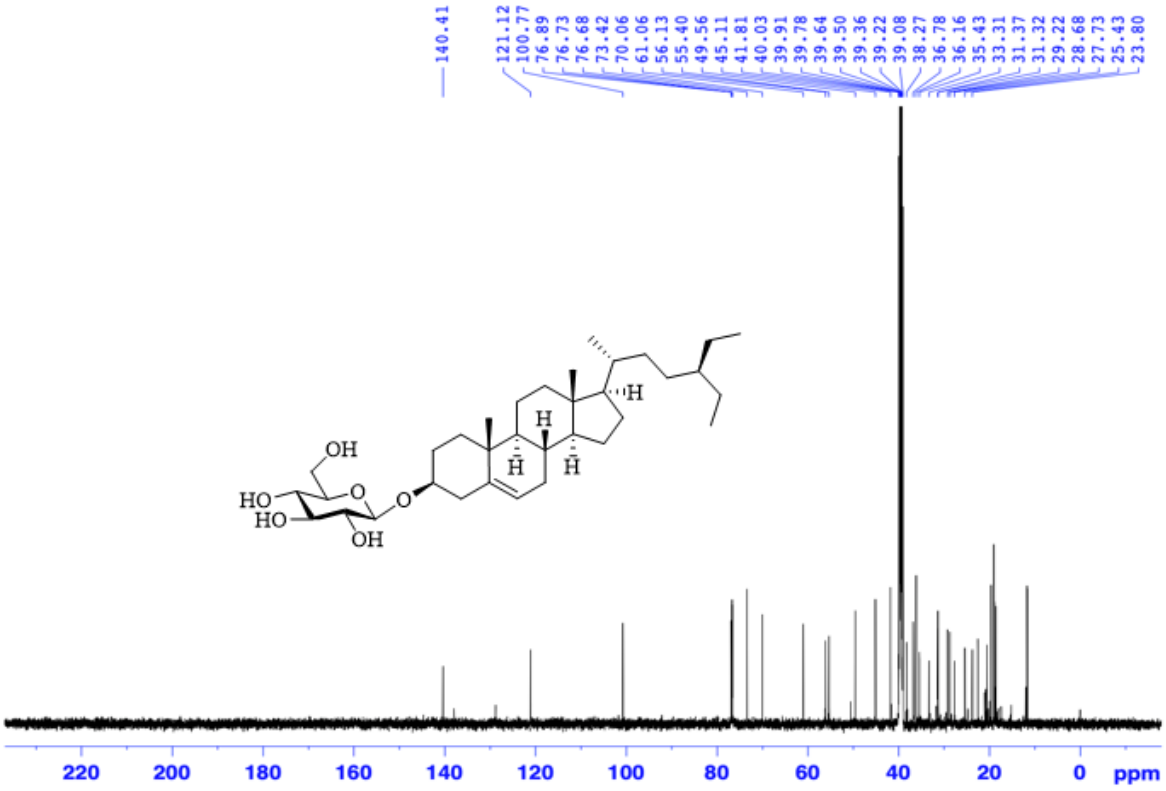

Figure S8: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol)

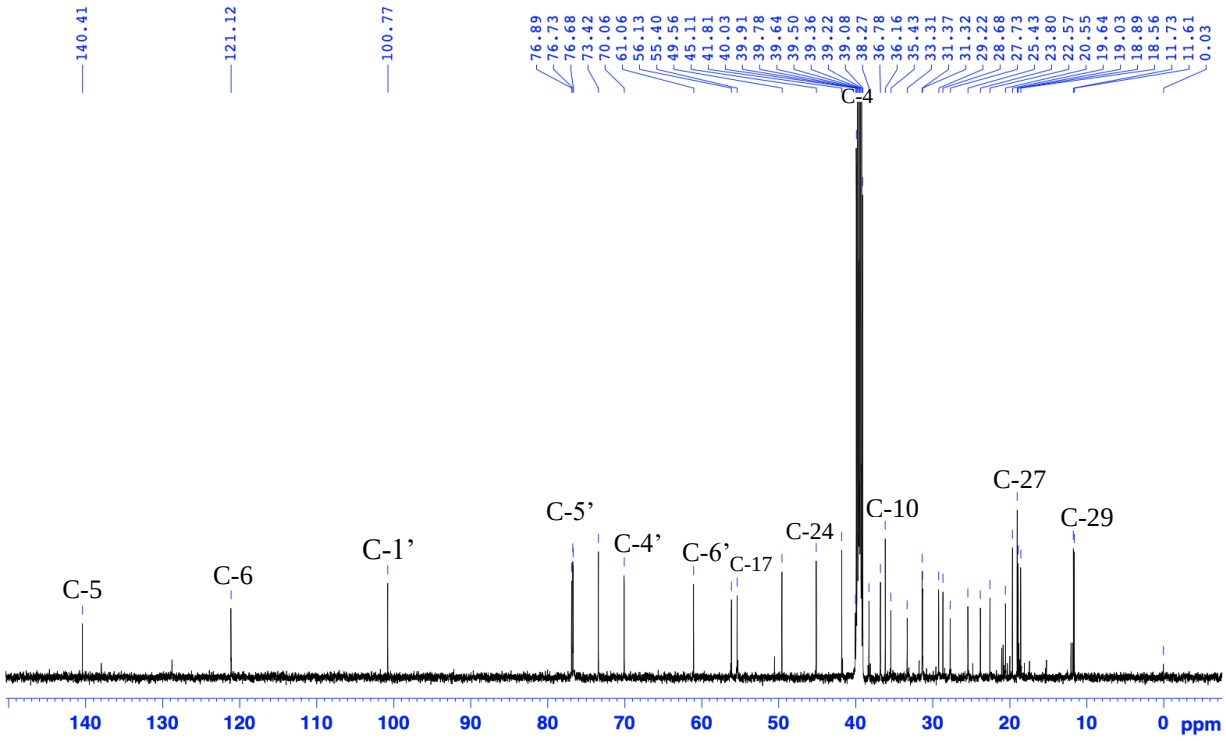

Figure S9: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol) (from δ_C 0 ppm to δ_C 140 ppm)

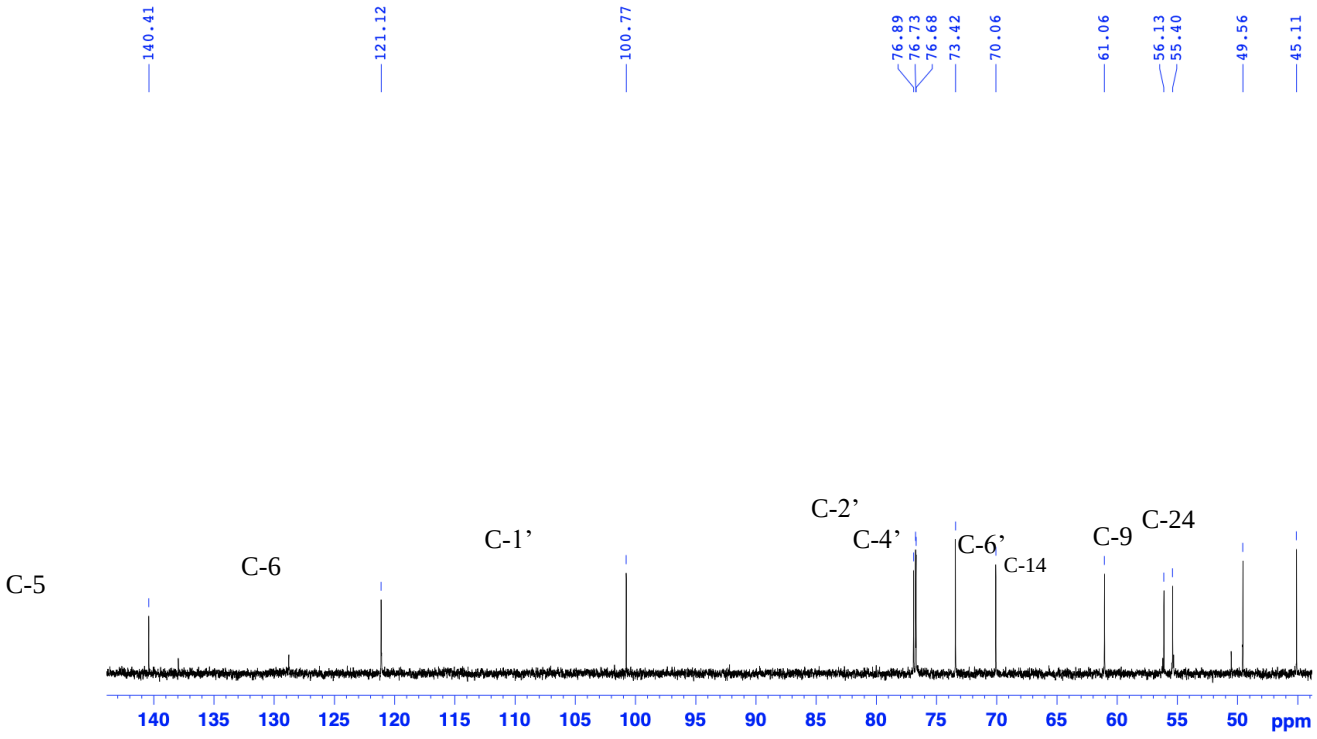

Figure S10: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol) (from δ_C 50 ppm to δ_C 140 ppm)

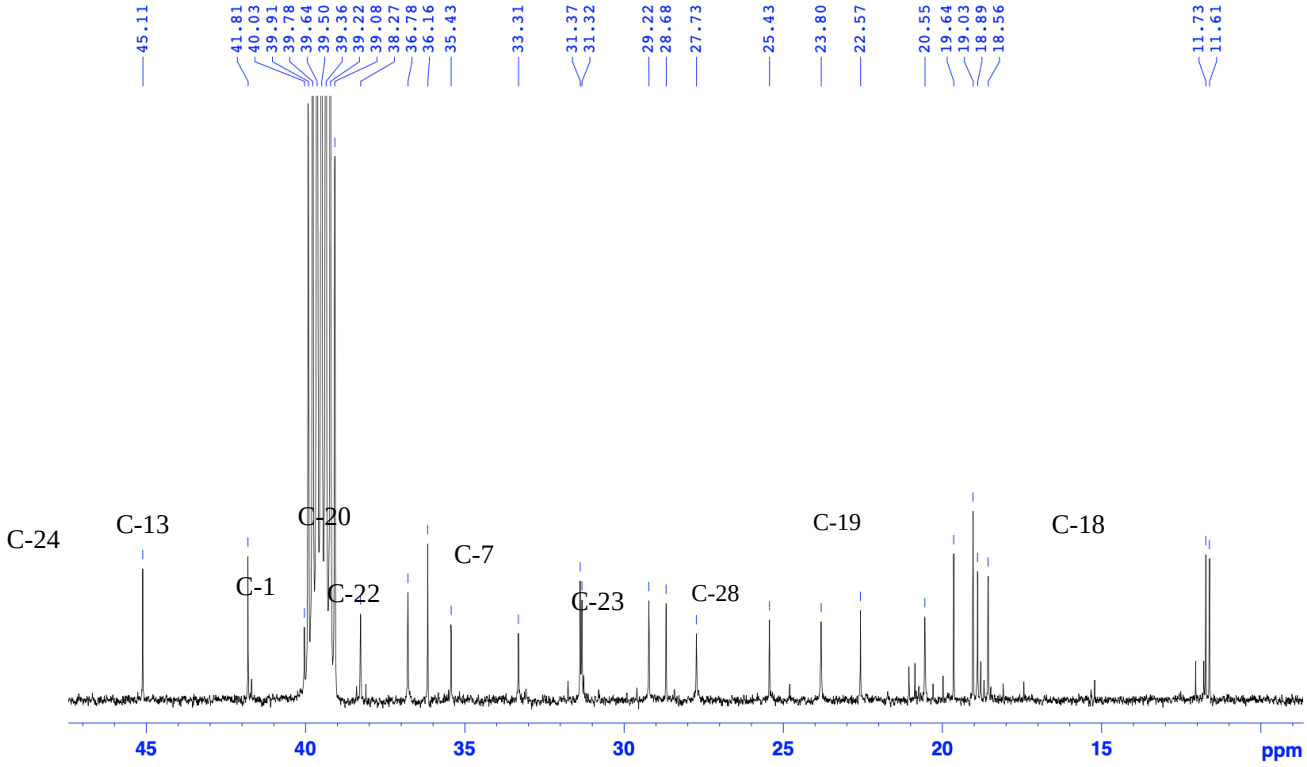

Figure S11: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **2** (daucosterol) (from δ_C 10 ppm to δ_C 47 ppm)

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

Position	Compound 3 (DMSO-d_6)		Allatonin (DMSO-d_6) [30]	
	^{13}C-NMR (125 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_H ppm
1-NH		10.53 (1H, *s*)		10.50 (1H, *s*)
2	156.7		157.6	
3-NH		8.04 (1H, *s*)		8.10 (1H, *s*)
4	62.4	5.25 (1H, *d*, 7.8 Hz)	62.7	5.30 (1H, *d*, 8.1 Hz)
5	173.6		174.0	
6-NH		6.88 (1H, *d*, 7.8 Hz)		6.90 (1H, *d*, 8.1 Hz)
7	157.3		157.1	
-NH_2		5,77 (2H, *s*)		5.80 (2H, *s*)

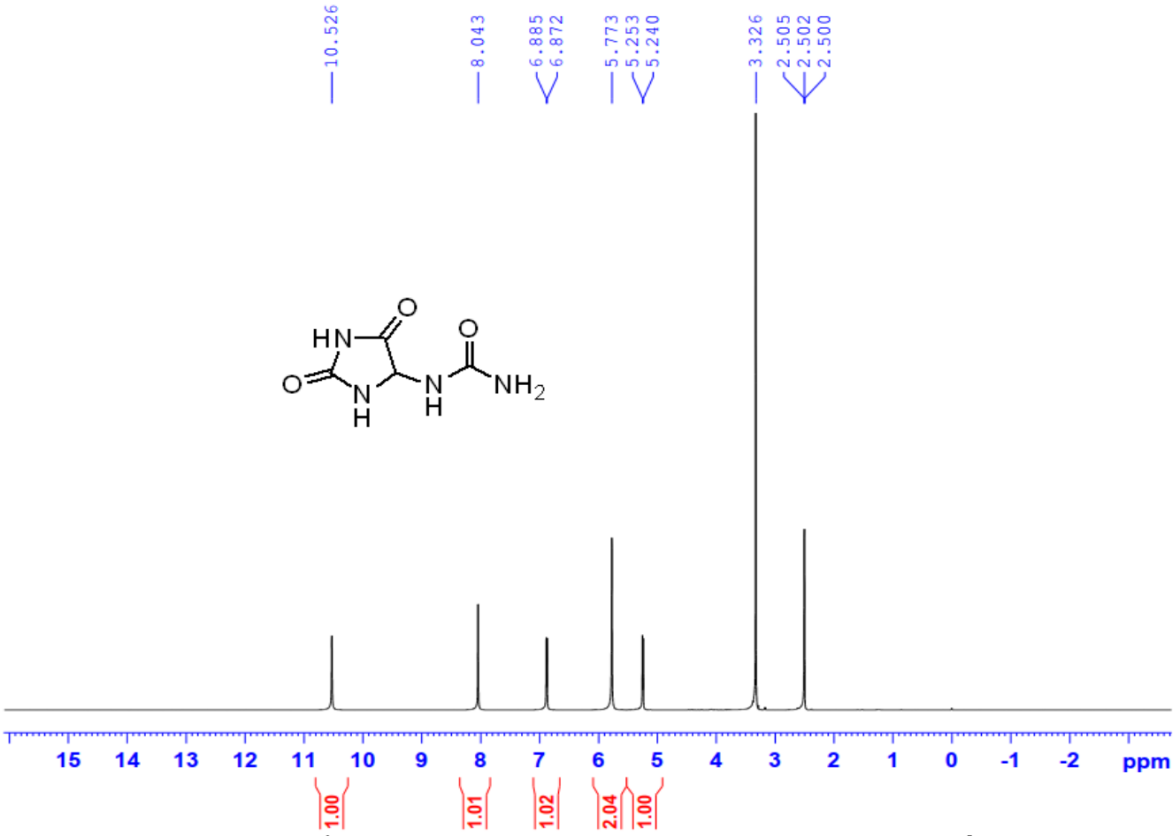

Figure S12: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **3** (allatonin)

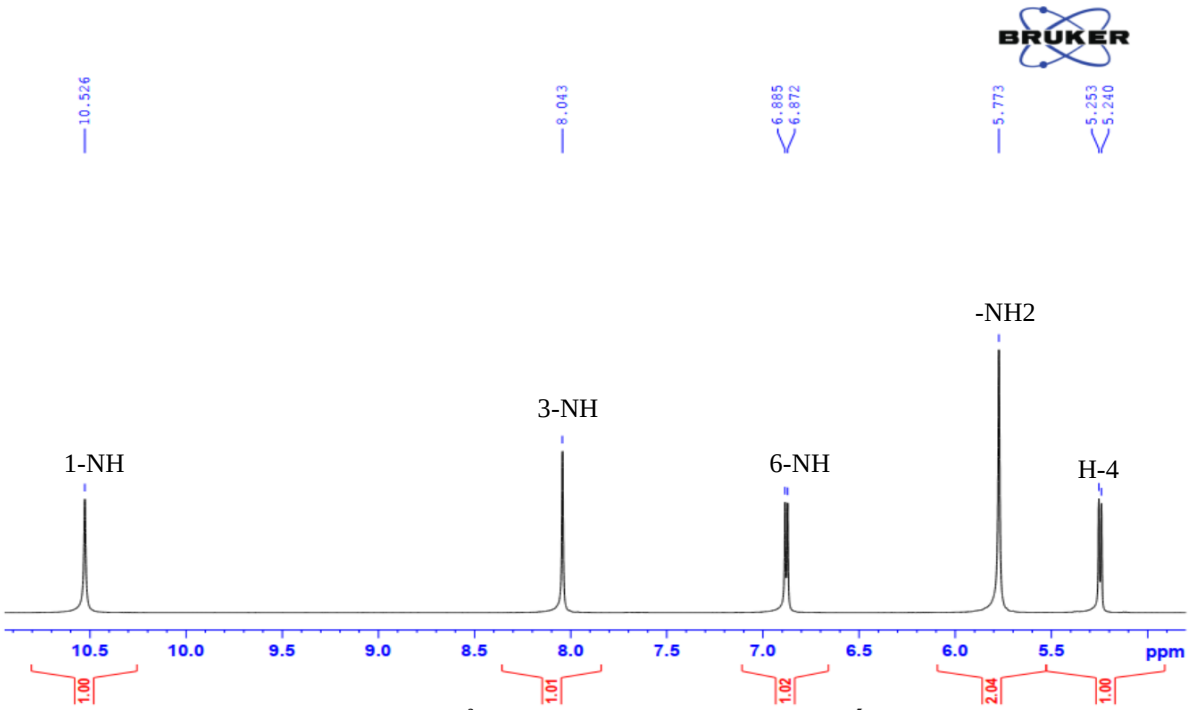

Figure S13: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **3** (allatonin) (from δ_H 5 ppm to δ_H 11 ppm)

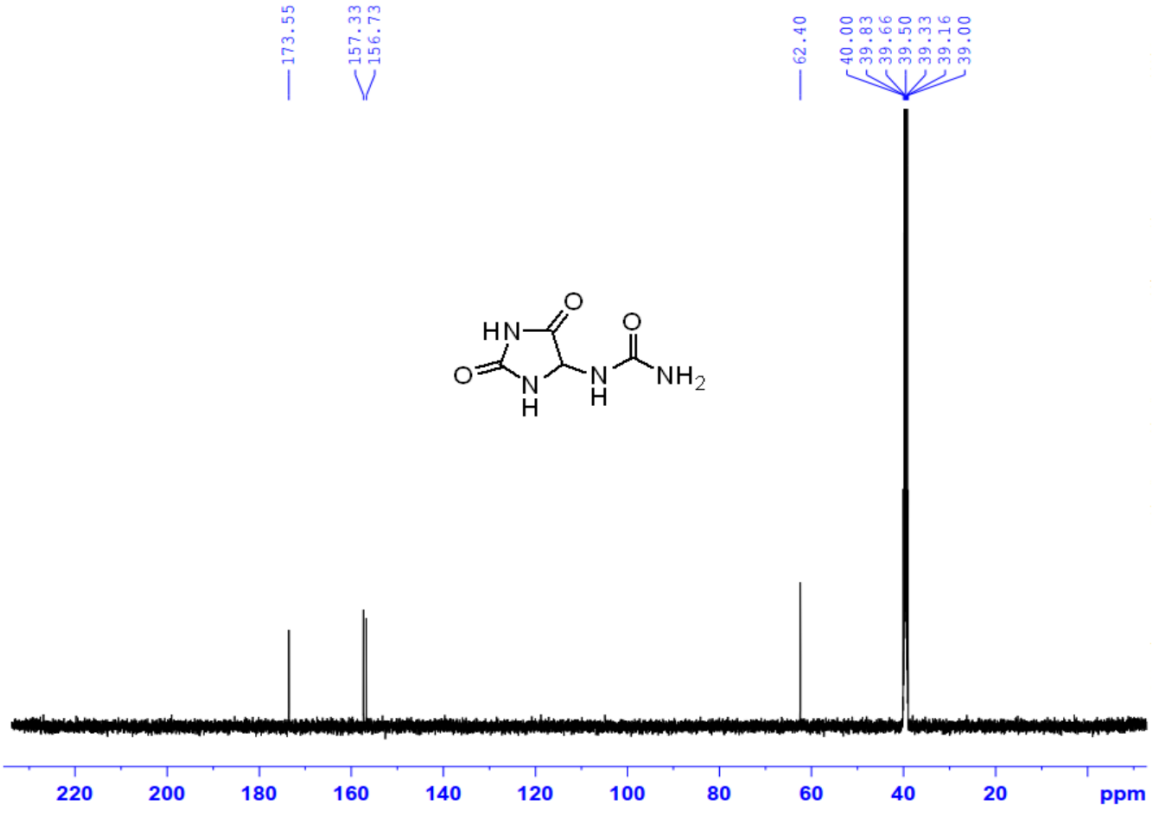

Figure S14: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **3** (allatonin)

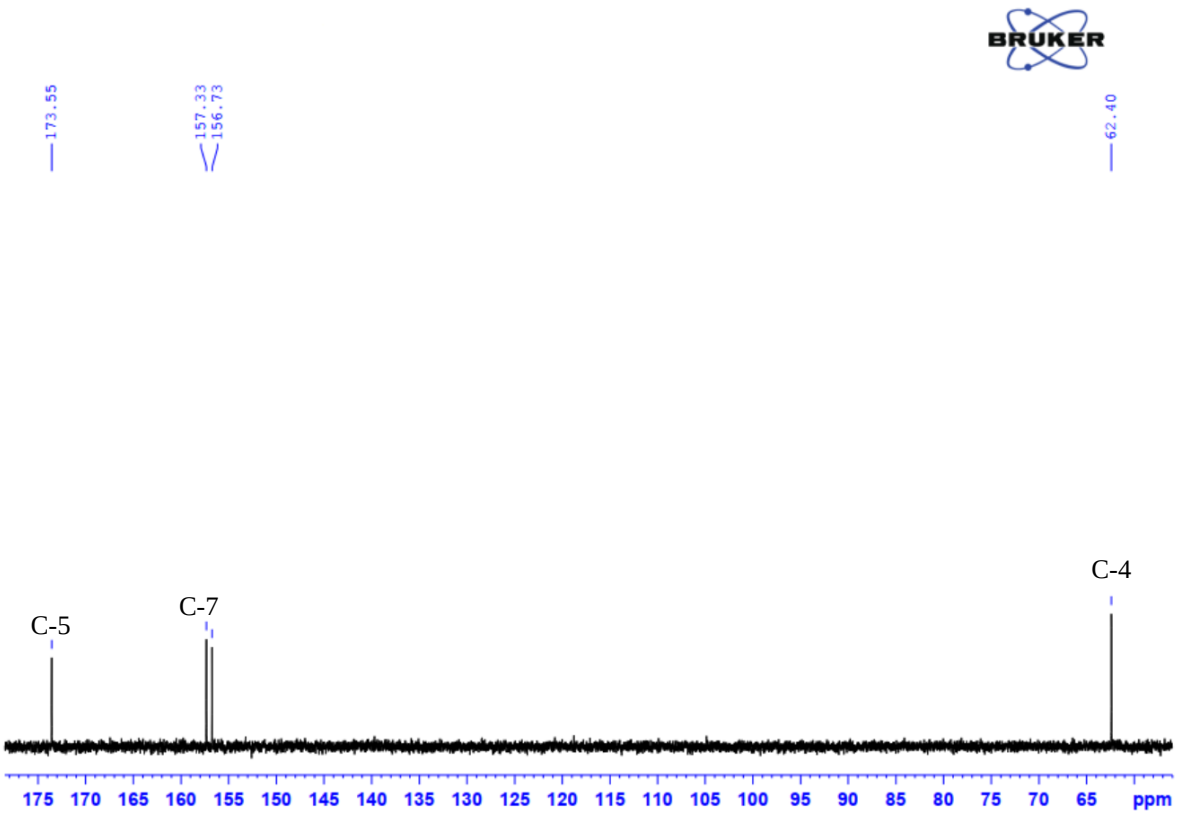

Figure S15: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **3** (allatonin) (from δ_C 60 ppm to δ_C 175 ppm)

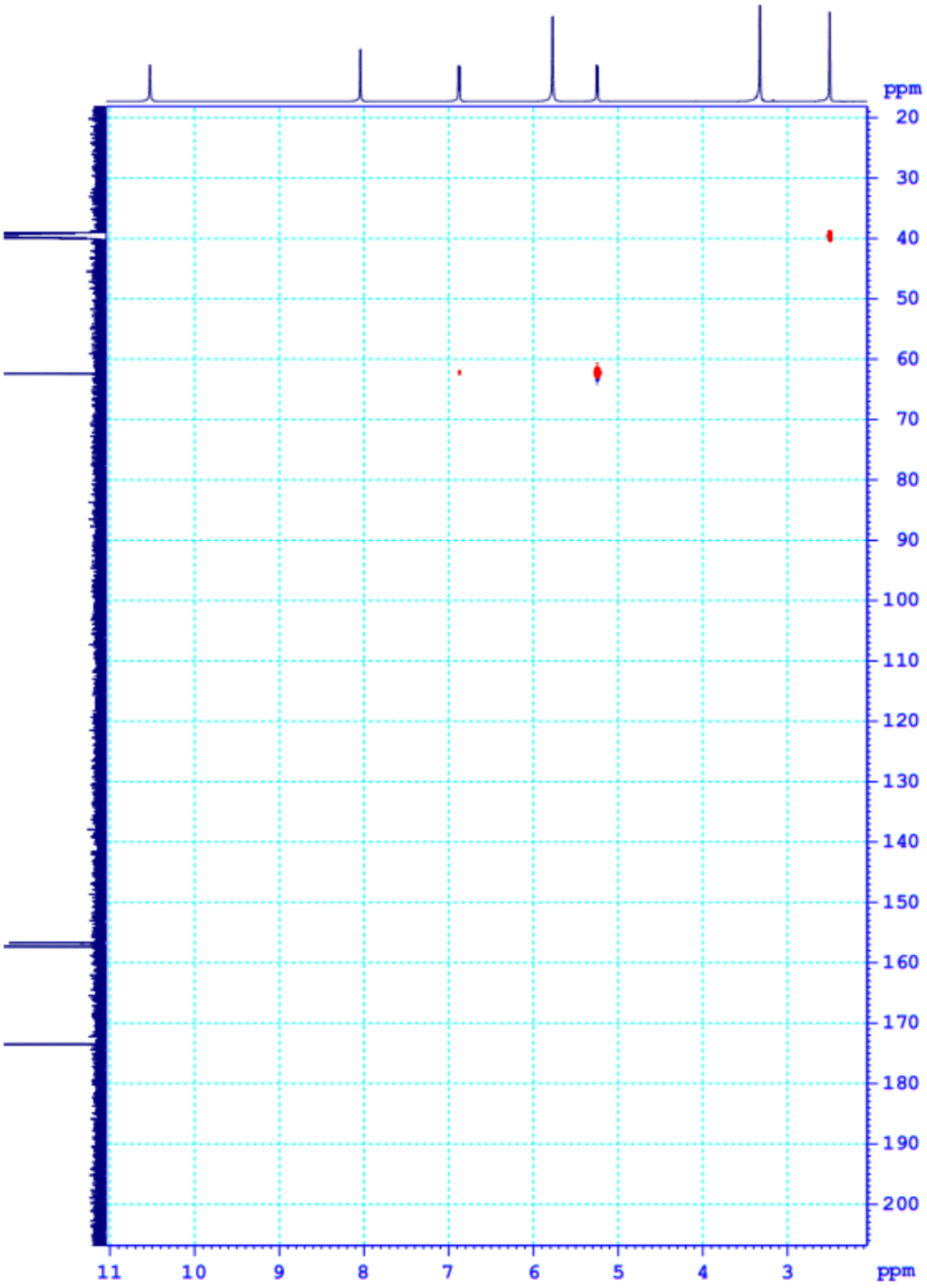

Figure S16: HSQC spectrum of compound **3** (allatonin)

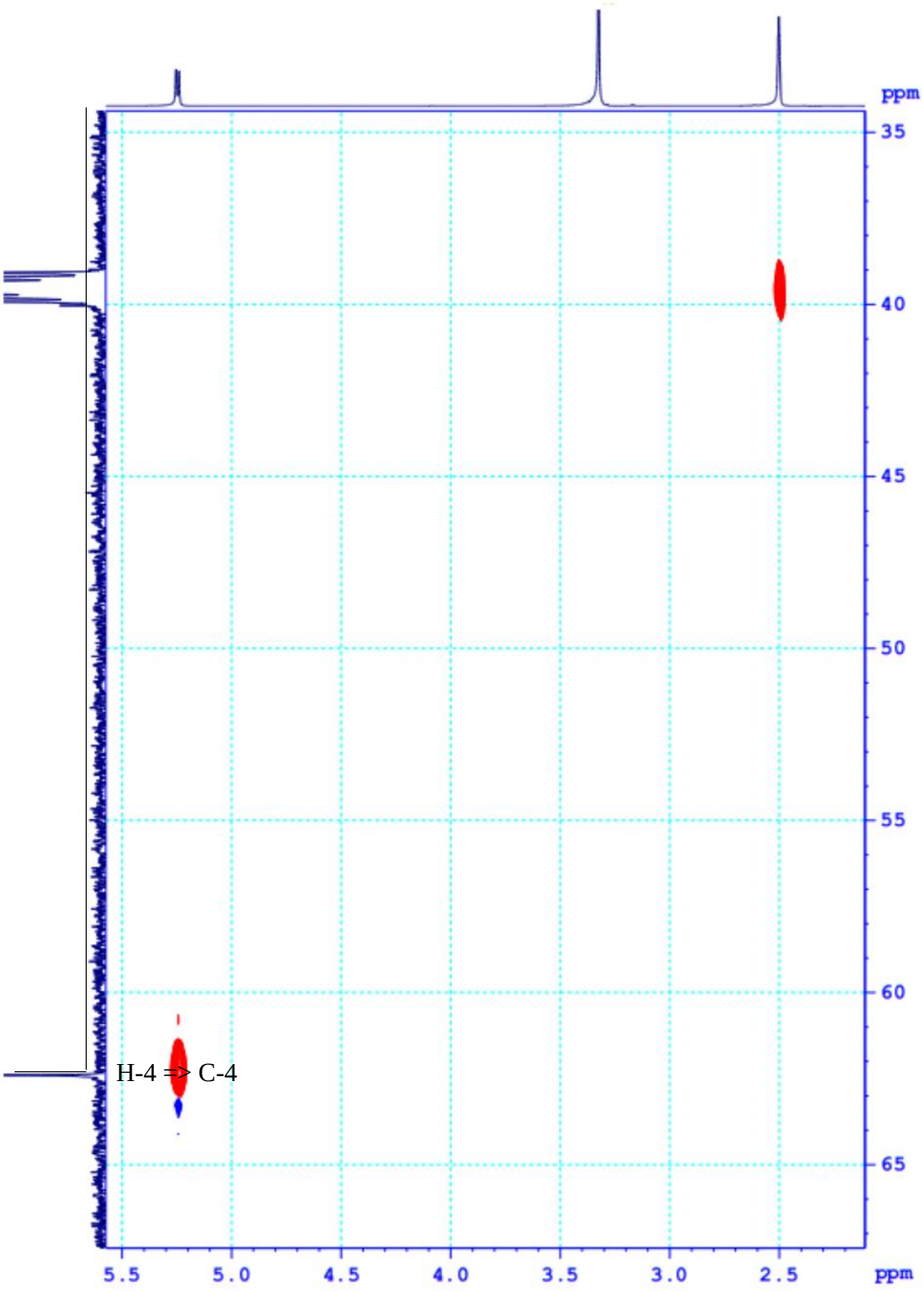

Figure S17: HSQC spectrum of compound **3** (allatonin) (from δ_C 35 ppm to δ_C 65 ppm)

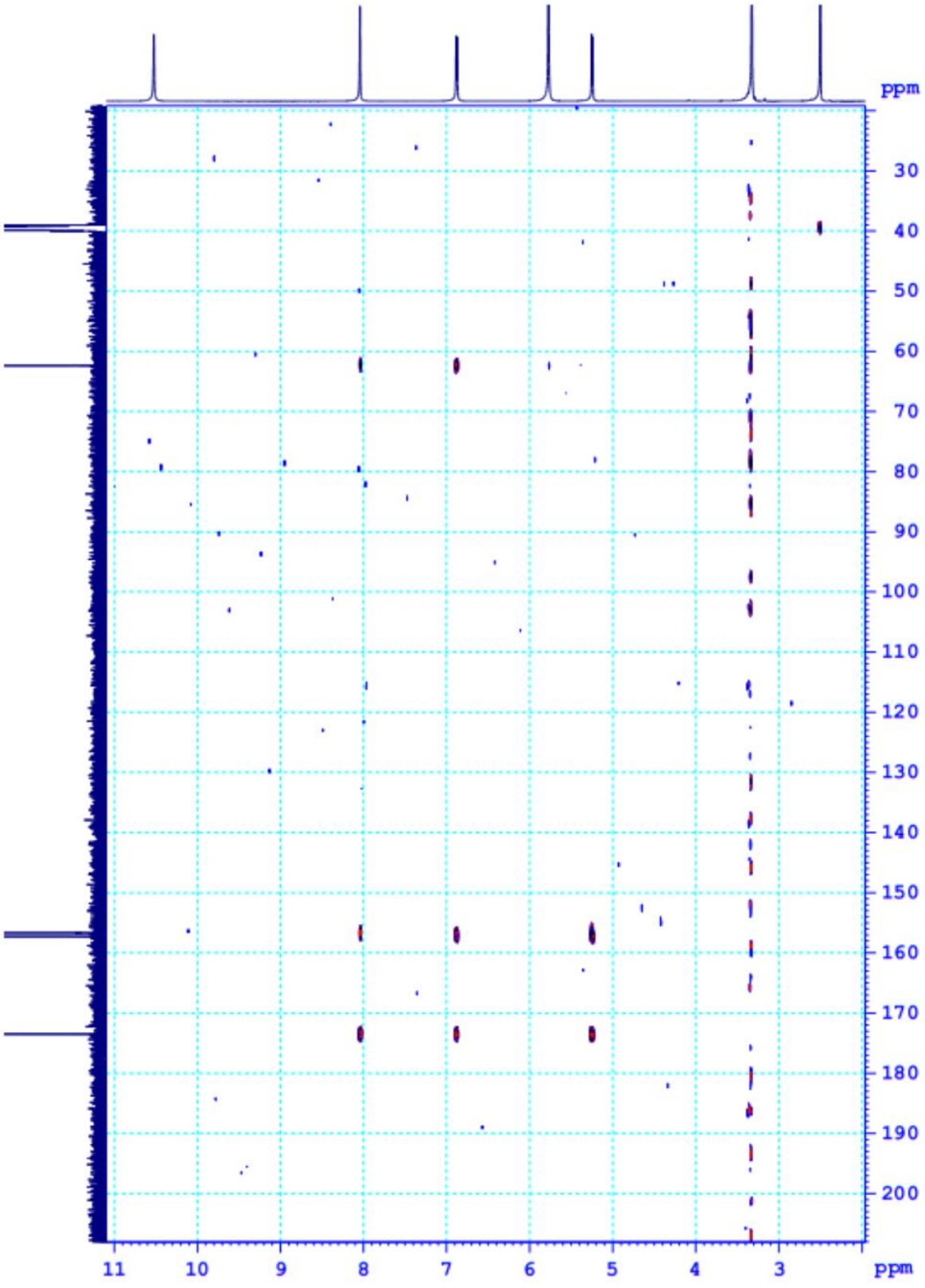

Figure S18: HMBC spectrum of compound **3** (allatonin)

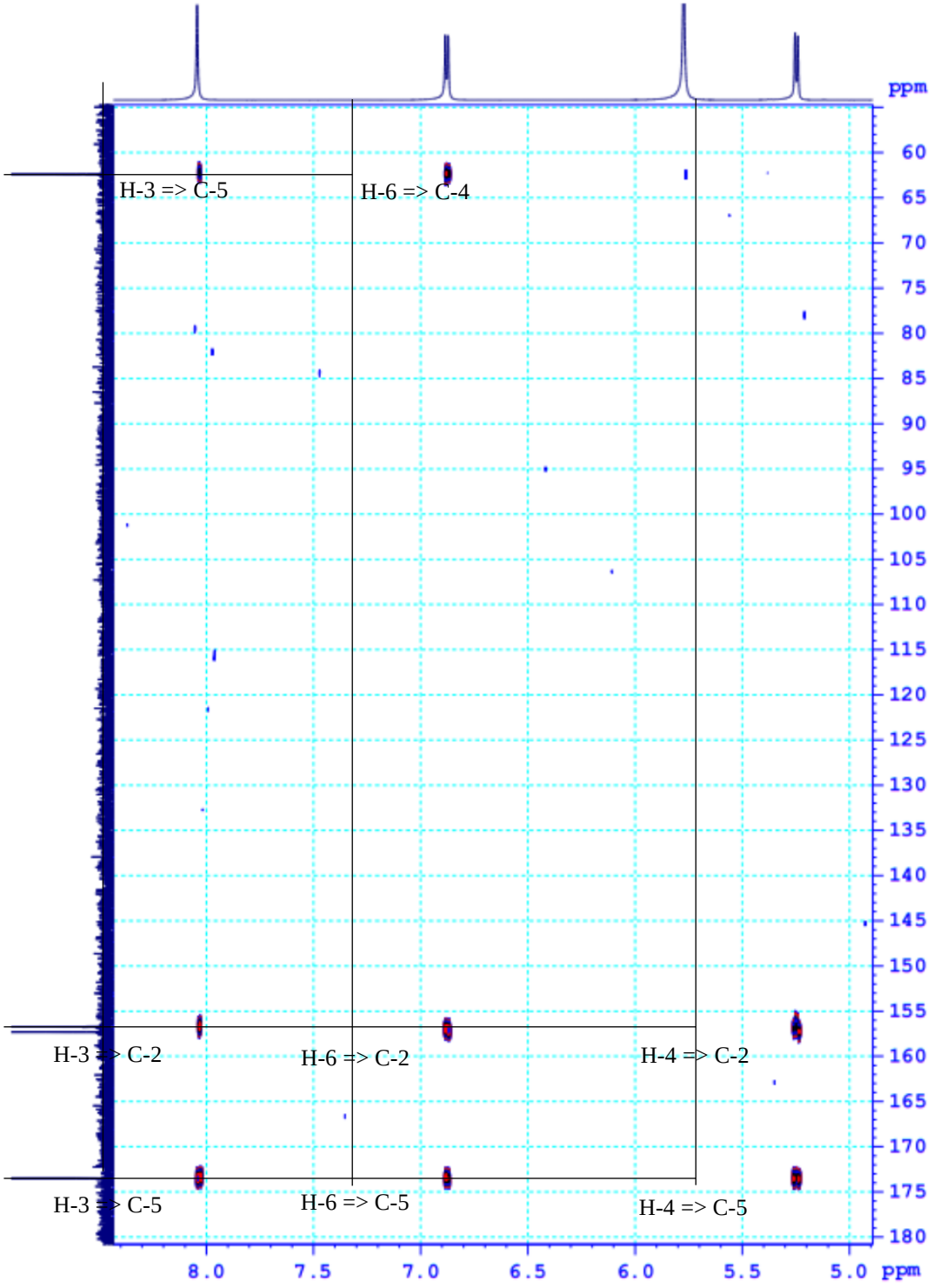

Figure S19: HMBC spectrum of compound **3** (allatonin) (from δ_C 60 ppm to δ_C 180 ppm)

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

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

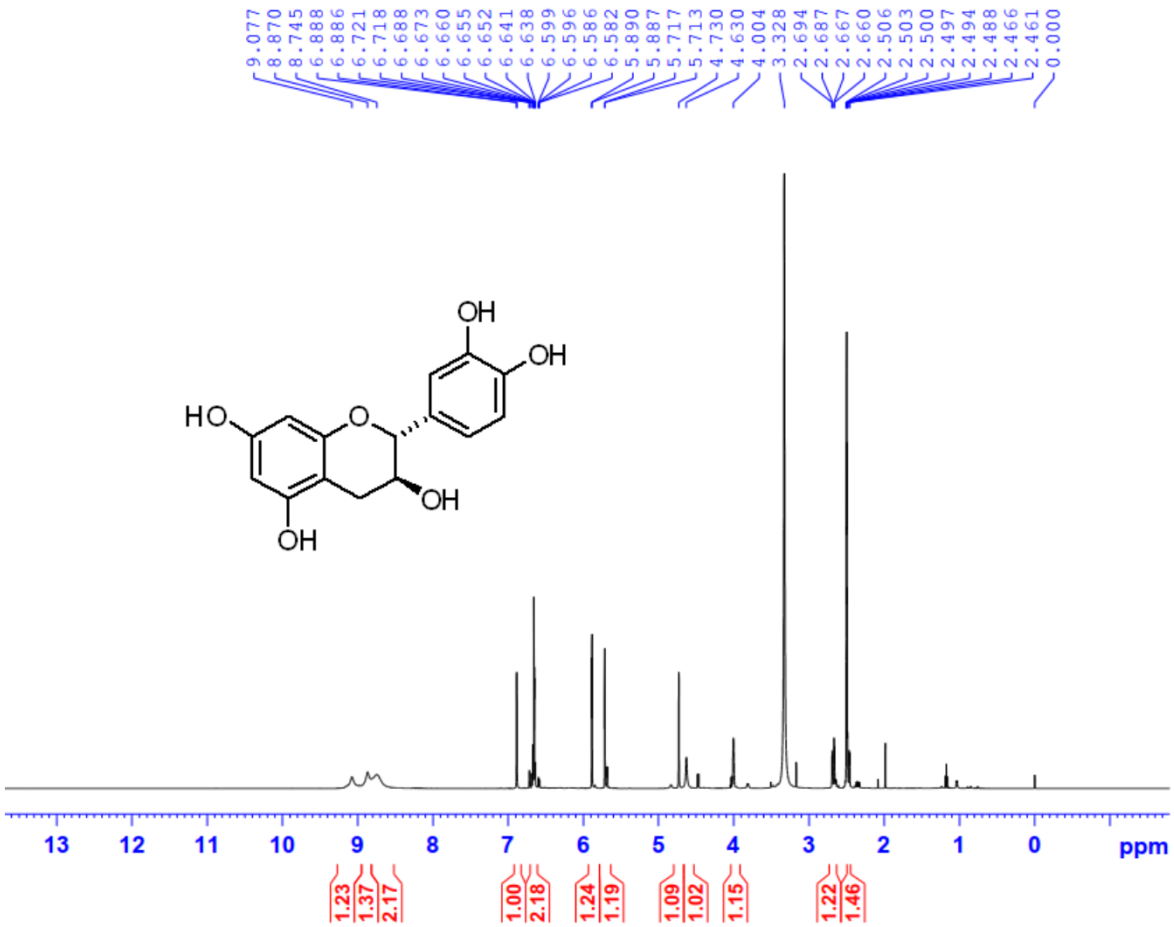

Figure S20: [1]H-NMR (600 MHz, DMSO-d_6) spectrum of compound **4** ((+)-catechin)

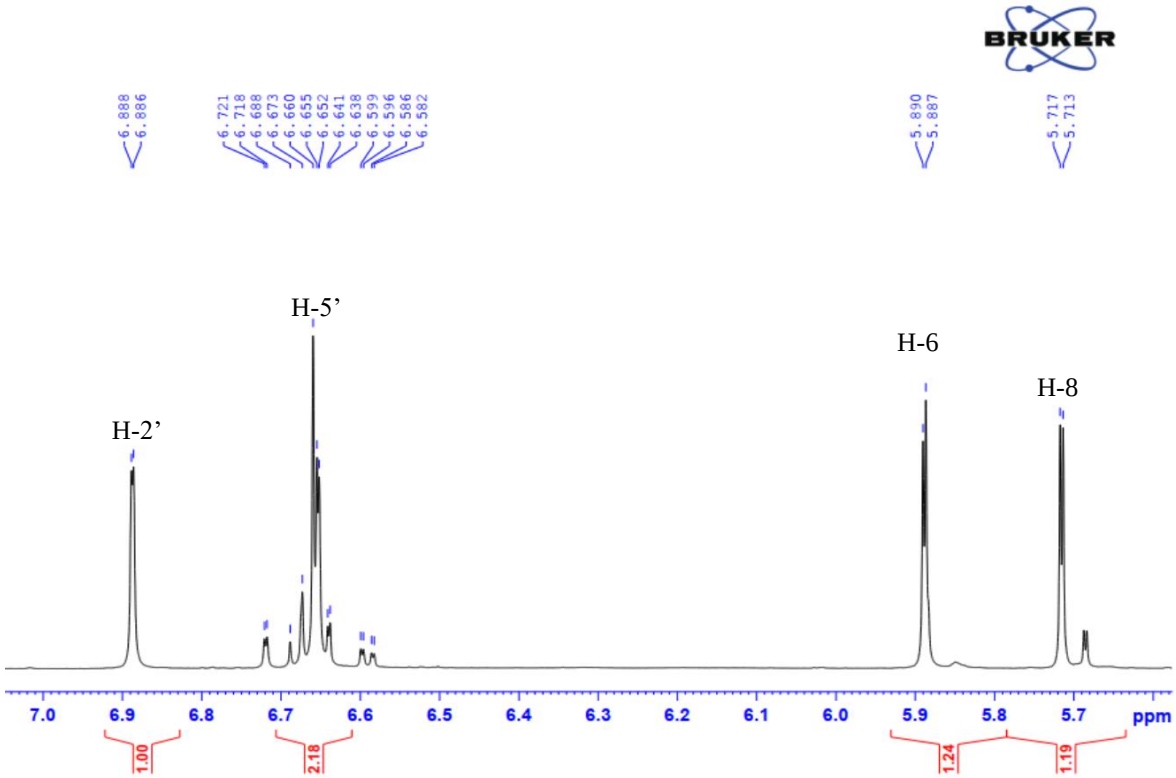

Figure S21: [1]H-NMR (600 MHz, DMSO-d_6) spectrum of compound **4** ((+)-catechin) (from δ_H 5.6 ppm to δ_H 7.0 ppm)

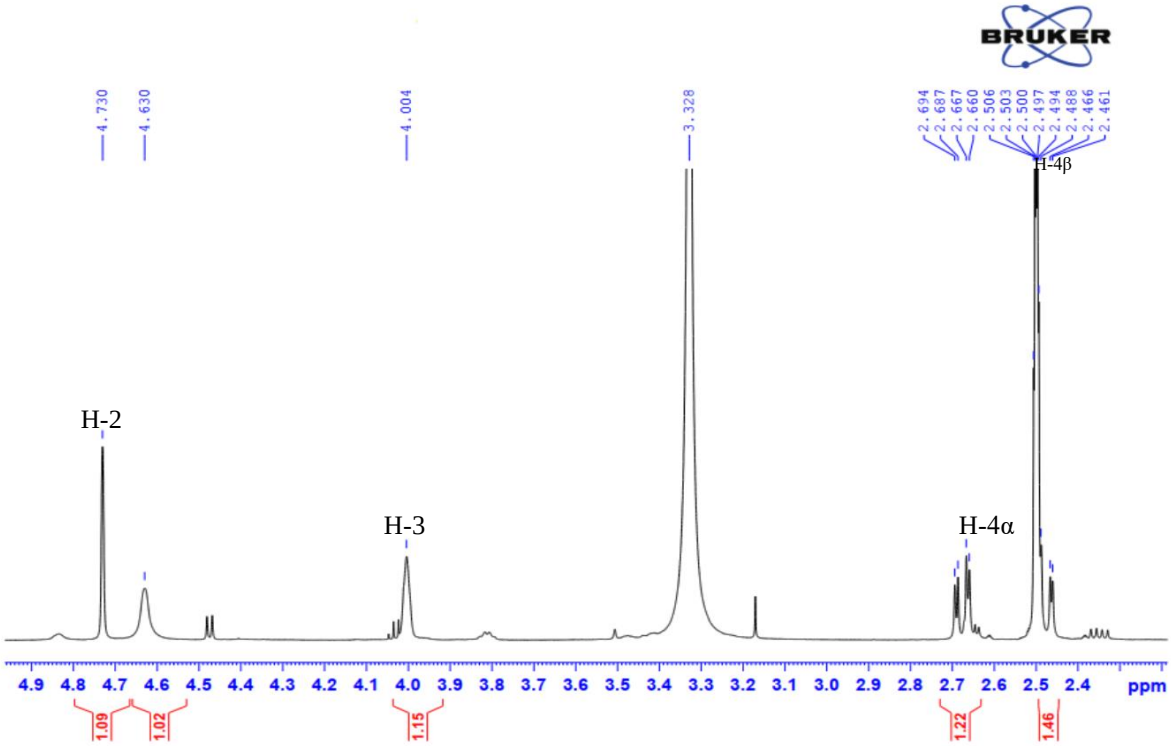

Figure S22: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **4** ((+)-catechin) (from δ_H 2.3 ppm to δ_H 4.9 ppm)

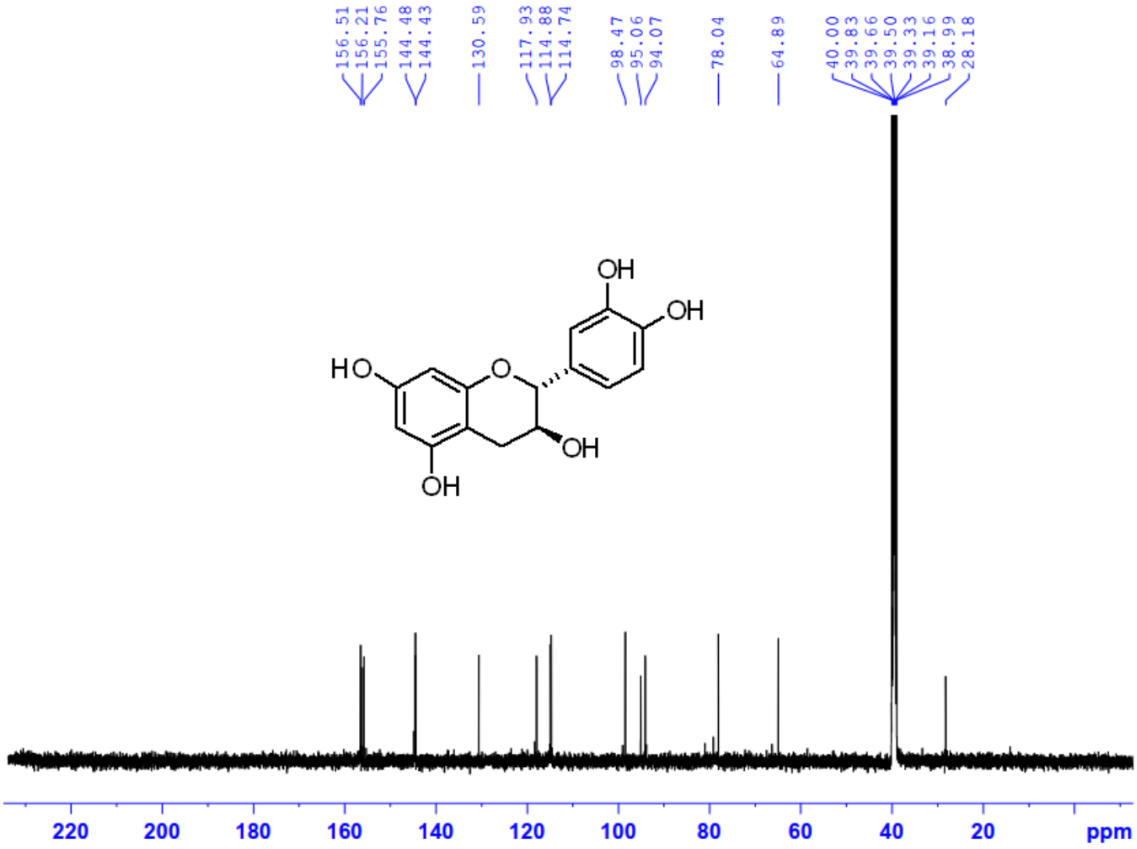

Figure S23: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **4** ((+)-catechin)

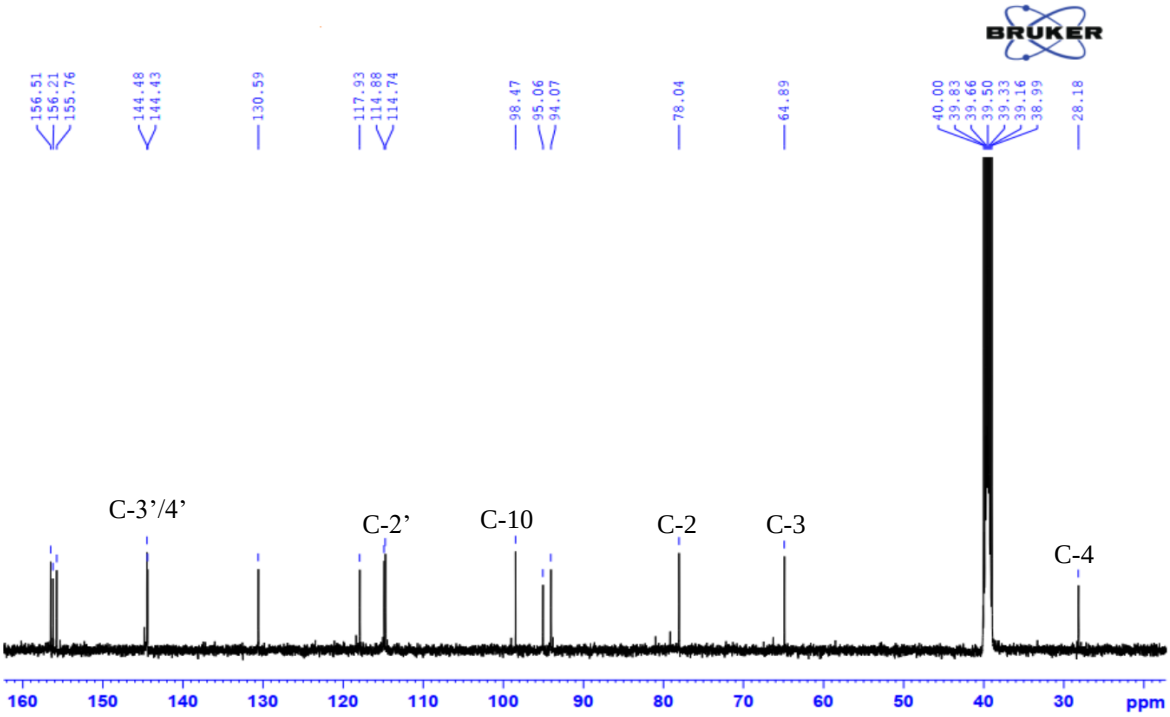

Figure S24: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **4** ((+)-catechin) (from δ_C 20 ppm to δ_C 160 ppm)

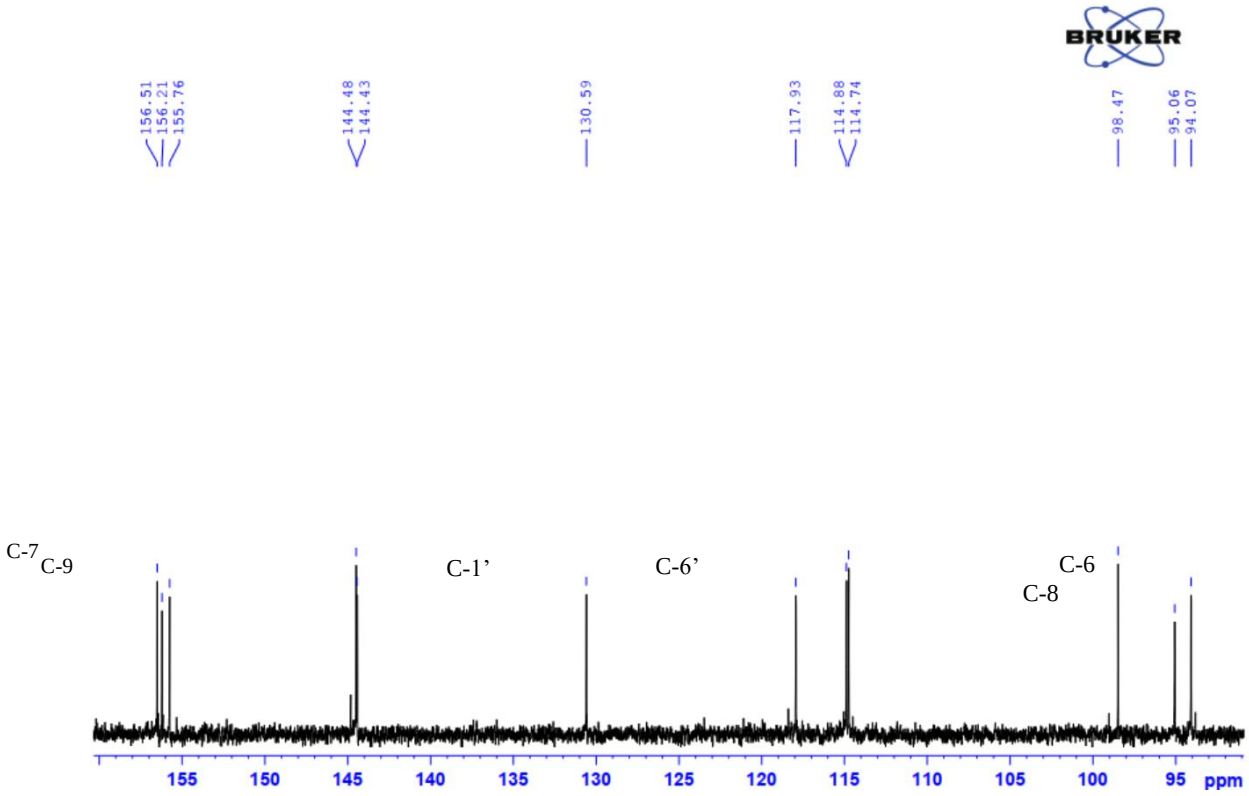

Figure S25: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **4** ((+)-catechin) (from δ_C 90 ppm to δ_C 160 ppm)

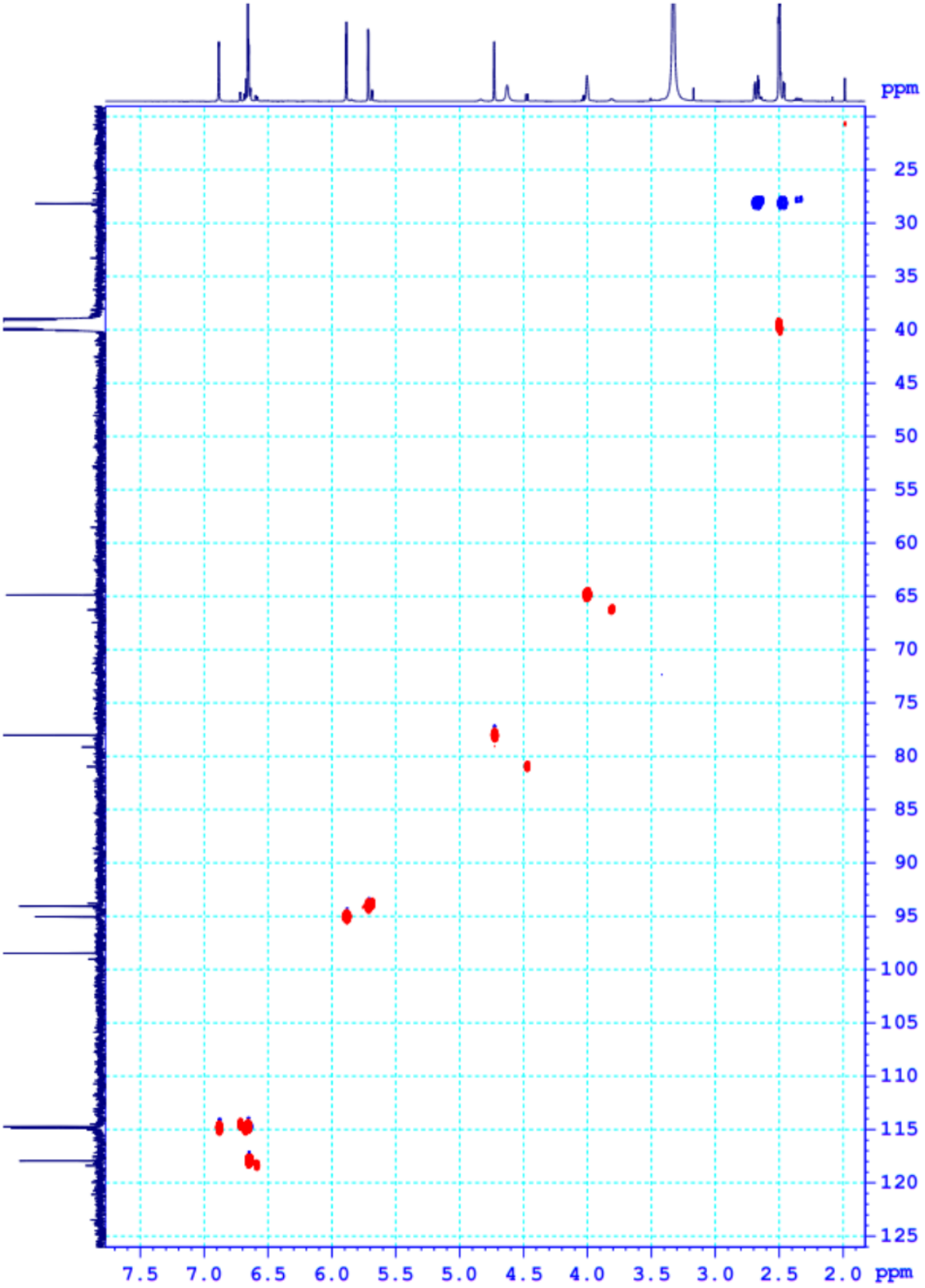

Figure S26: HSQC spectrum of compound **4** ((+)-catechin)

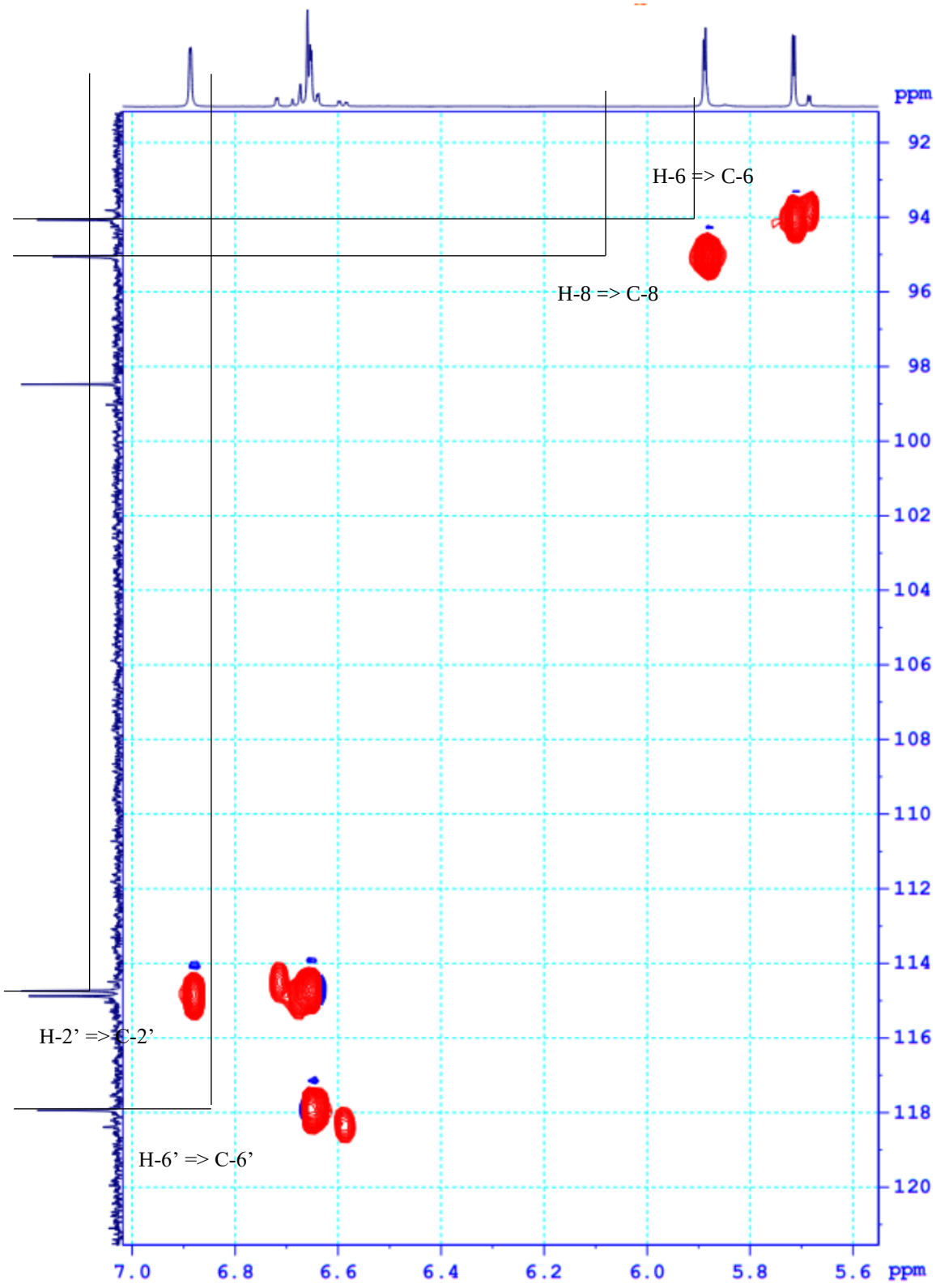

Figure S27: HSQC spectrum of compound **4** ((+)-catechin) (from δ_C 92 ppm to δ_C 120 ppm)

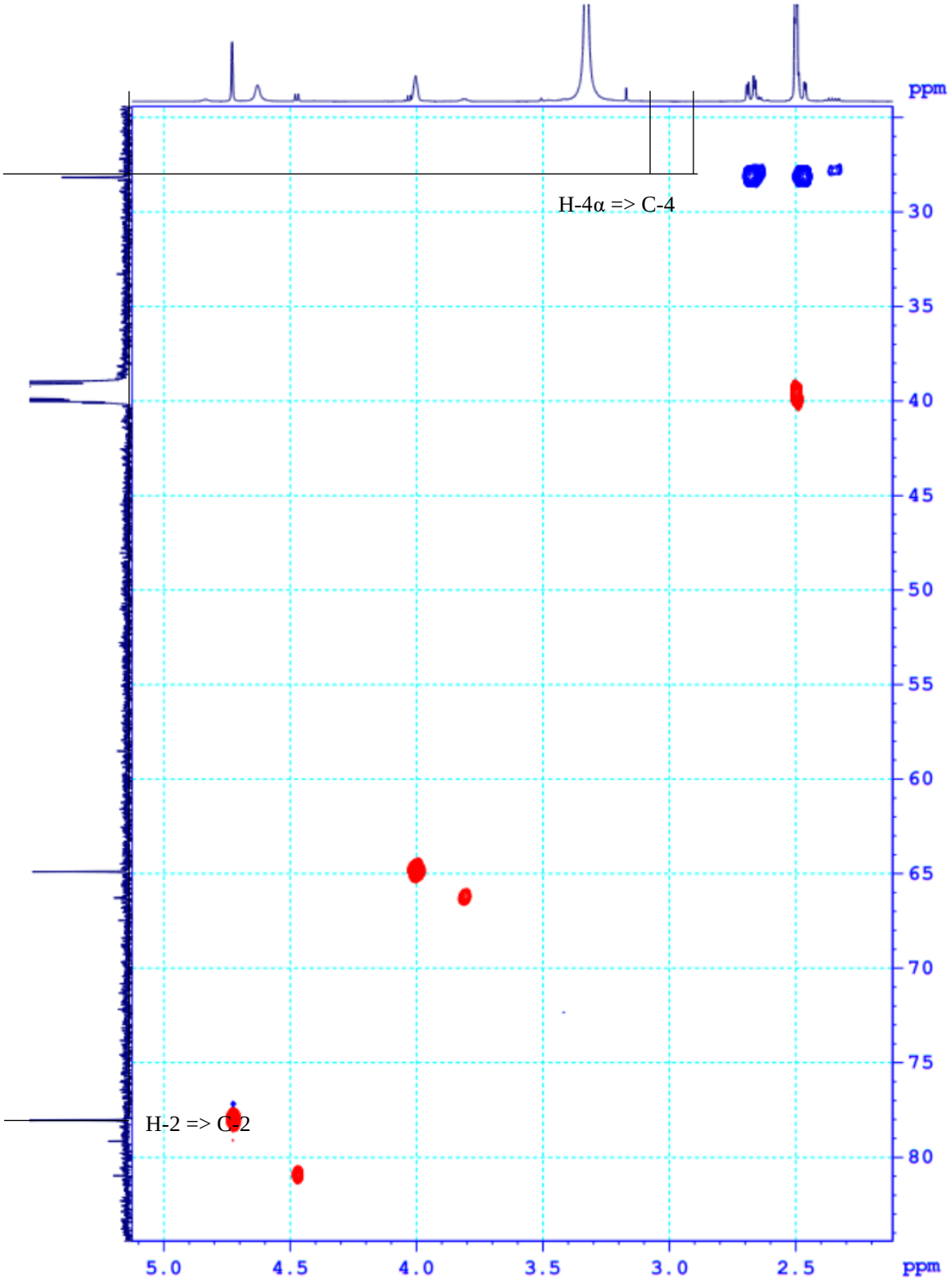

Figure S28: HSQC spectrum of compound **4** ((+)-catechin) (from δ_C 20 ppm to δ_C 90 ppm)

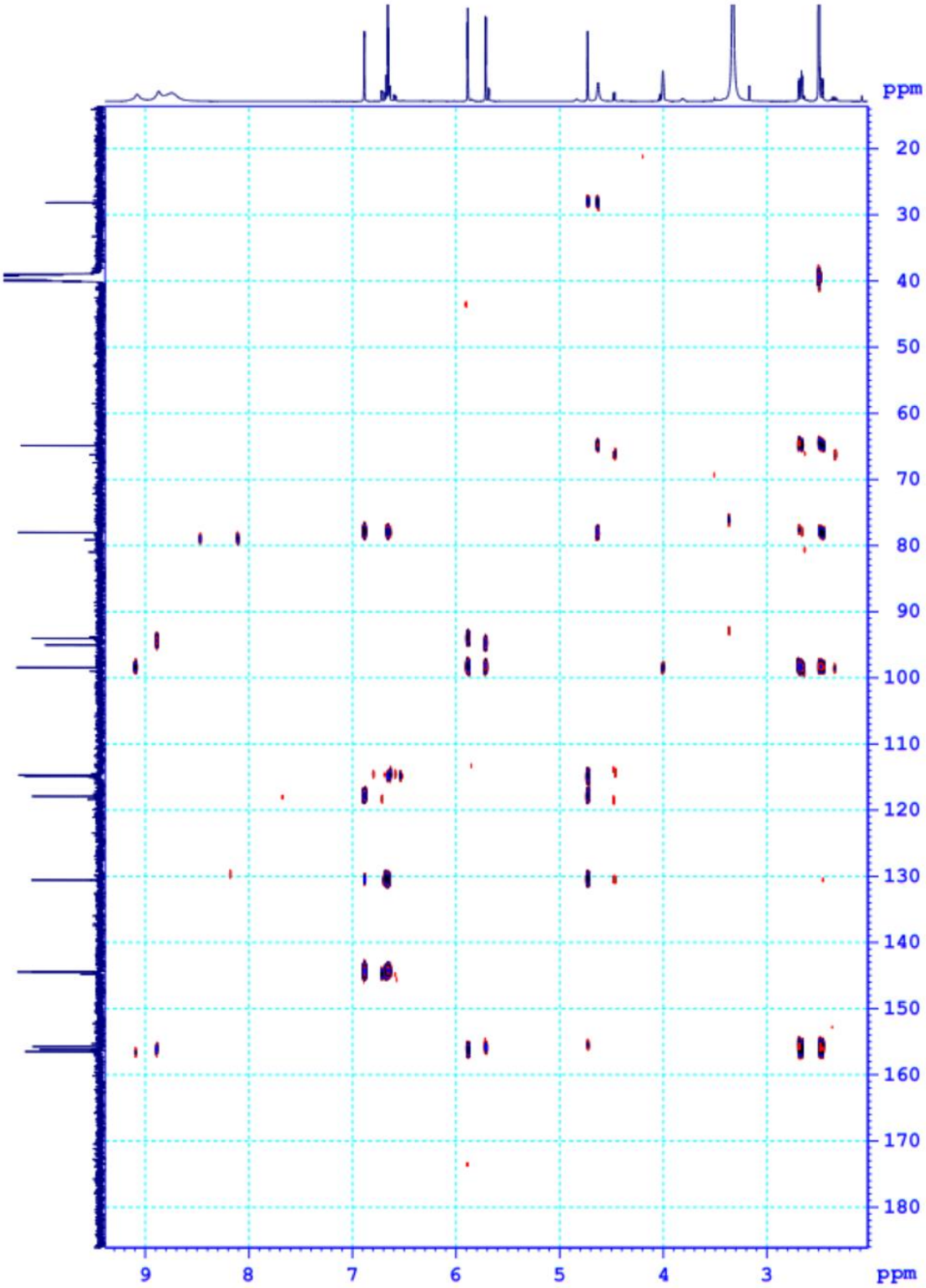

Figure S29: HMBC spectrum of compound **4** ((+)-catechin)

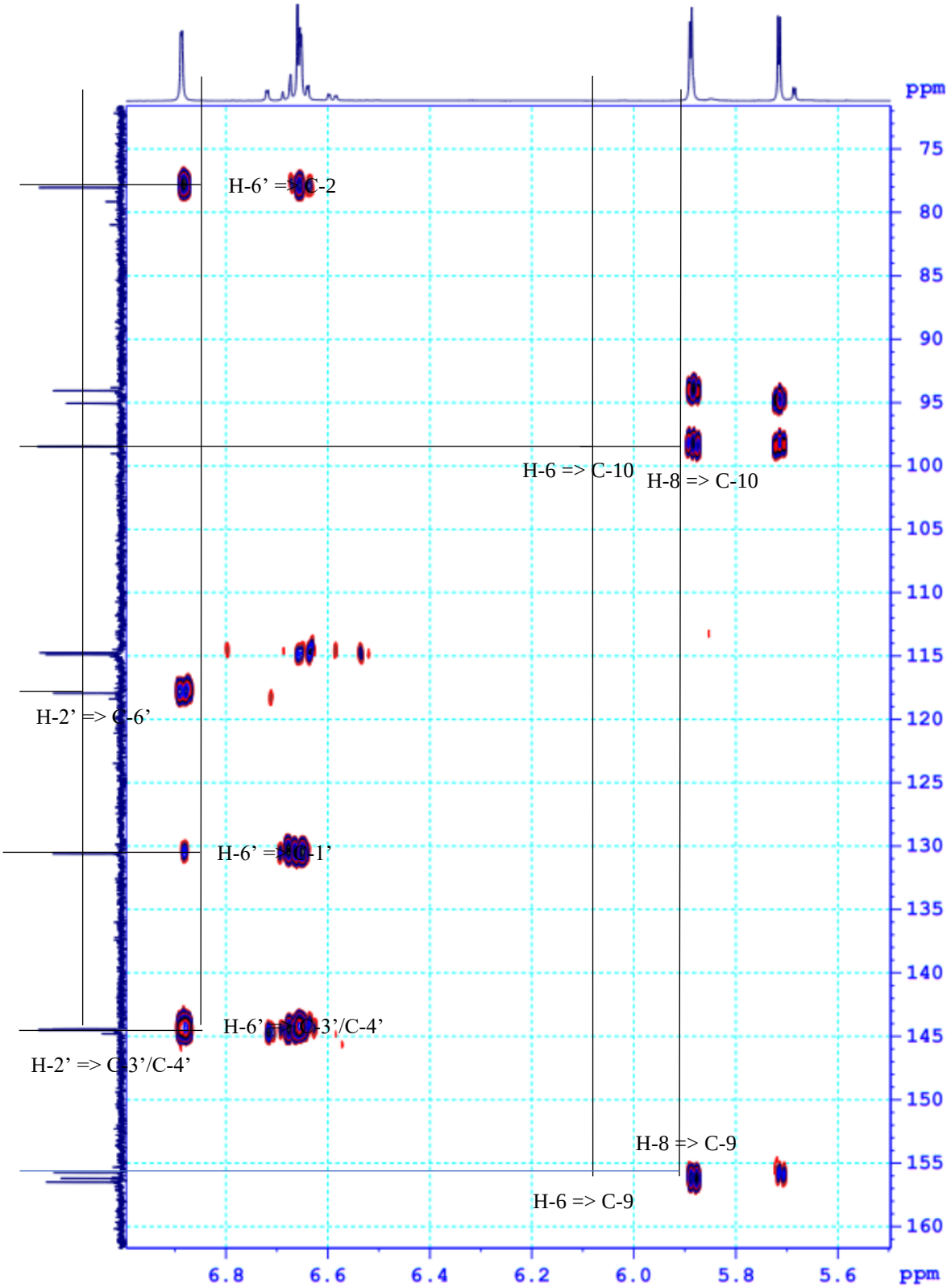

Figure S30: HMBC spectrum of compound **4** ((+)-catechin) (from δ_C 75 ppm to δ_C 160 ppm)

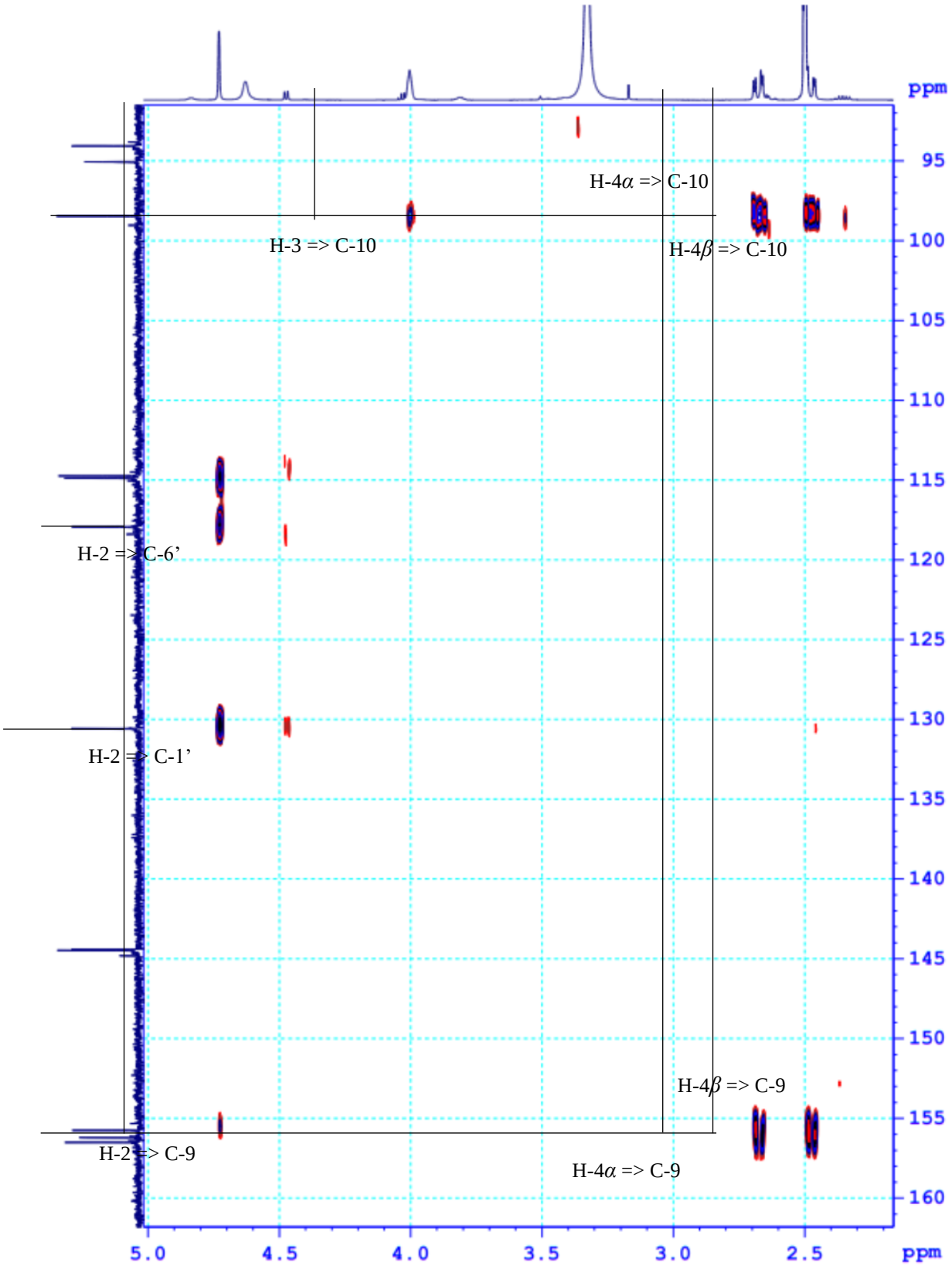

Figure S31: HMBC spectrum of compound **4** ((+)-catechin) (from δ_C 90 ppm to δ_C 160 ppm)

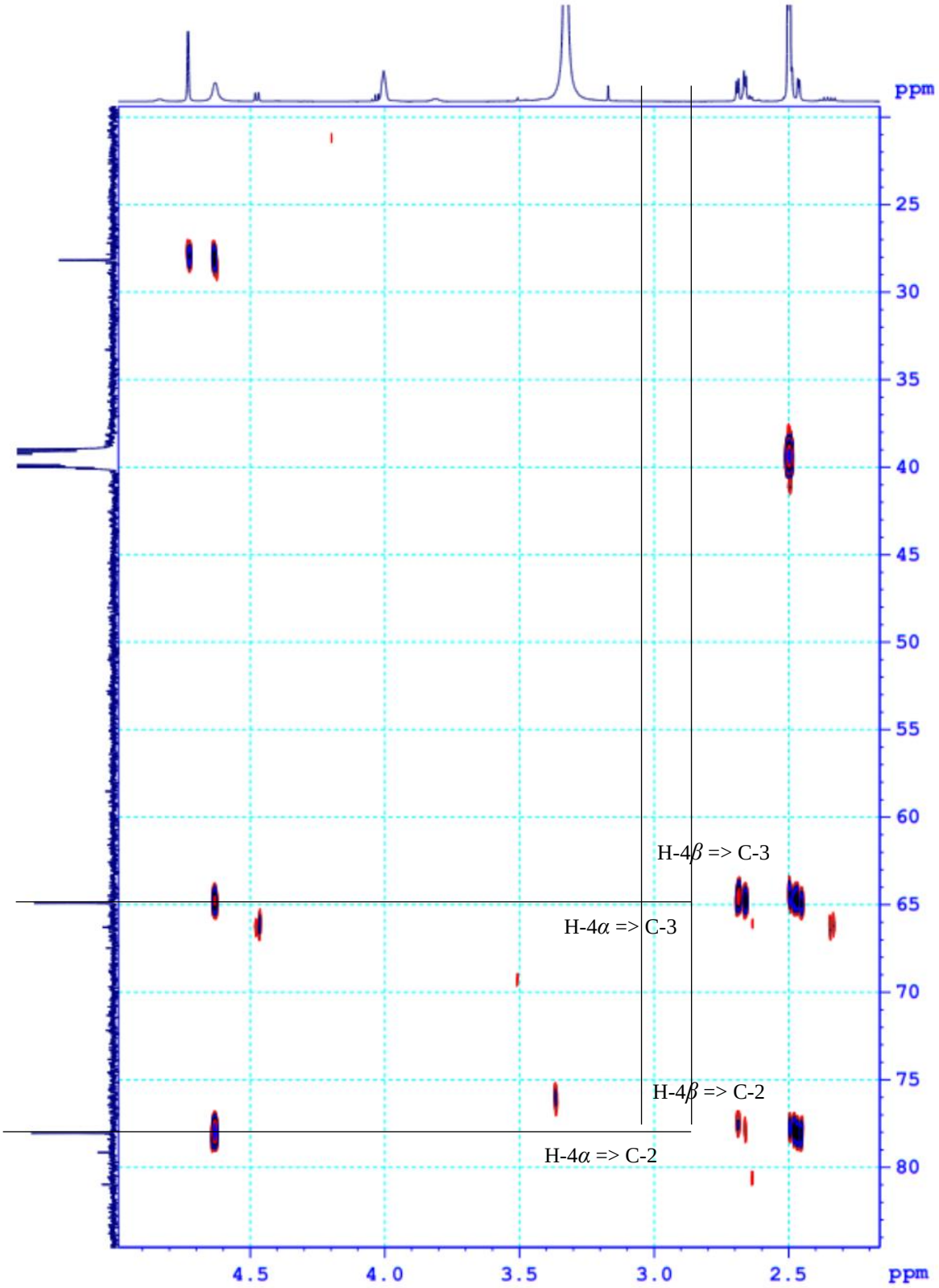

Figure S32: HMBC spectrum of compound **4** ((+)-catechin) (from δ_C 20 ppm to δ_C 90 ppm)

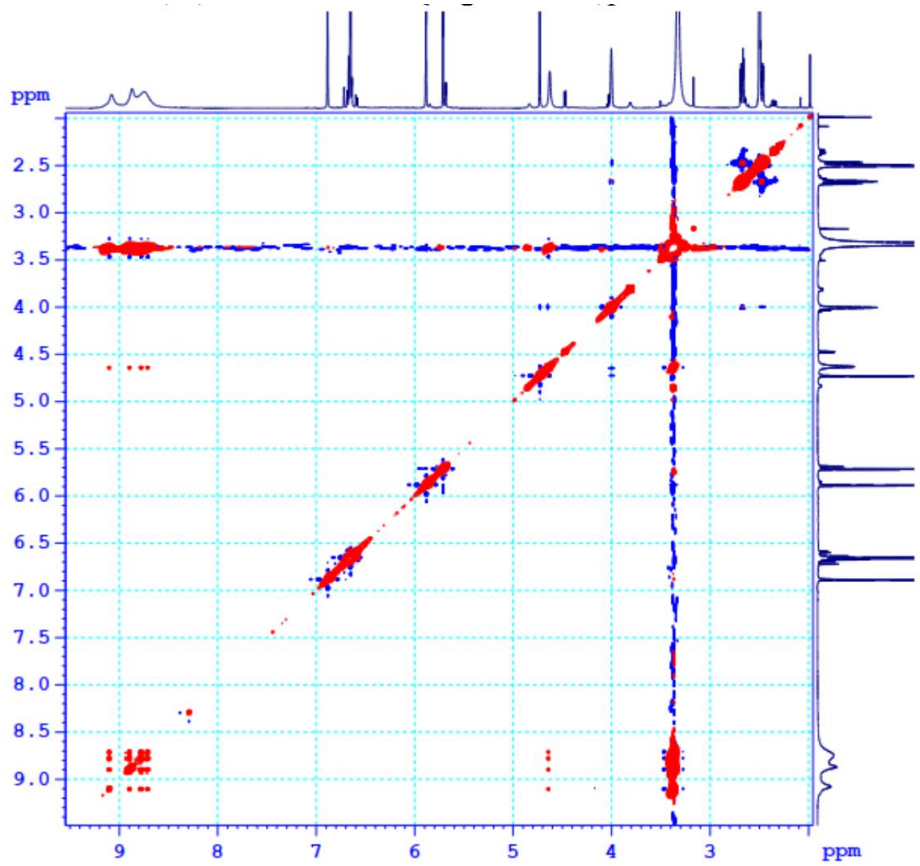

Figure S33: NOESY spectrum of compound **4** ((+)-catechin)

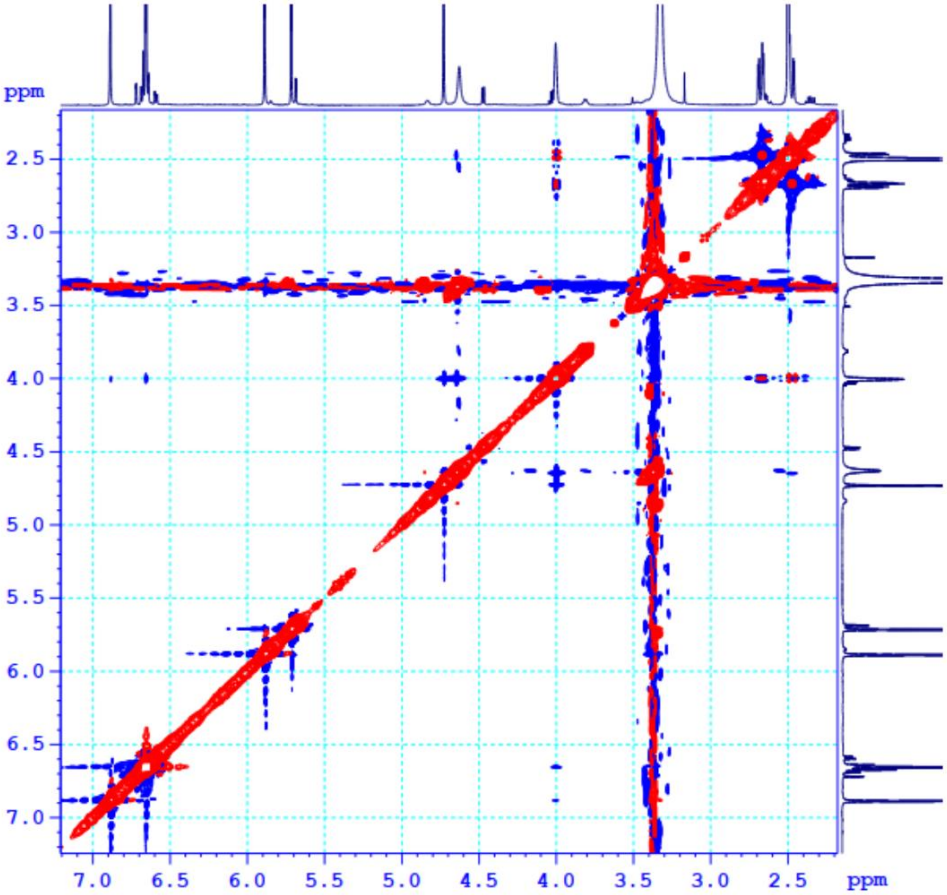

Figure S34: NOESY spectrum of compound **4** ((+)-catechin) (from δ_H 2.5 ppm to δ_C 7.0 ppm)

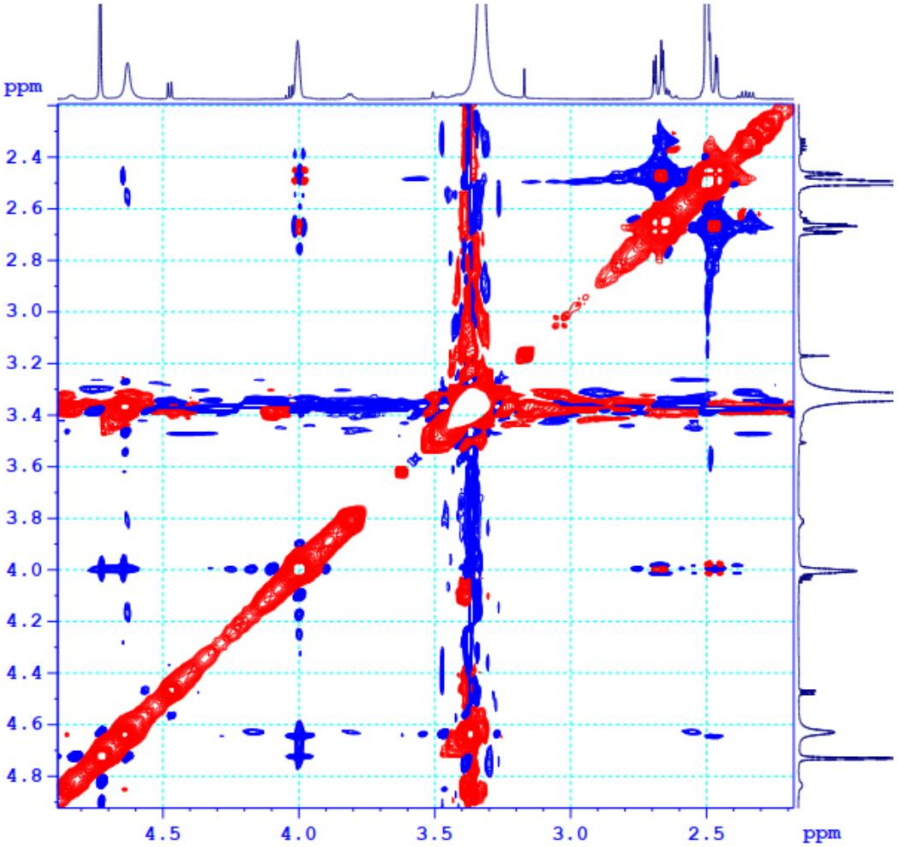

Figure S35: NOESY spectrum of compound **4** ((+)-catechin) (from δ_H 2.4 ppm to δ_H 4.8 ppm)

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

Position	Compound **5** (DMSO-d_6)		Apigenin (DMSO-d_6) [32]	
	^{13}C-NMR (150 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_H ppm
2	163.7	-	163.7	-
3	102.8	6.76 (1H, *s*)	102.8	6.75 (1H, *s*)
4	181.7	-	181.7	-
5	161.2	-	161.2	-
6	98.9	6.18 (1H, *d*, 1.8 Hz)	98.9	6.15 (1H, *d*, 1.9 hz)
7	164.2	-	164.5	-
8	94.0	6.47 (1H, *d*, 1.8 Hz)	94.0	6.44 (1H, *d*, 1.9 Hz)
9	157.3	-	157.3	-
10	103.6	-	103.5	-
1'	121.1	-	121.1	-
2'	128.5	7.92 (2H, *d*, 9.0 Hz)	128.5	7.91 (2H, *d*, 9.0 Hz)
3'	115.9	6.92 (2H, *d*, 9.0 Hz)	116.0	6.90 (2H, *d*, 9.0 Hz)
4'	161.4	-	161.4	-
5'	115.9	6.92 (2H, *d*, 9.0 Hz)	116.0	6.90 (2H, *d*, 9.0 Hz)
6'	128.5	7.92 (2H, *d*, 9.0 Hz)	128.5	7.91 (2H, d, 9.0 Hz)

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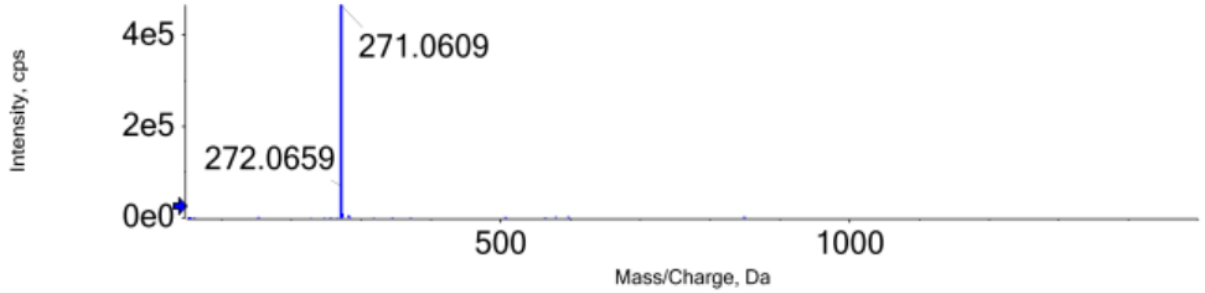
ANALYSIS REPORT

Injection details

Sample name	SAL	*Vial position*	38
Sample file name	SER. wiff2-YEN	*Inject volume*	5.00
Acquisition date	20/04/2023 10:47:59 AM	*Acquisition method*	**ESI _POS_SCAN**
Operator	CB21261708	*Instrument name*	X500R 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)

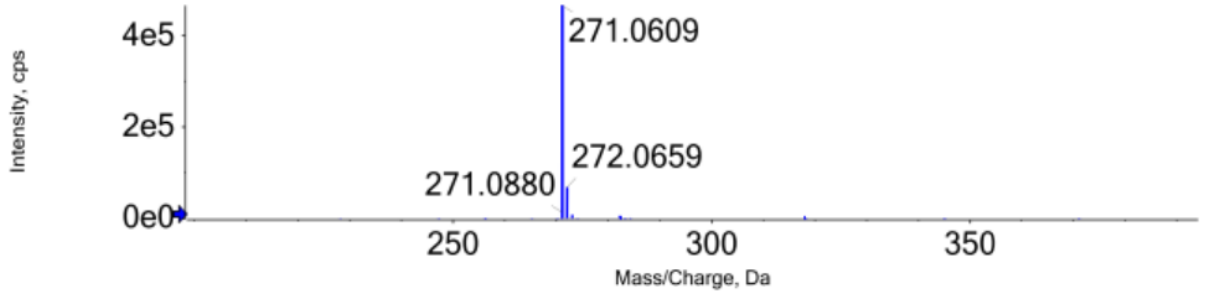


Figure S36: (+)ESI-MS spectrum of compound **5** (apigenin)

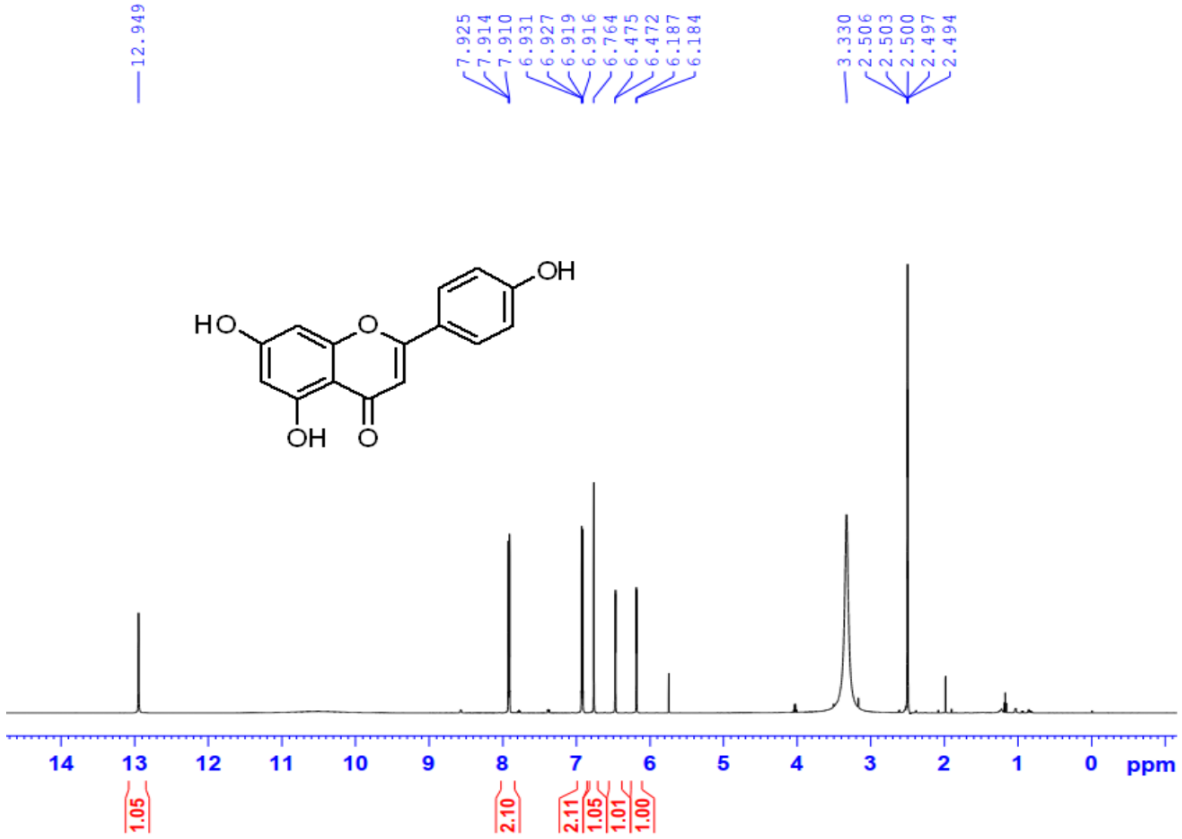


Figure S37: [1]H-NMR (600 MHz, DMSO-d_6) spectrum of compound **5** (apigenin)

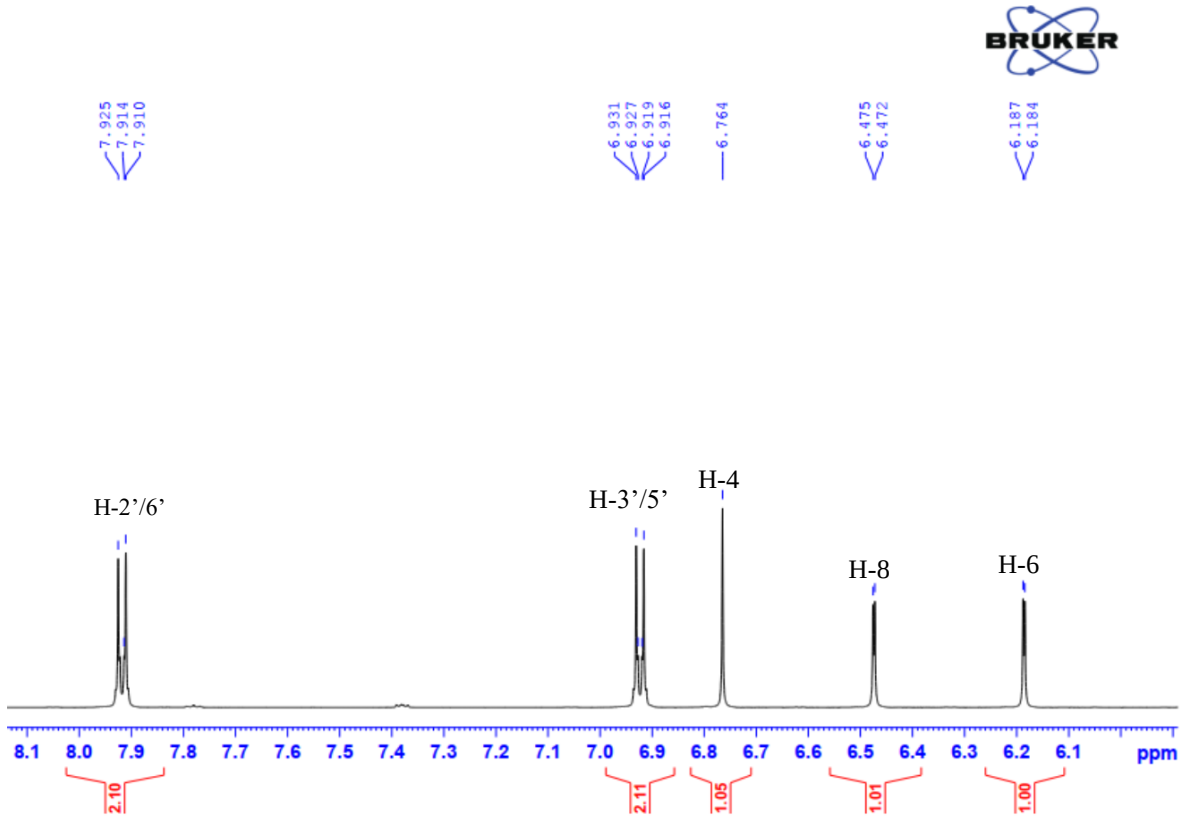


Figure S38: [1]H-NMR **(**600 MHz, DMSO-d_6**)** spectrum of compound **5** (apigenin) (from δ_H 6.0 ppm to δ_H 8.1 ppm)

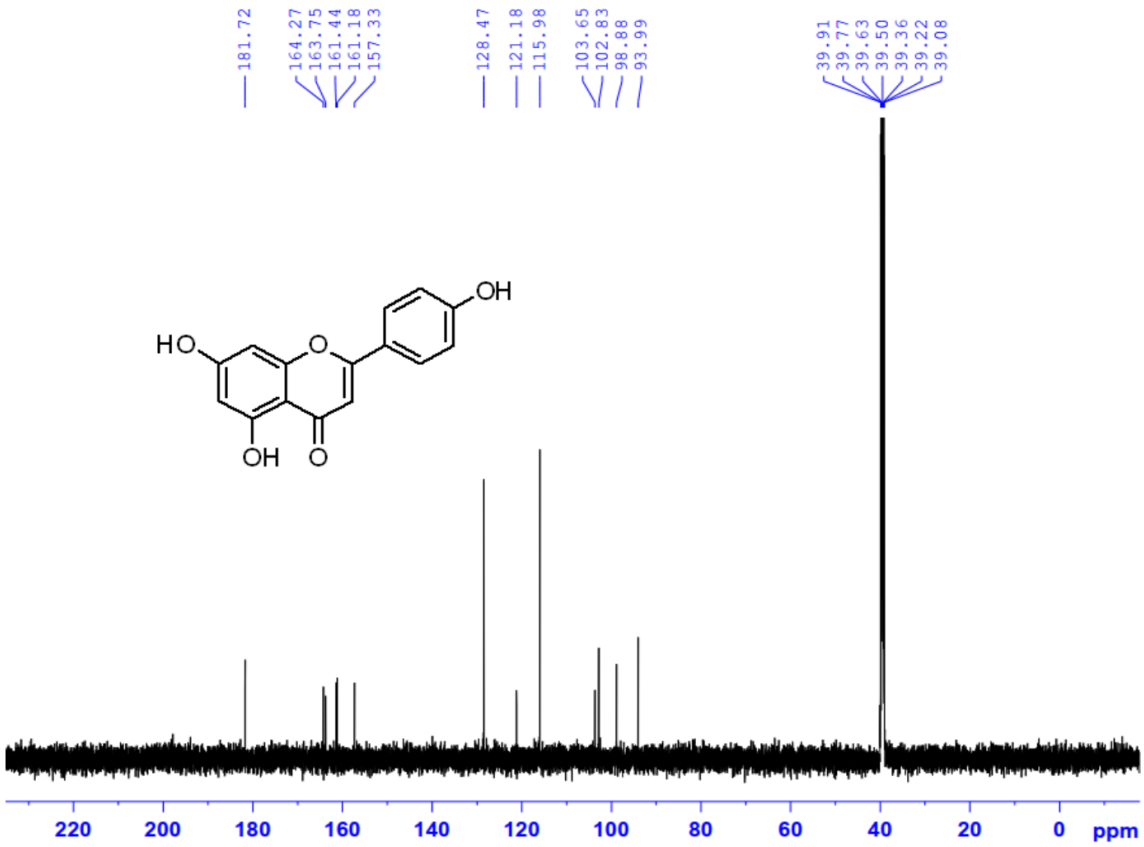


Figure S39: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **5** (apigenin)

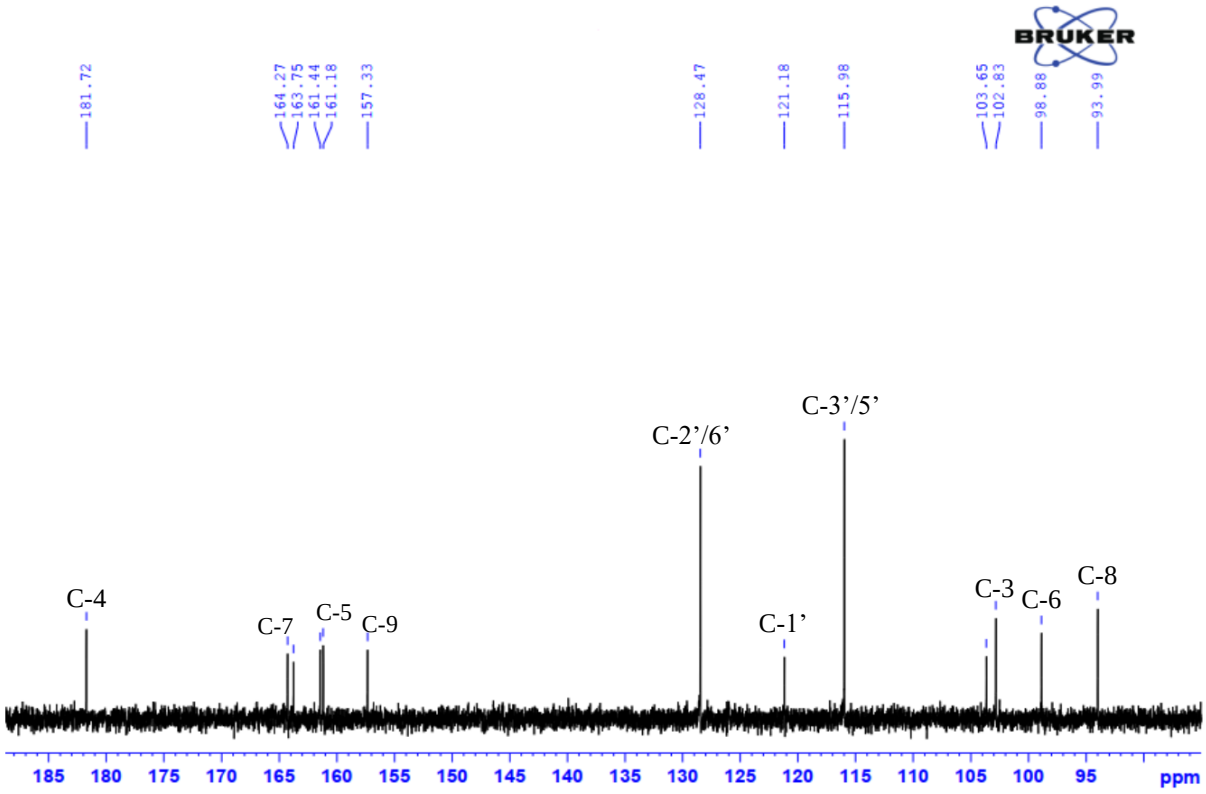


Figure S40: ^{13}C-NMR (150 MHz, DMSO-d_6**)** spectrum of compound **5** (apigenin) (from δ_C 90 ppm to δ_C 185 ppm)

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

Position	Compound **6** (DMSO-d_6)		Rutin (DMSO-d_6) [33]	
	^{13}C-NMR (150 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_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, *d*, 2.0 Hz)	99.9	6.20 (1H, *d*, 1.8 Hz)
7	164.6	-	165.9	-
8	93.6	6.36 (1H, *d*, 2.0 Hz)	94.8	6.39 (1H, *d*, 2.2 Hz)
9	156.5	-	159.3	-
10	103.7	-	105.6	-
1'	121.1	-	123.1	-
2'	116.2	7.55 (1H, *d*, 1.8 Hz)	117.6	7.66 (1H, *d*, 1.8 Hz)
3'	144.8	-	145.8	-
4'	148.5	-	149.7	-
5'	115.2	6.84 (1H, *d*, 8.4 Hz)	116.1	6.86 (1H, *d*, 8.0 Hz)
6'	121.6	7.53 (1H, *dd*, 8.4, 2.4 Hz)	123.5	7.60 (1H, *dd*, 8.0, 1.8 Hz)
1"	101.2	5.33 (1H, *d*, 7.2 Hz)	104.7	5.09 (1H, *d*, 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, *s*)	102.4	4.51 (1H, *d*, 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, *d*, 6.0 Hz)	17.9	1.11 (3H, *d*, 6.0 Hz)

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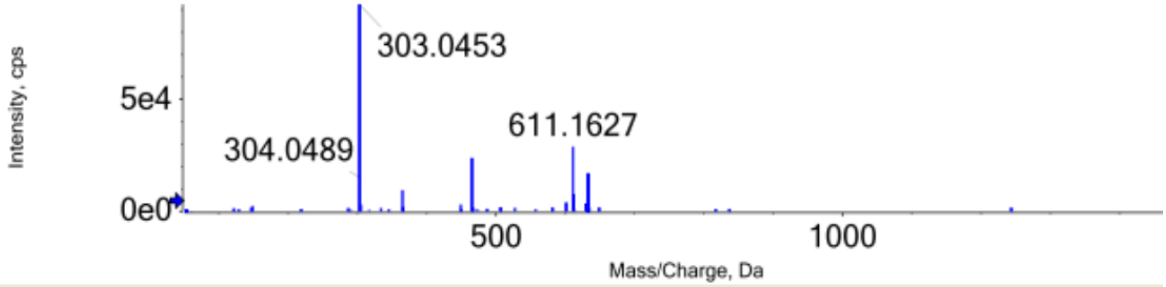
Injection details

Sample name	SAL	*Vial position*	37
Sample file name	SER. wiff2-YEN	*Inject volume*	5.00
Acquisition date	20/04/2023 10:43:32 AM	*Acquisition method*	**ESI _POS_SCAN**
Operator	CB21261708	*Instrument name*	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

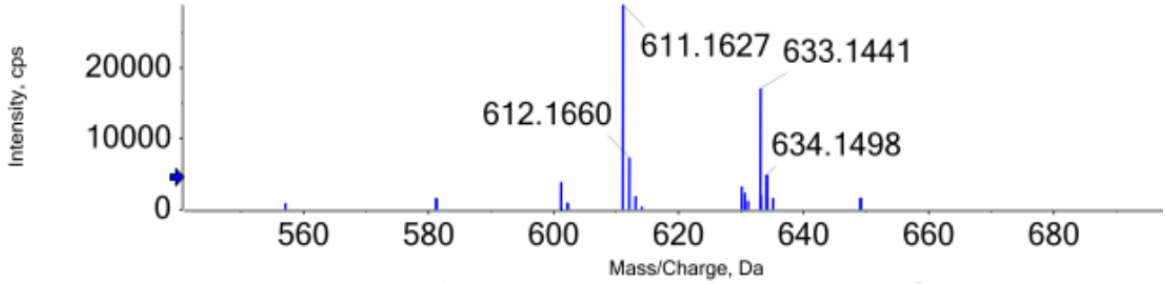


Figure S41: (+)ESI-MS spectrum of compound **6**

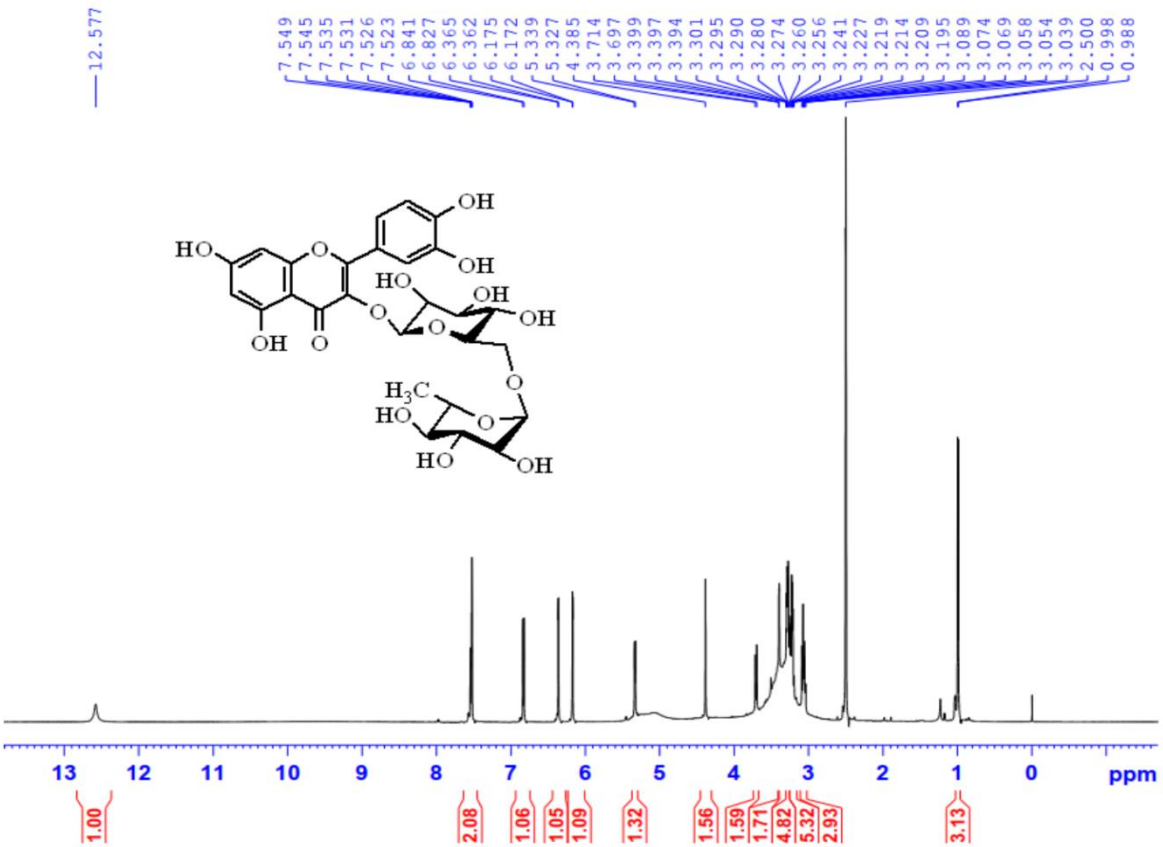


Figure S42: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **6** (rutin)

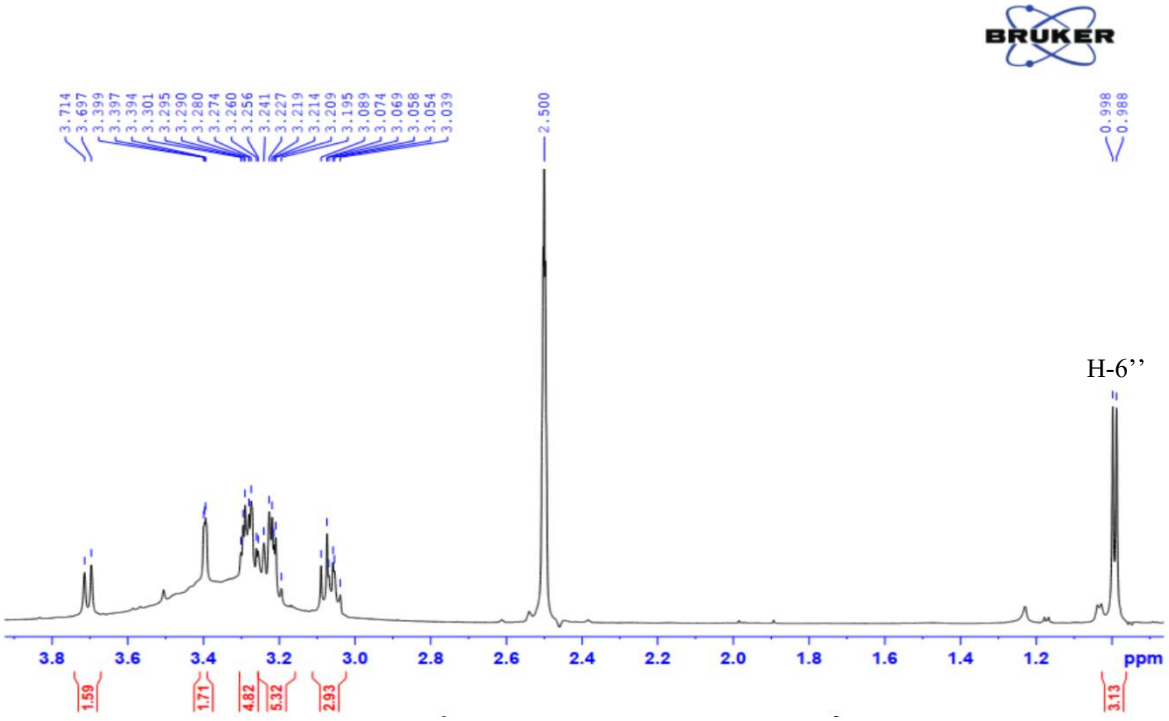


Figure S43: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **6** (rutin) (from $\delta_{\mathbf{H}}$ 1.0 ppm to δ_{H} 3.8 ppm)

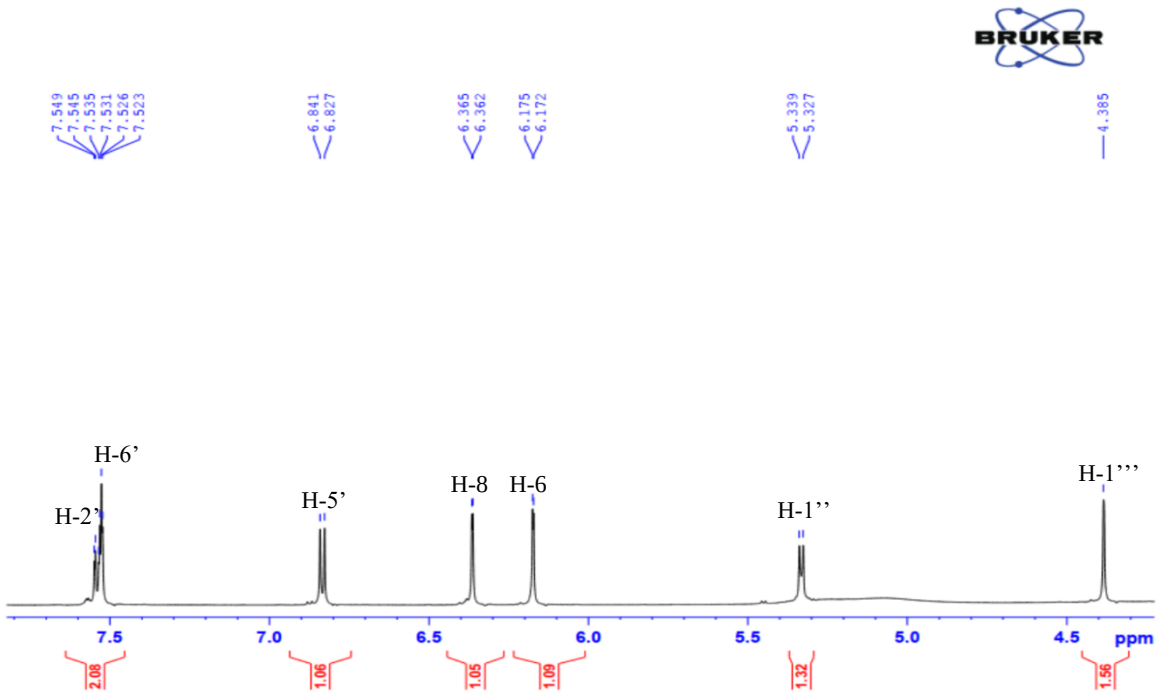


Figure S44: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of compound **6** (rutin) (from δ_H 4.3 ppm to δ_H 7.7 ppm)

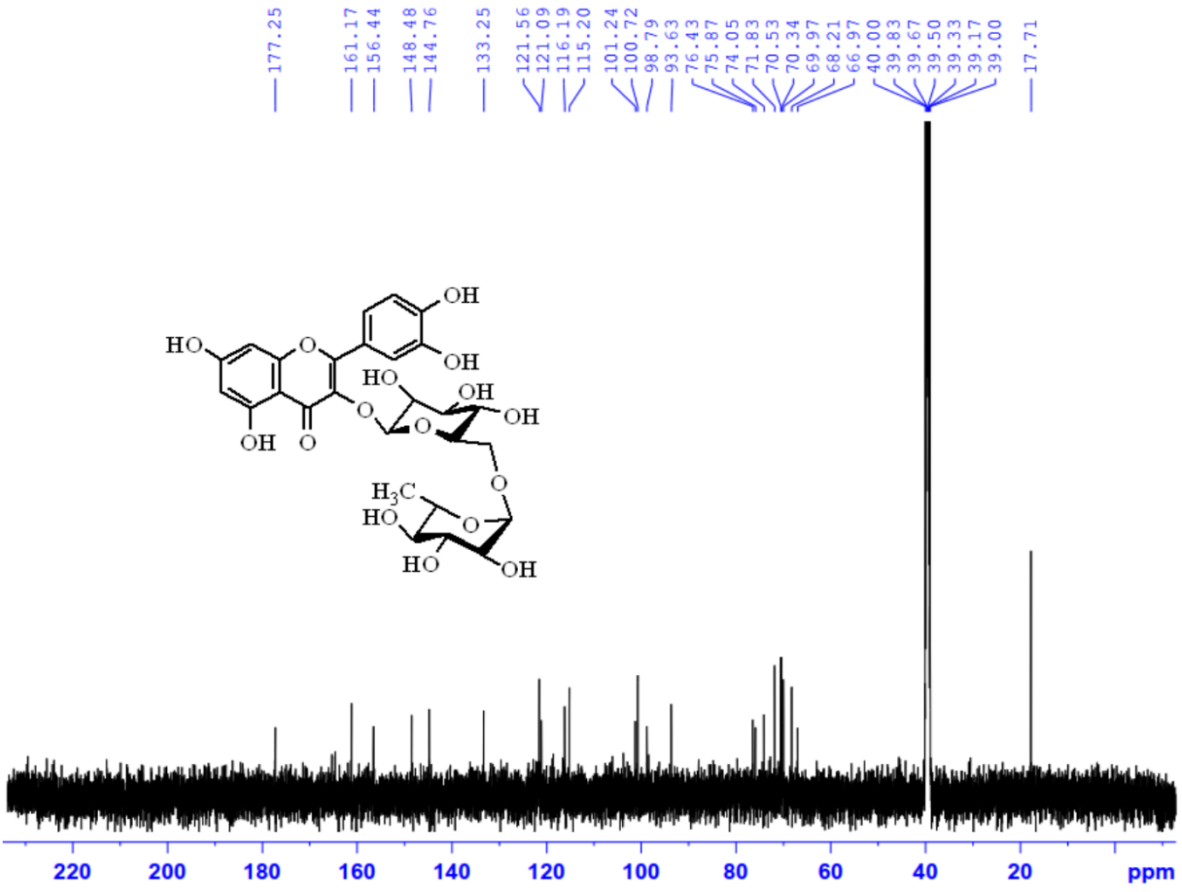


Figure S45: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **6** (rutin)

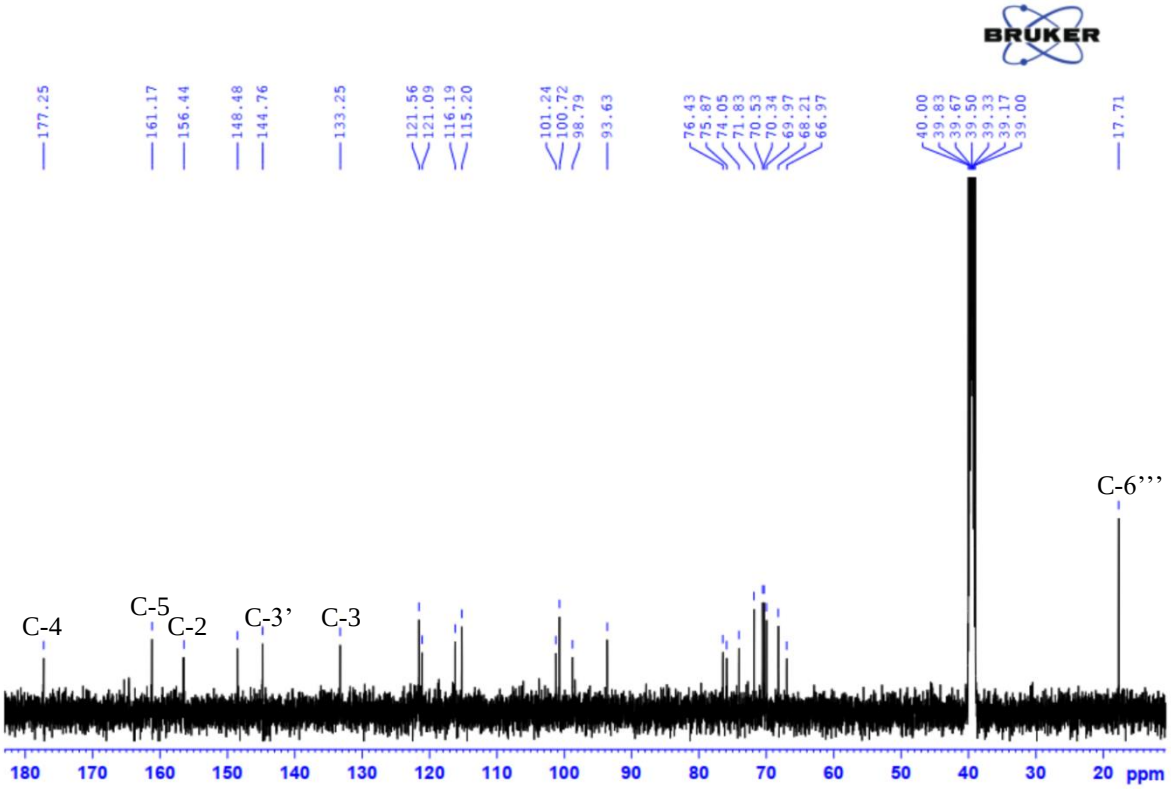


Figure S46: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **6** (rutin) (from δ_C 15 ppm to δ_C 180 ppm)

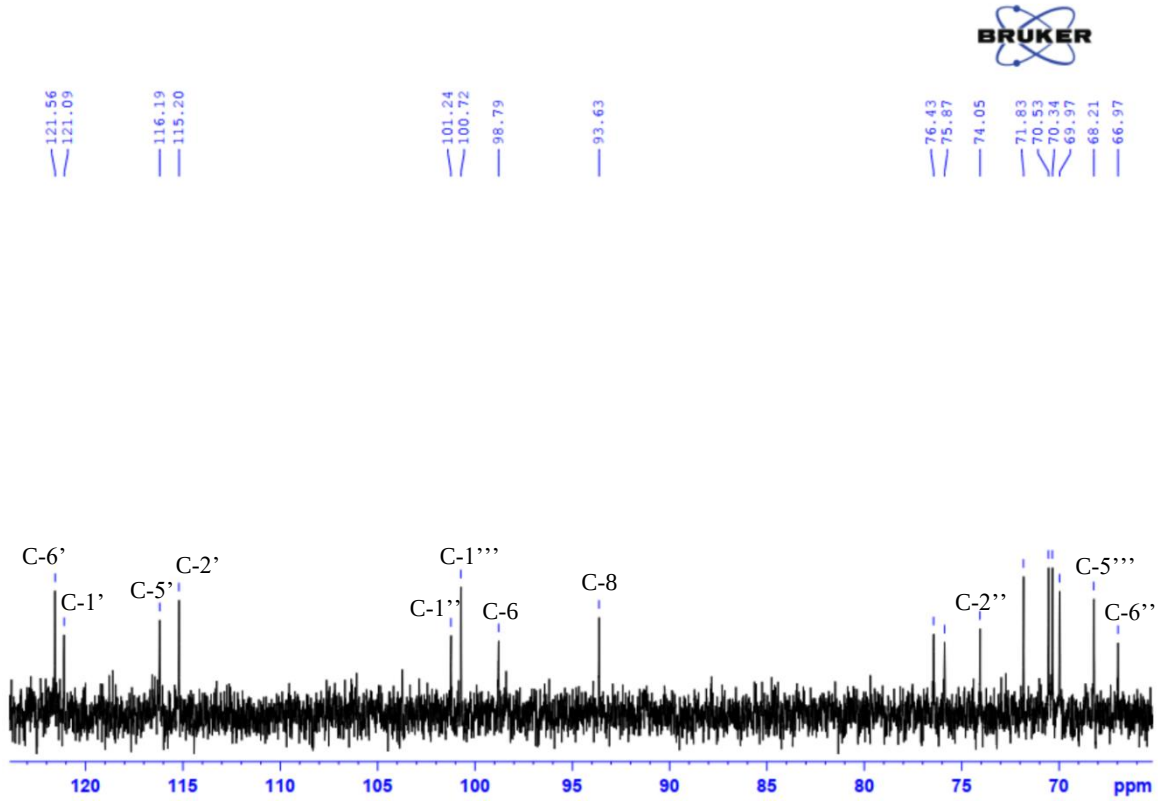


Figure S47: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of compound **6** (rutin) (from δ_C 60 ppm to δ_C 125 ppm)

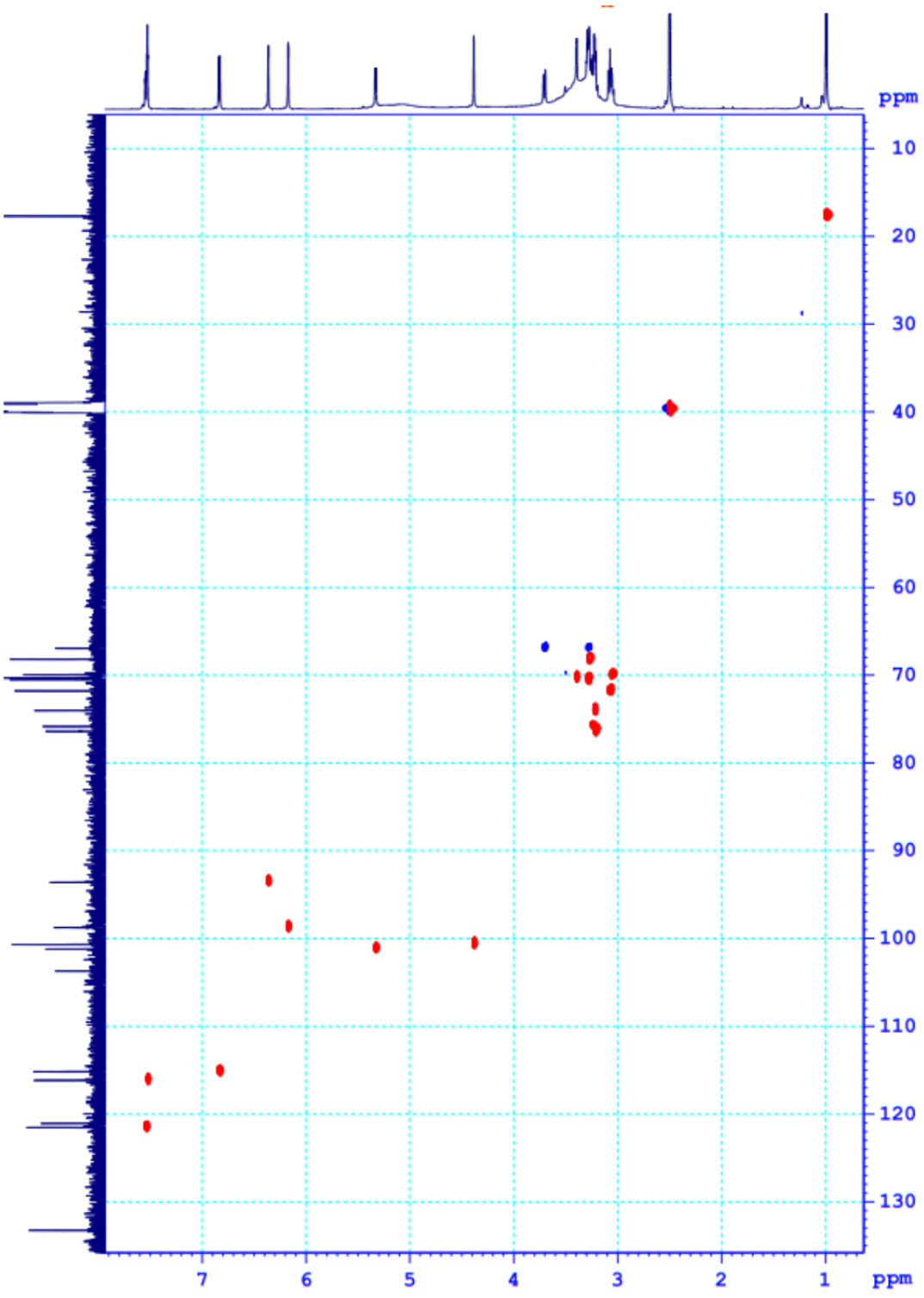


Figure S48: HSQC spectrum of compound **6** (rutin)

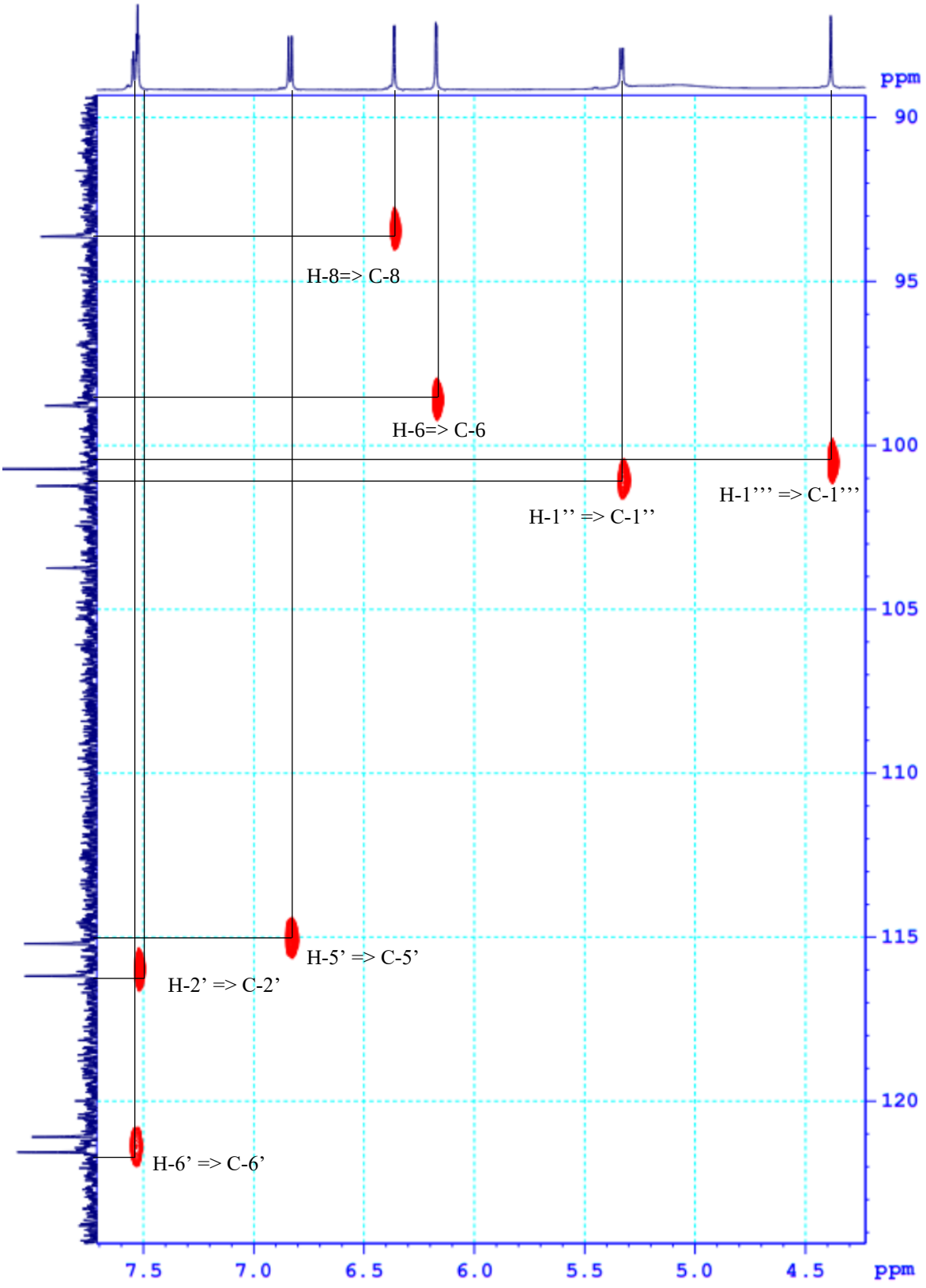


Figure S49: HSQC spectrum of compound **6** (rutin) (from δ_C 90 ppm to δ_C 125 ppm)

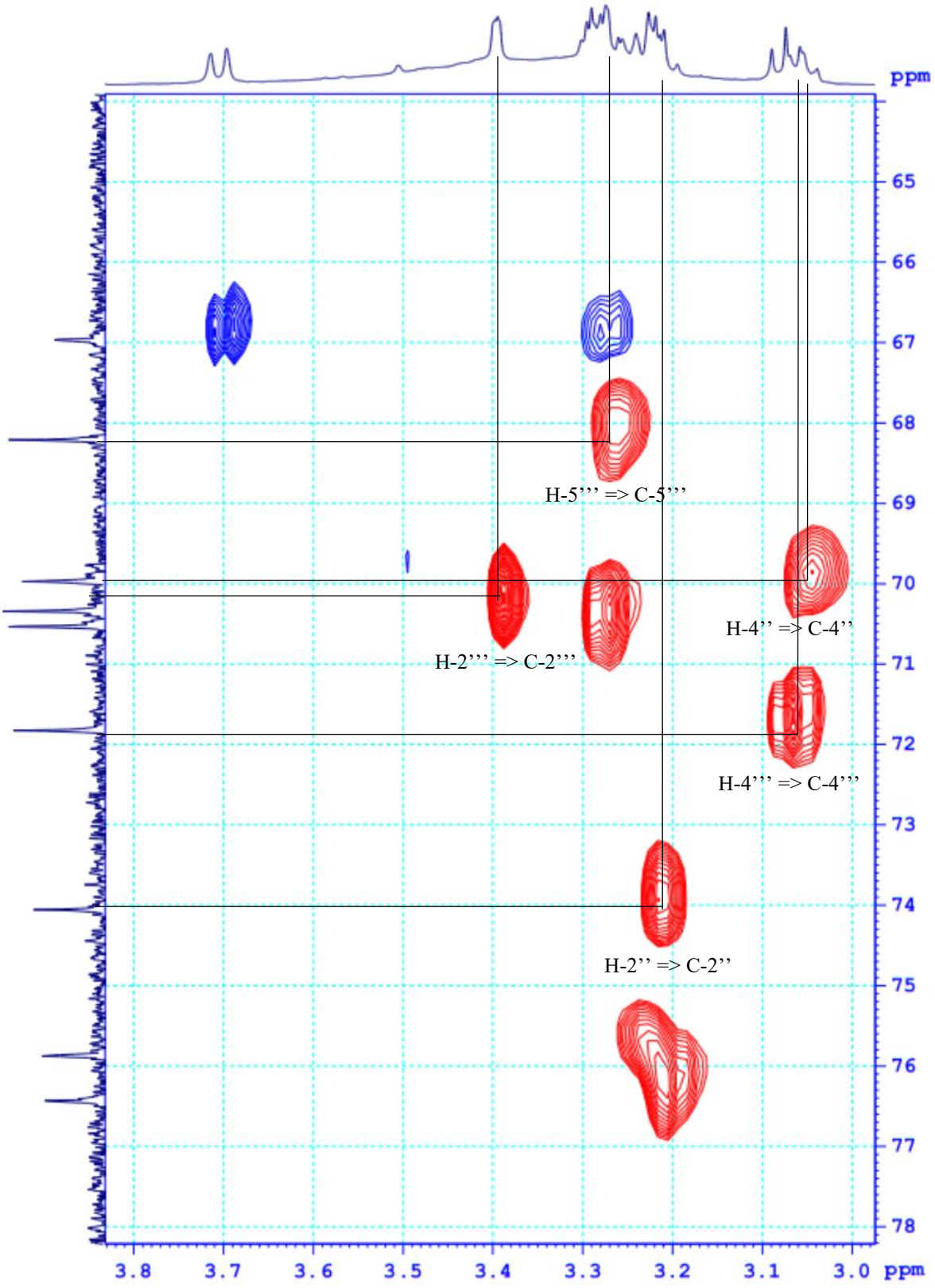


Figure S50: HSQC spectrum of compound **6** (rutin) (from δ_C 64 ppm to δ_C 78 ppm)

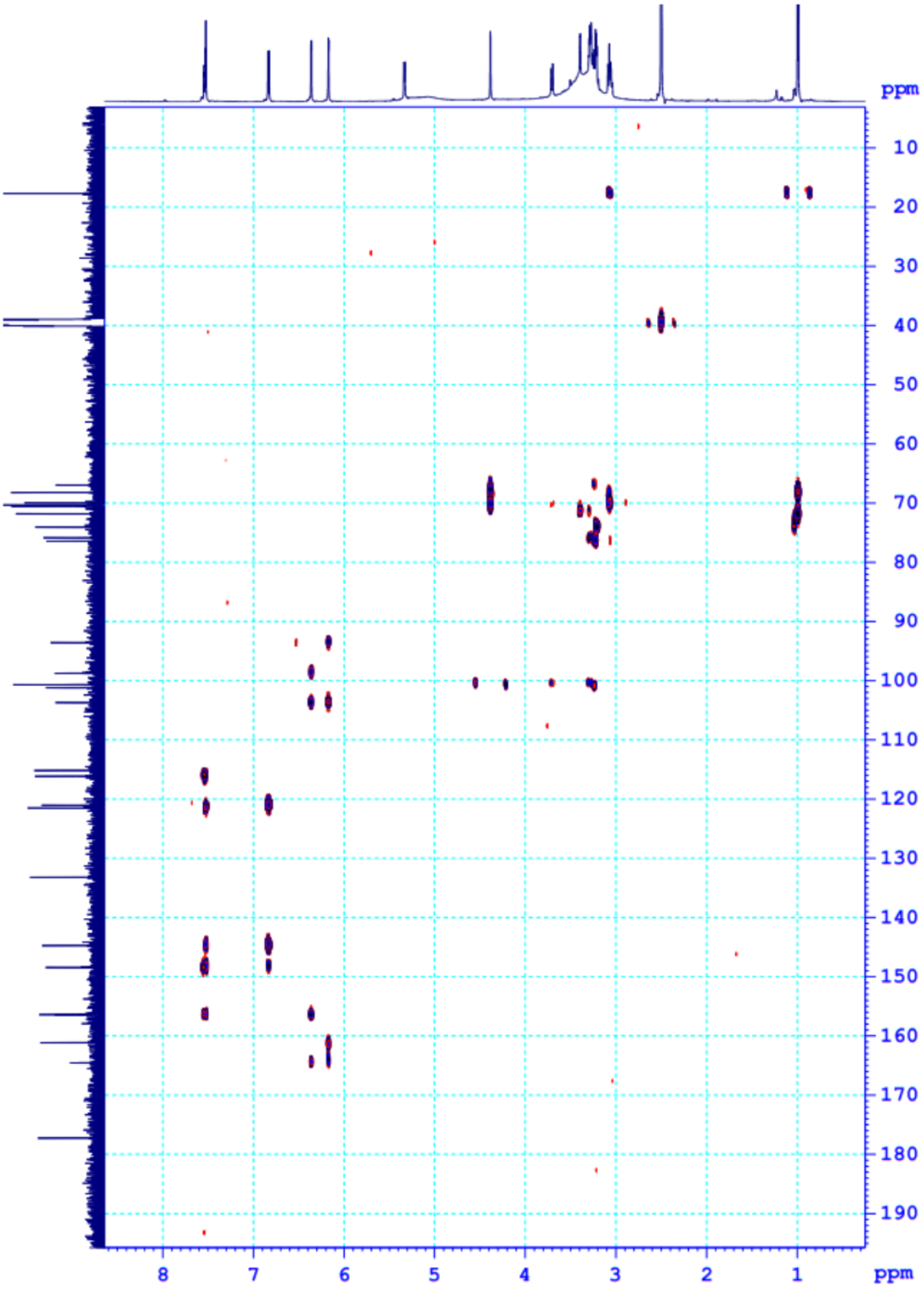


Figure S51: HMBC spectrum of compound **6** (rutin)

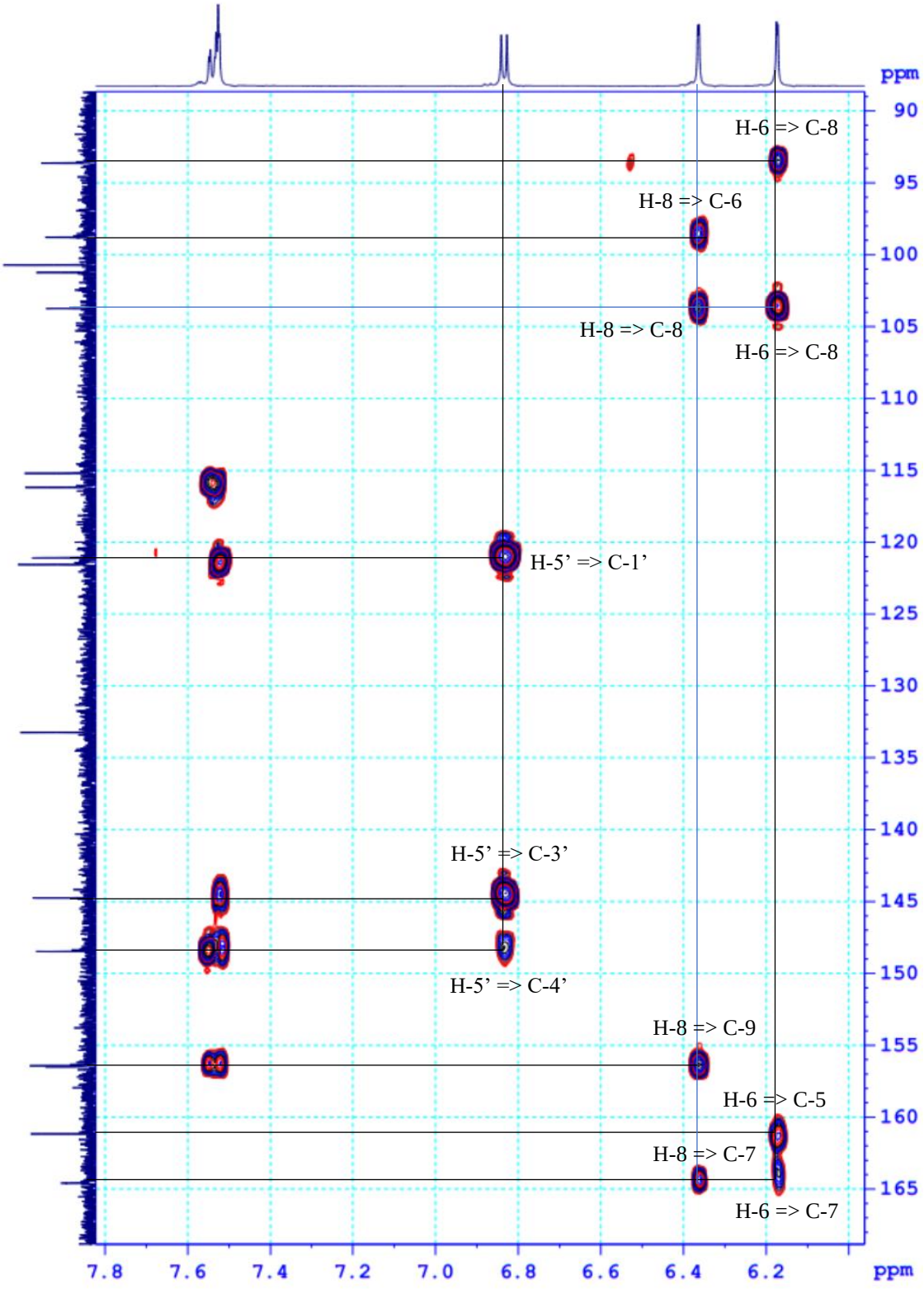


Figure S52: HMBC spectrum of compound **6** (rutin) (from δ_C 90 ppm to δ_C 165 ppm)

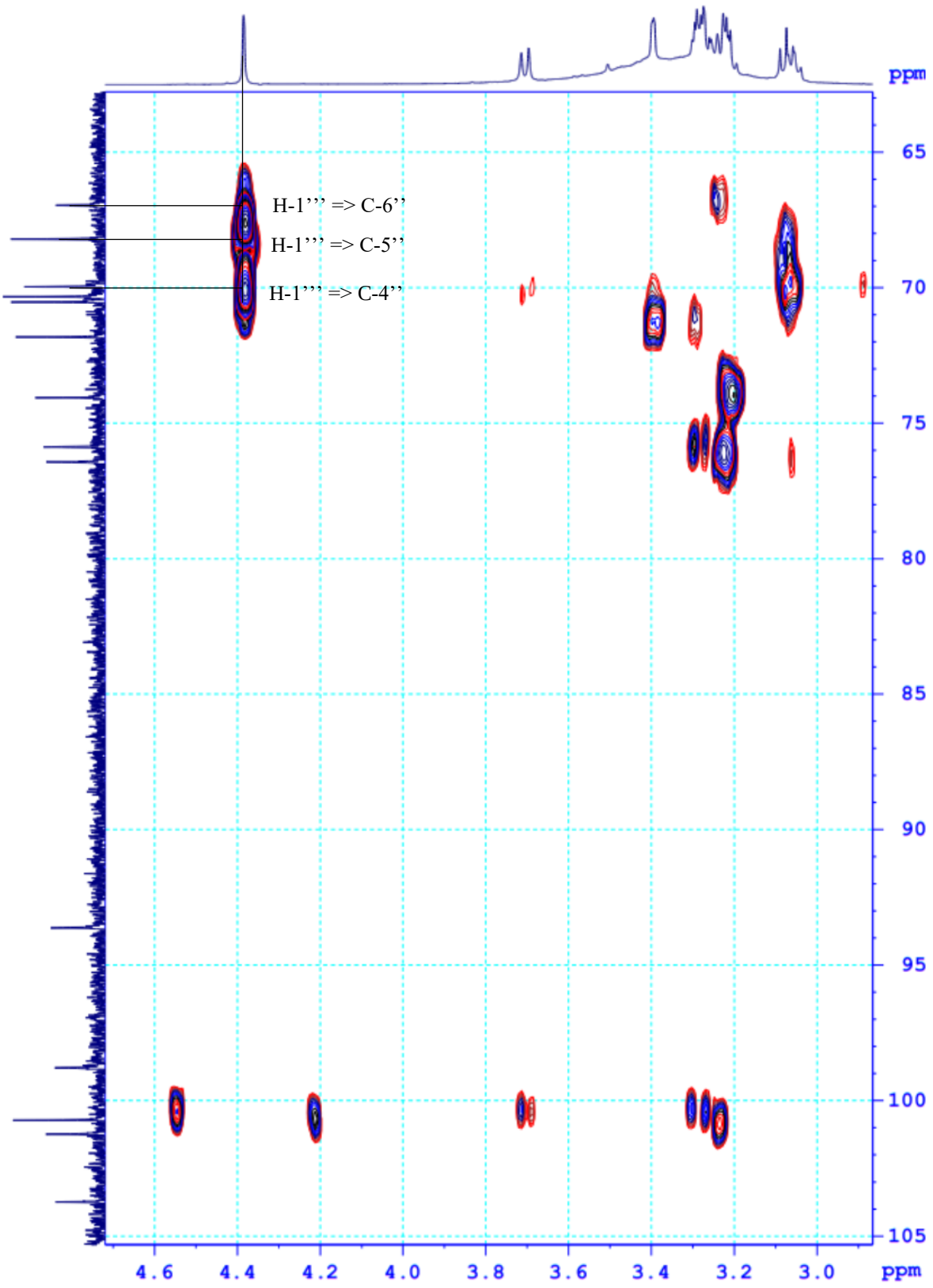


Figure S53: HMBC spectrum of compound **6** (rutin) (from δ_C 65 ppm to δ_C 105 ppm)

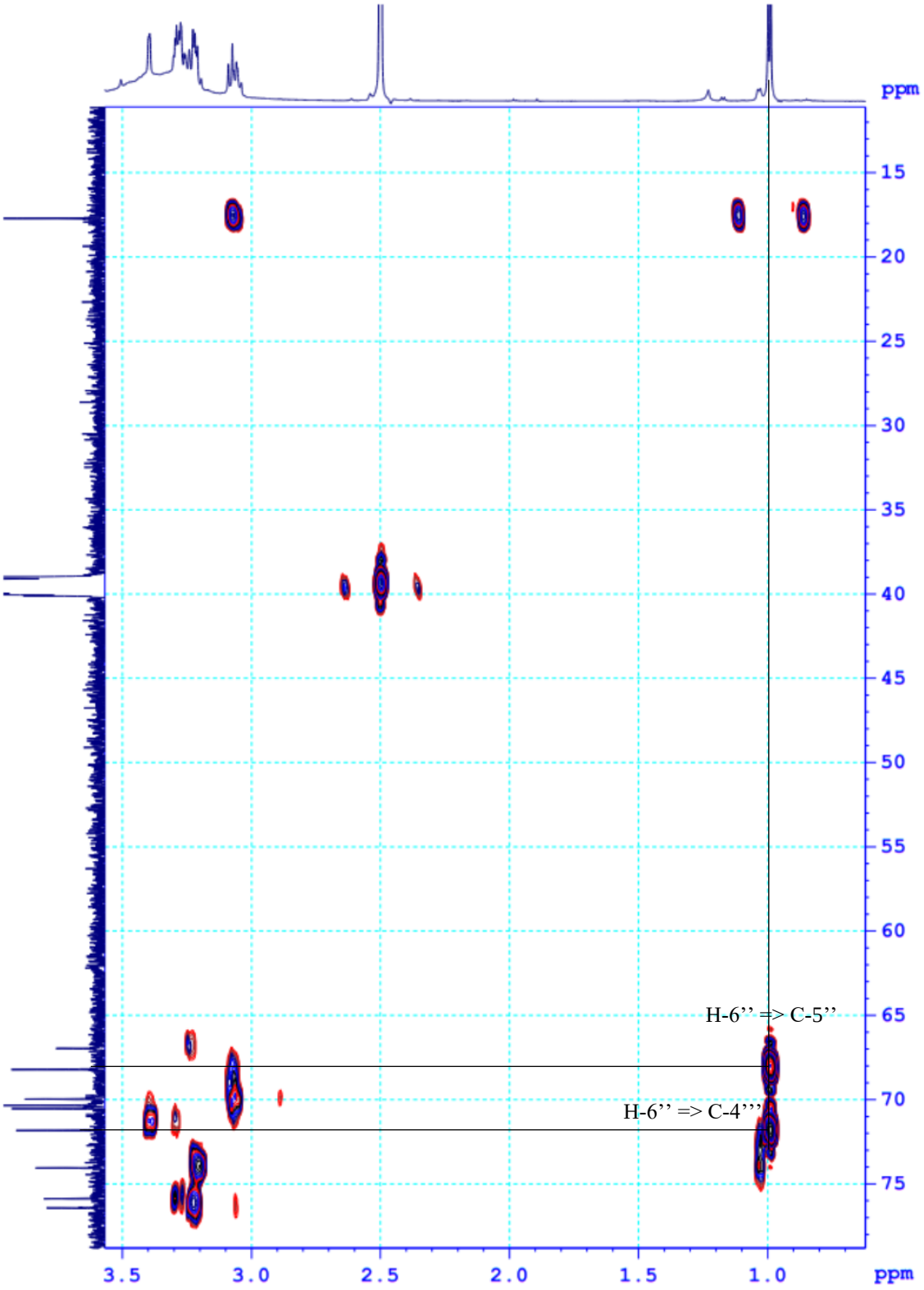


Figure S54: HMBC spectrum of compound **6** (rutin) (from δ_C 15 ppm to δ_C 75 ppm)

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

Position	Compound **7** (MeOD)		Isatin ($CDCl_3$) [34,35]	
	^{13}C-NMR (125 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_H ppm
1-NH	-	-	-	8.01
2	161.4	-	159.5	-
3	185.4	-	184.6	-
3*α*	119.4	-	117.9	-
4	124.4	7.60 (1H, *td*, 7.8, 1.2 Hz)	122.9	7.63
5	126.0	7.12 (1H, *td*, 7.8, 0.6 Hz)	124.8	7.13
6	139.5	7.56 (1H, *dd*, 7.8, 0.6 Hz)	138.5	7.57
7	113.4	6.96 (1H, *d*, 8.4 Hz)	112.4	6.91
7*α*	152.0	-	150.9	-

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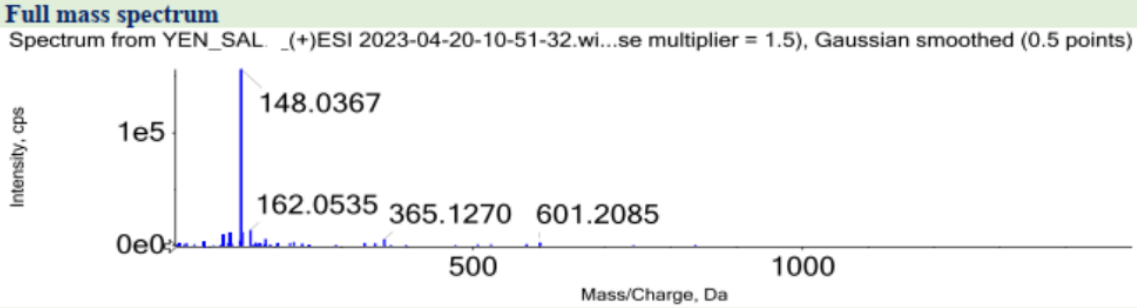
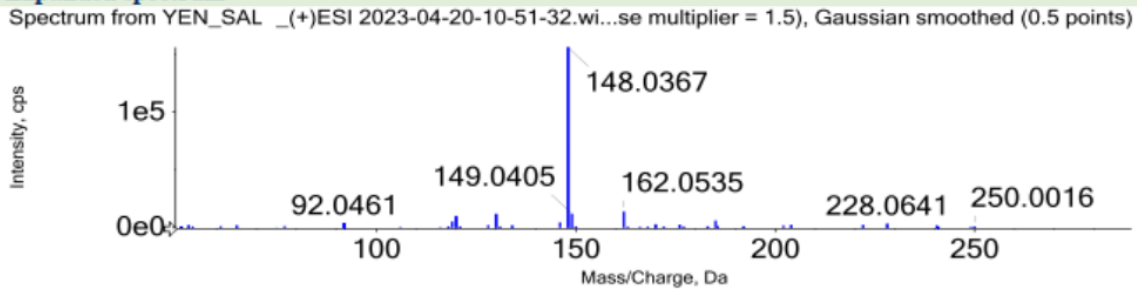
Injection details

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*	**ESI _POS_SCAN**
Operator	CB21261708	*Instrument name*	X500R QTOF

Full mass spectrum



Expanded spectrum



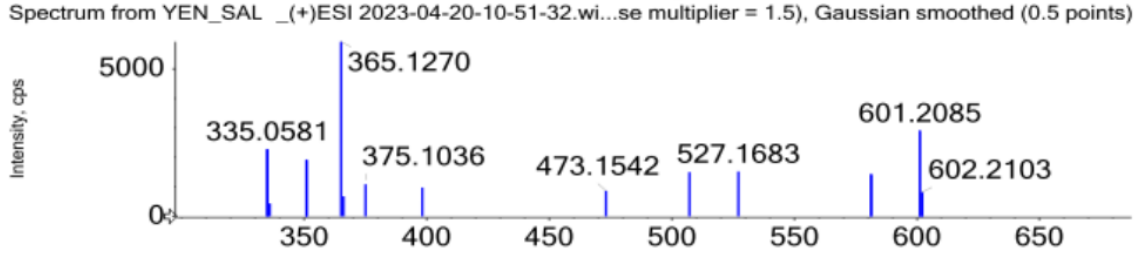


Figure S55: (+)ESI-MS spectrum of compound **7** (isatin)

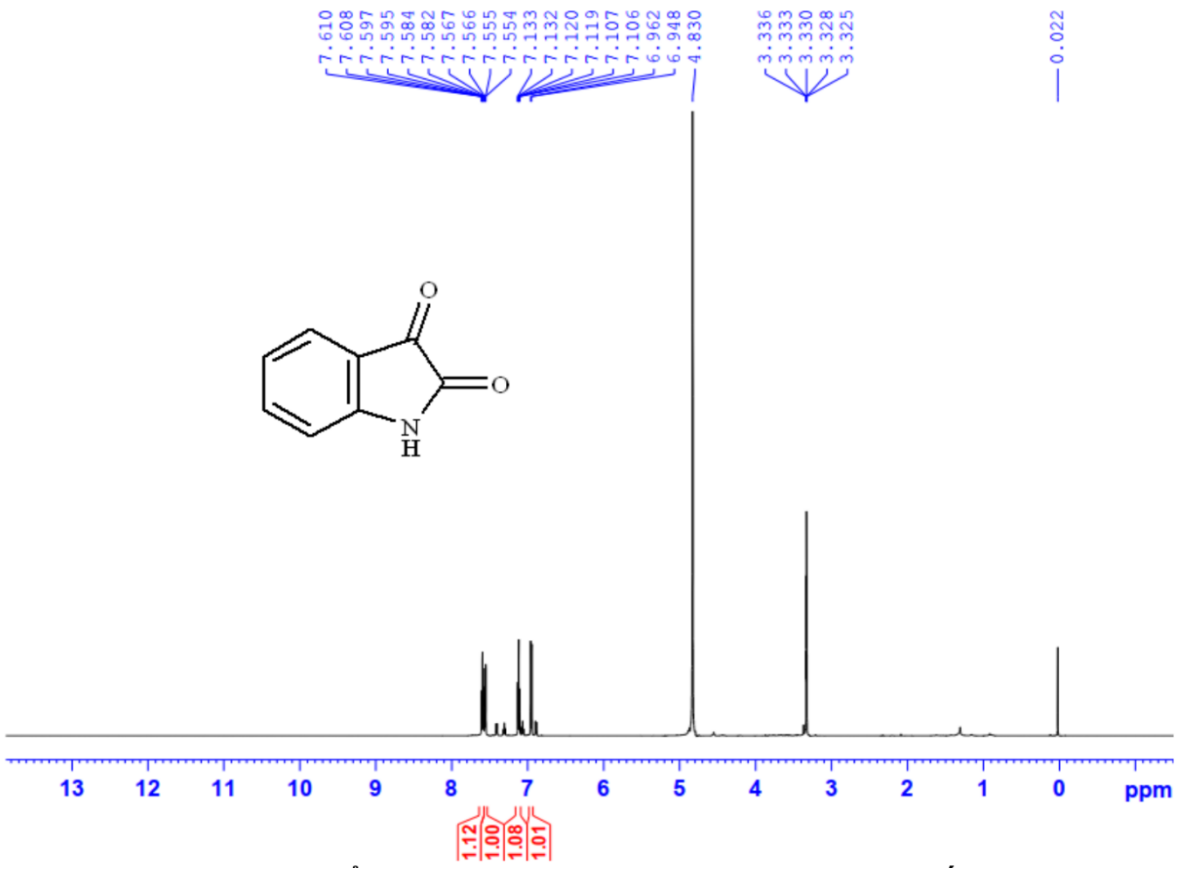


Figure S56: [1]H-NMR (600 MHz, MeOD) spectrum of compound **7** (isatin)

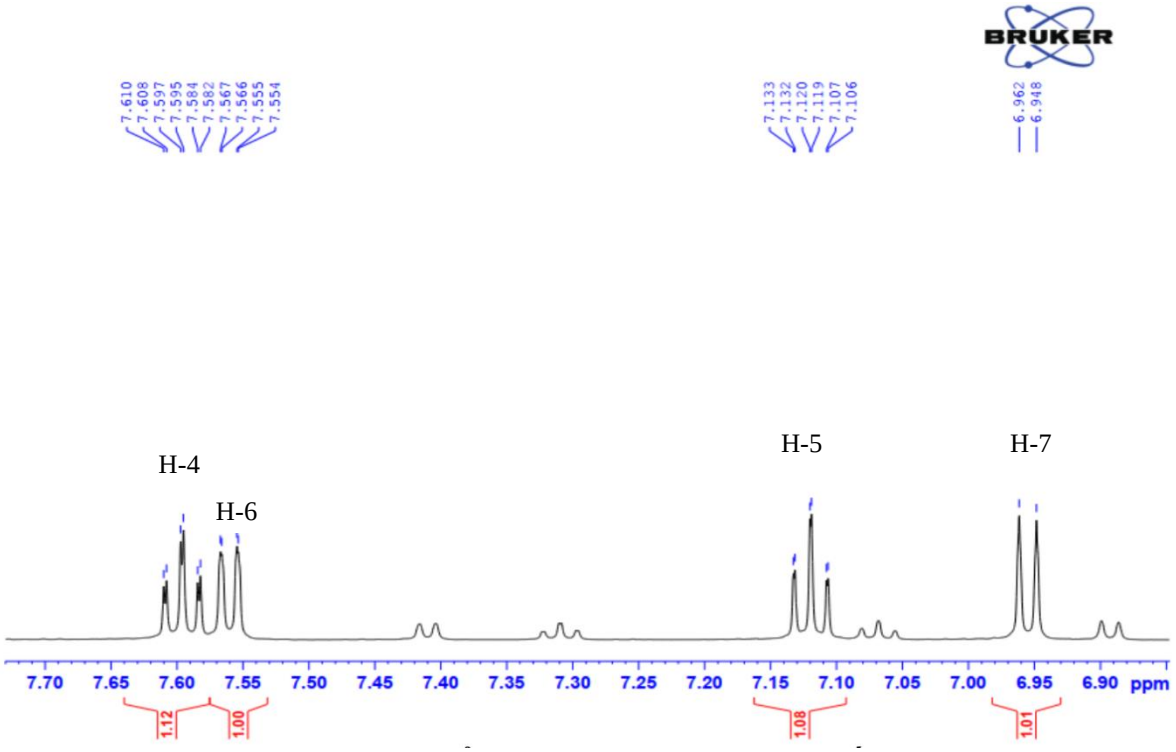


Figure S57: [1]H-NMR spectrum of compound **7** (isatin) (from δ_H 6.9 ppm to δ_H 7.7 ppm)

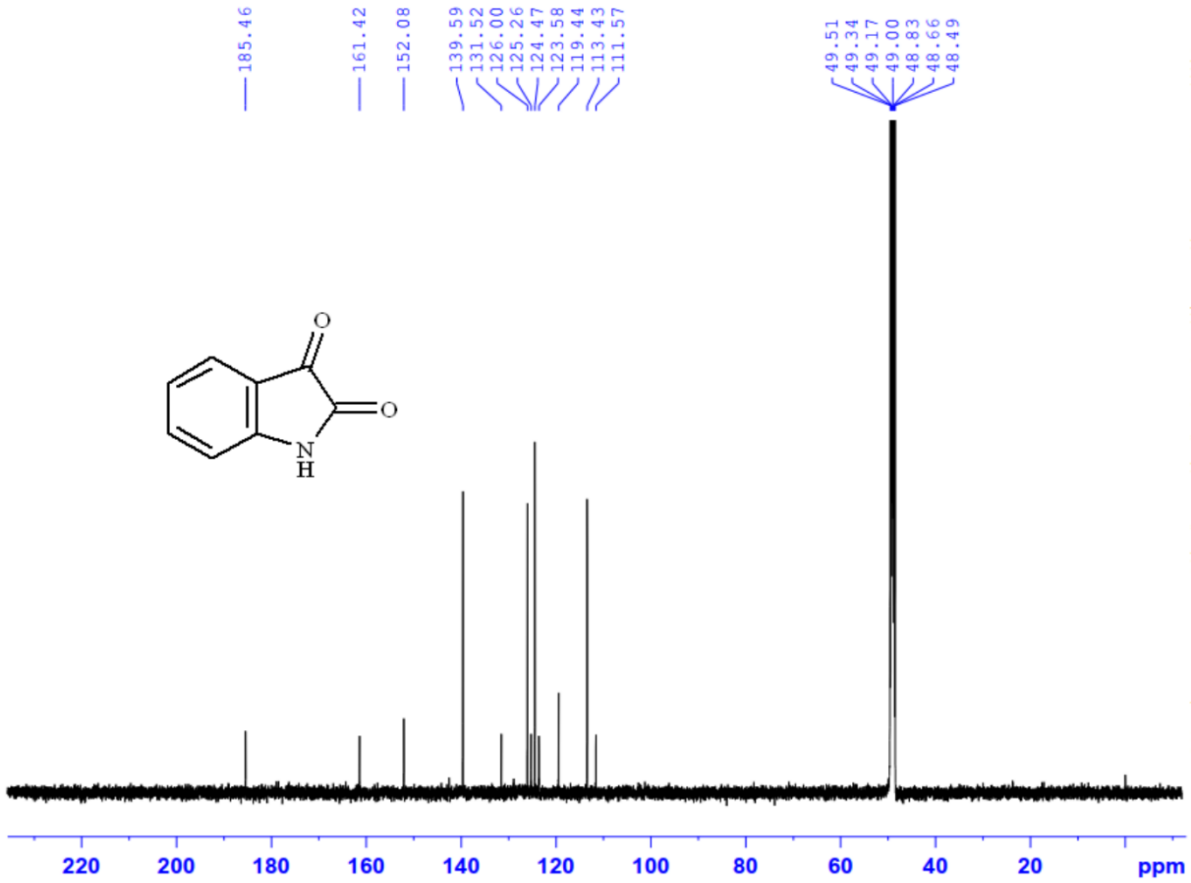


Figure S58: ^{13}C-NMR (150MHz, MeOD) spectrum of compound **7** (isatin)

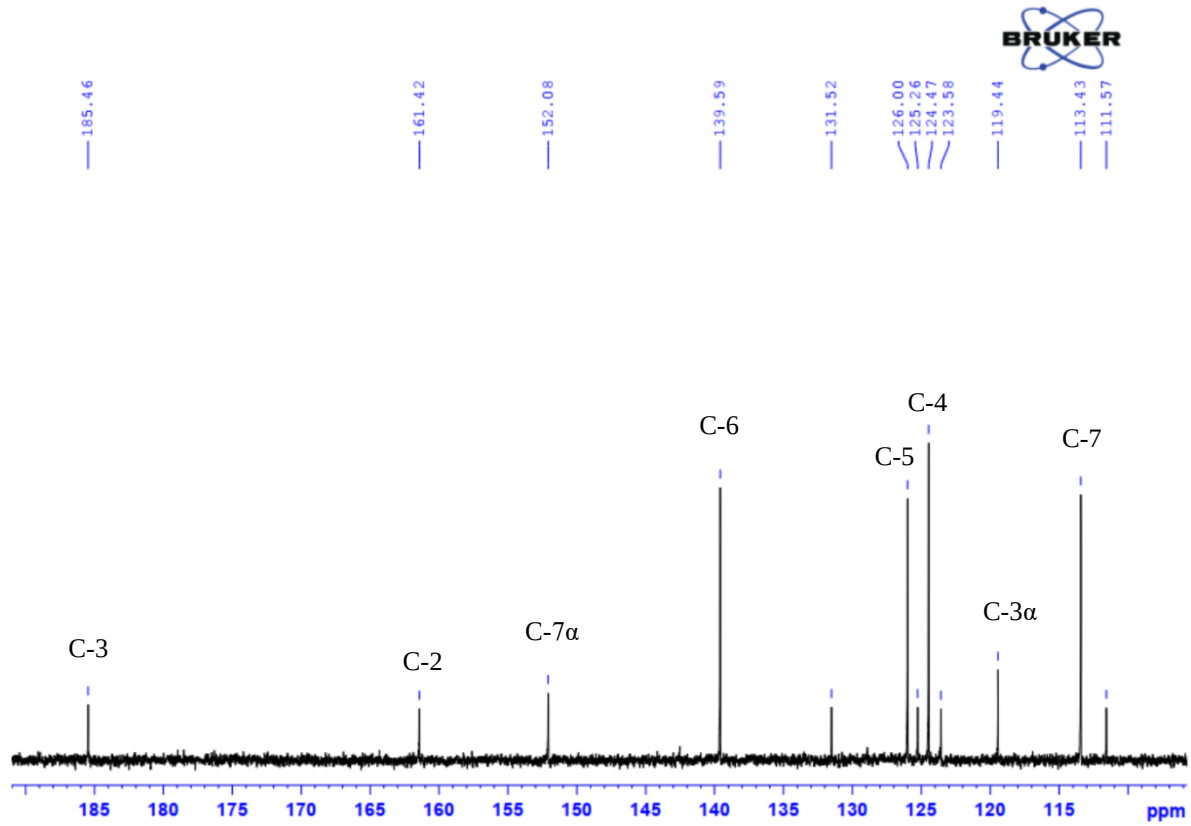


Figure S59: ^{13}C-NMR spectrum of compound **7** (isatin) (from δ_C 110 ppm to δ_C 185 ppm)

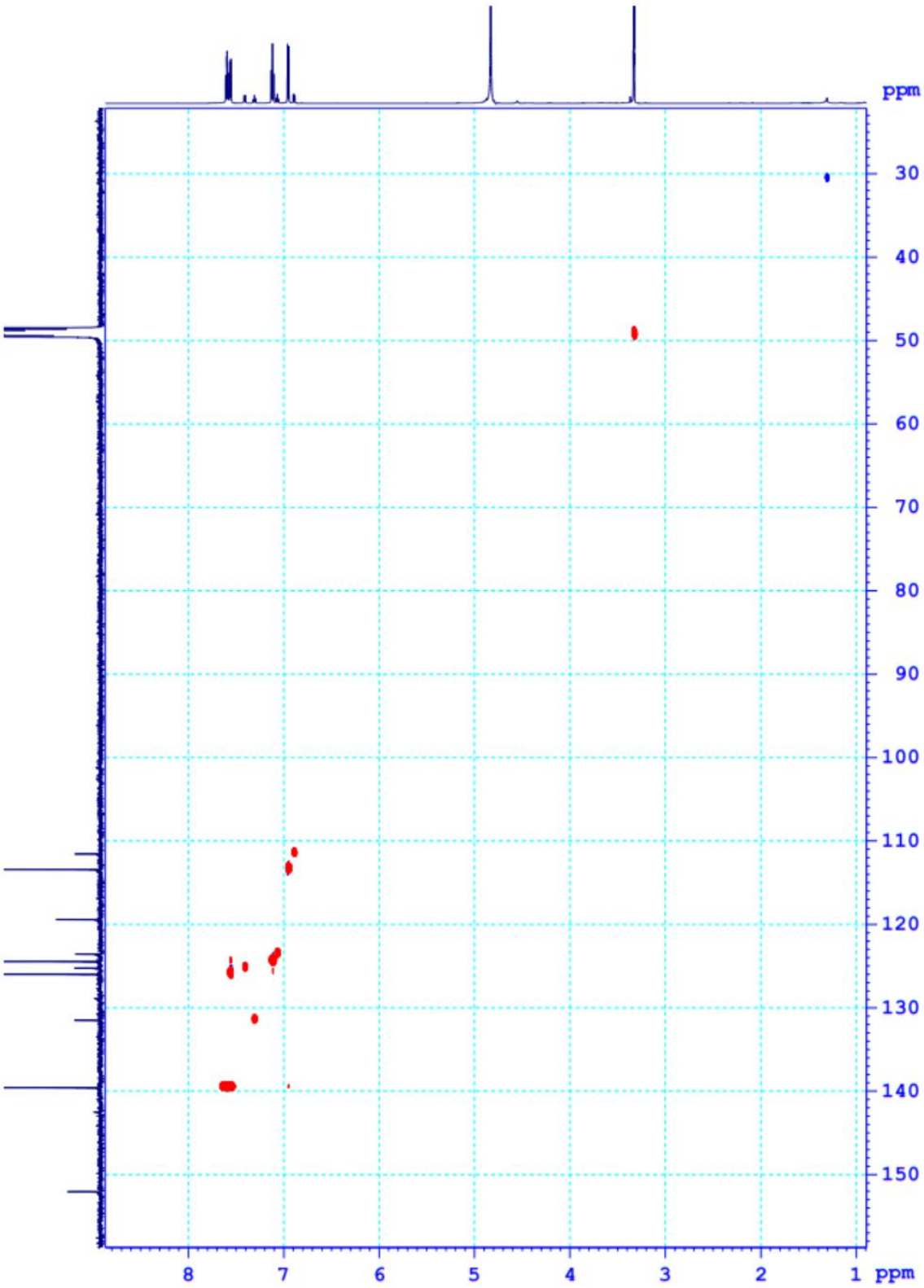


Figure S60: HSQC spectrum of compound **7** (isatin)

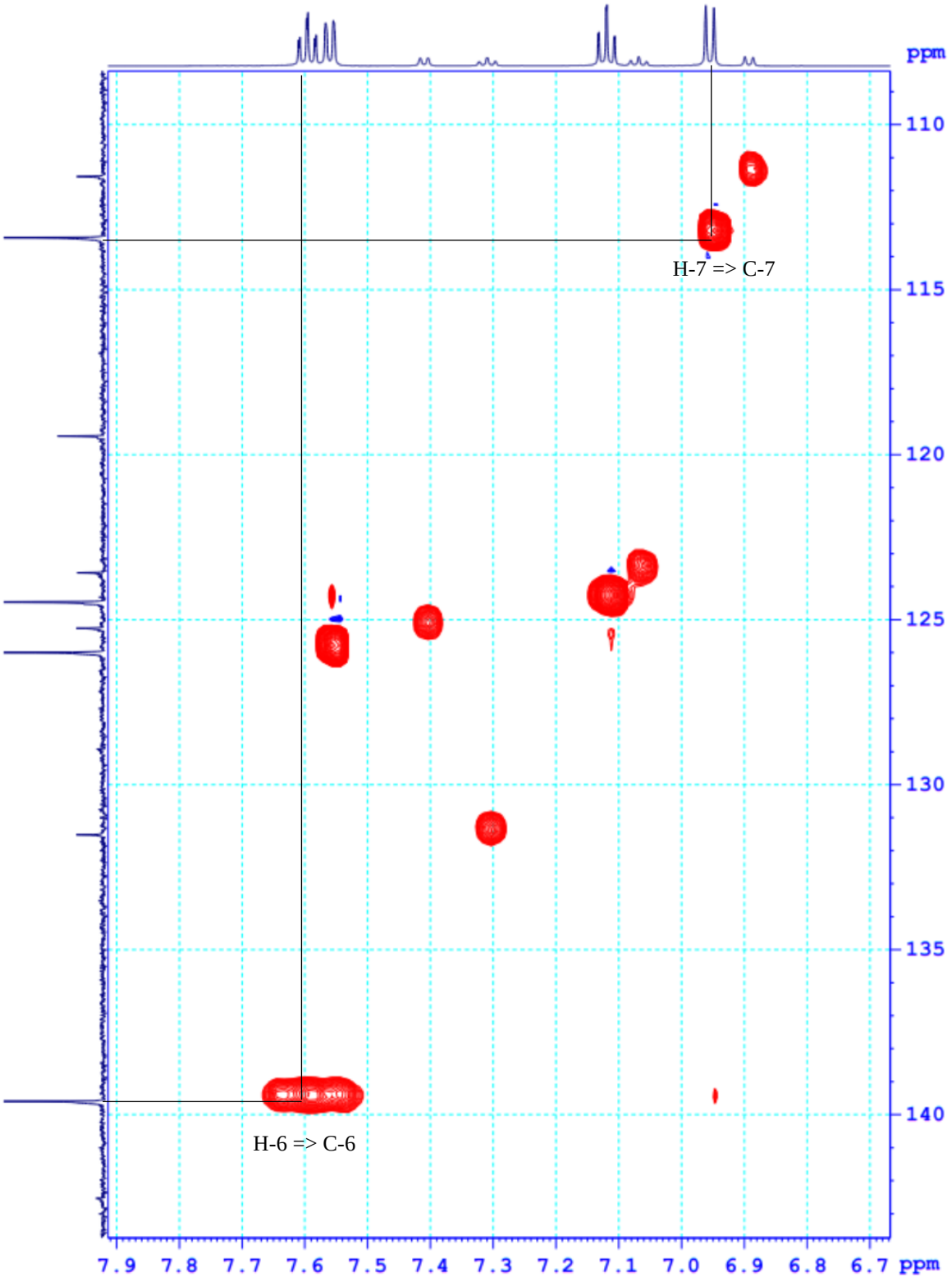


Figure S61: HSQC spectrum of compound **7** (isatin) (from δ_C110 ppm to δ_C 140 ppm)

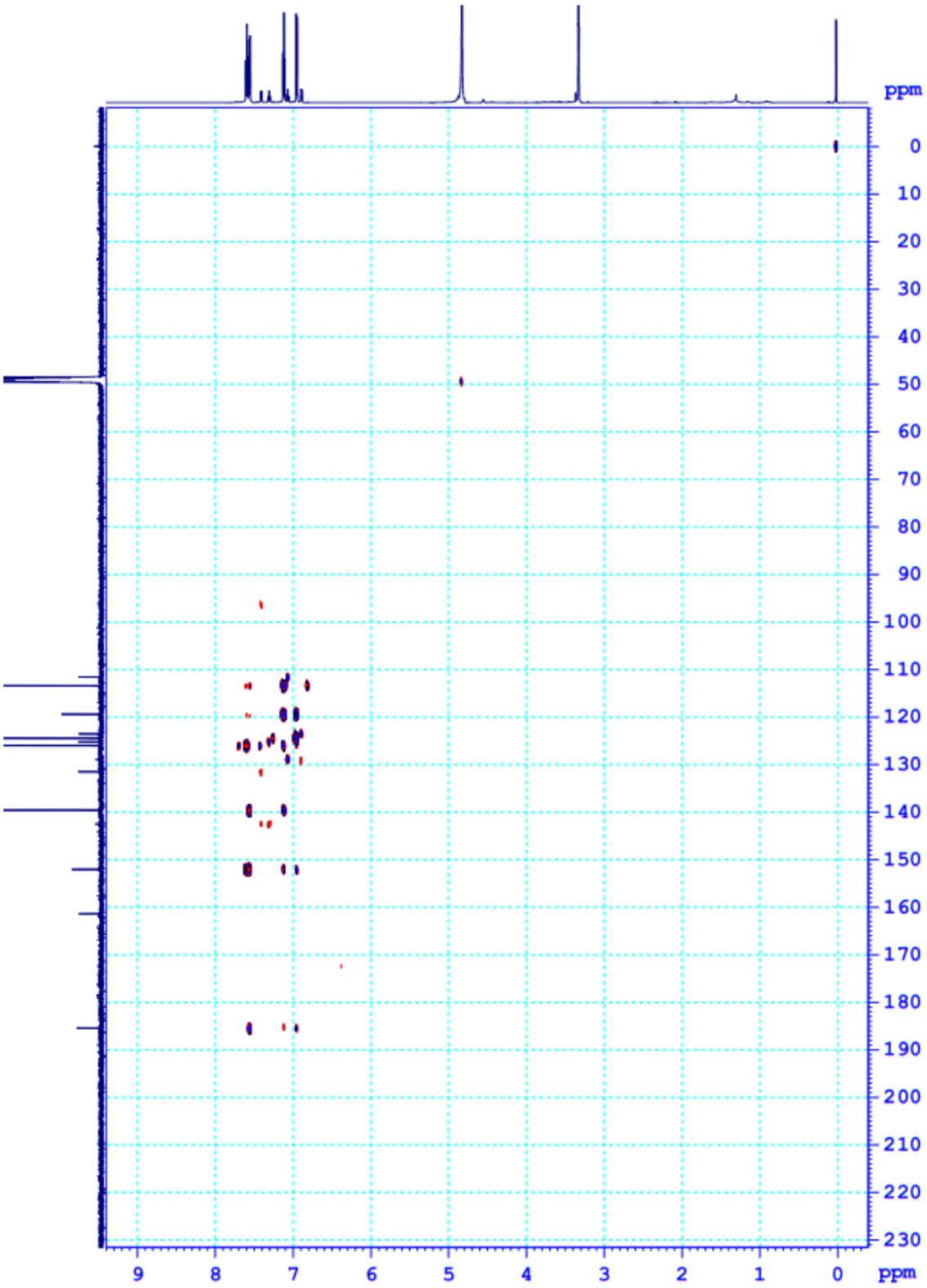


Figure S62: HMBC spectrum of compound **7** (isatin)

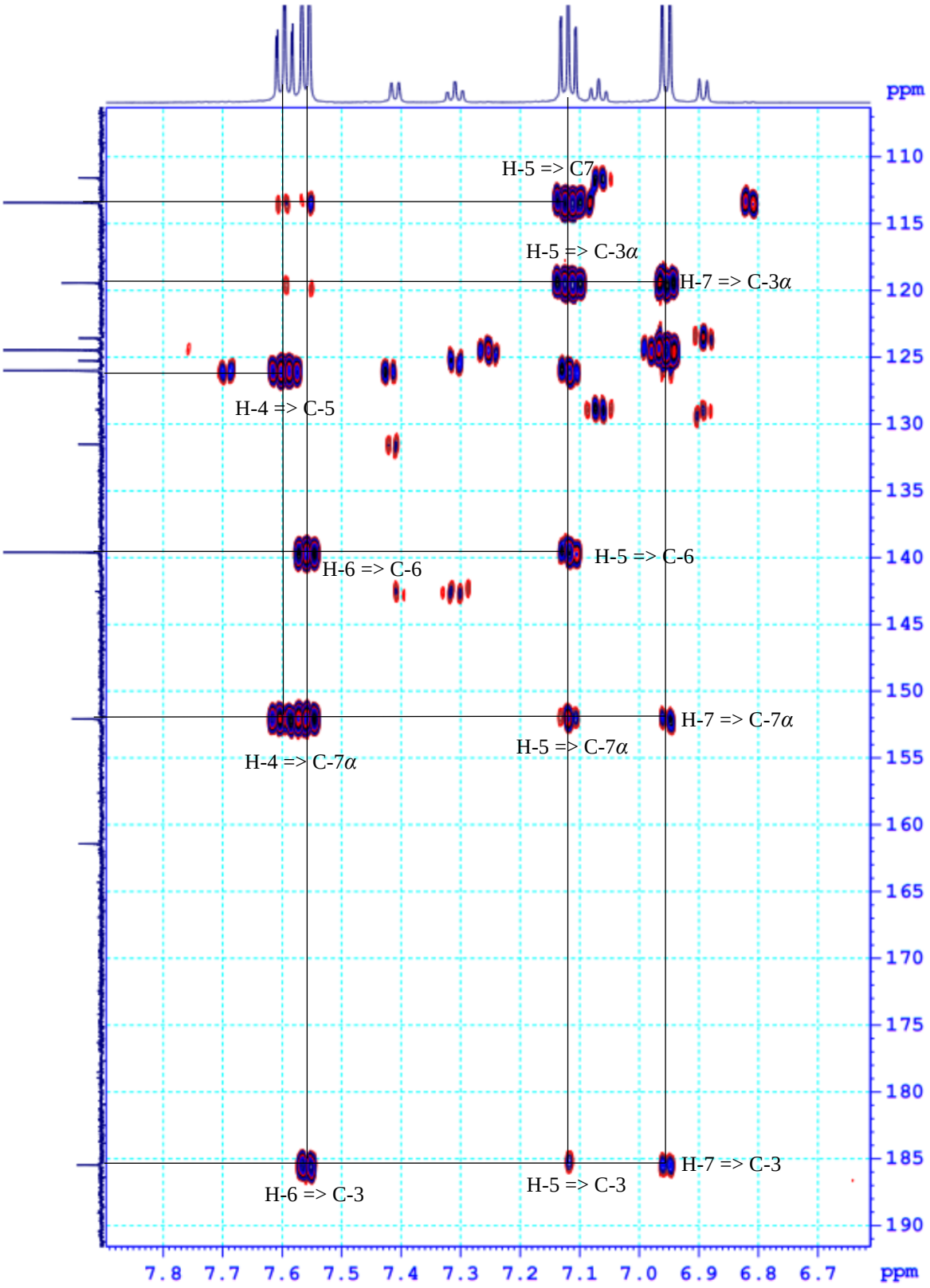


Figure S63: HMBC spectrum of compound **7** (isatin) (from δ_C 110 ppm to δ_C 190 ppm)

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

Position	Compound **8** (MeOD)		3-hydroxy-3-(2-oxopropyl)indolin-2-one ($CDCl_3$) [36]	
	^{13}C-NMR (125 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (100 MHz) δ_C ppm	**^{1}H-NMR** (400 MHz) δ_H ppm
1-NH	-		-	
2	181.1	-	179.8	-
3	74.8	-	76.2	-
3*α*	124.8	-	125.3	7.63 (1H, *d*, 7.8 Hz)
4	123.4	7.02 (1H, *td*, 1.2 Hz, 7.8 Hz)	123.0	7.07 (1H, *t*, 7.4 Hz)
5	130.7	7.25 (1H, *td*, 1.2 Hz, 7.8 Hz)	128.2	7.37 (1H, *d*, 7.6 Hz)
6	111.2	6.89 (1H, *d*, 7.8 Hz)	112.7	6.89 (1H, *d*, 7.6 Hz)
7	143.6	7.33 (1H, *dd*, 0.6 Hz, 7.2 Hz)	137.0	-
7*α*	132.3	-	132.3	-
8	51.1	3.36 (1H, *d*, 16.8 Hz) 3.19 (1H, *d*, 16.8 Hz)	49.5	3.20 (1H, *d*, 17.2 Hz) 2.98 (1H, *d*, 17.2 Hz)
9	207.4	-	207.4	-
10	30.7	2.09 (3H, *s*)	31.6	2.22 (3H, *s*)

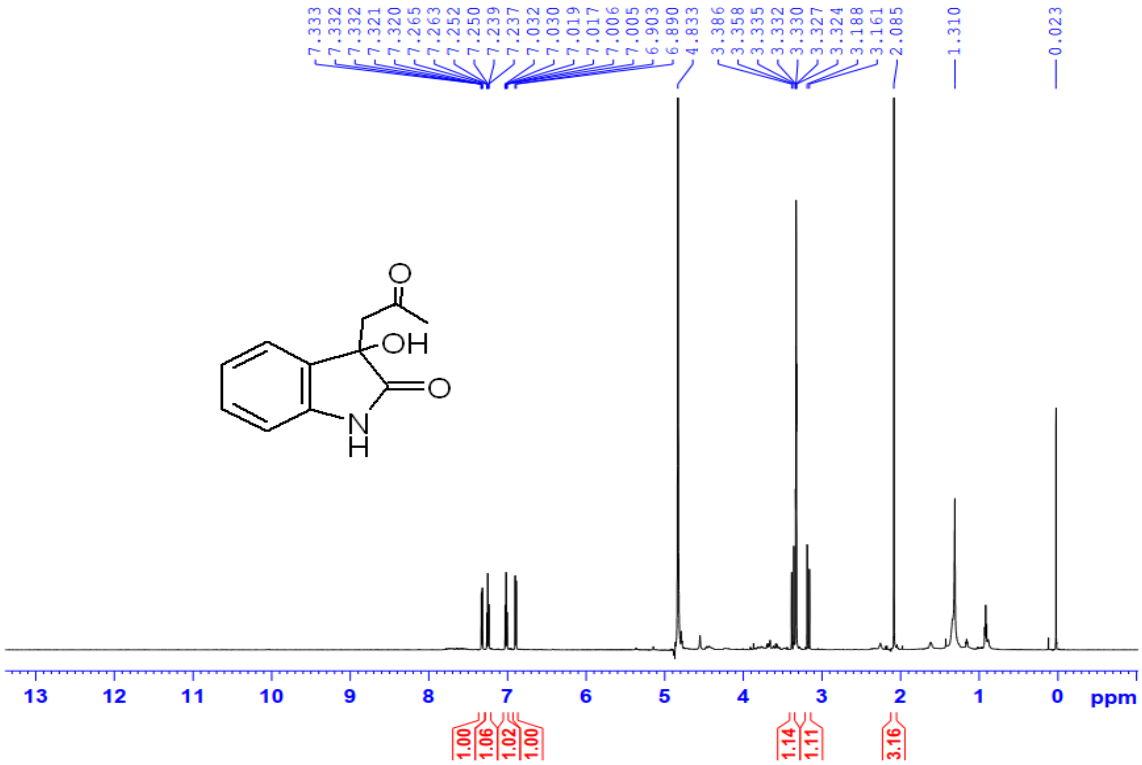


Figure S64: [1]H-NMR (600 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one).

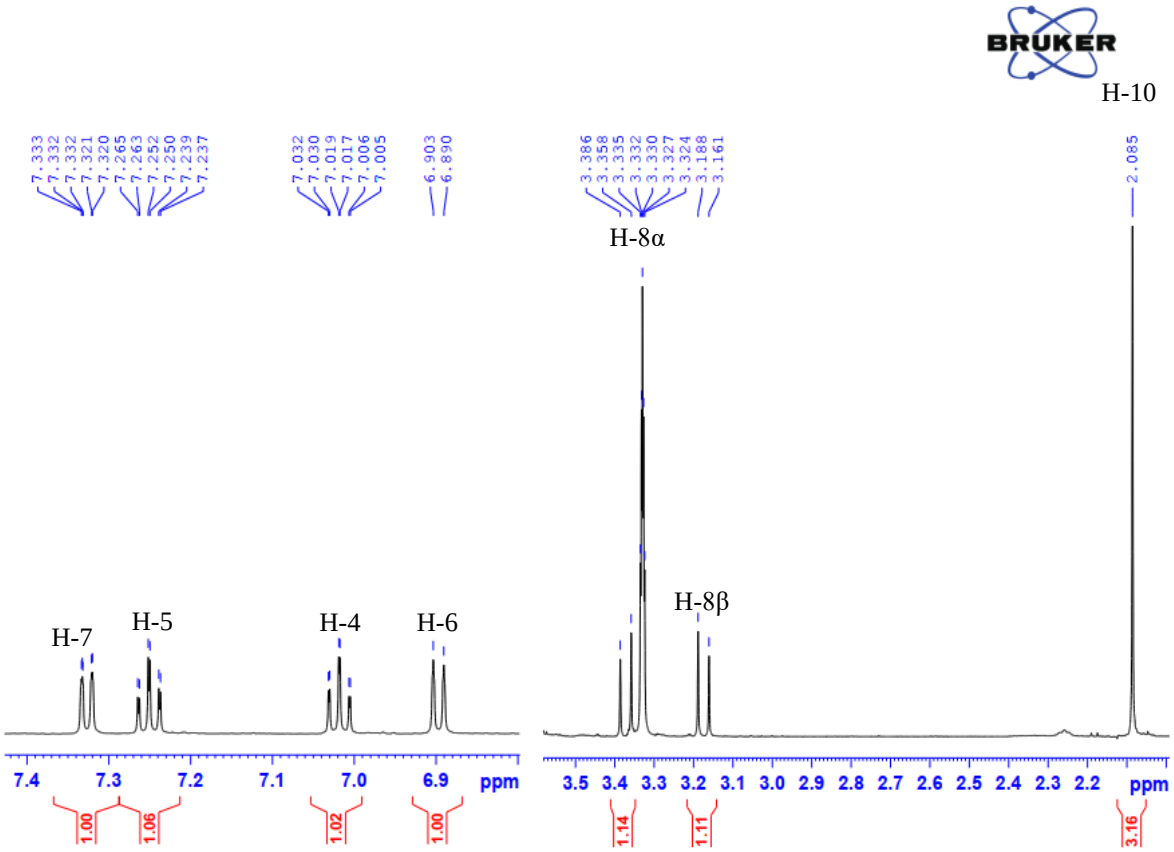


Figure S65: [1]H-NMR (600 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from δ_H 2.0 ppm to δ_H 7.4 ppm)

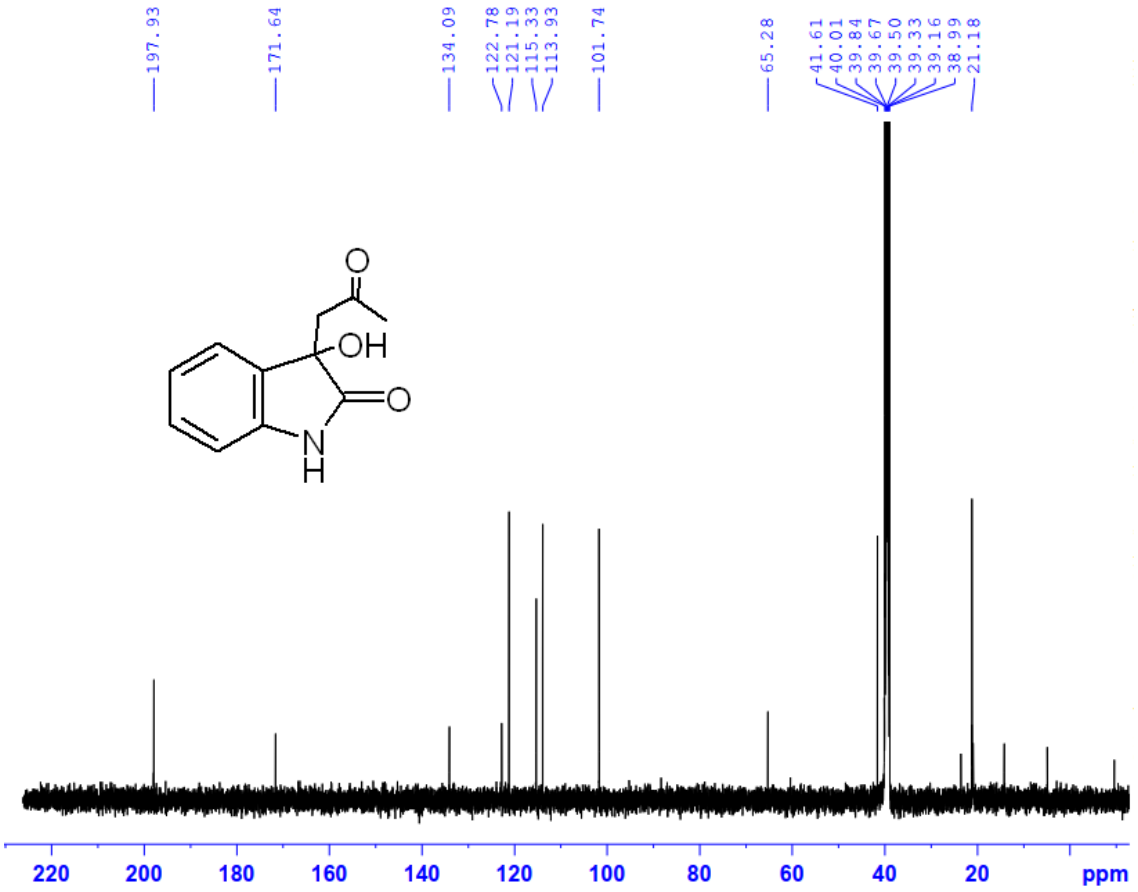


Figure S66: ^{13}C-NMR (150 MHz, MeOD) spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)

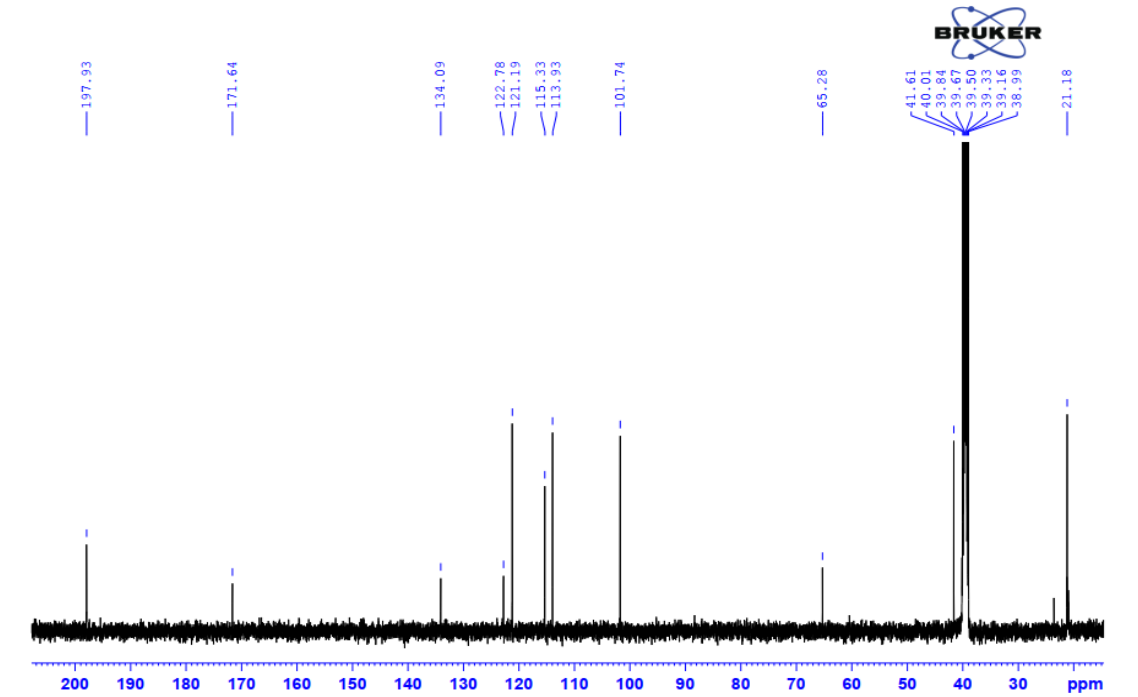


Figure S67: ^{13}C-NMR spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from δ_C 20 ppm to δ_C 200 ppm)

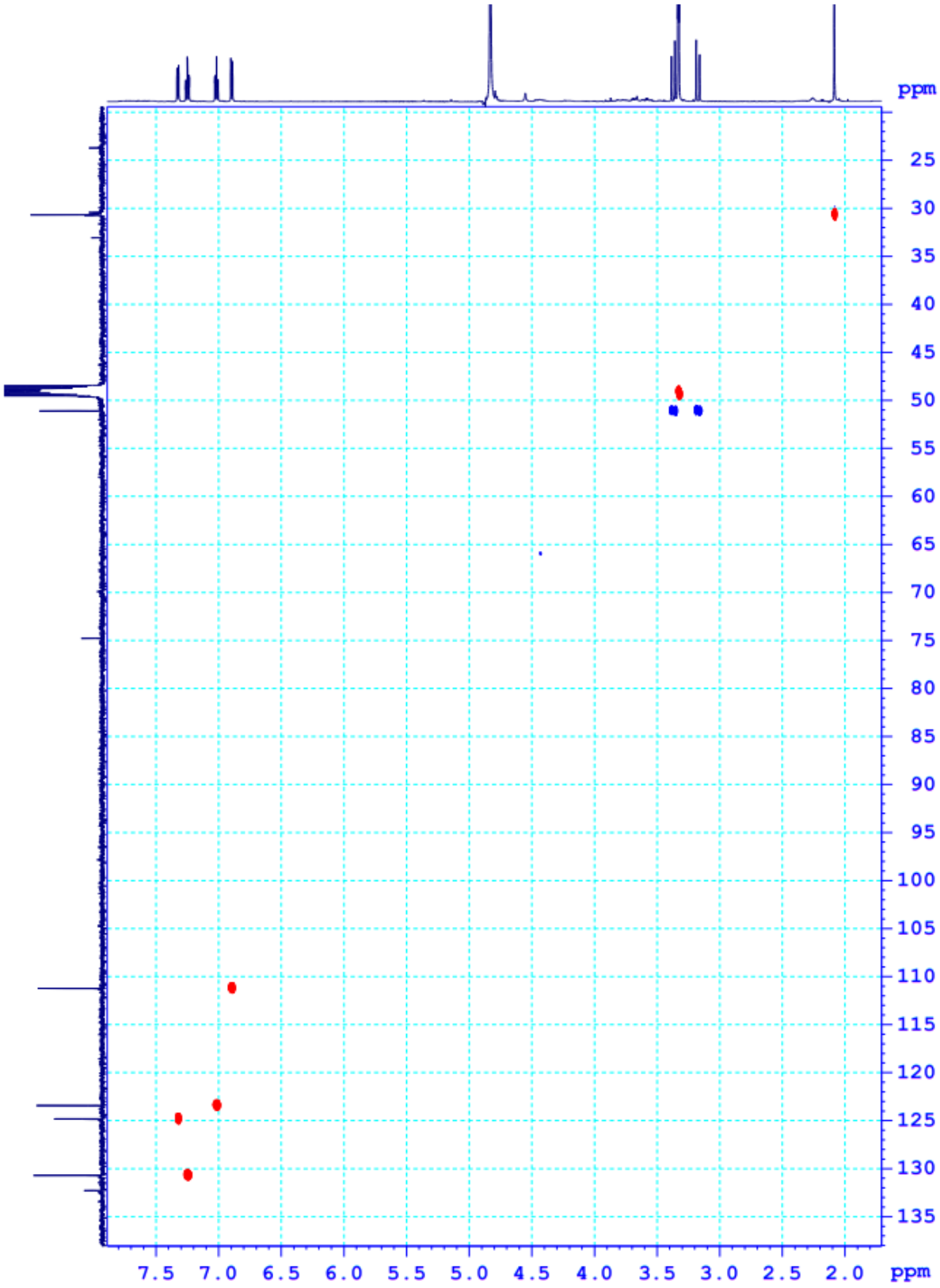


Figure S68: HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)

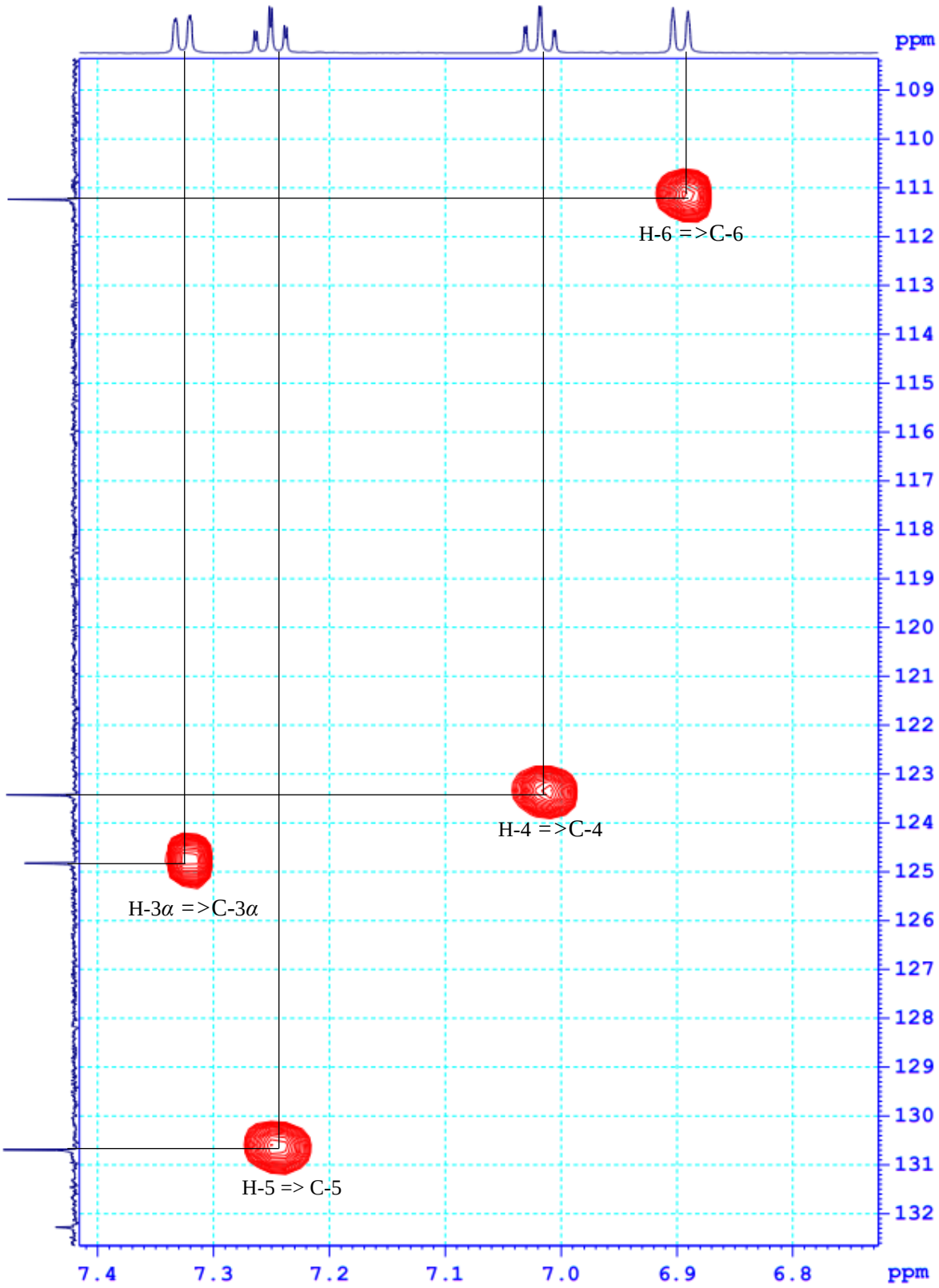


Figure S69: HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) (from δ_C109 ppm to δ_C 132 ppm)

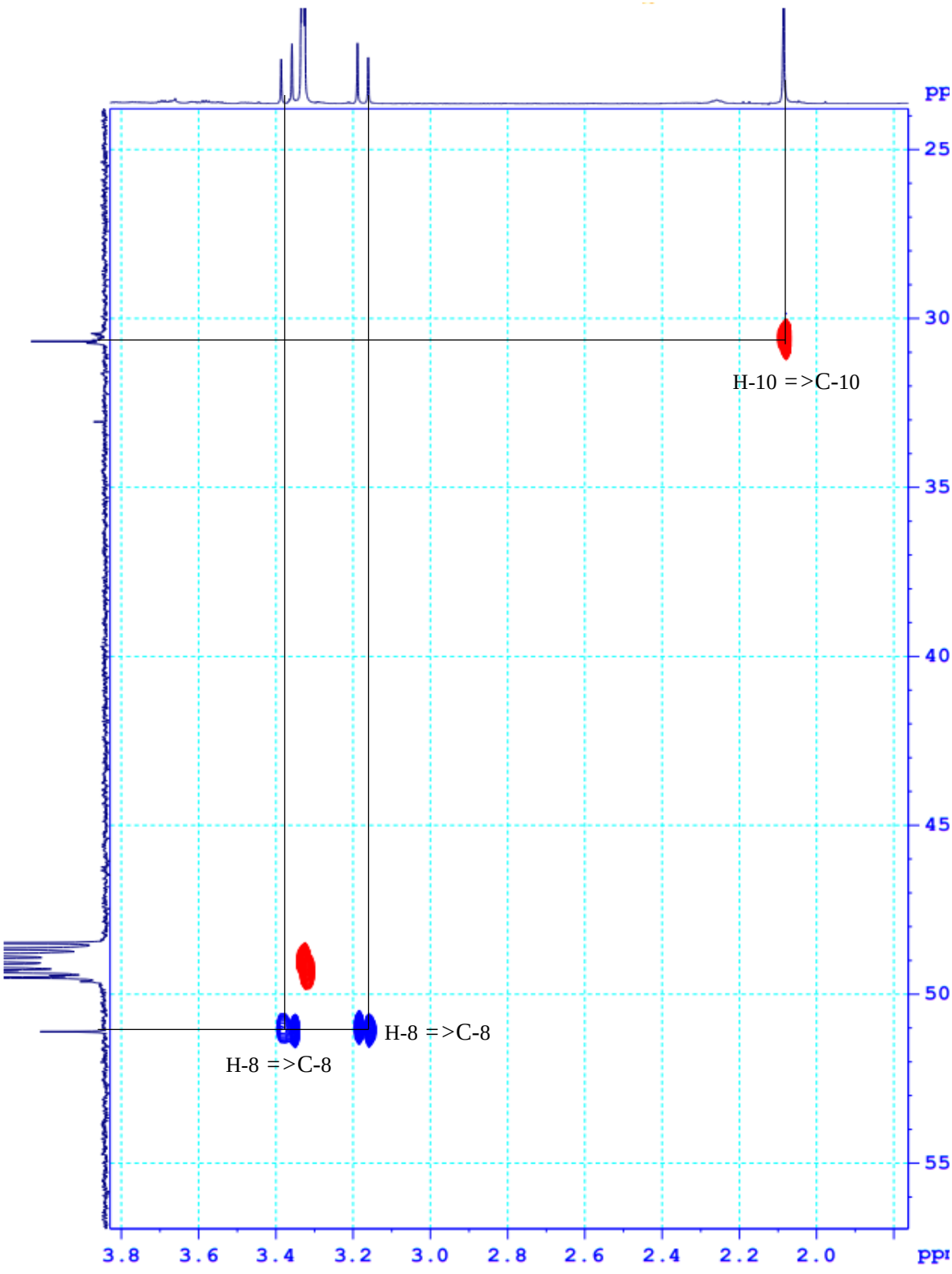


Figure S70: HSQC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) **(**from δ_C 25 ppm to δ_C 55 ppm)

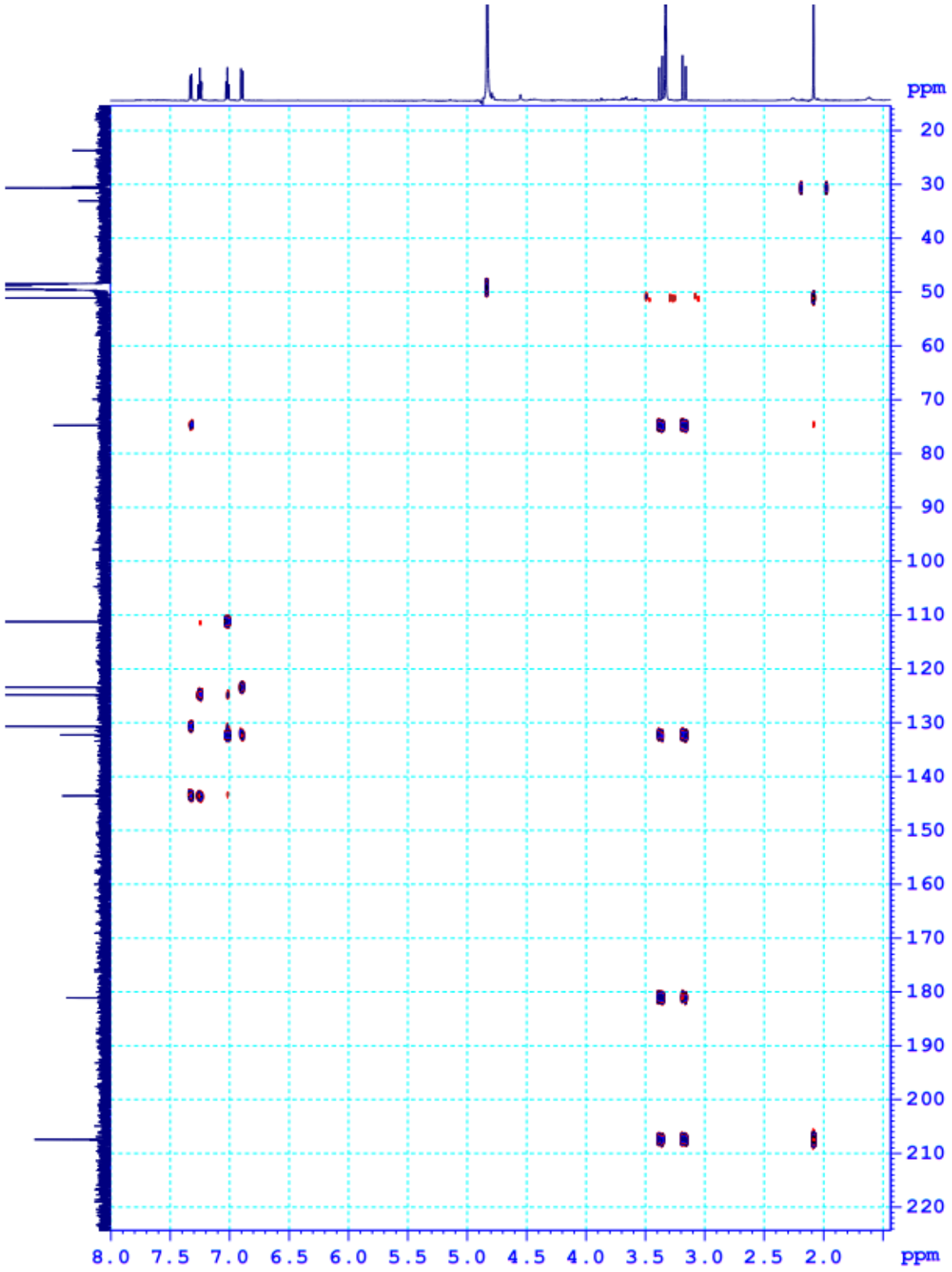


Figure S71: HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one)

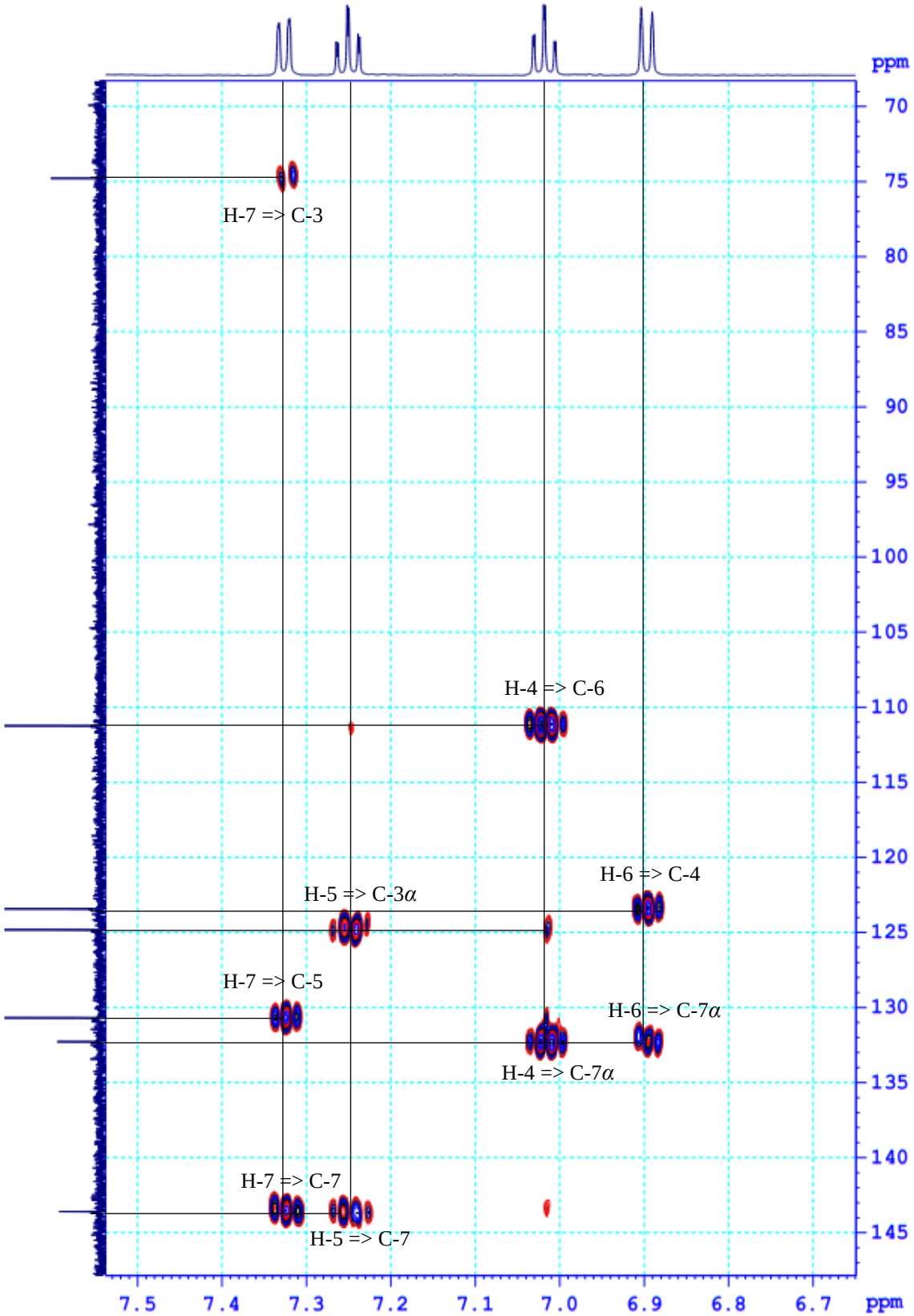


Figure S72: HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) **(**from δ_C 70 ppm to δ_C 145 ppm)

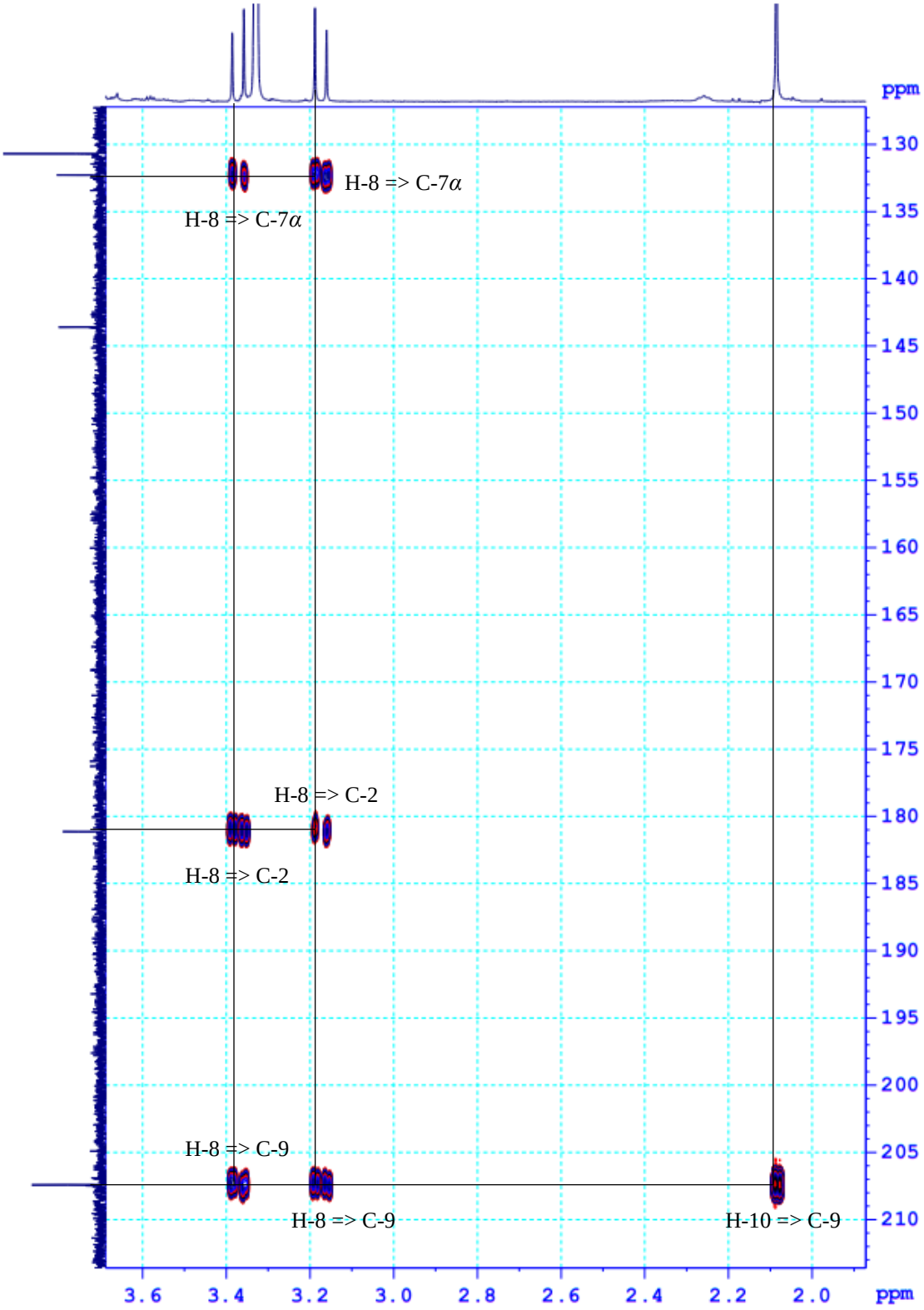


Figure S73: HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) **(**from δ_C 130 ppm to δ_C 210 ppm)

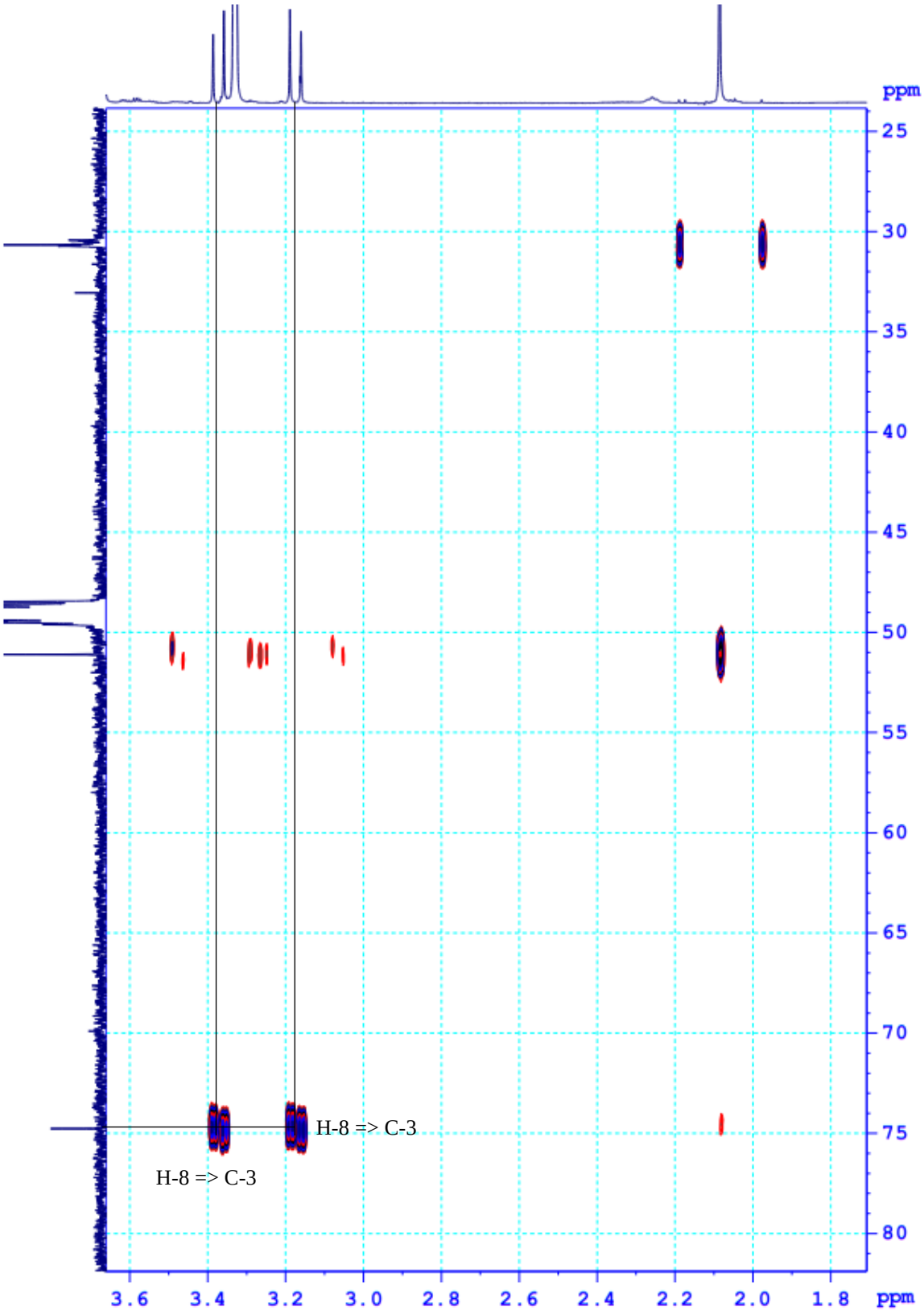


Figure S74: HMBC spectrum of compound **8** (3-hydroxy-3-(2-oxopropyl)indolin-2-one) **(**from δ_C 25 ppm to δ_C 80 ppm)

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

Position	Compound **9** (MeOD)		benzoic acid ($CDCl_3$) [37]	
	^{13}C-NMR (125 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (100 MHz) δ_C ppm	**^{1}H-NMR** (400 MHz) δ_H ppm
1	131.9	-	129.3	-
2 & 6	130.7	8.02 (2H, *dd*)	130.2	8.13 (2H, *d*, 7.4 Hz)
3 & 5	129.4	7.46 (2H, *m*)	128.5	7.47 (2H, *t*, 7.4 Hz)
4	134.0	7.58 (1H, *m*)	133.8	7.61 (1H, *t*, 7.4 Hz)
1'	169.9	-	172.4	-

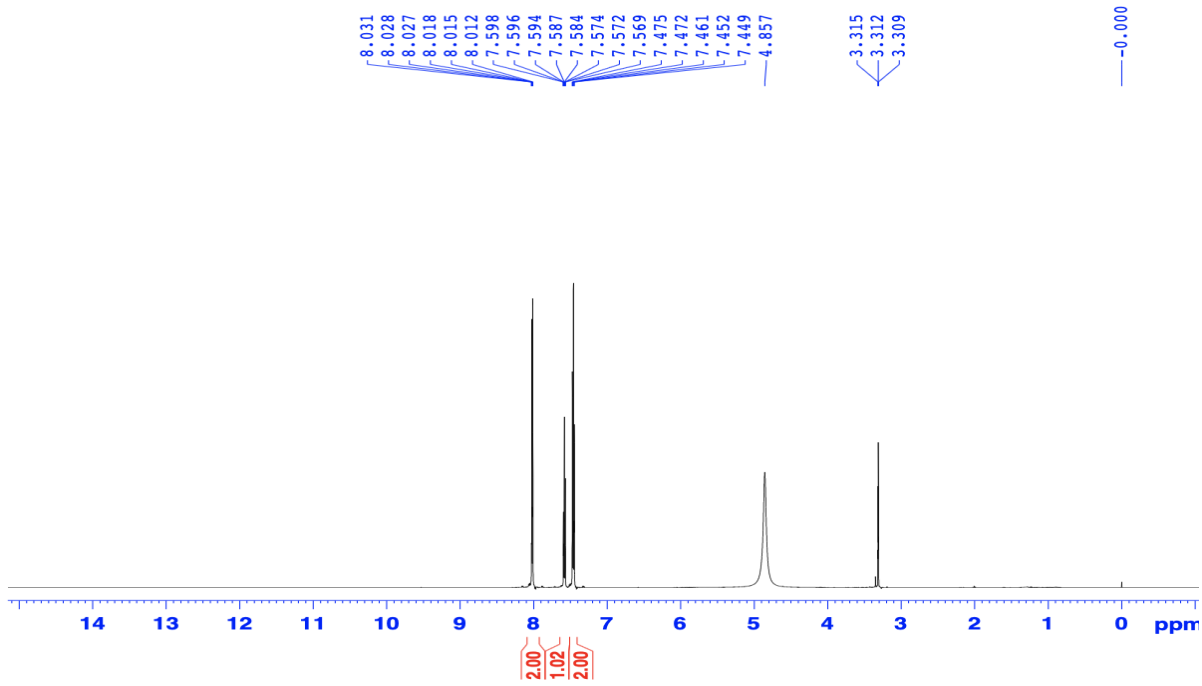


Figure S75: ^{1}H-NMR (600 MHz, MeOD) spectrum of compound **9** (benzoic acid)

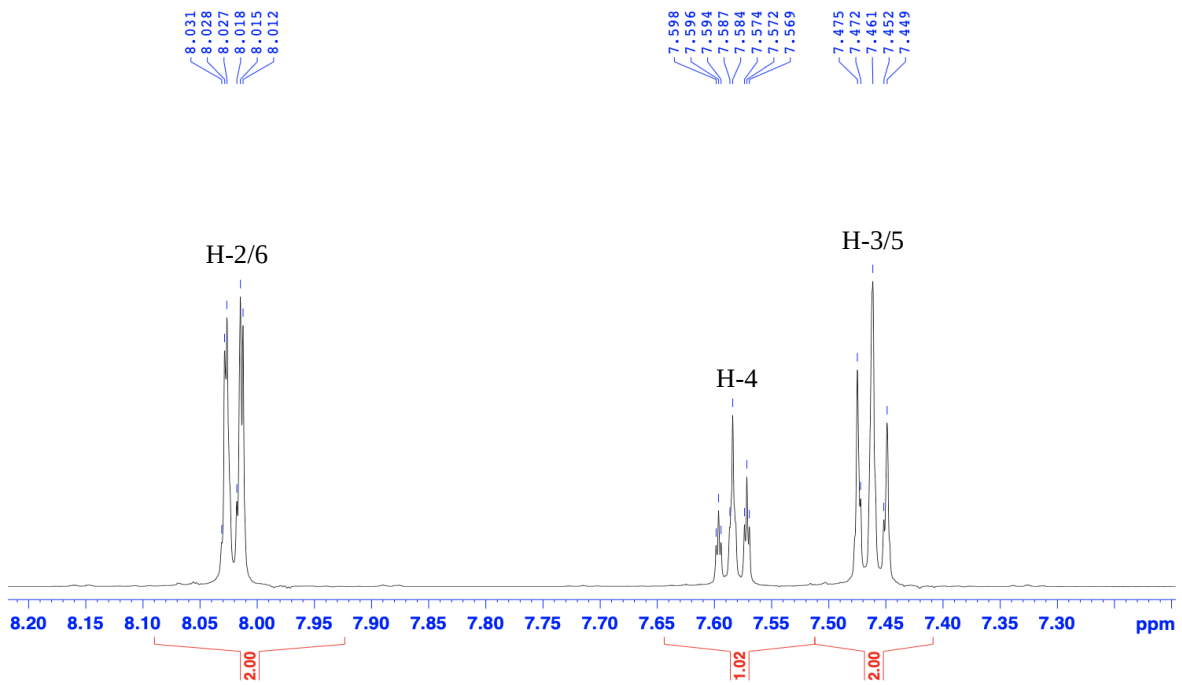


Figure S76: [1]H-NMR spectrum of compound **9** (benzoic acid) (from δ_H 7.3 ppm to δ_H 8.2 ppm)

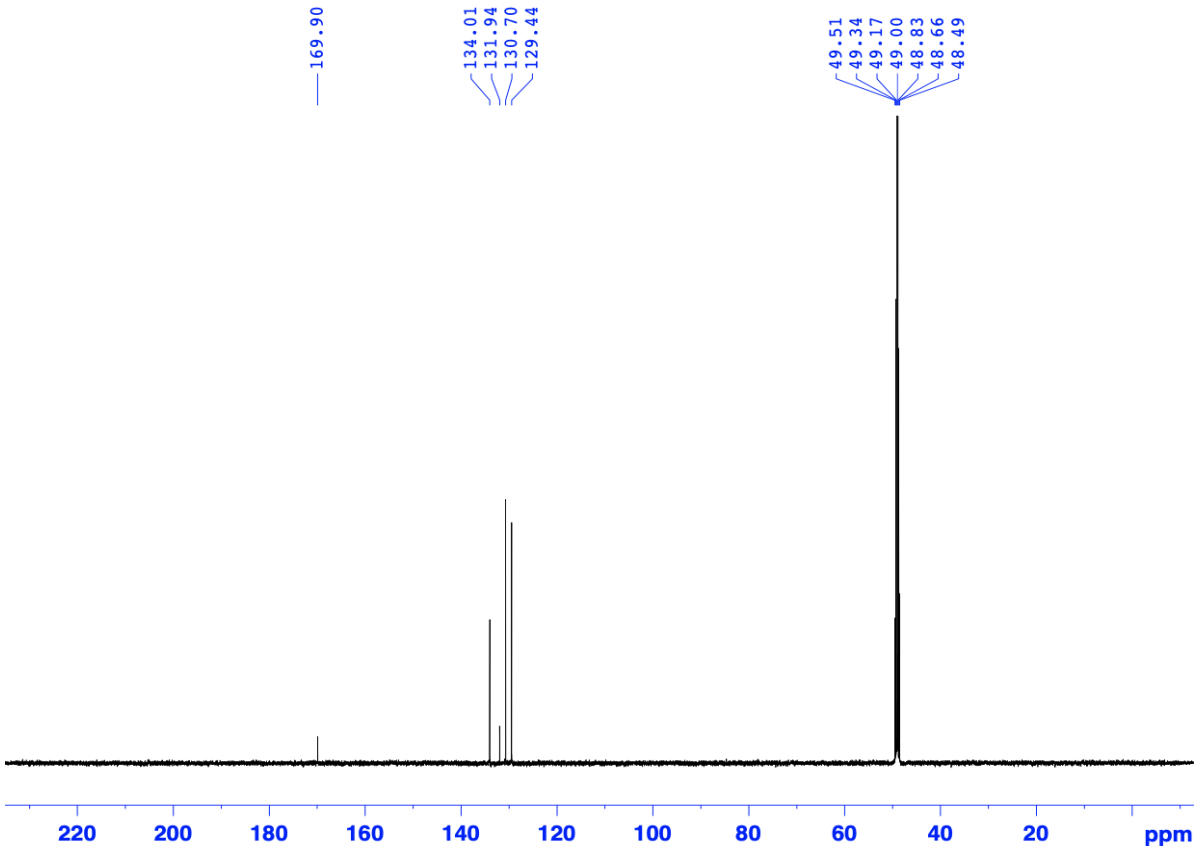


Figure S77: [13]C-NMR (150 MHz, MeOD) spectrum of compound **9** (benzoic acid)

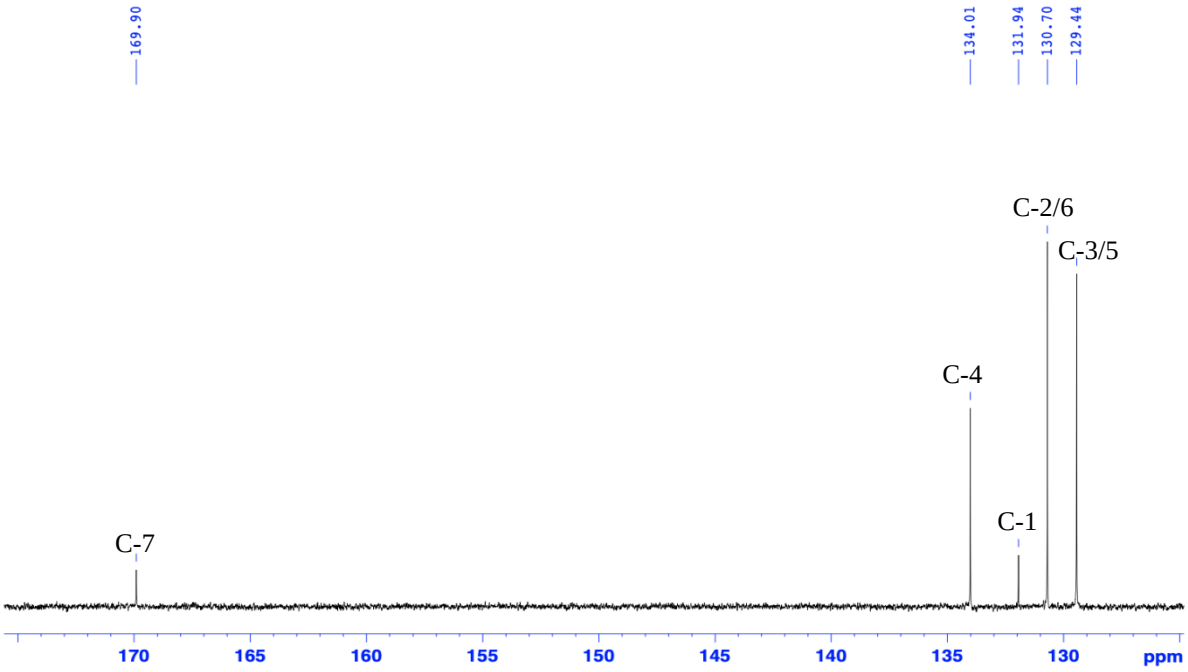


Figure S78: ^{13}C-NMR spectrum of compound **9** (benzoic acid) **(**from δ_C 130 ppm to δ_C 170 ppm)

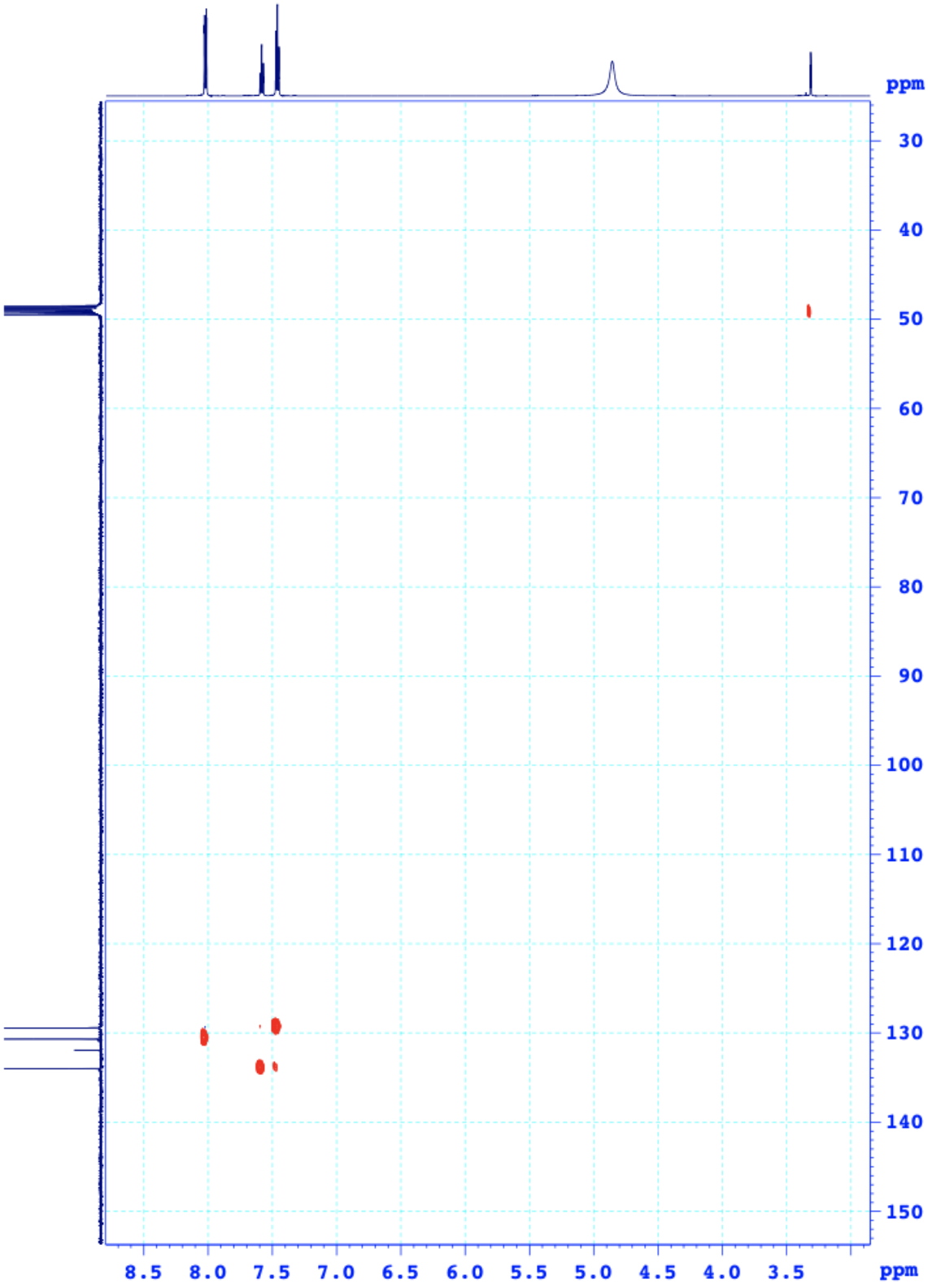


Figure S79: HSQC spectrum of compound 9 (benzoic acid)

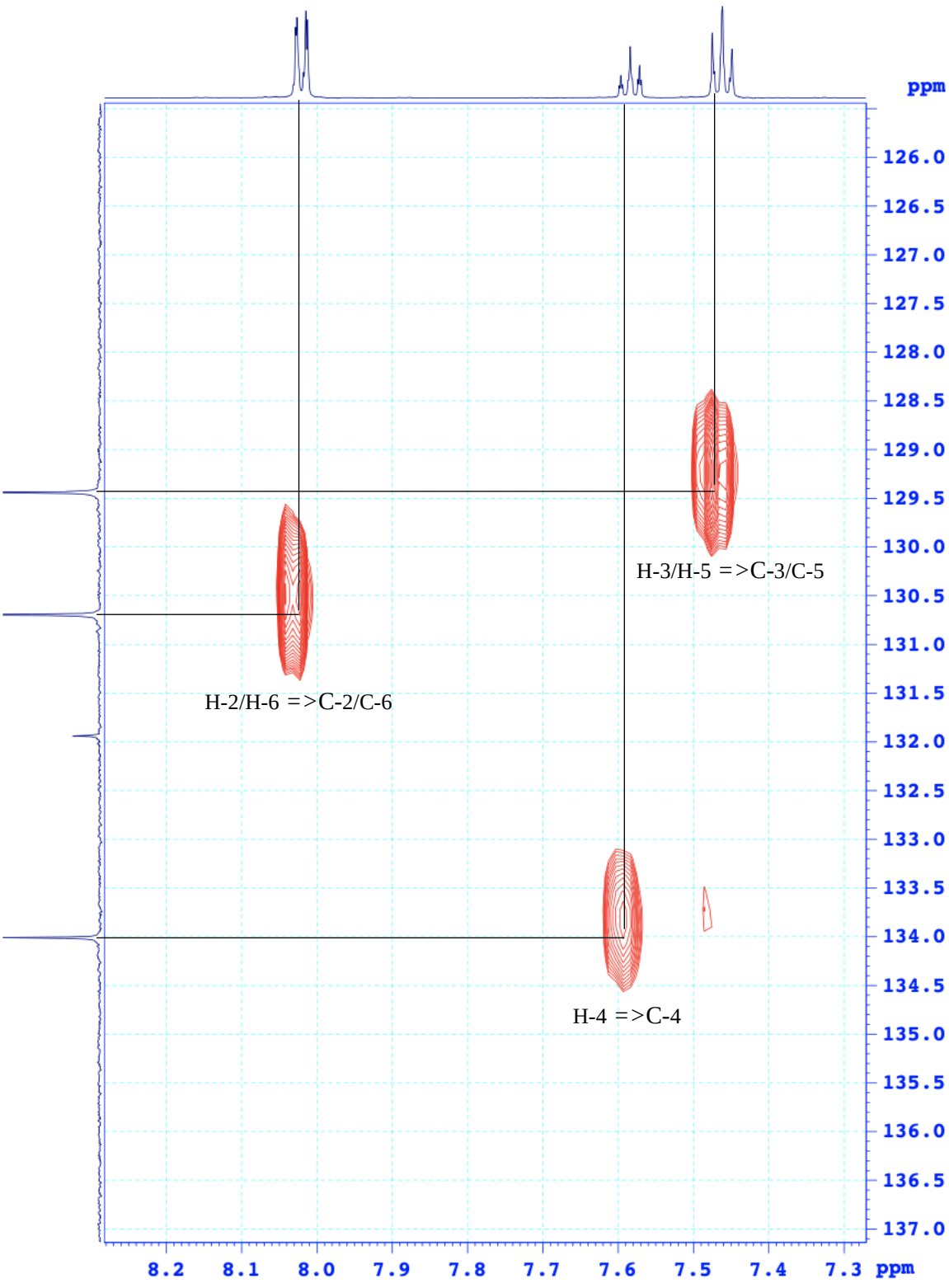


Figure S80: HSQC spectrum of compound **9** (benzoic acid) **(**from δ_C 126 ppm to δ_C 137 ppm)

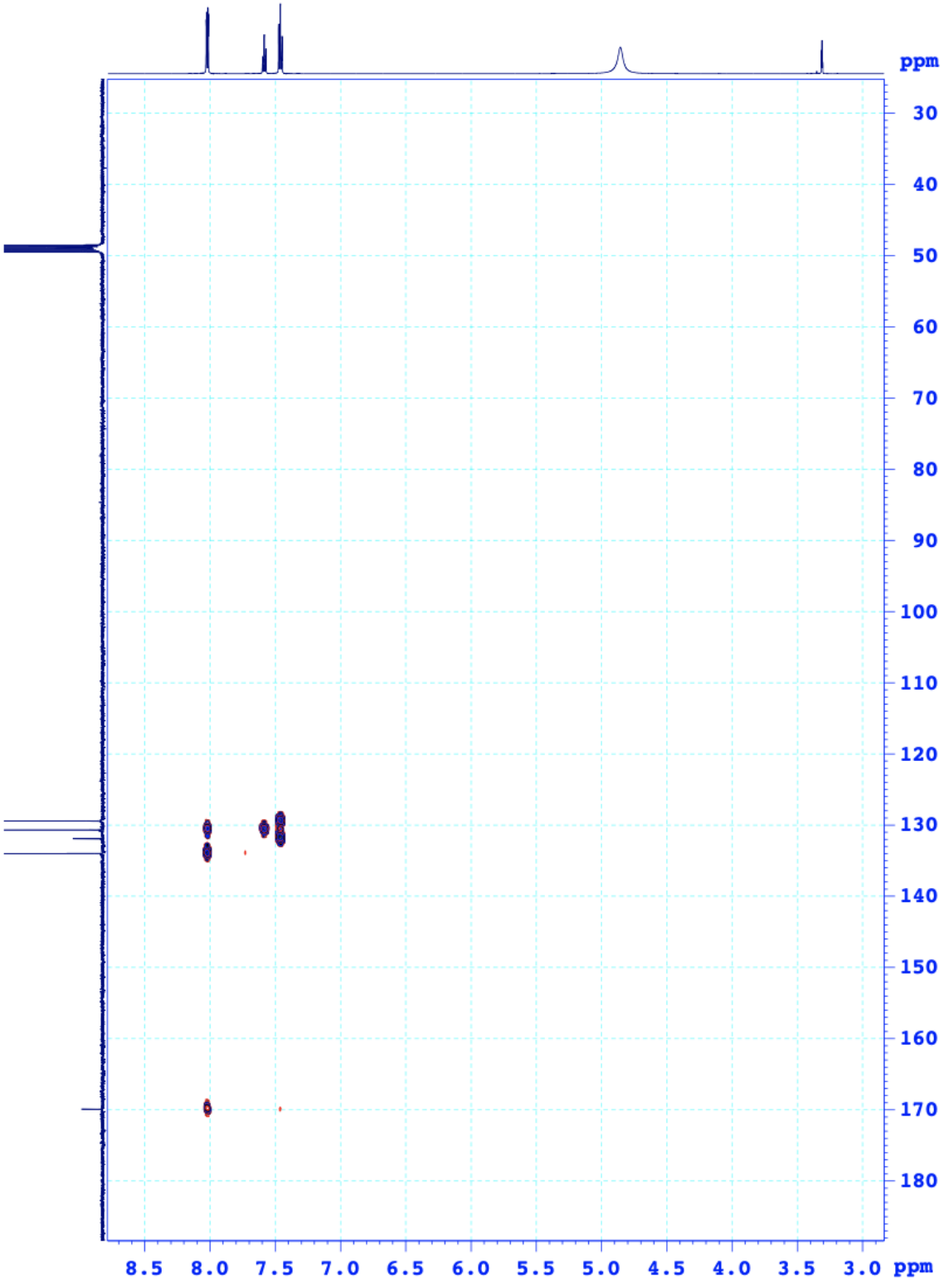


Figure S81: HMBC spectrum of compound 9 (benzoic acid)

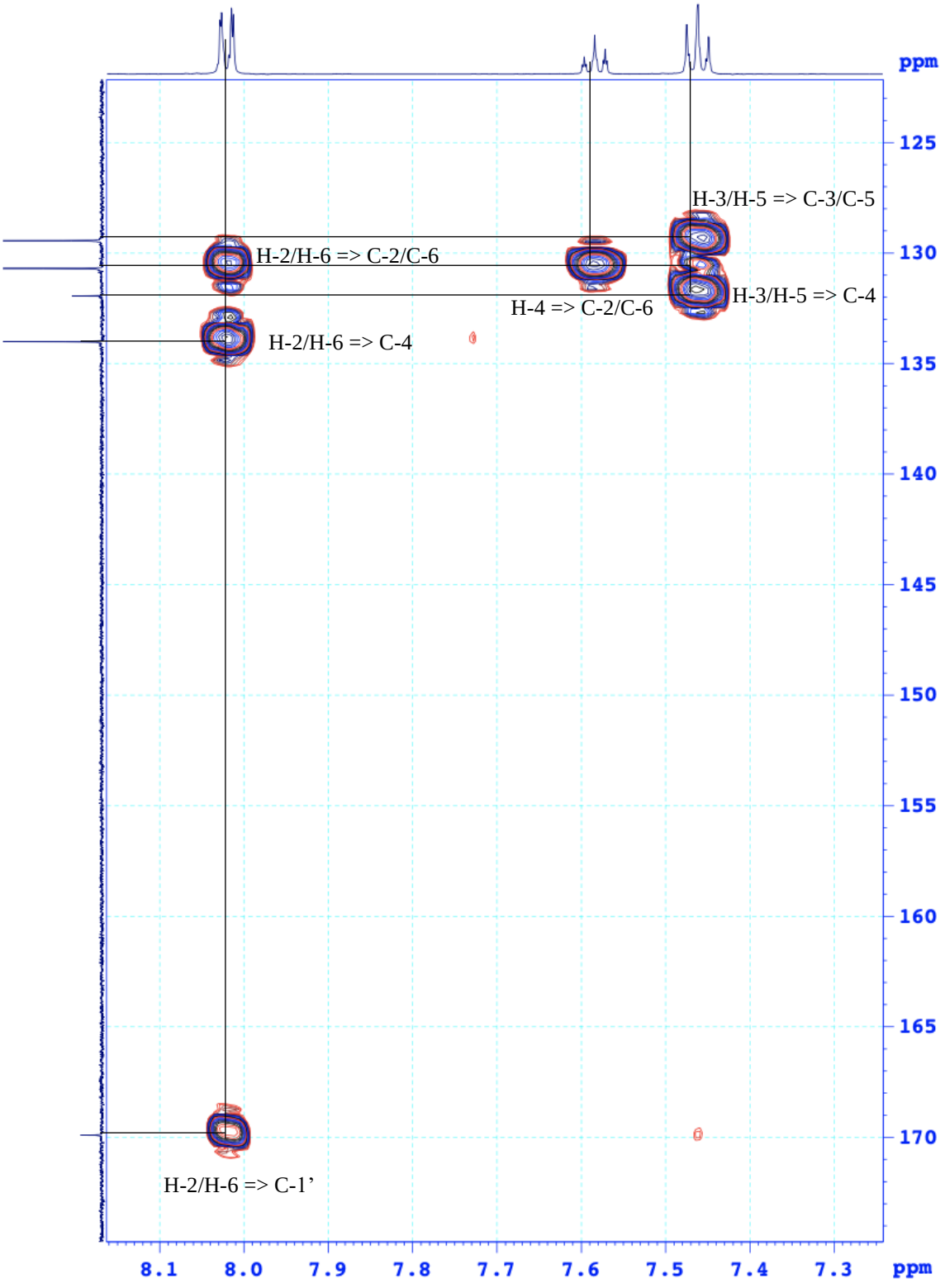


Figure S82: HMBC spectrum of compound **9** (benzoic acid) **(**from δ_C 125 ppm to δ_C 170 ppm)

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

Position	Compound **10** (DMSO-d_6)		Ethylene glycol dibenzoate ($CDCl_3$) [38]	
	^{13}C-NMR (150 MHz) δ_C ppm	^{1}H-NMR (600 MHz) δ_H ppm	^{13}C-NMR (125 MHz) δ_C ppm	^{1}H-NMR (500 MHz) δ_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, *d*, 2.0 Hz)	99.9	6.20 (1H, *d*, 1.8 Hz)
7	164.6	-	165.9	-
8	93.6	6.36 (1H, *d*, 2.0 Hz)	94.8	6.39 (1H, *d*, 2.2 Hz)
9	156.5	-	159.3	-
10	103.7	-	105.6	-
1'	121.1	-	123.1	-
2'	115.2	7.55 (1H, *d*, 1.8 Hz)	117.6	7.66 (1H, *d*, 1.8 Hz)
3'	144.8	-	145.8	-
4'	148.5	-	149.7	-
5'	116.2	6.84 (1H, *d*, 8.4 Hz)	116.1	6.86 (1H, *d*, 8.0 Hz)
6'	121.6	7.53 (1H, *dd*, 8.4, 2.4 Hz)	123.5	7.60 (1H, *dd*, 8.0, 1.8 Hz)
1"	101.2	5.33 (1H, *d*, 7.2 Hz)	104.7	5.09 (1H, *d*, 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, *s*)	102.4	4.51 (1H, *d*, 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, *d*, 6.0 Hz)	17.9	1.11 (3H, *d*, 6.0 Hz)

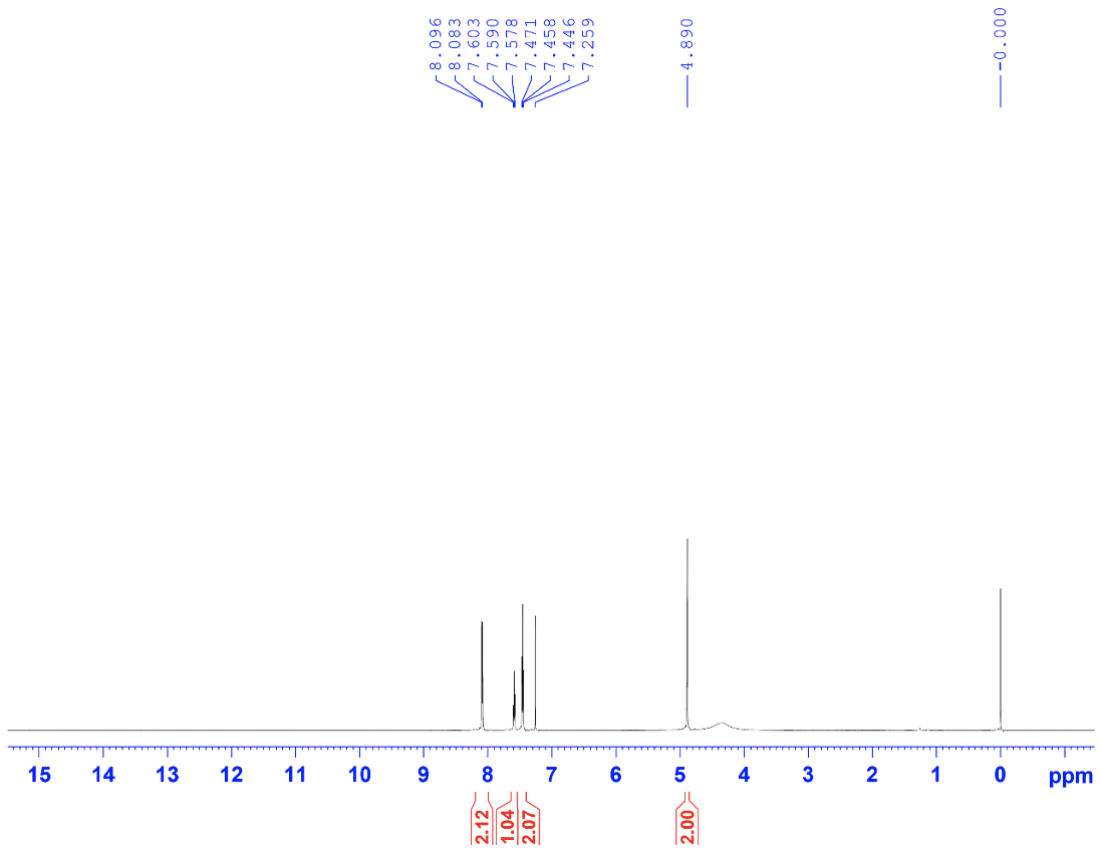


Figure S83: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of compound **10** (ethylene glycol dibenzoate)

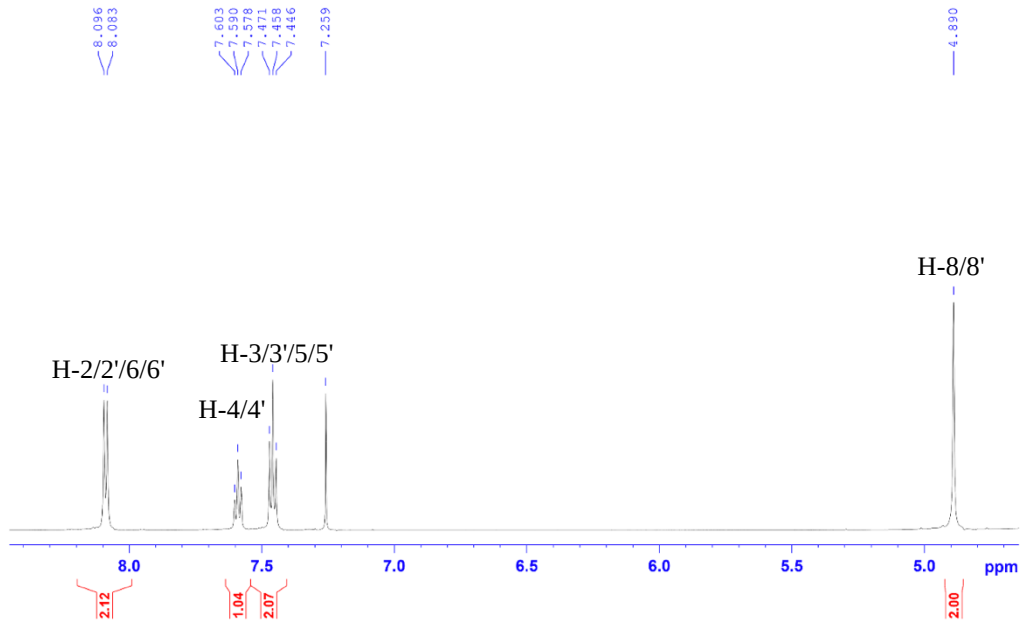


Figure S84: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of compound **10** (ethylene glycol dibenzoate) (from δ_H 4.7 ppm to δ_H 8.5 ppm)

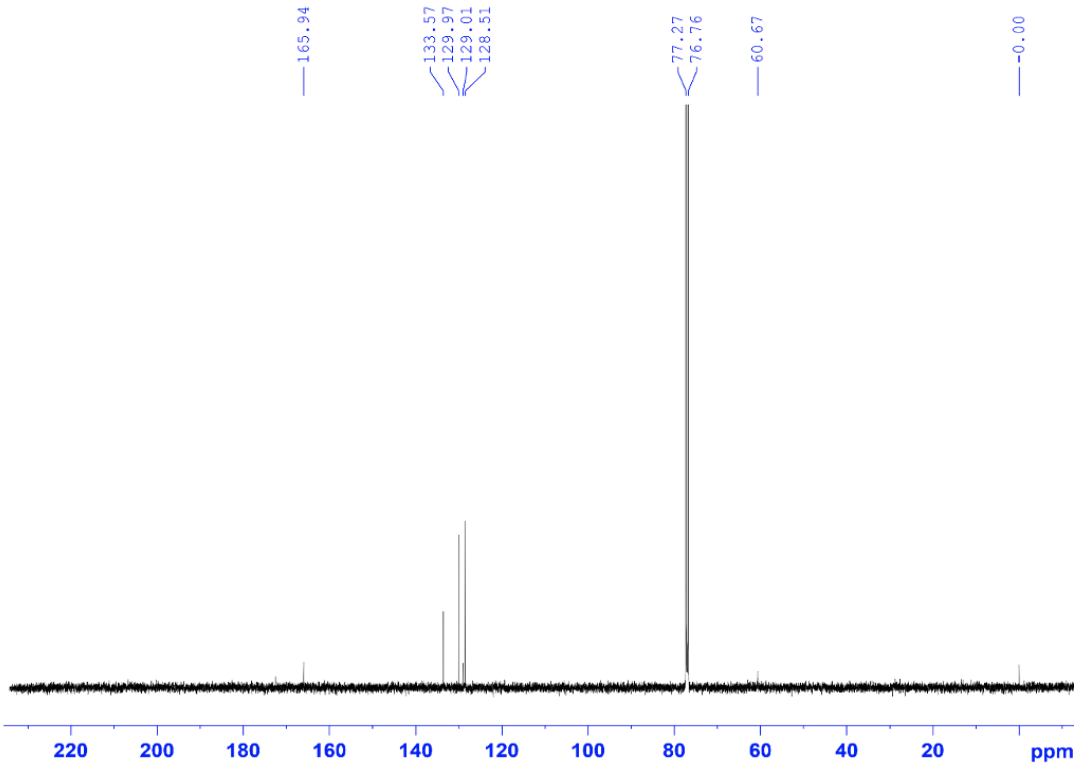


Figure S85: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of compound **10** (ethylene glycol dibenzoate)

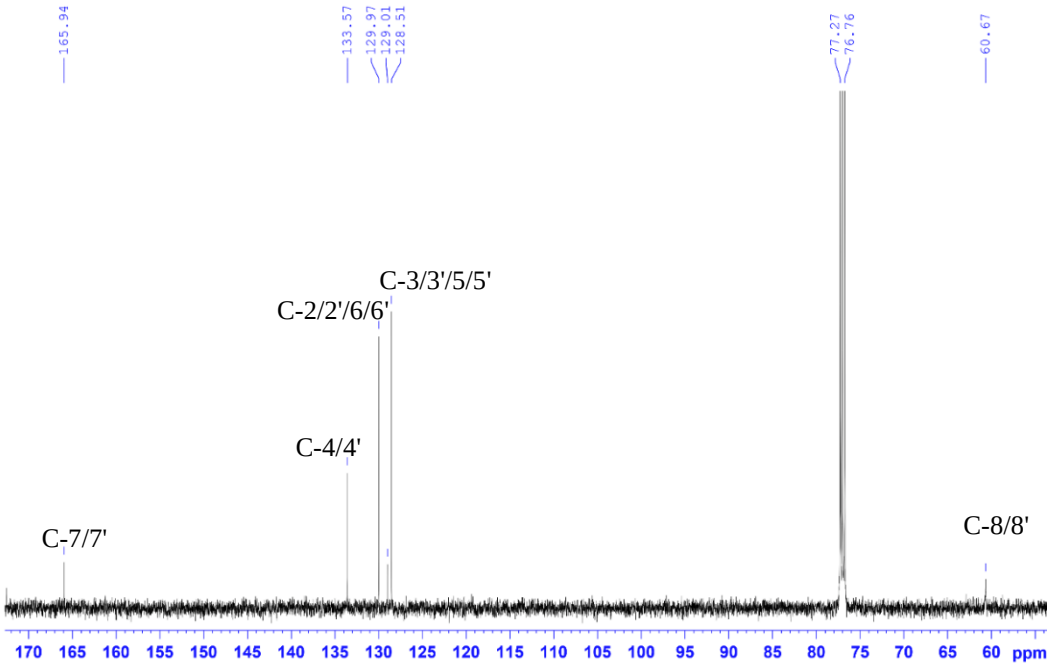


Figure S86: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of compound **10** (ethylene glycol dibenzoate) **(**from δ_C 60 ppm to δ_C 170 ppm)

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

Position	Compound **11** (MeOD)		Nicotiflorin (MeOD) [39]	
	^{13}C-NMR (150 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_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, *d*, 1.8 Hz)	100.1	6.23 (1H, *d*, 2.1 Hz)
7	166.2	-	166.4	-
8	95.0	6.42 (1H, *d*, 1.8 Hz)	95.0	6.43 (1H, *d*, 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, *d*, 9.0 Hz)	132.4	8.10 (2H, *d*, 8.9 Hz)
3' & 5'	116.1	6.92 (2H, *d*, 9.0 Hz)	116.1	6.93 (2H, *d*, 8.9 Hz)
4'	161.5	-	161.5	-
1"	104.6	5.15 (1H, *d*, 7.2 Hz)	104.6	5.00 (1H, *d*, 7.4 Hz)
2"	75.8	3.47 (3H, *m*)	75.8	3.41-3.49 (*m*)
3"	78.2	3.47 (3H, *m*)	78.1	3.41-3.49 (*m*)
4"	72.1	3.65 (1H, *brs*)	72.1	3.28-3.33 (*m*)
5"	77.2	3.36 (1H, *ddd*, 1.2 Hz, 6.6 Hz, 10.8 Hz)	77.2	3.41-3.49 (*m*)
6"	68.6	3.84 (1H, *dd*, 1.2 Hz, 10.8 Hz) 3.40 (1H, *dd*, 6.0 Hz, 10.8 Hz)	68.6	3.83 (1H, *d*, 9.6 Hz) 3.41-3.49 (*m*)
1'"	102.4	4.54 (1H, *d*, 1.2 Hz)	102.4	4.53 (1H, *d*, 1.3 Hz)
2'"	71.5	3.29 (2H, *m*)	71.4	3.67 (1H, *dd*, 1.6 Hz, 3.4 Hz)
3'"	72.3	3.54 (1H, *dd*, 3.6 Hz, 9.6 Hz)	72.3	3.56 (1H, *dd*, 3.5 Hz, 9.5 Hz)
4'"	73.9	3.29 (2H, *m*)	73.9	3.29-3.36 (*m*)
5'"	69.7	3.47 (3H, *m*)	69.7	3.46-3.50 (*m*)
6'"	17.9	1.14 (3H, *d*, 6.0 Hz)	17.9	1.16 (3H, *d*, 6.2 Hz)

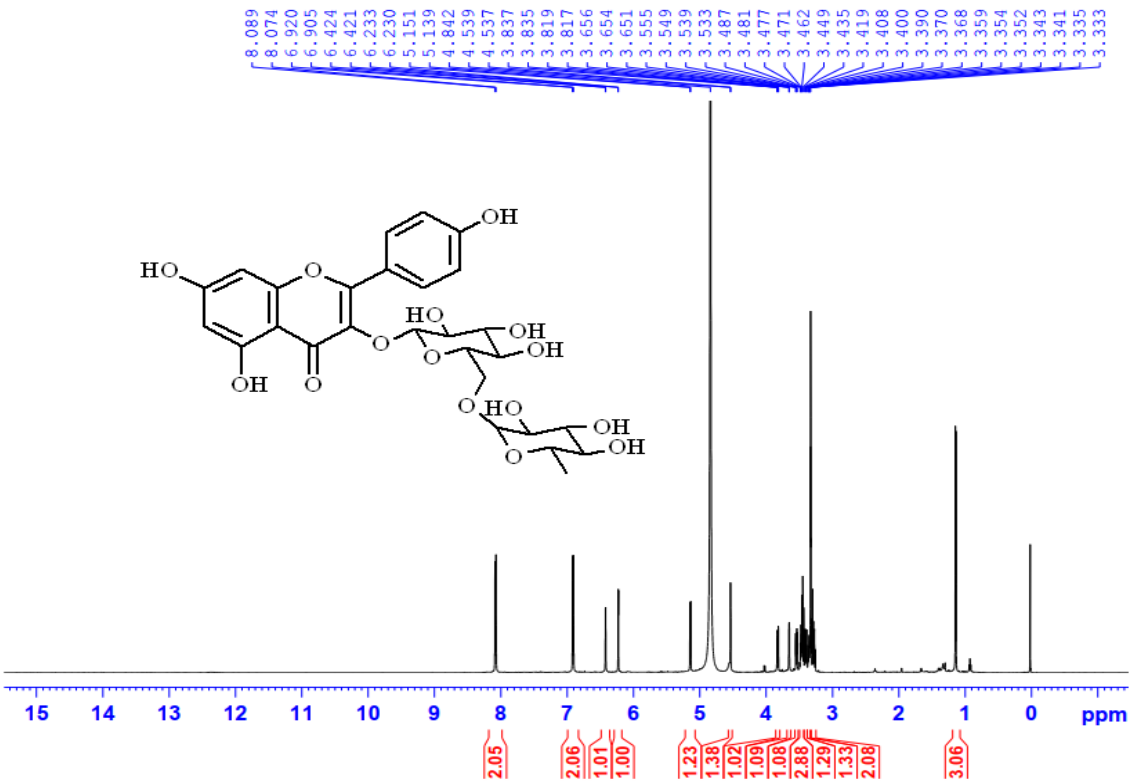


Figure S87: ^{1}H-NMR (600 MHz, MeOD**)** spectrum of compound **11** (nicotiflorin)

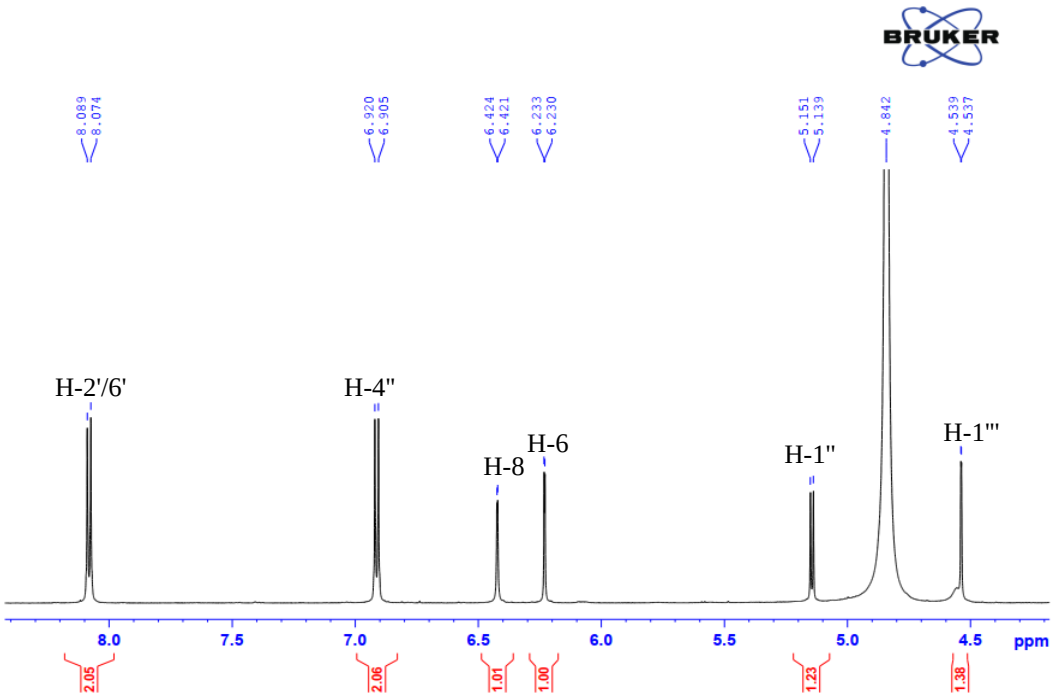


Figure S88: ^{1}H-NMR (600 MHz, MeOD**)** spectrum of compound **11** (nicotiflorin) (from δ_H 4.5 ppm to δ_H 8.0 ppm)

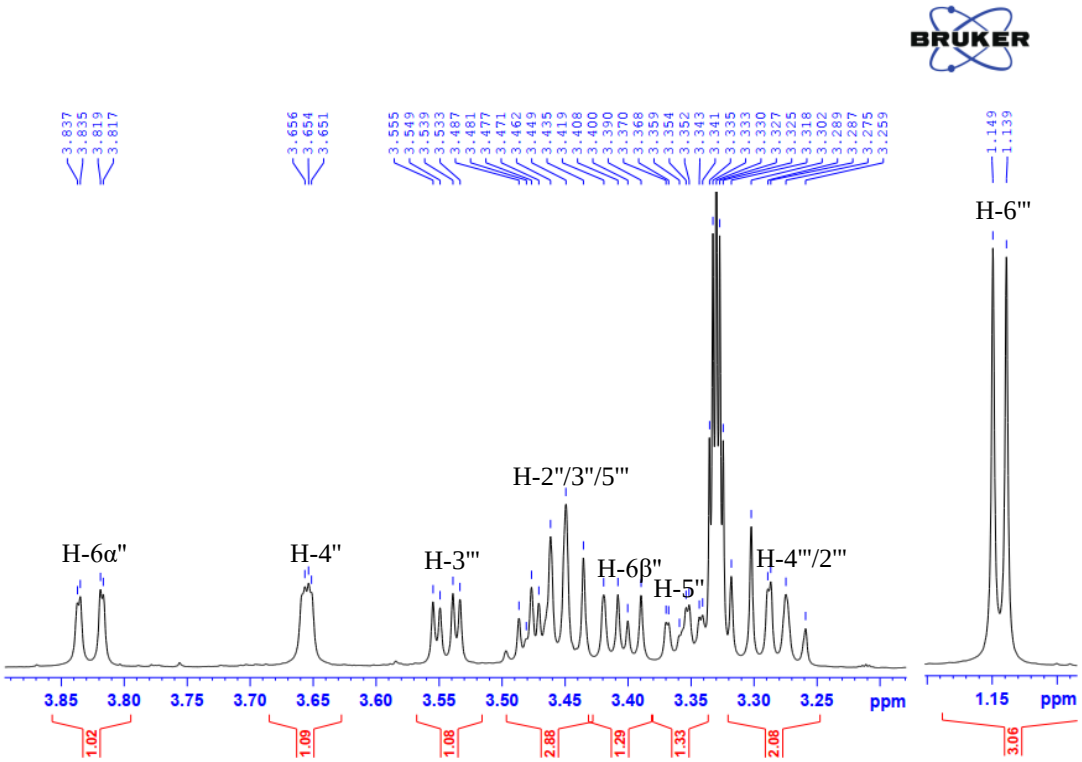


Figure S89: [1]H-NMR (600 MHz, MeOD**)** spectrum of compound **11** (nicotiflorin) (from δ_H 1.10 ppm

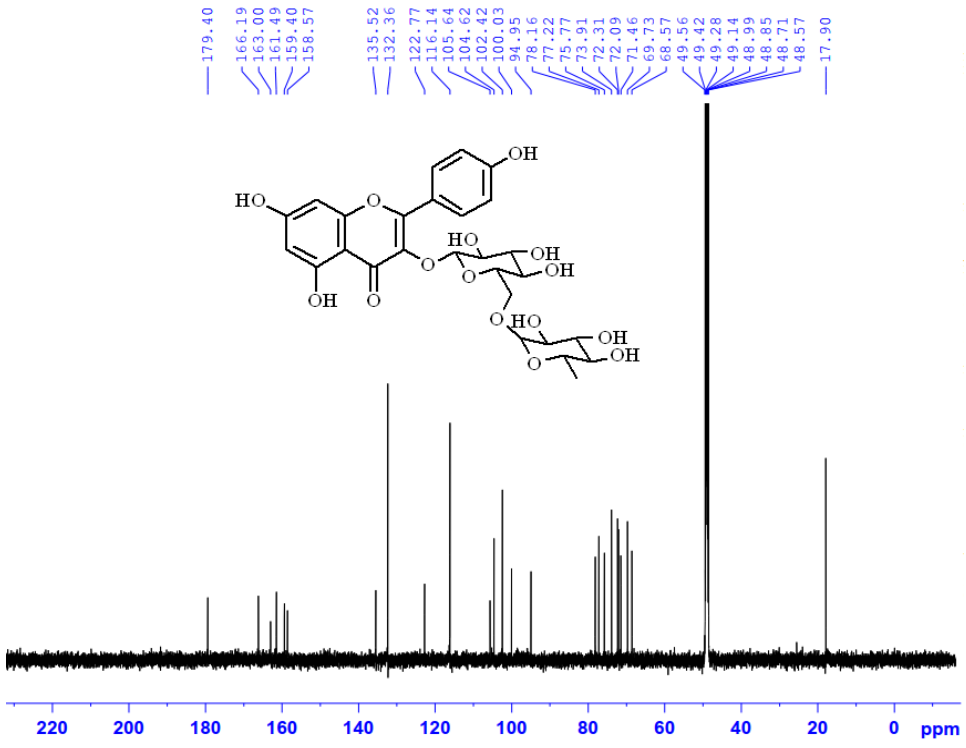


Figure S90: [13]C-NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin)

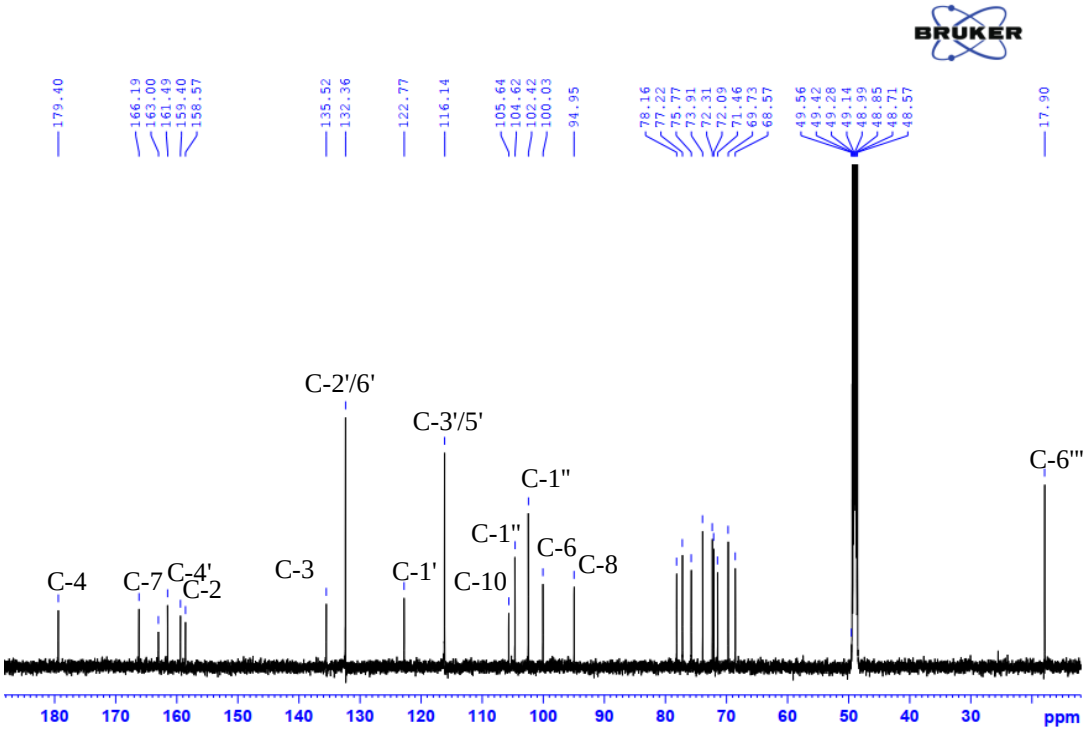


Figure S91: ^{13}C-NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin) (from δ_C 20 ppm to δ_C 180 ppm)

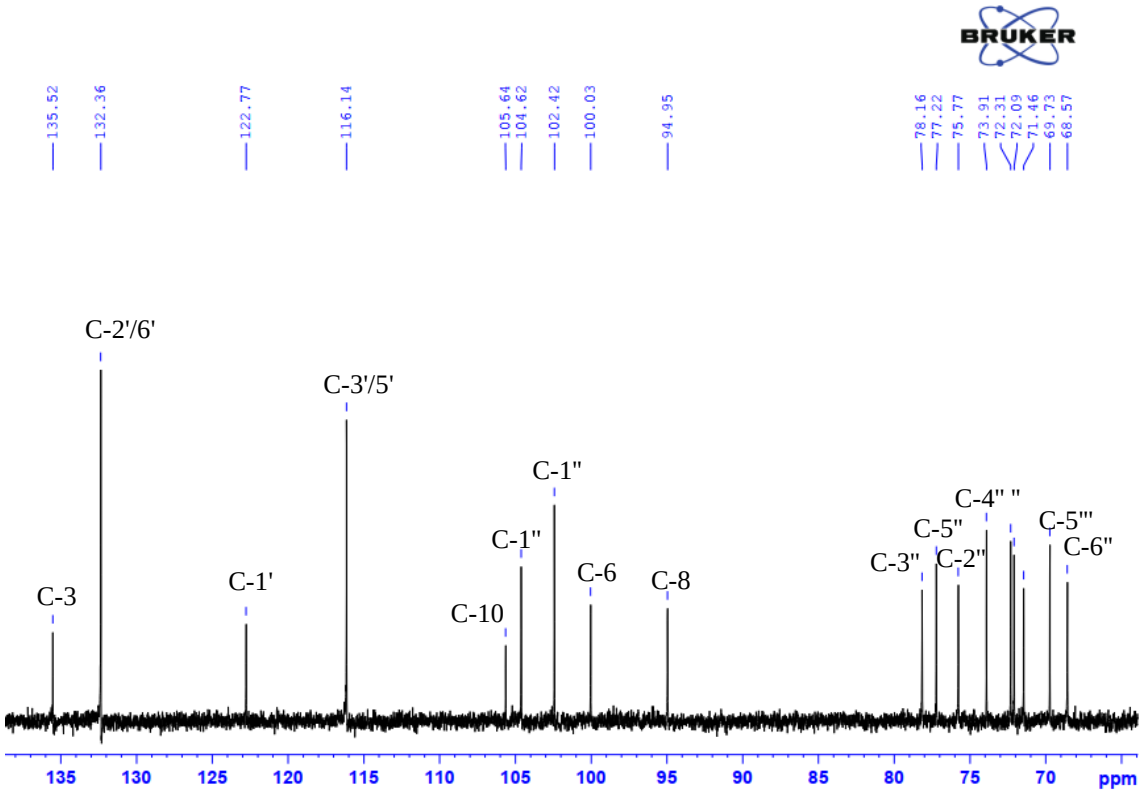


Figure S92: ^{13}C-NMR (150 MHz, MeOD) spectrum of compound **11** (nicotiflorin**)** (from δ_C 65 ppm to δ_C 135 ppm**)**

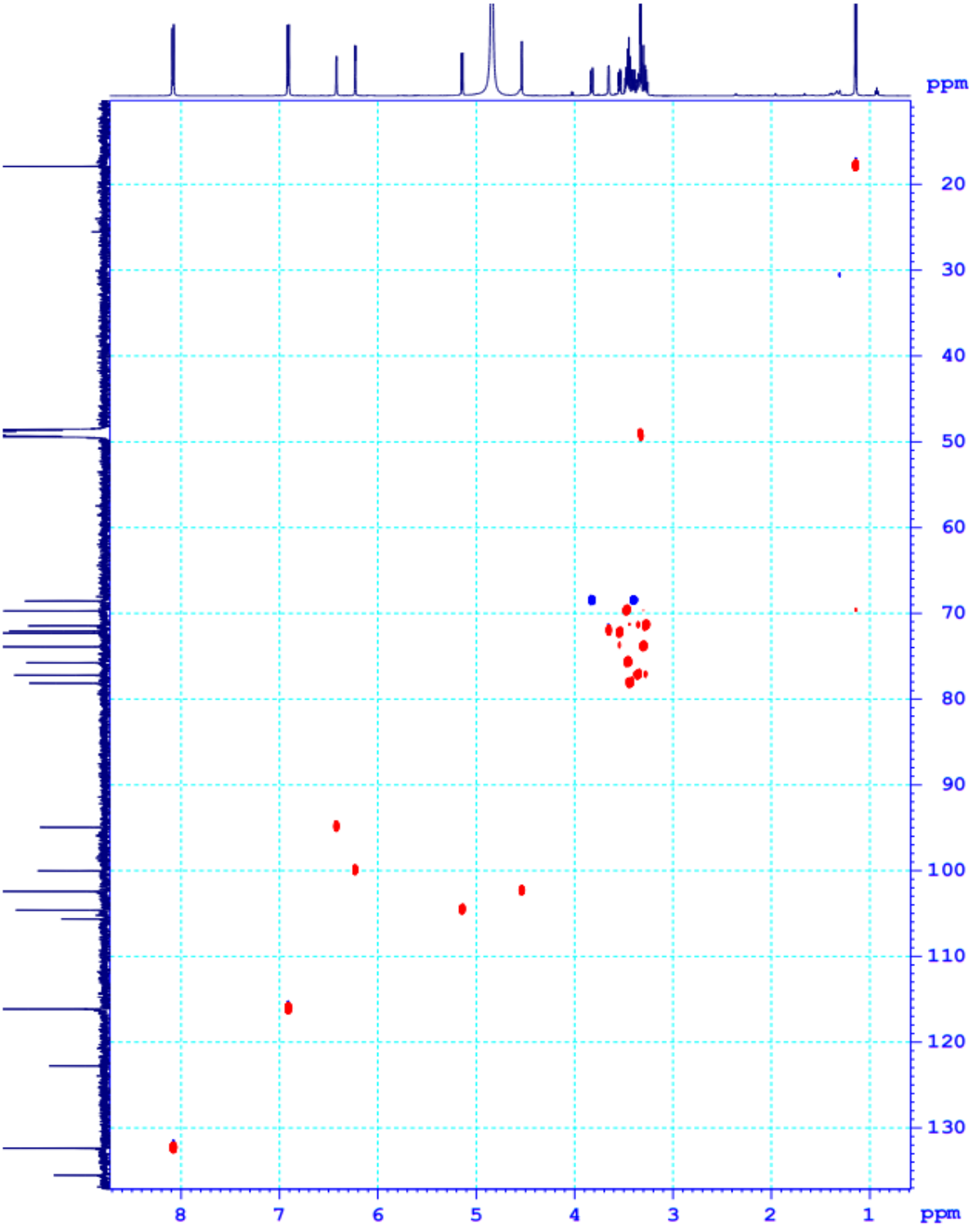


Figure S93: HSQC spectrum of compound **11** (nicotiflorin)

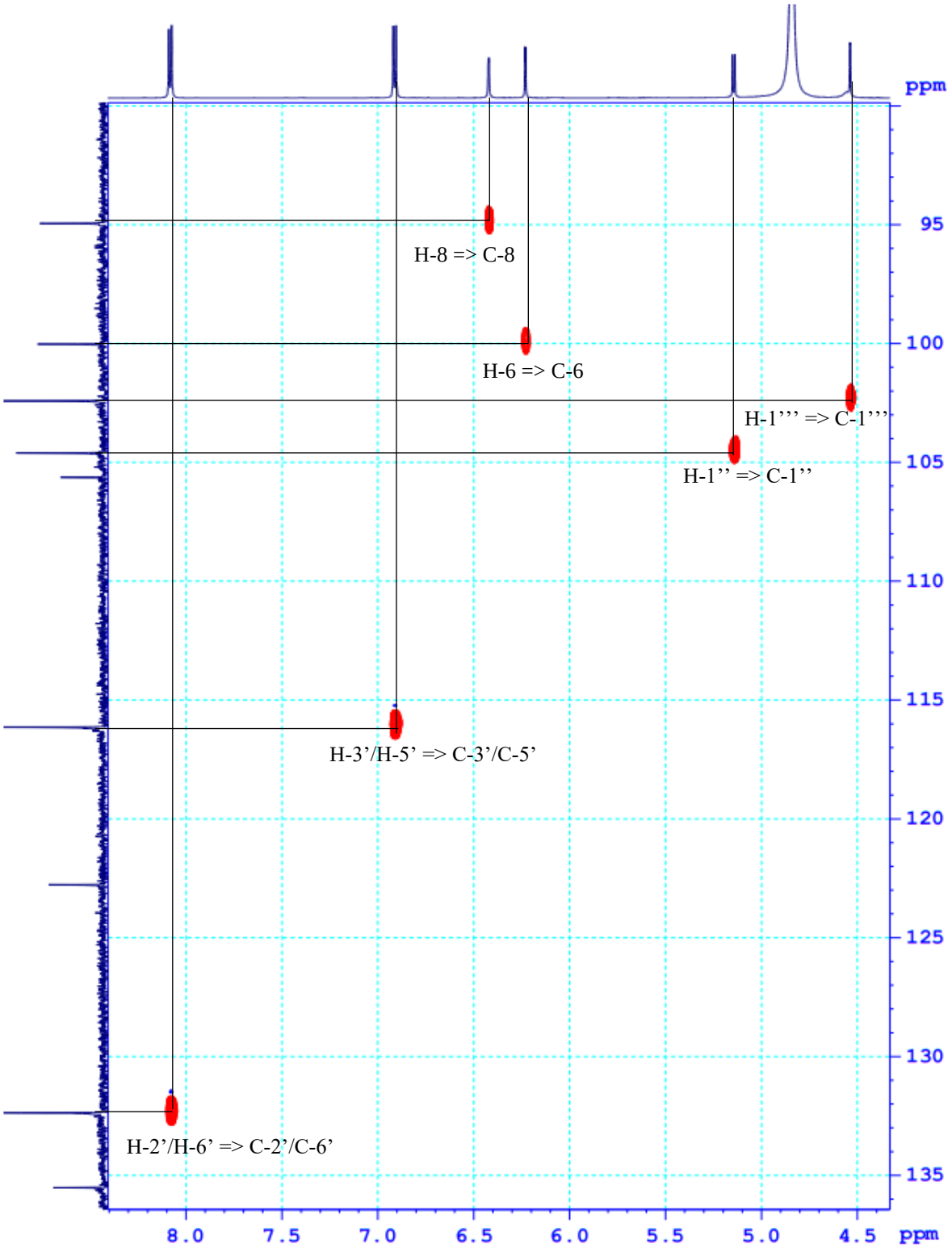


Figure S94: HSQC spectrum of compound **11** (nicotiflorin) (from δ_C 90 ppm to δ_C 135 ppm)

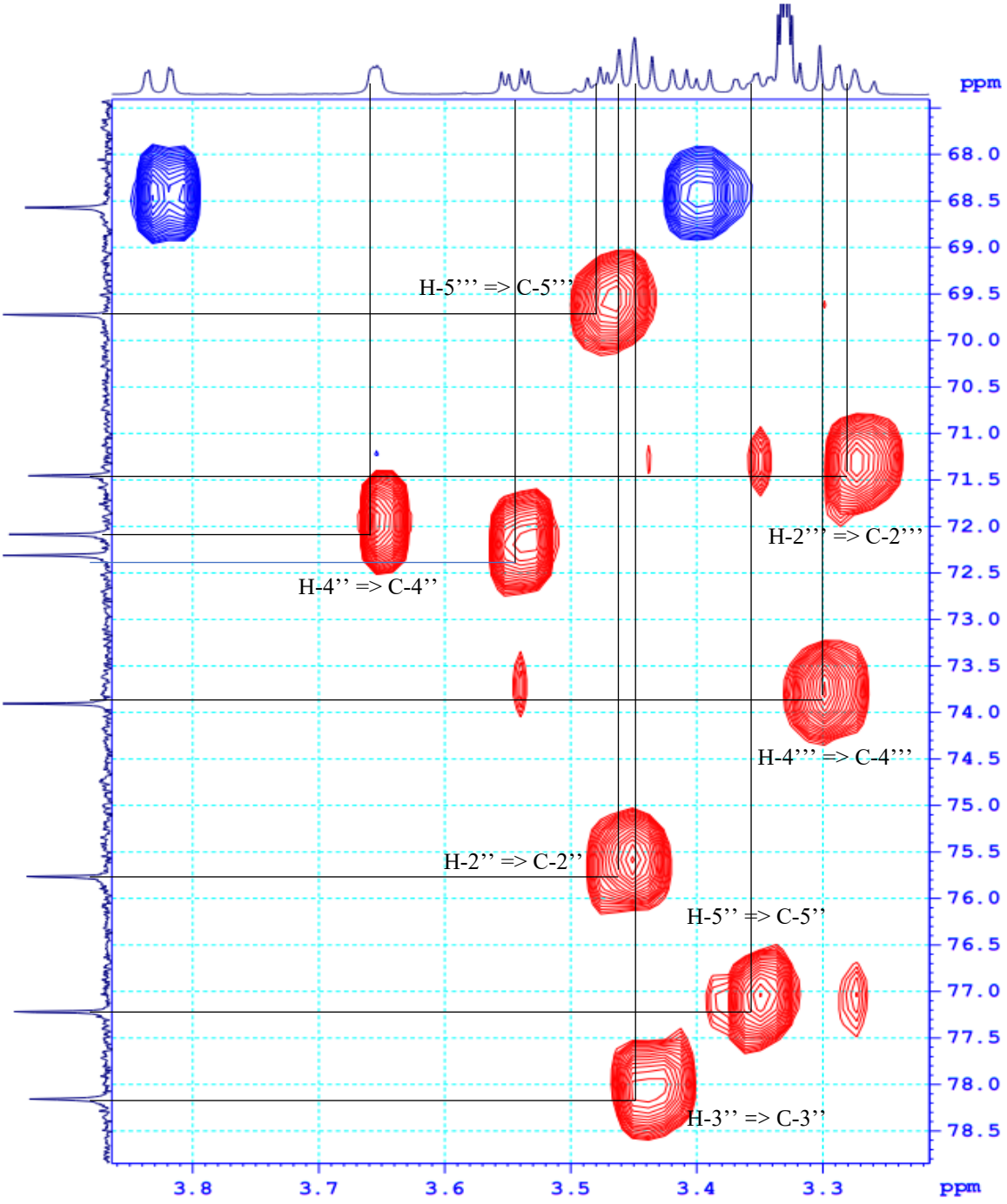


Figure S95: HSQC spectrum of compound **11** (nicotiflorin) (from δ_C 67.5 ppm to δ_C 78.5 ppm)

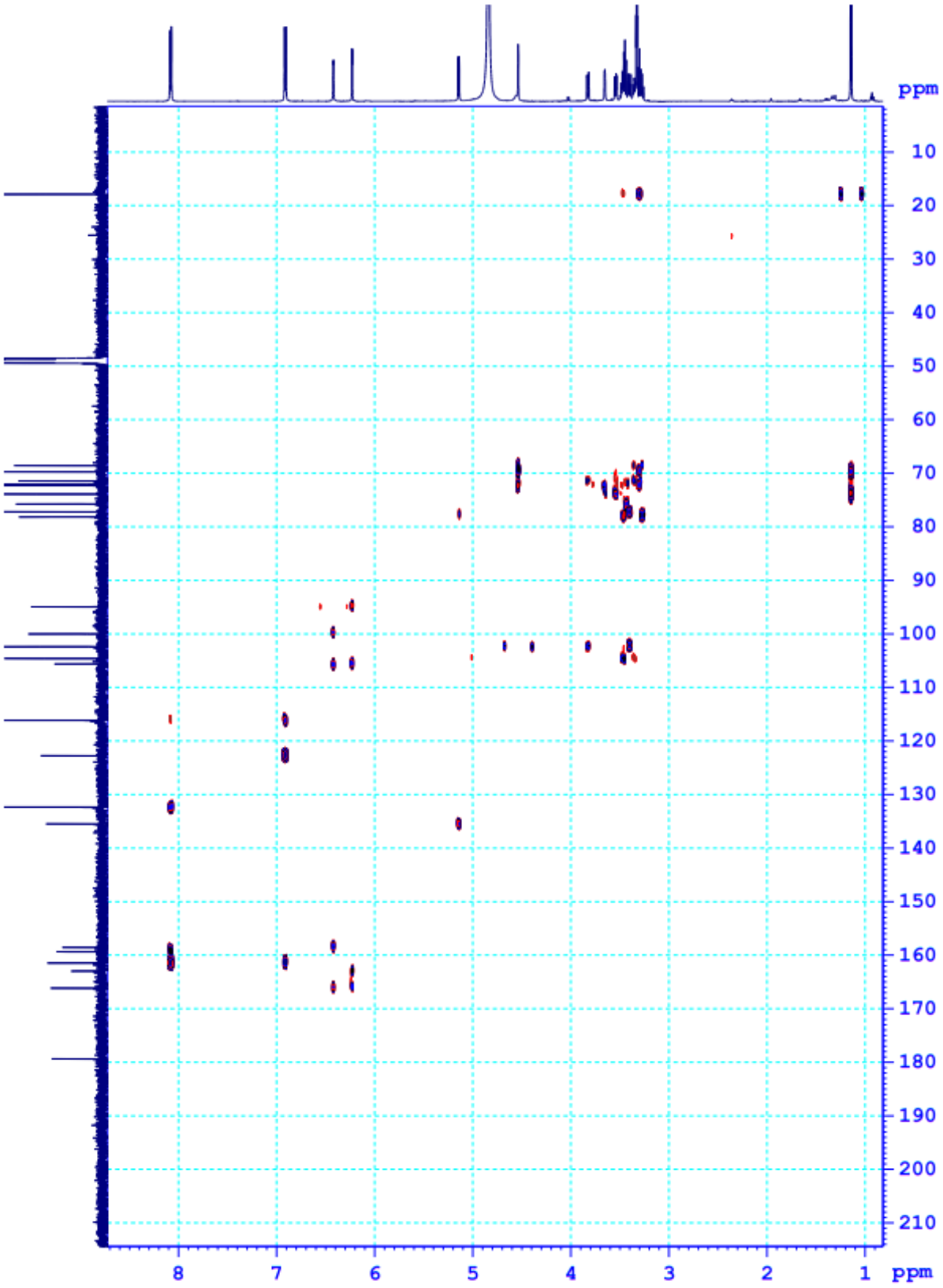


Figure S96: HMBC spectrum of compound **11** (nicotiflorin)

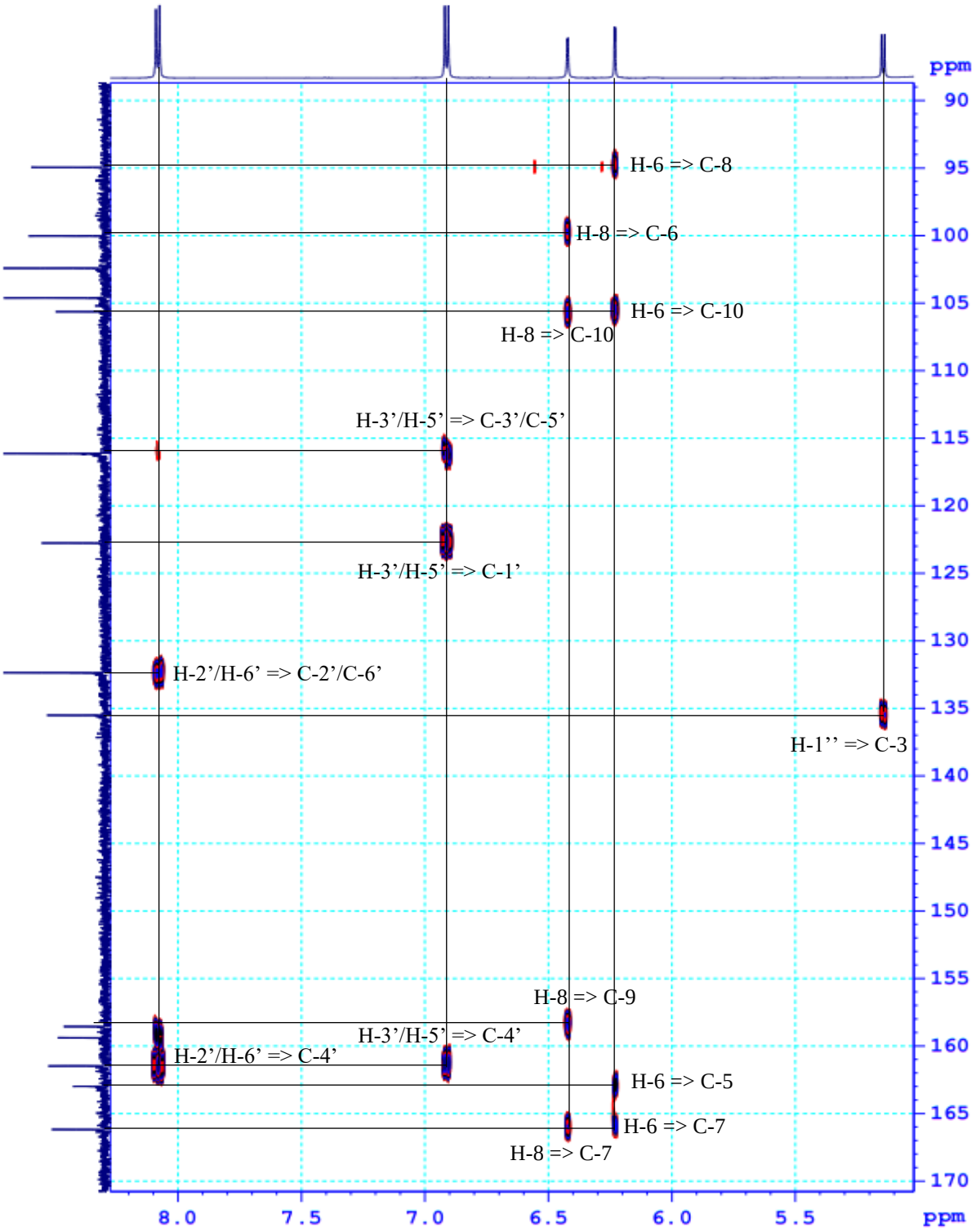


Figure S97: HMBC spectrum of compound **11** (nicotiflorin) (from δ_C 90 ppm to δ_C 170 ppm)

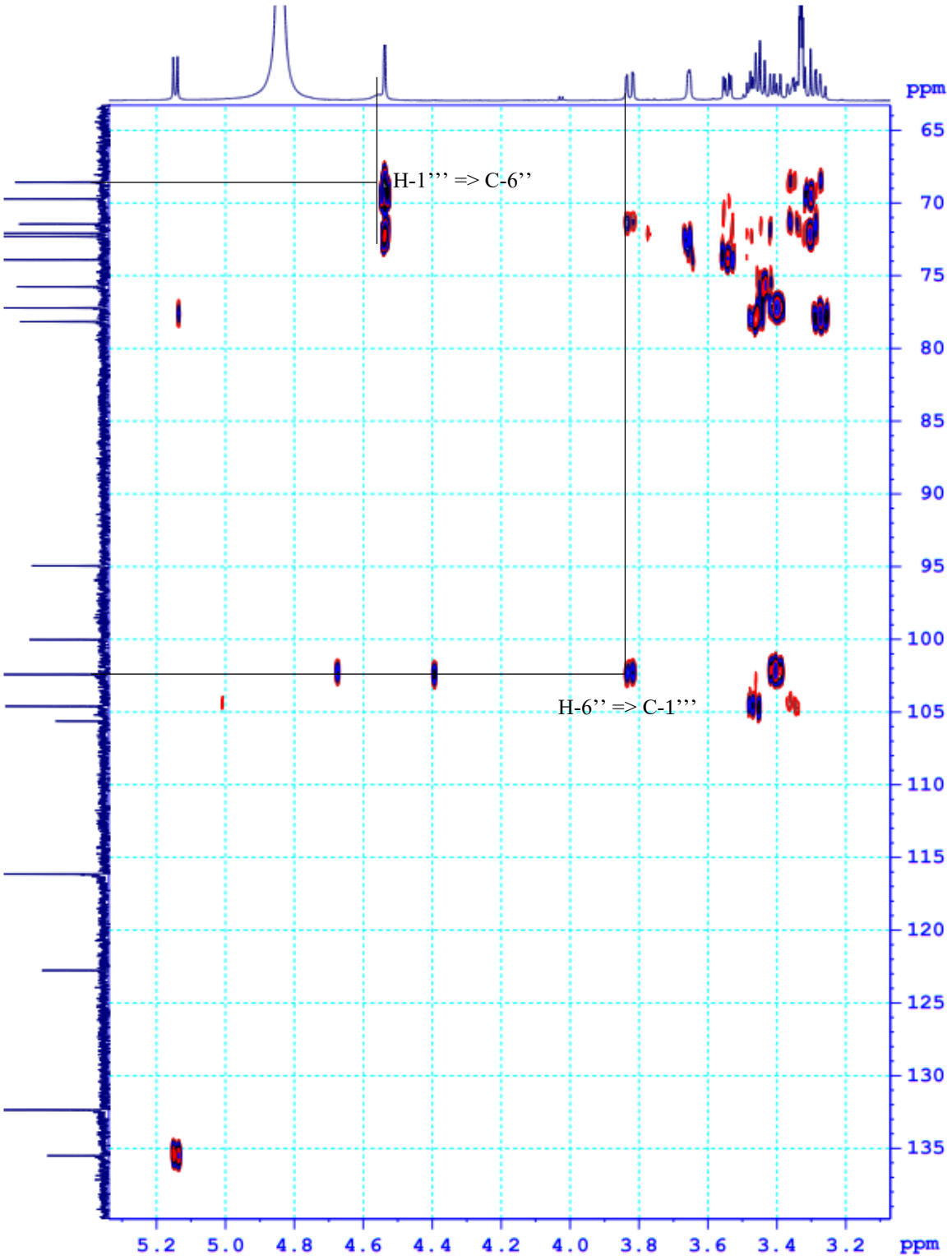


Figure S98: HMBC spectrum of compound **11** (nicotiflorin) (from δ_C 65 ppm to δ_C 140 ppm)

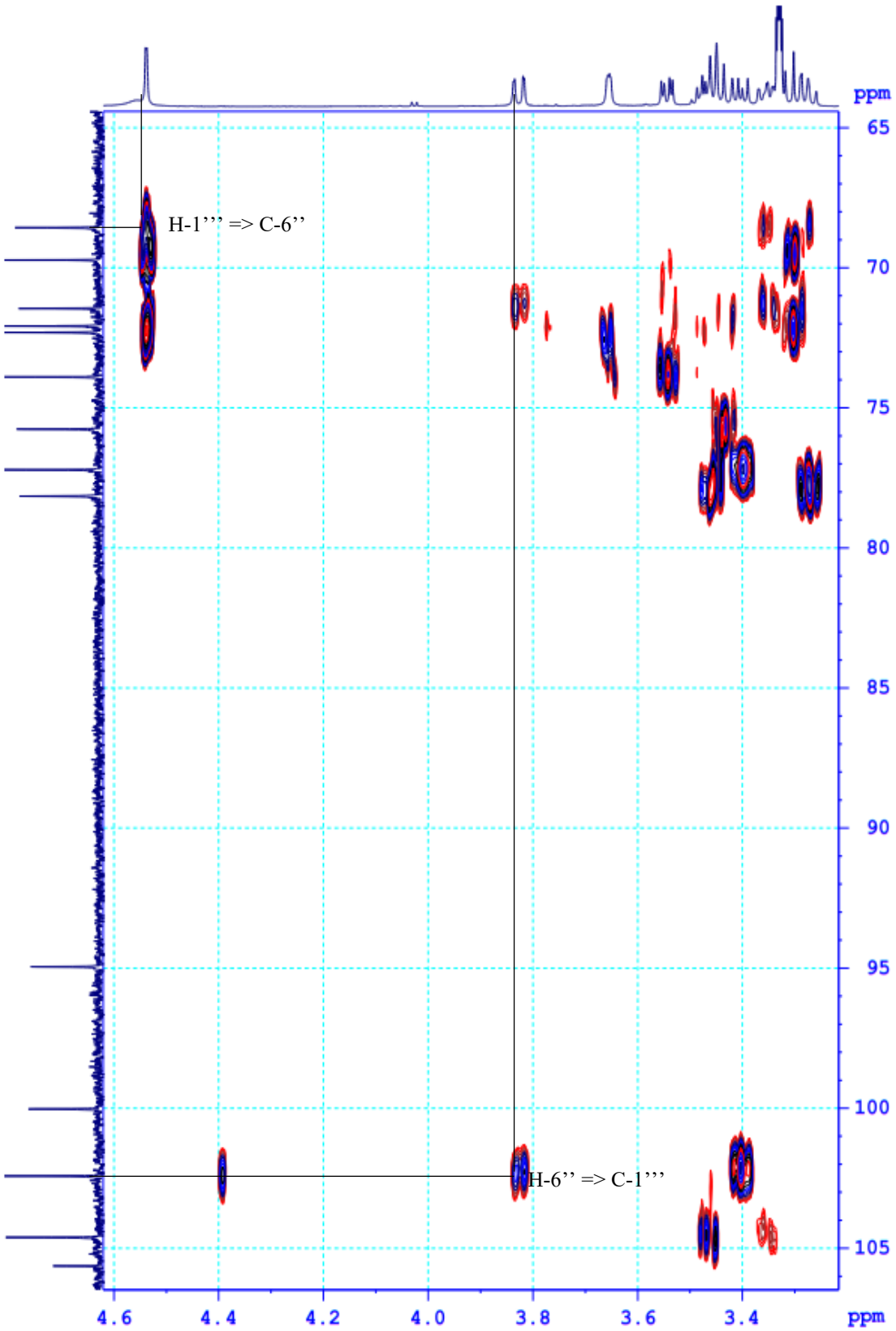


Figure S99: HMBC spectrum of compound **11** (nicotiflorin) (from δ_C 65 ppm to δ_C 105 ppm)

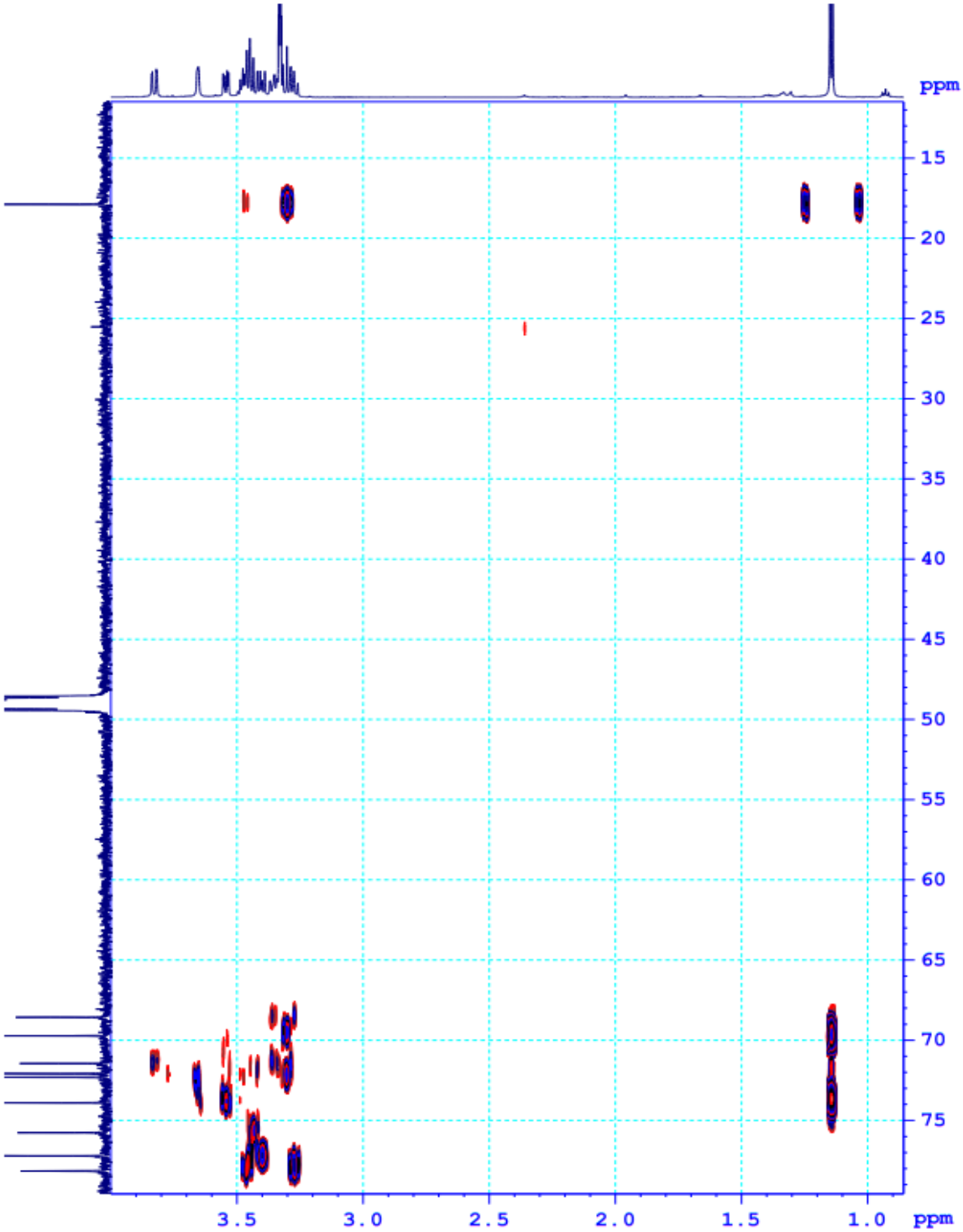


Figure S100: HMBC spectrum of compound **11 (**nicotiflorin) (from δ_C 15 ppm to δ_C 80 ppm)

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

Position	Compound **12** (D_2O)		3,3',4,4'-tetrahydroxybiphenyl ($CDCl_3$) [40]	
	^{13}C-NMR (150 MHz) δ_C ppm	**^{1}H-NMR** (600 MHz) δ_H ppm	**^{13}C-NMR** (125 MHz) δ_C ppm	**^{1}H-NMR** (500 MHz) δ_H ppm
1 & 1'	128.8	-	134.8	-
2 & 2'	117.0	7.33 (1H, *brd*, 8.4 Hz)	116.5	6.97 (1H, *d*, 2.0 Hz)
3 & 3'	143.3	-	145.2	
4 & 4'	147.1	-	146.3	
5 & 5'	115.4	6.88 (1H, *d*, 8.4 Hz)	114.6	6.77 (2H, *d*, 8.0 Hz)
6 & 6'	122.5	7.38 (1H, *d*, 1.8 Hz)	118.9	6.85 (2H, *dd*, 8.0 Hz, 2.0 Hz)

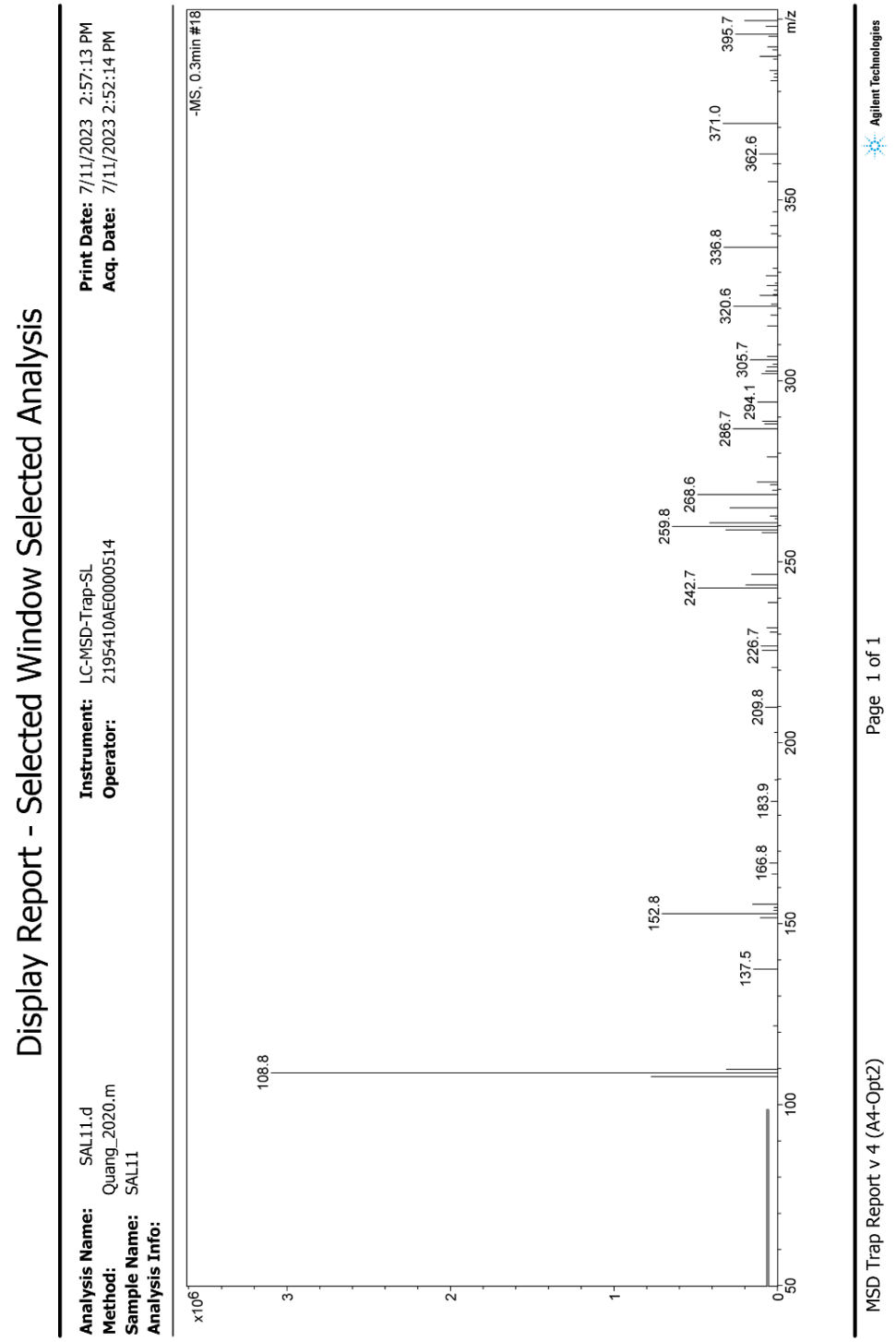


Figure S101: (-)-ESI-MS spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)

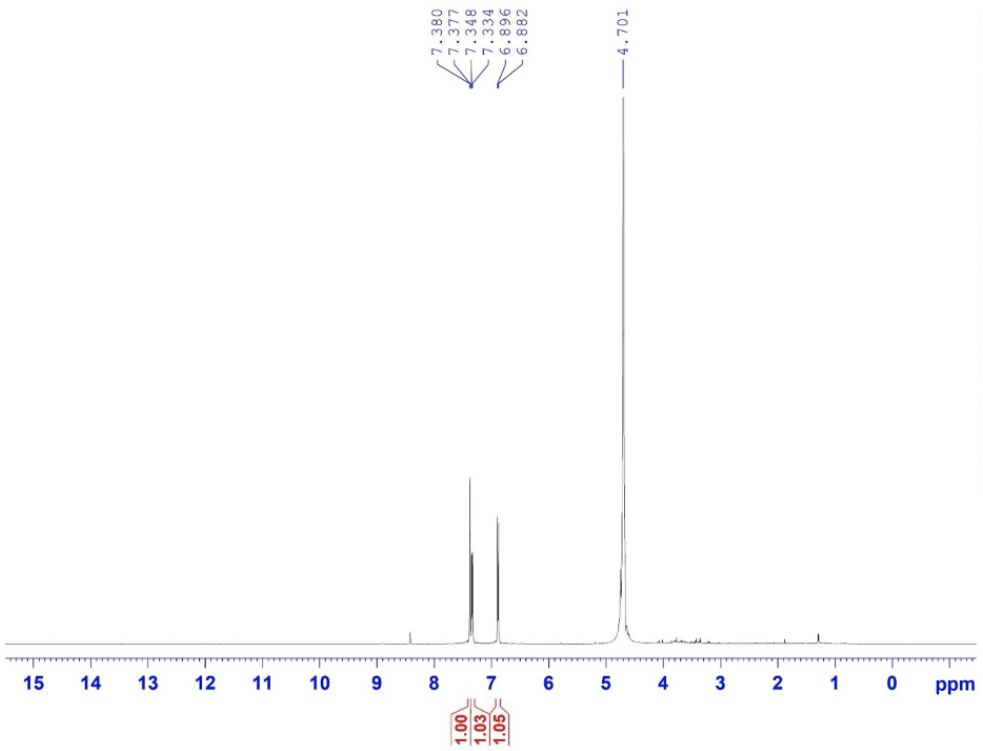


Figure S102: [1]H-NMR (600 MHz, D_2O) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)

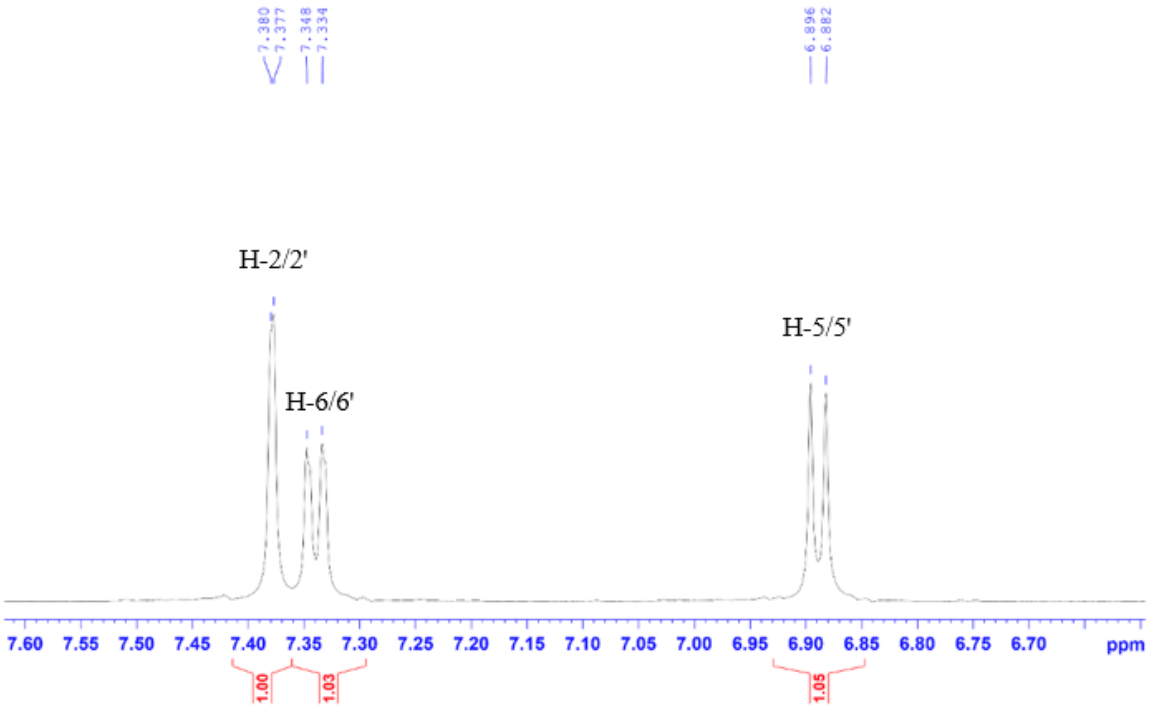


Figure S103: [1]H-NMR (600 MHz, D_2O) spectrum of compound 12 (3,3',4,4'tetrahydroxybiphenyl) (from δ_H 6.6 ppm to δ_H 7.6 ppm)

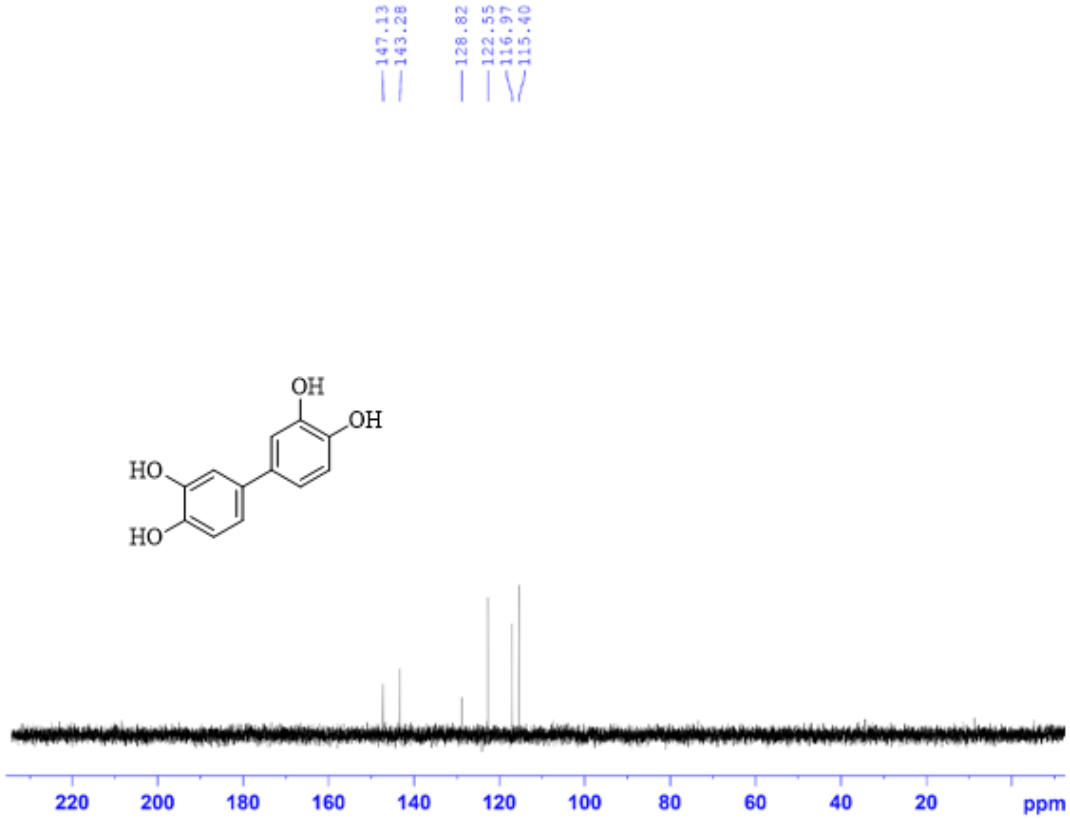


Figure S104: ^{13}C-NMR (150 MHz, D_2O) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)

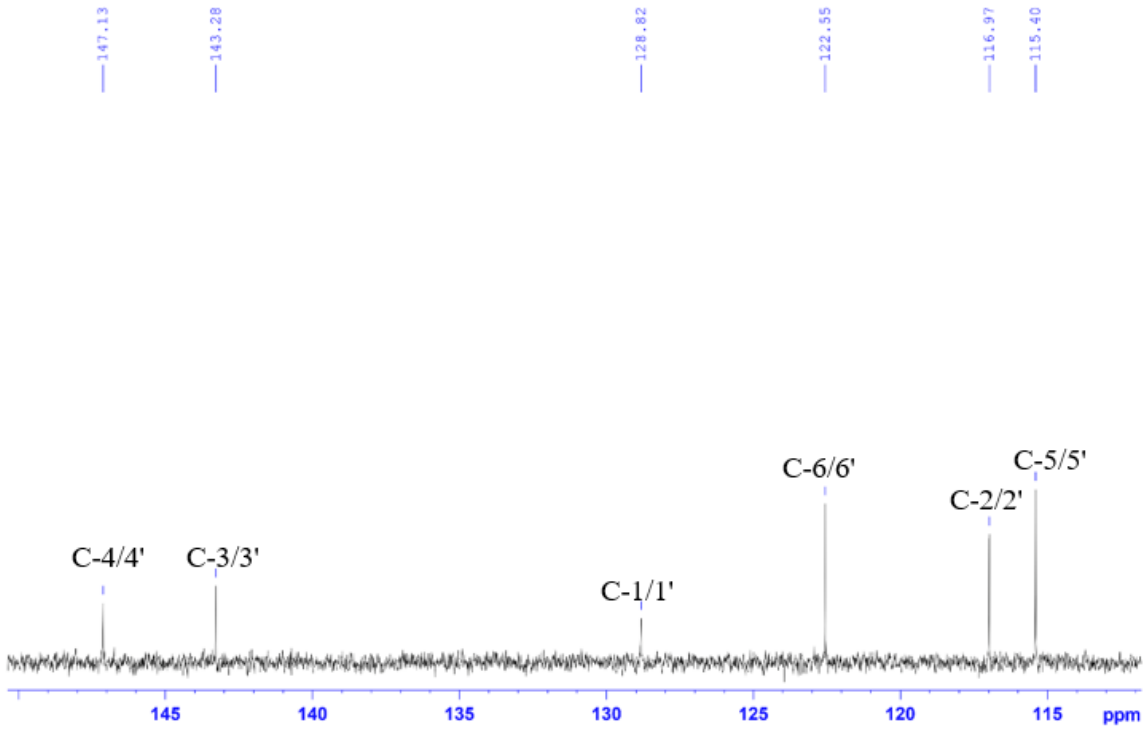


Figure S105: ^{13}C-NMR (150 MHz, D_2O) spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl) **(**from δ_C 115 ppm to δ_C 150 ppm)

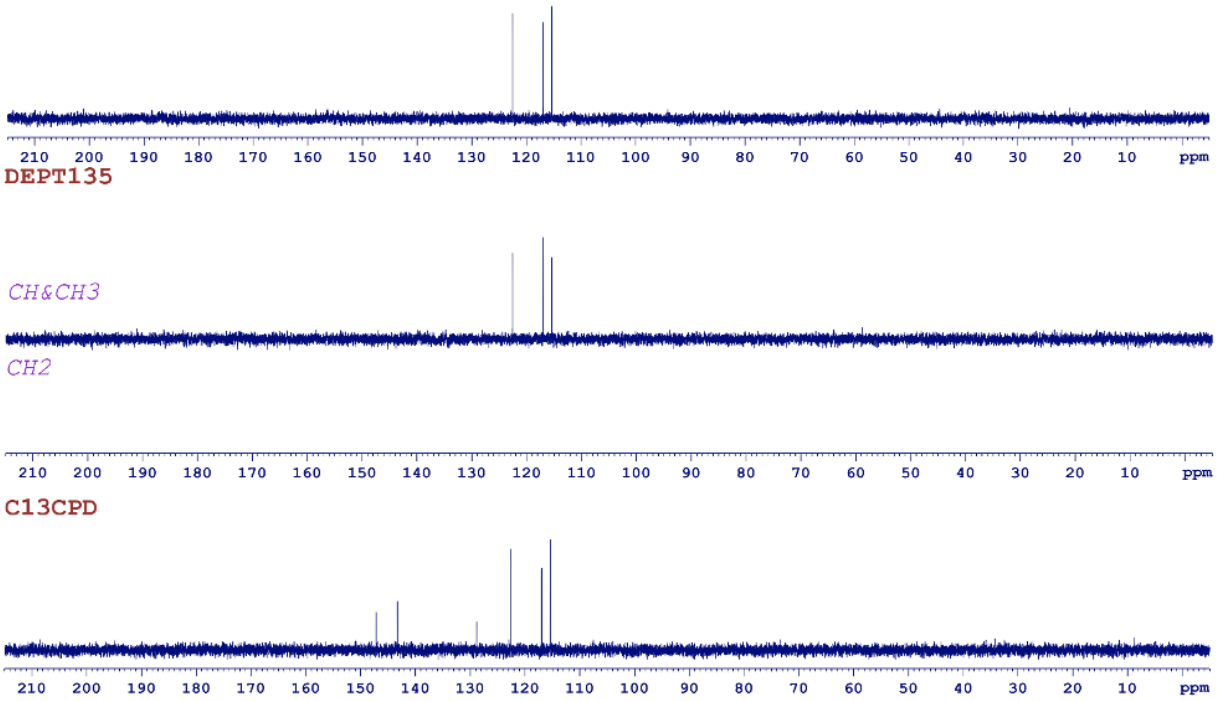


Figure S106: DEPT-90 spectrum of compound **12** (3,3',4,4'-tetrahydroxybiphenyl)

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