Supplementary material

Phytochemical Analysis and Dermo-Cosmetic Evaluation of *Cymbidium* sp. (Orchidaceae) cultivation by-products

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Table S1: NMR data of compounds **1**, **2**, **3**, and **4** in $CDCl_3$ (600 MHz, δ ppm).

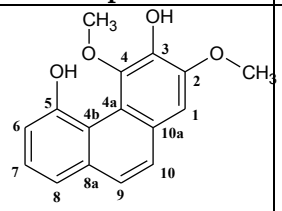
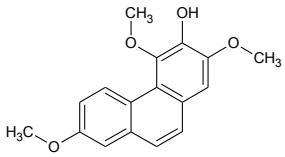
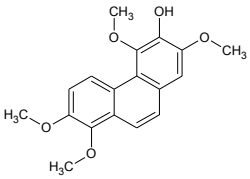
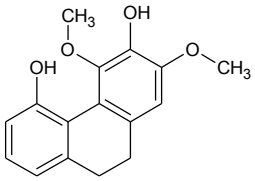
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	^{1}H (*J* in Hz)	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**
1	7.17 s	106.0	7.08 s	104.2	7.03 s	104.7	6.71 s	107.8
2		146.9		146.1		146.7		145.6
3		138.9		138.7		138.9		136.6
4		140.8		143.5		144.0		141.9
4a		117.1		118.6		118.6		118.9
4b		117.7		123.0		124.8		117.3
5		154.3	9.33 d (9.3)	128.1	9.13 d (9.5)	117.8		153.0
6	7.22 dd (7.8/1.4)	115.7	7.25 m	116.6	7.28 d (9.5)	116.7	6.96 dd (7.8/1.2)	118.0
7	7.49 t (7.8)	127.1		156.9		148.7	7.16 t (7.8)	128.3
8	7.41 dd (7.8/1.4)	120.3	7.23 m	108.2		143.1	6.85 dd (7.8/1.2)	119.7
8a		134.6		132.9		127.6	2.72 m (2H)	140.4
9	7.58 d (8.8)	126.9	7.53 d (8.9)	125.1	7.93 d (9.3)	125.5	2.66 m (2H)	31.0
10	7.50 d (8.8)	126.1	7.58 d (8.9)	127.0	7.54 d (9.3)	126.8		30.6
10a		127.4		125.5		126.1		132.1
(2)-OCH_3	4.08 s	56.2	4.05 s	55.9	4.00 s	56.1	3.95 s	56.2
(4)-OCH_3	3.84 s	62.1	3.95 s	59.5	3.89 s	60.2	3.76 s	61.7
(6)-OCH_3								
(7)-OCH_3			3.95 s	55.1	3.97 s	55.9		
(8)-OCH_3					3.94 s	61.4		
(3)-OH	5.95 s		5.97 s				5.52 s	
(5)-OH	10.27 s						8.55 s	

Table S2: NMR data of compounds **5**, **6** and **7** in $CDCl_3$ (600 MHz, δ ppm)

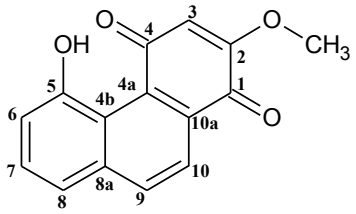
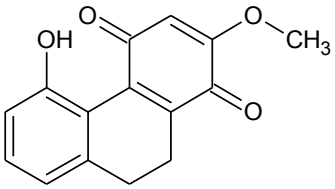
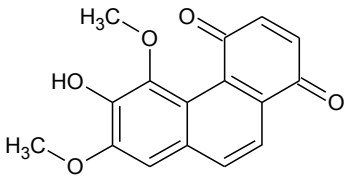
	Compound 5		**Compound 6**		**Compound 7**	
						
	^{1}H (*J* in Hz)	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**
1	-	180.0	-	180.3	-	185.0
2	-	158.9	-	158.1	6.84 d (10.2)	135.2
3	6.29 s	111.4	6.04 s	107.9	7.07 d (10.2)	140.3
4	-	191.6	-	191.1	-	186.1
4a	-	129.9	-	138.5	-	131.7
4b	-	121.4	-	116.9	-	119.6
5	-	155.7	-	154.8	-	142.0
6	7.25 dd (7.8/1.4)	117.4	6.91 dd (7.6/1.2)	118.7	-	140.4
7	7.59 t (7.8)	130.9	7.22 t (7.6)	131.8	-	150.5
8	7.43 dd (7.8/1.4)	120.8	6.78 dd (7.6/1.2)	119.7	6.99 s	102.3
8a	-	138.9	-	140.0	-	131.8
9	8.16 d (8.7)	137.2	2.70 (2H) m	27.8	7.89 d (8.4)	132.2
10	8.19 d (8.7)	121.8	2.65 (2H) m	20.7	7.95 d (8.4)	120.2
10a	-	132.4	-	142.6	-	131.3
(2)-OCH_3	3.98 s	56.4	3.90 s	55.9	-	-
(5)-OH	12.22 s	-	9.81 s	-	-	-
(6)-OH		-	-	-	6.21 brs	-
(5)-OCH_3		-	-	-	3.93 s	60.2
(7)-OCH_3		-	-	-	4.07 s	56.1

Table S3: NMR data of compounds **8**, **9**, and **10** in $CDCl_3$ (600 MHz, δ ppm).

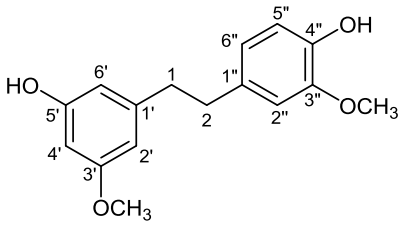
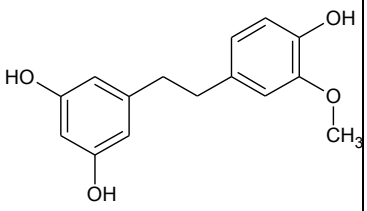
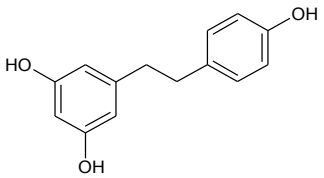
	Compound 8		**Compound 9**		**Compound 10**	
						
	^{1}H (*J* in Hz)	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**
1	2.81 m	37.4	2.79 m	37.0	2.77 m	36.4
2	2.83 m	38.4	2.82 m	37.6	2.82 m	37.5
1′	-	144.7	-	144.9	-	144.8
2′	6.25 brds	108.2	6.22	108.1	6.23 d (2.2)	107.8
3′	-	161.0	-	156.5	-	155.2
4′	6.25 brds	99.2	6.19 t (2.2)	100.3	6.18 t (2.2)	100.2
5′	-	156.8	-	156.5	-	155.2
6′	6.32 t (1.7)	107.0	6.22 m	108.1	6.23 d (2.2)	107.8
1′′	-	133.8	-	133.4	-	133.6
2′′	6.62 d (2.0)	111.4	6.61 d (2.0)	111.2	7.03 d (8.5)	129.1
3′′	-	146.5	-	146.4	6.74 d (8.5)	114.9
4′′	-	143.9	-	143.8	-	154.1
5′′	6.83 d (8.3)	114.4	6.82 d (7.9)	114.3	6.74 d (8.5)	114.9
6′′	6.68 dd (8.3/2.0)	121.2	6.67 dd (7.9/2.0)	121.2	7.03 d (8.5)	129.1
(3′)-OCH_3	3.75 s	55.4	-	-		
(3′′)-OCH_3	3.84 s	56.0	3.84 s	55.6		
(3′)-OH	-		4.75 brds			
(5′)-OH	4.63 s		4.75 brds			
(4′′)-OH	5.46 s		5.45 s			

Table S4: NMR data of compounds **11** and **12** in $CDCl_3$ (600 MHz, δ ppm).

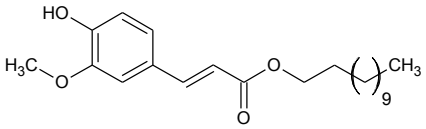
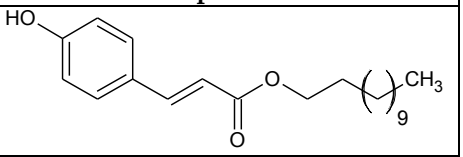
	Compound 11		**Compound 12**	
				
	^{1}H (*J* in Hz)	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**
1	-	127.2	-	127.7
2	7.04 d (1.9)	108.9	7.43 d (8.7)	129.9
3	-	146.7	6.83 d (8.7)	115.9
4	-	147.9	-	157.6
5	6.92 d (8.1)	114.2	6.83 d (8.7)	115.9
6	7.07 dd (8.1/1.9)	122.6	7.43 d (8.7)	129.9
7	7.61 d (15.8)	144.1	7.62 d (15.8)	144.3
8	6.29 d (15.8)	115.4	6.30 d (15.8)	116.1
9	-	167.6	-	167.5
1′	4.19 t (6.8) 2H	64.1	4.18 t (6.8) 2H	64.6
2′	1.69 m 2H	28.0	1.69 m 2H	28.3
3′	1.39 m 2H	25.6	1.39 m 2H	25.9
4′-11′	1.25-1.27 m	22.1-31.2	1.25-1.27 m	22.1-31.2
12′	0.88 t (6.9)	13.4	0.88 t (6.9)	14.1
-OCH_3	3.93 s	55.3	-	

Table S5: NMR data of compounds **13** in $CDCl_3$ (600 MHz, δ ppm).

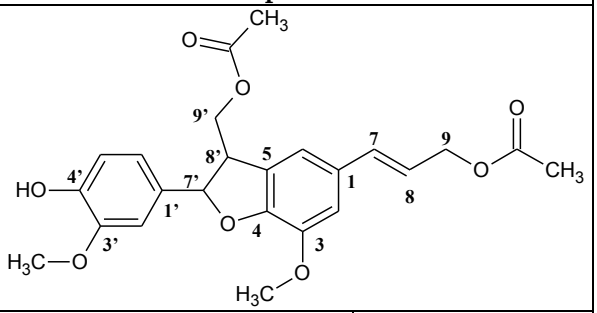
	Compound 13	
		
	^{1}H (*J* in Hz)	**^{13}C**
1	-	130.2
2	6.88 m	110.2
3	-	144.0
4	-	147.8
5	-	127.2
6	6.88 m	114.8
7	6.60 d (15.9)	133.9
8	6.15 dt (15.9/6.5)	120.7
9	4.71 d (6.5)	64.6
1′	-	131.8
2′	6.88 m	108.2
3′	-	146.2
4′	-	145.7
5′	6.88 m	113.8
6′	6.88 m	119.0
7′	5.47 d (7.3)	88.2
8′	3.77 m	49.8
9′	4.43 dd (11.0/5.6) 4.31 dd (11.0/7.3)	64.7
(3)-OCH_3	3.90 s	55.4
(3′)-OCH_3	3.86 s	55.4
(9)-$CO\underline{CH_3}$	2.02 s	20.1
(9′)-$CO\underline{CH_3}$	2.10 s	20.4
(9)-$\underline{C}OCH_3$	-	170.2
(9′)-$\underline{C}OCH_3$	-	170.4
(4′)-OH	5.61 s	-

Table S6: NMR data of compounds **14** in $CDCl_3$ (600 MHz, δ ppm).

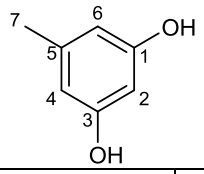
	Compound 14	
		
	^{1}H (*J* in Hz)	**^{13}C**
1	-	156.9
2	6.17 t (*J* = 2.3 Hz)	100.1
3	-	156.9
4	6.24 d (*J* = 2.2 Hz)	108.9
5	-	141.1
6	6.24 d (*J* = 2.2 Hz)	108.9
7	2.24 s (3H)	21.5

Table S7: NMR data of compounds **15** and **16** in $CDCl_3$ (600 MHz, δ ppm).

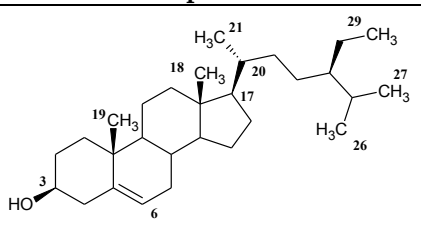
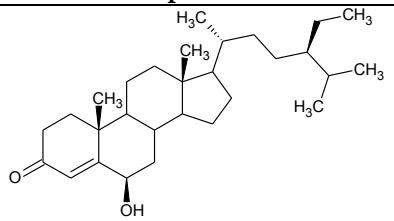
	Compound 15		**Compound 16**	
				
	^{1}H (*J* in Hz)	**^{13}C**	**^{1}H (*J* in Hz)**	**^{13}C**
1	1.89 m 1.15 m	37.2	2.03 m 1.71 ddd (15.0/14.2/4.2)	37.25
2	1.85 m 1.56 m	31.6	2.52 ddd (17.1/15.0/5.0) 2.37 ddd (17.1/4.2/1.0)	34.2
3	3.53 m	71.8	-	200.3
4	2.28 m	42.3	5.82 s	126.6
5	-	140.7	-	168.4
6	5.35 m	121.7	4.34 brds	73.4
7	1.53 m	31.9	2.00 m / 1.24 m	38.6
8	1.93 m	31.9	1.95 m	30.1
9	0.98 m	50.1	0.90 m	53.6
10	-	36.5	-	37.9
11	1.51 m	21.1	1.49 m (2H)	21.0
12	2.03 m / 1.19 m	39.7	2.03 m / 1.15 m	39.7
13	-	42.3	-	42.4
14	1.00 m	56.7	1.01 m	55.9
15	1.61 m / 1.13 m	24.3	1.61 m / 1.13 m	24.5
16	1.86 m / 1.35 m	28.2	1.86 m / 1.30 m	28.3
17	1.10 m	56.0	1.12 m	56.2
18	0.68 s	11.8	0.74 s	11.6
19	1.00 s	19.4	1.38 s	19.6
20	1.37 m	36.1	1.35 m	36.3
21	0.92 d (6.5)	18.8	0.92 d (6.6)	18.7
22	1.35 m / 1.04 m	33.9	1.31 m / 1.01 m	34.1
23	1.20 m	26.0	1.16 m	26.3
24	1.97 m	45.8	0.93 m	45.9
25	1.70 m	29.1	1.66 m	29.4
26	0.84 d (6.5)	19.8	0.81 d (6.8)	19.6
27	0.81 d (6.5)	19.0	0.84 d (6.9)	19.1
28	1.27 m / 1.21 m	23.0	1.27 m / 1.21 m	23.2
29	0.85 t (7.5)	12.0	0.85 t (7.5)	11.9

Table S8: P-values after one-way Anova by Dunnett's multiple comparisons test against the positive control on collagenase assay.

Dunnett's multiple comparisons test	Significant	Summary	P Value
Phosphoramidon vs. Flowers DCM	Yes	****	<0.0001
Phosphoramidon vs. Flowers EtoAc	Yes	****	<0.0001
Phosphoramidon vs. Flowers EtOH: H2O	No	ns	0.0848
Phosphoramidon vs. Leaves DCM	No	ns	0.1652
Phosphoramidon vs. Leaves EtoAc	Yes	****	<0.0001
Phosphoramidon vs. Leaves EtOH: H2O	Yes	****	<0.0001
Phosphoramidon vs. Pseudobulbs DCM	Yes	****	<0.0001
Phosphoramidon vs. Pseudobulbs EtoAc	Yes	****	<0.0001
Phosphoramidon vs. Pseudobulbs EtOH: H2O	No	ns	0.9959
Phosphoramidon vs. Roots DCM	No	ns	0.9994
Phosphoramidon vs. Roots EtoAc	Yes	****	<0.0001
Phosphoramidon vs. Roots EtOH: H2O	Yes	****	<0.0001

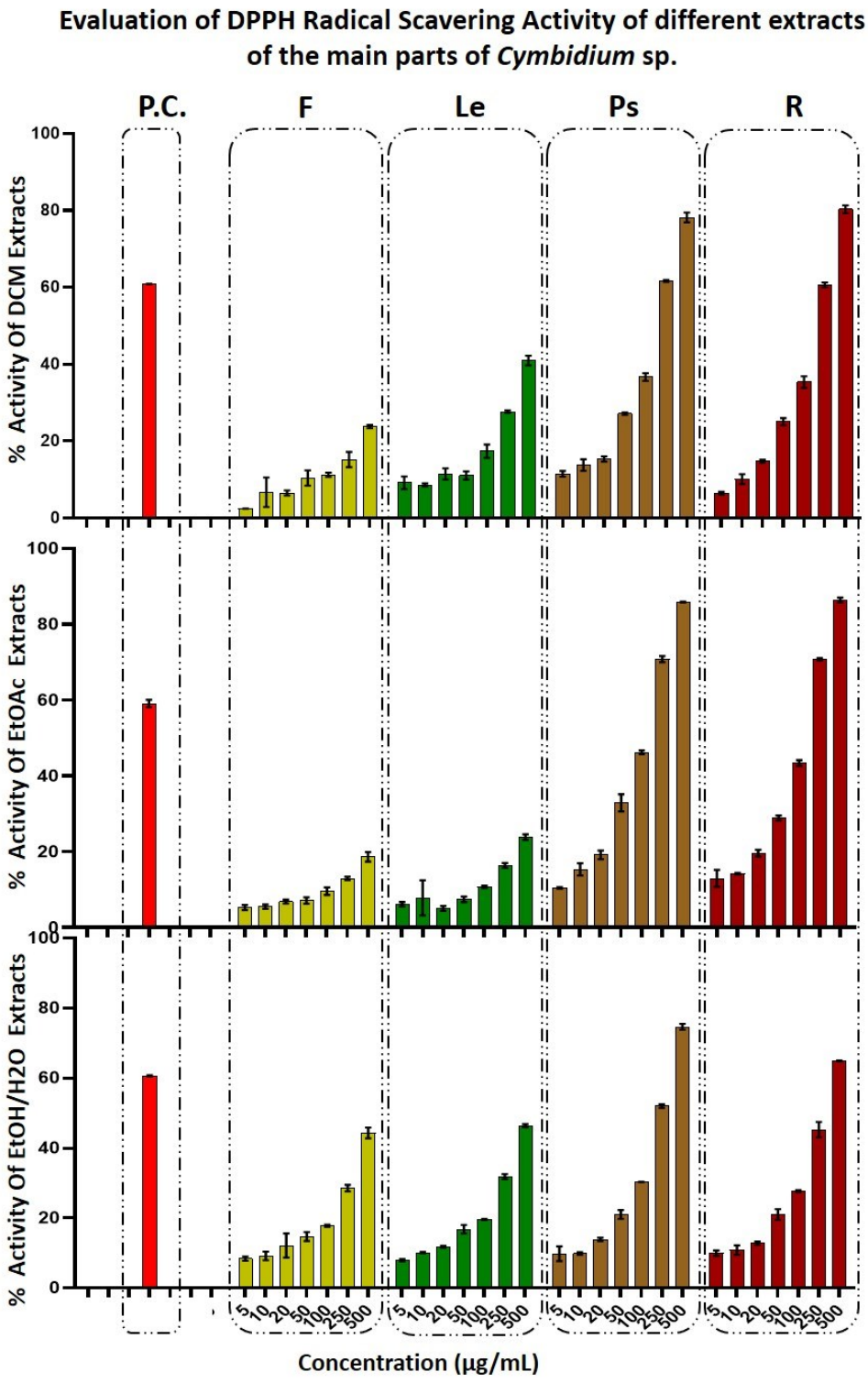


Figure S1: Determination of DPPH radical scavenging activity of DCM, EtOAc, and EtOH/H_2O extracts of Flowers, Leaves, Pseudobulbs, and Roots of *Cymbidium* sp. All experiments were performed in triplicate. Data are expressed as mean ±SD (n=3, $p<0.05$) for all tested dosages.

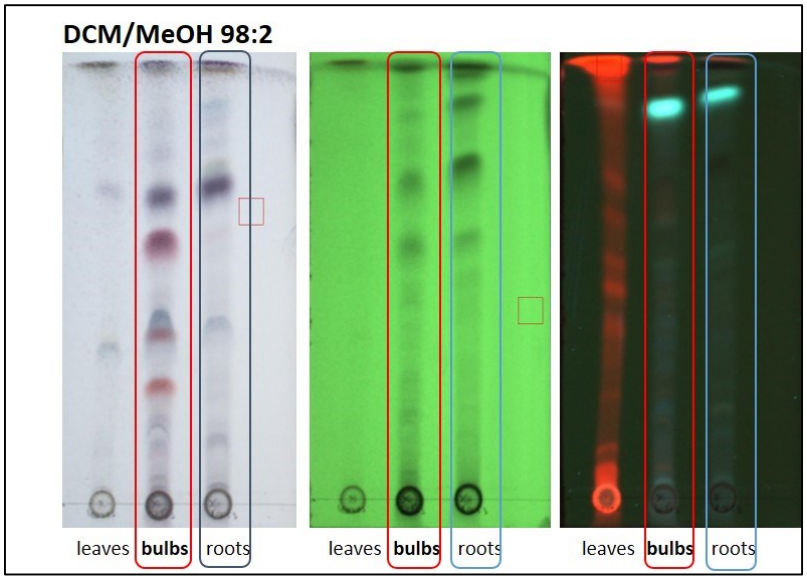


Figure S2: TLC chromatograms of EtOAc total extracts from *Cymbidium* sp. pseudobulbs (red) and roots (blue) in DCM/MeOH 98:2 (Left: vis, center: UV-254nm, right: UV-366nm).

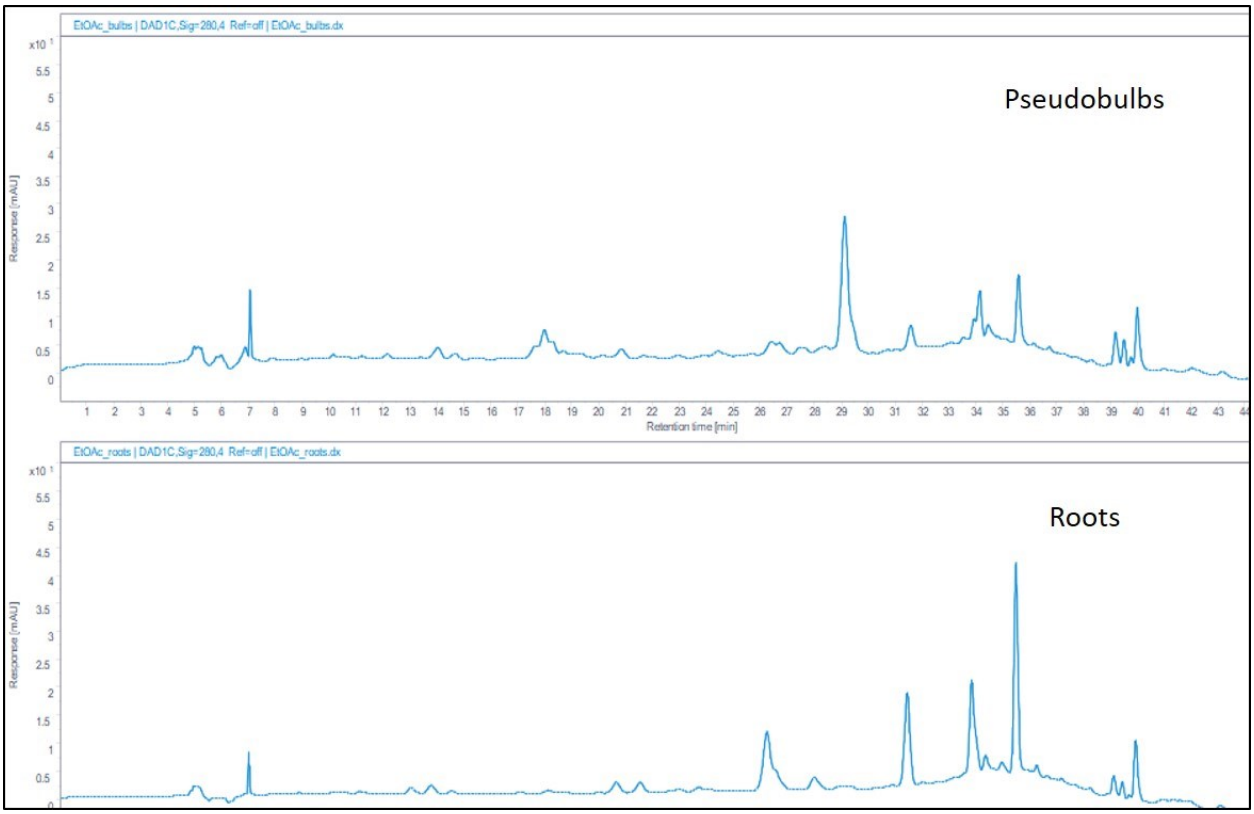


Figure S3. HPLC-DAD chromatogram of EtOAc total extracts from *Cymbidium* sp. bulbs and roots at 280 nm.

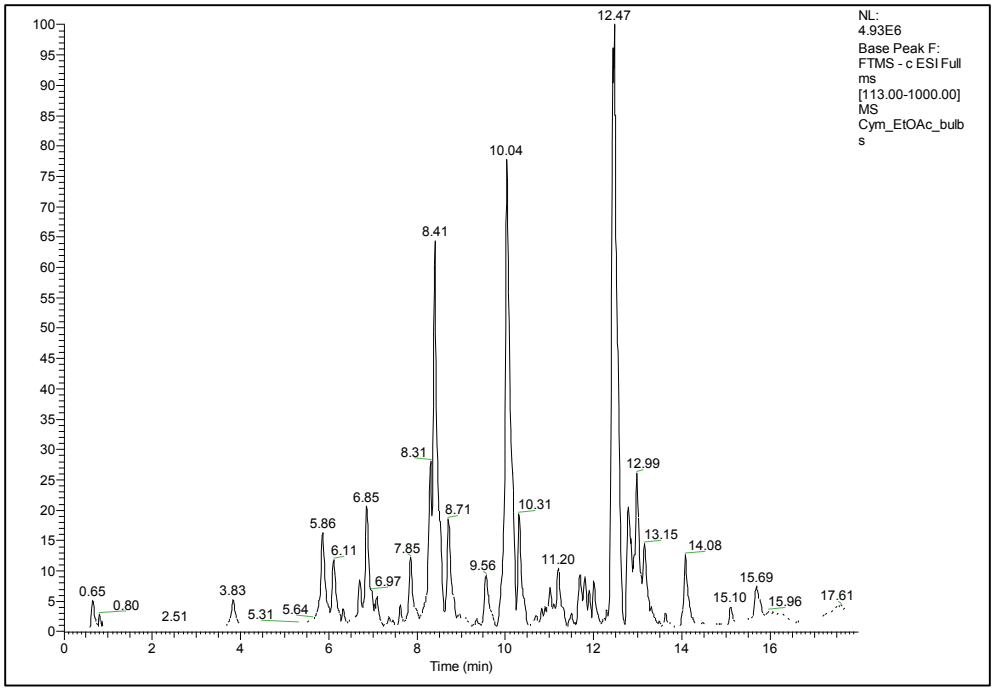


Figure S4: BP–UPLC-HRMS chromatogram of EtOAc total extract from *Cymbidium* sp. pseudobulbs.

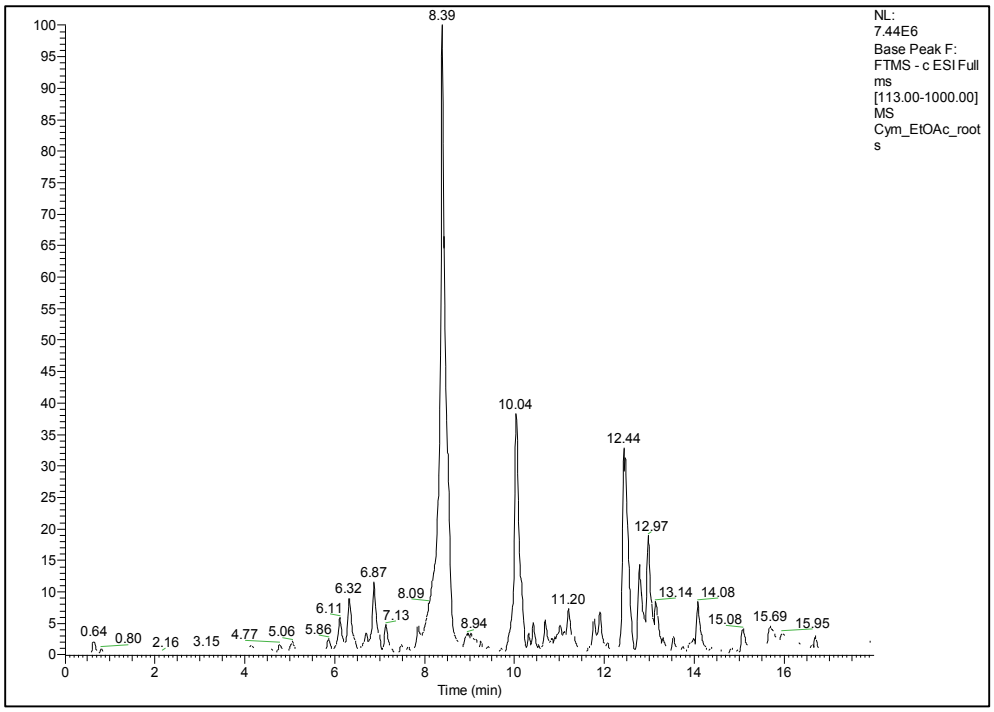


Figure S5: BP–UPLC-HRMS chromatogram of EtOAc total extract from *Cymbidium* sp. roots.

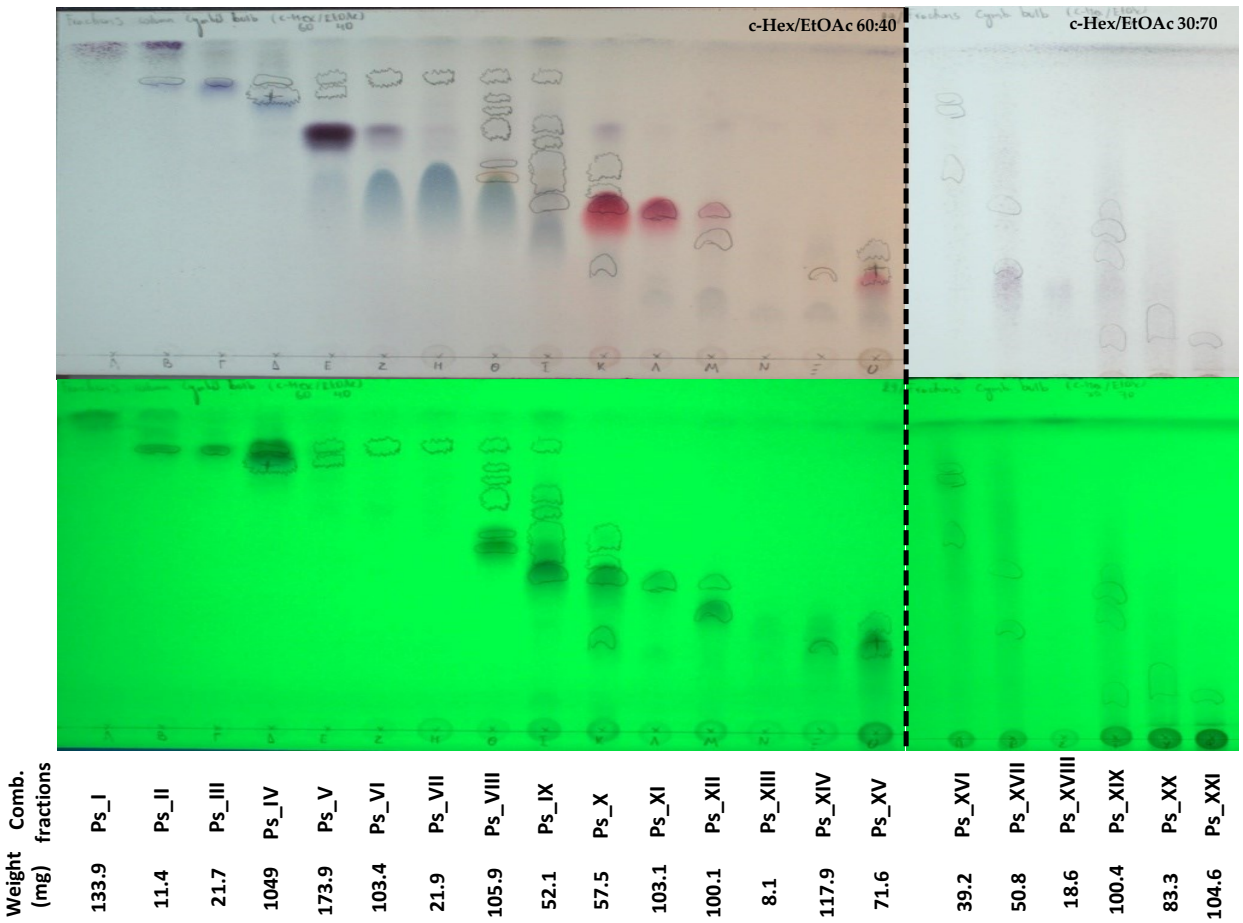
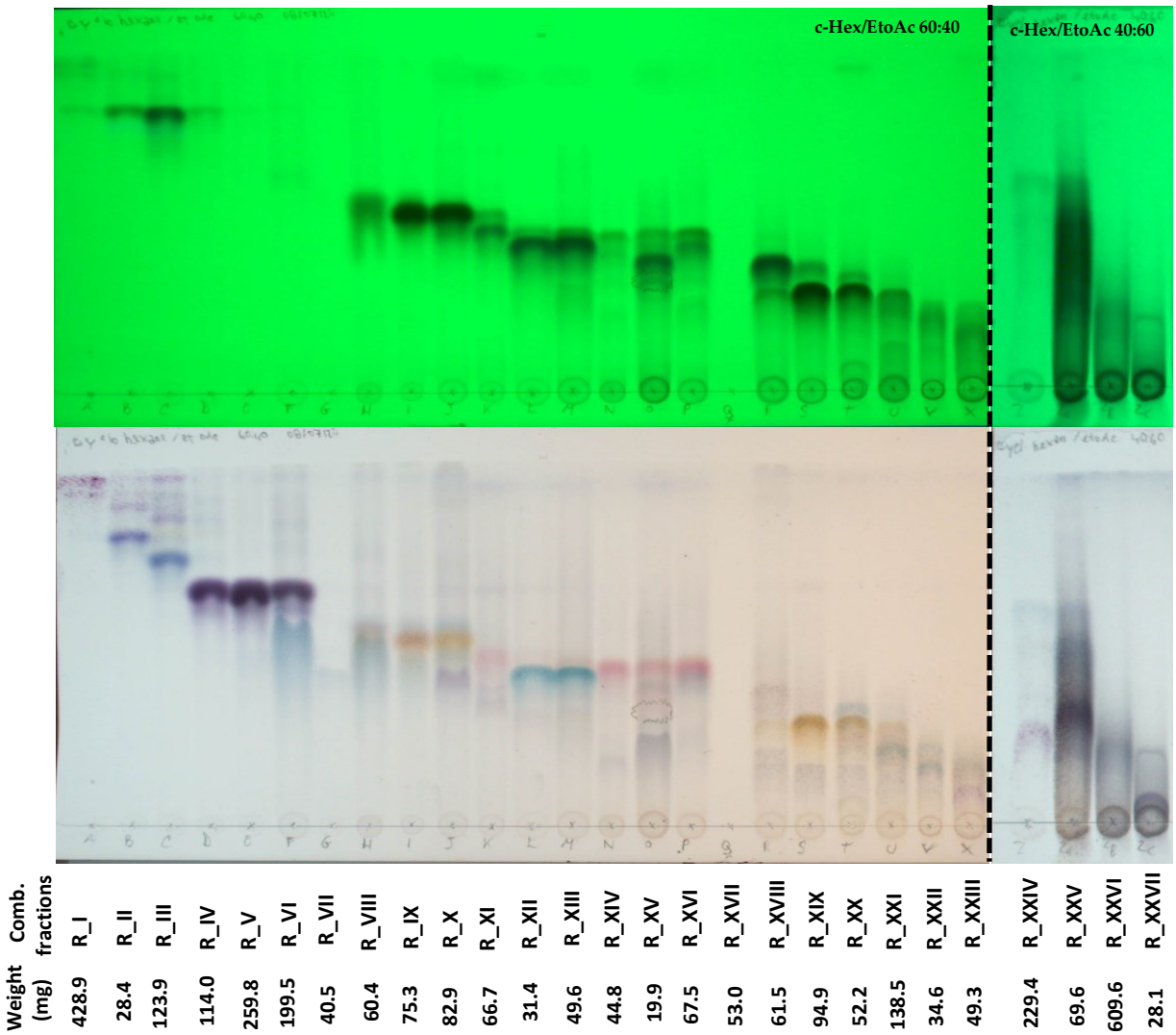


Figure S6: TLC chromatogram and weights of combined fractions obtained from the EtOAc pseudobulb extract through silica gel CC. Bottom: under UV lamp at 254 nm; Top: at Vis after spraying the plate with vanillin-sulfuric acid reagent and heating.



Comb. fractions	R_I	R_II	R_III	R_IV	R_V	R_VI	R_VII	R_VIII	R_IX	R_X	R_XI	R_XII	R_XIII	R_XIV	R_XV	R_XVI	R_XVII	R_XVIII	R_XIX	R_XX	R_XXI	R_XXII	R_XXIII	R_XXIV	R_XXV	R_XXVI	R_XXVII
Weight (mg)	428.9	28.4	123.9	114.0	259.8	199.5	40.5	60.4	75.3	82.9	66.7	31.4	49.6	44.8	19.9	67.5	53.0	61.5	94.9	52.2	138.5	34.6	49.3	229.4	69.6	609.6	28.1

Figure S7: TLC chromatogram and weights of combined fractions obtained from the EtOAc root extract through silica gel CC. Top: under UV lamp at 254 nm; Bottom: at Vis after spraying the plate with vanillin-sulfuric acid reagent and heating.

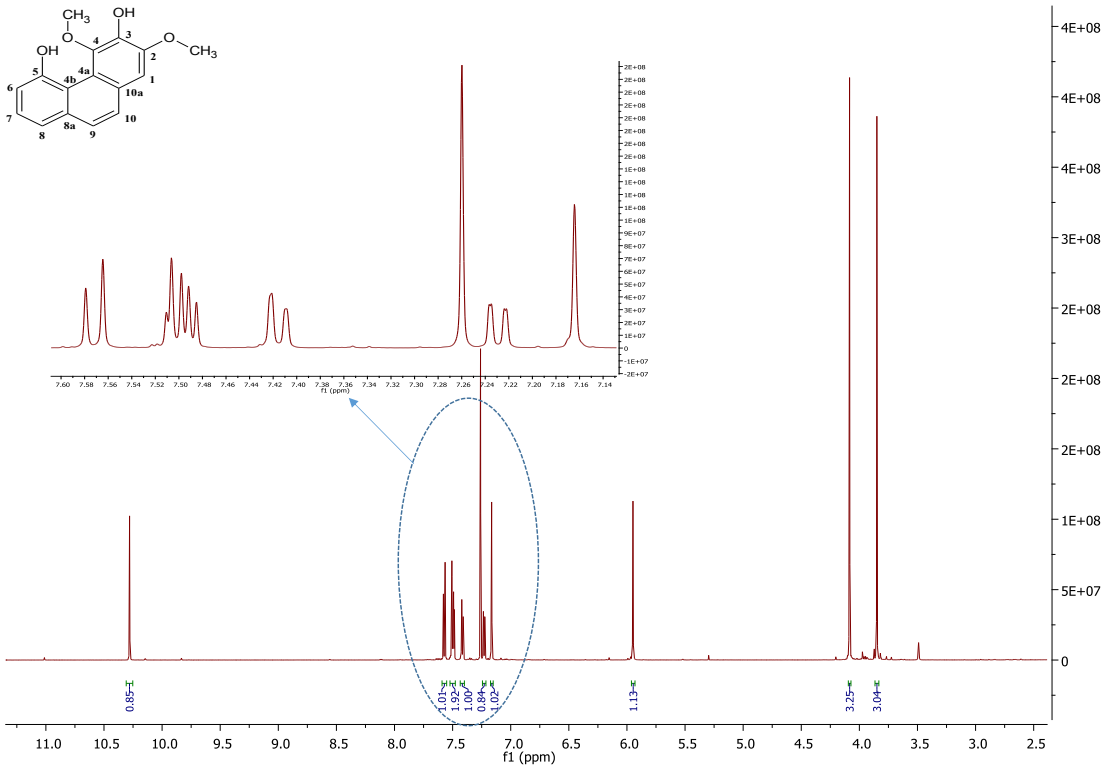


Figure S8a: ^{1}H-NMR spectrum of **compound 1** recorded in $CDCl_3$ at 600 MHz.

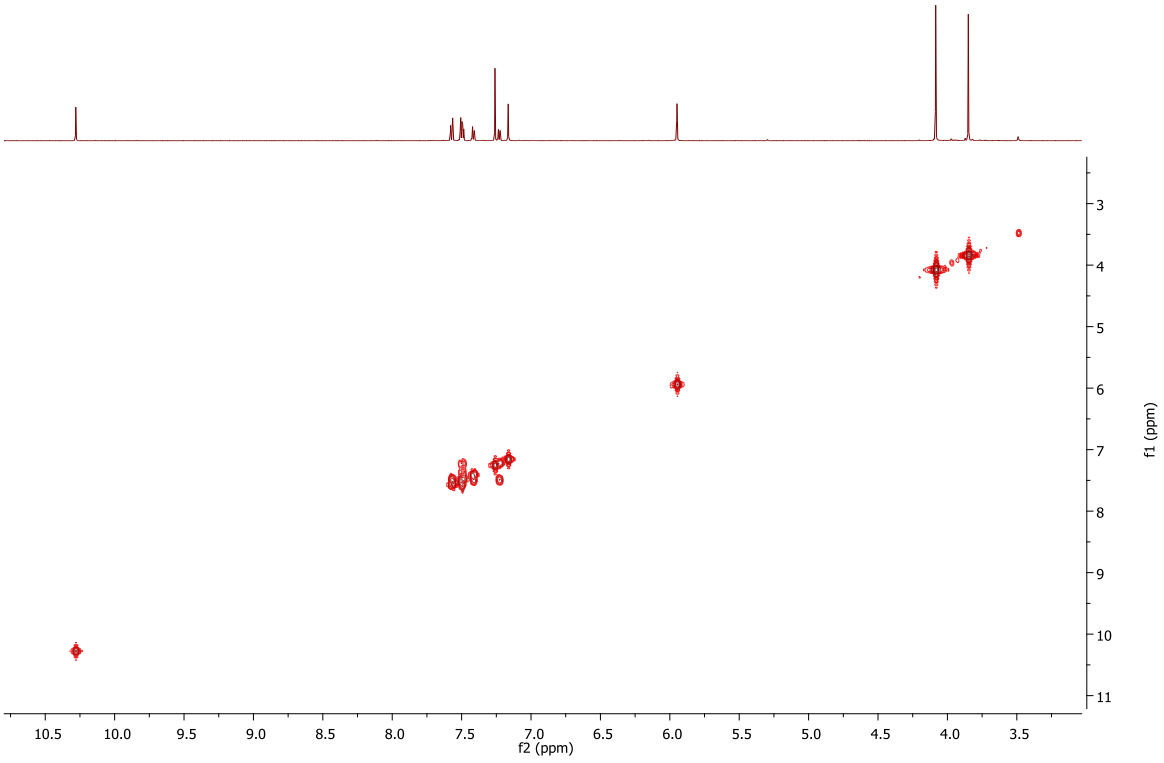


Figure S8b: COSY spectrum of **compound 1** recorded in $CDCl_3$ at 600 MHz.

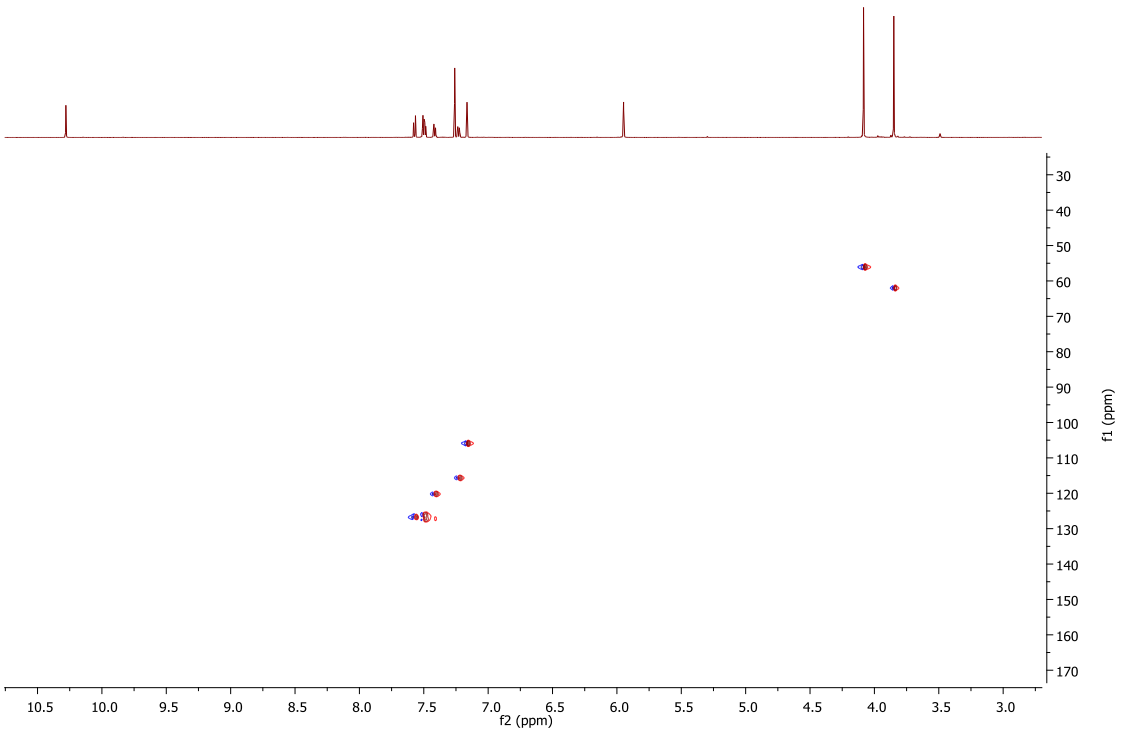


Figure S8c: HSQC-DEPT spectrum of **compound 1** recorded in $CDCl_3$ at 600 MHz.

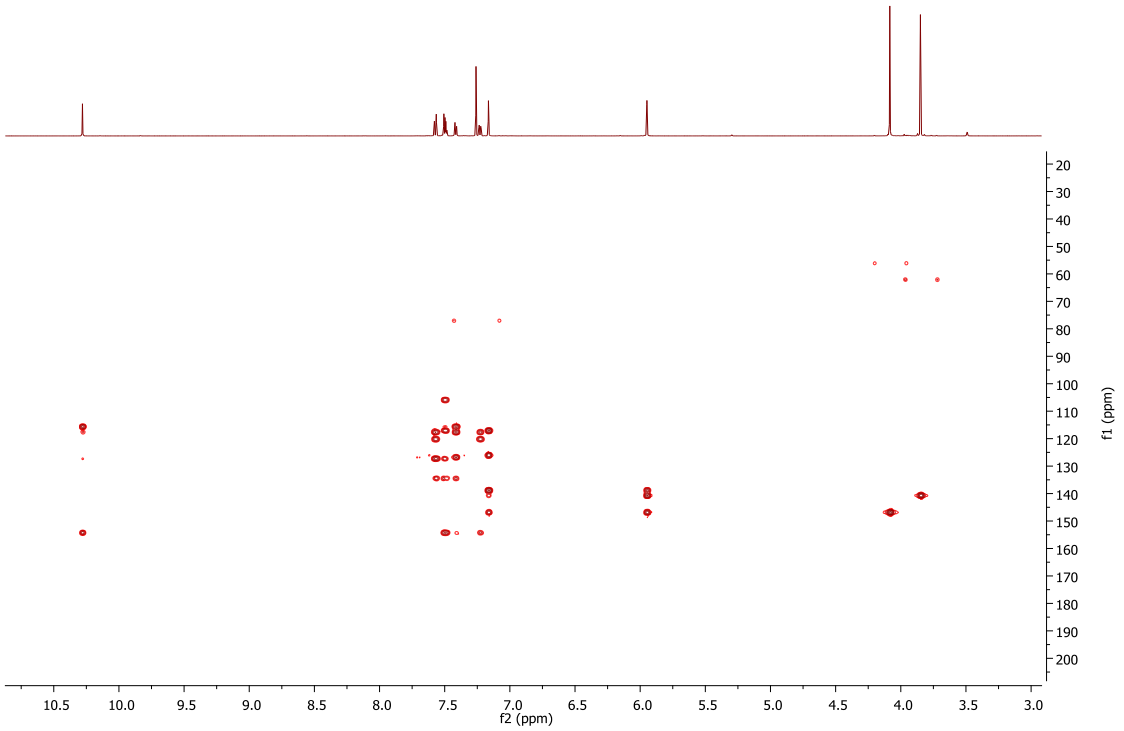


Figure S8d: HMBC spectrum of **compound 1** recorded in $CDCl_3$ at 600 MHz.

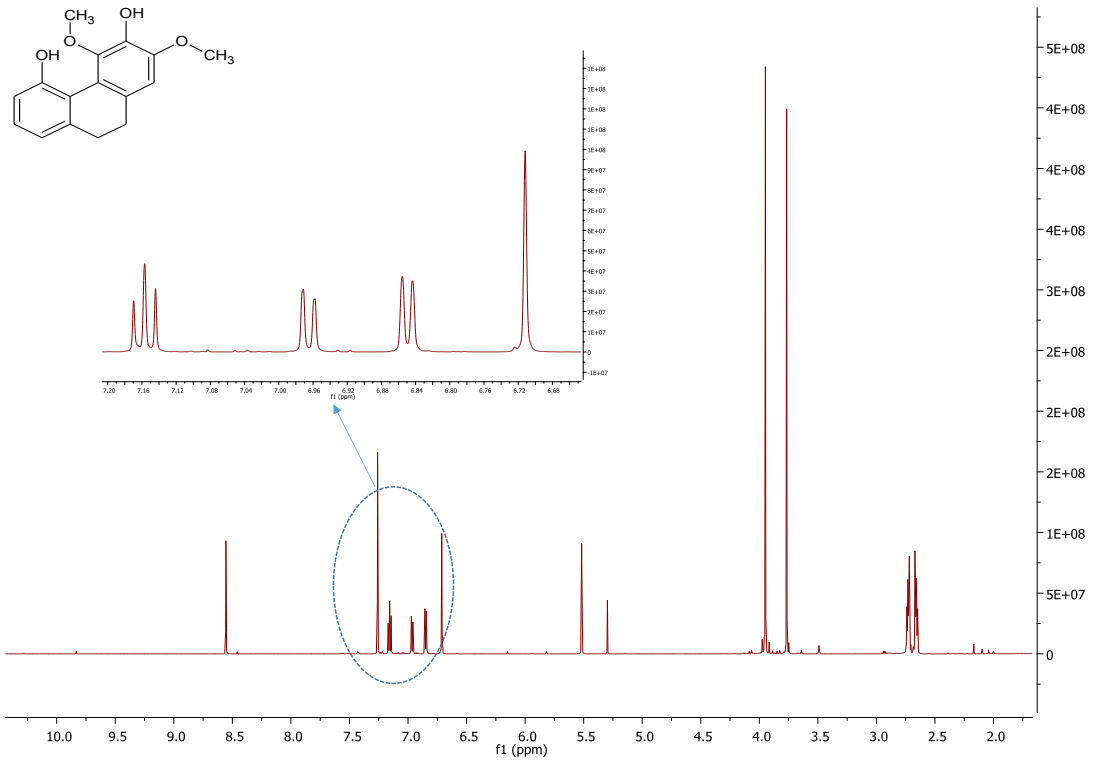


Figure S9a: ^{1}H-NMR spectrum of **compound 4** recorded in $CDCl_3$ at 600 MHz.

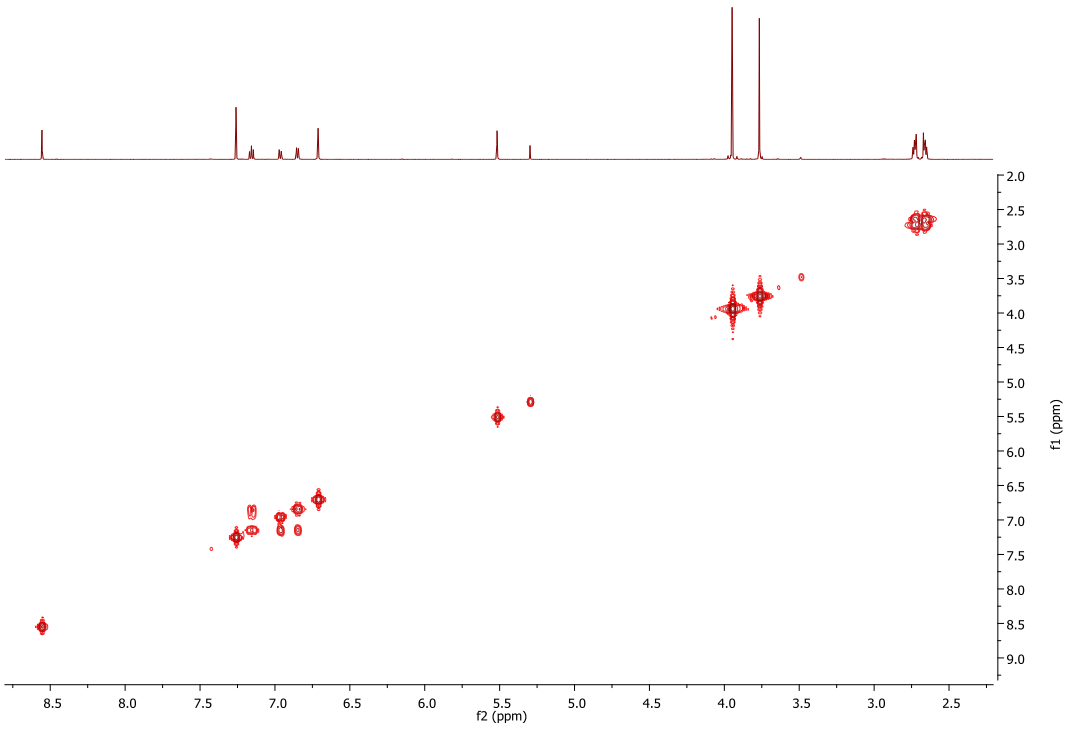


Figure S9b: COSY spectrum of **compound 4** recorded in $CDCl_3$ at 600 MHz.

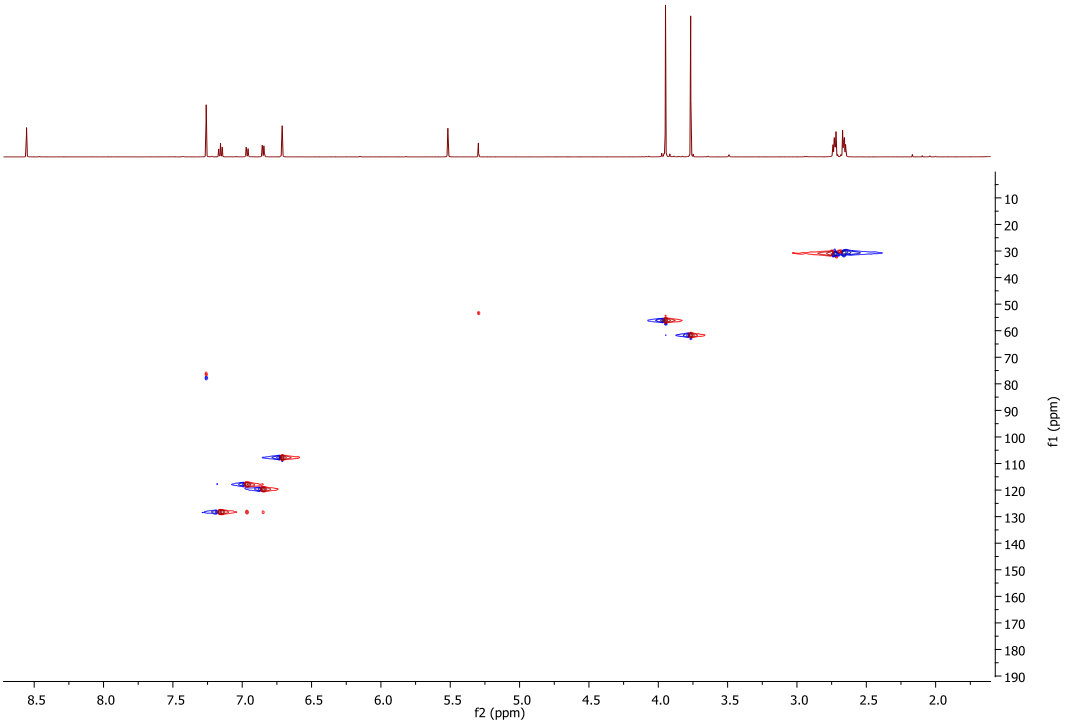


Figure S9c: HSQC-DEPT spectrum of **compound 4** recorded in $CDCl_3$ at 600 MHz.

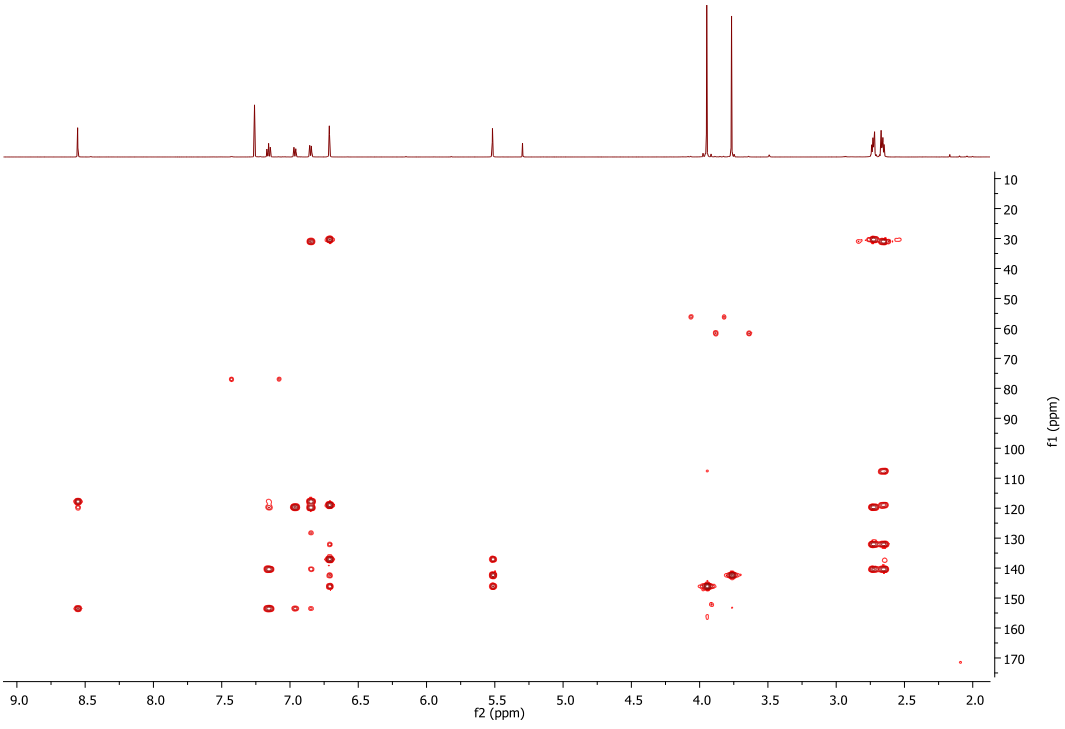


Figure S9d: HMBC spectrum of **compound 4** recorded in $CDCl_3$ at 600 MHz.

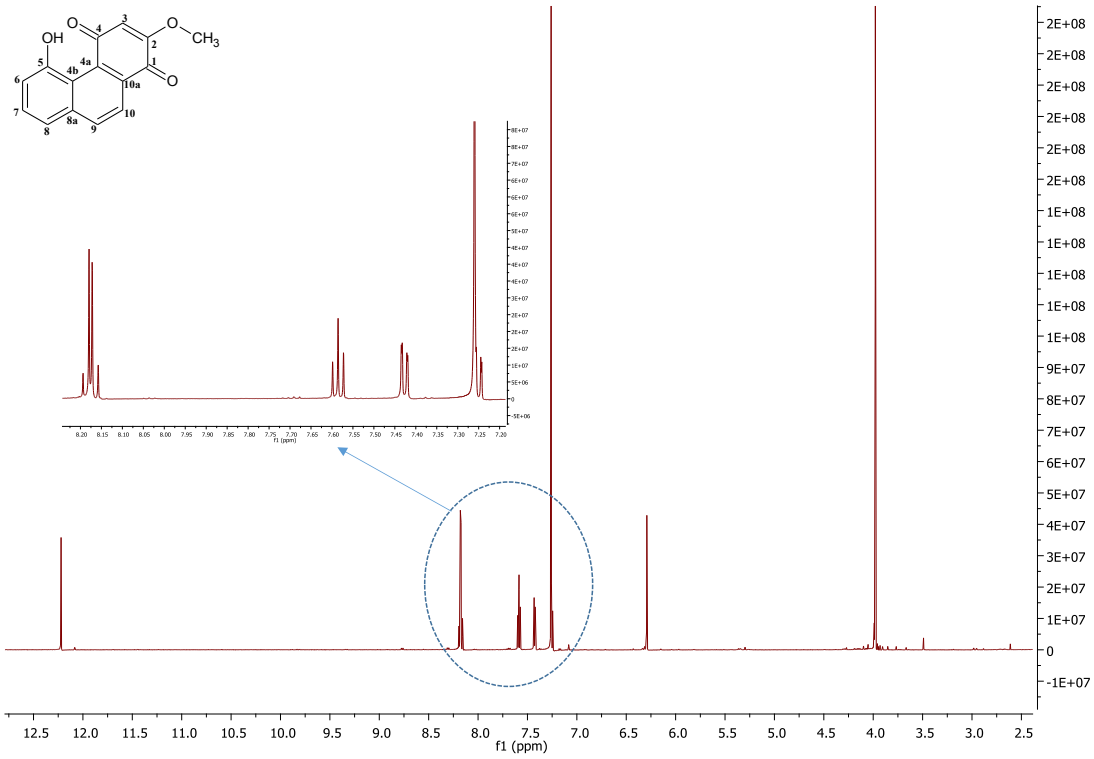


Figure S10a: ^{1}H-NMR spectrum of **compound 5** recorded in $CDCl_3$ at 600 MHz.

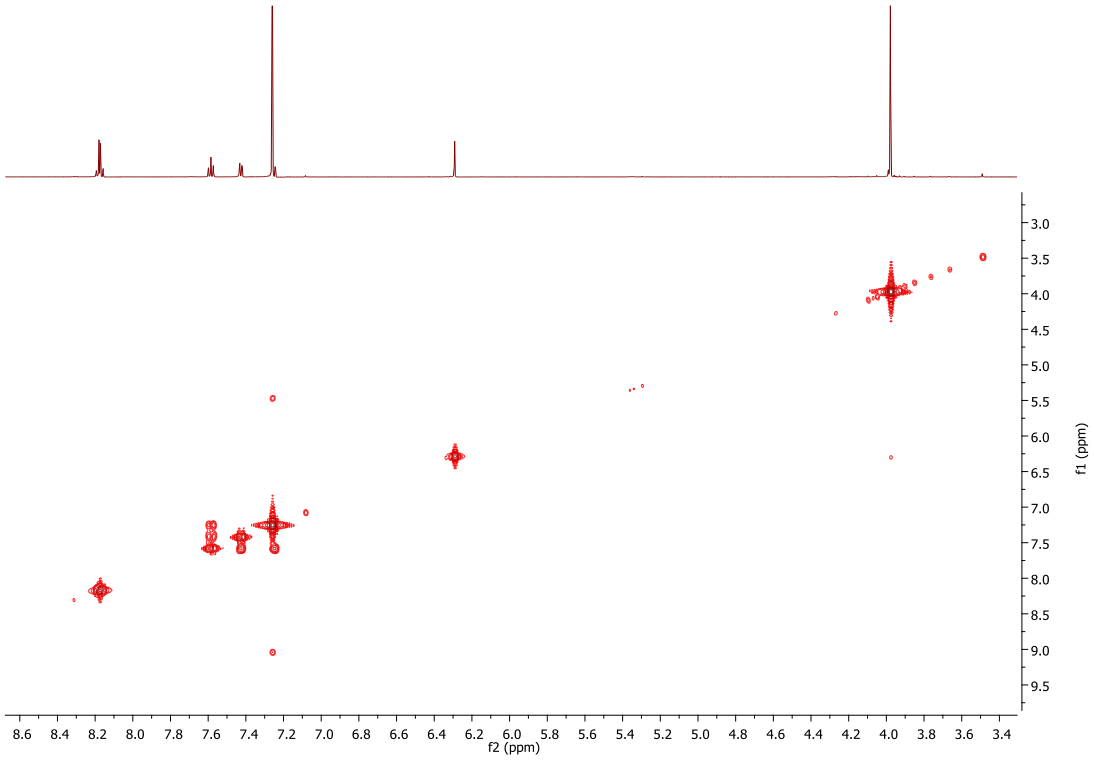


Figure S10b: COSY spectrum of **compound 5** recorded in $CDCl_3$ at 600 MHz.

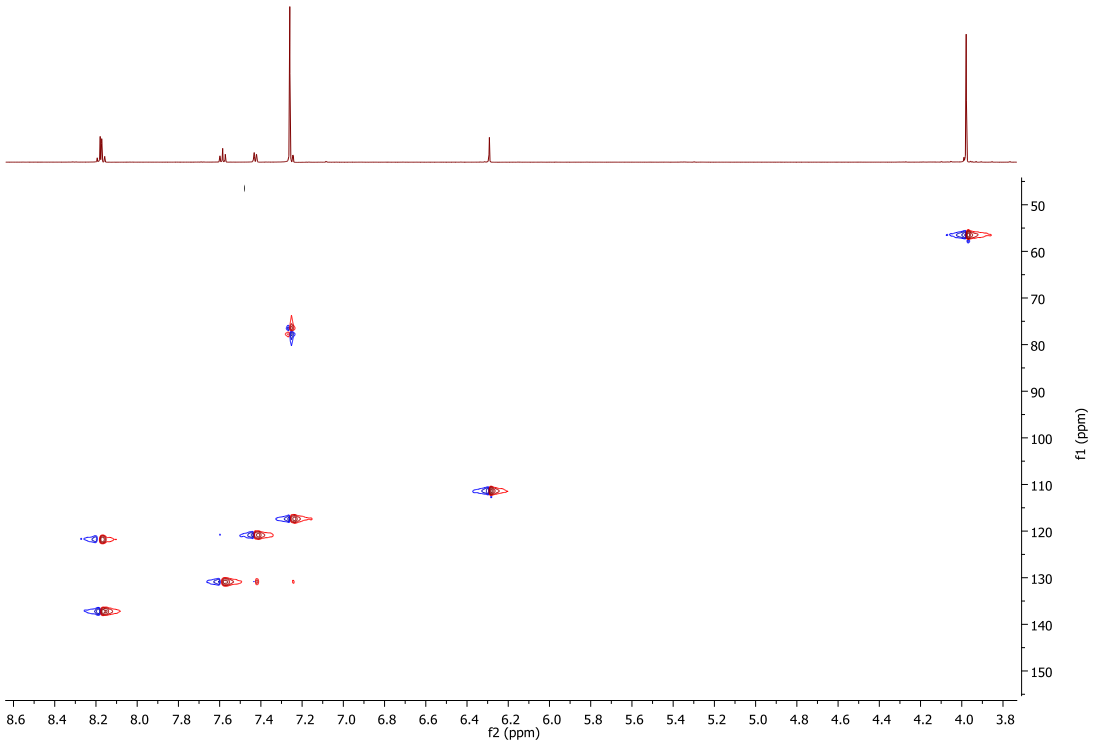


Figure S10c: HSQC-DEPT spectrum of **compound 5** recorded in $CDCl_3$ at 600 MHz.

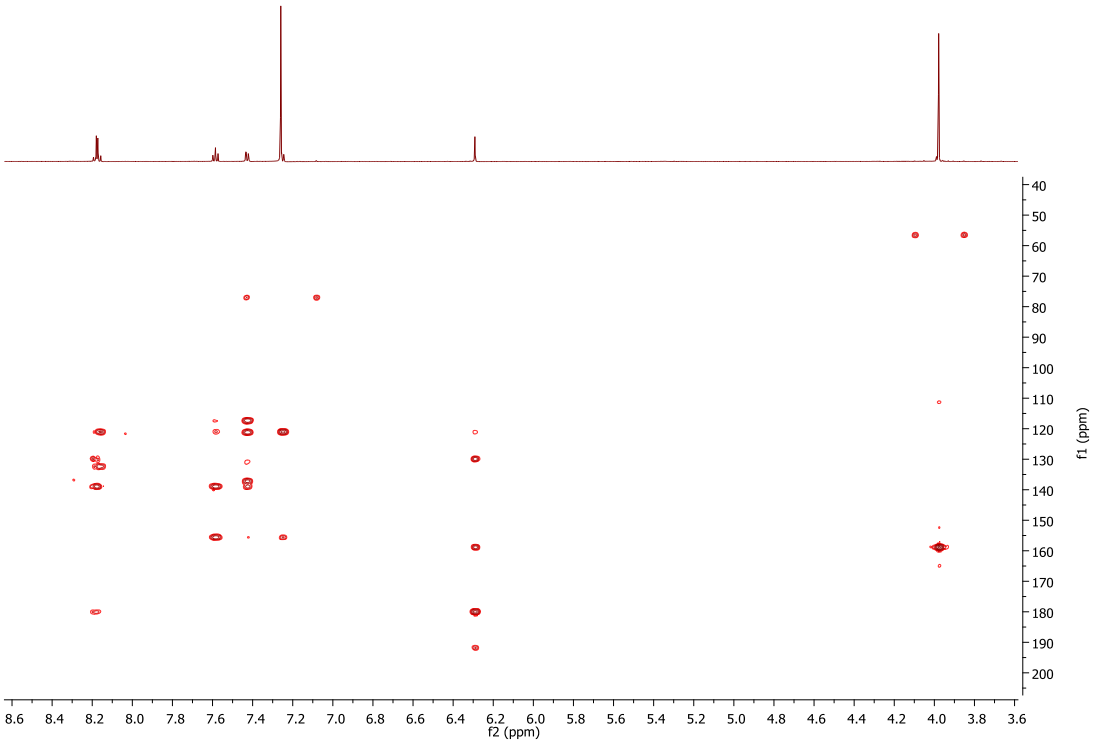


Figure S10d: HMBC spectrum of **compound 5** recorded in $CDCl_3$ at 600 MHz.

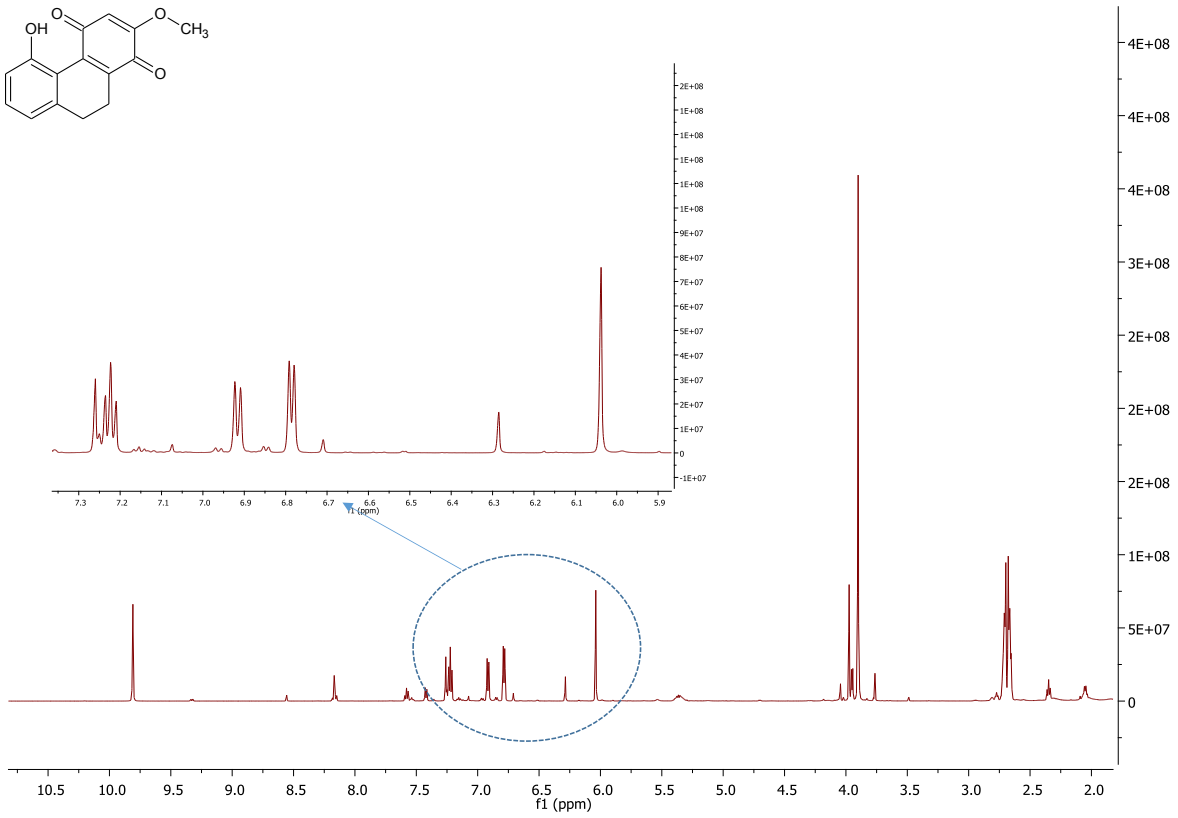


Figure S11: ^{1}H-NMR spectrum of **compound 6** recorded in $CDCl_3$ at 600 MHz.

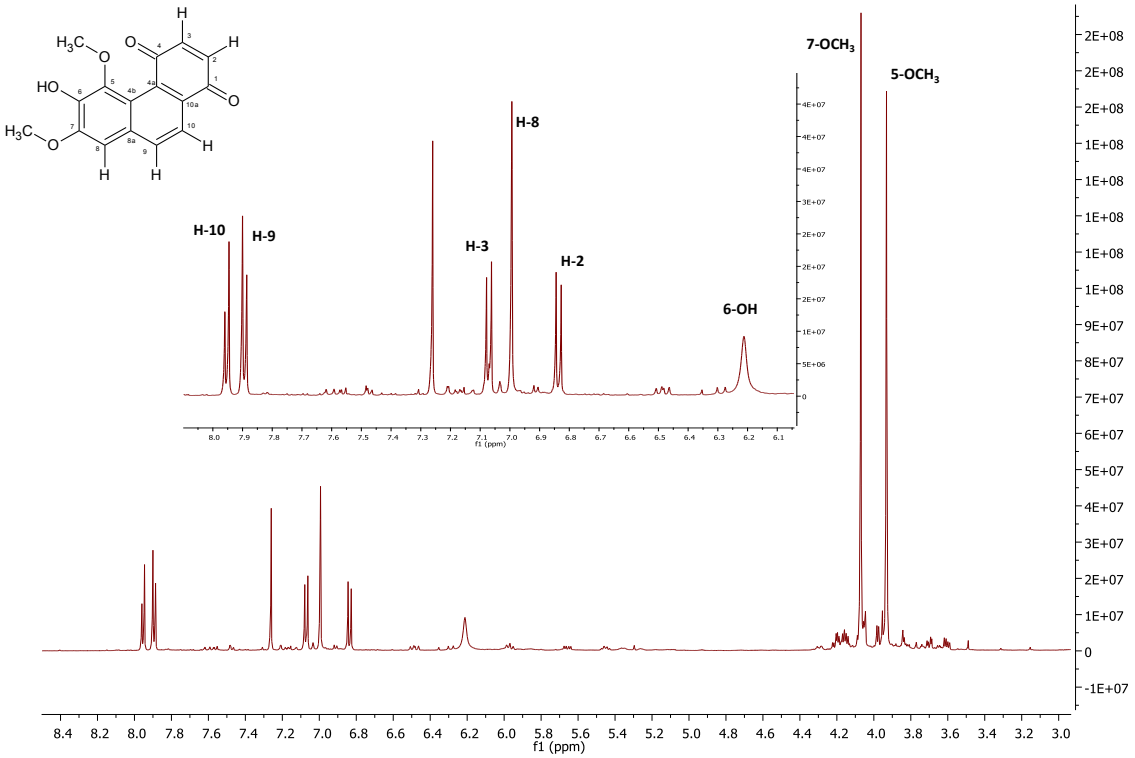


Figure S12a: ^{1}H-NMR spectrum of **compound 7** recorded in $CDCl_3$ at 600 MHz.

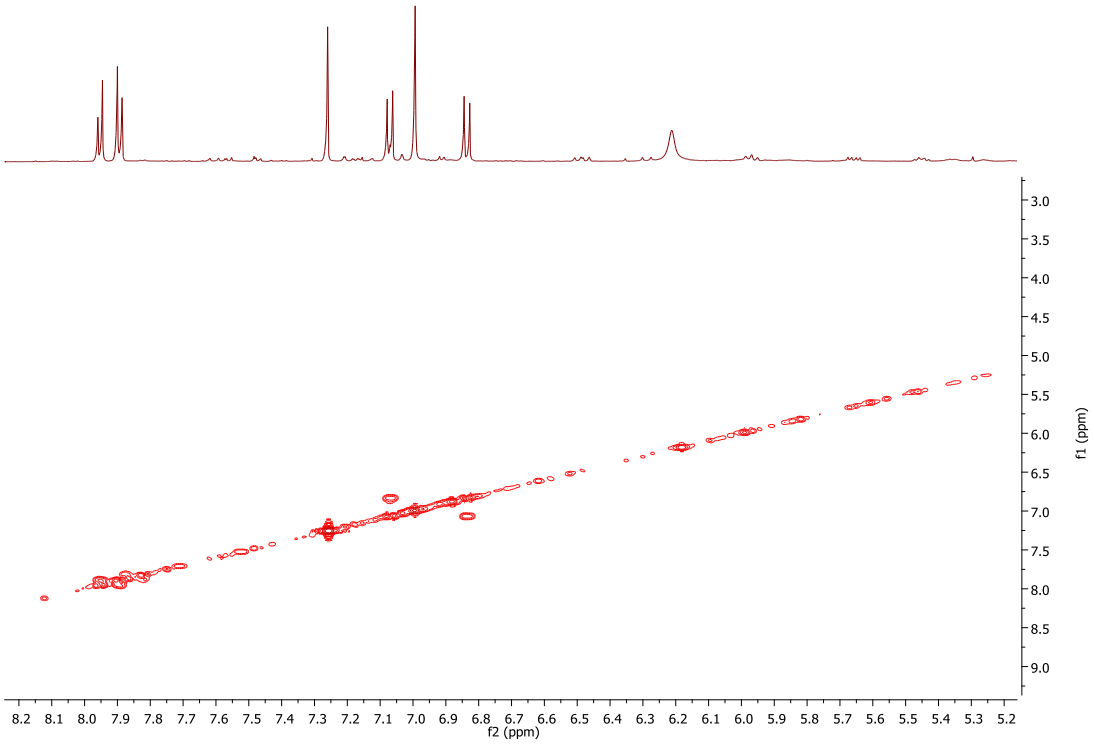


Figure S12b: COSY spectrum of **compound 7** recorded in $CDCl_3$ at 600 MHz.

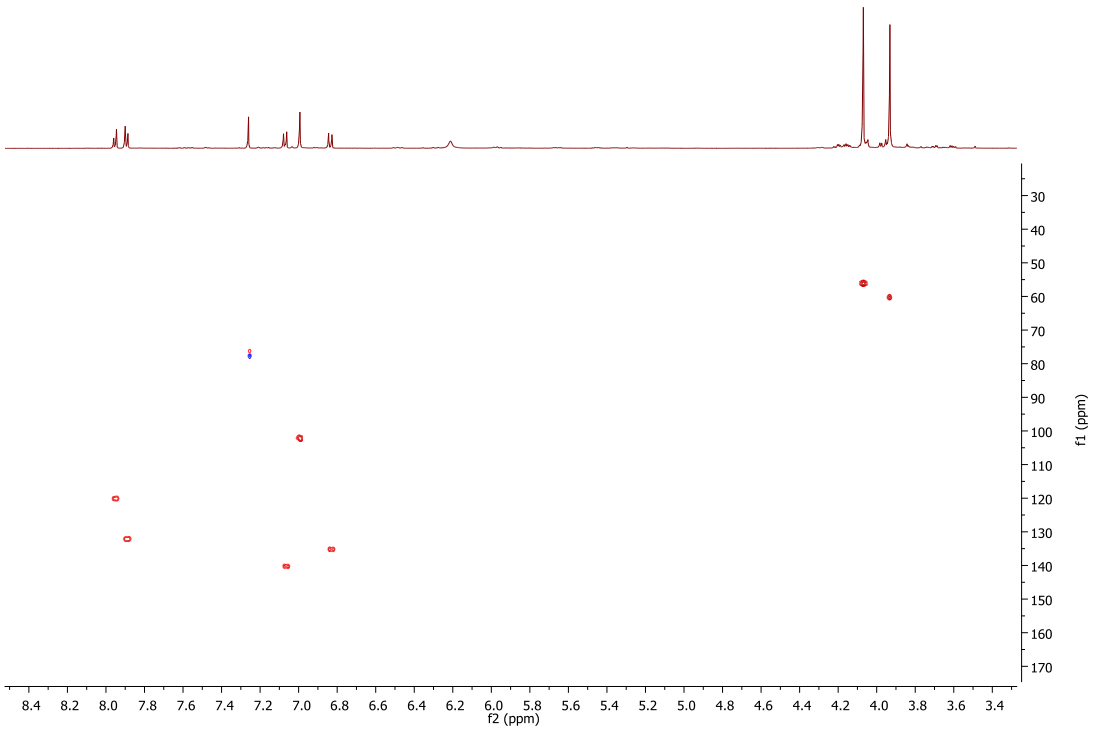


Figure S12c: HSQC-DEPT spectrum of **compound 7** recorded in $CDCl_3$ at 600 MHz.

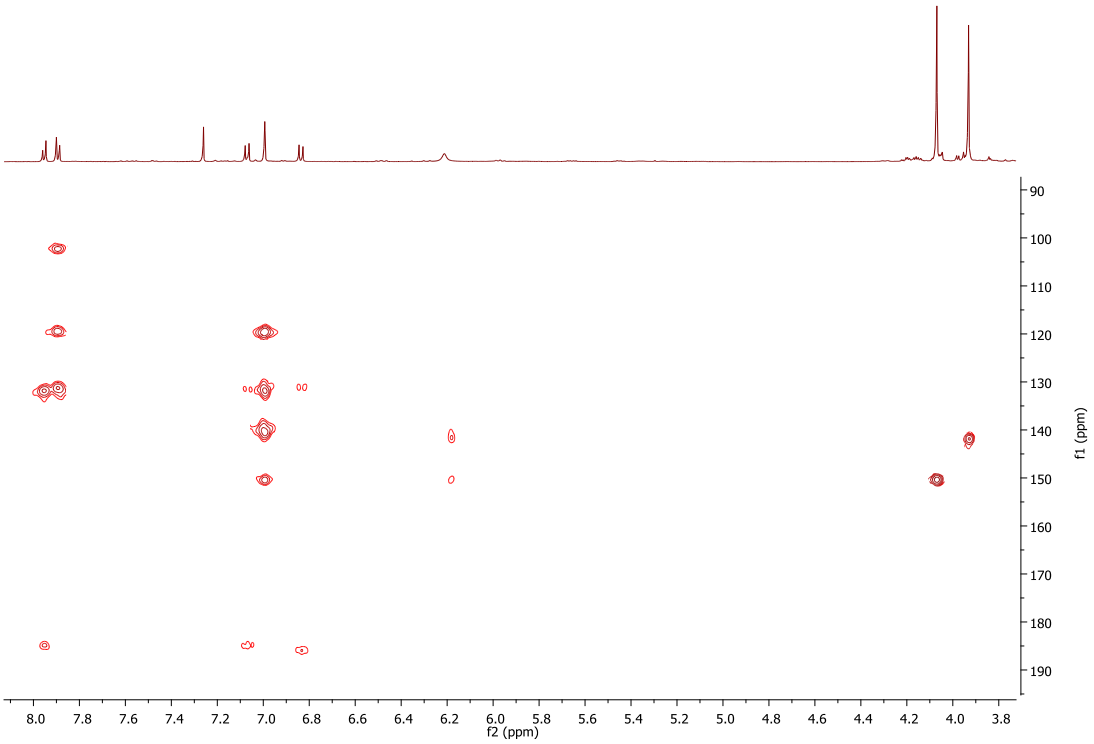


Figure S12d: HMBC spectrum of **compound 7** recorded in $CDCl_3$ at 600 MHz.

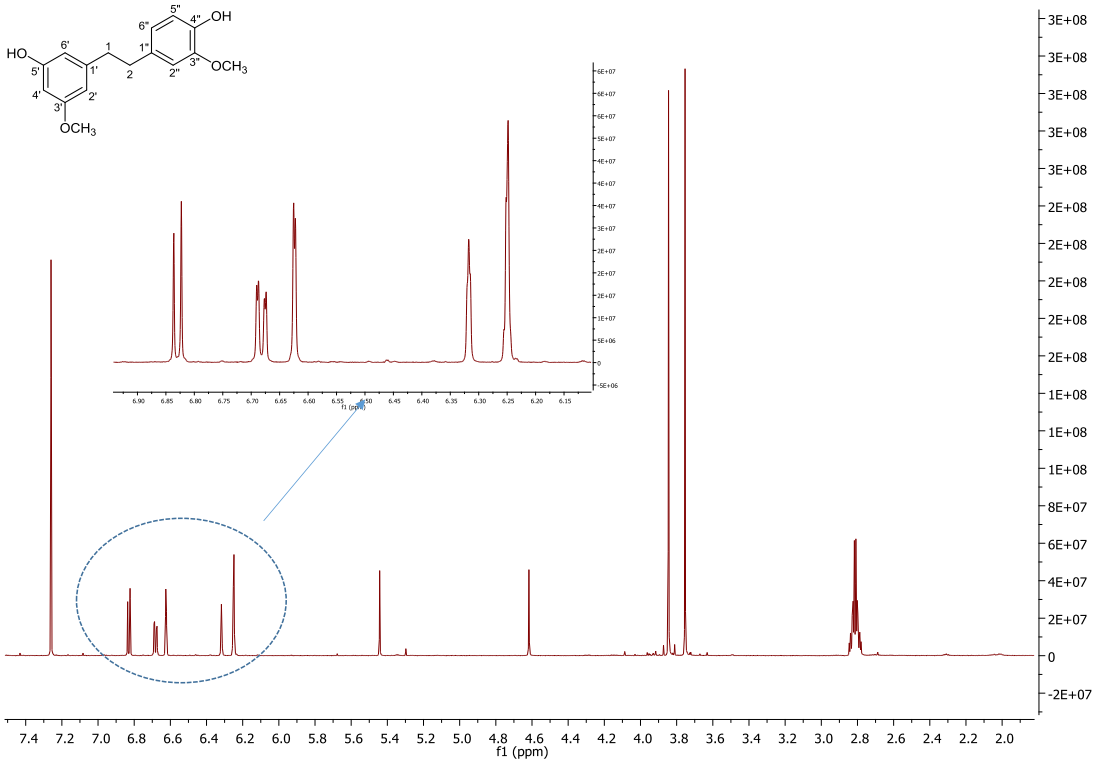


Figure S13a: ^{1}H-NMR spectrum of **compound 8** recorded in $CDCl_3$ at 600 MHz.

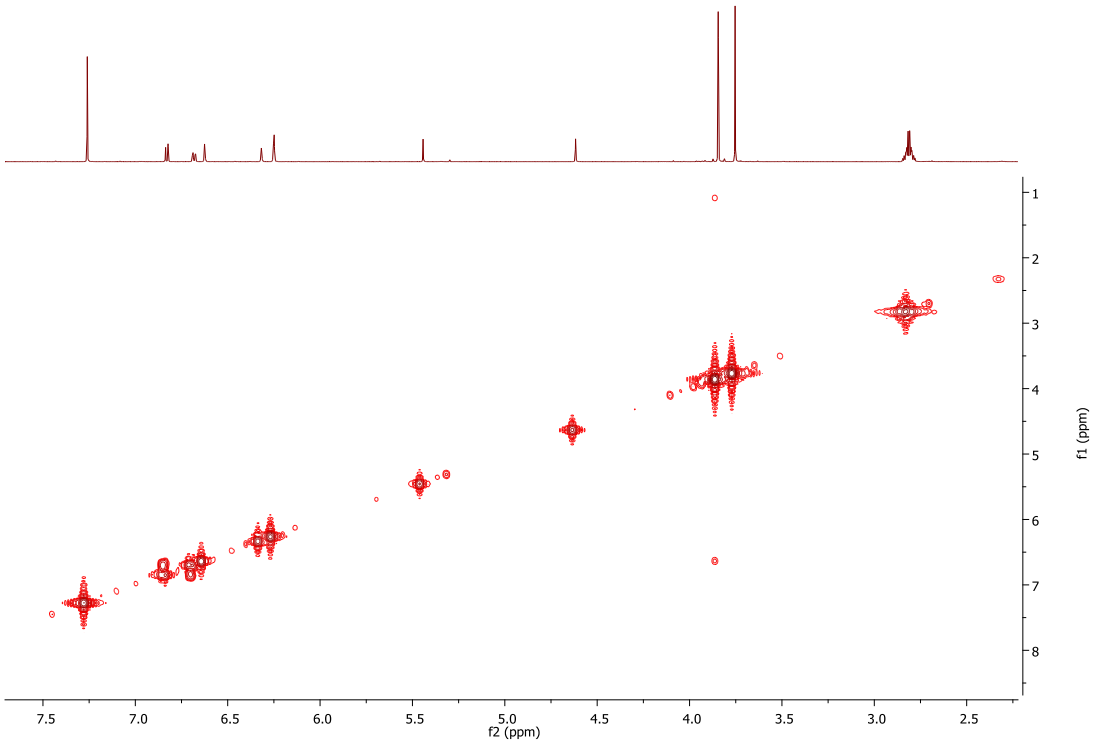


Figure S13b: COSY spectrum of **compound 8** recorded in $CDCl_3$ at 600 MHz.

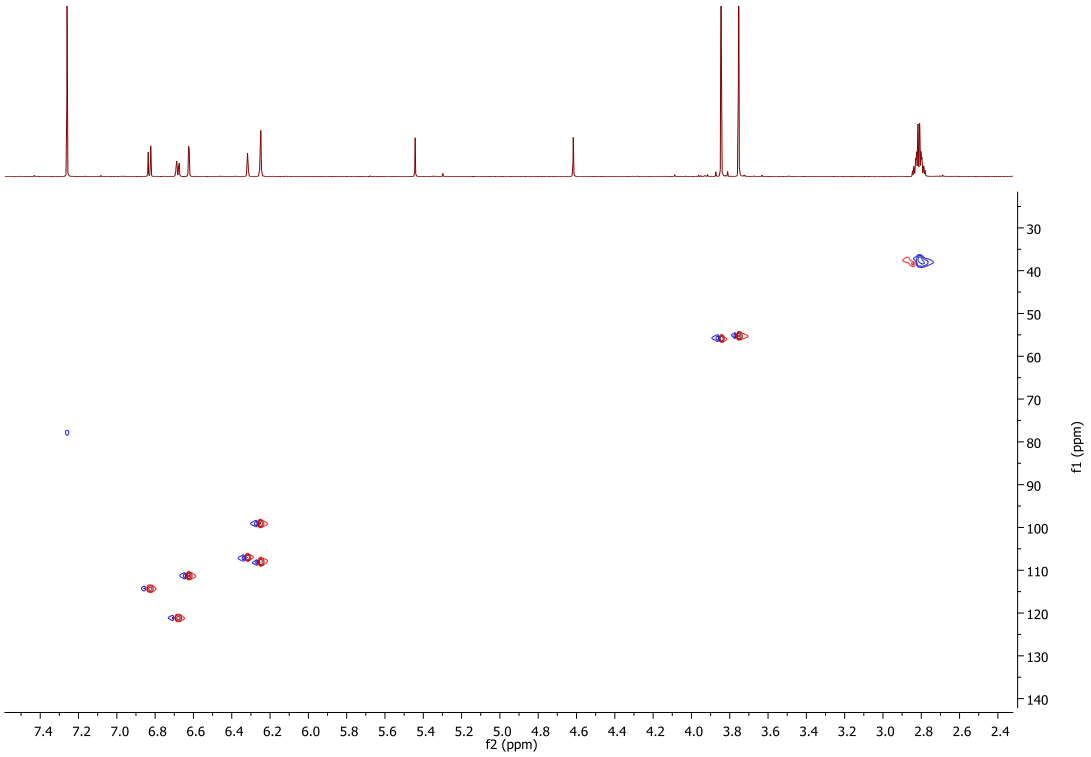


Figure S13c: HSQC-DEPT spectrum of **compound 8** recorded in $CDCl_3$ at 600 MHz.

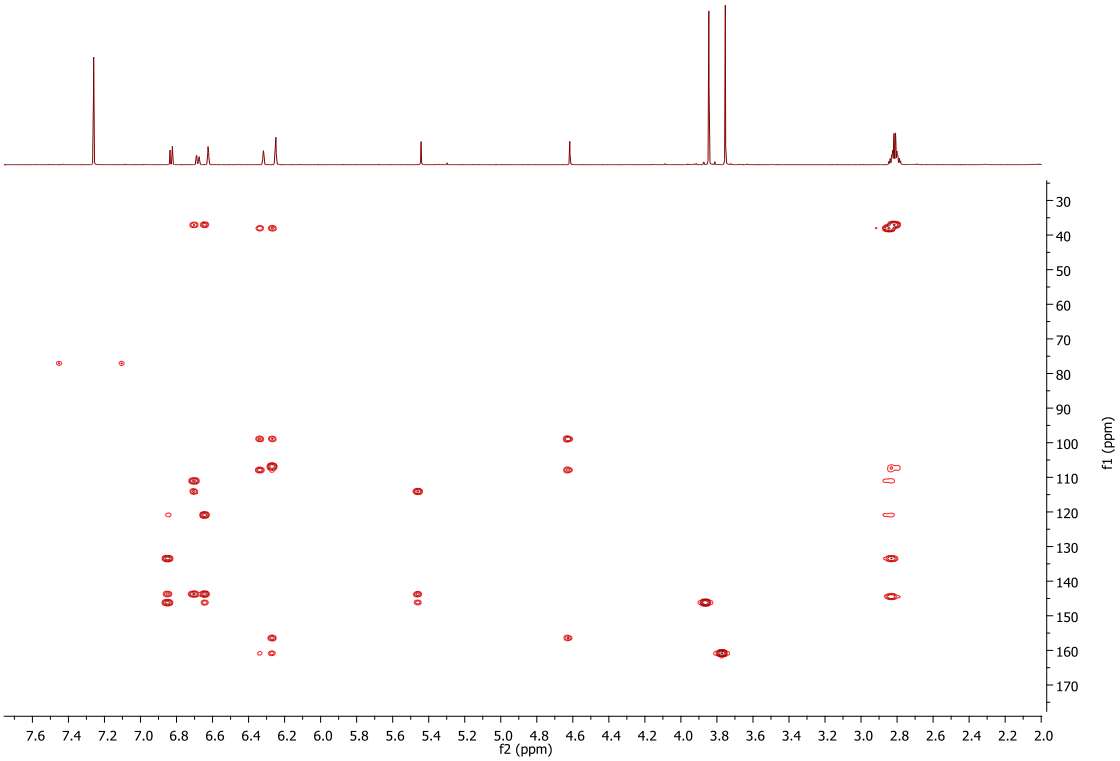


Figure S13d: HMBC spectrum of **compound 8** recorded in $CDCl_3$ at 600 MHz.

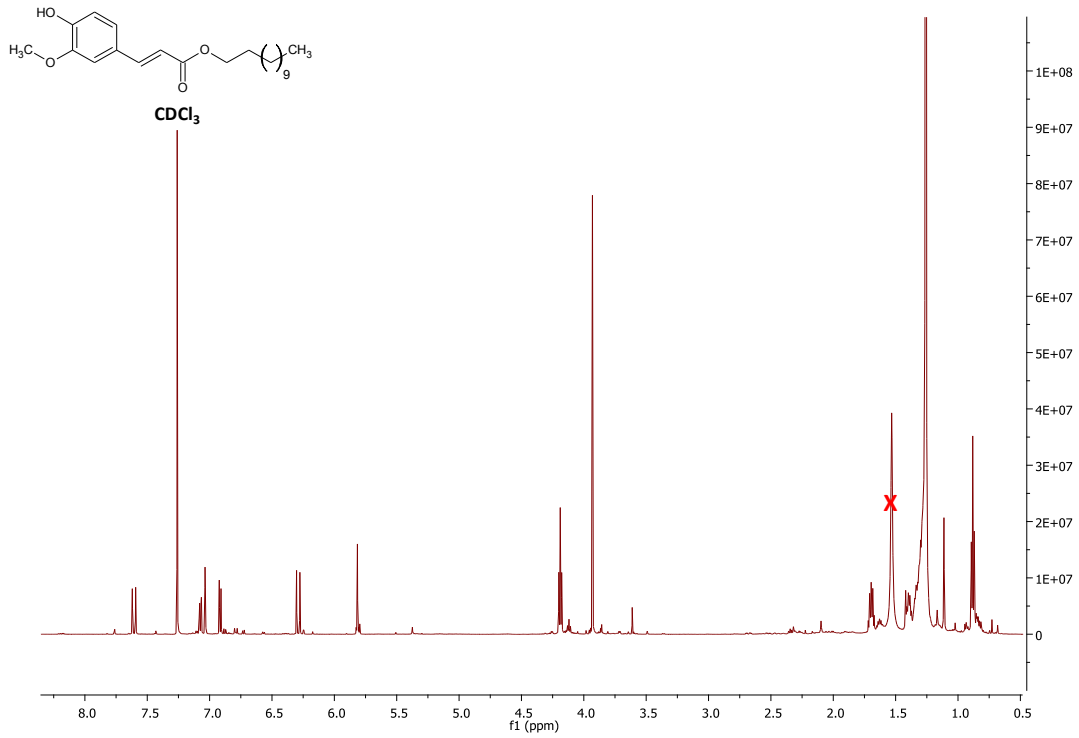


Figure S14a: ^{1}H-NMR spectrum of **compound 11** recorded in $CDCl_3$ at 600 MHz.

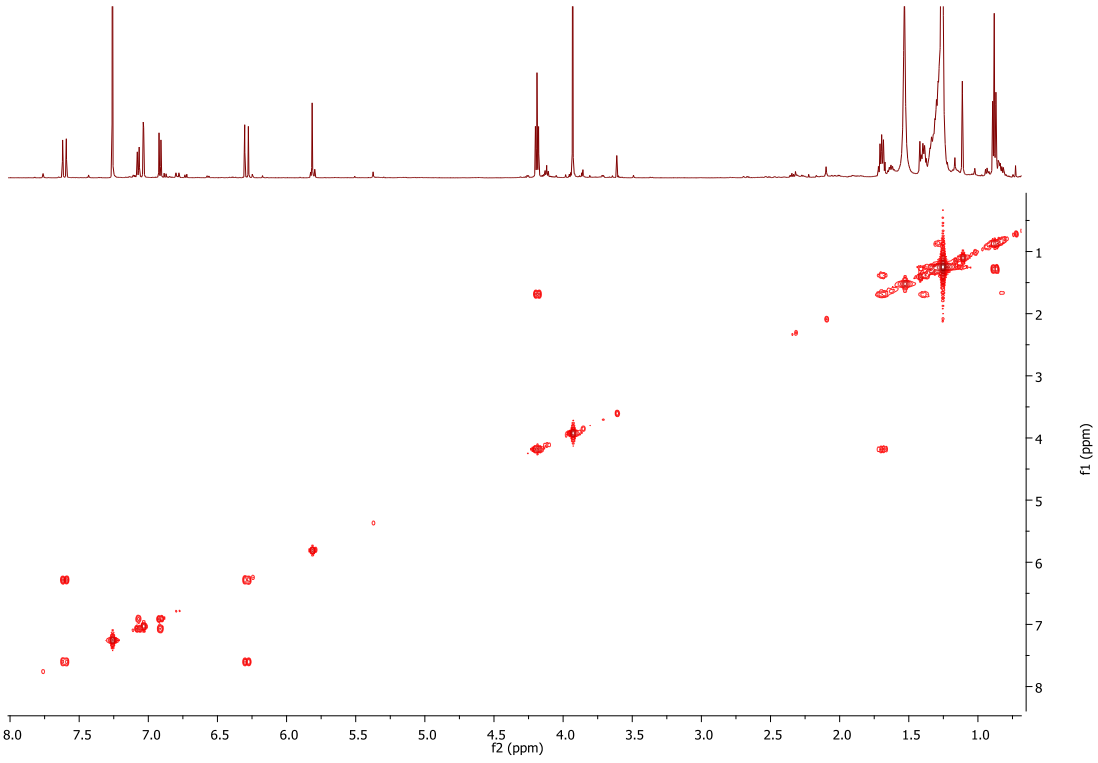


Figure S14b: COSY spectrum of **compound 11** recorded in $CDCl_3$ at 600 MHz.

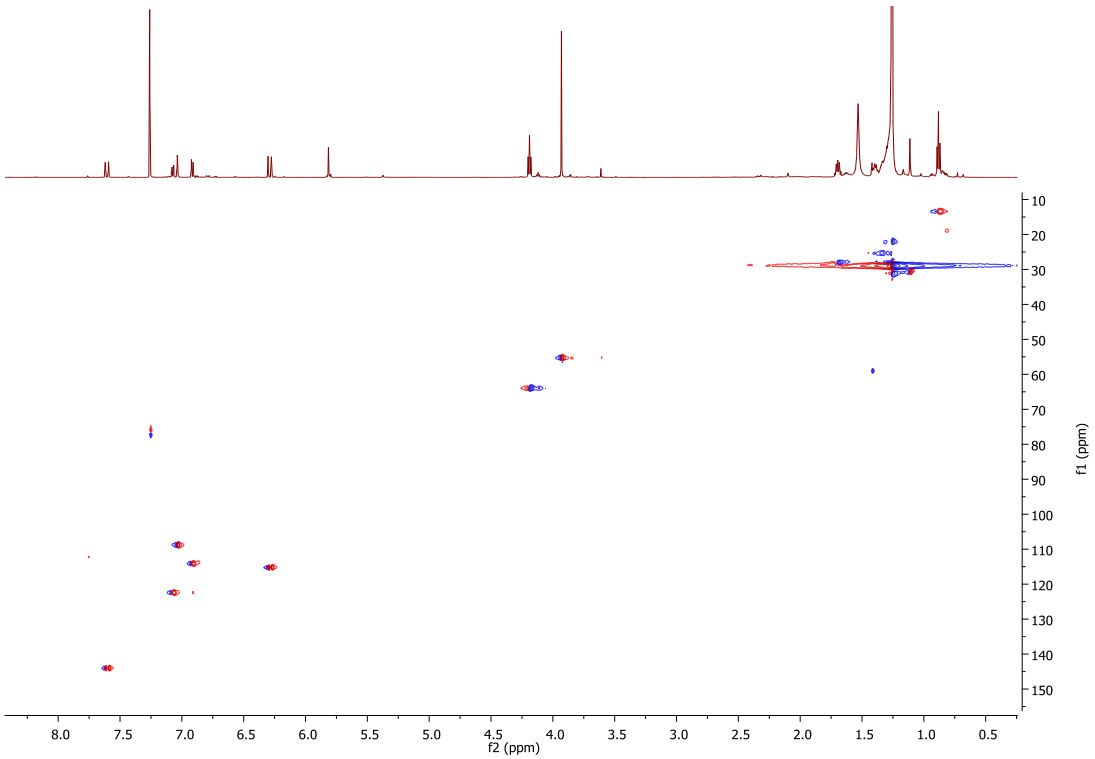


Figure S14c: HSQC-DEPT spectrum of **compound 11** recorded in $CDCl_3$ at 600 MHz.

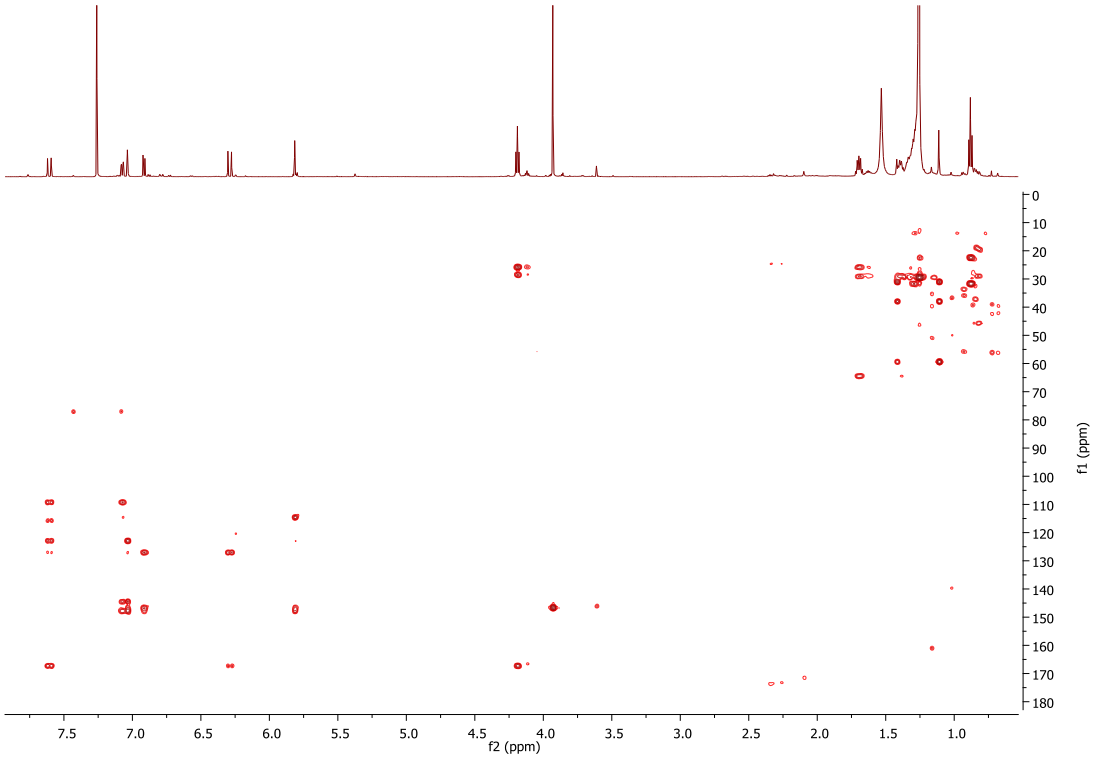


Figure S14d: HMBC spectrum of **compound 11** recorded in $CDCl_3$ at 600 MHz.

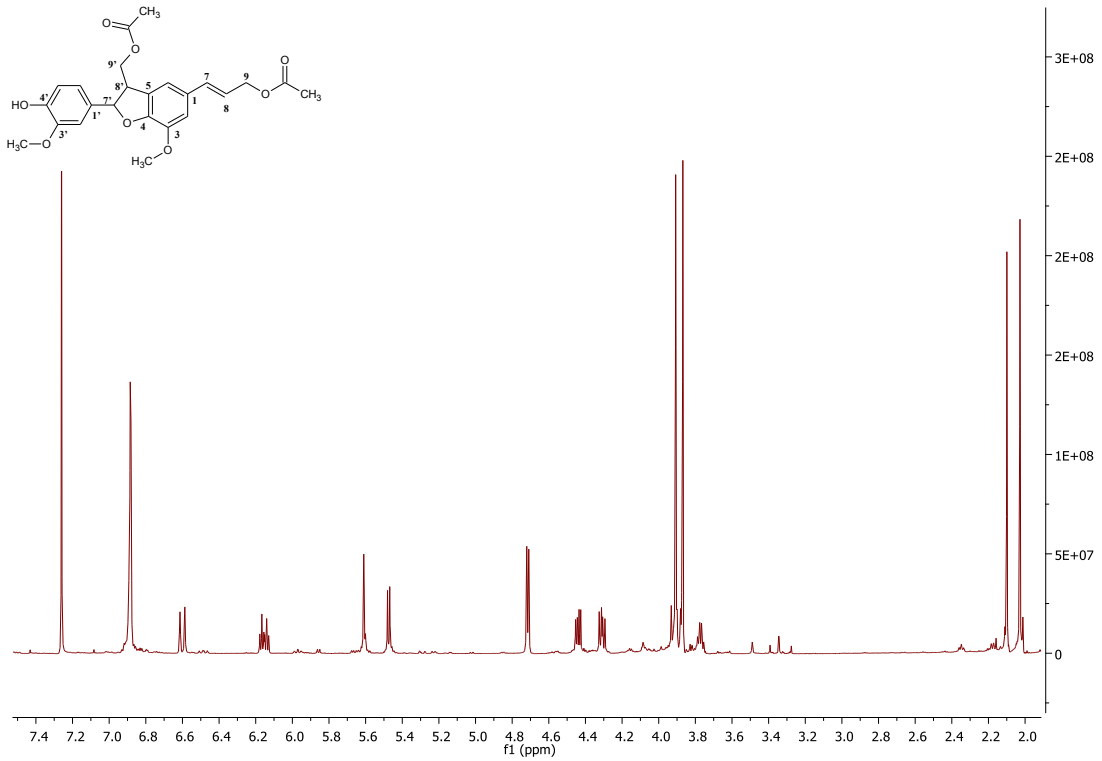


Figure S15a: ^{1}H-NMR spectrum of **compound 13** recorded in $CDCl_3$ at 600 MHz.

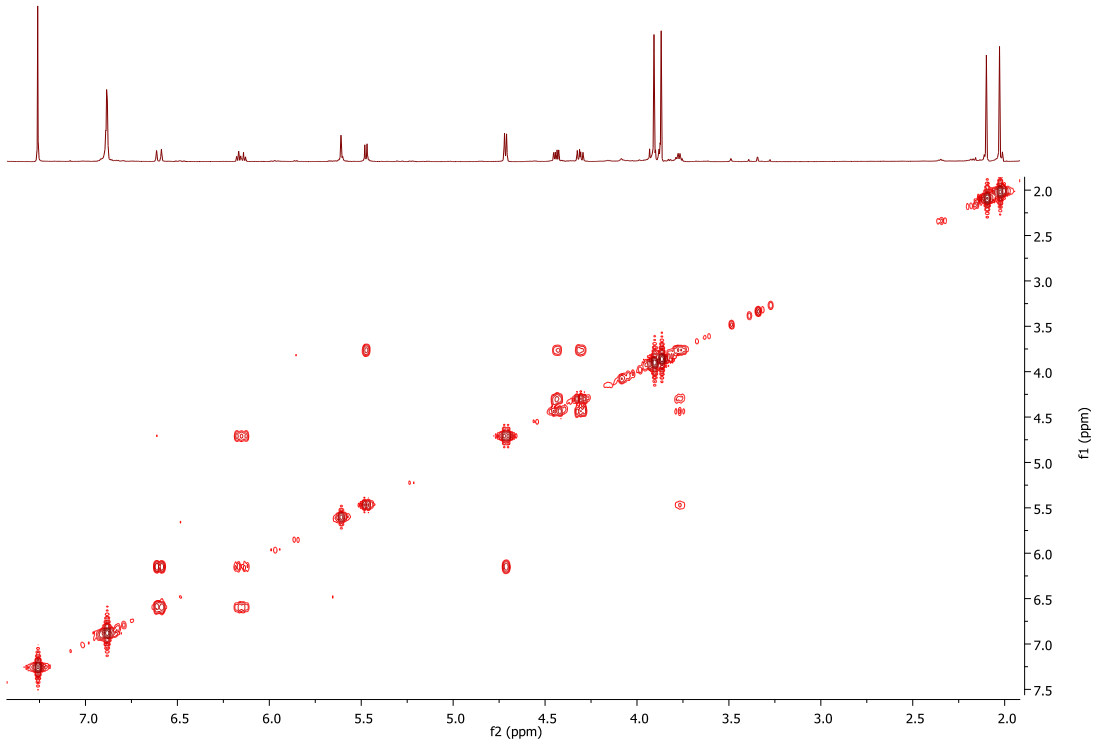


Figure S15b: COSY spectrum of **compound 13** recorded in $CDCl_3$ at 600 MHz.

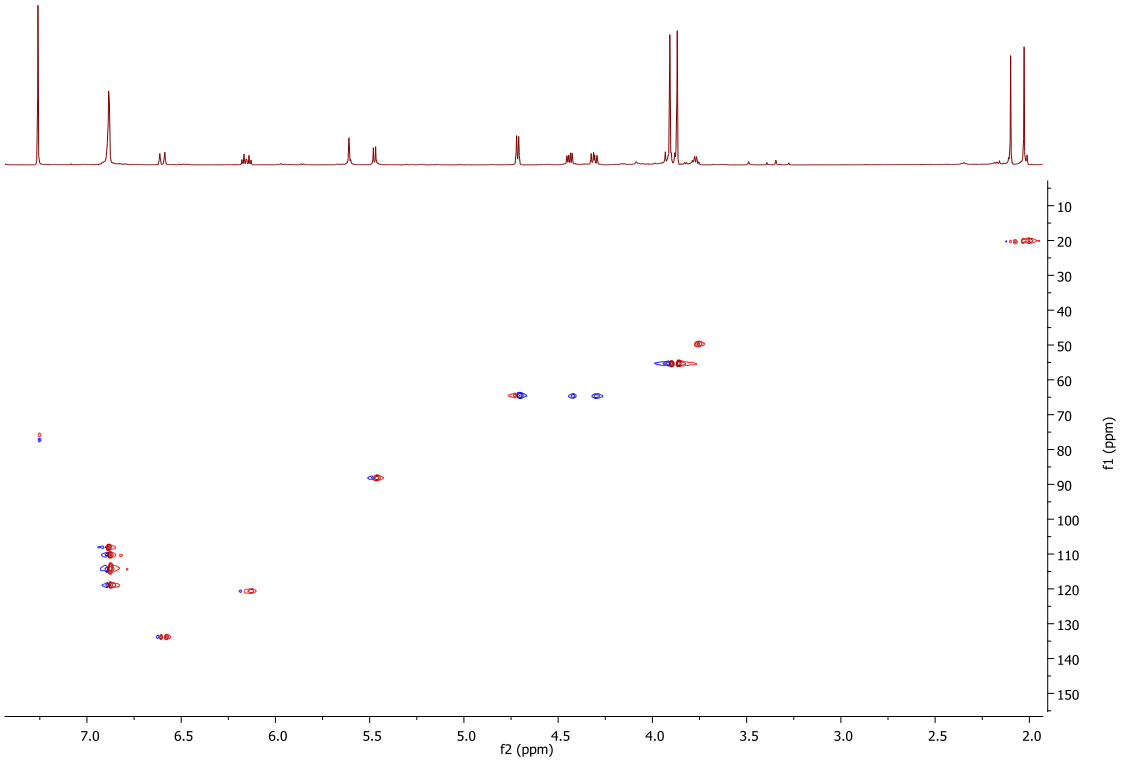


Figure S15c: HSQC-DEPT spectrum of **compound 13** recorded in $CDCl_3$ at 600 MHz.

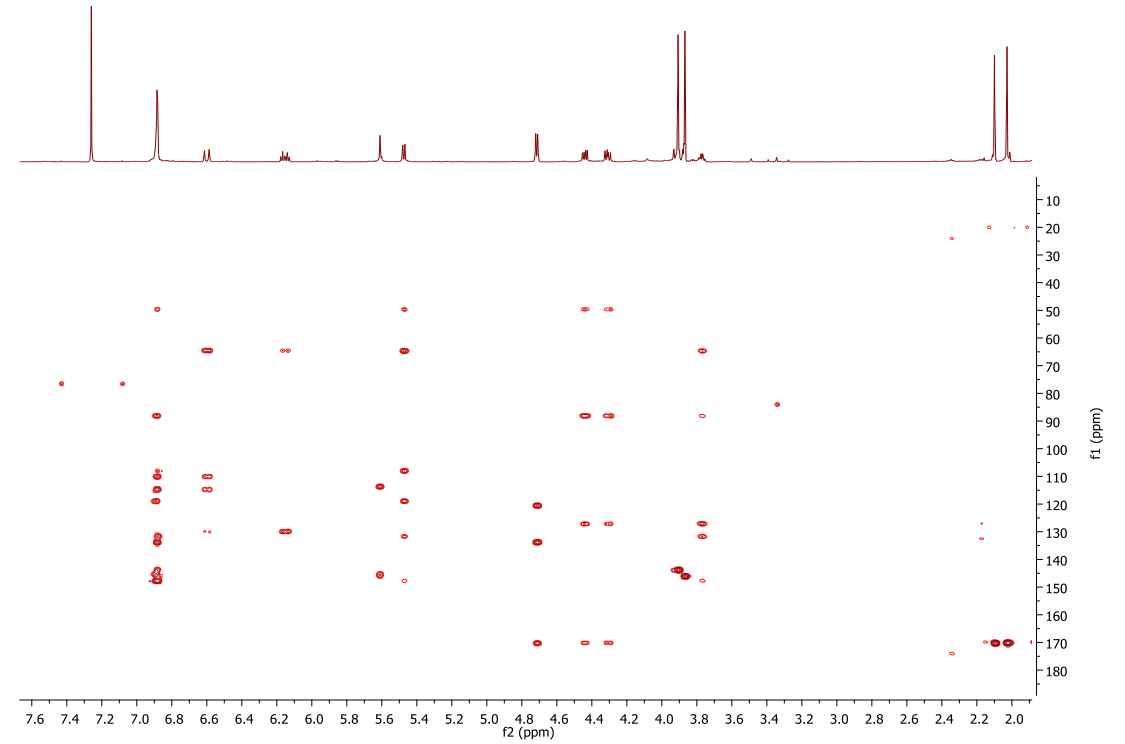


Figure S15d: HMBC spectrum of **compound 13** recorded in $CDCl_3$ at 600 MHz.

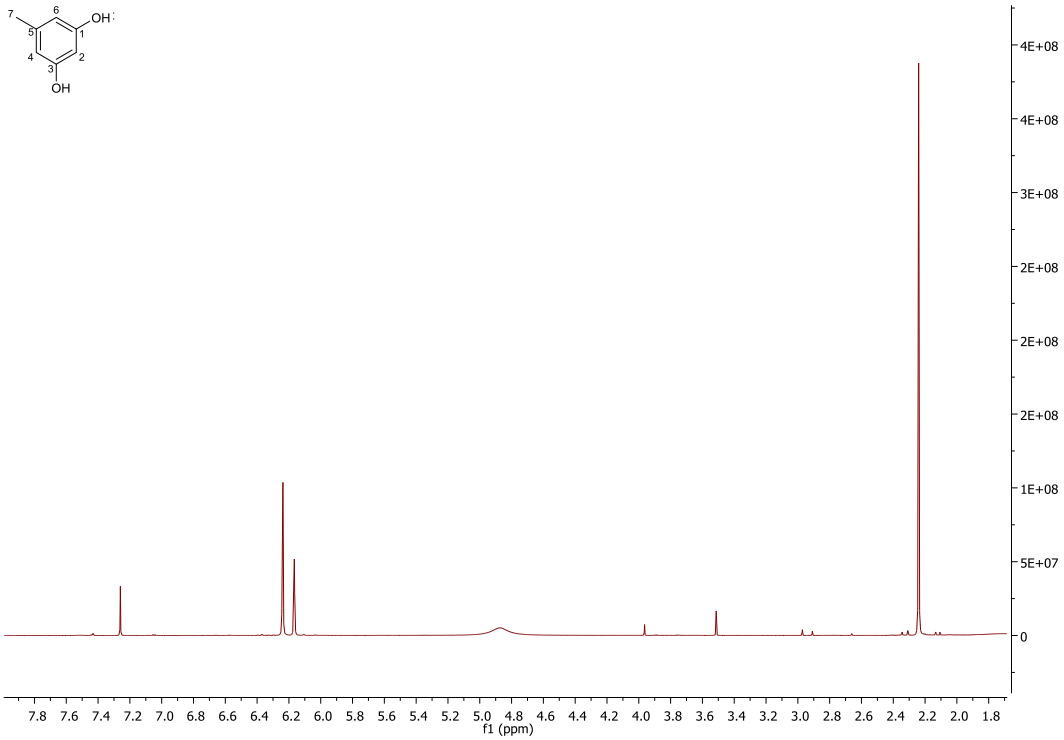


Figure S16a: ^{1}H-NMR spectrum of **compound 14** recorded in $CDCl_3$ at 600 MHz.

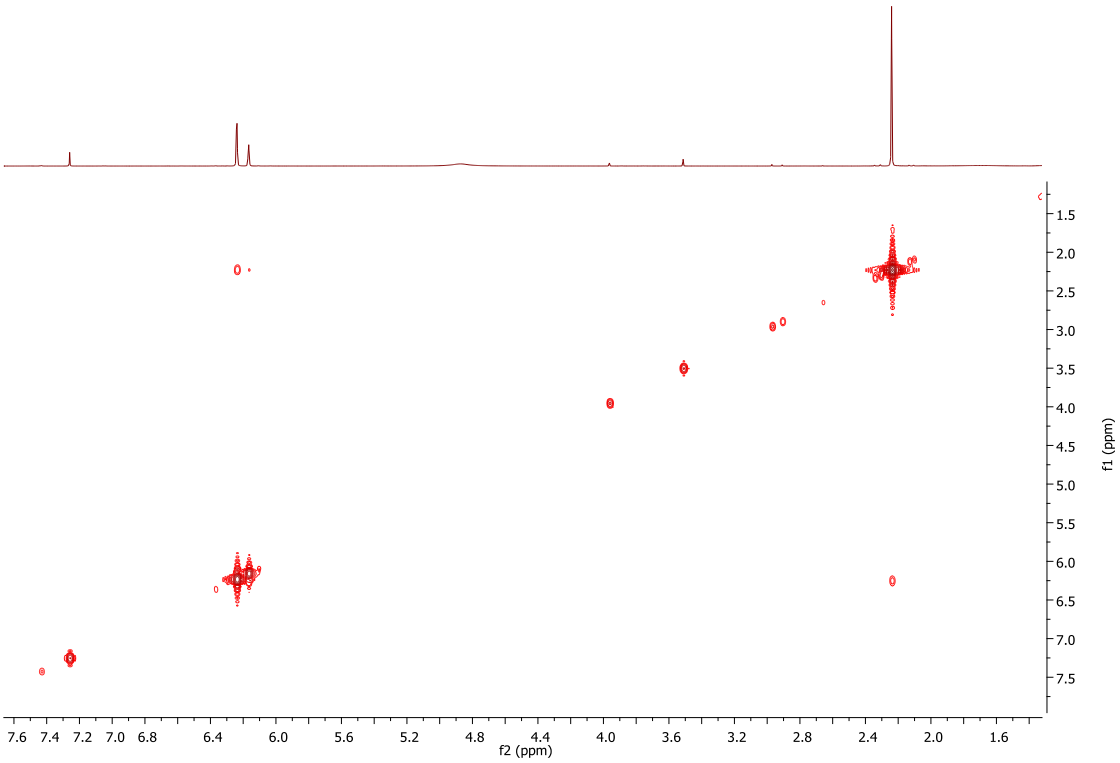


Figure S16b: COSY spectrum of **compound 14** recorded in $CDCl_3$ at 600 MHz.

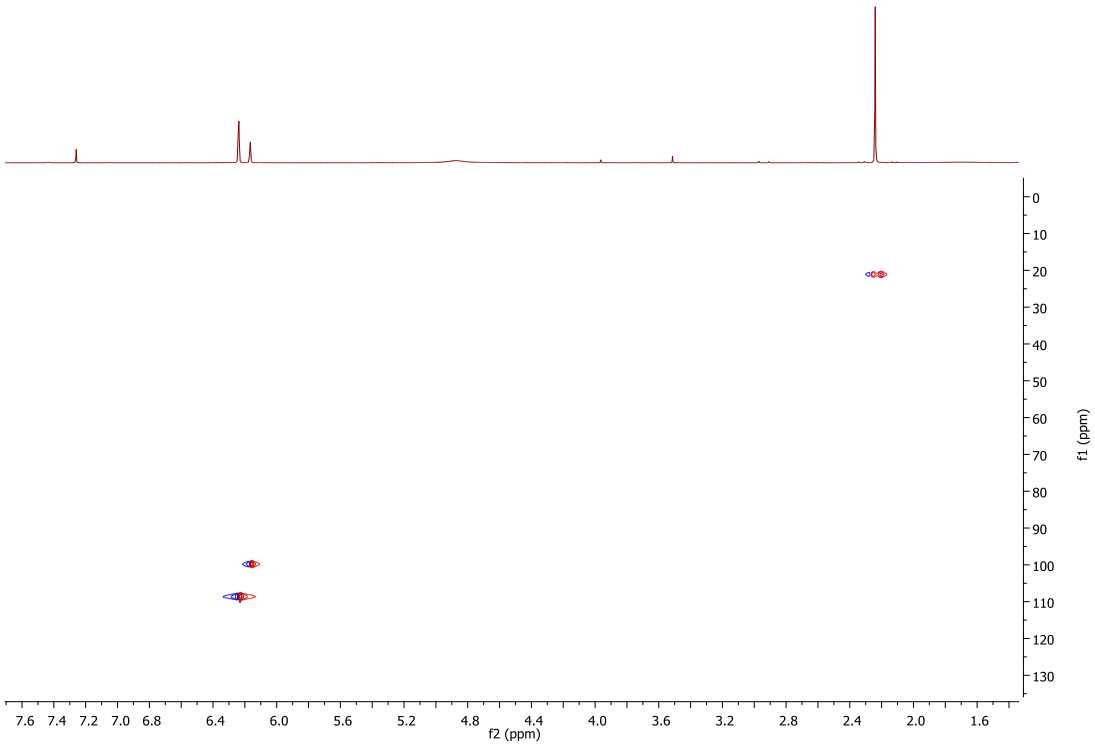


Figure S16c: HSQC-DEPT spectrum of **compound 14** recorded in $CDCl_3$ at 600 MHz.

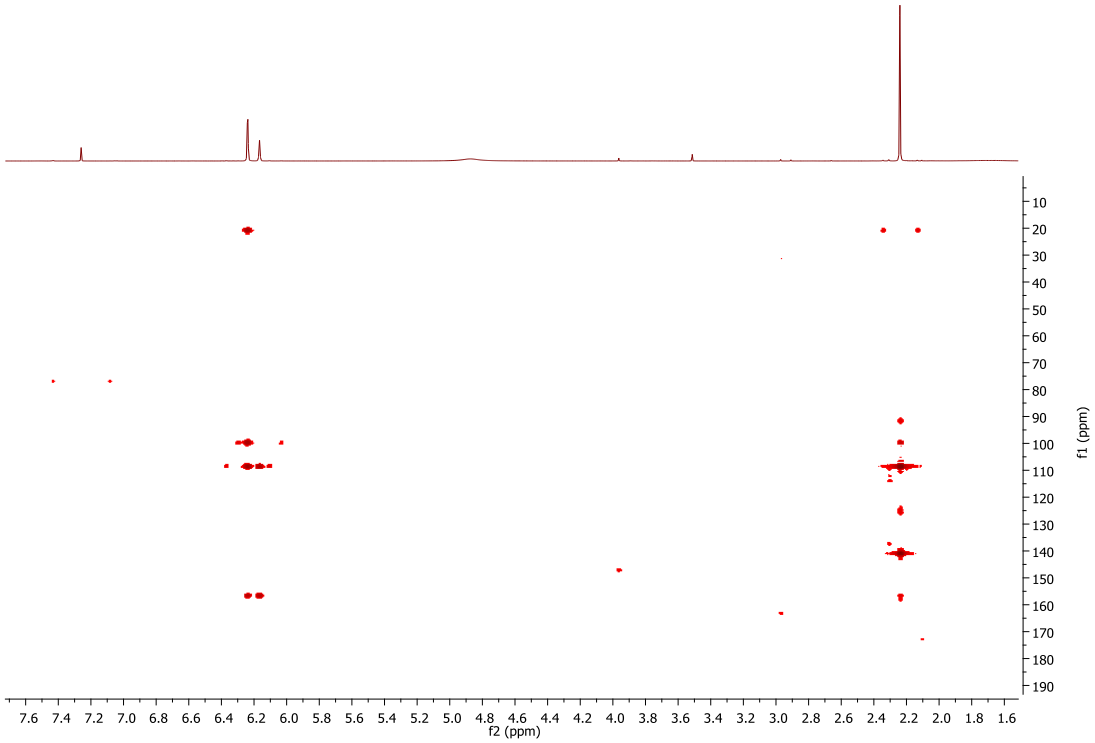


Figure S16d: HMBC spectrum of **compound 14** recorded in $CDCl_3$ at 600 MHz.

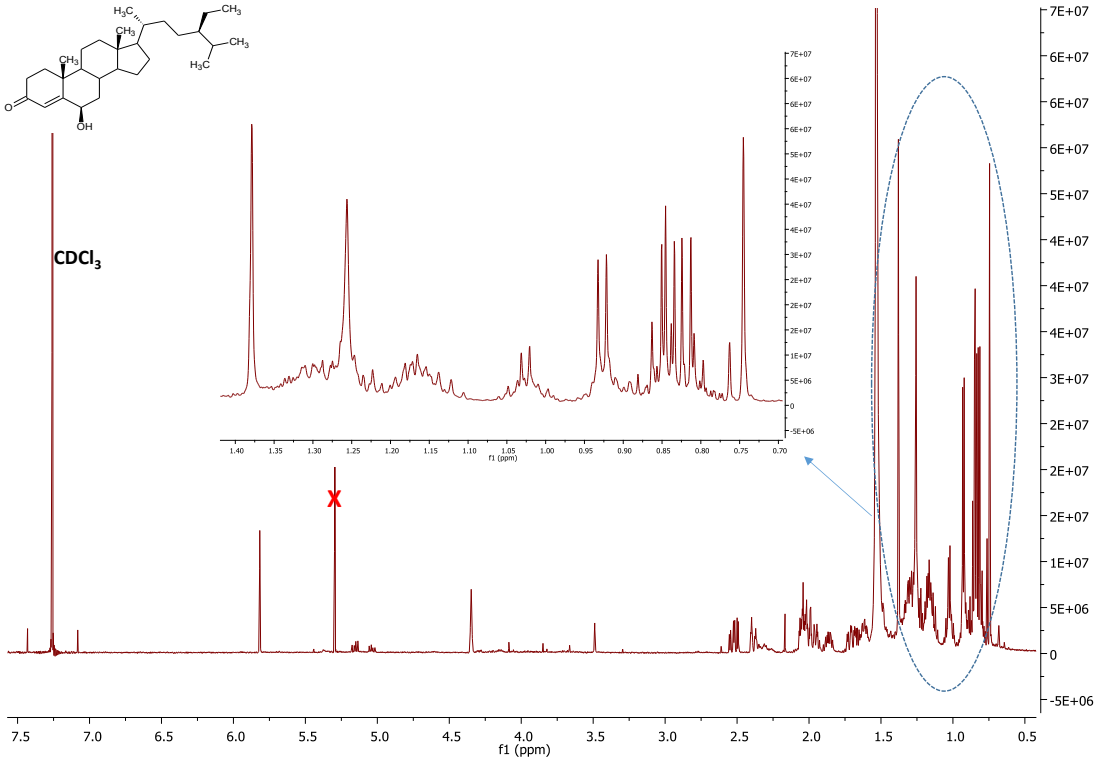


Figure S17a: ^{1}H-NMR spectrum of **compound 16** recorded in $CDCl_3$ at 600 MHz.

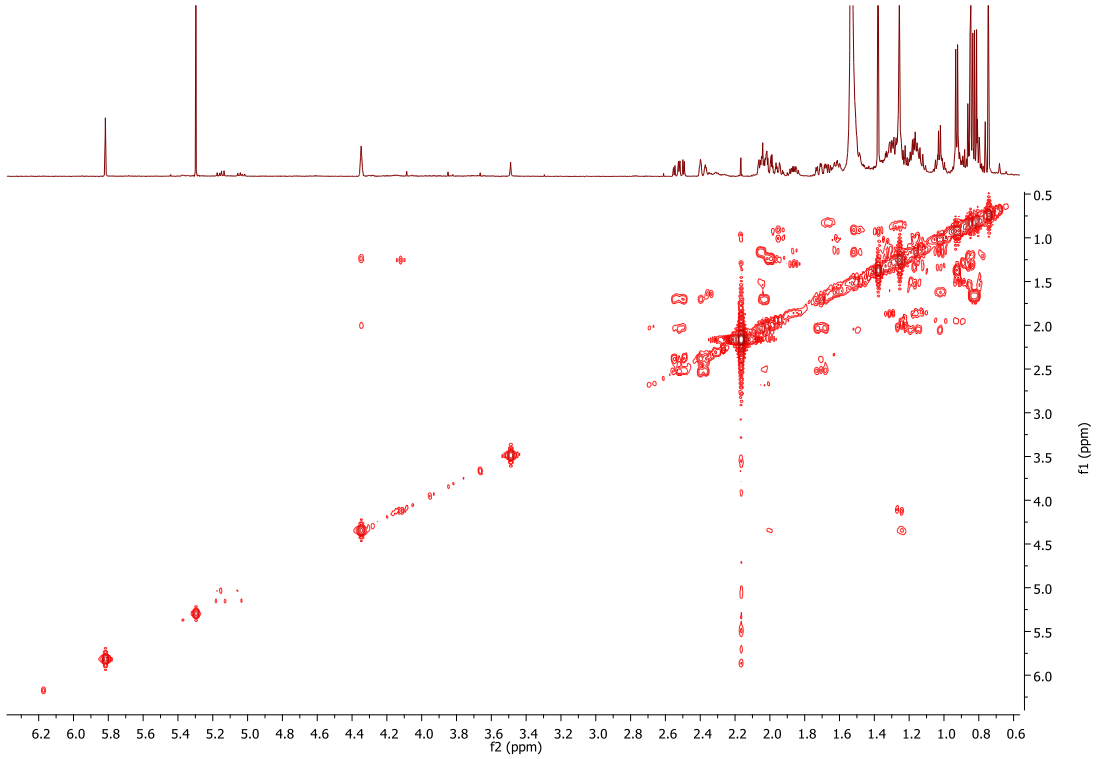


Figure S17b: COSY spectrum of **compound 16** recorded in $CDCl_3$ at 600 MHz.

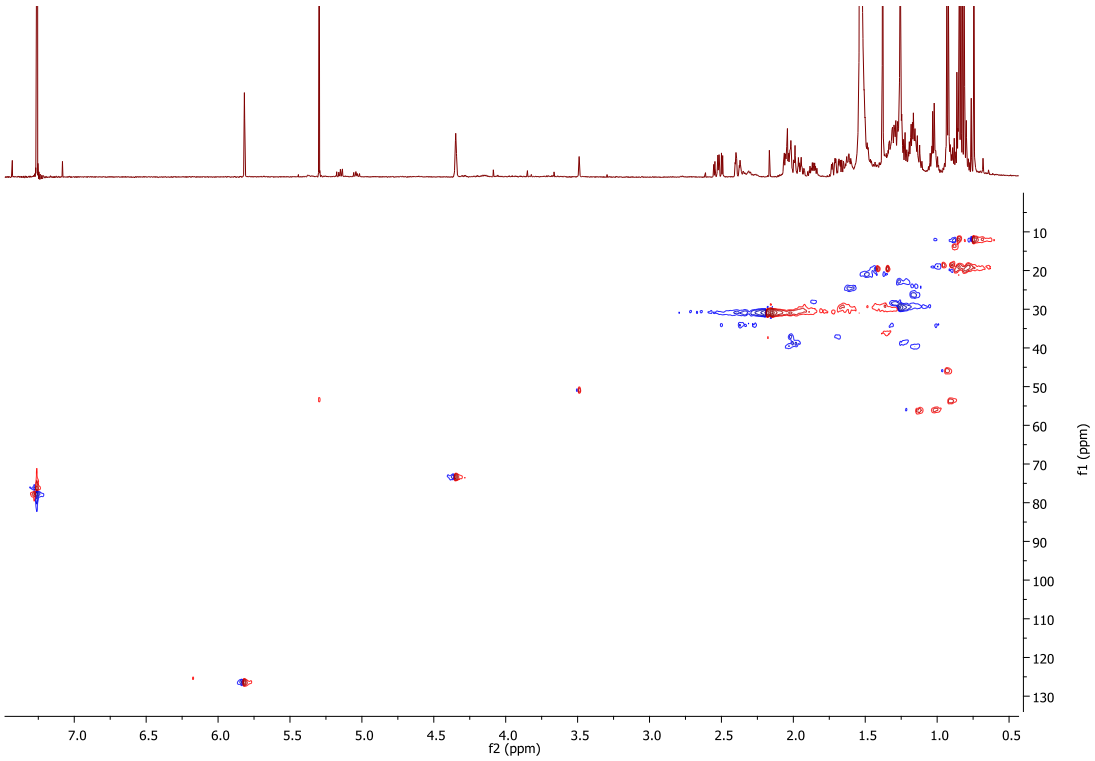


Figure S17c: HSQC-DEPT spectrum of **compound 16** recorded in $CDCl_3$ at 600 MHz.

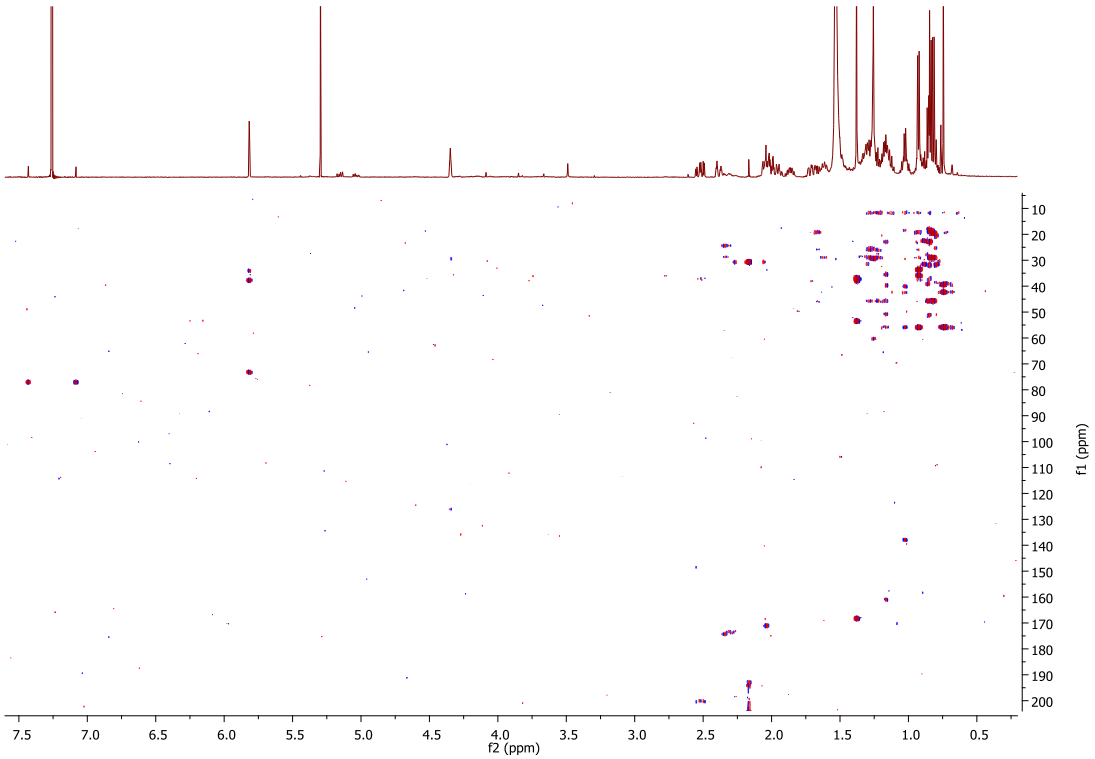


Figure S17d: HMBC spectrum of **compound 16** recorded in $CDCl_3$ at 600 MHz.