Supplementary Material

Total synthesis of prenylated acylphloroglucinols: faberiones A, B, and E

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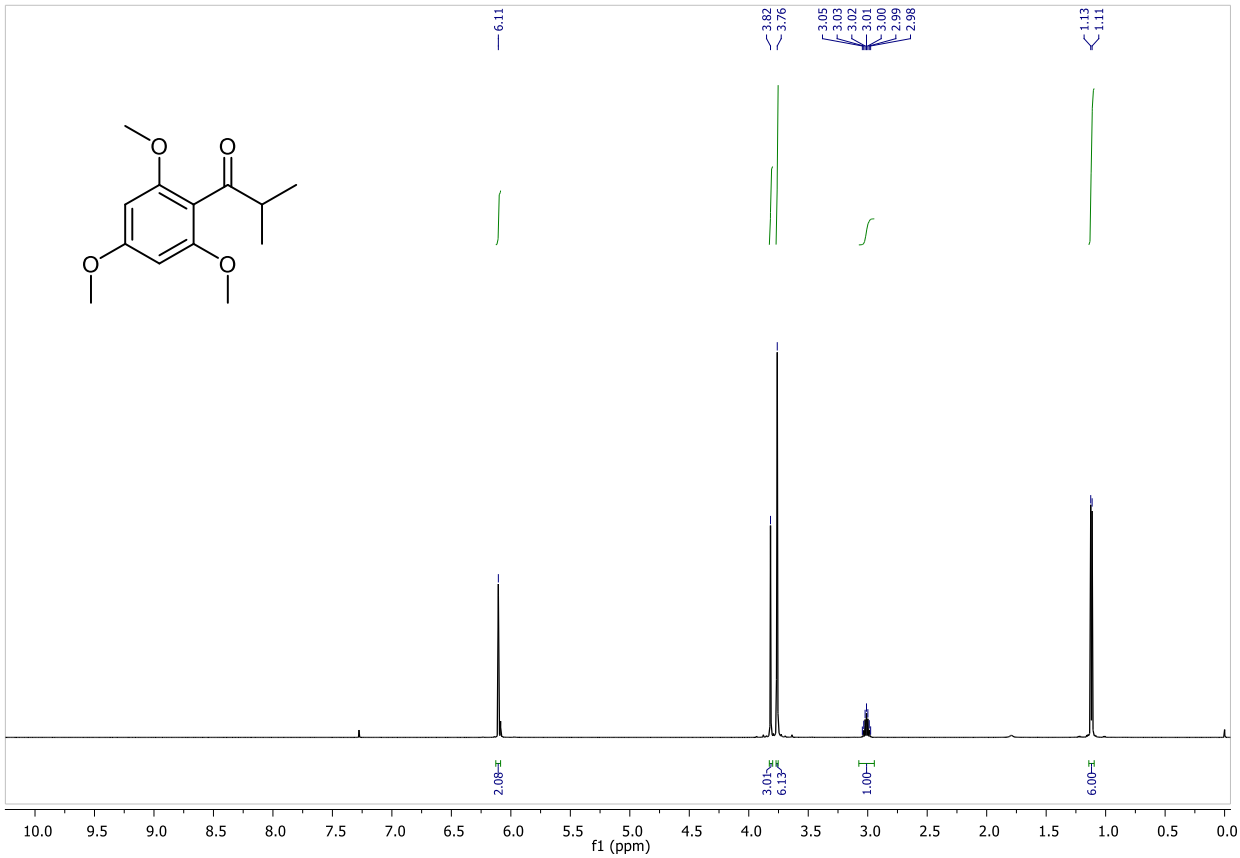

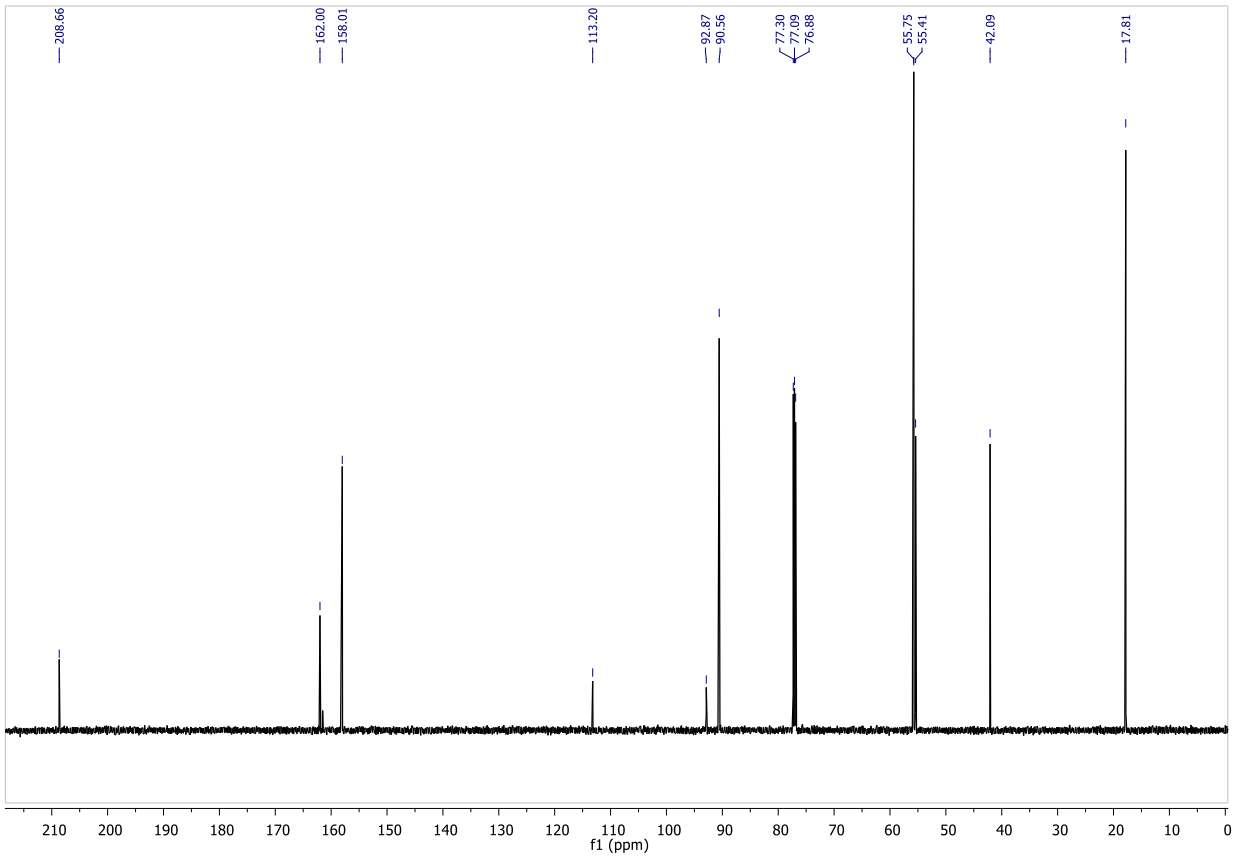

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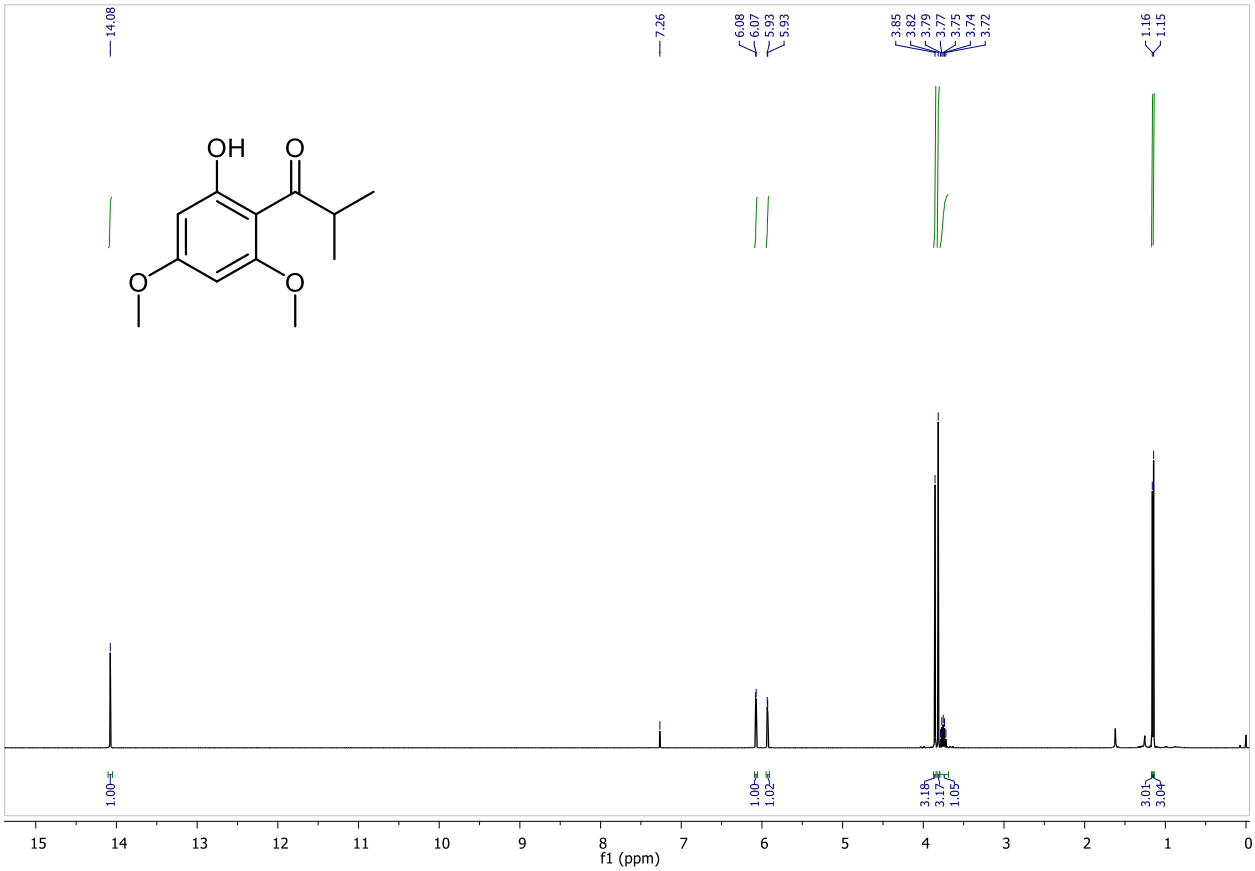
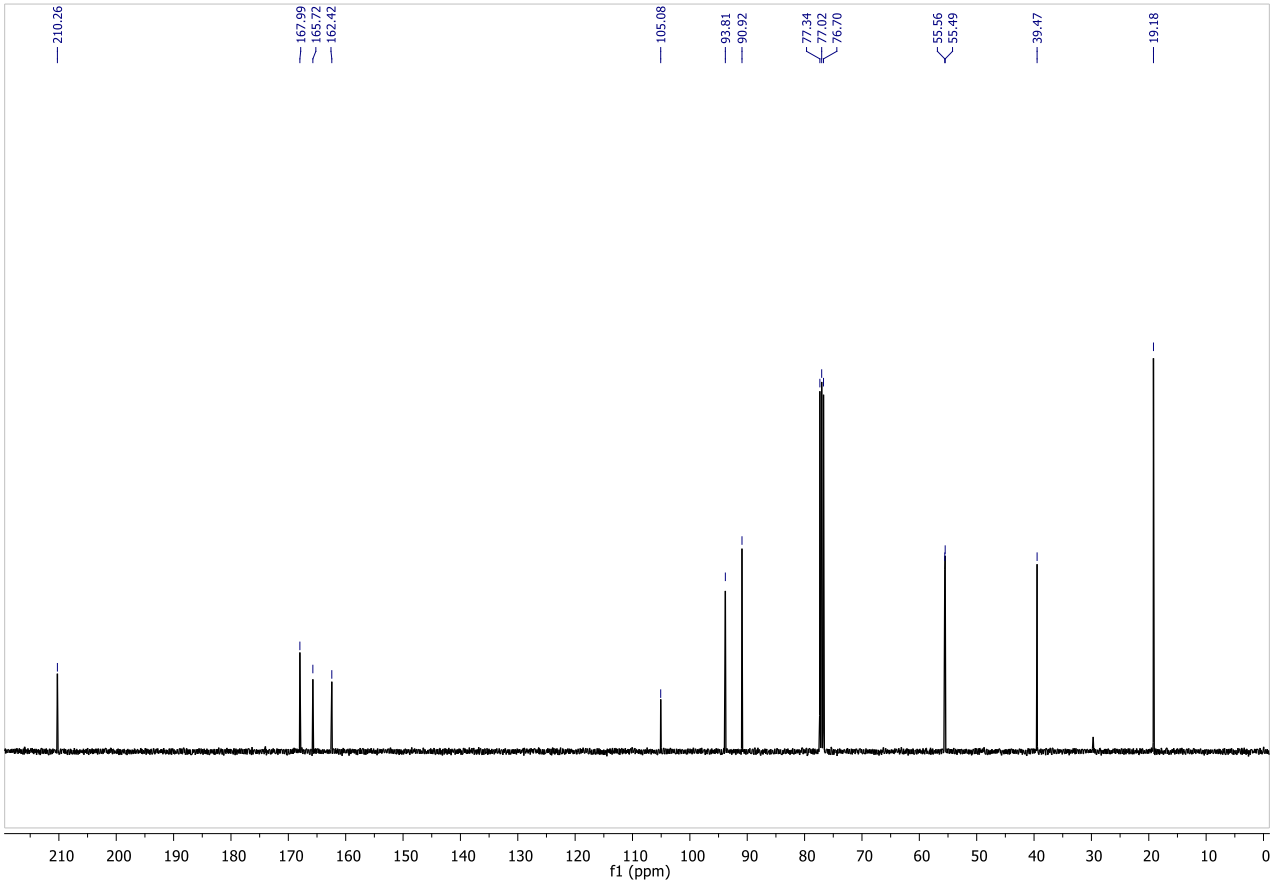
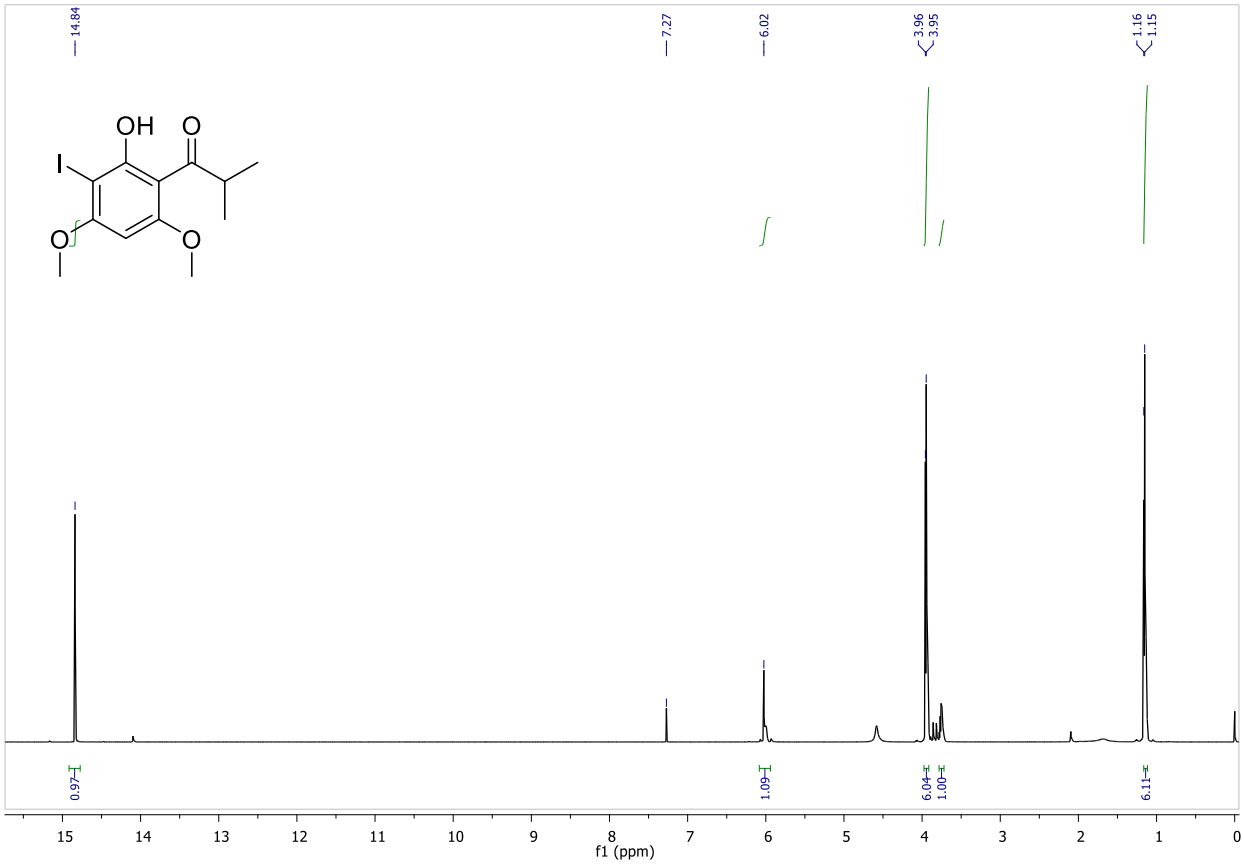
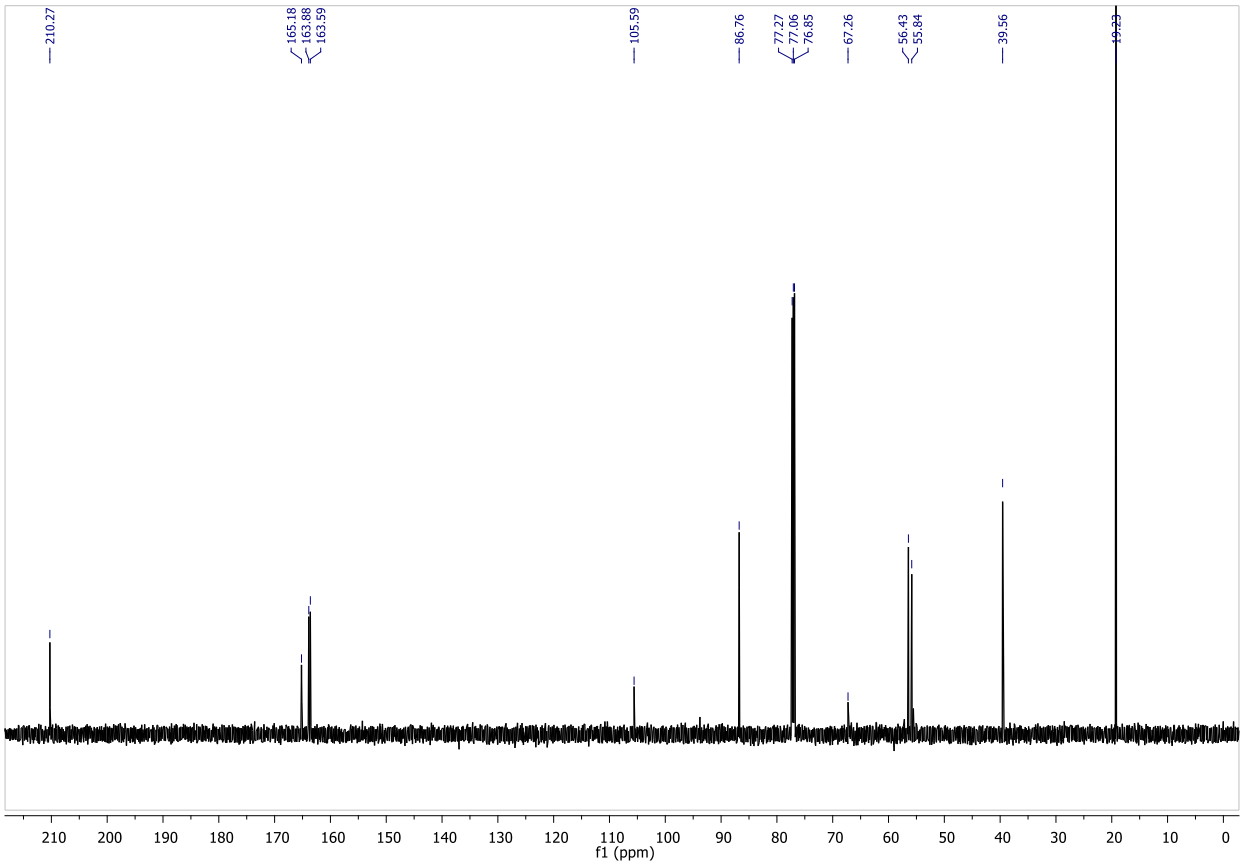




^{1}H and ^{13}C NMR spectrum of compound **9a** in $CDCl_3$





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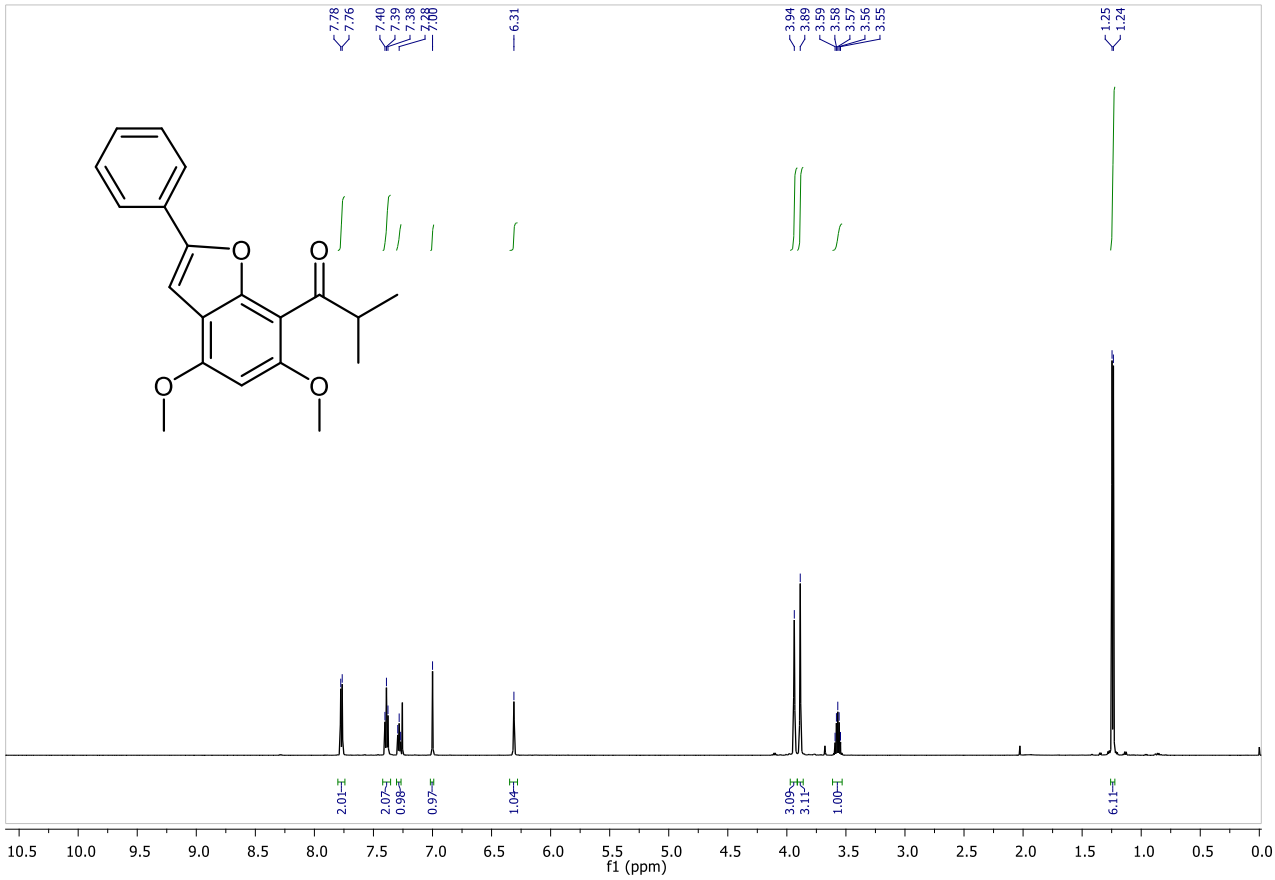
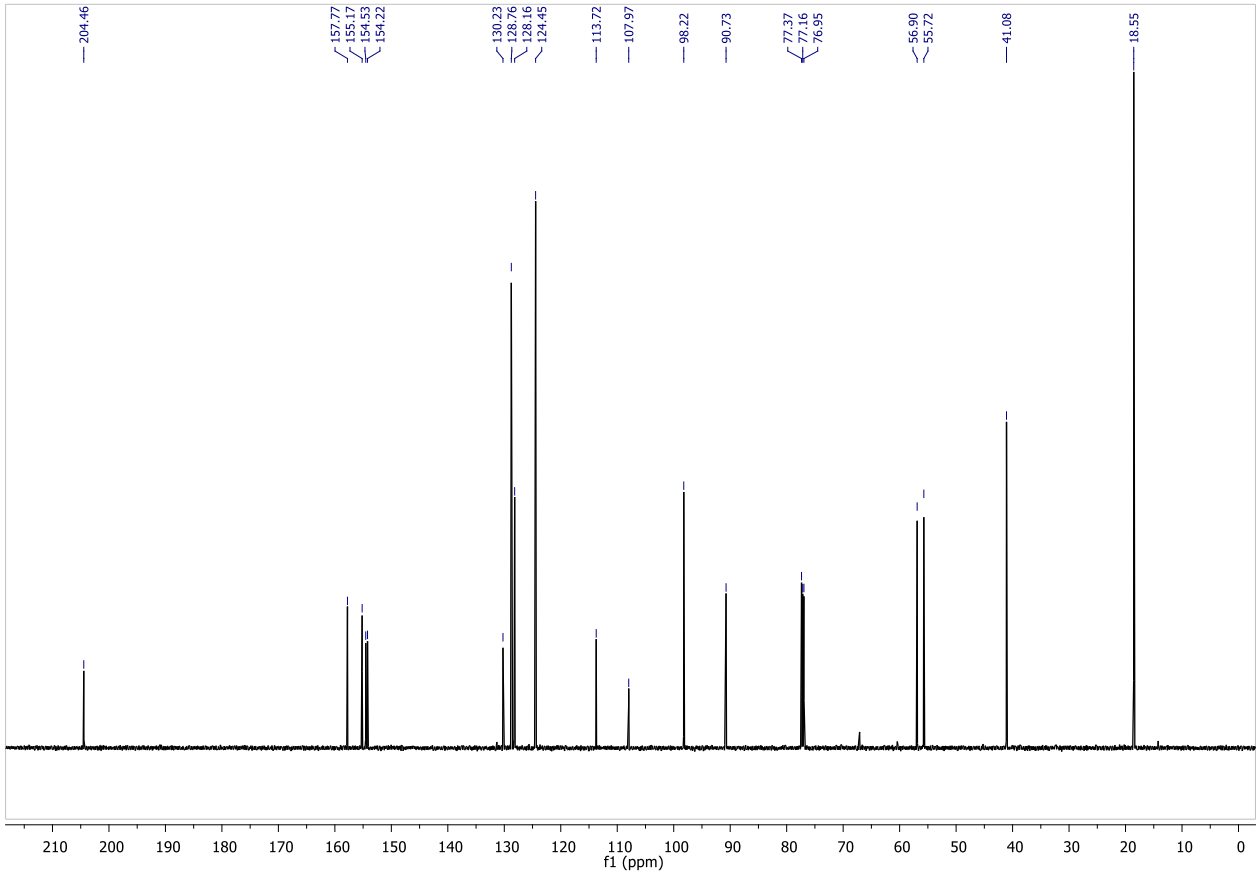
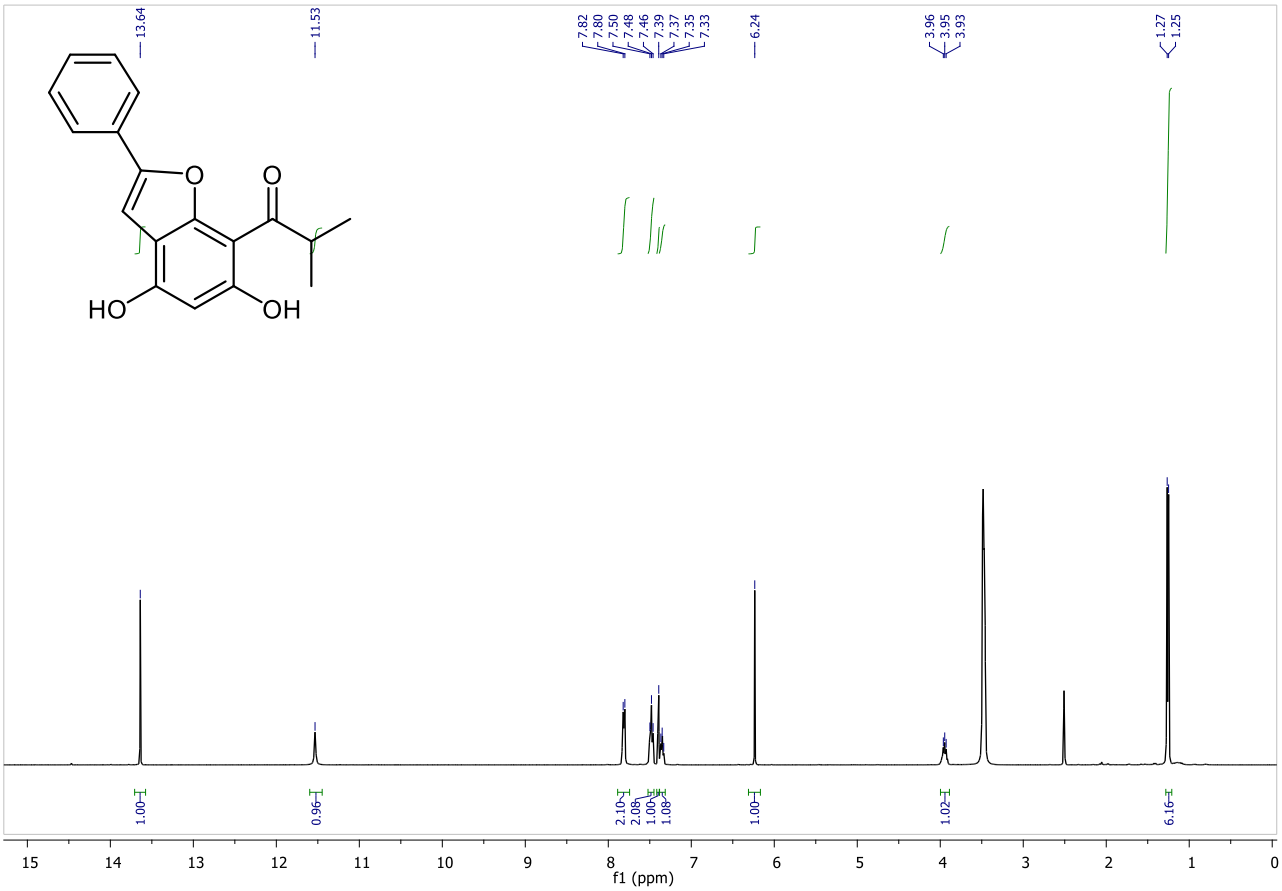
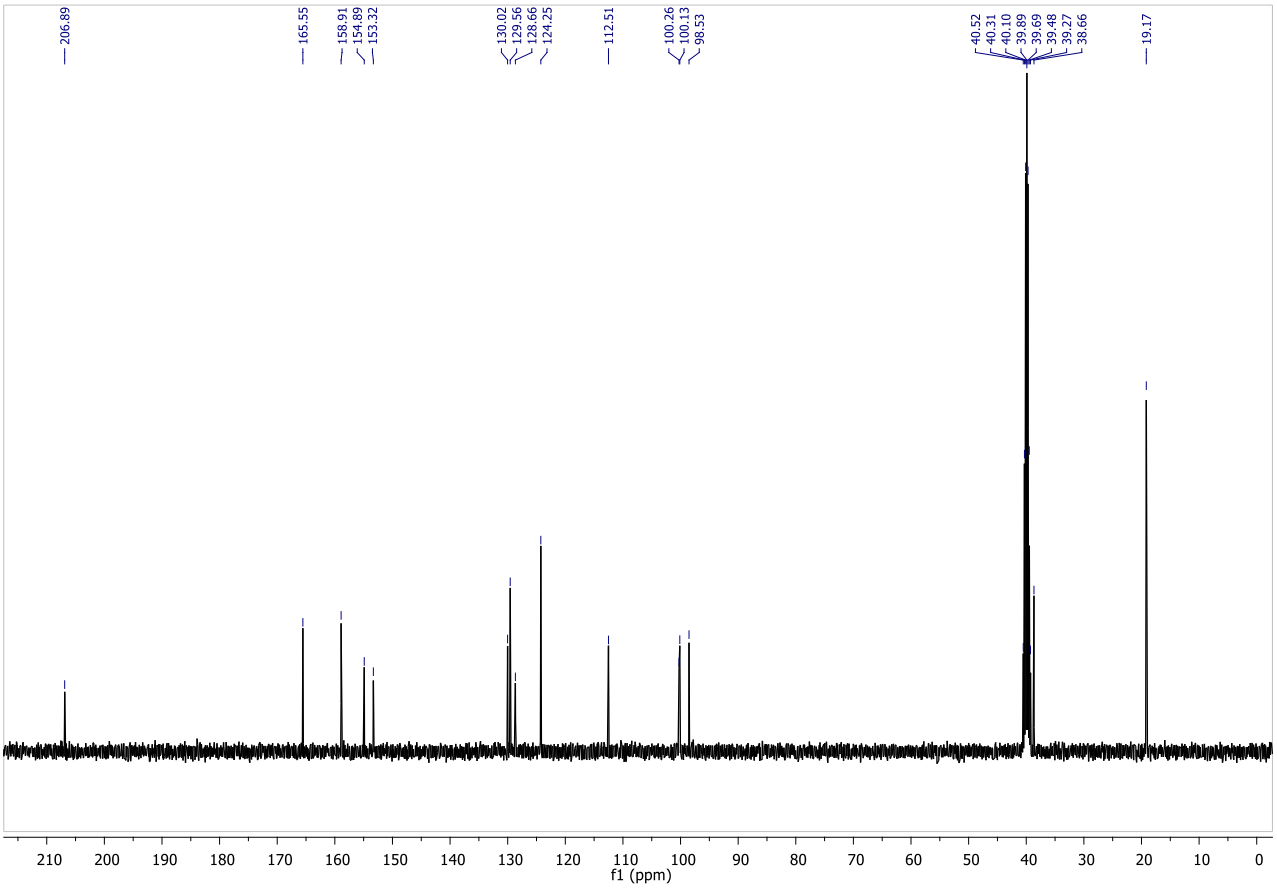




^{1}H and ^{13}C NMR spectrum of compound **7a** in DMSO-d_6





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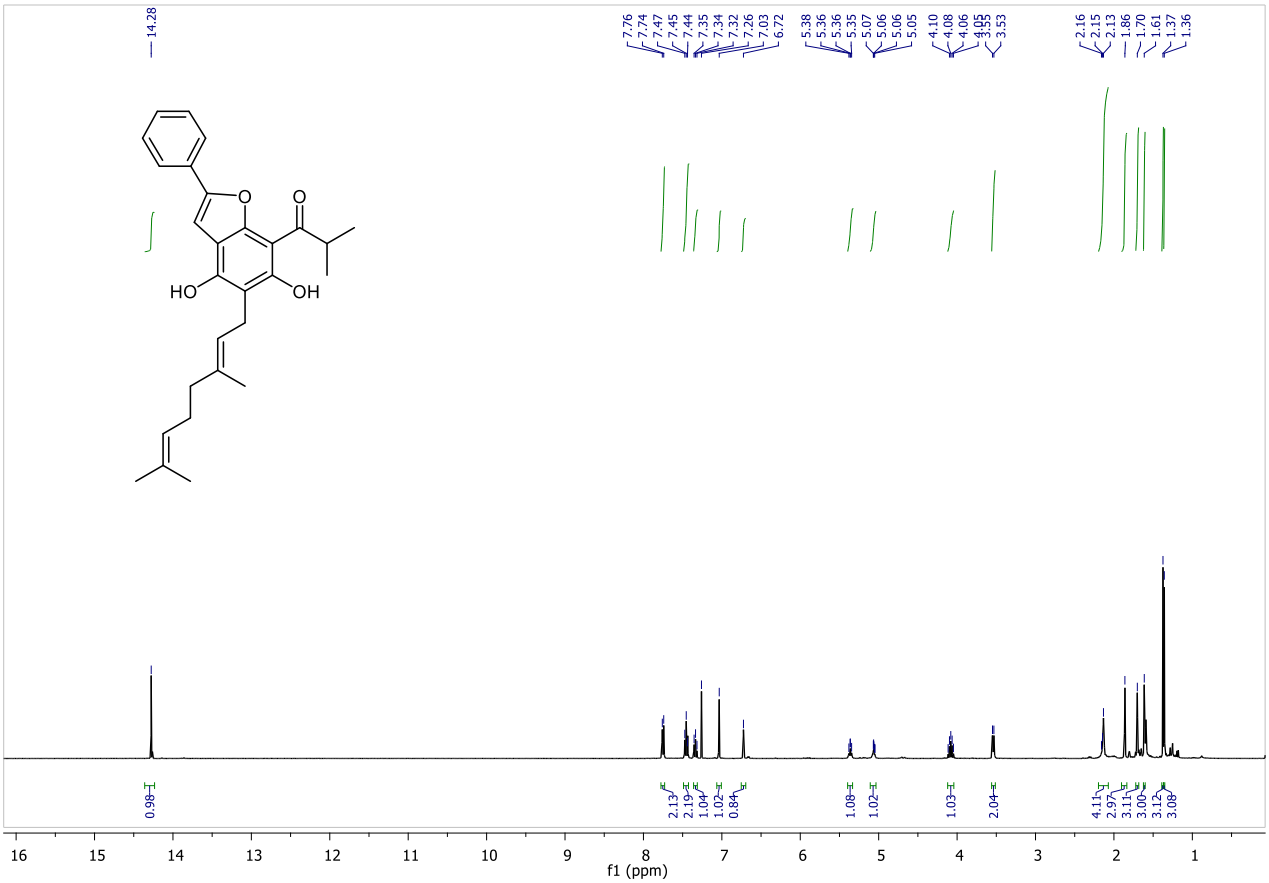
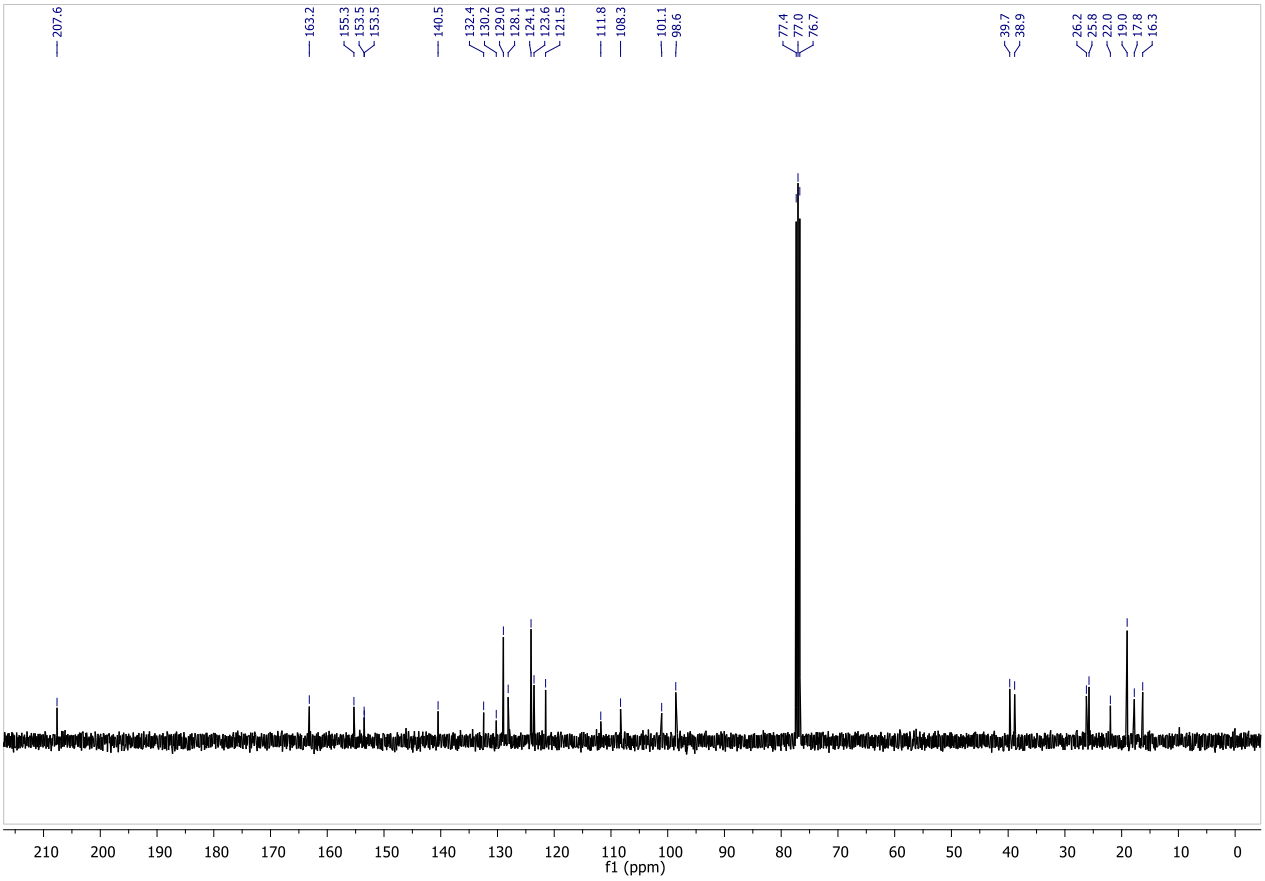
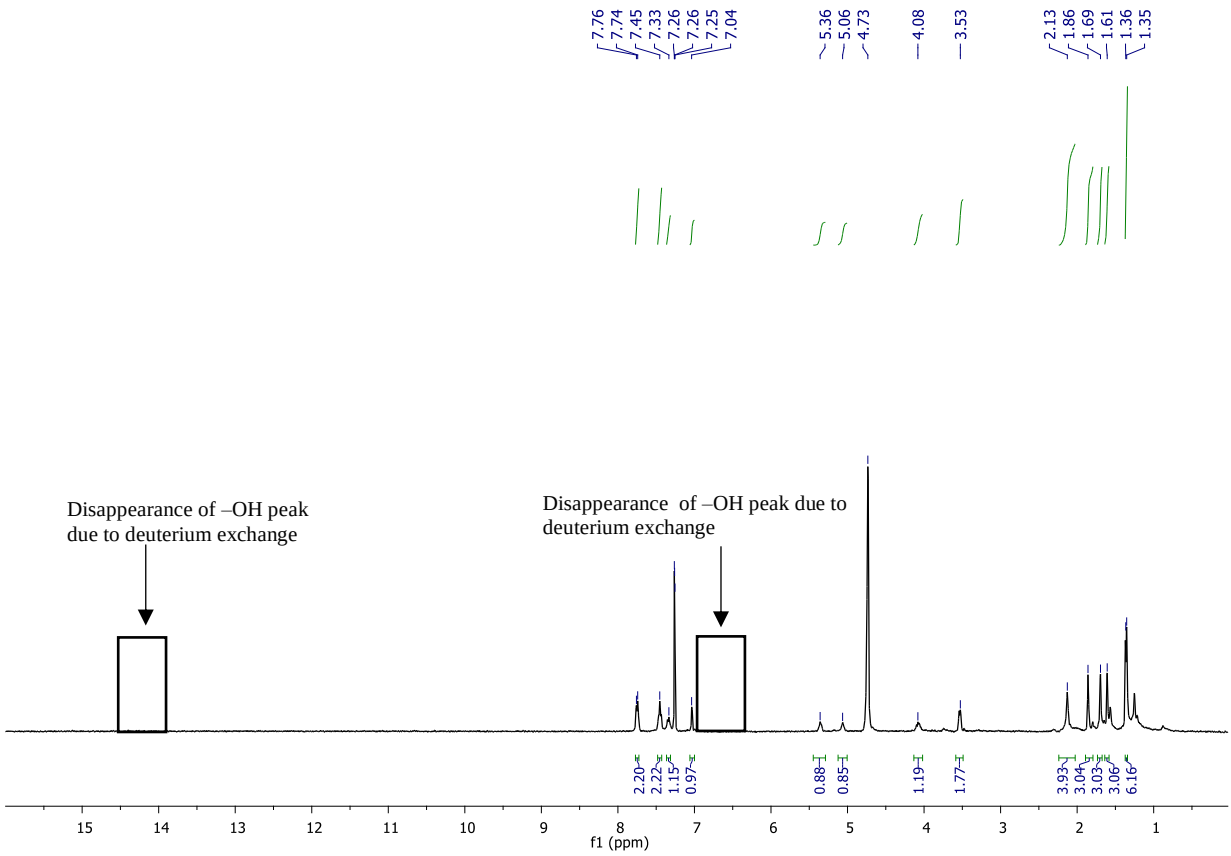
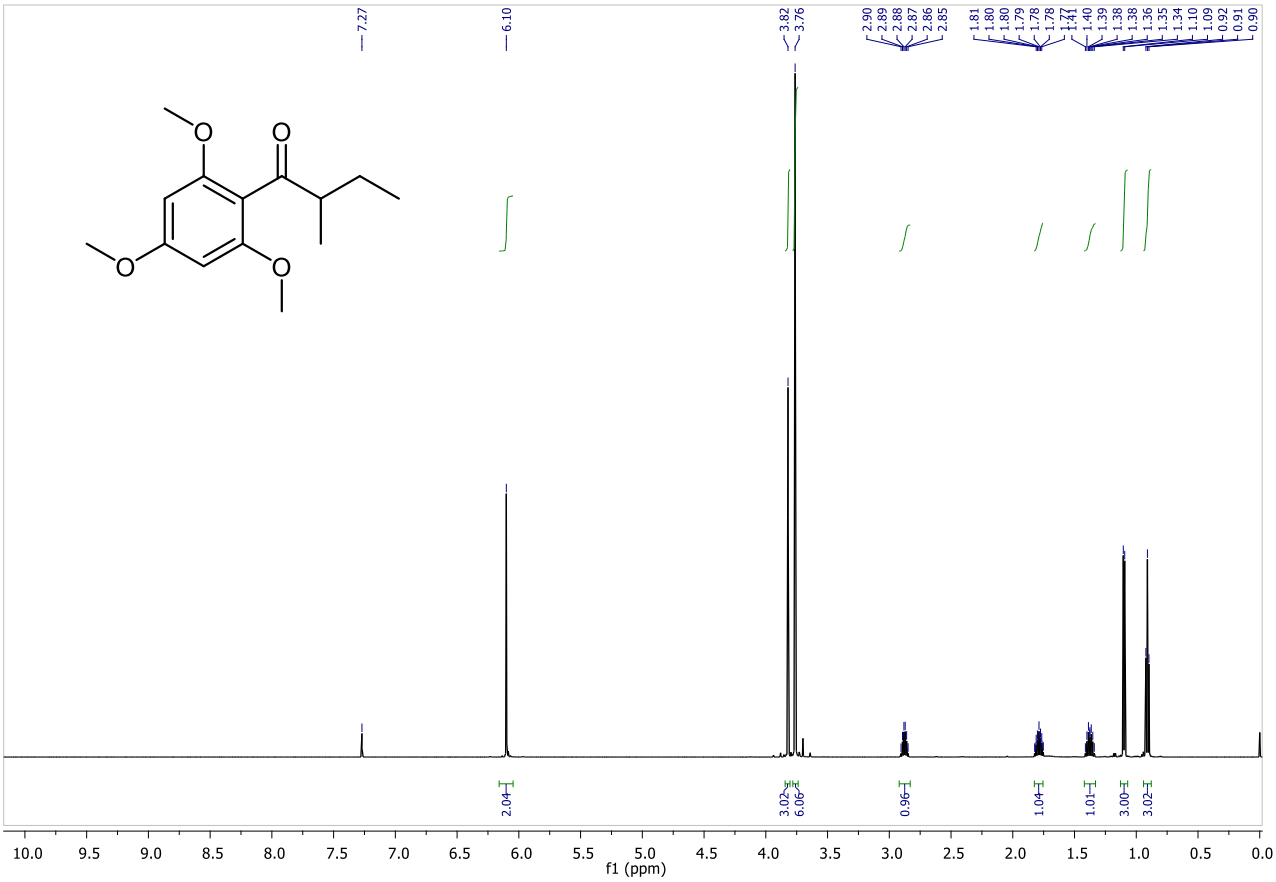


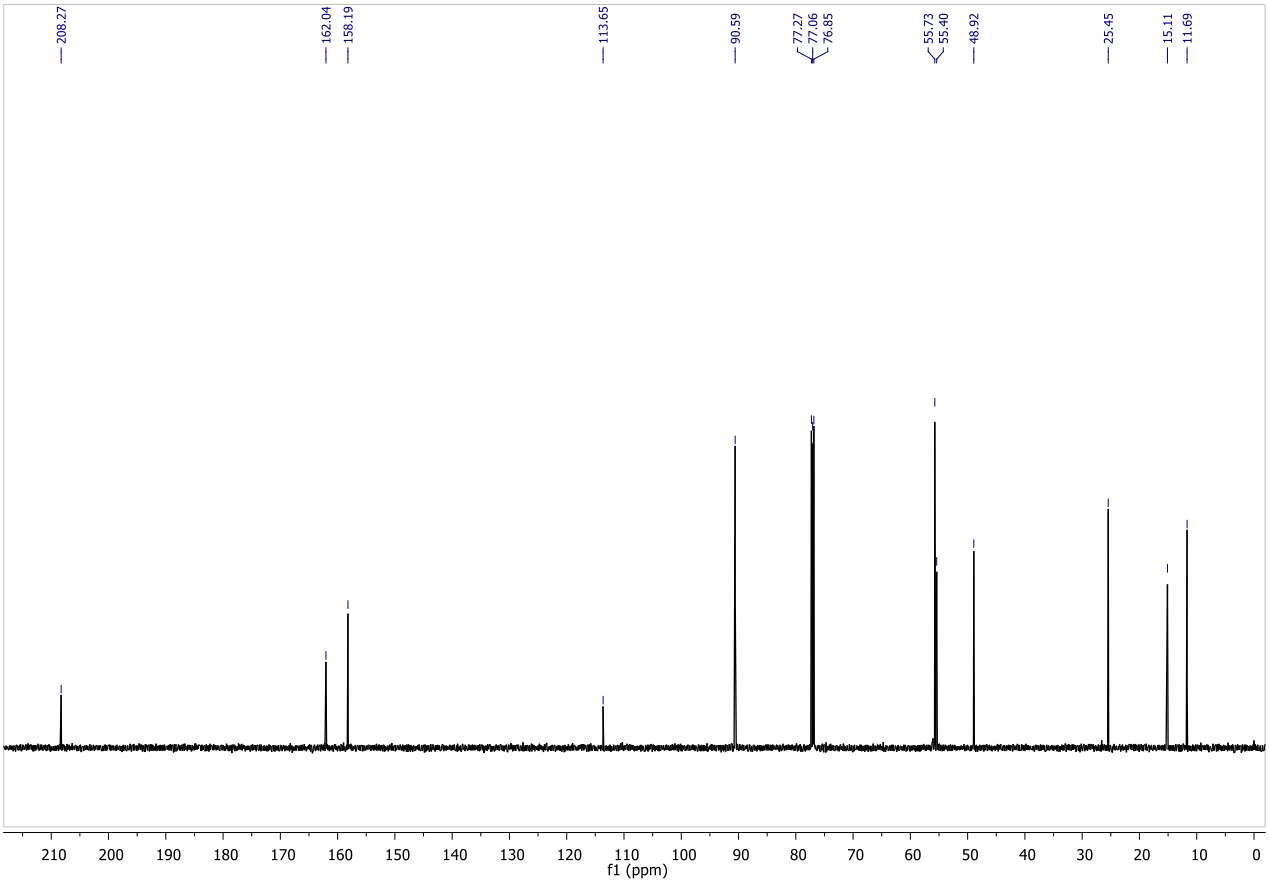


Deuterium exchange NMR of faberione A **1** in $CDCl_3$+D_2O

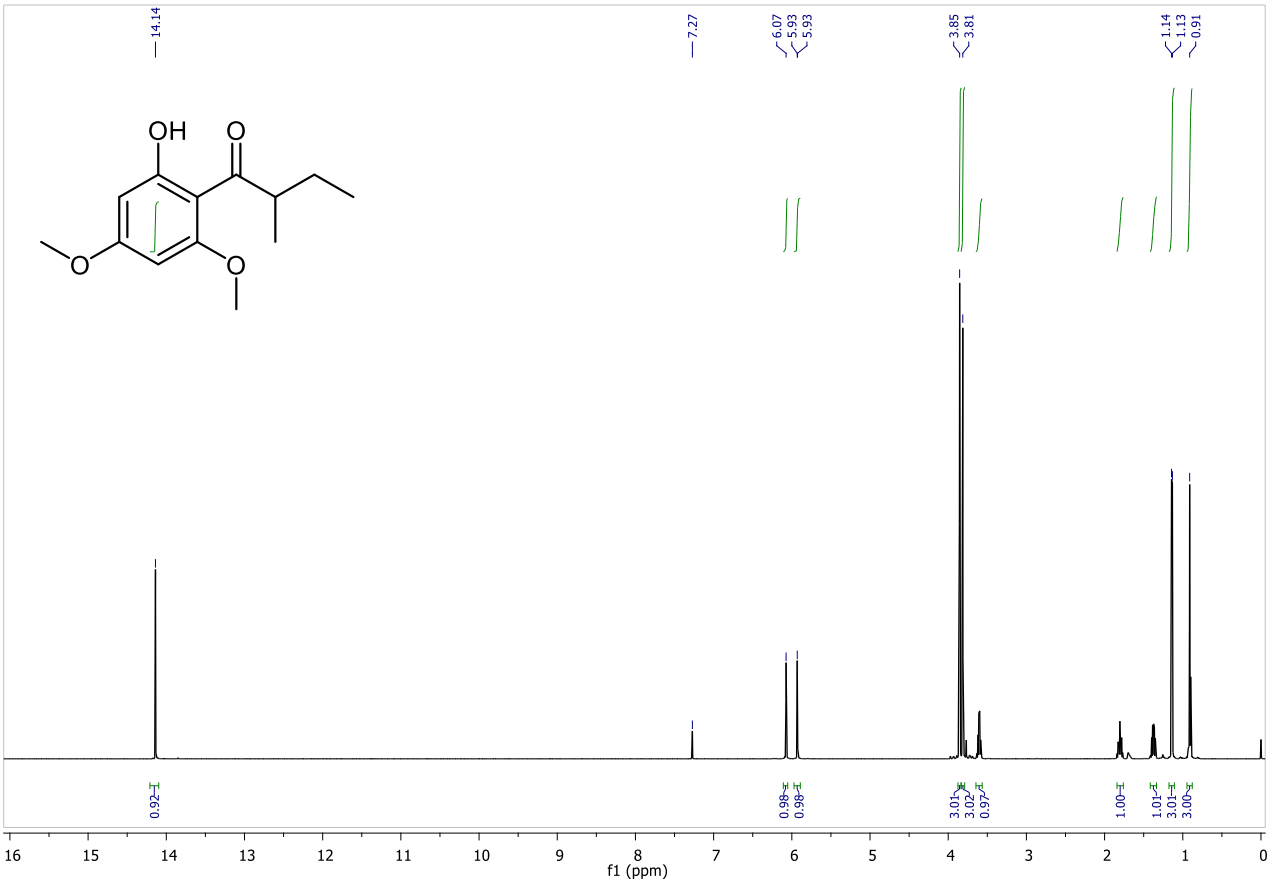


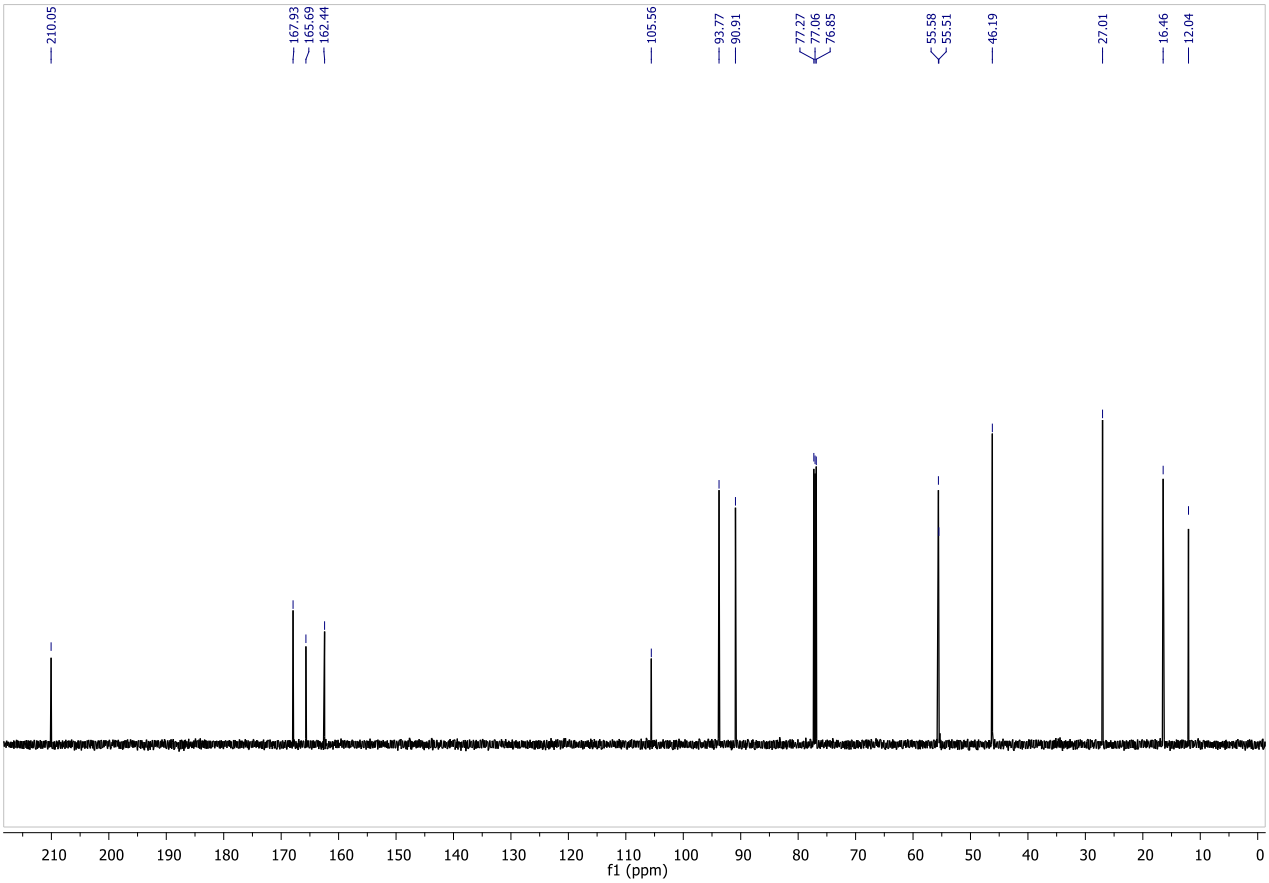
^{1}H and ^{13}C NMR spectrum of compound **11b** in $CDCl_3$



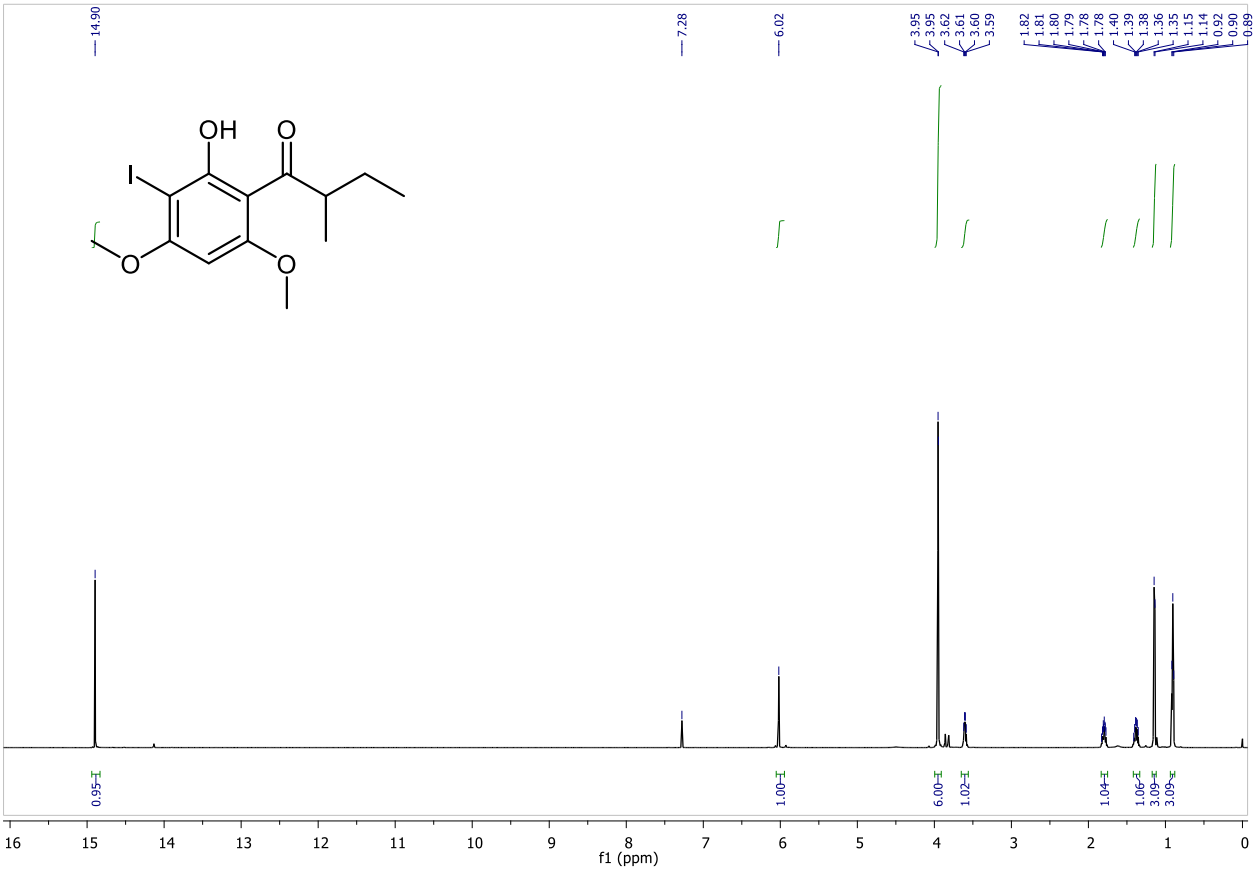


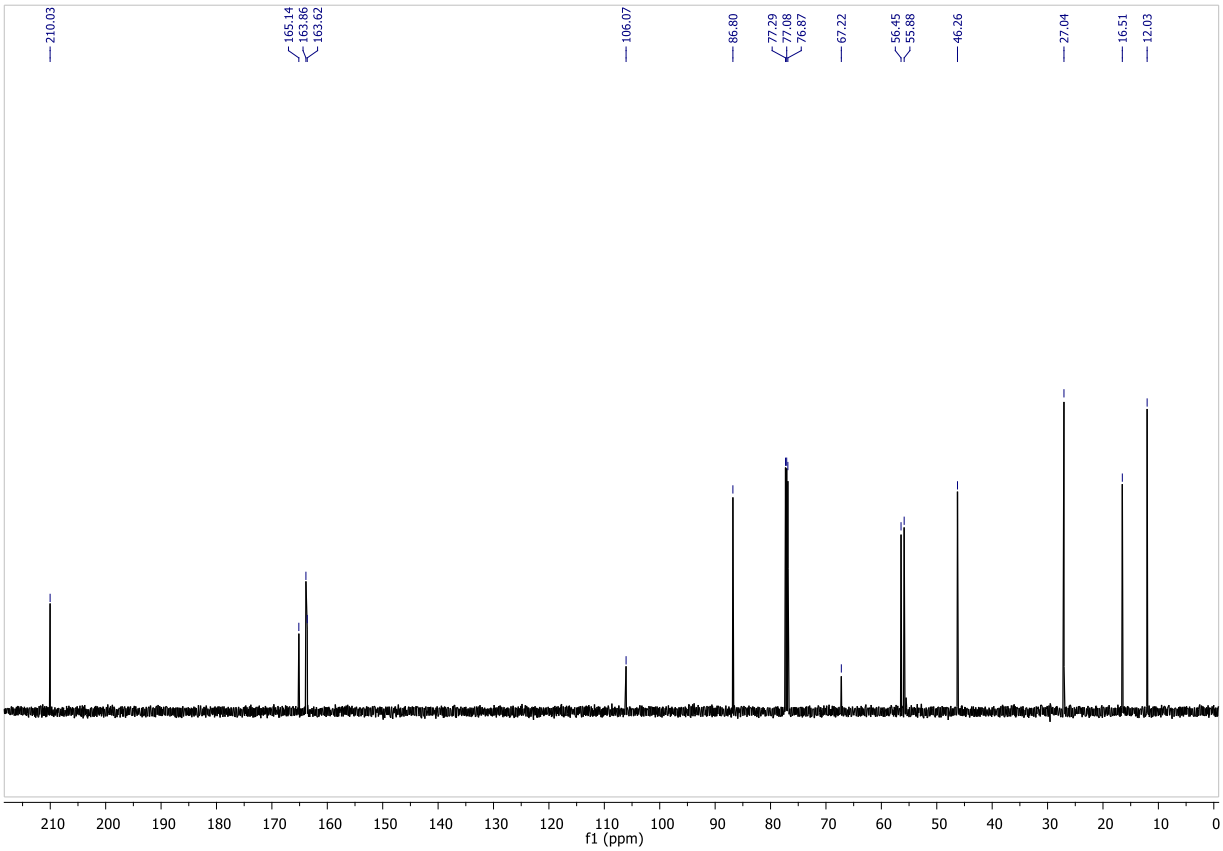
^{1}H and ^{13}C NMR spectrum of compound **10b** in $CDCl_3$



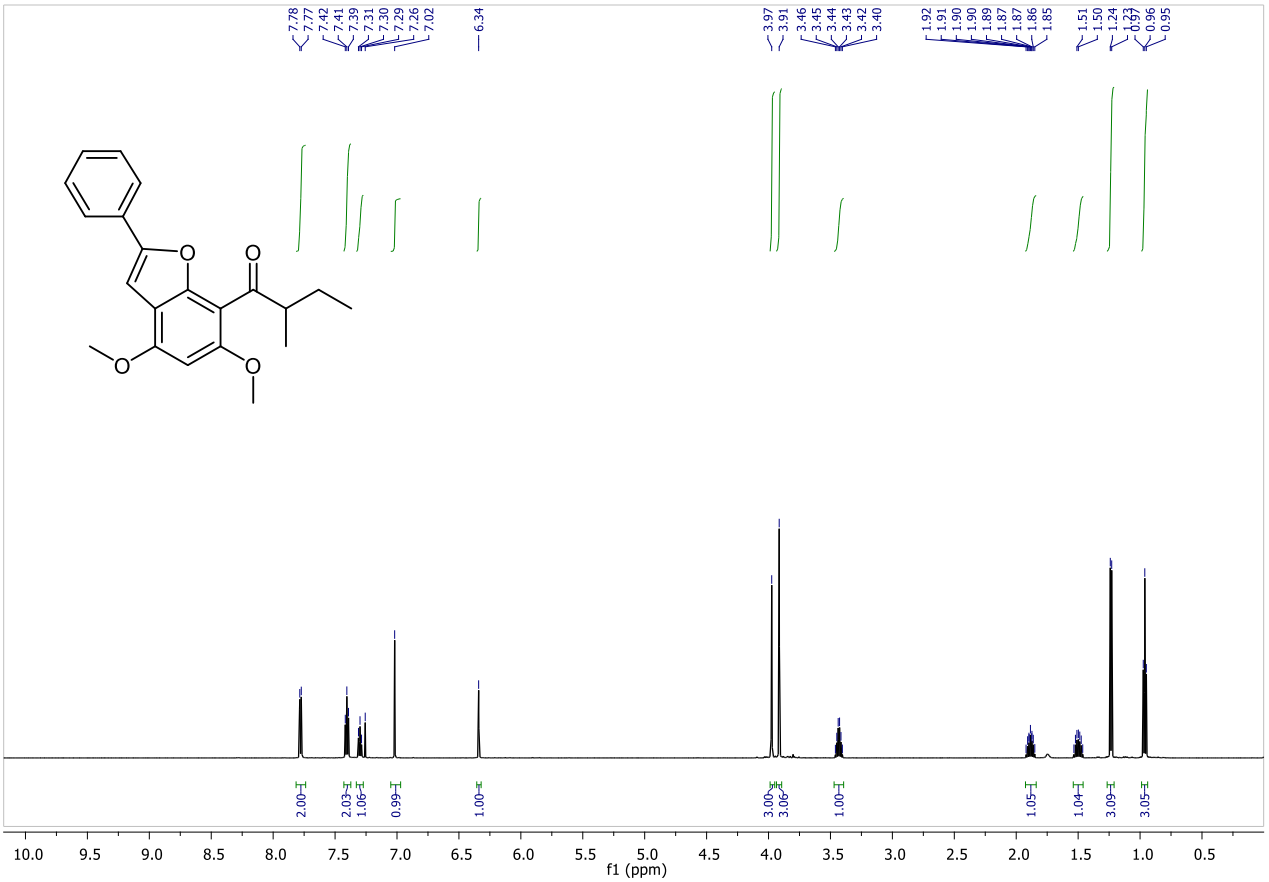


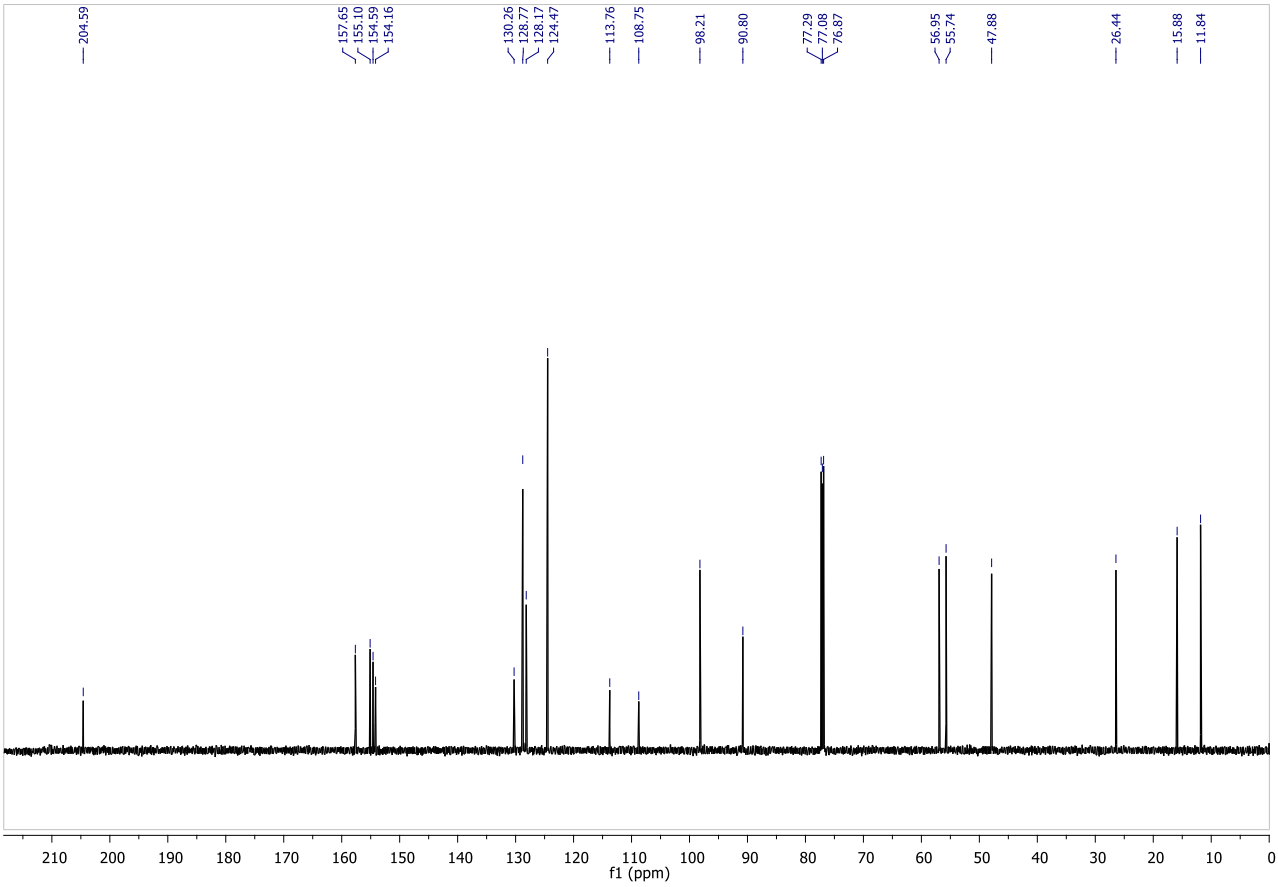
^{1}H and ^{13}C NMR spectrum of compound **9b** in $CDCl_3$



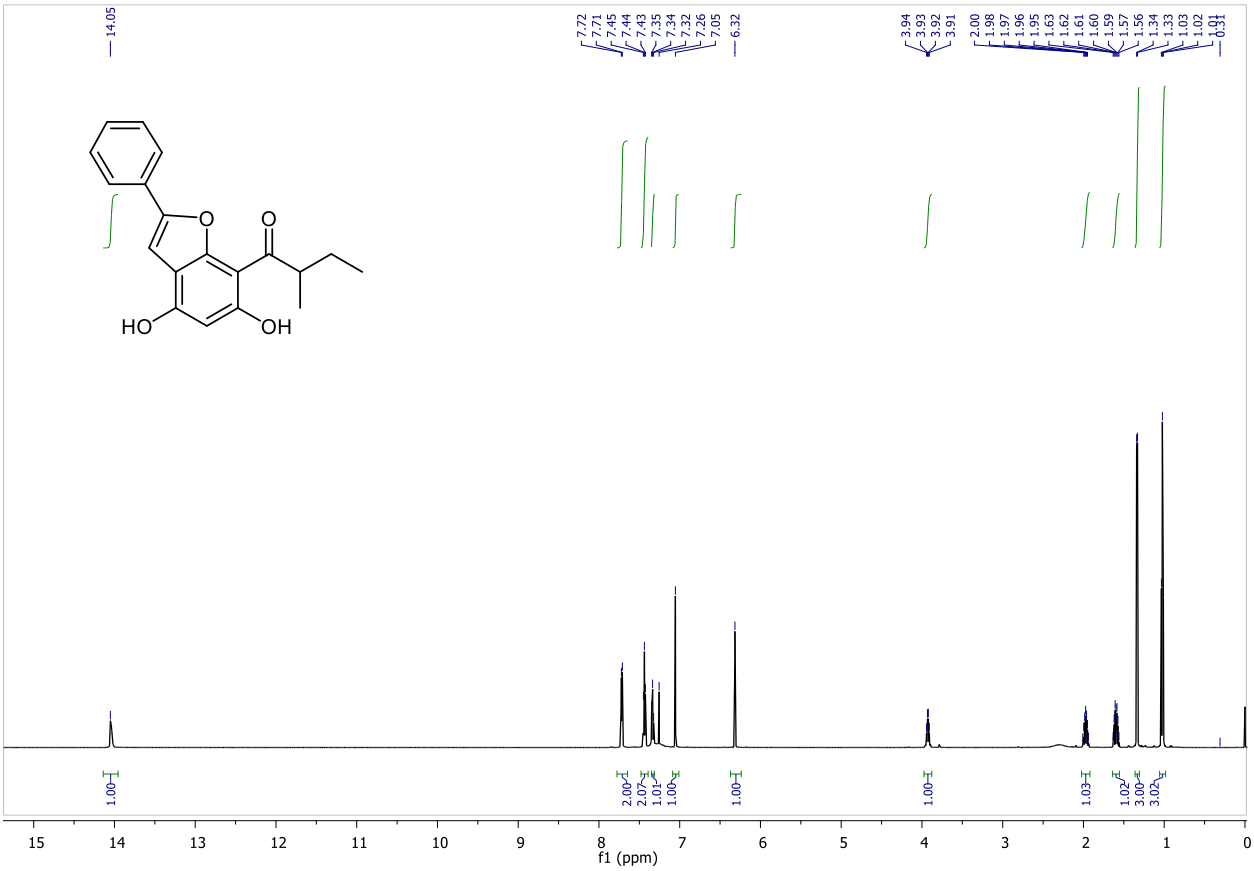


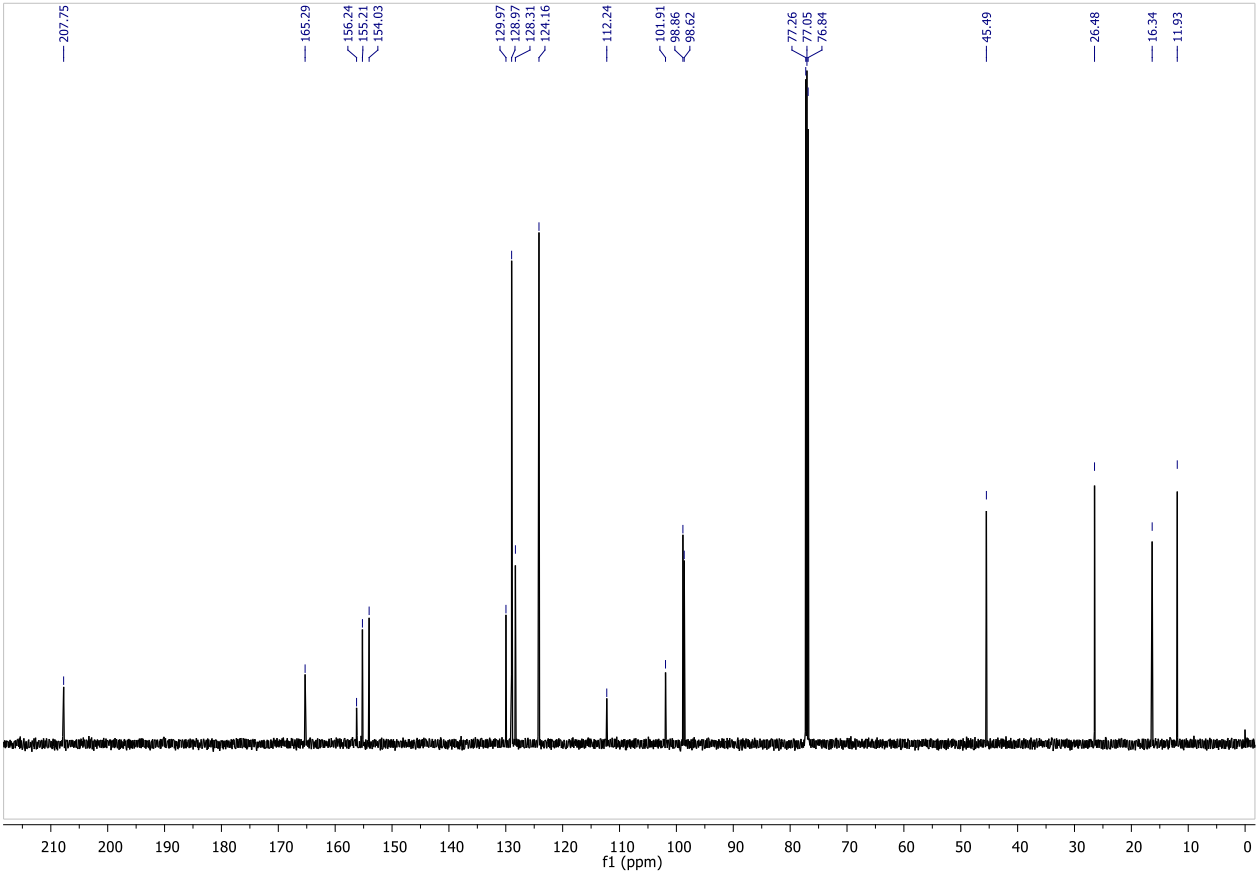
^{1}H and ^{13}C NMR spectrum of compound **8b** in $CDCl_3$



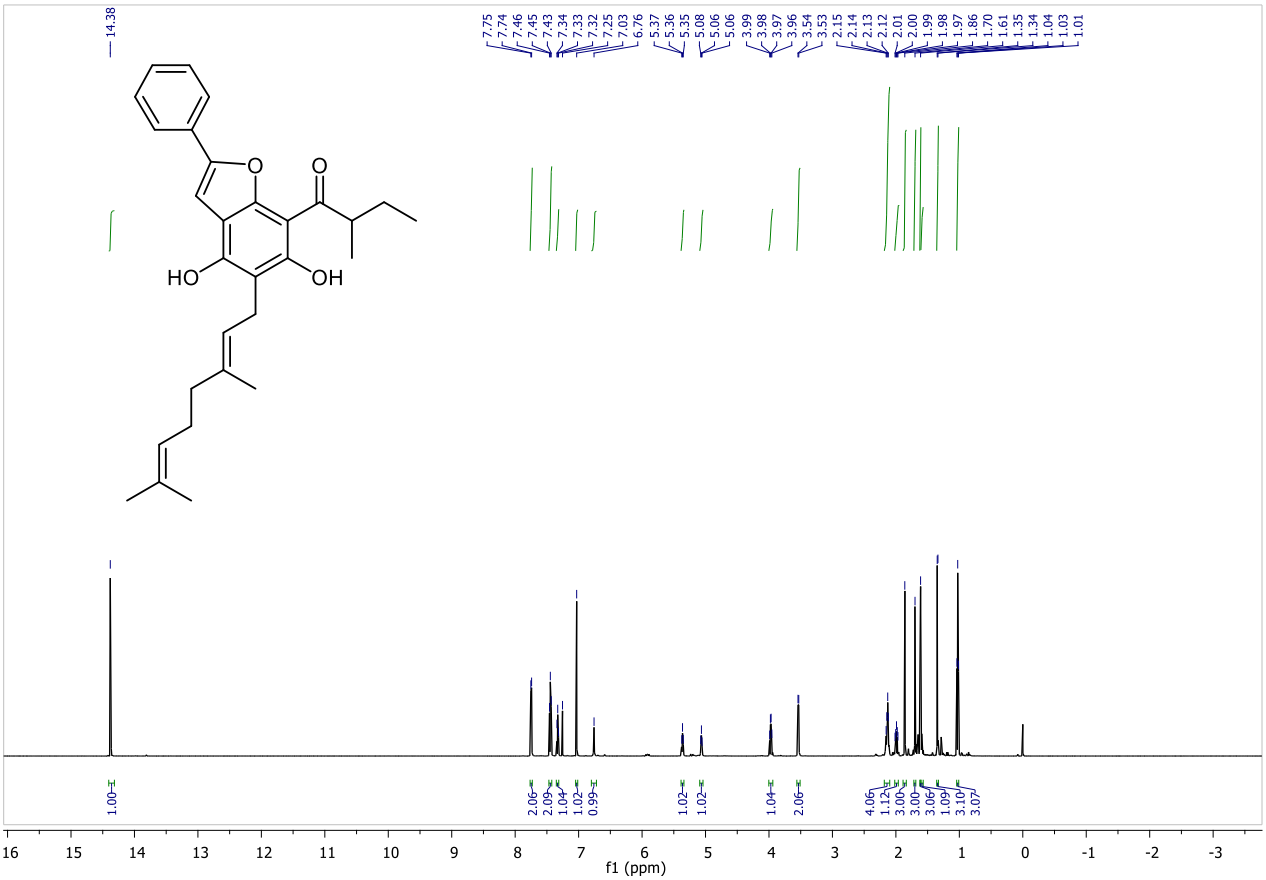


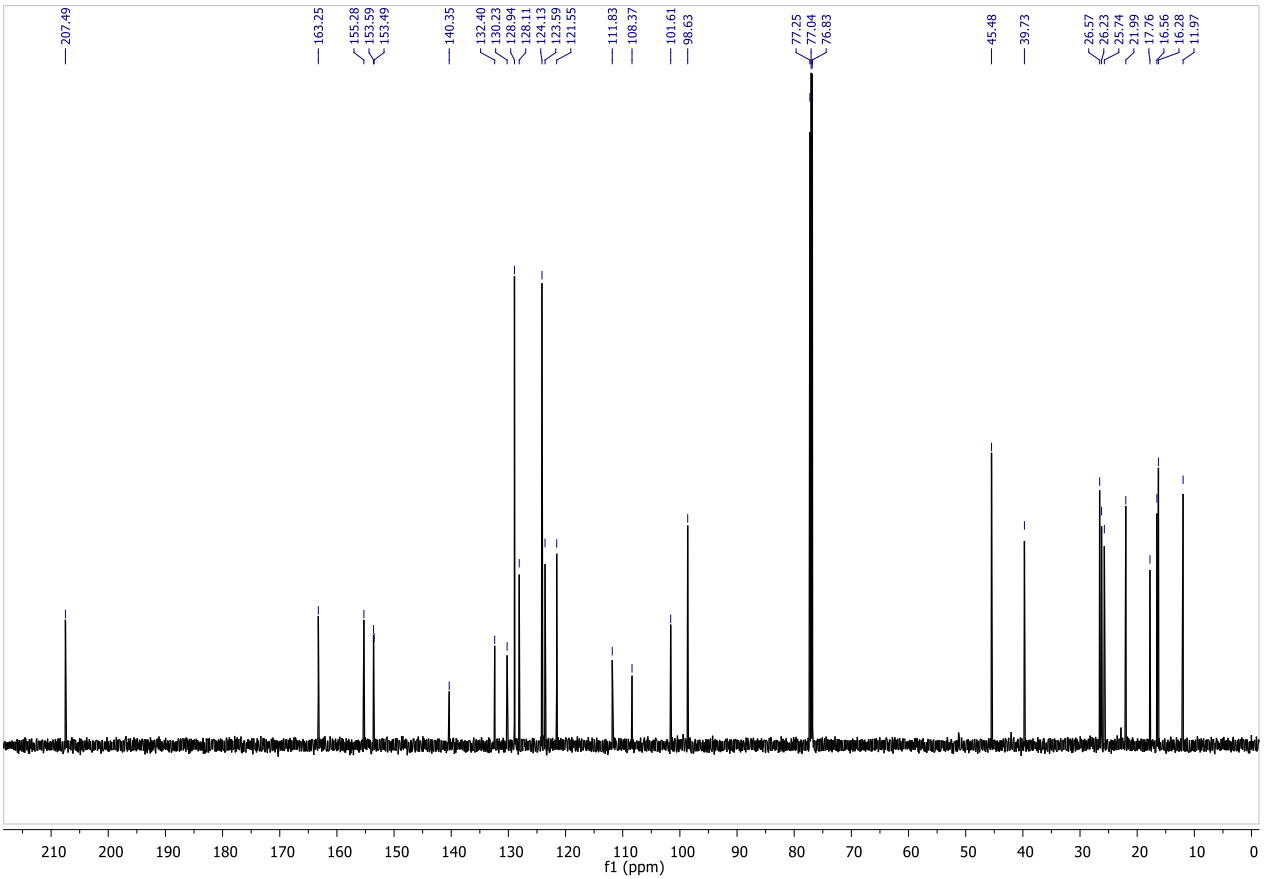
^{1}H and ^{13}C NMR spectrum of compound **7b** in $CDCl_3$



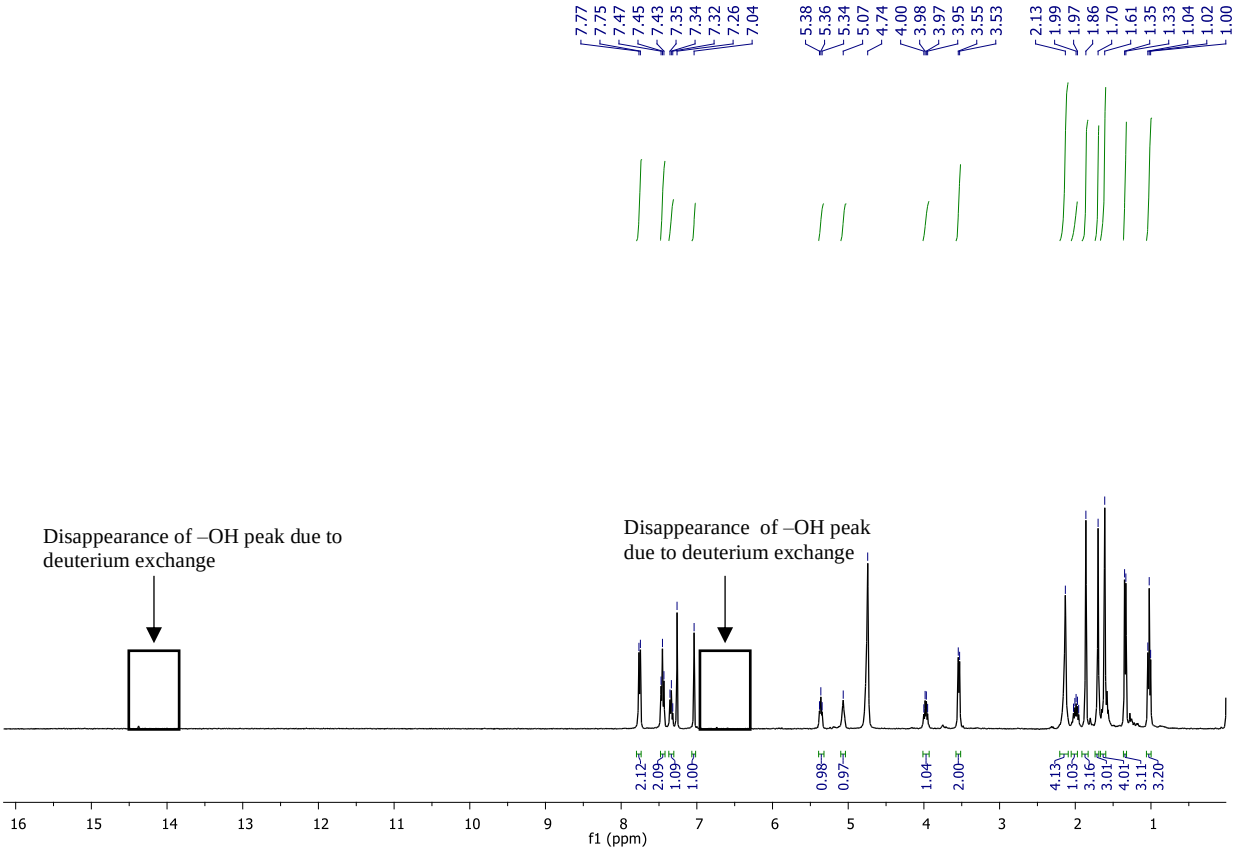


^{1}H and ^{13}C NMR spectrum of faberione B **2** in $CDCl_3$

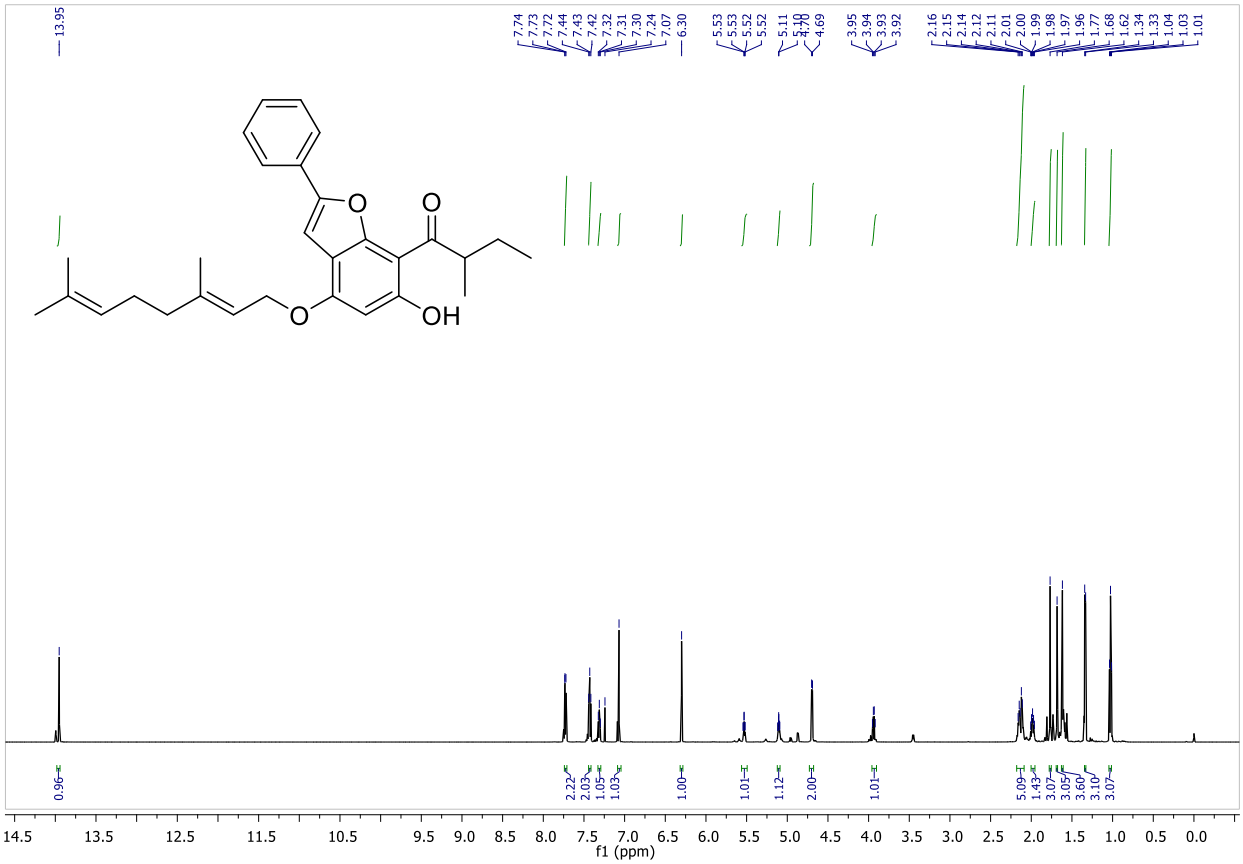


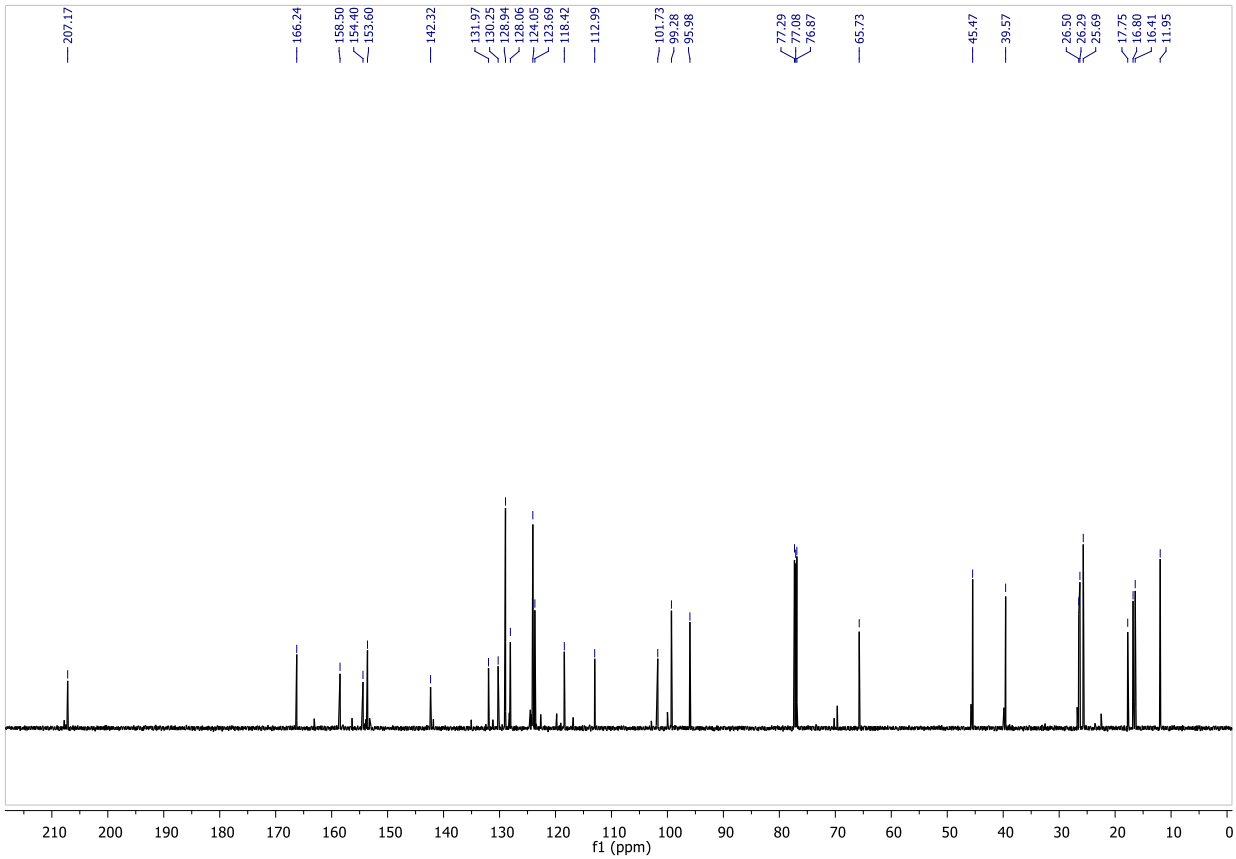


Deuterium exchange NMR of faberione B **2** in $CDCl_3$+D_2O

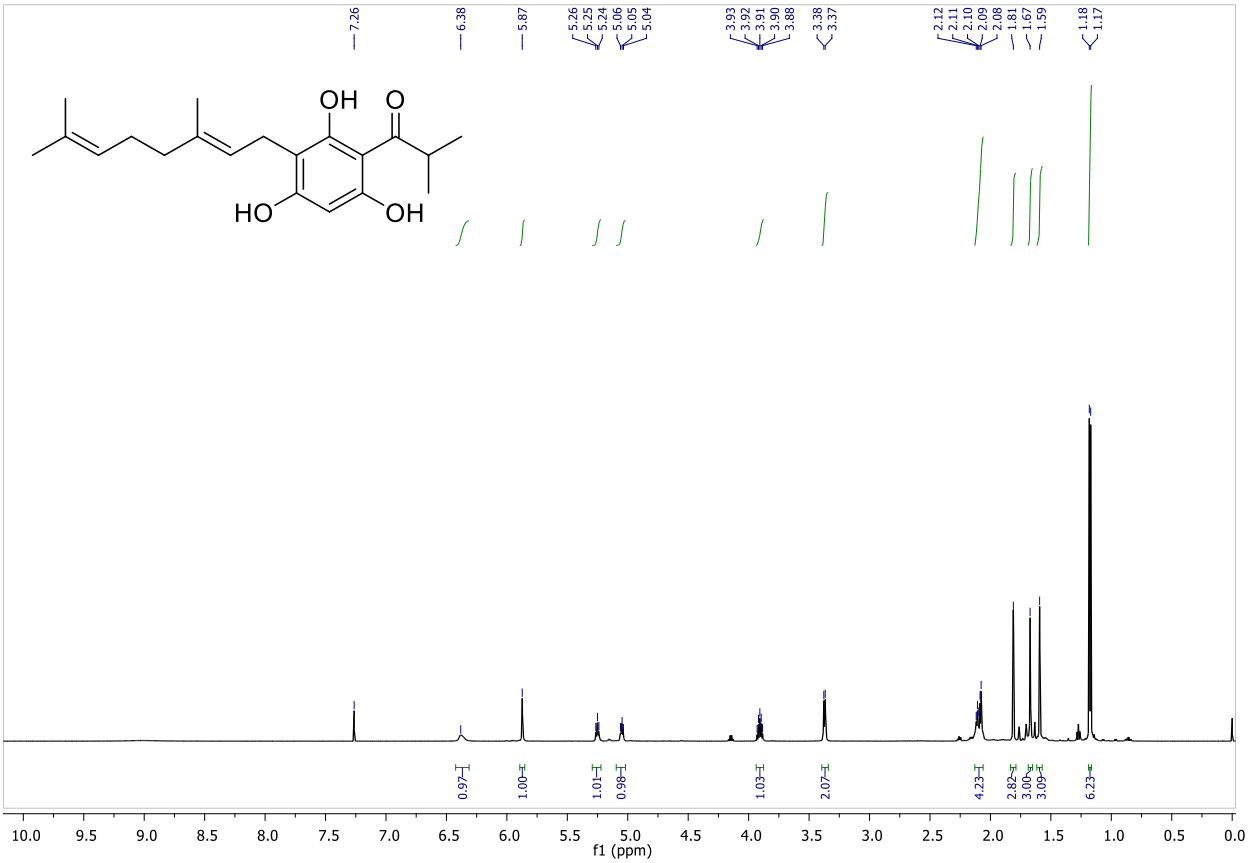


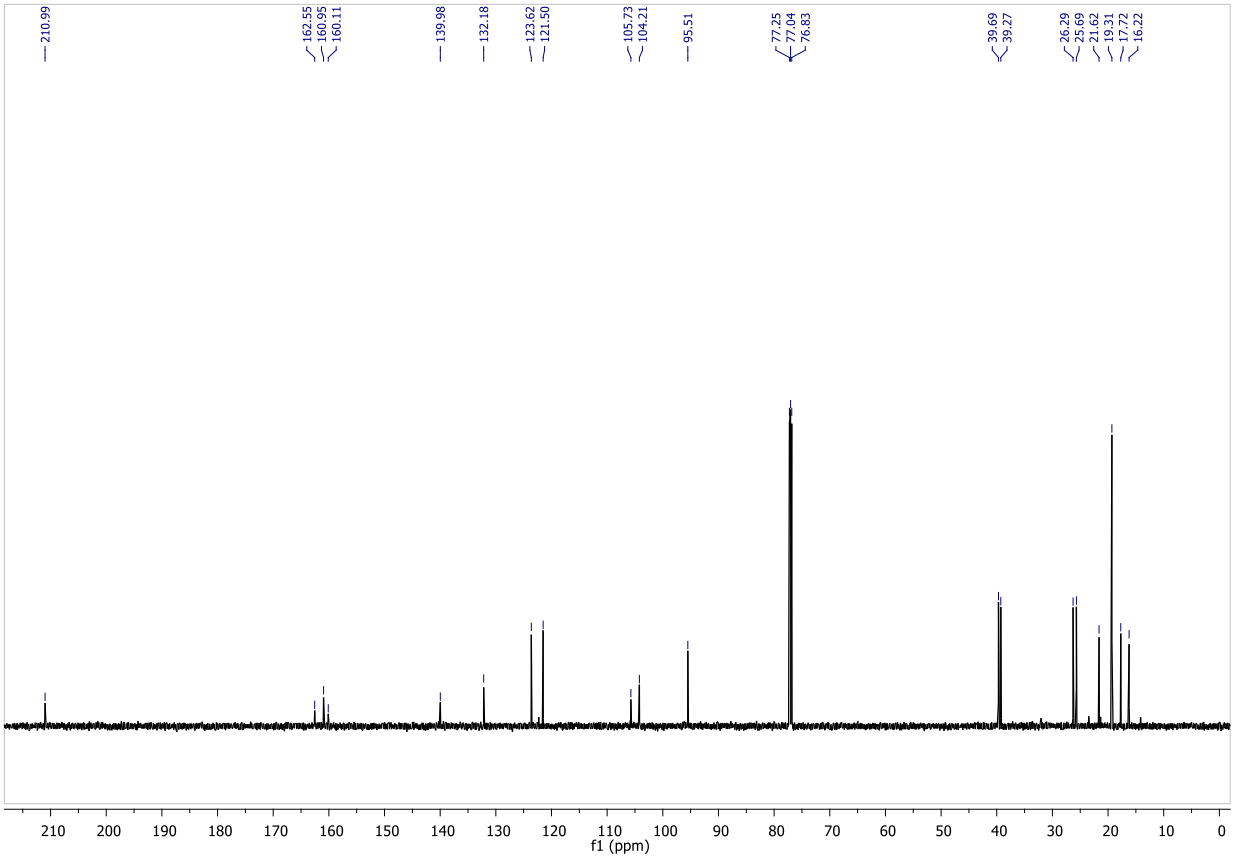
^{1}H and ^{13}C NMR spectrum of compound **12** in $CDCl_3$



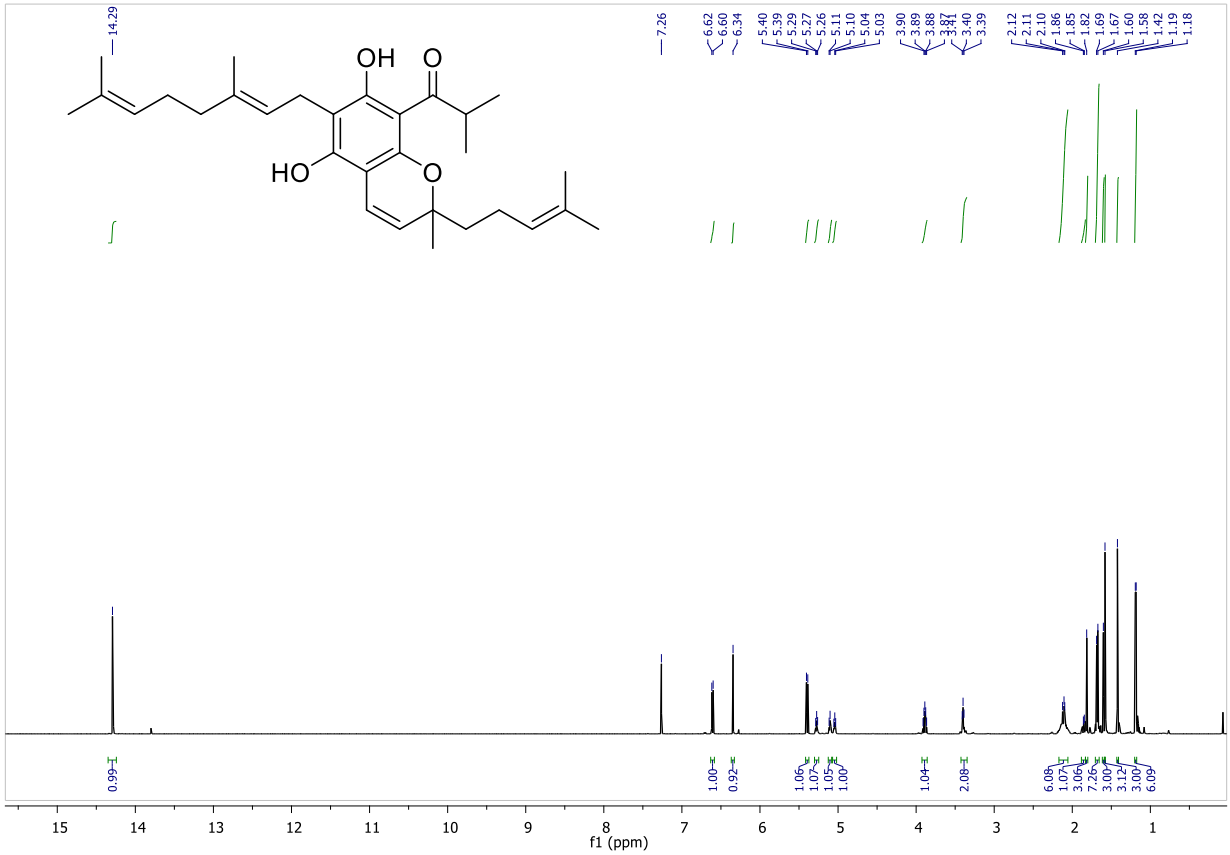


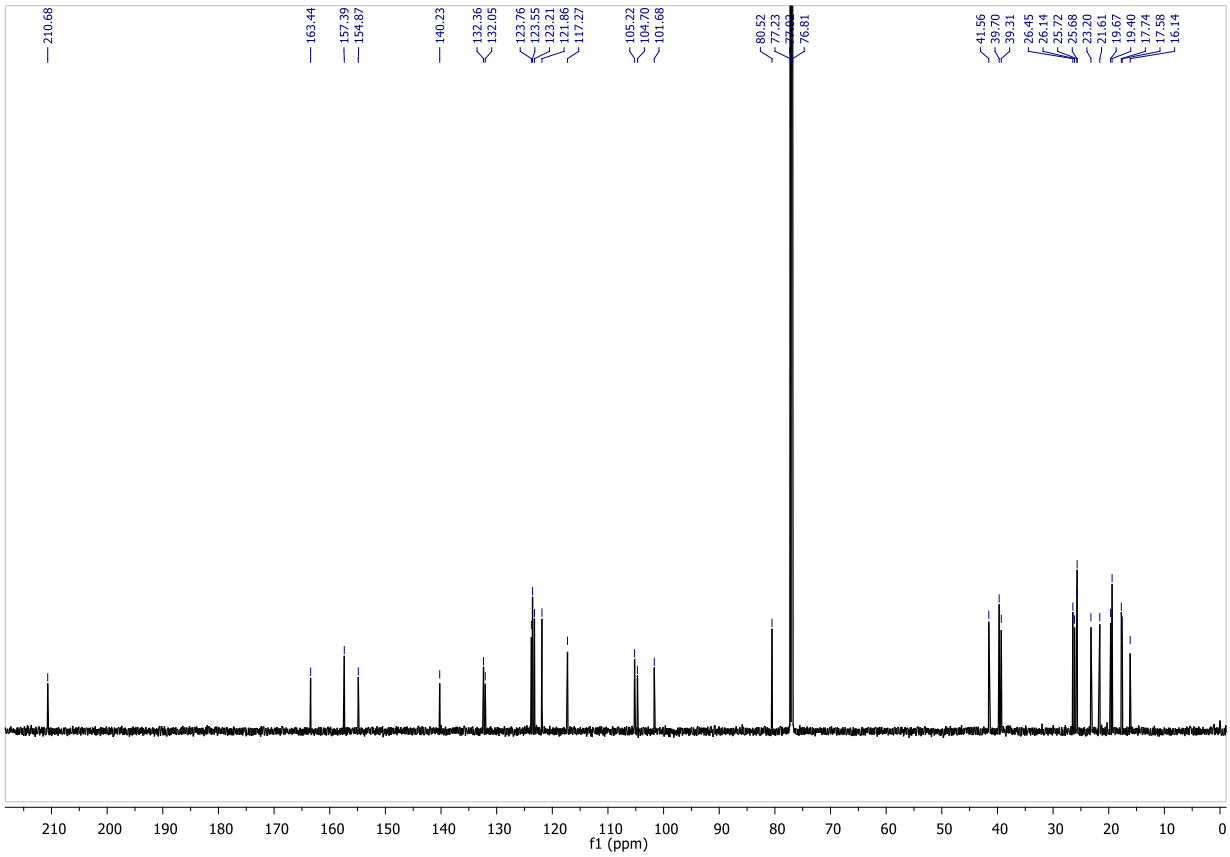
^{1}H and ^{13}C NMR spectrum of compound **13** in $CDCl_3$



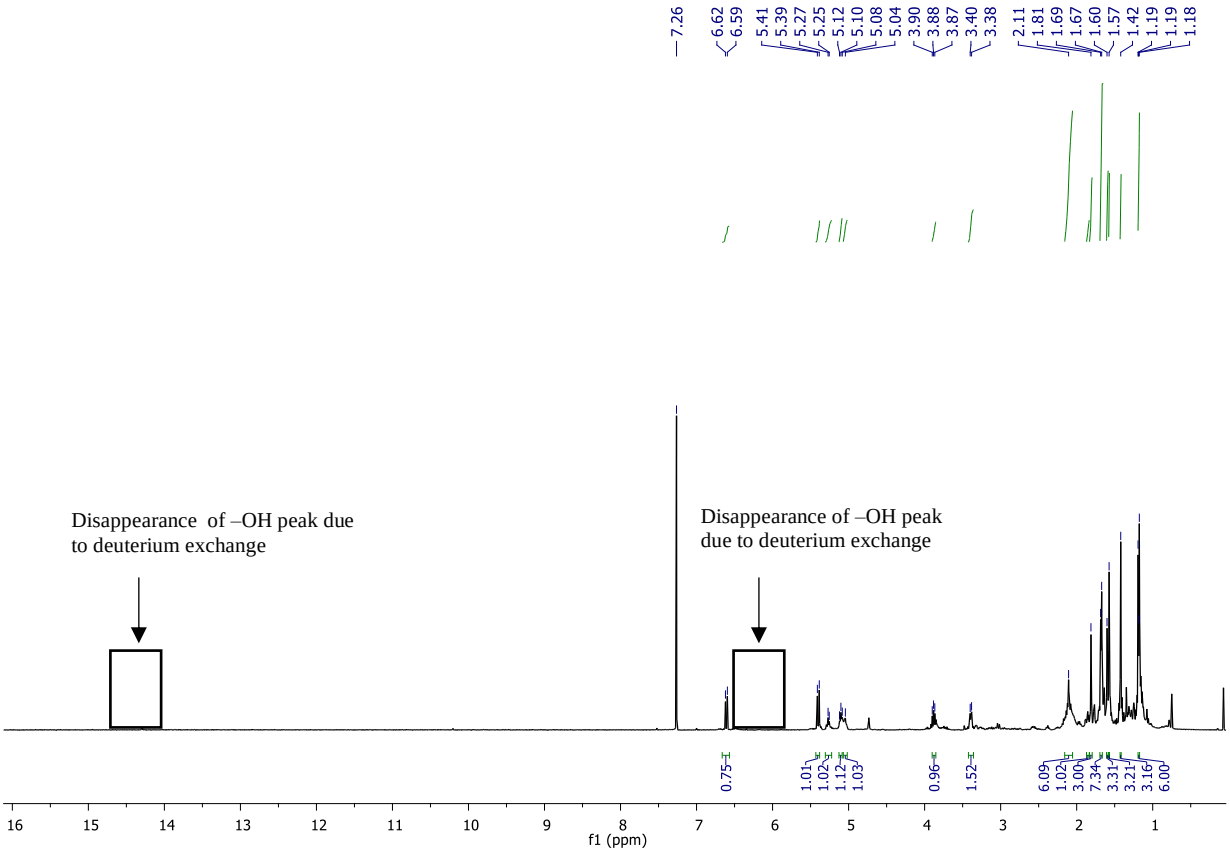


^{1}H and ^{13}C NMR spectrum of faberione E **3** in $CDCl_3$

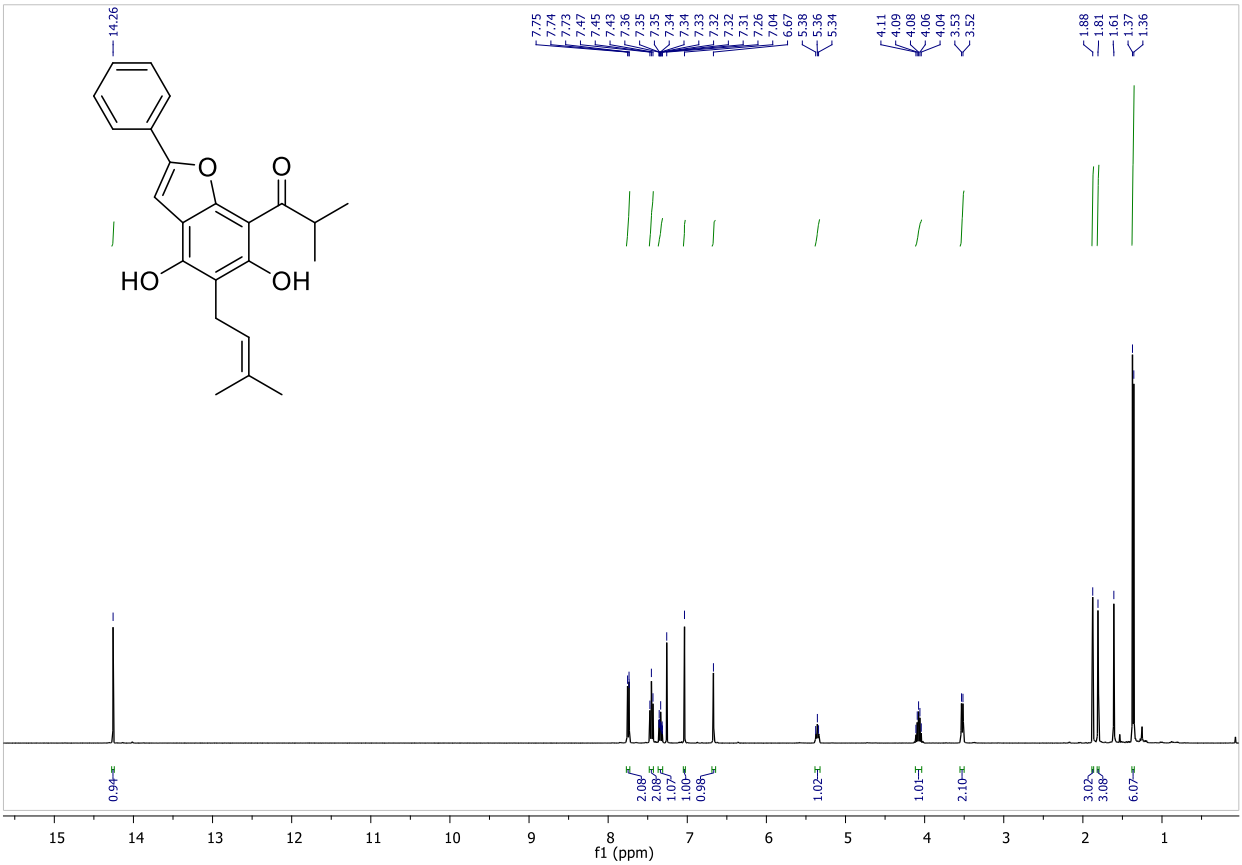


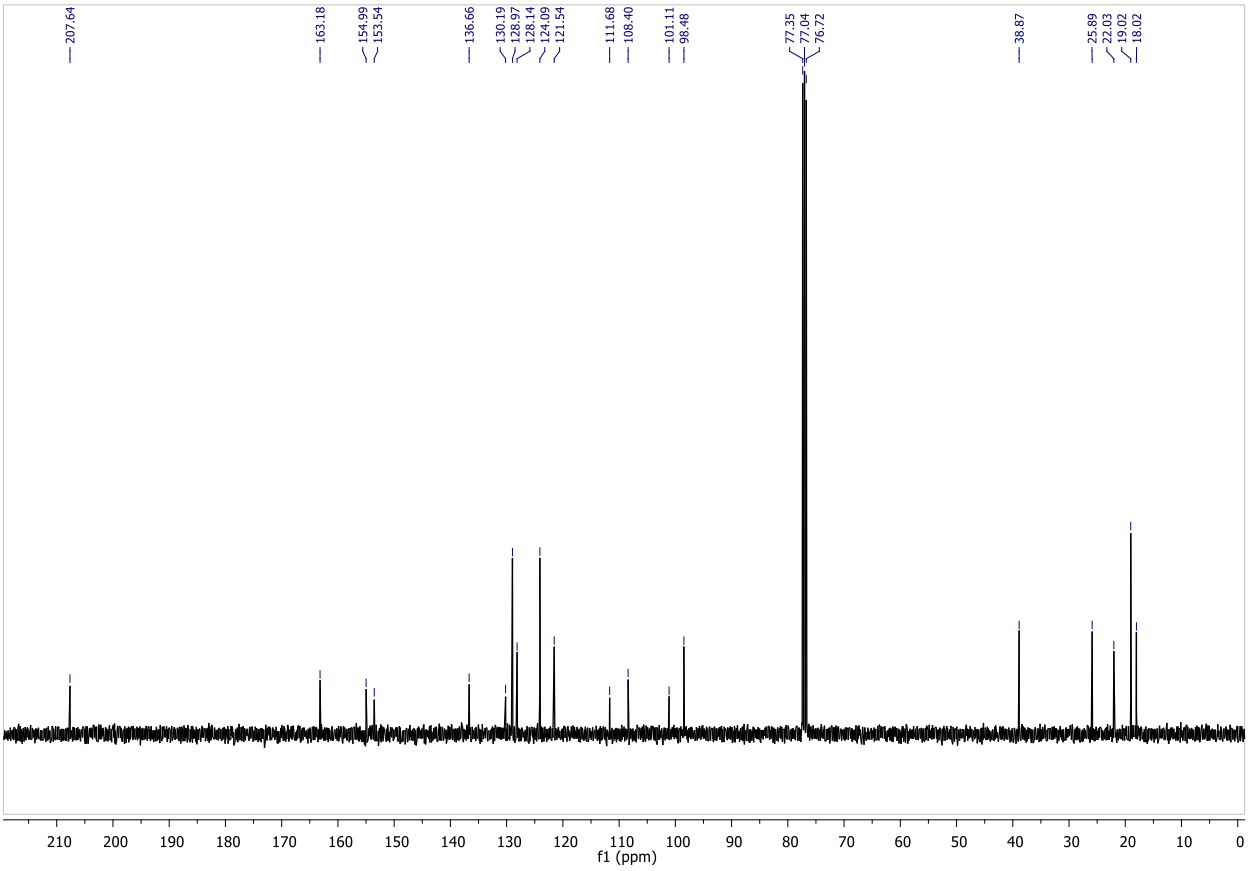


Deuterium exchange NMR of faberione E **3** in $CDCl_3$+D_2O

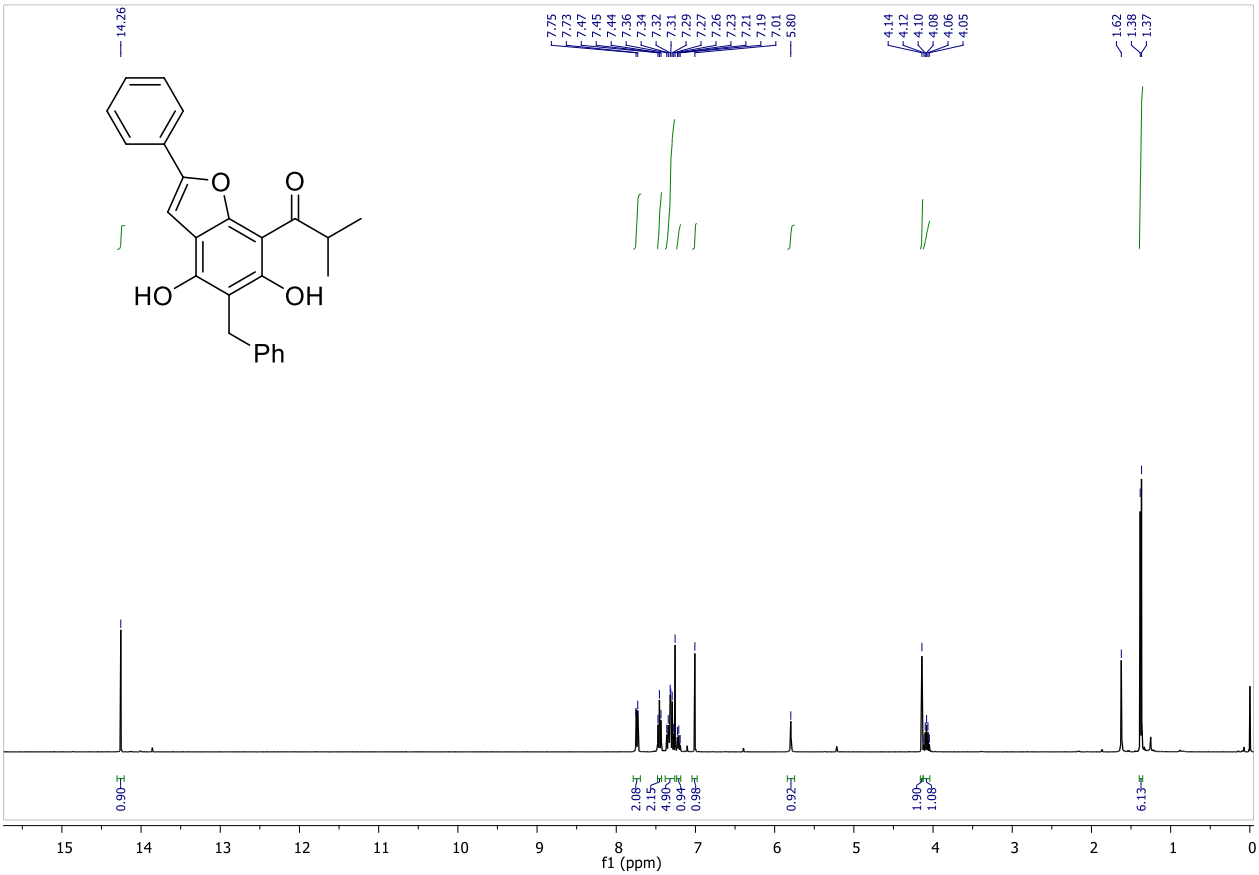


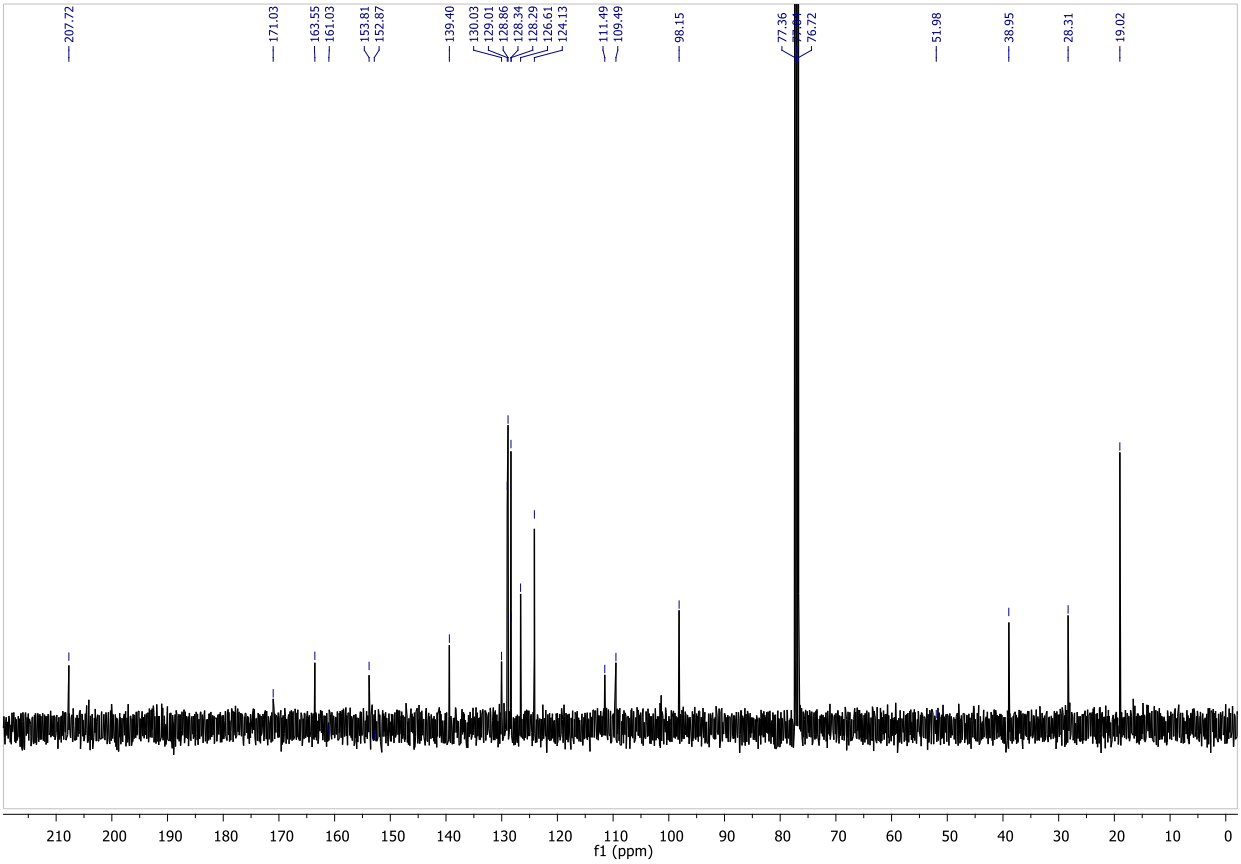
^{1}H and ^{13}C NMR spectrum of compound **1a** in $CDCl_3$



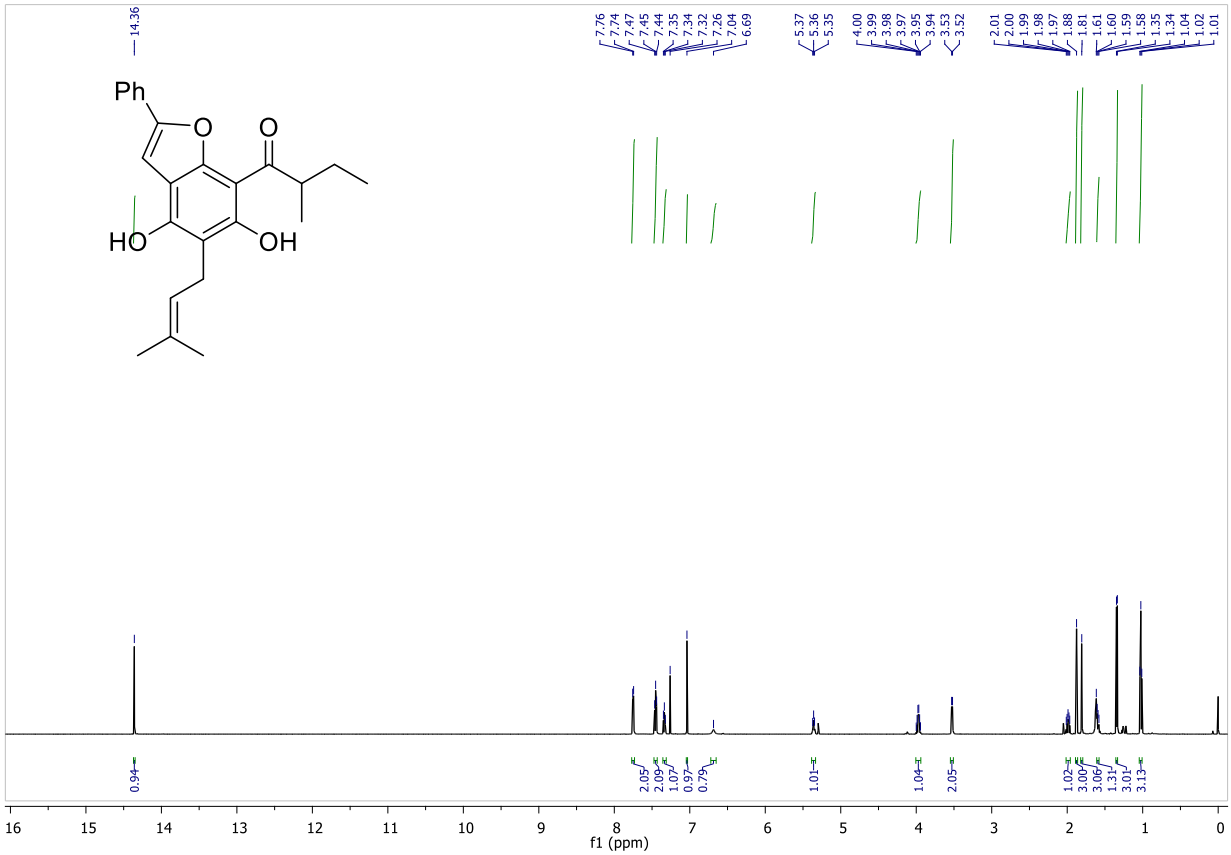


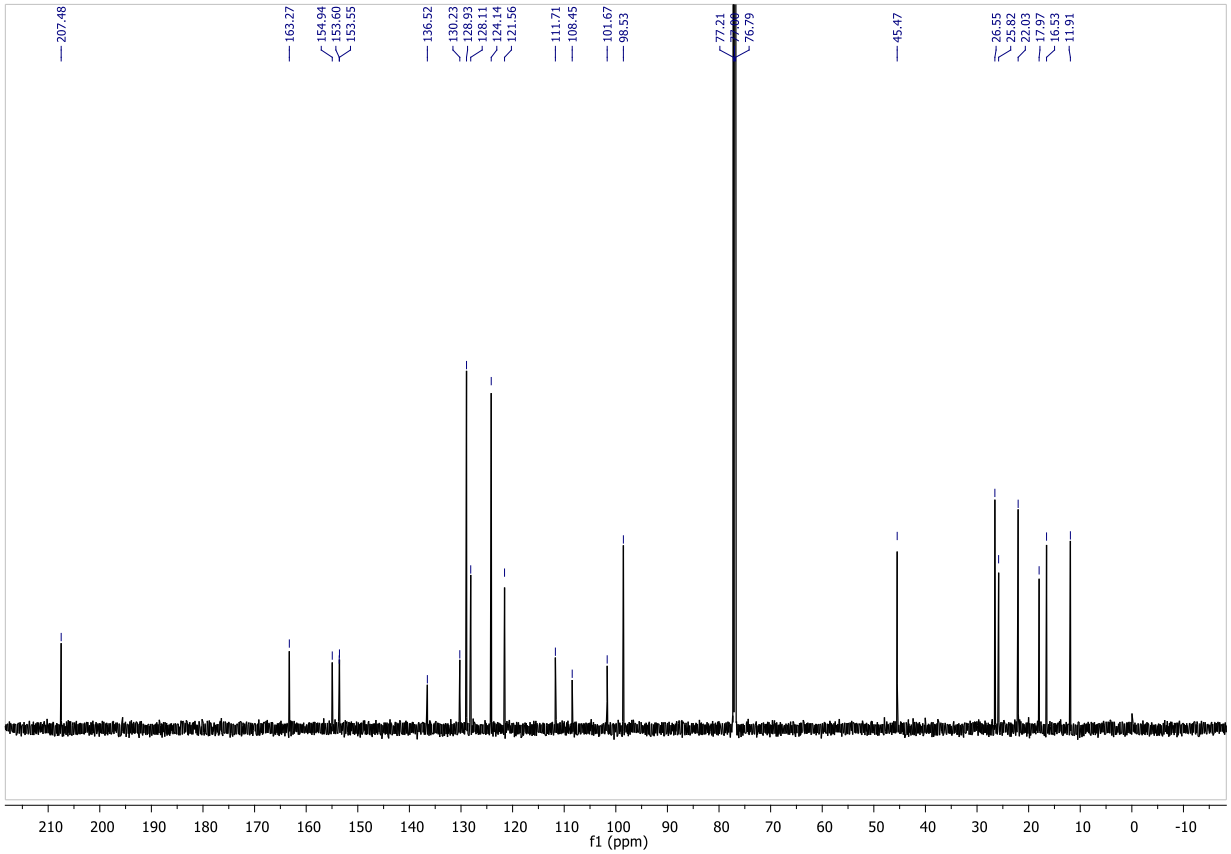
^{1}H and ^{13}C NMR spectrum of compound **1b** in $CDCl_3$



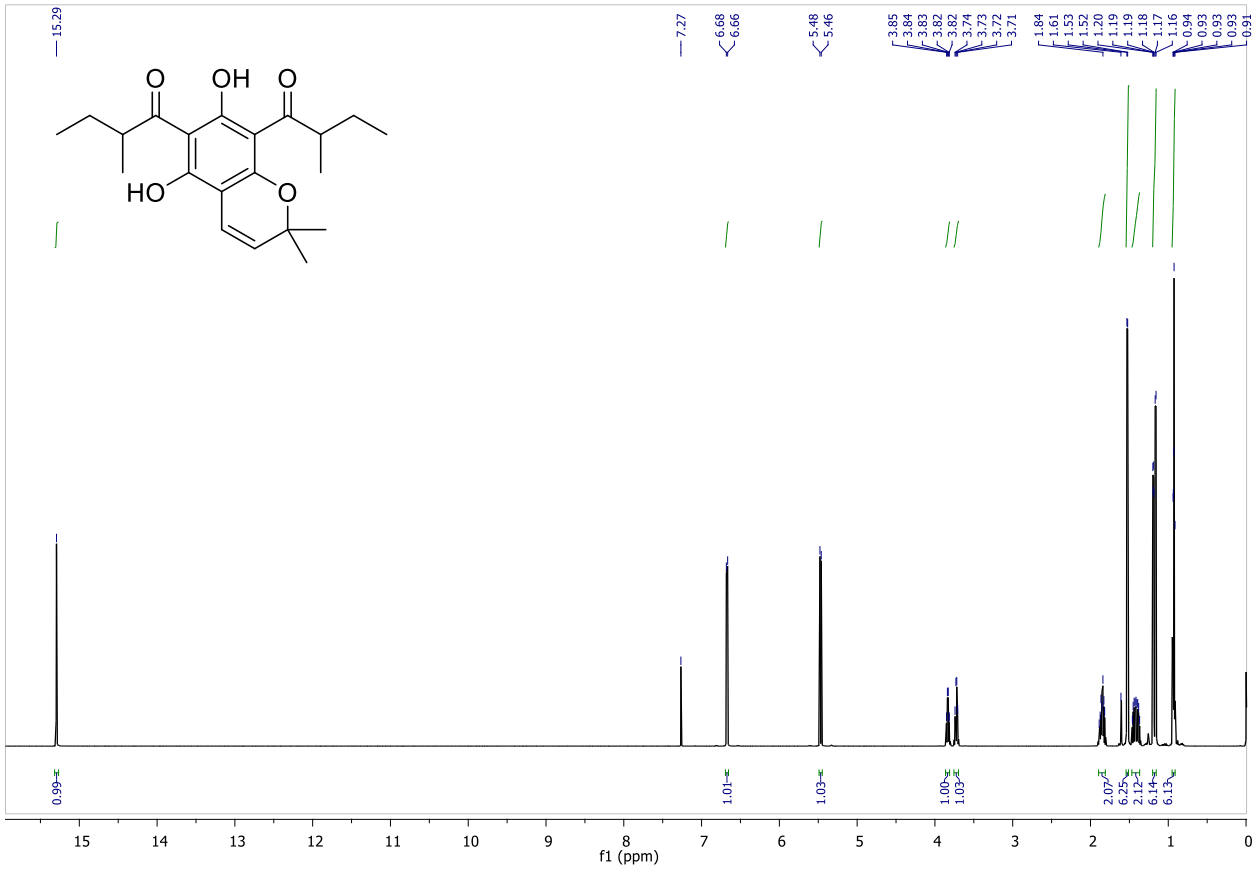


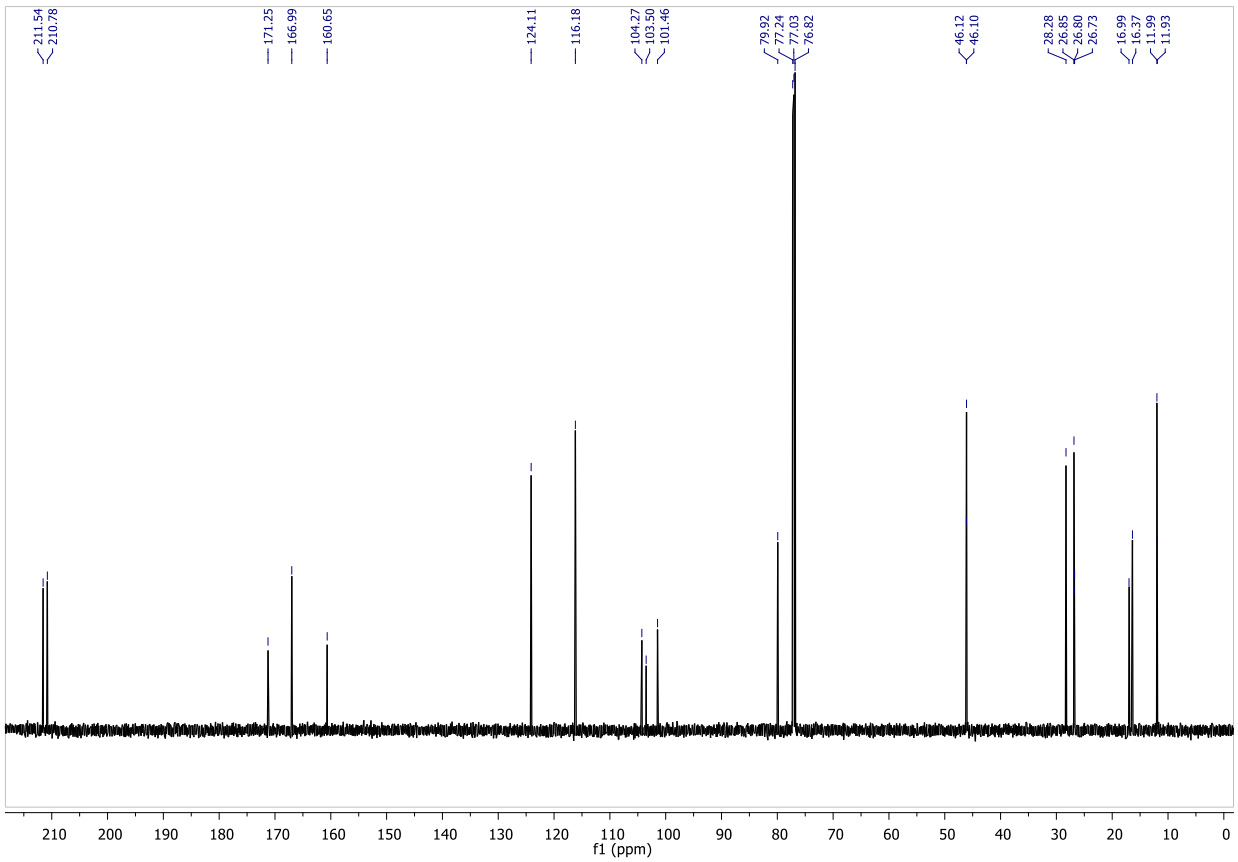
^{1}H and ^{13}C NMR spectrum of compound **2a** in $CDCl_3$



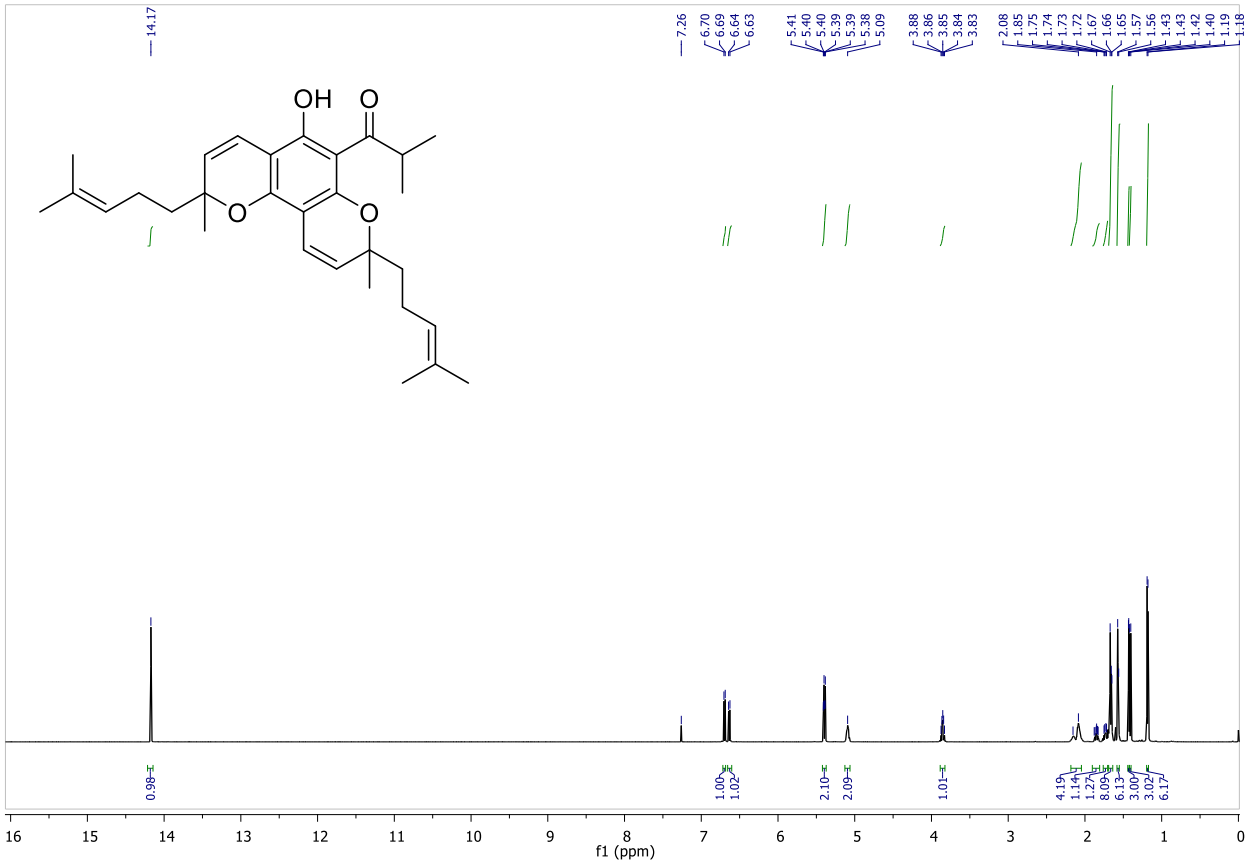


^{1}H and ^{13}C NMR spectrum of compound **3a** in $CDCl_3$





^{1}H and ^{13}C NMR spectrum of compound **3b** in $CDCl_3$



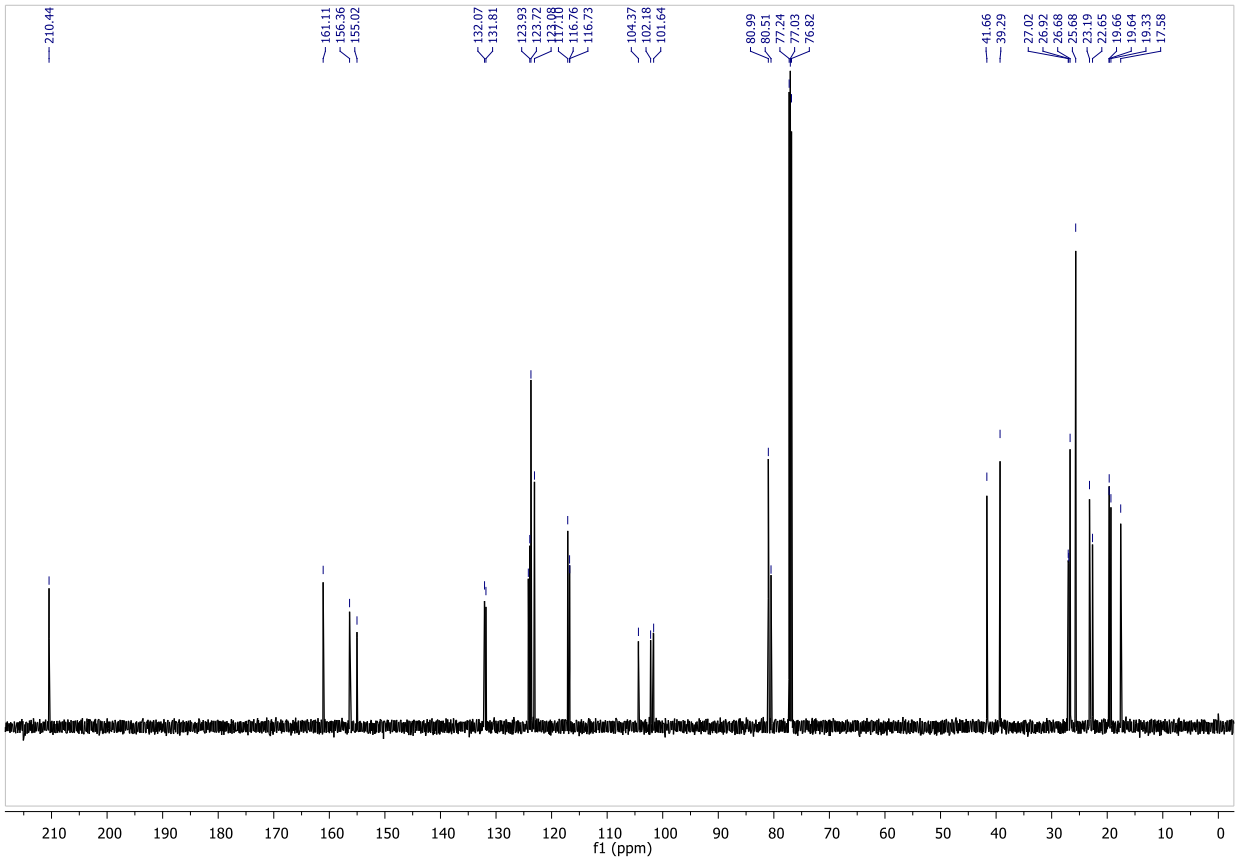
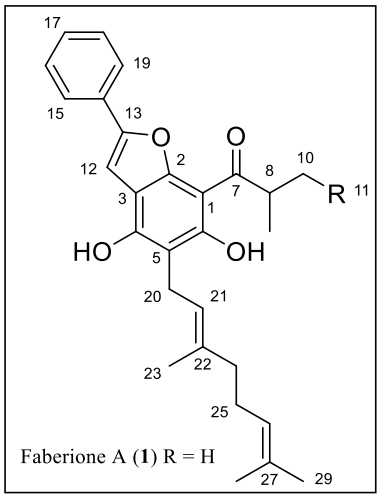
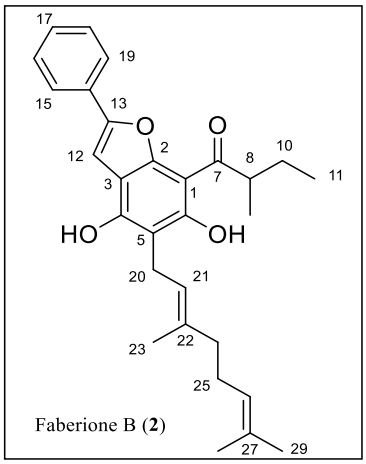


Table 1. ^{1}H and ^{13}C NMR data comparison of isolated faberione A (1) with synthetic faberione A data in $CDCl_3$



Position	Faberione A (Isolated)		Faberione A (Synthetic)	
	δ_H (mult. J/Hz) 600 MHz	δ_C 150 MHz	δ_H (mult. J/Hz) 400 MHz	δ_C 100 MHz
1		101.1, C		101.1, C
2		153.5, C		153.5, C
3		111.8, C		111.8, C
4		155.3, C		155.3, C
5		108.3, C		108.3, C
6		163.2, C		163.2, C
7		207.6, C		207.6, C
8	4.06 (sept, *J* = 6.8, 1H)	38.9, CH	4.04-4.12 (m, 1H)	38.9, CH
9	1.35 (d, *J*=6.8, 3H)	19.0, CH_3	1.37 (d, *J*=6.8, 3H)	19.0, CH_3
10	1.35 (d, *J*=6.8, 3H)	19.0, CH_3	1.37 (d, *J*=6.8, 3H)	19.0, CH_3
12	7.01 (s, 1H)	98.6, CH	7.03 (s, 1H)	98.6, CH
13		153.4, C		153.5, C
14		130.2, C		130.2, C
15, 19	7.73 (d, *J*=7.6, 2H)	124.1, CH	7.75 (d, *J*=7.4, 2H)	124.1, CH
16, 18	7.43 (t, *J*=7.6, 2H)	129.0, CH	7.45 (t, *J*=7, 2H)	129.0, CH
17	7.32 (t, *J*=7.6, 1H)	128.1, CH	7.34 (t, *J*=7.4, 1H)	128.1, CH
20	3.52 (brd, *J*=7.2, 2H)	22.0, CH_2	3.54 (brd, *J*=7.2, 2H)	22.0, CH_2
21	5.34 (t, *J*= 7.2, 1H)	121.5, CH	5.36 (t, *J*=7.5, 1H)	121.5, CH
22		140.5, C		140.5, C
23	1.84 (s, 3H)	16.3, CH_3	1.86 (s, 3H)	16.3, CH_3
24	2.11 overlap	39.7, CH_2	2.13-2.16 (m, 2H) overlap	39.7, CH_2
25	2.13, m	26.2, CH_2	2.13-2.16 (m, 2H) overlap	26.2, CH_2
26	5.04 (t, *J*= 6.1, 1H)	123.6, CH	5.06 (t, *J*= 5.4, 1H)	123.6, CH
27		132.5, C		132.4, C
28	1.68 (s, 3H)	25.8, CH_3	1.70 (s, 3H)	25.8, CH_3
29	1.59 (s, 3H)	17.8, CH_3	1.61 (s, 3H)	17.8, CH_3
30	14.26 (s, 1H) (OH-6)		14.28 (s, 1H) (OH-6)	
31	6.68 (brs, 1H) (OH-4)		6.72 (brs, 1H) (OH-4)	

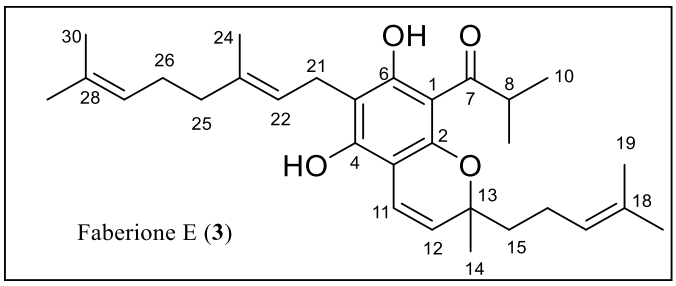
Table 2. ^{1}H and ^{13}C NMR data comparison of isolated faberione B (2) with synthetic faberione B data in $CDCl_3$



Faberione B (**2**)

Position	Faberione B (Isolated)		Faberione B (Synthetic)	
	δ_H (mult. J/Hz) 600 MHz	δ_C 150 MHz	δ_H (mult. J/Hz) 600s MHz	δ_C 150 MHz
1		101.6, C		101.6, C
2		153.5, C		153.5, C
3		111.8, C		111.8, C
4		155.3, C		155.3, C
5		108.3, C		108.4, C
6		163.2, C		163.2, C
7		207.5, C		207.5, C
8	3.95 (m, 1H)	45.5, CH	3.96-3.99 (m, 1H)	45.5, CH
9	1.32 (d, *J*= 6.8, 3H)	16.6, CH_3	1.34 (d, *J*= 6.8, 3H)	16.6, CH_3
10	1.97 (m, 1H), 1.57 (m, 1H)	26.6, CH_2	1.96-2.02 (m, 1H), 1.57-1.61 (m, 1H)	26.6, CH_2
11	1.00 (t, *J*= 7.2, 3H)	12.0, CH_3	1.03 (t, *J*= 7.2, 3H)	12.0, CH_3
12	7.01 (s, 1H)	98.6, CH	7.03 (s, 1H)	98.6, CH
13		153.5, C		153.6, C
14		130.2, C		130.2, C
15, 19	7.74 (d, *J*= 7.6, 2H)	124.1, CH	7.75 (d, *J*= 7.2, 2H)	124.1, CH
16, 18	7.43 (t, *J*= 7.6, 2H)	129.0, CH	7.45 (t, *J*= 7.2, 2H)	128.94, CH
17	7.32 (t, *J*= 7.6, 1H)	128.1, CH	7.33 (t, *J*= 7.4, 1H)	128.1, CH
20	3.52 (brd, *J*= 7.2, 2H)	22.0, CH_2	3.54 (brd, *J*= 7.2, 2H)	22.0, CH_2
21	5.35 (t, *J*= 7.2, 1H)	121.5, CH	5.36 (t, *J*= 7.2, 1H)	121.5, CH
22		140.5, C		140.4, C
23	1.84 (s, 3H)	16.3, CH_3	1.86 (s, 3H)	16.3, CH_3
24	2.11 (m, 2H) overlap	39.7, CH_2	2.12-2.15 (m, 2H) overlap	39.7, CH_2
25	2.14 (m, 2H)	26.2, CH_2	2.12-2.15 (m, 2H) overlap	26.2, CH_2
26	5.04 (t, *J*= 6.7, 1H)	123.5, CH	5.07 (t, *J*= 6.2, 1H)	123.6, CH
27		132.5, C		132.4, C
28	1.68 (s, 3H)	25.8, CH_3	1.70 (s, 3H)	25.7, CH_3
29	1.61 (s, 3H)	17.8, CH_3	1.61 (s, 3H)	17.8, CH_3
30	14.37 (s, 1H)		14.38 (s, 1H)	
31	6.69 (brs, 1H)		6.76 (brs, 1H)	

Table 3. ^{1}H and ^{13}C NMR data comparison of isolated faberione E (3) with synthetic faberione E data in $CDCl_3$



Position	Faberione E (Isolated)		Faberione E (Synthetic)	
	δ_H (mult. J/Hz) 600 MHz	δ_C 150 MHz	δ_H (mult. J/Hz) 600 MHz	δ_C 150 MHz
1		104.7, C		104.7, C
2		154.9, C		154.9, C
3		101.7, C		101.7, C
4		157.4, C		157.4, C
5		105.2, C		105.2, C
6		163.4, C		163.4, C
7		210.7, C		210.7, C
8	3.86 (sept, *J*= 6.8, 1H)	39.3, CH	3.89 (sept, *J*= 6.7, 1H)	39.3, CH
9	1.17 (d, *J*= 6.8, 3H)	19.4, CH_3	1.19 (d, *J*= 6.8, 3H)	19.4, CH_3
10	1.16 (d, *J*= 6.8, 3H)	19.7, CH_3	1.18 (d, *J*= 6.8, 3H)	19.7, CH_3
11	6.58 (d, *J*= 10.0, 1H)	117.3, CH	6.61 (d, *J*= 10.0, 1H)	117.3, CH
12	5.37 (d, *J*= 10.0, 1H)	123.2, CH	5.40 (d, *J*= 10.0, 1H)	123.2, CH
13		80.5, C		80.5, C
14	1.65-1.85 (m, 2H) overlape	41.6, CH_2	1.68-1.85 (m, 2H) overlape	41.6, CH_2
15	1.40 (s, 3H)	26.5, CH_3	1.42 (s, 3H)	26.5, CH_3
16	2.04-2.12 (m, 2H)	23.2, CH_2	2.06-2.17 (m, 2H)	23.2, CH_2
17	5.08 (t, *J*= 7.1, 1H)	123.8, CH	5.11 (t, *J*= 7.1, 1H)	123.8, CH
18		132.1, C		132.1, C
19	1.65 (s, 3H)	25.8, CH_3	1.68 (s, 3H)	25.7, CH_3
20	1.55 (s, 3H)	17.6, CH_3	1.58 (s, 3H)	17.6, CH_3
21	3.39 (m, 2H)	21.6, CH_2	3.39-3.41 (m, 2H)	21.6, CH_2
22	5.25 (t, *J*= 6.9, 1H)	121.9, CH	5.27 (t, *J*= 6.9, 1H)	121.9, CH
23		140.3, C		140.2, C
24	1.79 (s, 3H)	16.2, CH_3	1.82 (s, 3H)	16.1, CH_3
25	2.07 (m, 2H) overlape	39.7, CH_2	2.07-2.17 (m, 2H) overlape	39.7, CH_2
26	2.10 (m, 2H) overlape	26.1, CH_2	2.07-2.17 (m, 2H) overlape	26.1, CH_2
27	5.02 (t, *J*= 6.3, 1H)	123.5, CH	5.04 (t, *J*= 6.8, 1H)	123.5, CH
28		132.4, C		132.4, C
29	1.67 (s, 3H)	25.7, CH_3	1.68 (s, 3H)	25.7, CH_3
30	1.58 (s, 3H)	17.8, CH_3	1.60 (s, 3H)	17.7, CH_3
31	14.28 (s, 1H)	OH-6	14.29 (s, 1H)	
32	6.33 (brs, 1H)	OH-4	6.34 (brs, 1H)	

