Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Total Synthesis of Nafuredin B

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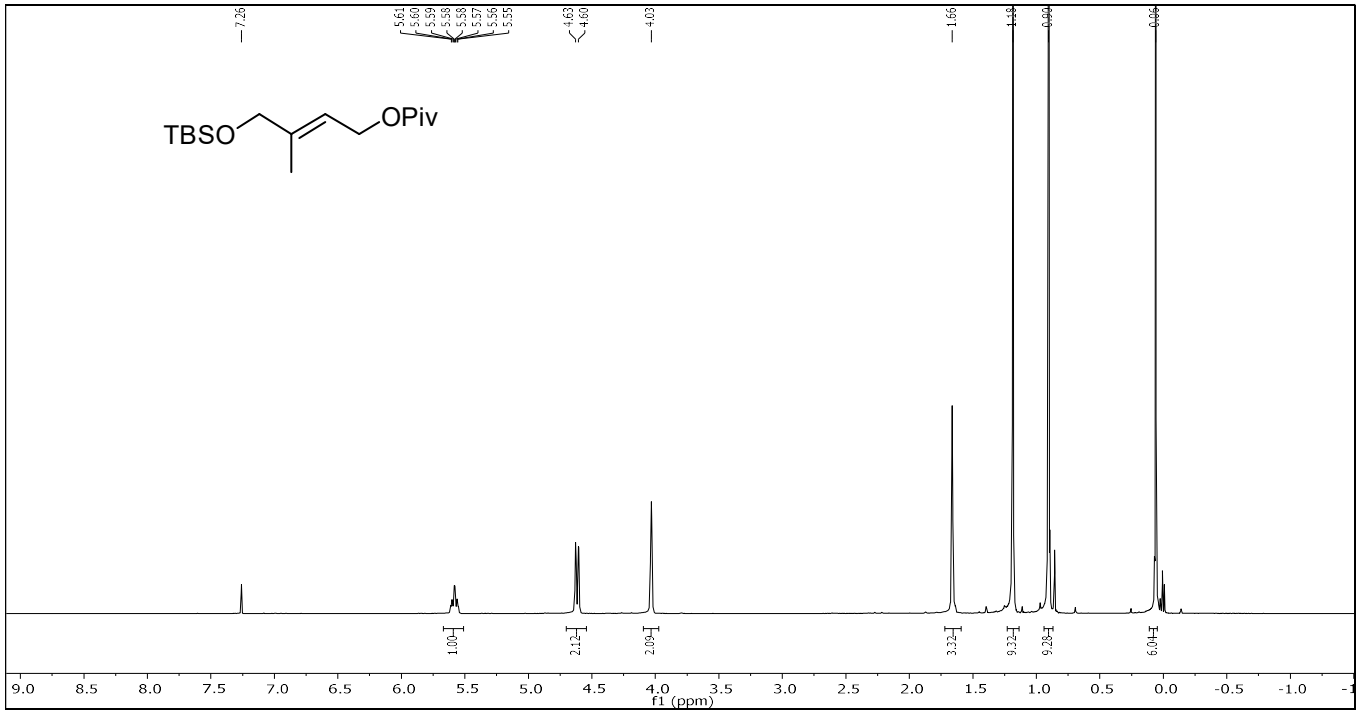
Supporting Information

1. Table S1: ^{1}H and ^{13}C NMR Comparison between Synthetic and Isolated Nafuridin B

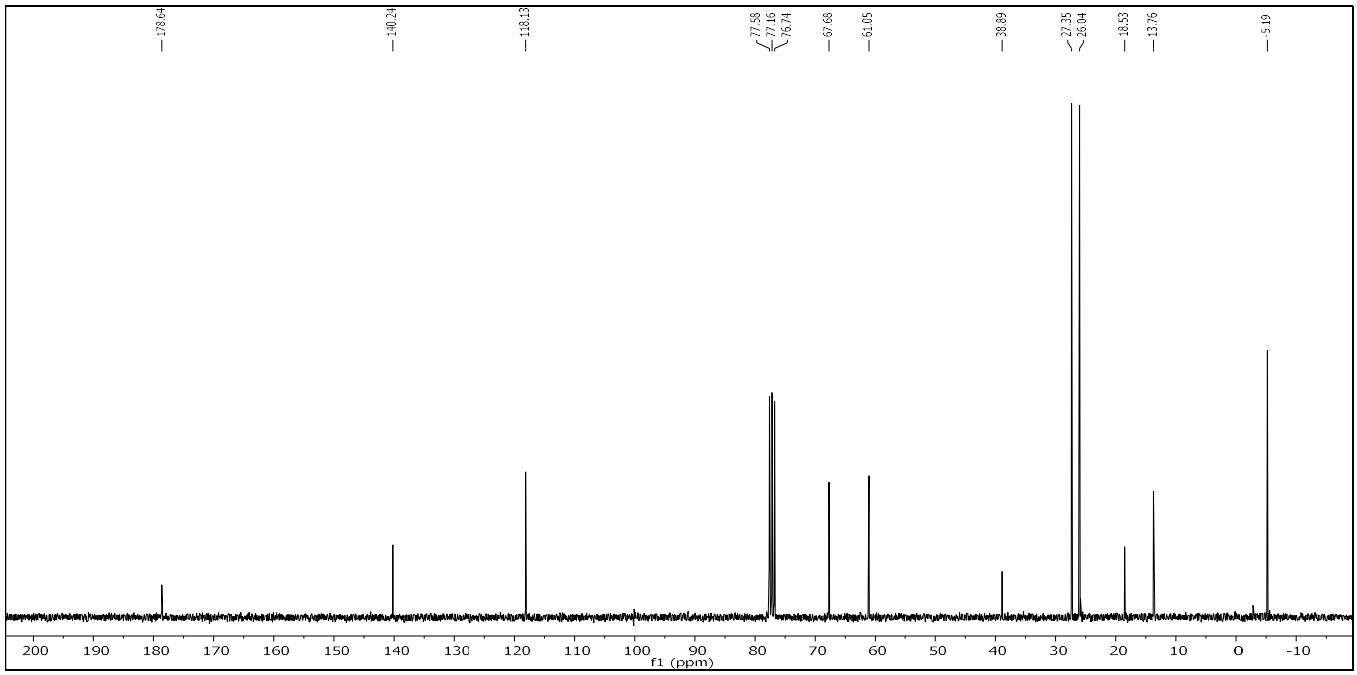
Position	Isolated compound δ_H in ppm, (J in Hz)	Synthetic compound δ_H in ppm, (J in Hz)	Isolated compound δ_C in ppm	Synthetic compound δ_C in ppm
1			163.3	163.3
2	5.83, d (9.8)	5.85, d (9.8)	118.0	118.1
3	6.89, d (9.8)	6.88, d (9.7)	156.3	156.2
4			68.0	68.0
5	4.73, d (6.7)	4.74, d (6.5)	84.4	84.3
6	5.64, m	5.70, m	124.5	124.5
7	6.30, dd (10.5, 14.8)	6.31, dd (10.5, 15.2)	134.7	134.7
8	6.08, dd (10.5, 15.3)	6.10, dd (10.6, 15.3)	127.7	127.7
9	5.68, m	5.75, m	142.1	142.2
10	2.41, m	2.42, m	34.7	34.7
11	2.04, m, 1.95, dd (7.6, 13.3)	2.06, m, 1.95, dd (7.7, 13.4)	47.3	47.3
12			134.5	134.5
13	5.73, dd (10.8, 14.8)	5.67, d (8.9)	126.9	126.9
14	6.16, dd (10.8, 15.1)	6.18, dd (10.7, 15.2)	125.2	125.2
15	5.43, dd (7.8, 15.1)	5.44, dd (7.8, 15.1)	138.4	138.5
16	2.07, m	2.07, m	38.4	38.4
17	1.27, m	1.28, m	29.7	29.7
18	0.81, d (7.4)	0.81, t (7.4)	12.1	12.1
19	1.09, s	1.10, s	21.4	21.5
20	0.92, d (6.7)	0.93, d (6.9)	20.1	20.1
21	1.67, s	1.67, s	16.7	16.7
22	0.94, d (6.7)	0.95, d (6.6)	20.5	20.5

2. Copies of 1H-NMR, 13C-NMR, 2D-NMR and HRMS Spectra

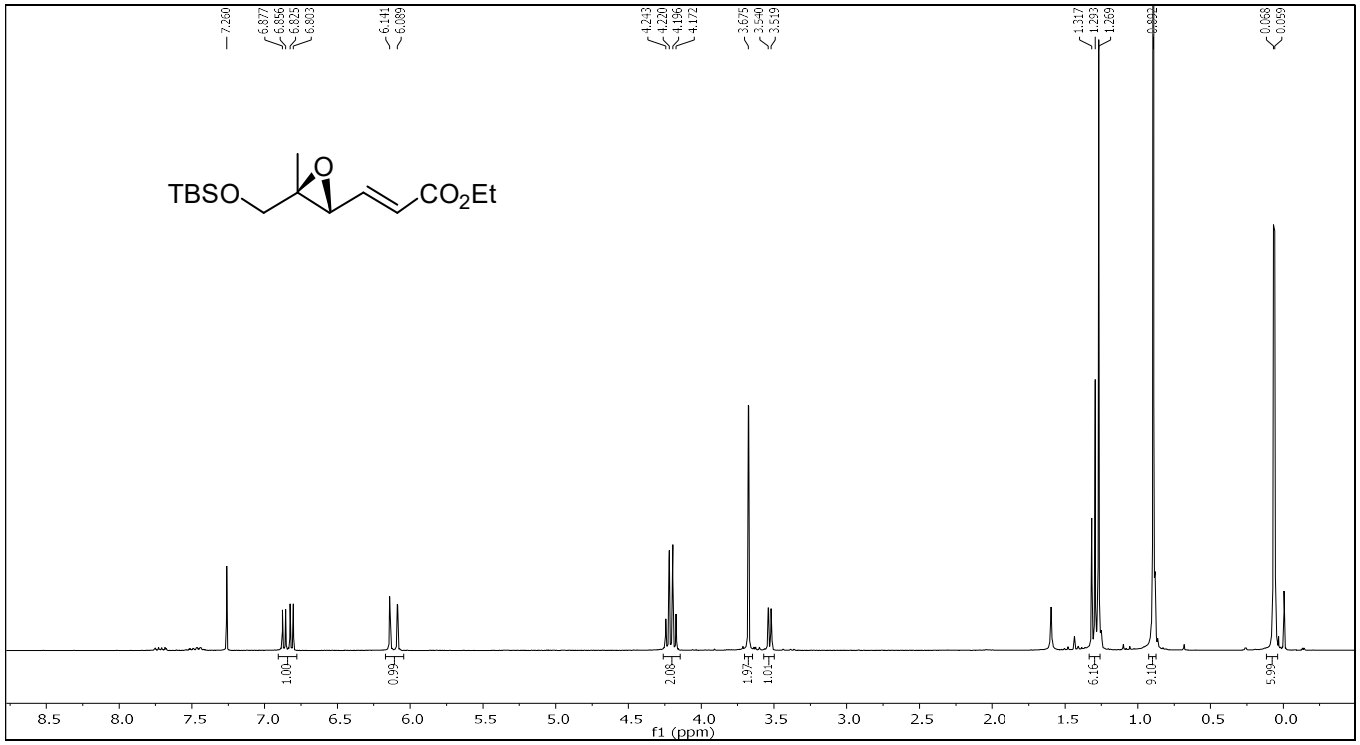
^{1}H-NMR spectrum of compound 13 (300 MHz, $CDCl_3$):



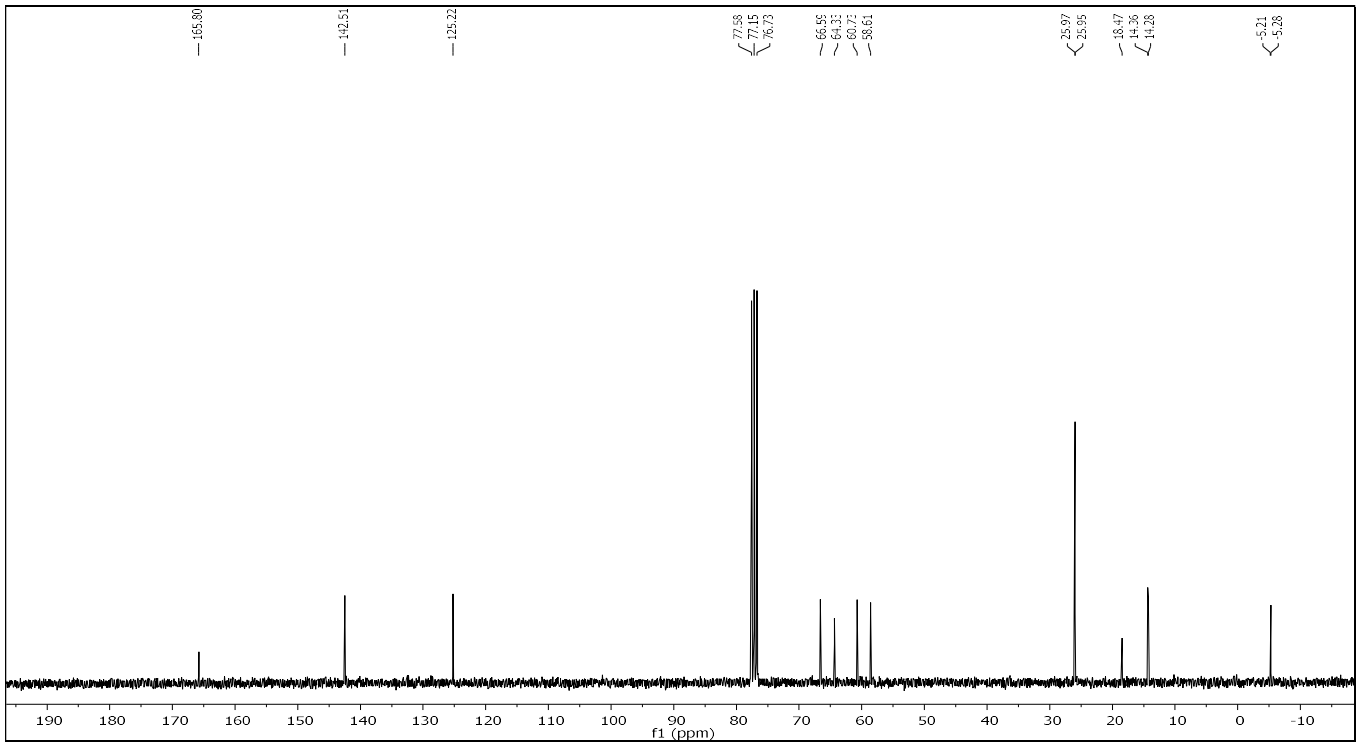
^{13}C-NMR spectrum of compound 13 (75 MHz, $CDCl_3$):



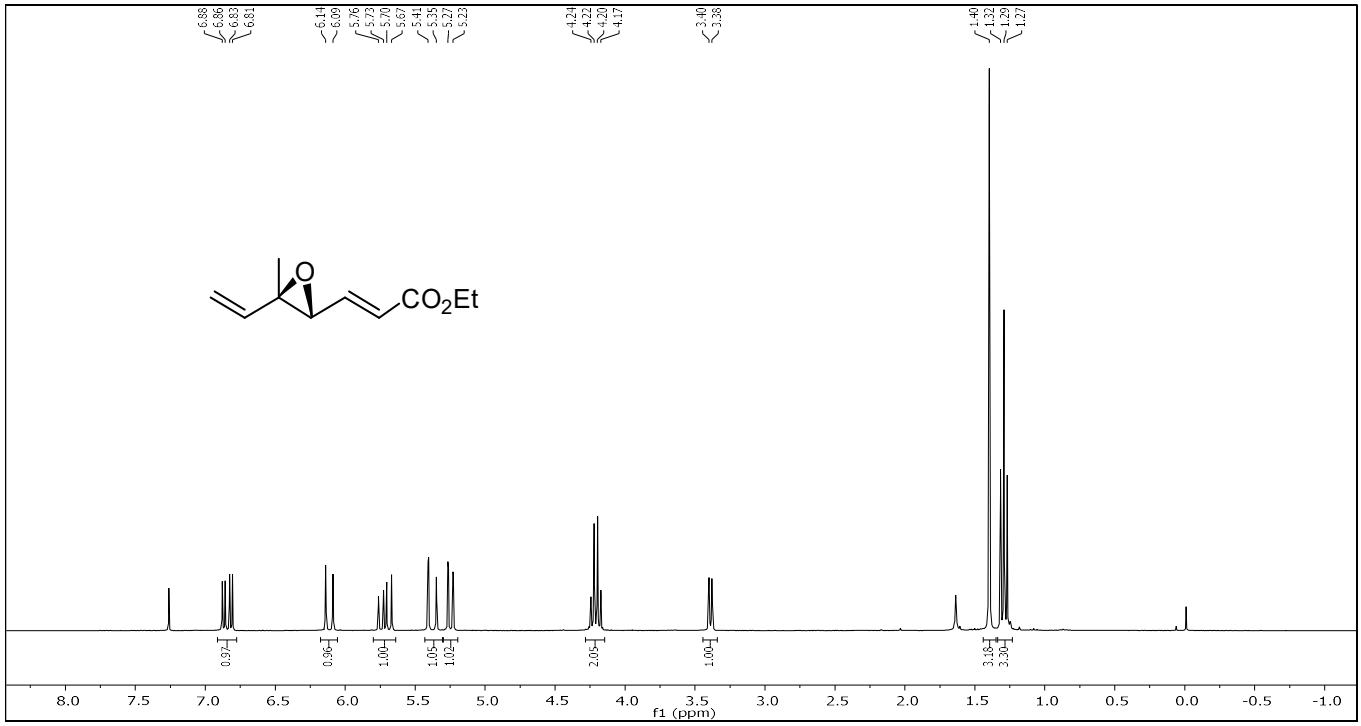
^{1}H-NMR spectrum of compound 14 (300 MHz, $CDCl_3$):



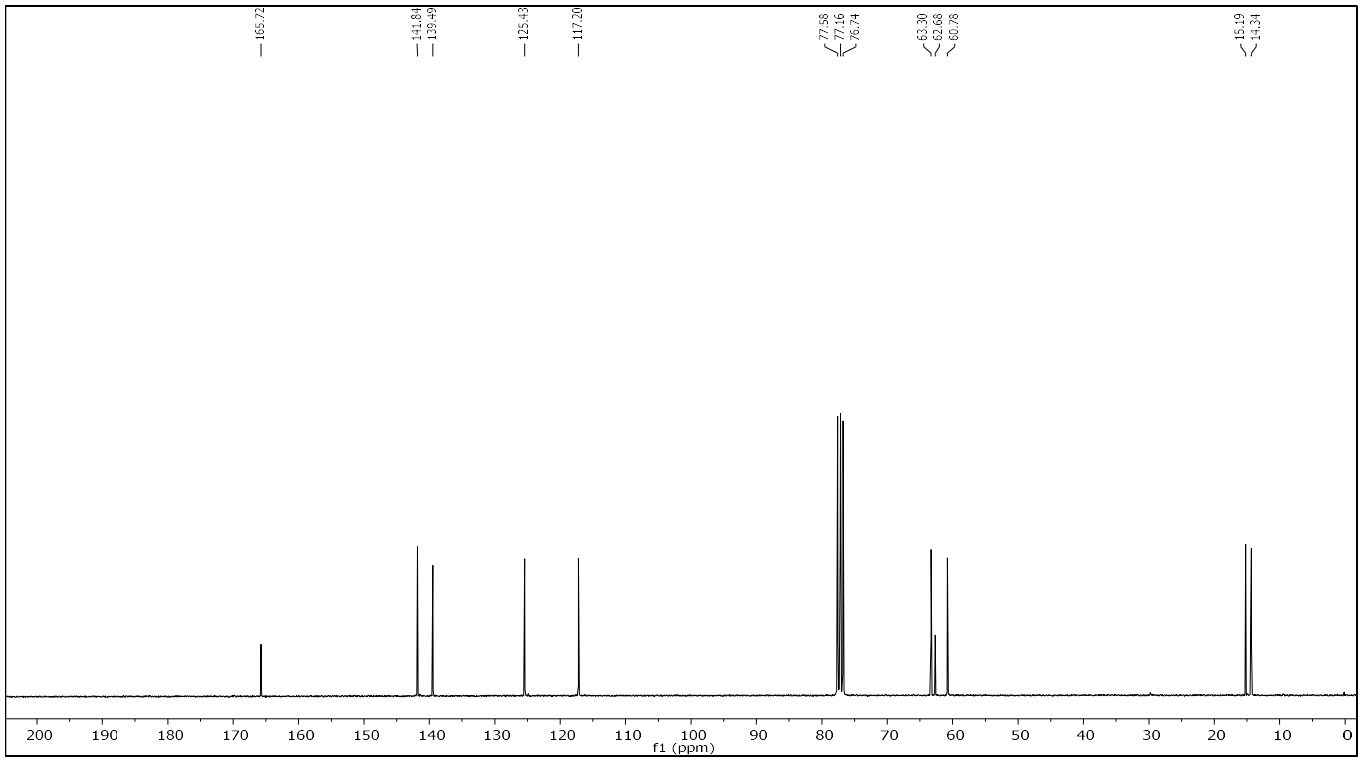
^{13}C-NMR spectrum of compound 14 (75 MHz, $CDCl_3$):



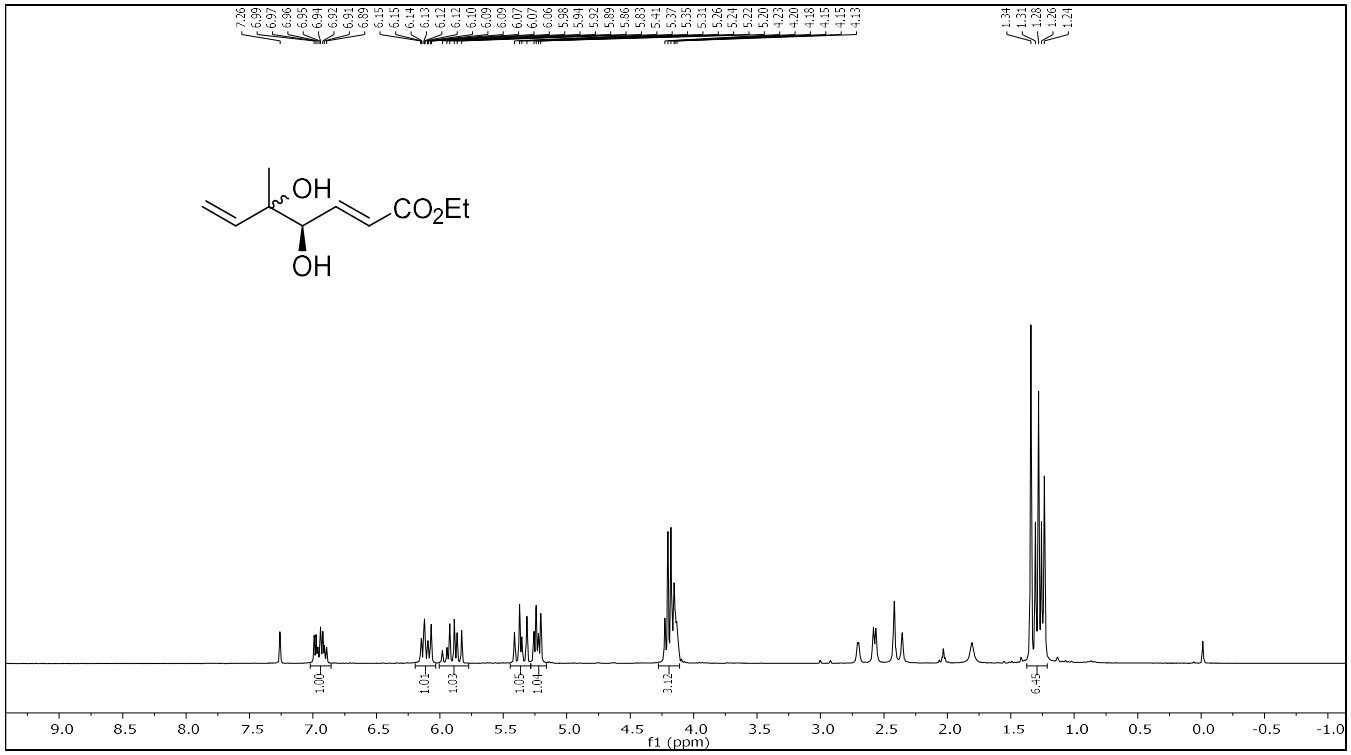
^{1}H-NMR spectrum of compound 11 (300 MHz, $CDCl_3$):



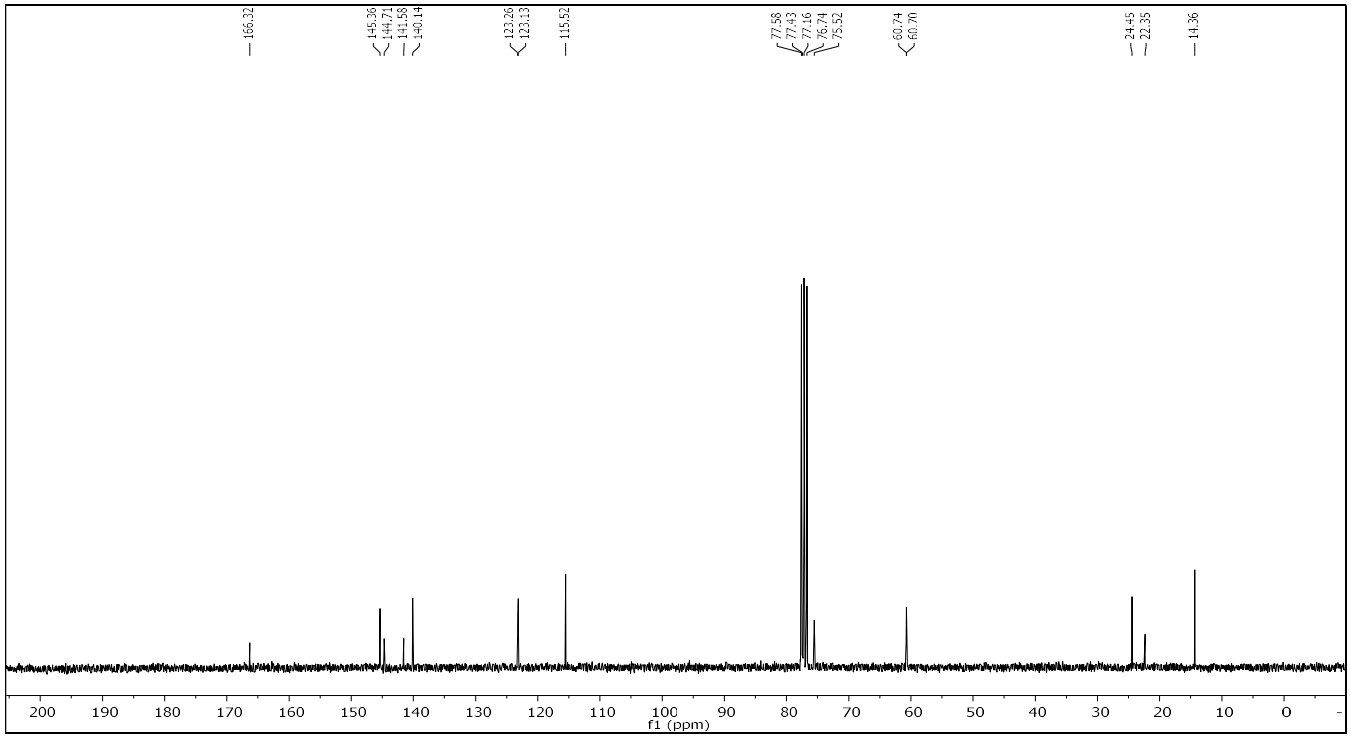
^{13}C-NMR spectrum of compound 11 (75 MHz, $CDCl_3$):



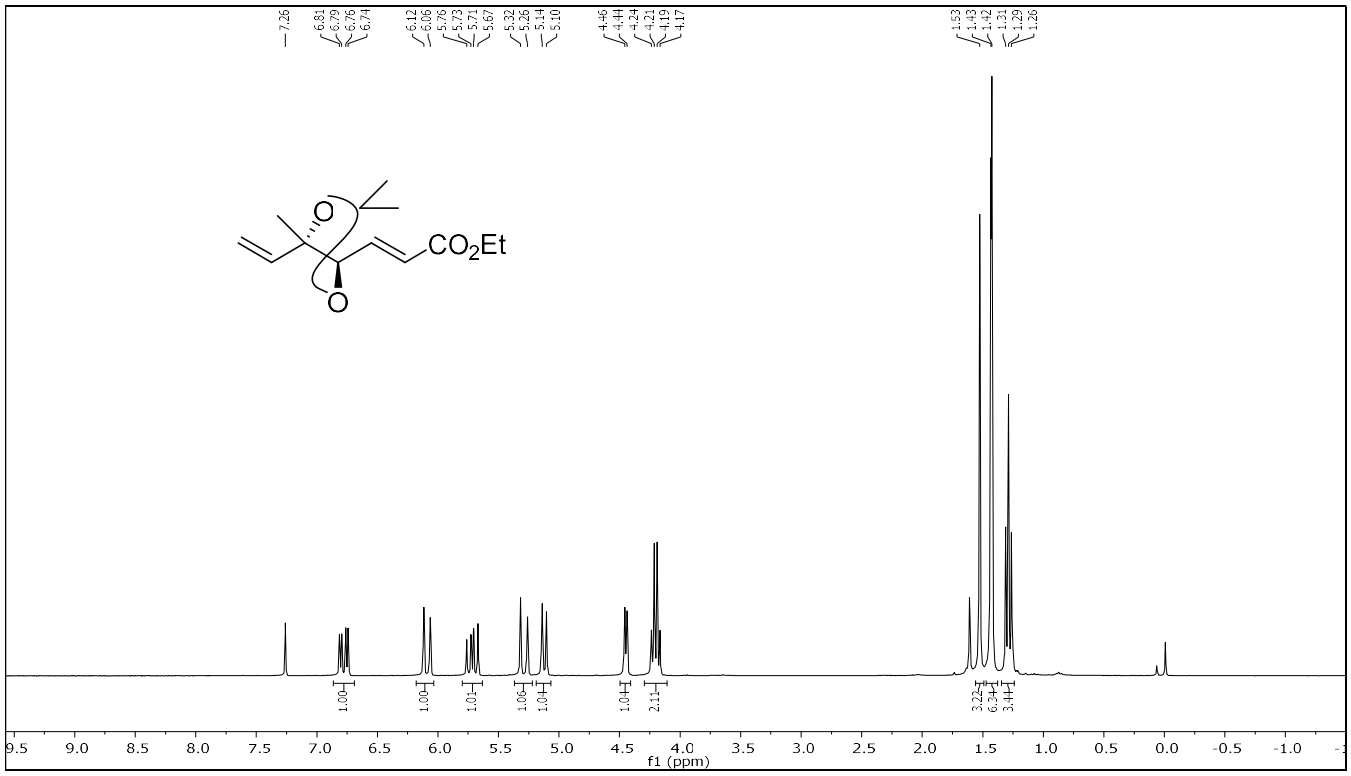
^{1}H-NMR spectrum of compound 15a/15b (300 MHz, $CDCl_3$):



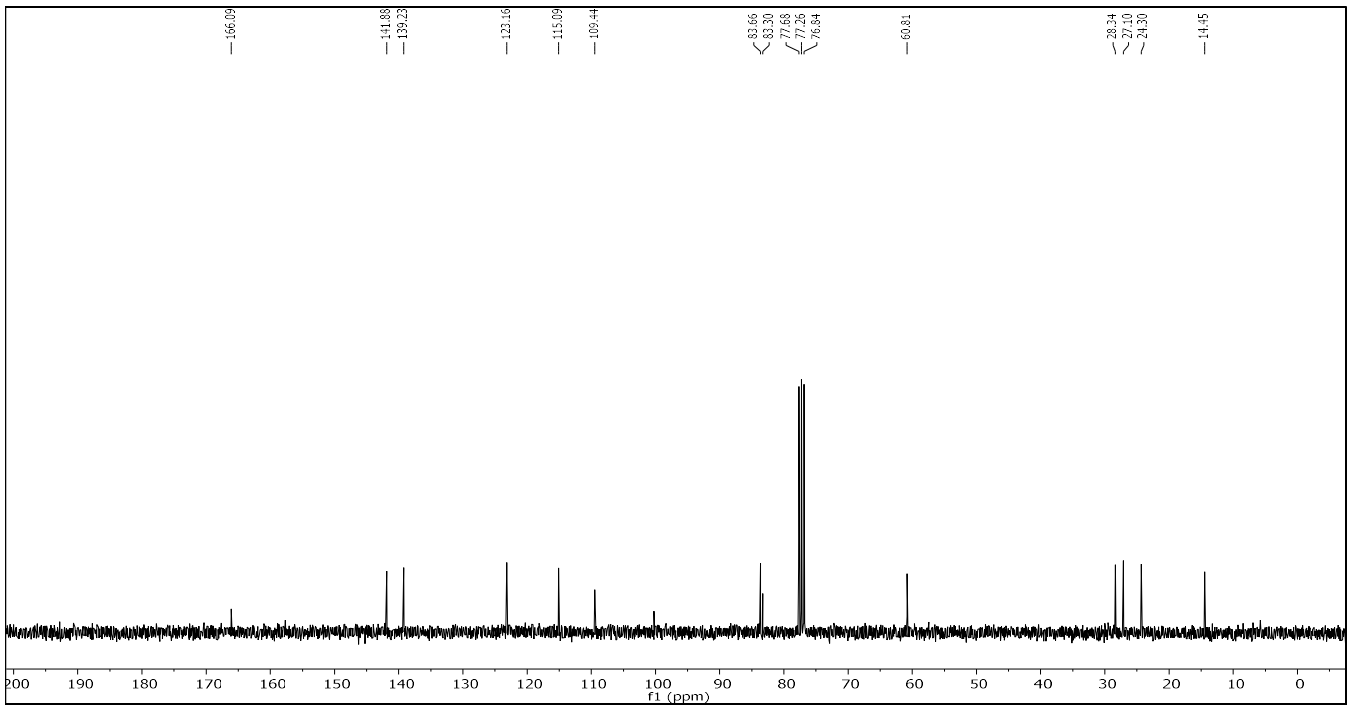
^{13}C-NMR spectrum of compound 15a/15b (75 MHz, $CDCl_3$):



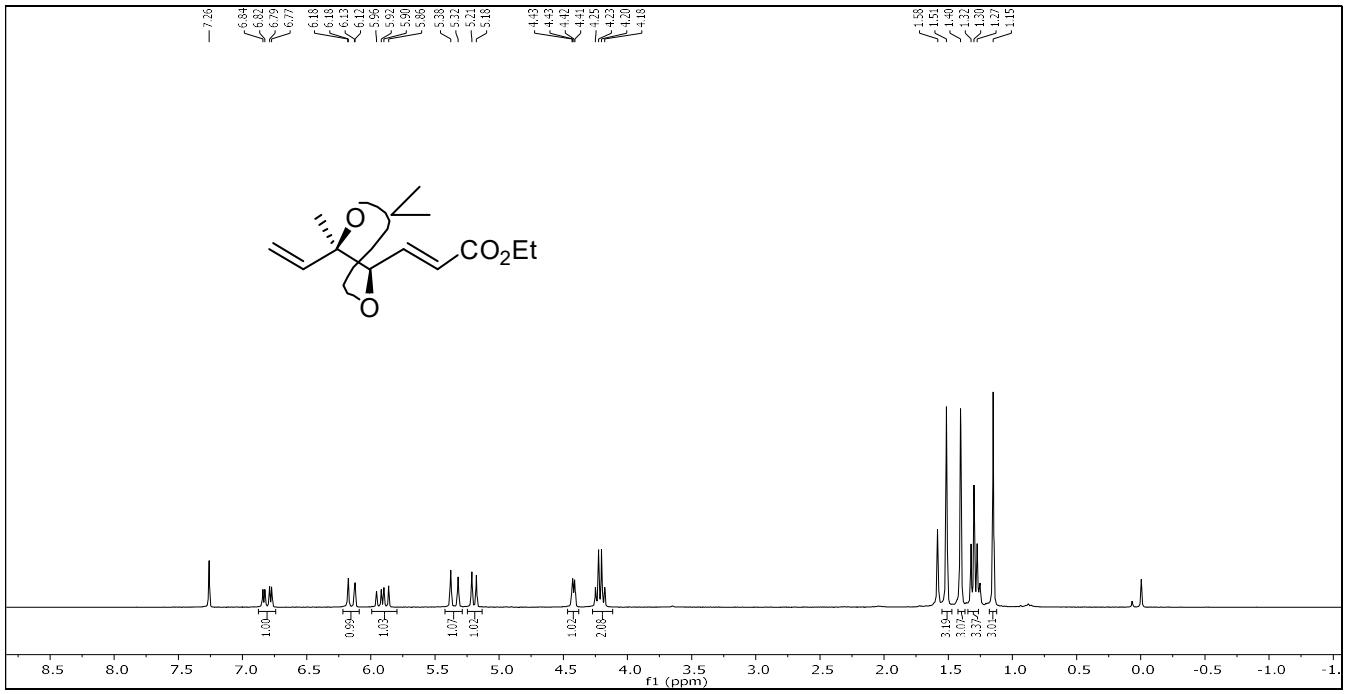
^{1}H-NMR spectrum of compound 16a (300 MHz, $CDCl_3$):



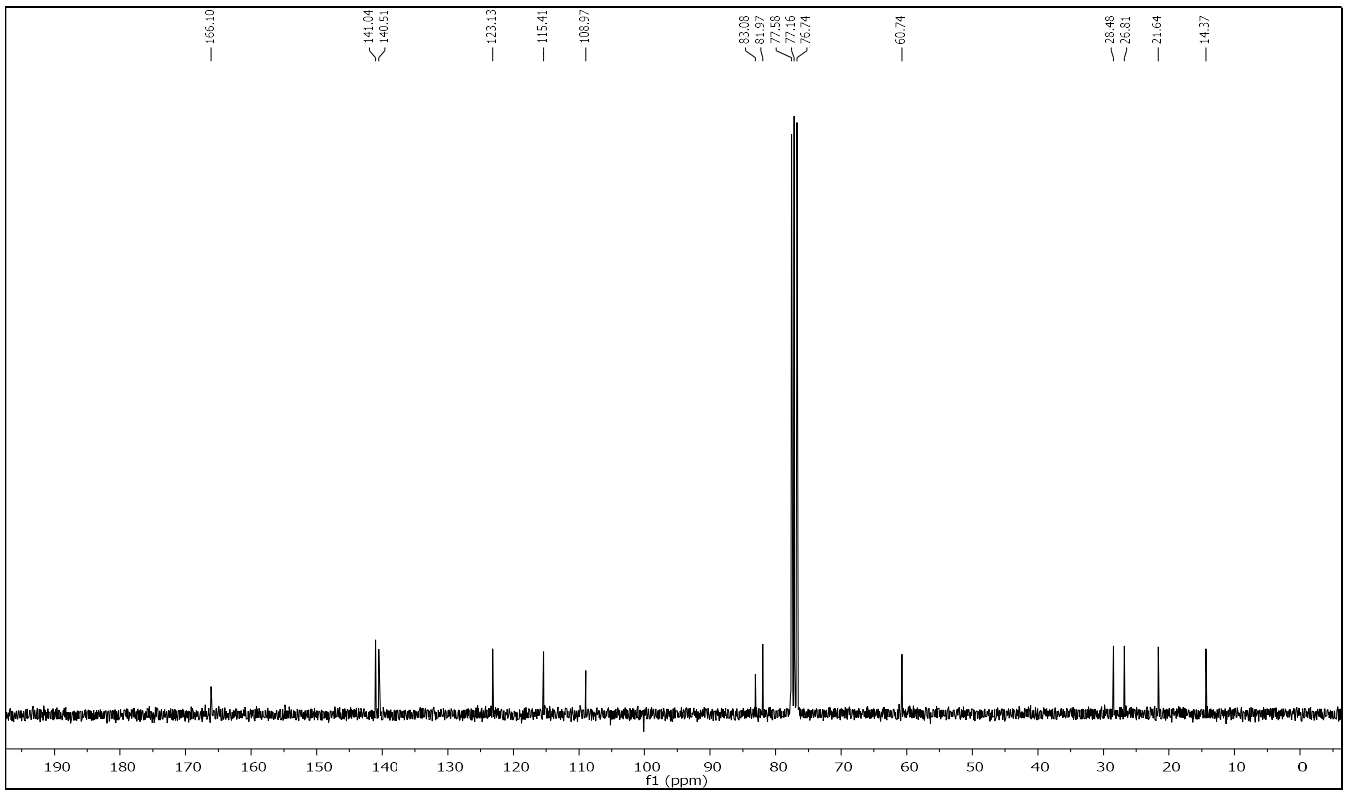
^{13}C-NMR spectrum of compound 16a (75 MHz, $CDCl_3$):



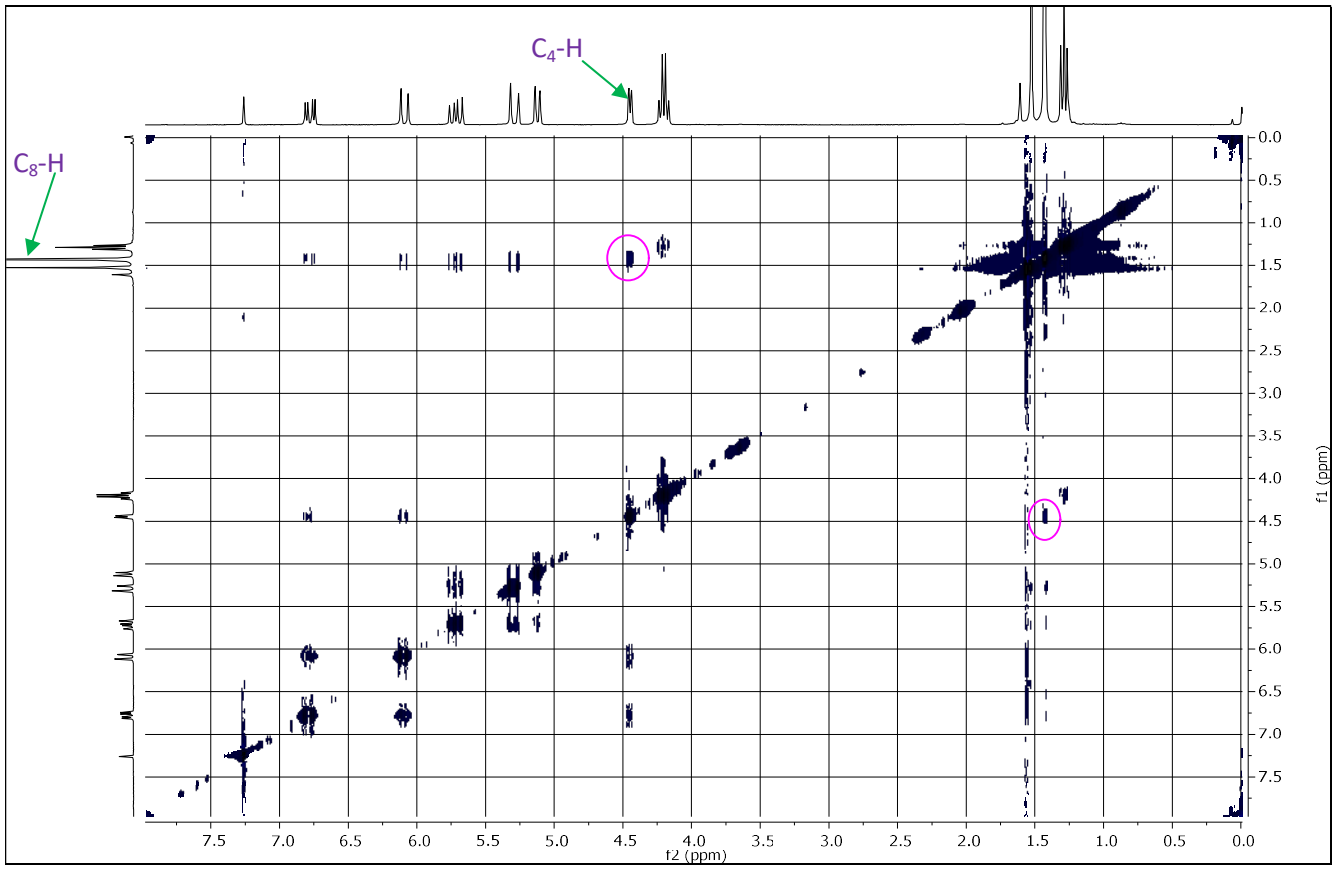
^{1}H-NMR spectrum of compound 16b (300 MHz, $CDCl_3$):

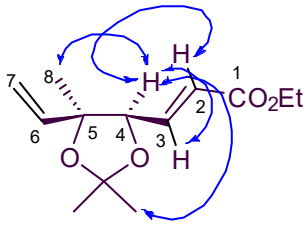


^{13}C-NMR spectrum of compound 16b (75 MHz, $CDCl_3$):



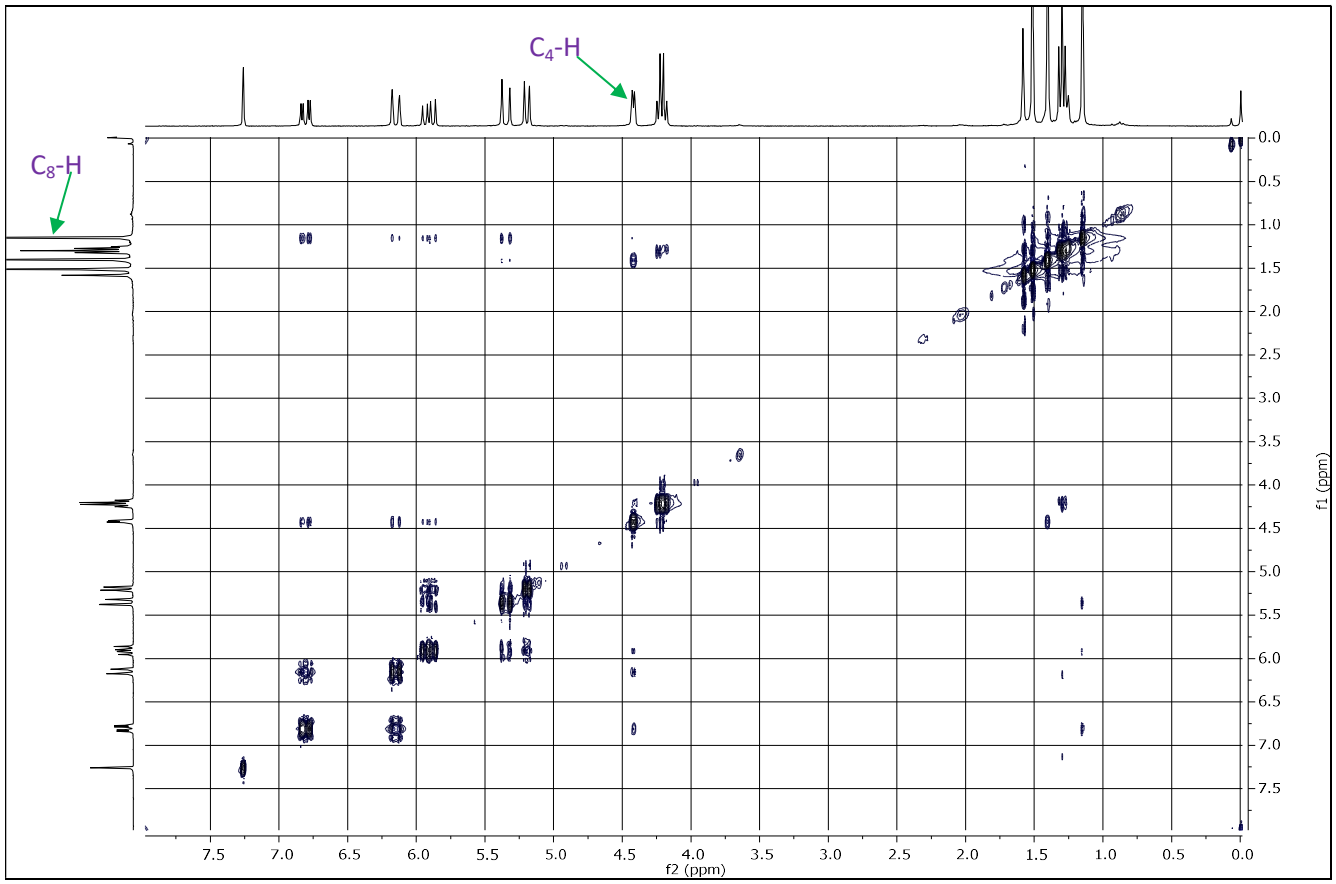
NOESY spectrum of compound 16a (300 MHz, $CDCl_3$):

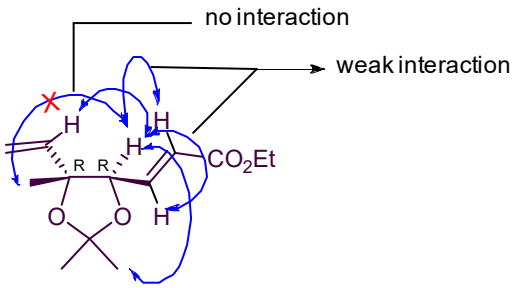




17a

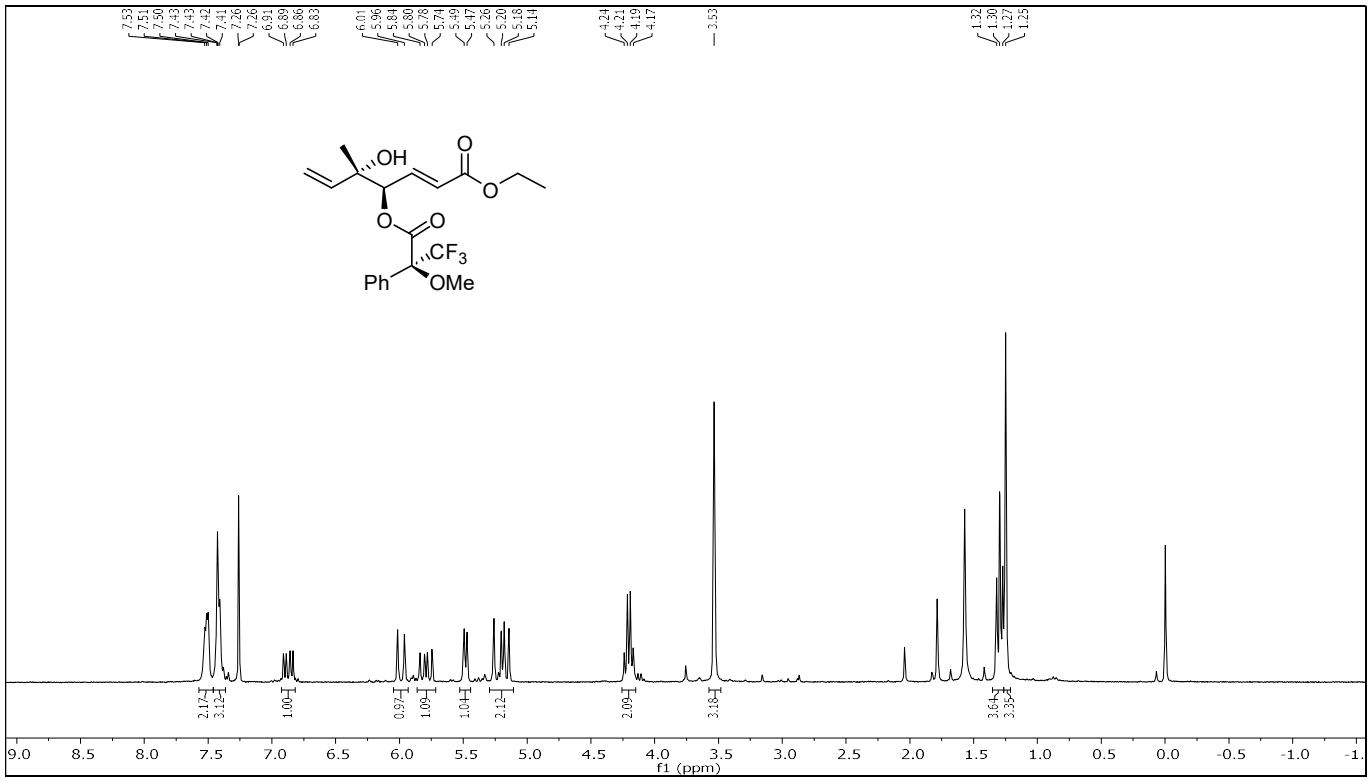
NOESY spectrum of compound 16b (300 MHz, $CDCl_3$):



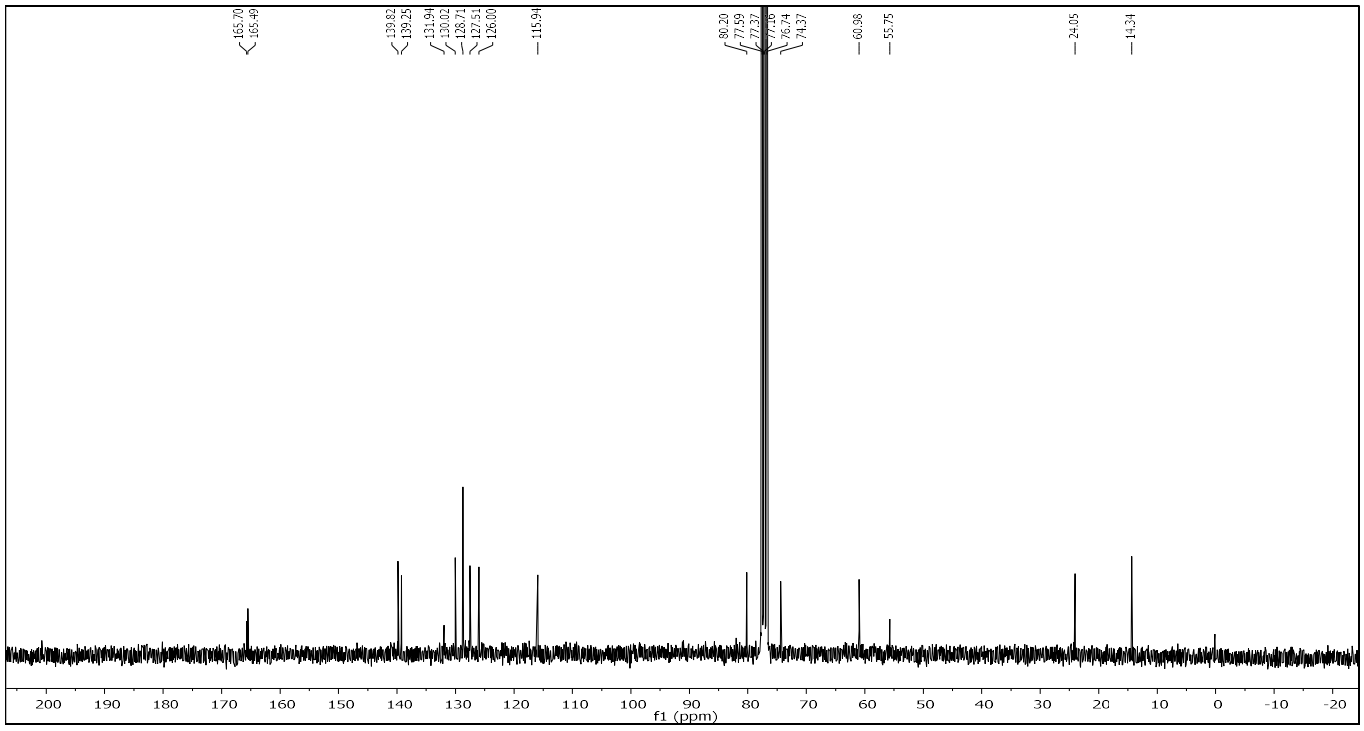


17b

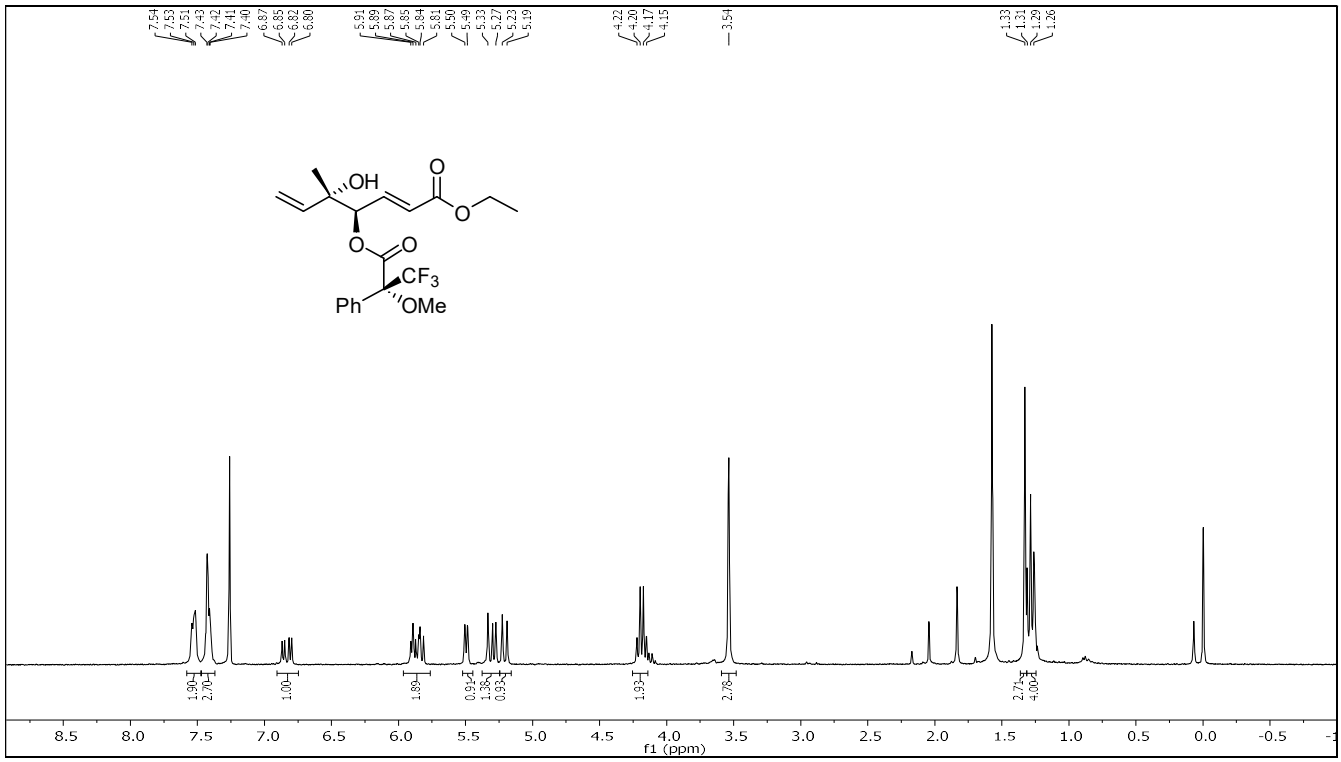
^{1}H-NMR spectrum of compound 17a (300 MHz, $CDCl_3$):



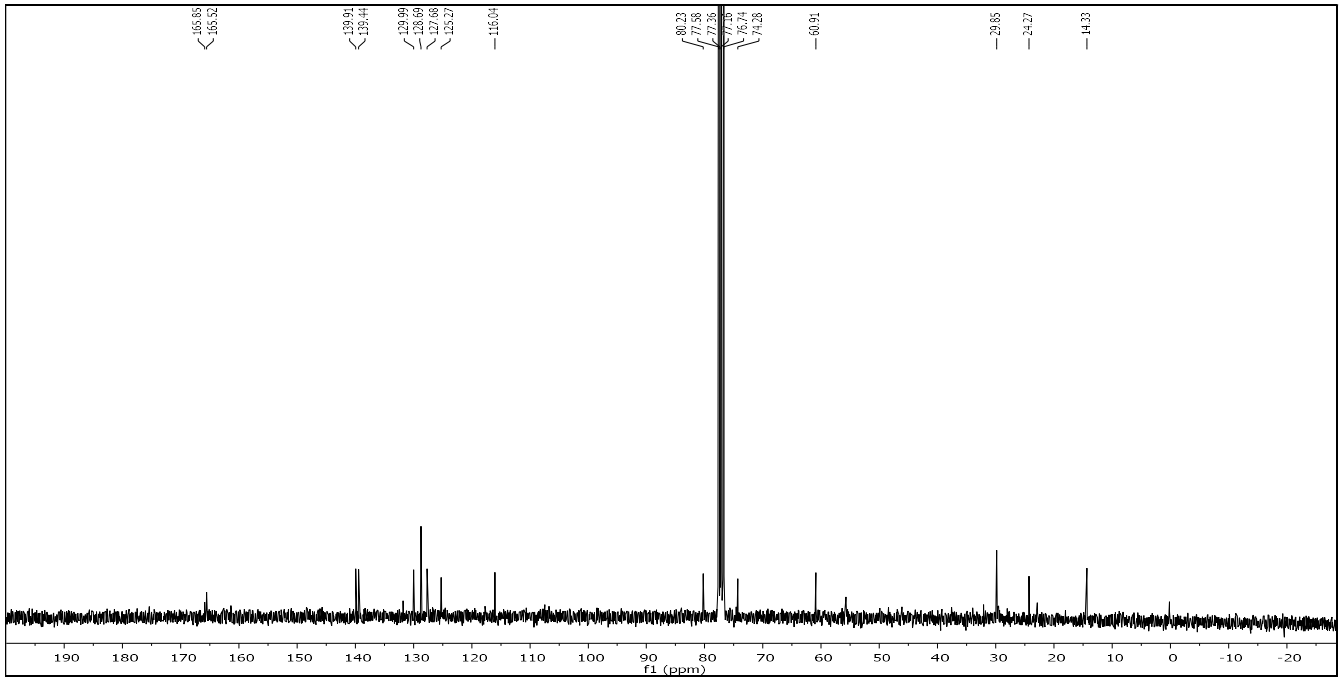
^{13}C-NMR spectrum of compound 17a (75 MHz, $CDCl_3$):



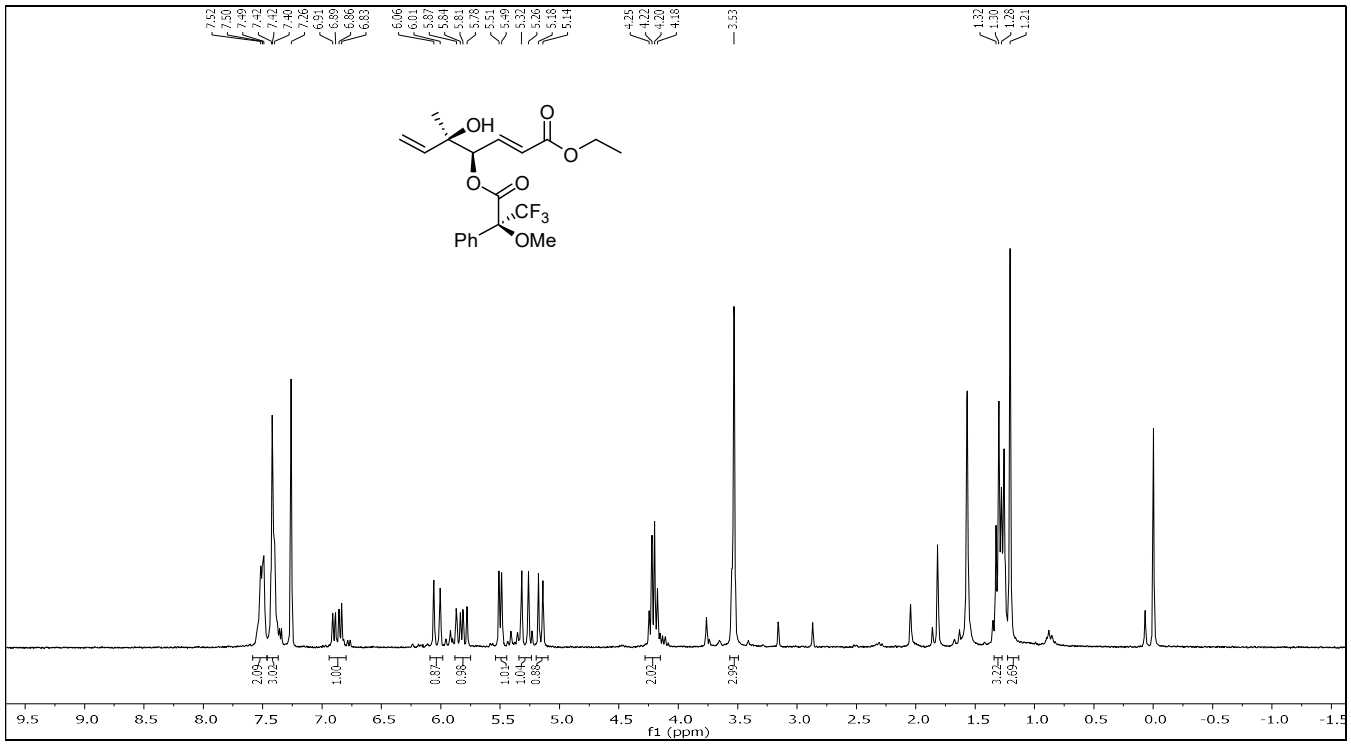
^{1}H-NMR spectrum of compound 17b (300 MHz, $CDCl_3$):



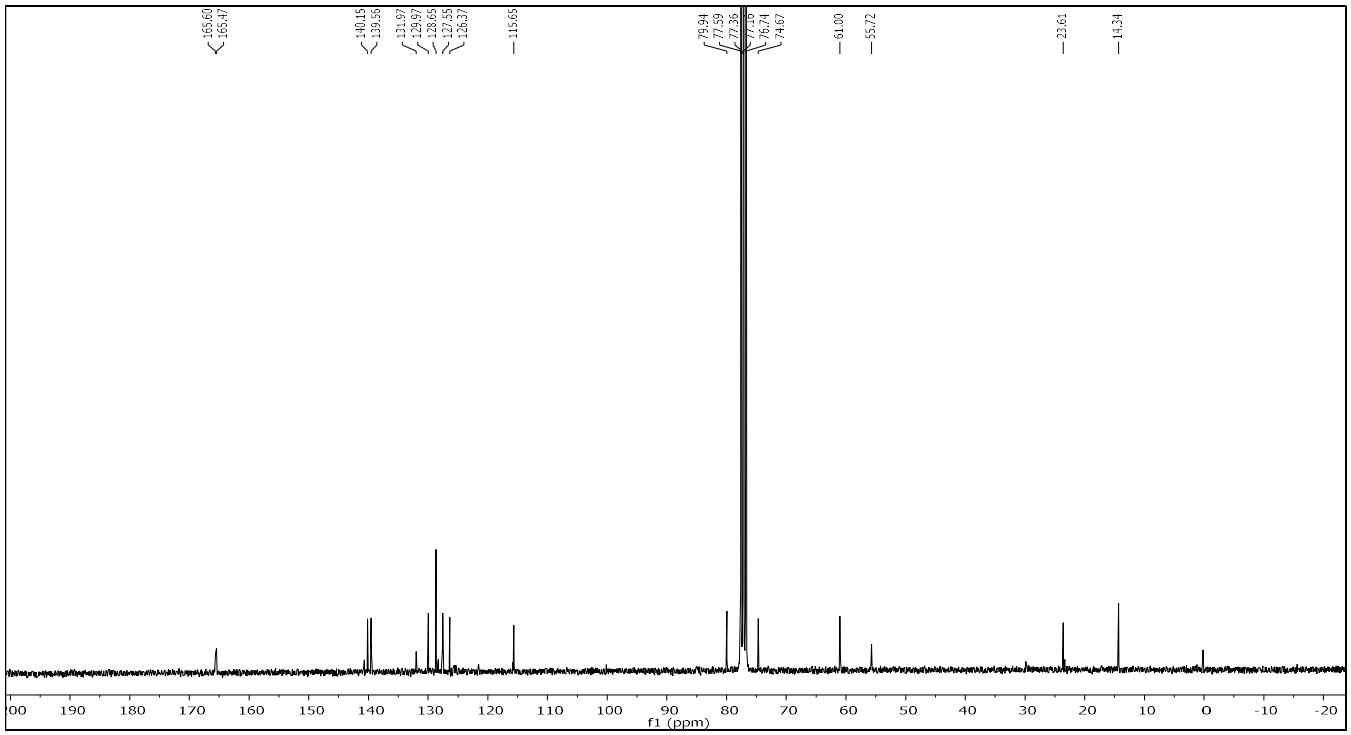
^{13}C-NMR spectrum of compound 17b (75 MHz, $CDCl_3$):



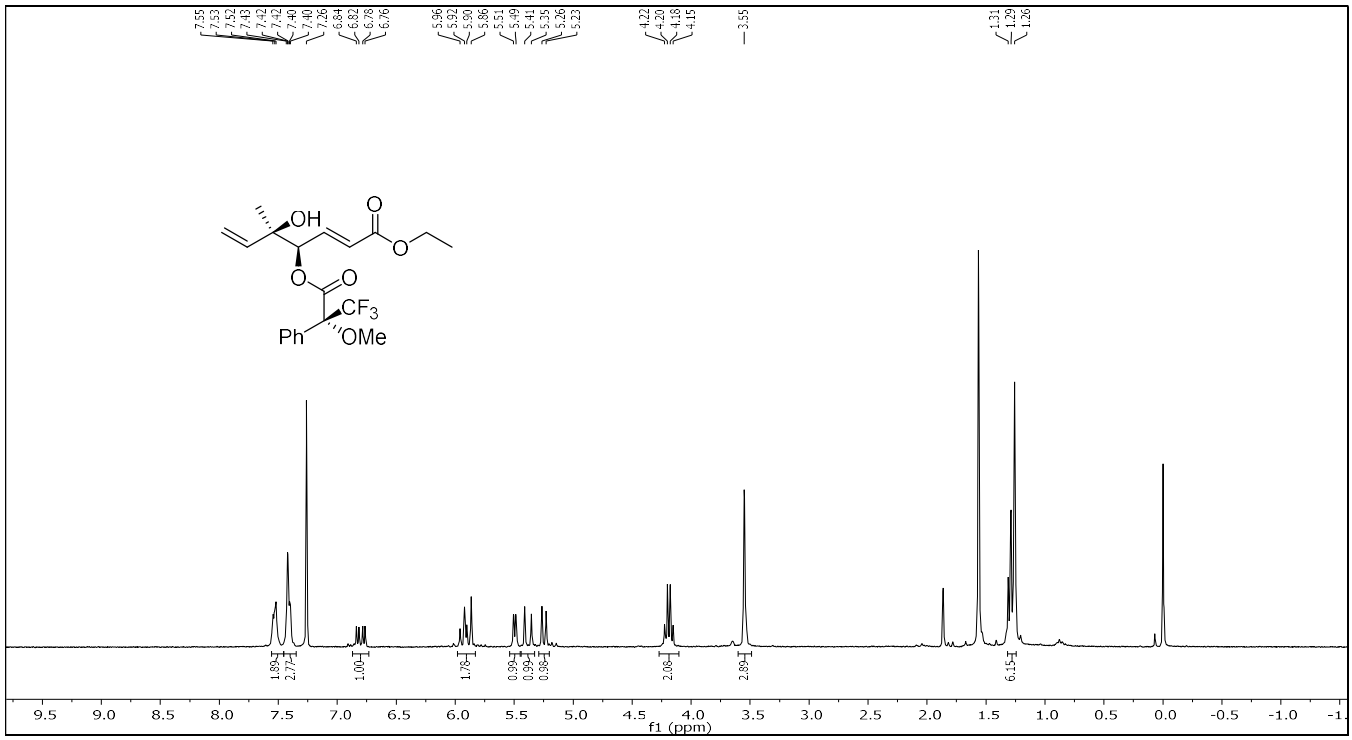
^{1}H-NMR spectrum of compound 18a (300 MHz, $CDCl_3$):



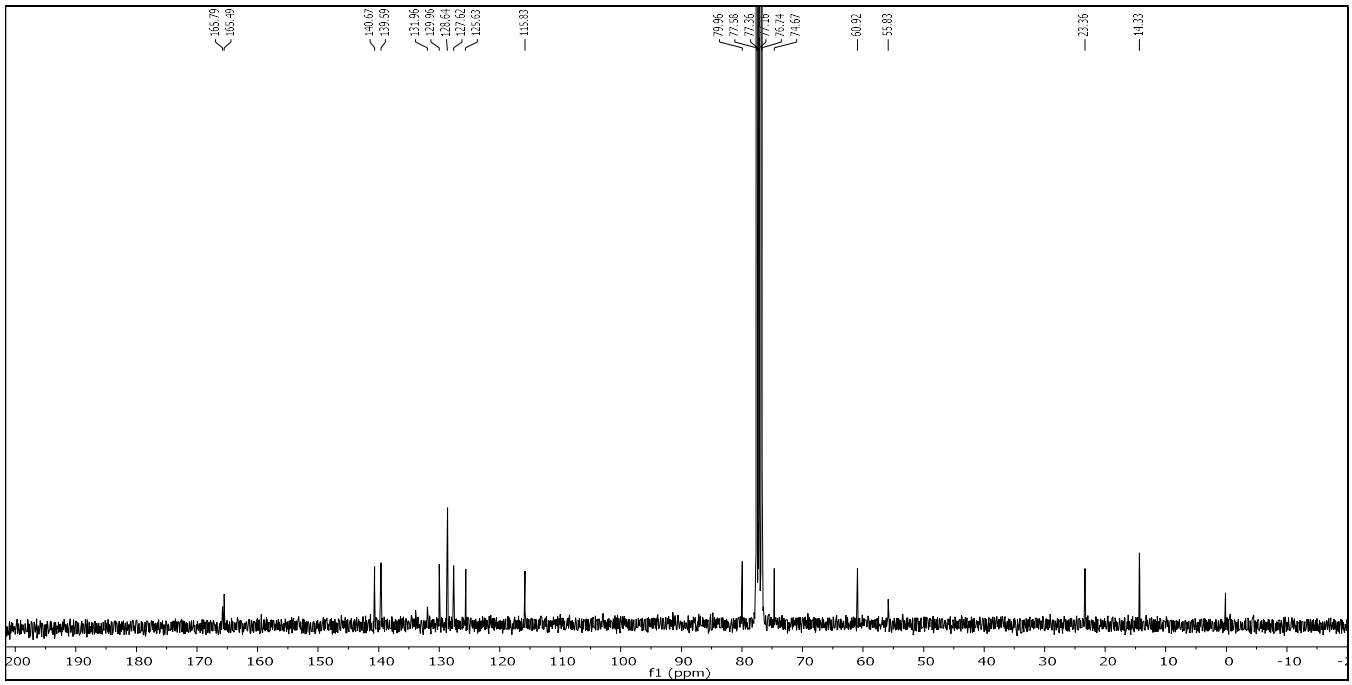
^{13}C-NMR spectrum of compound 18a (75 MHz, $CDCl_3$):



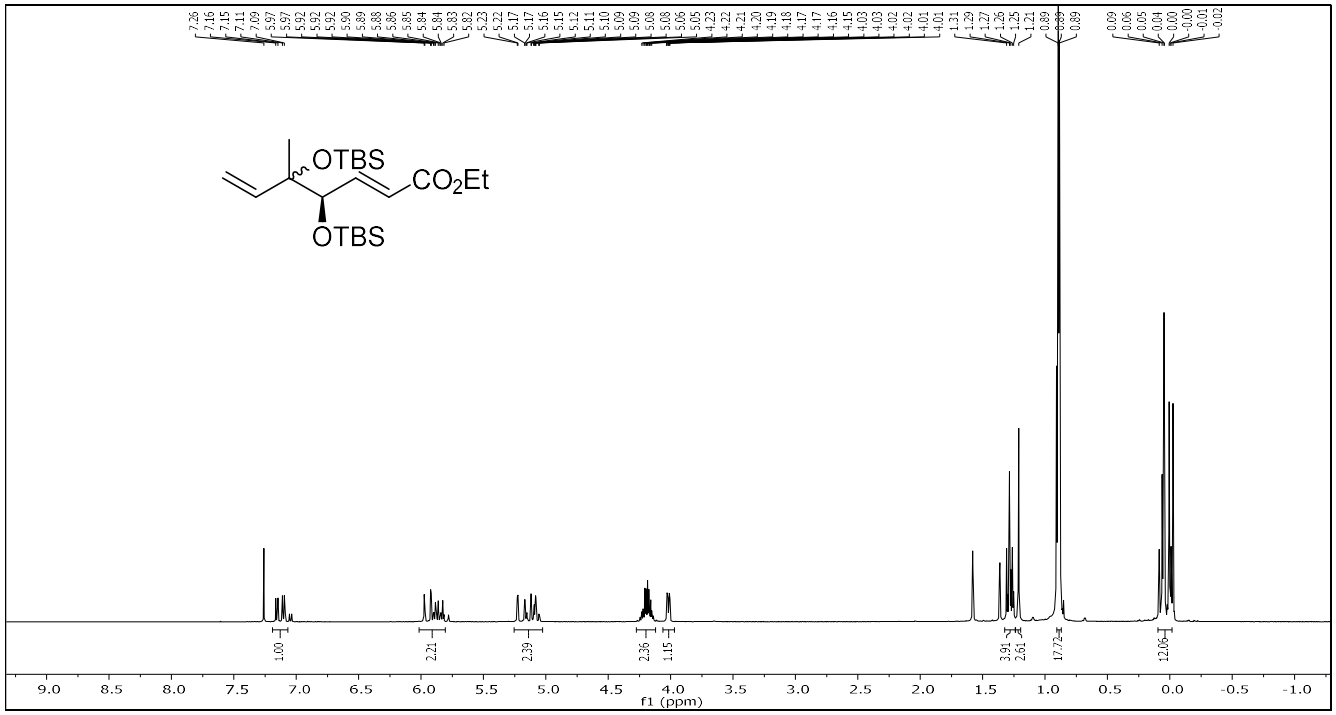
^{1}H-NMR spectrum of compound 18b (300 MHz, $CDCl_3$):



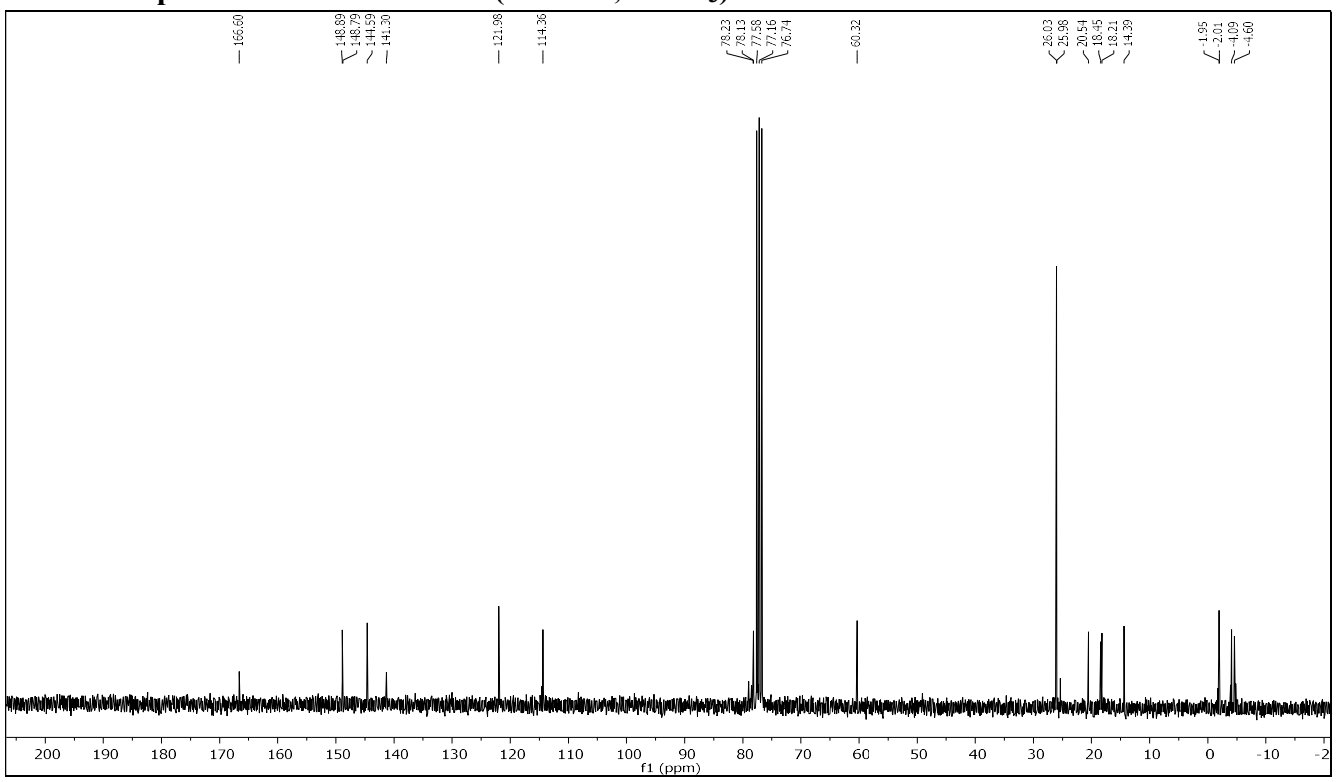
^{13}C-NMR spectrum of compound 18b (75 MHz, $CDCl_3$):



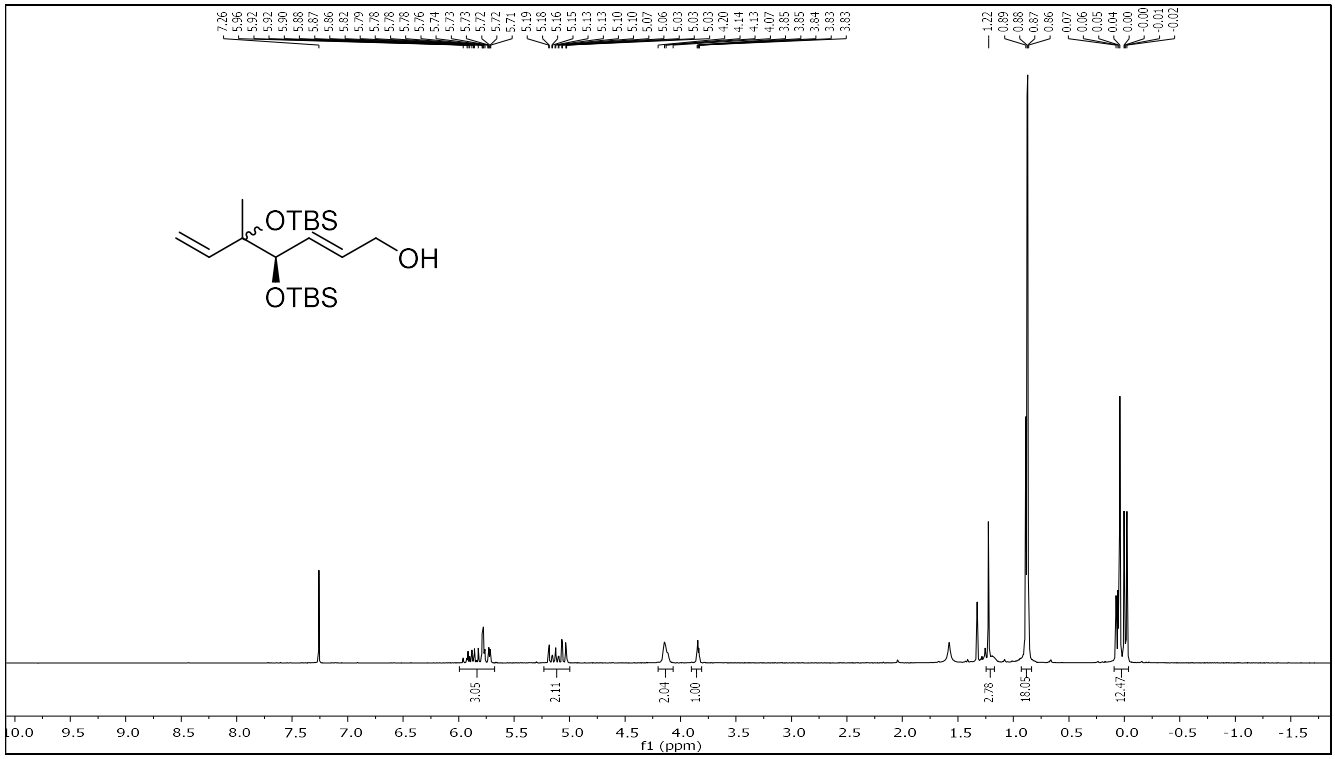
^{1}H-NMR spectrum of di-TBS ester (300 MHz, $CDCl_3$):



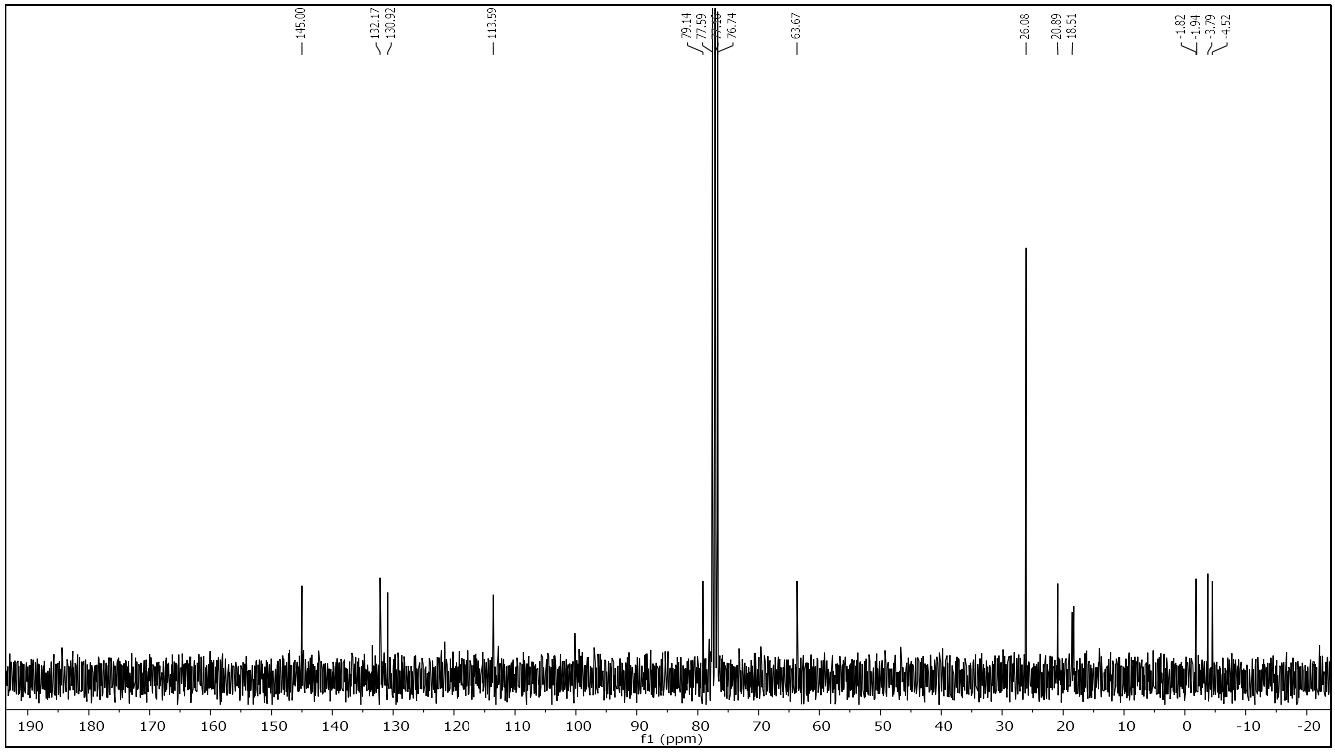
^{13}C-NMR spectrum of di-TBS ester (75 MHz, $CDCl_3$):



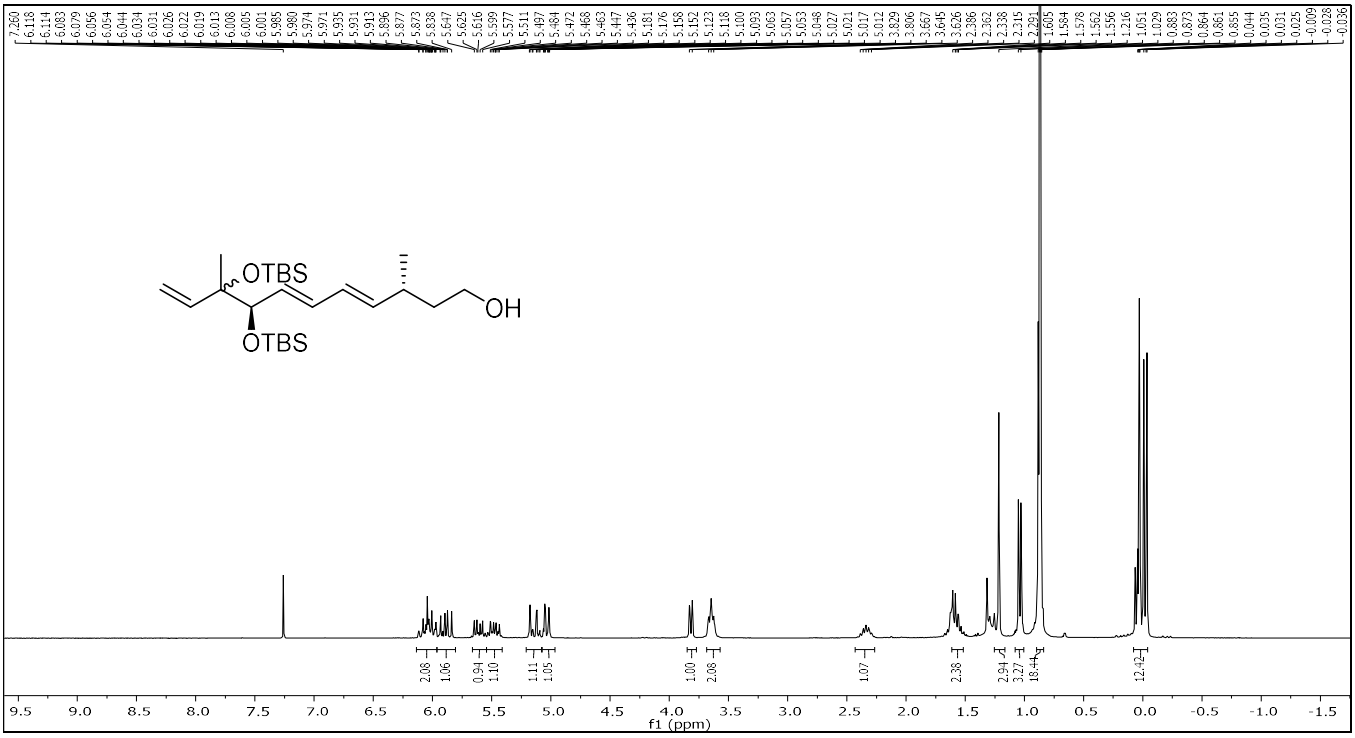
^{1}H-NMR spectrum of di-TBS alcohol (300 MHz, $CDCl_3$):



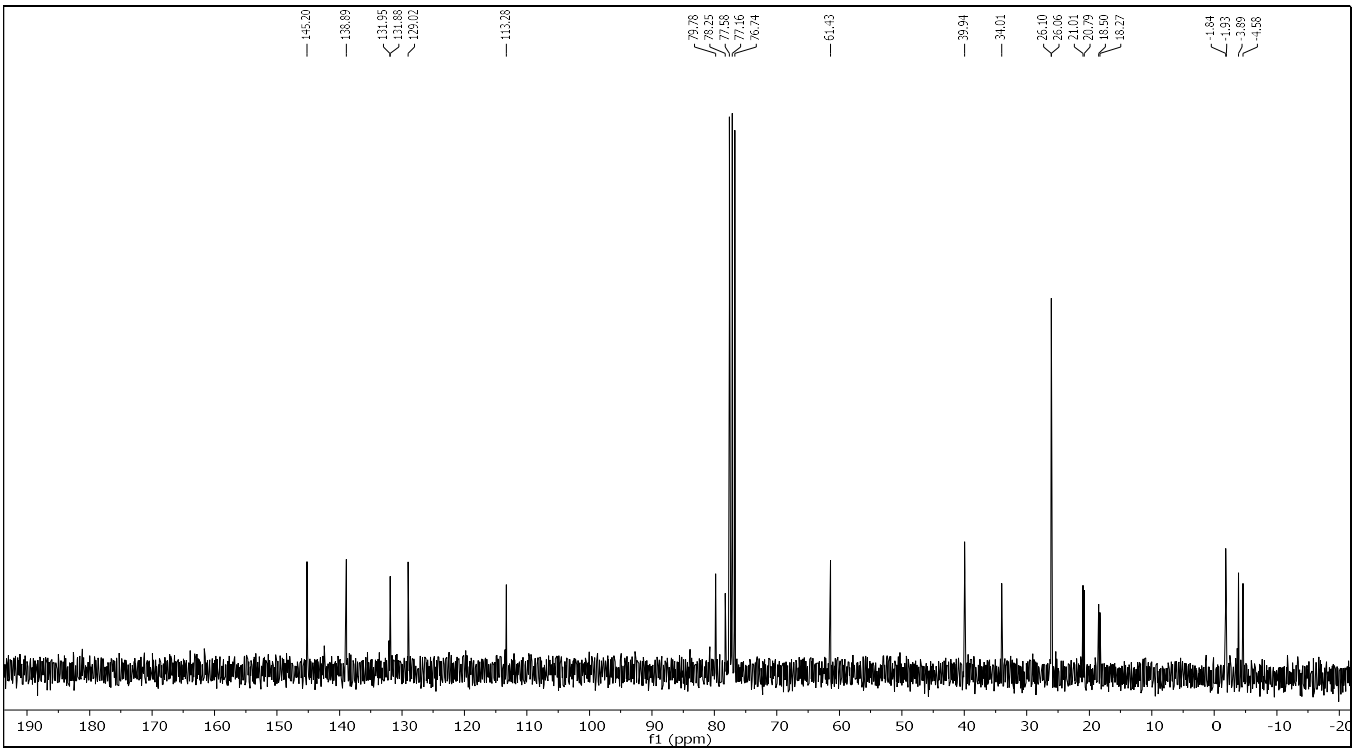
^{13}C-NMR spectrum of di-TBS alcohol (75 MHz, $CDCl_3$):



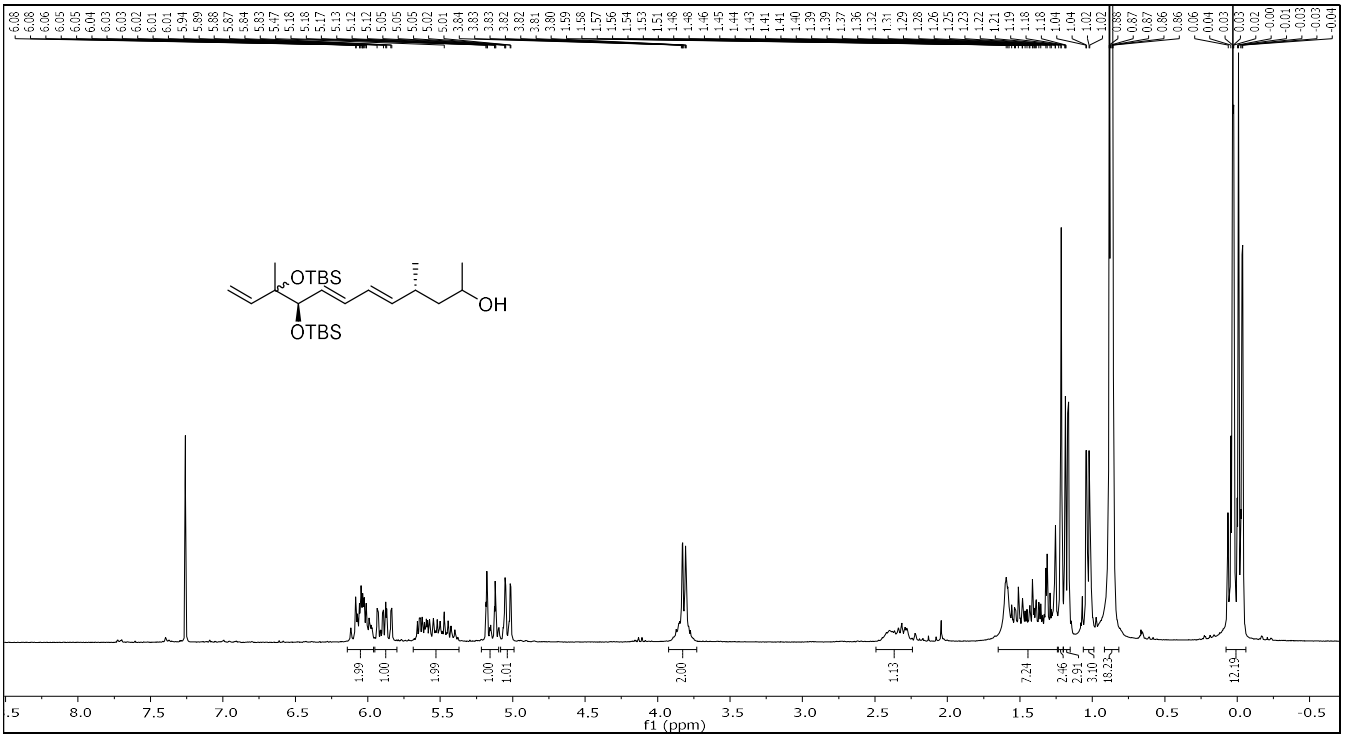
^{1}H-NMR spectrum of compound 19a/19b (300 MHz, $CDCl_3$):



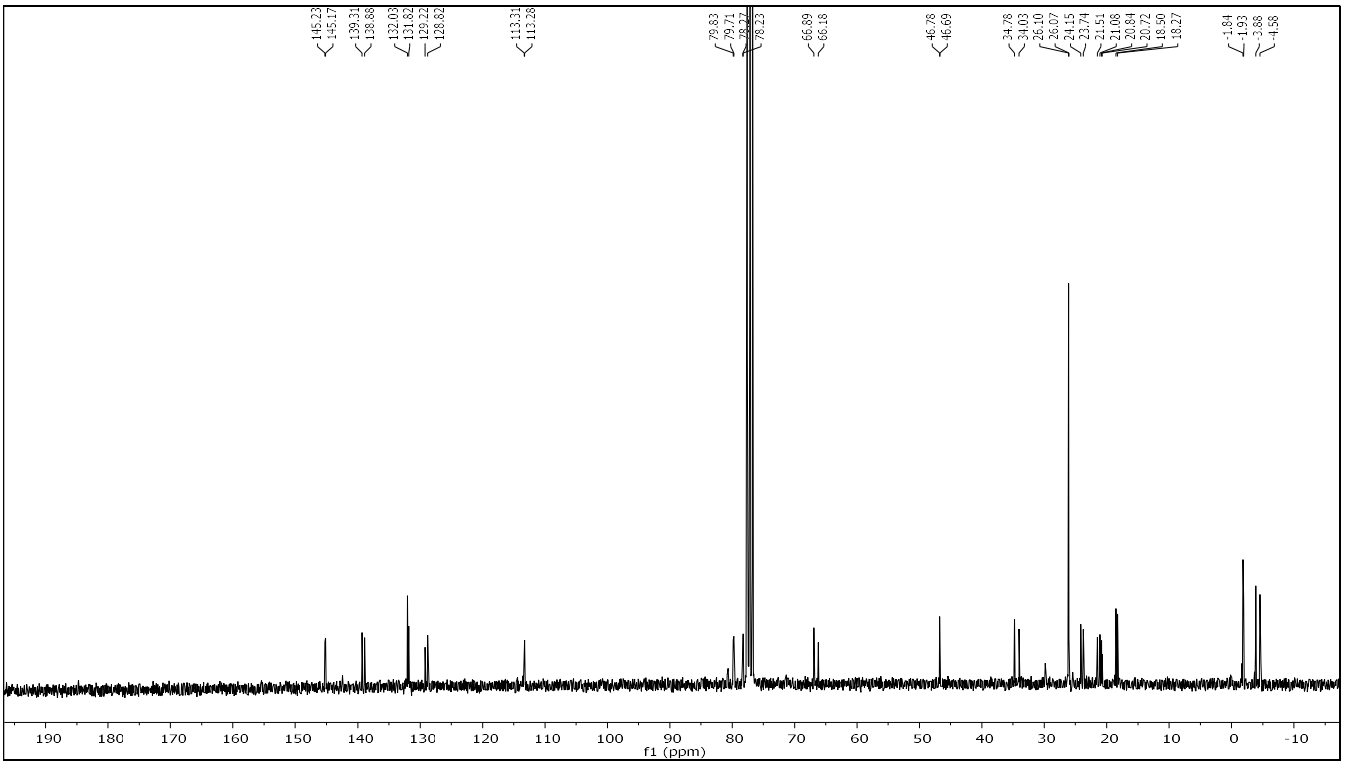
^{13}C-NMR spectrum of compound 19a/19b (75 MHz, $CDCl_3$):



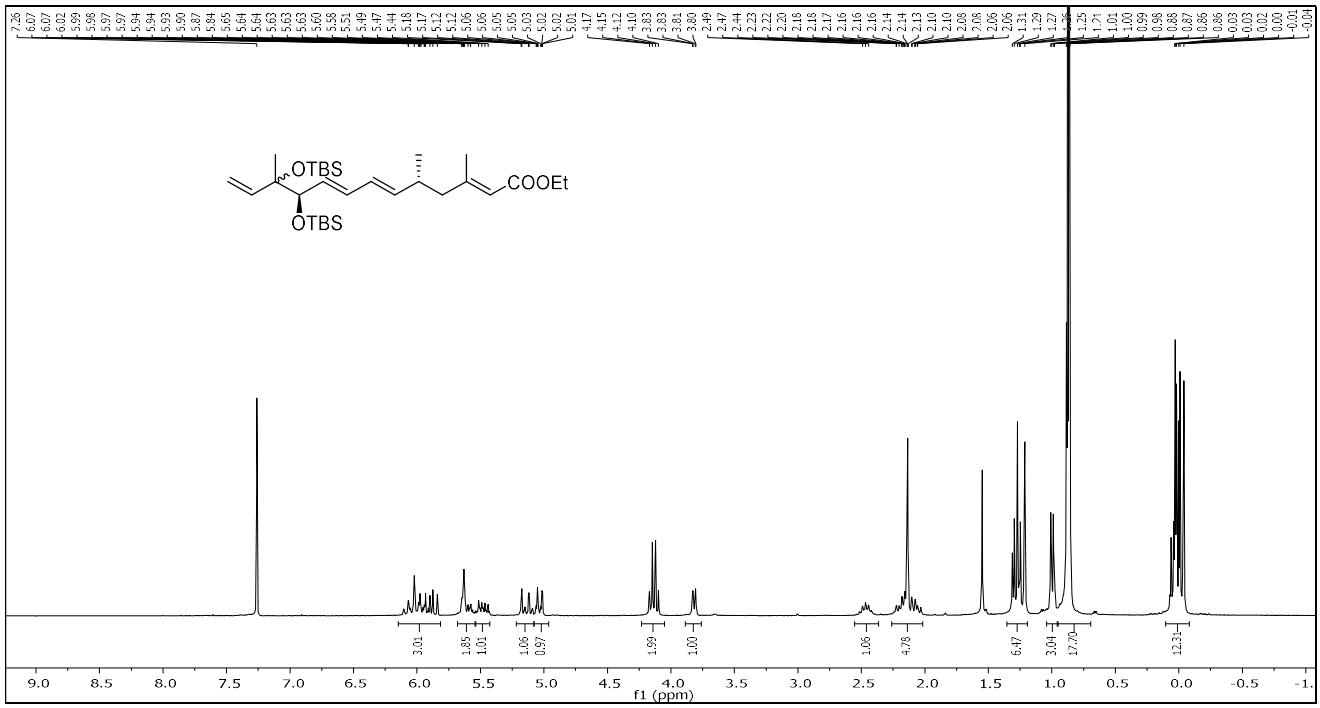
^{1}H-NMR spectrum of compound 20a/20b (300 MHz, $CDCl_3$):



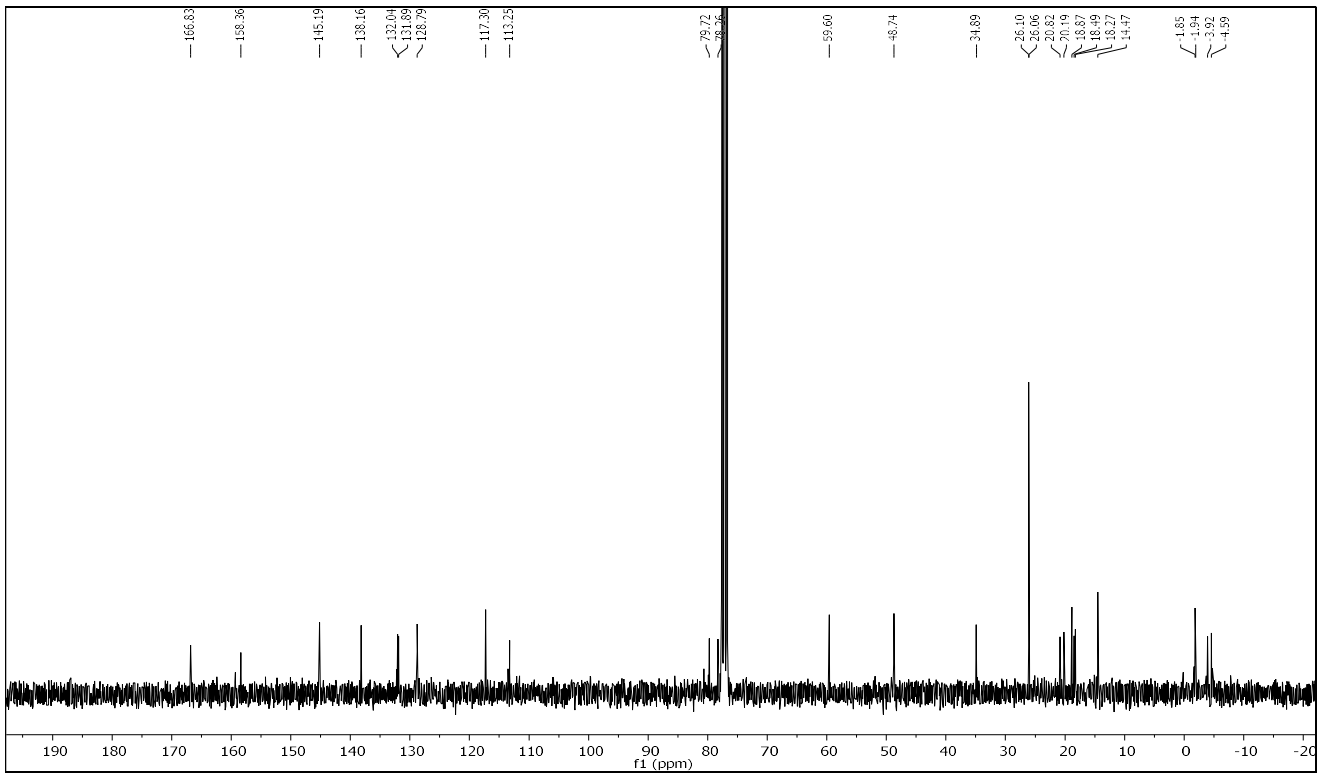
^{13}C-NMR spectrum of compound 20a/20b (75 MHz, $CDCl_3$):



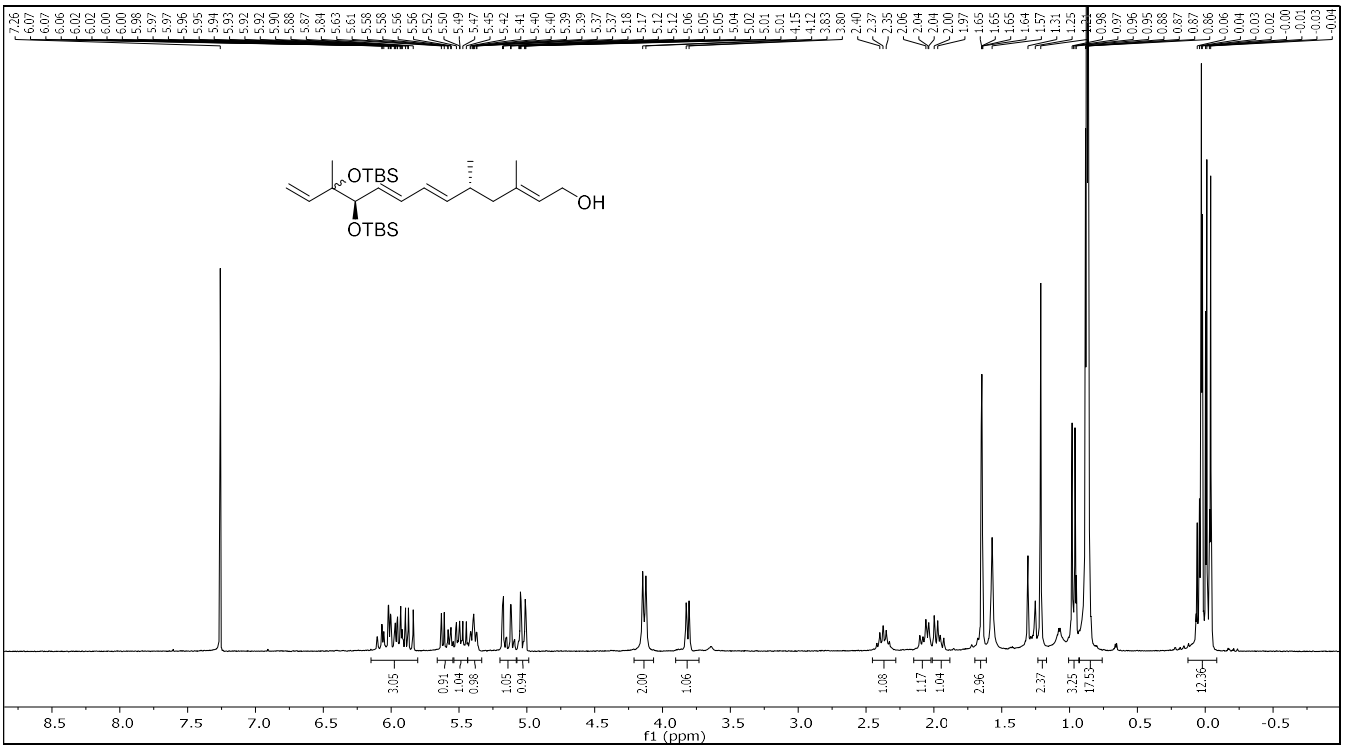
^{1}H-NMR spectrum of compound 21a/21b (300 MHz, $CDCl_3$):



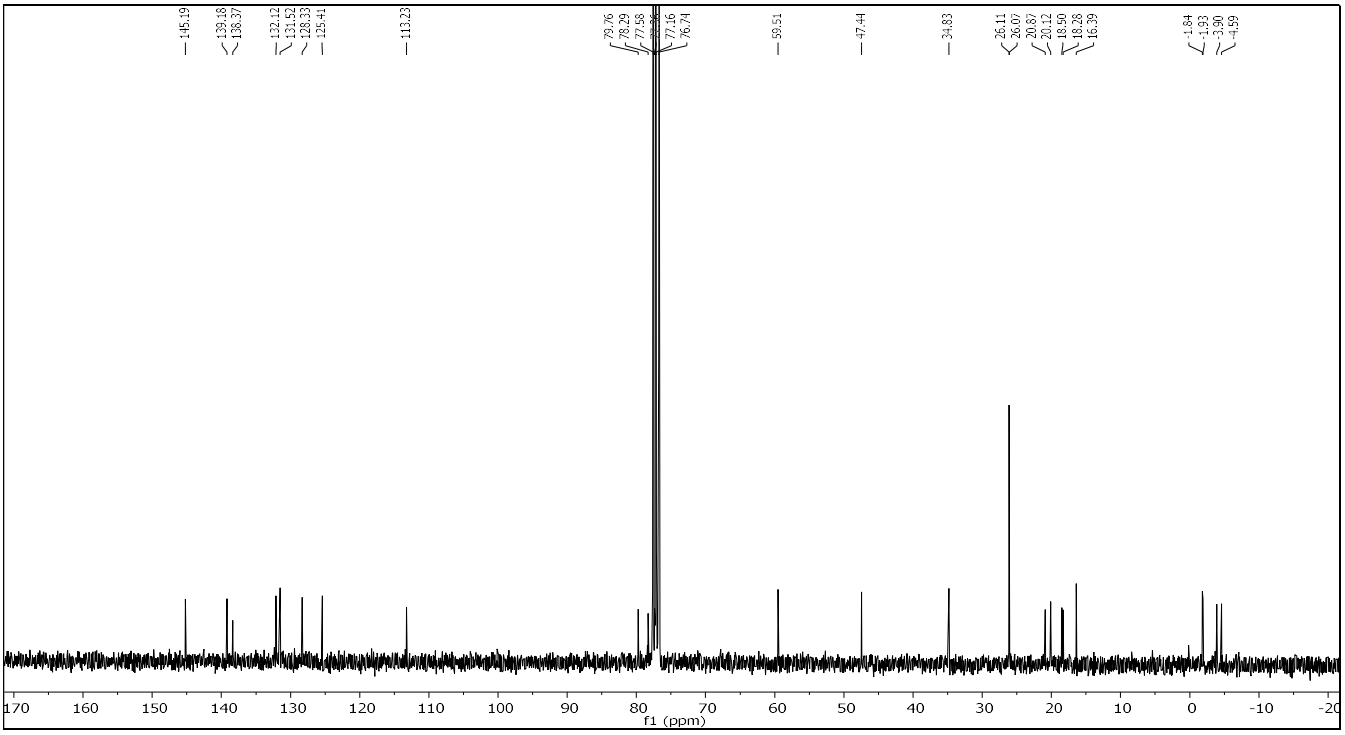
^{13}C-NMR spectrum of compound 21a/21b (75 MHz, $CDCl_3$):



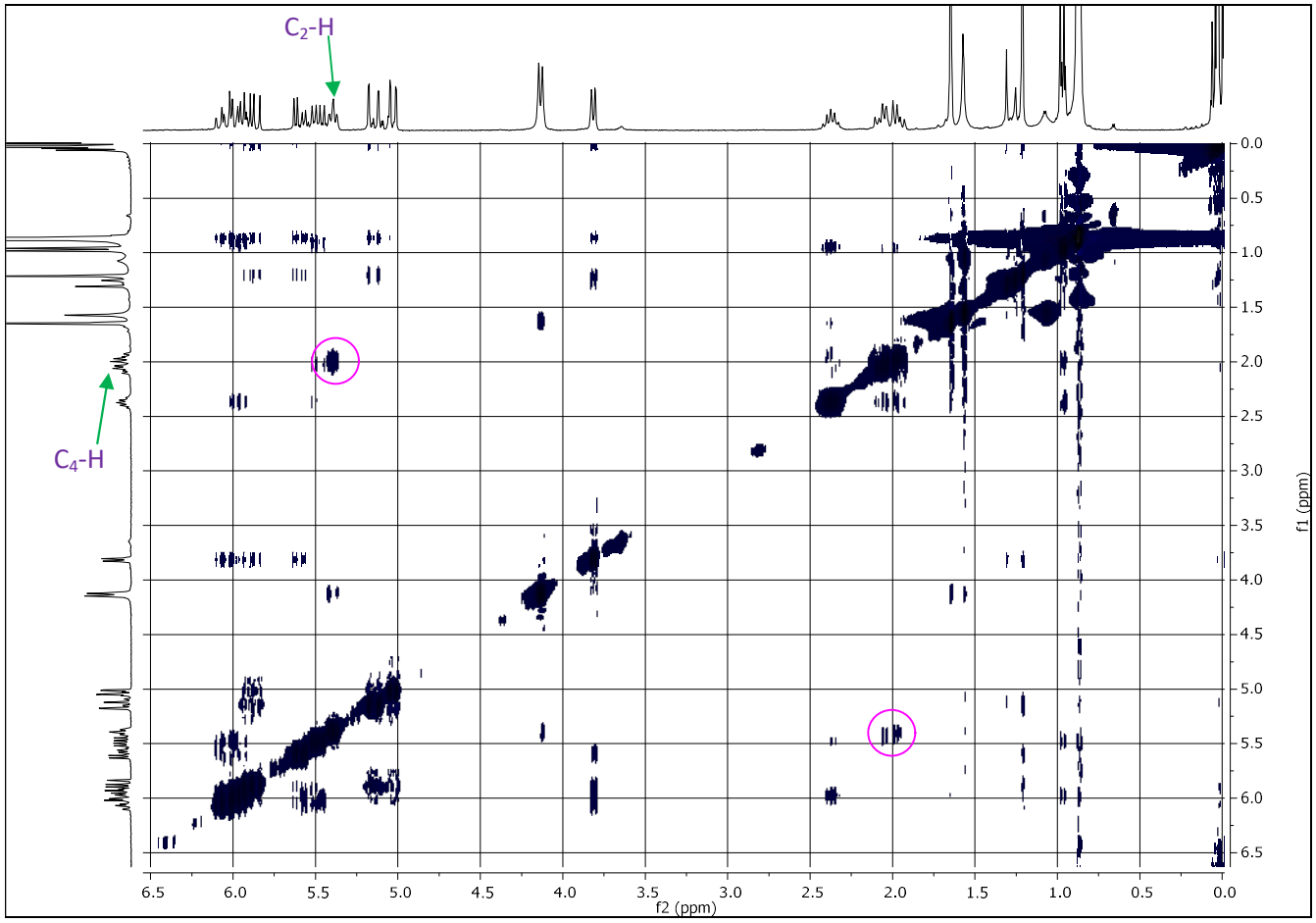
^{1}H-NMR spectrum of compound 22a/22b (300 MHz, $CDCl_3$):

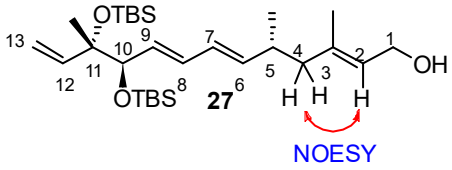


^{13}C-NMR spectrum of compound 22a/22b (75 MHz, $CDCl_3$):

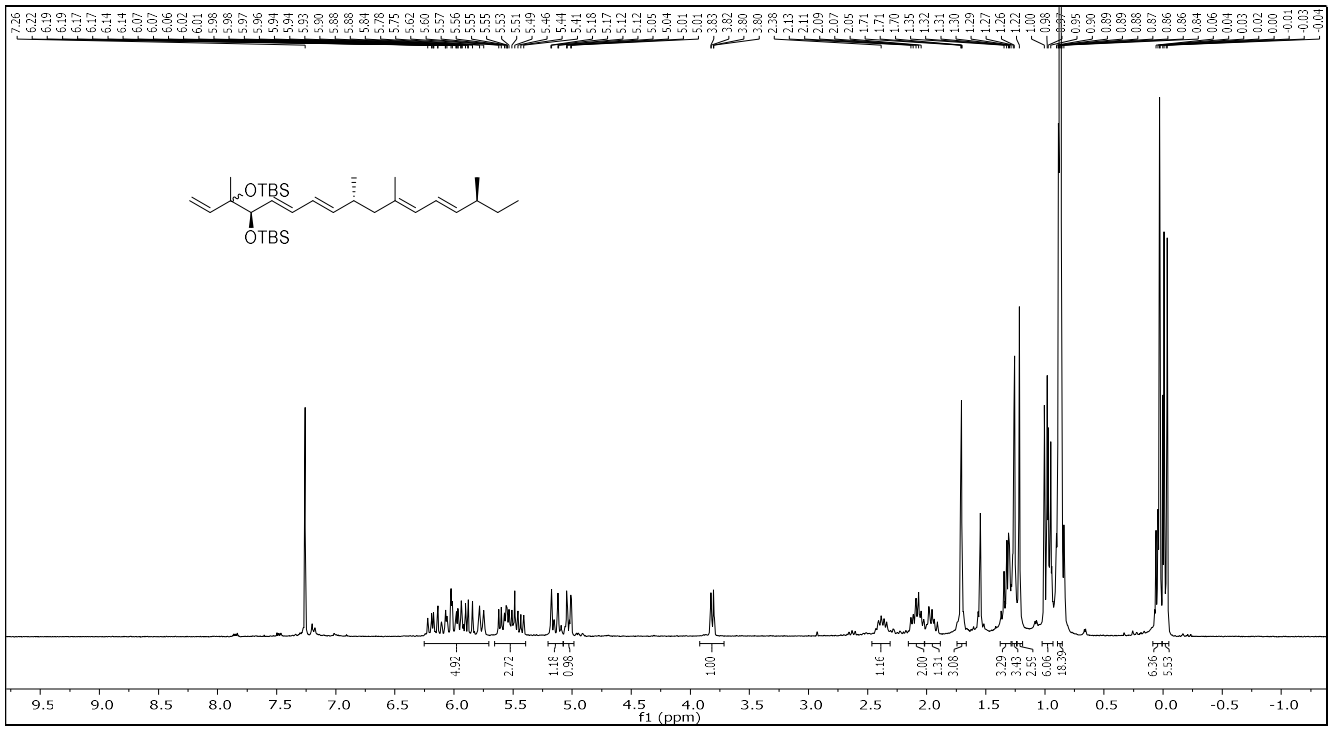


NOESY - spectrum of compound 22a/22b (300 MHz, $CDCl_3$):

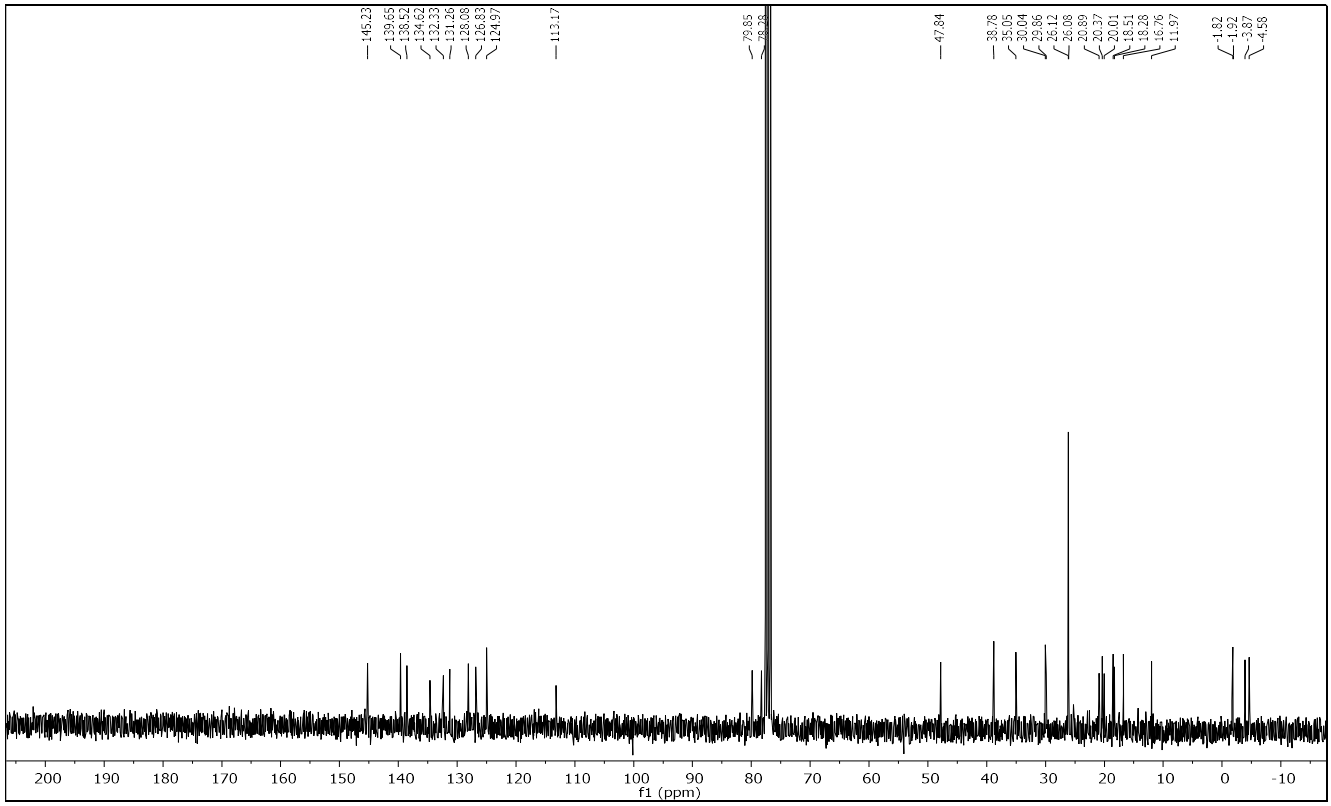




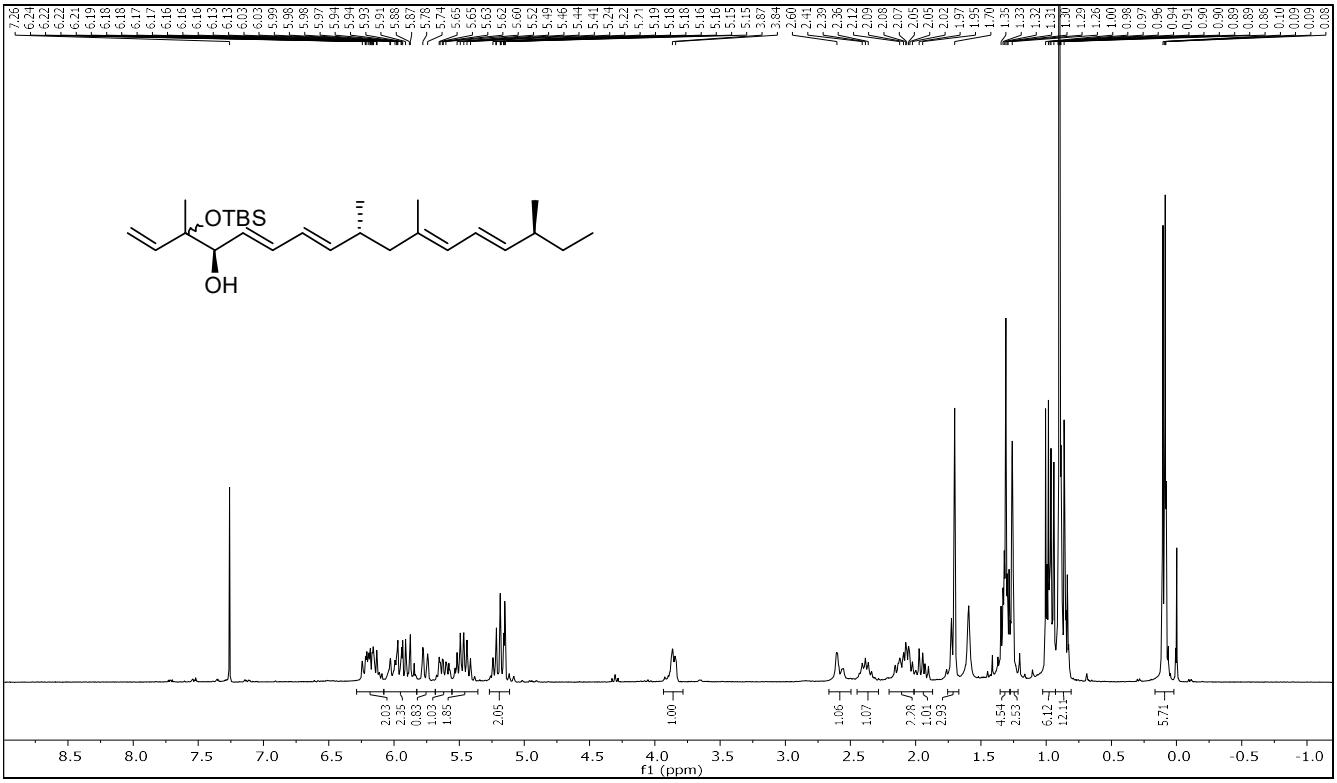
^{1}H-NMR spectrum of compound 23a/23b (300 MHz, $CDCl_3$):



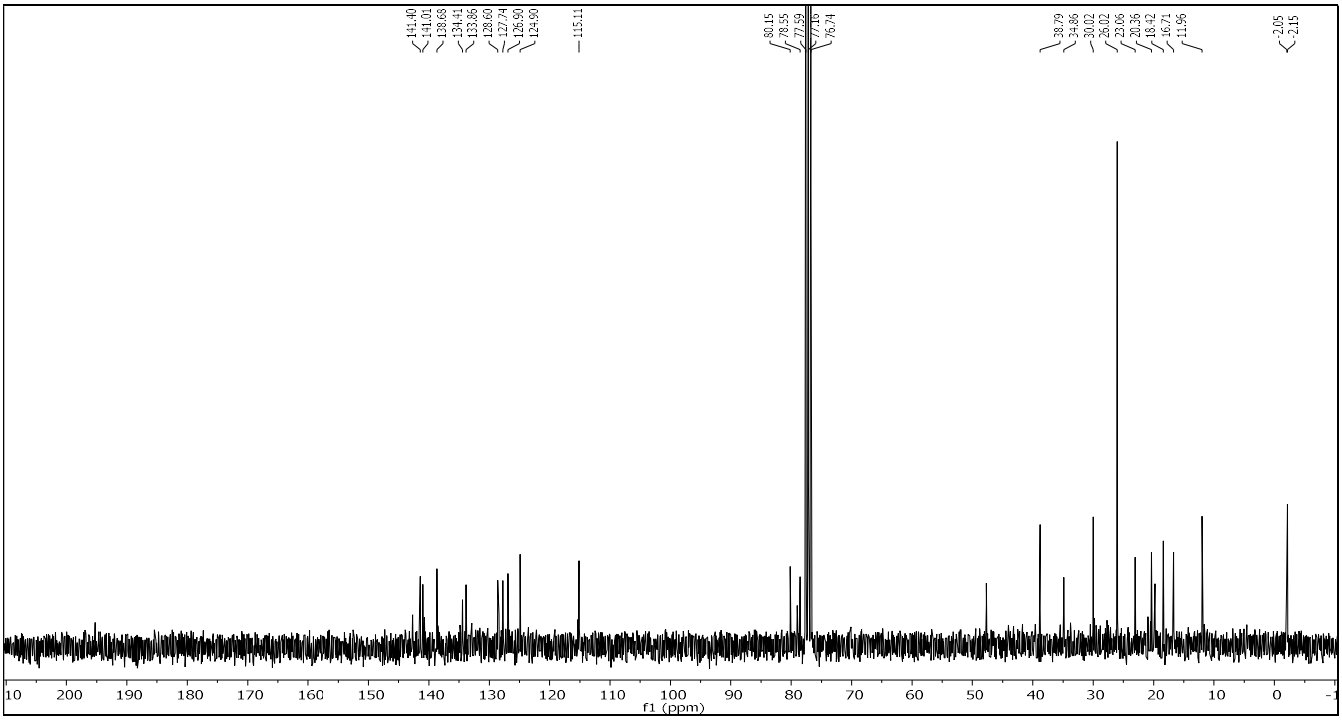
^{13}C-NMR spectrum of compound 23a/23b (75 MHz, $CDCl_3$):



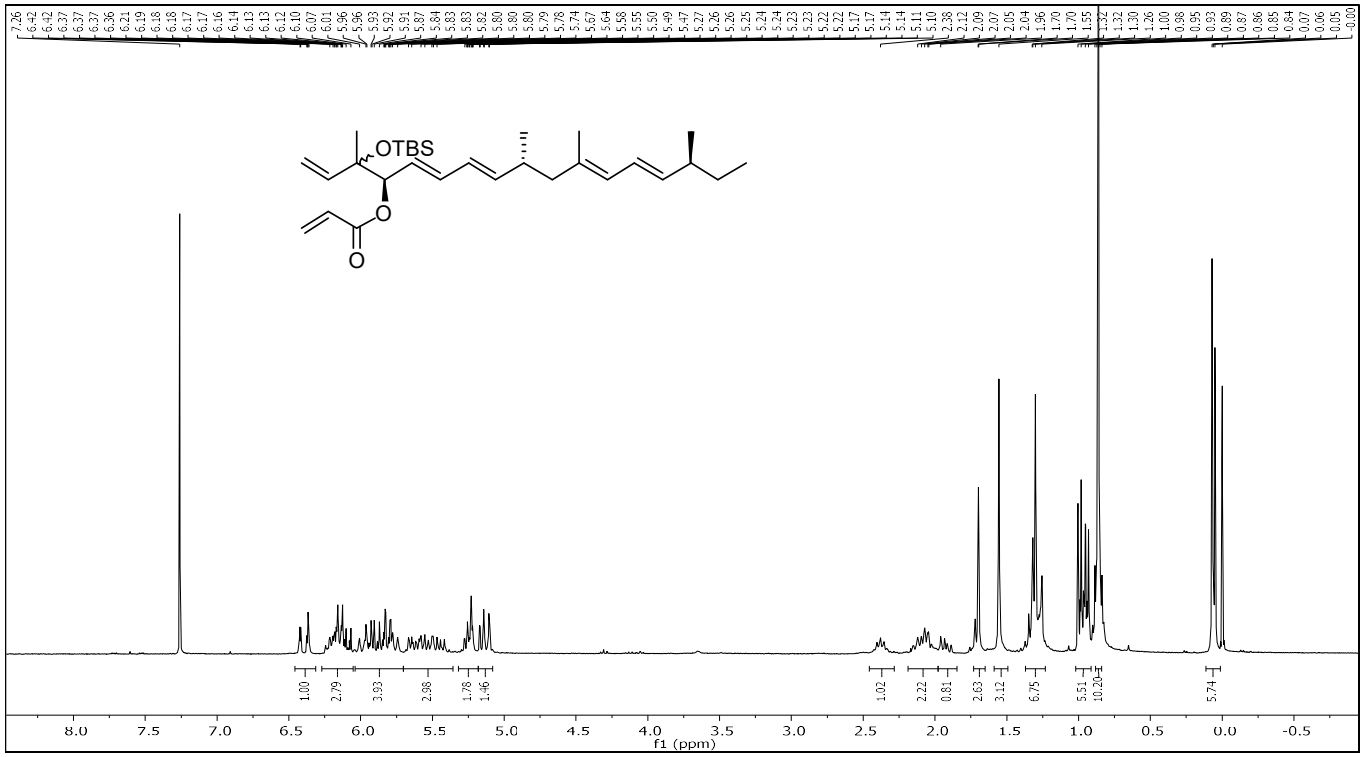
^{1}H-NMR spectrum of compound 24a/24b (300 MHz, $CDCl_3$):



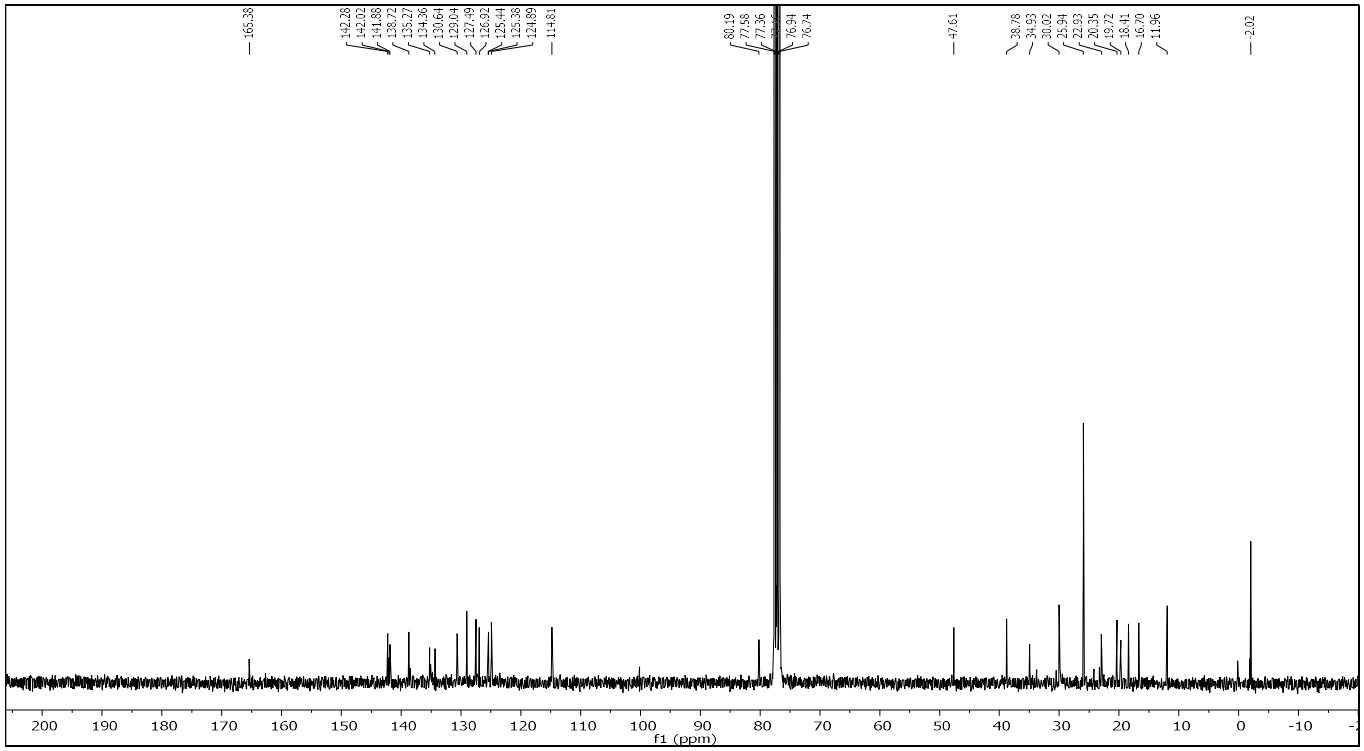
^{13}C-NMR spectrum of compound 24a/24b (75 MHz, $CDCl_3$):



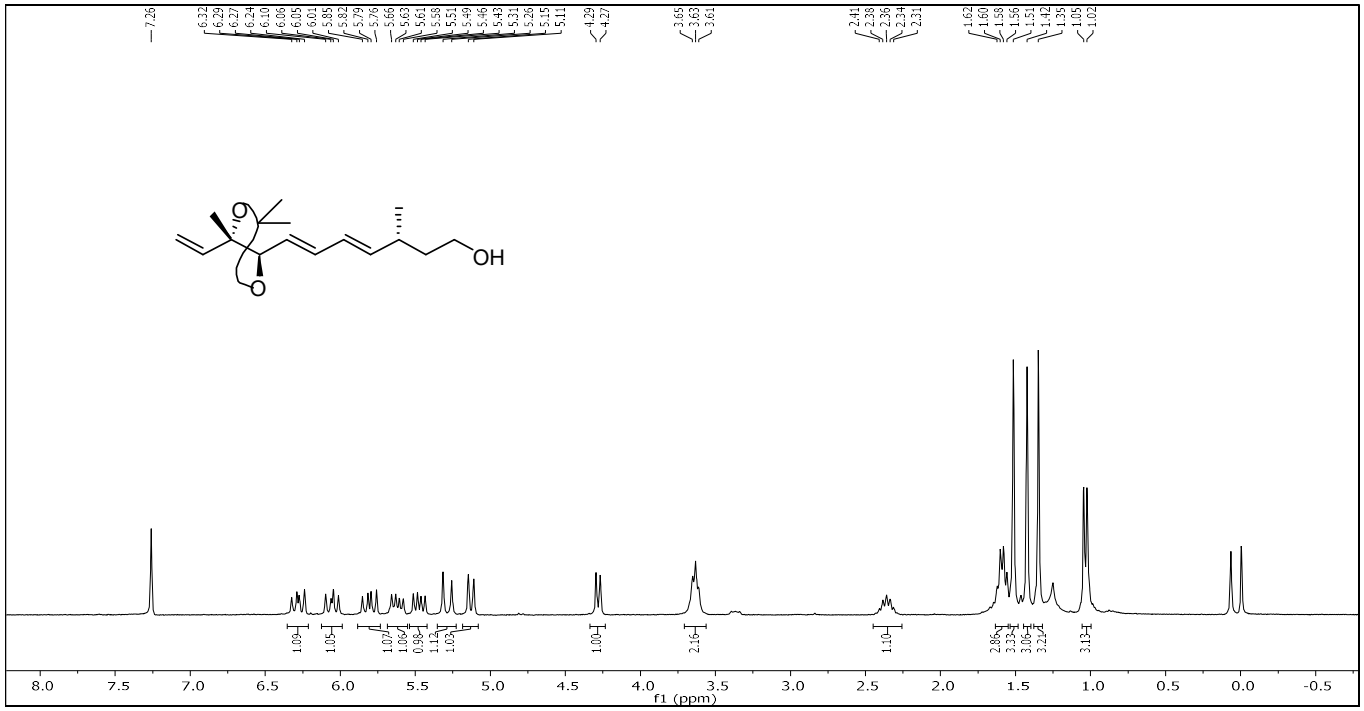
^{1}H-NMR spectrum of compound 6a/6b (300 MHz, $CDCl_3$):



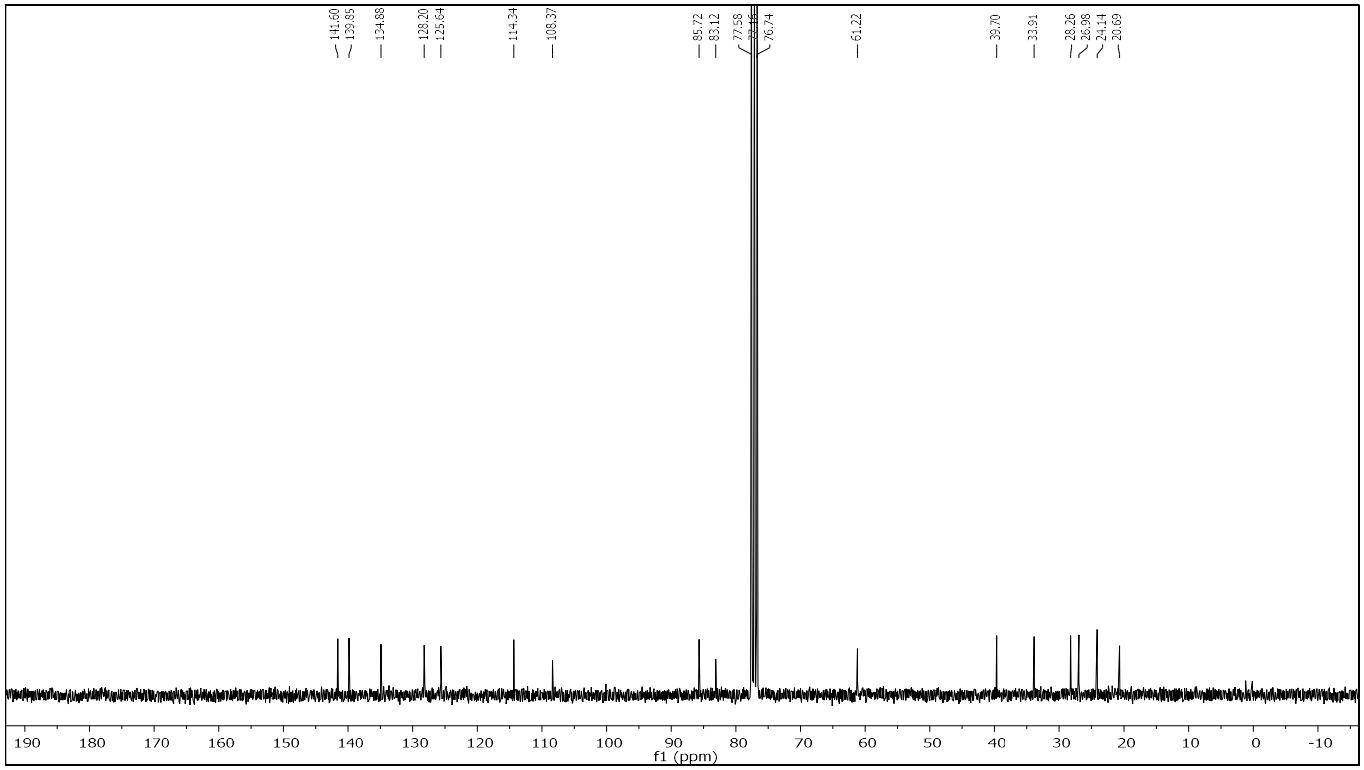
^{13}C-NMR spectrum of compound 6a/6b (75 MHz, $CDCl_3$):



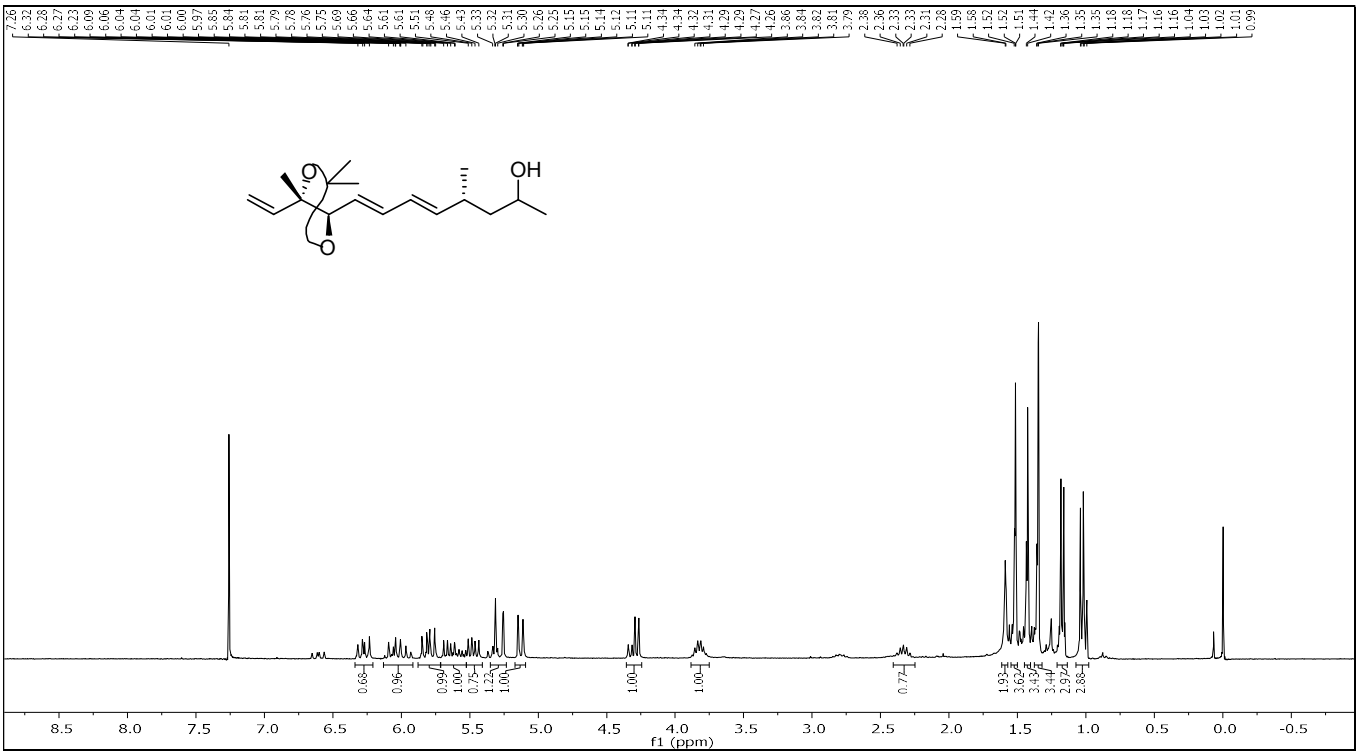
^{1}H-NMR spectrum of compound 25 (300 MHz, $CDCl_3$):



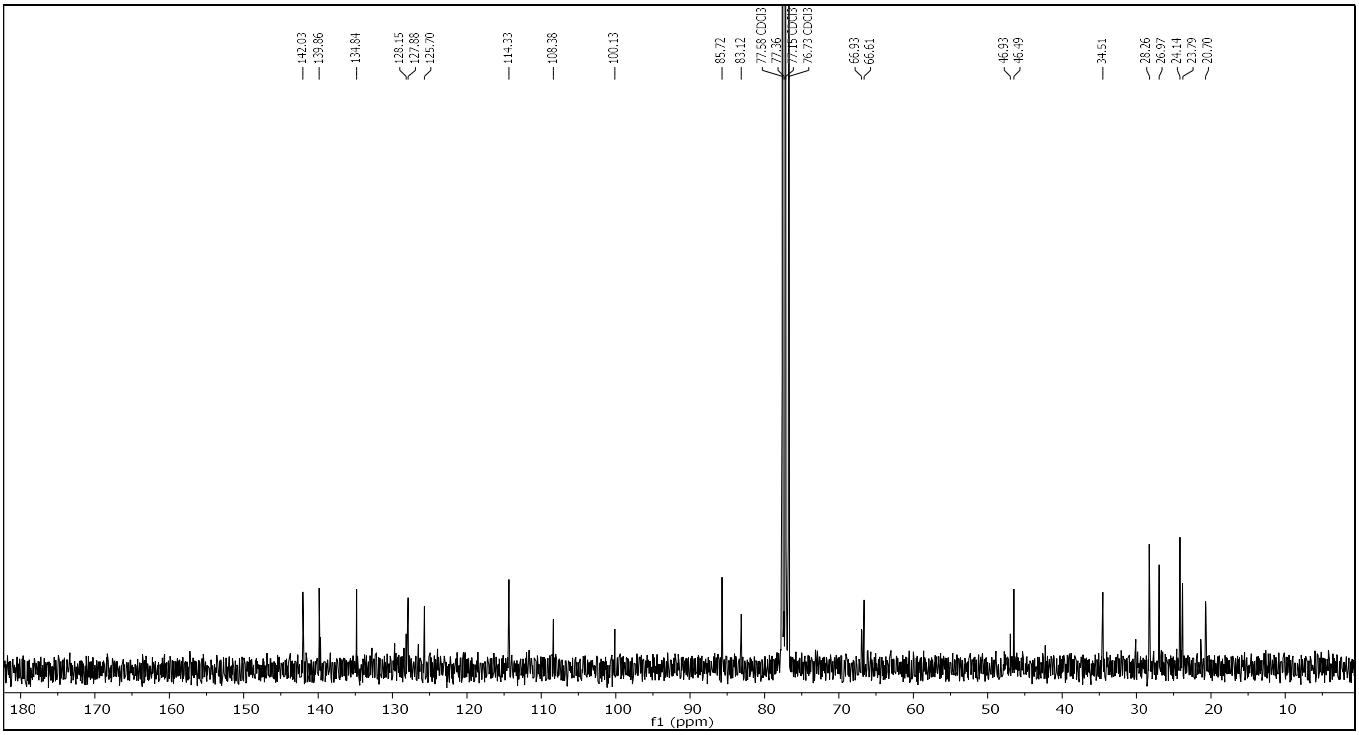
^{13}C-NMR spectrum of compound 25 (75 MHz, $CDCl_3$):



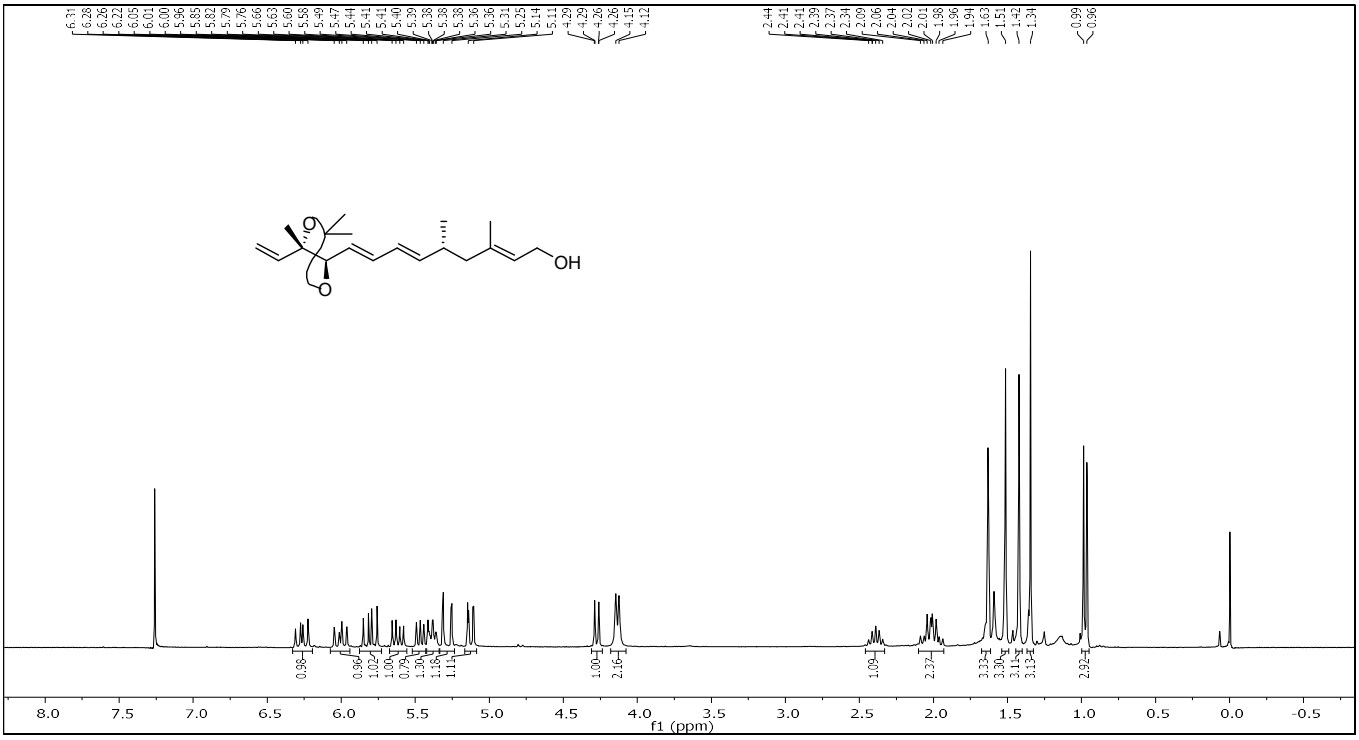
^{1}H-NMR spectrum of compound 26 (300 MHz, $CDCl_3$):



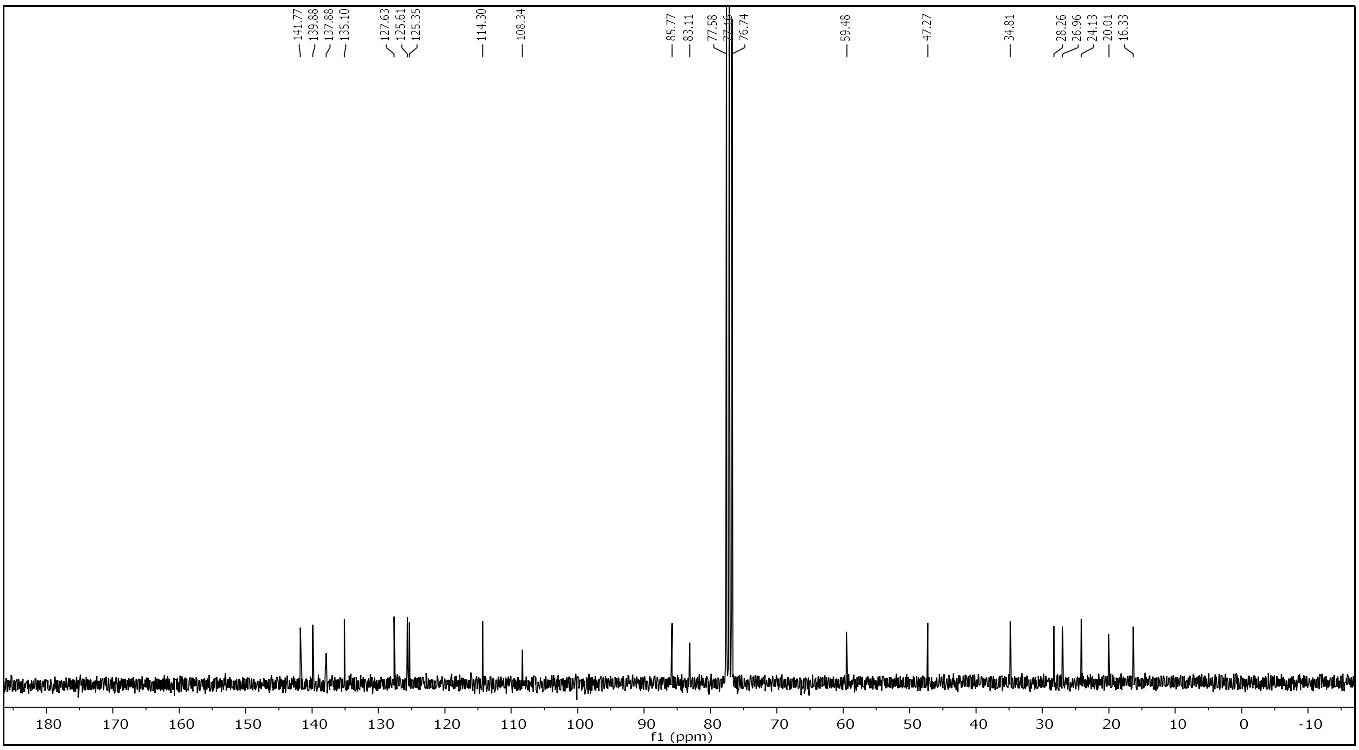
^{13}C-NMR spectrum of compound 26 (75 MHz, $CDCl_3$):



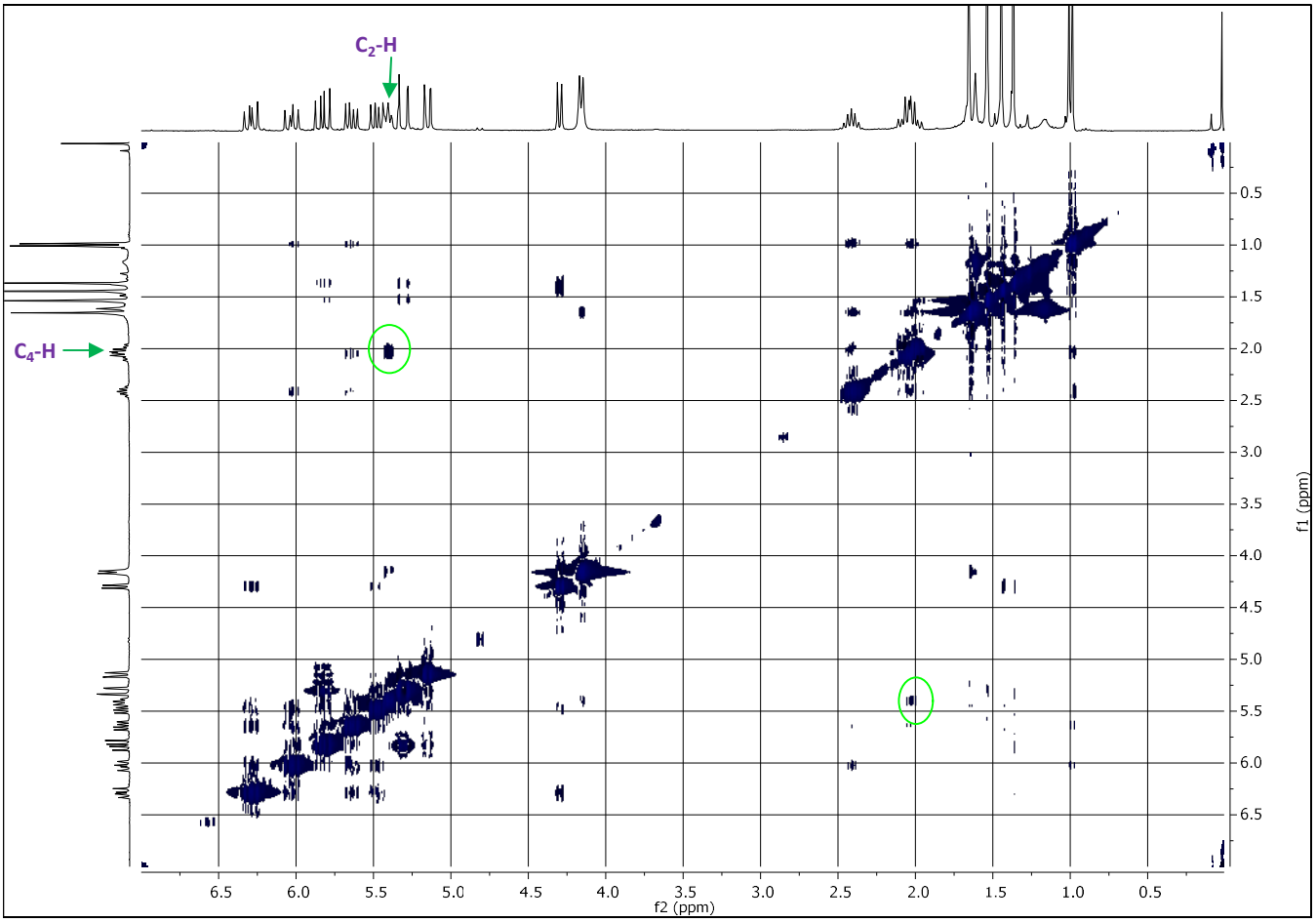
^{1}H-NMR spectrum of compound 27 (300 MHz, $CDCl_3$):

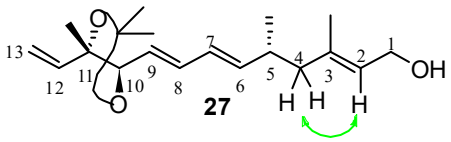


^{13}C-NMR spectrum of compound 27 (75 MHz, $CDCl_3$):

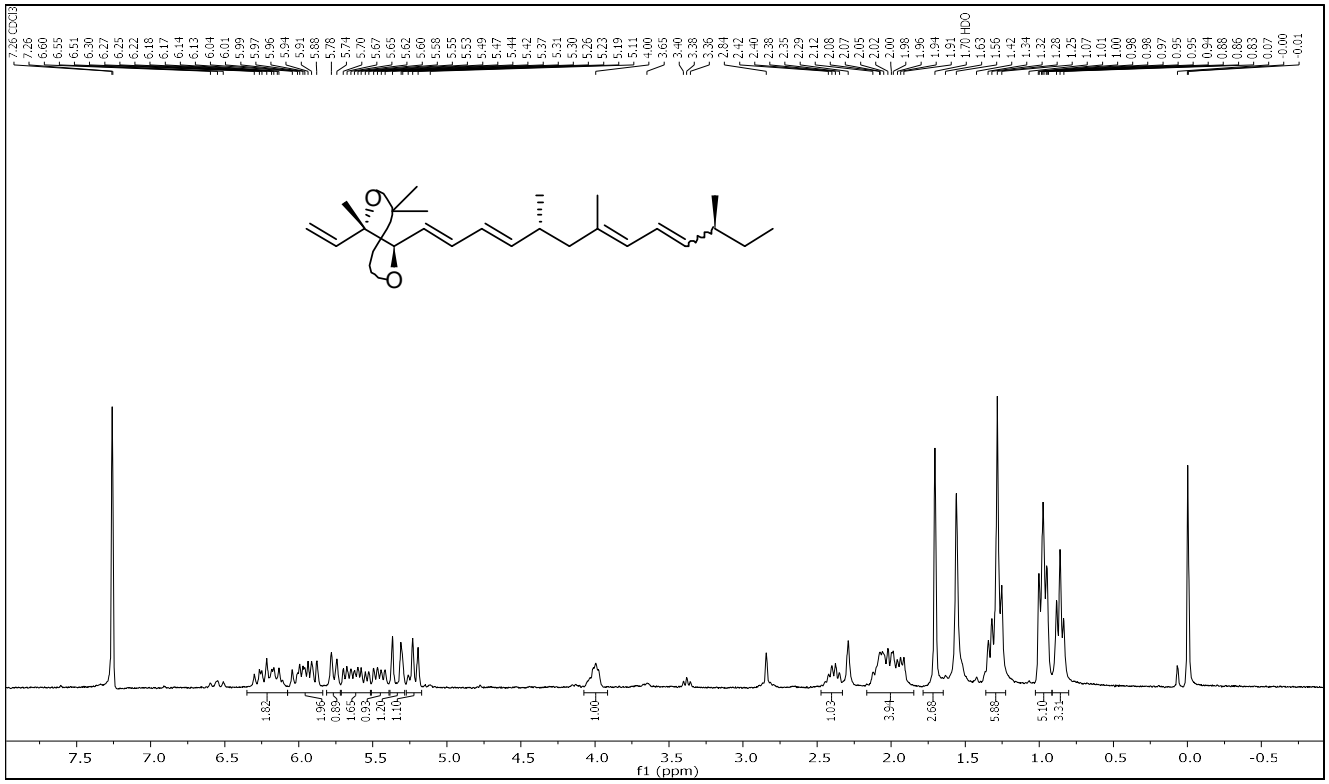


NOESY- spectrum of compound 27 (300 MHz, $CDCl_3$):

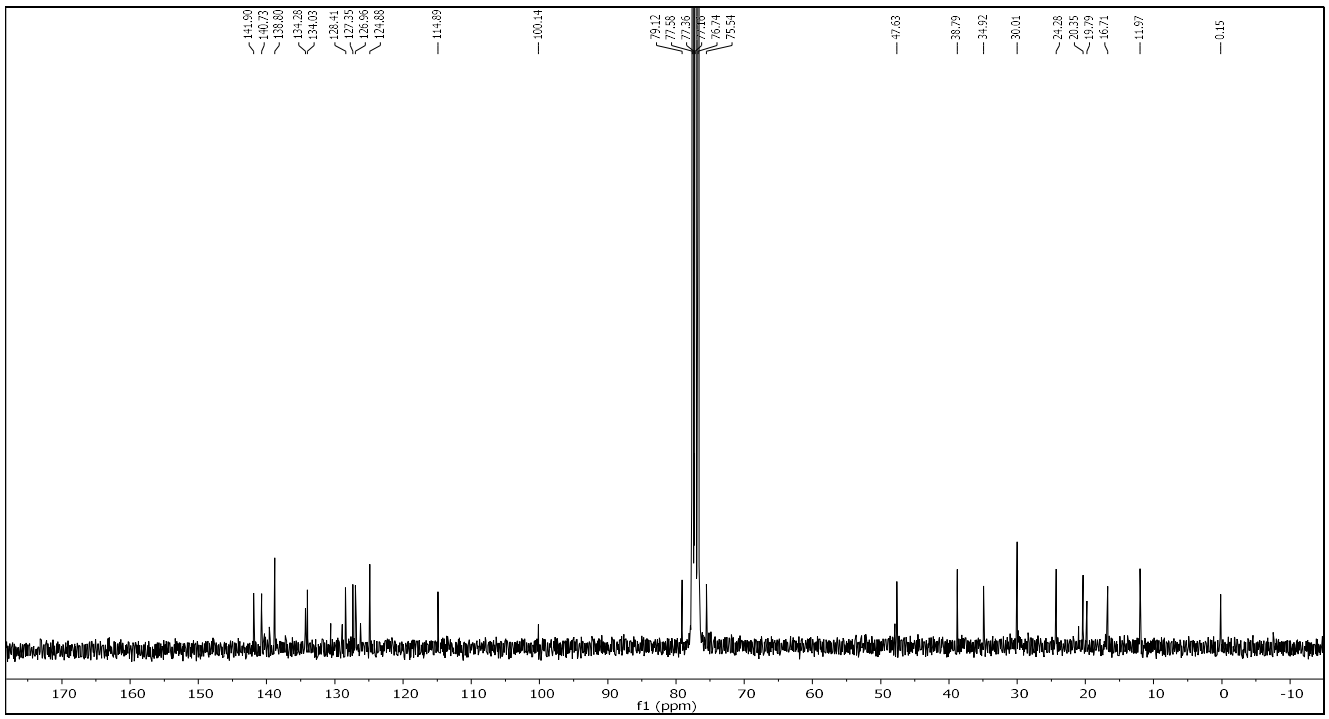




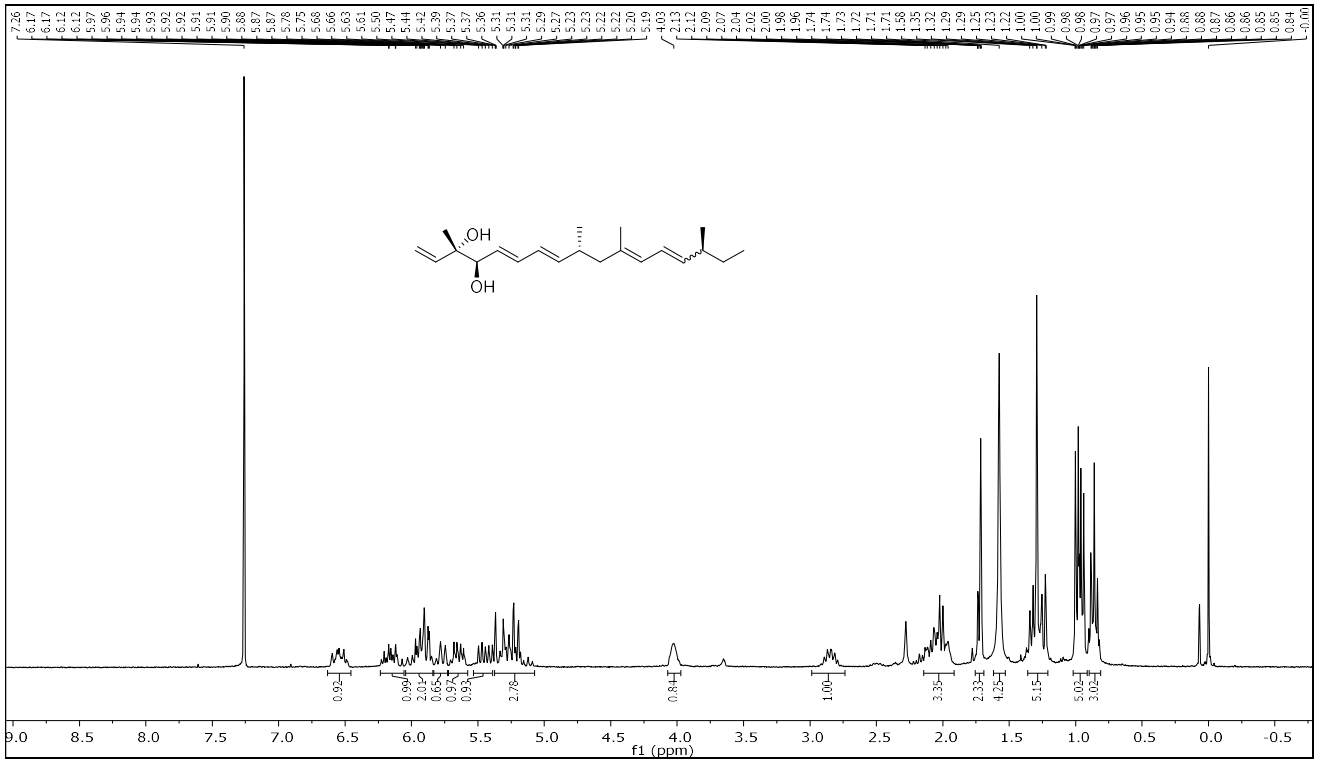
^{1}H-NMR spectrum of compound 28 (300 MHz, $CDCl_3$):



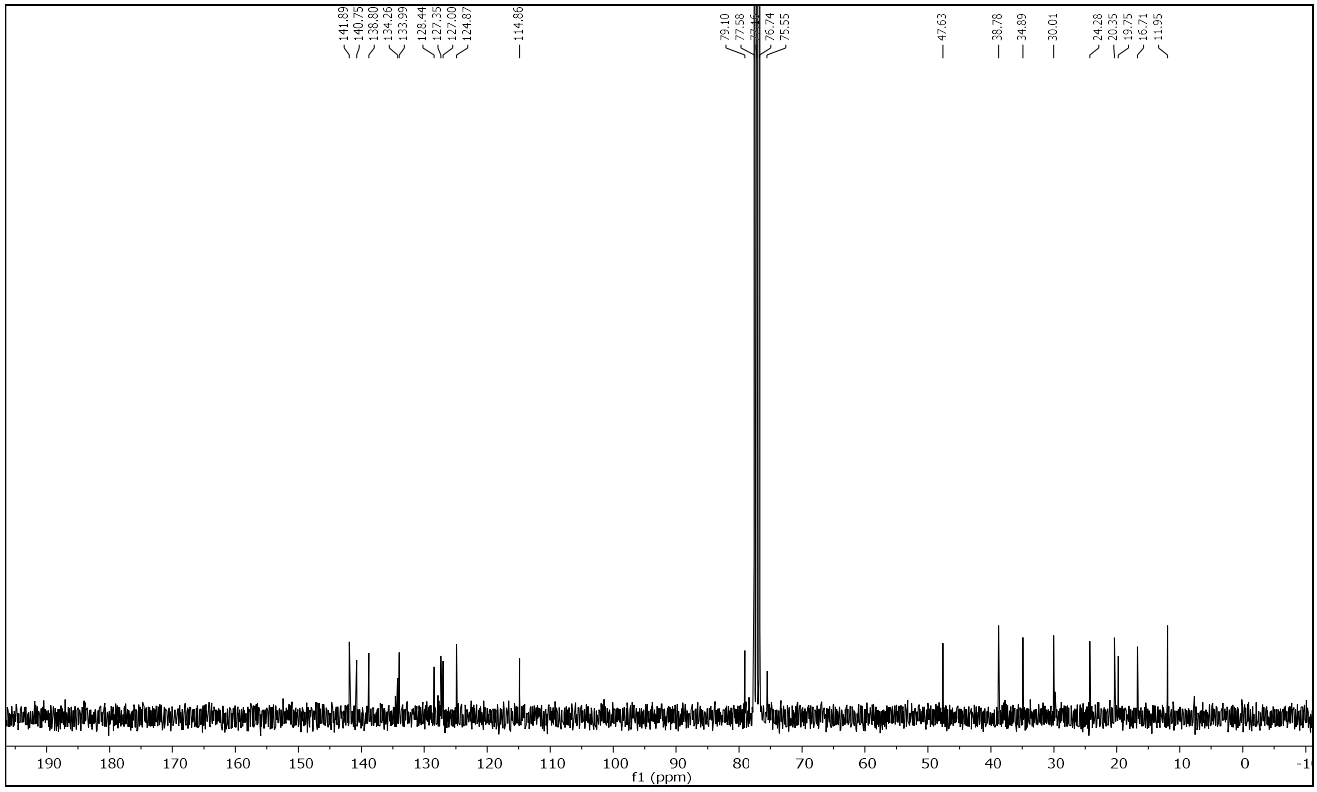
^{13}C-NMR spectrum of compound 28 (75 MHz, $CDCl_3$):



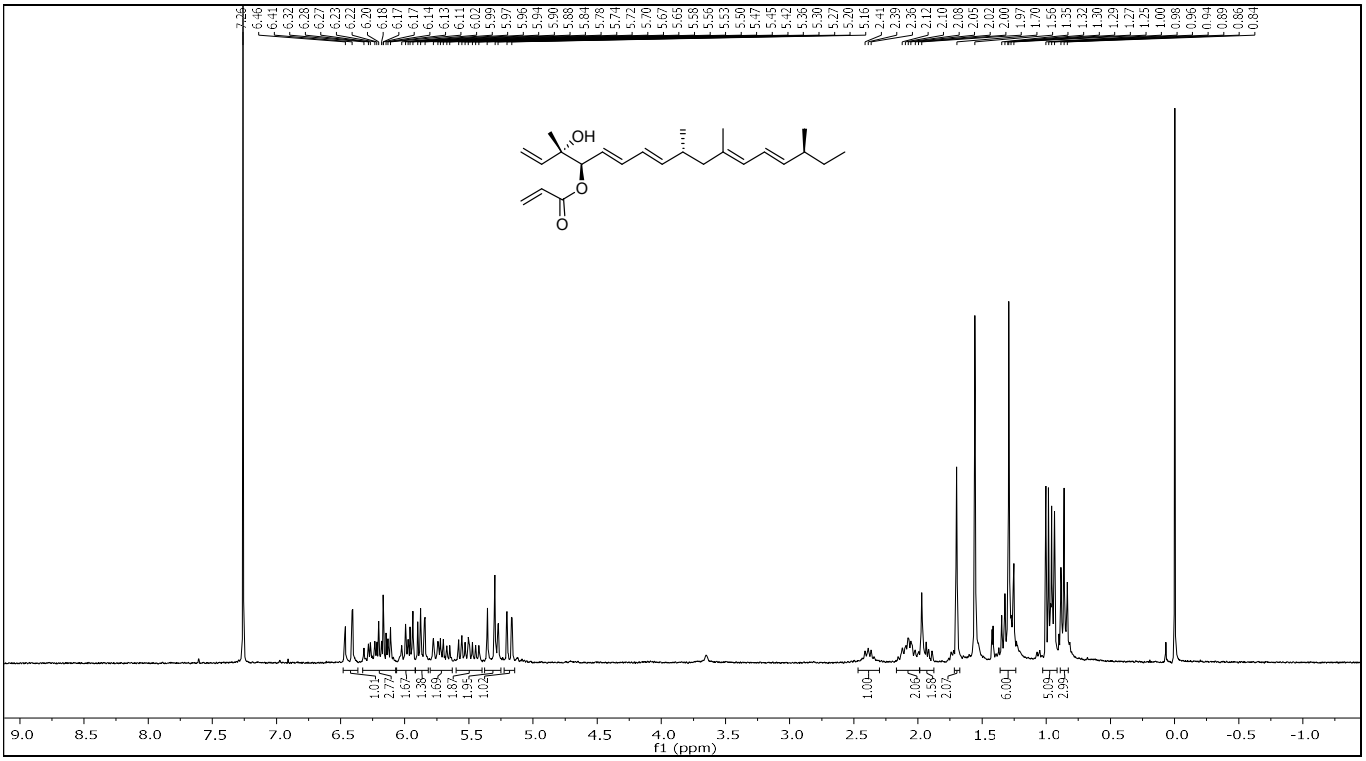
^{1}H-NMR spectrum of compound 29 (300 MHz, $CDCl_3$):



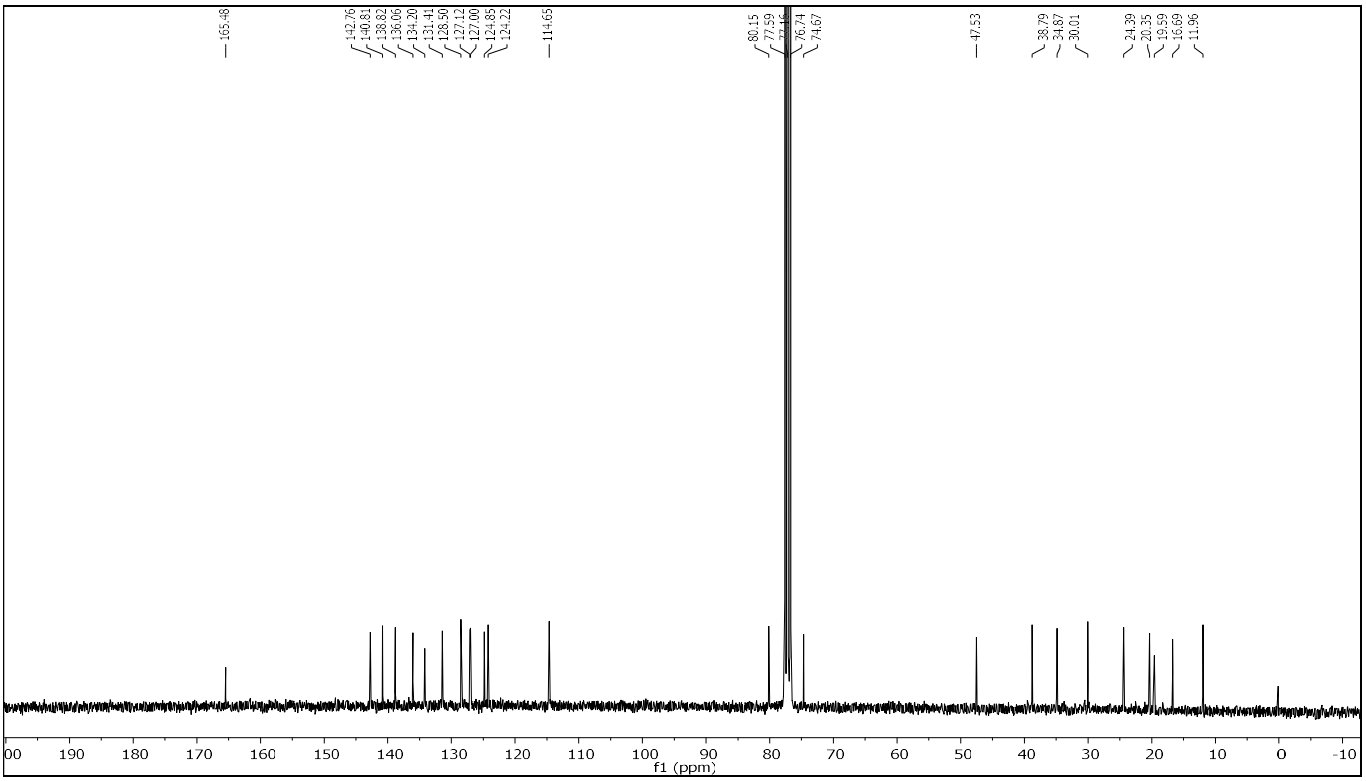
^{13}C-NMR spectrum of compound 29 (75 MHz, $CDCl_3$):



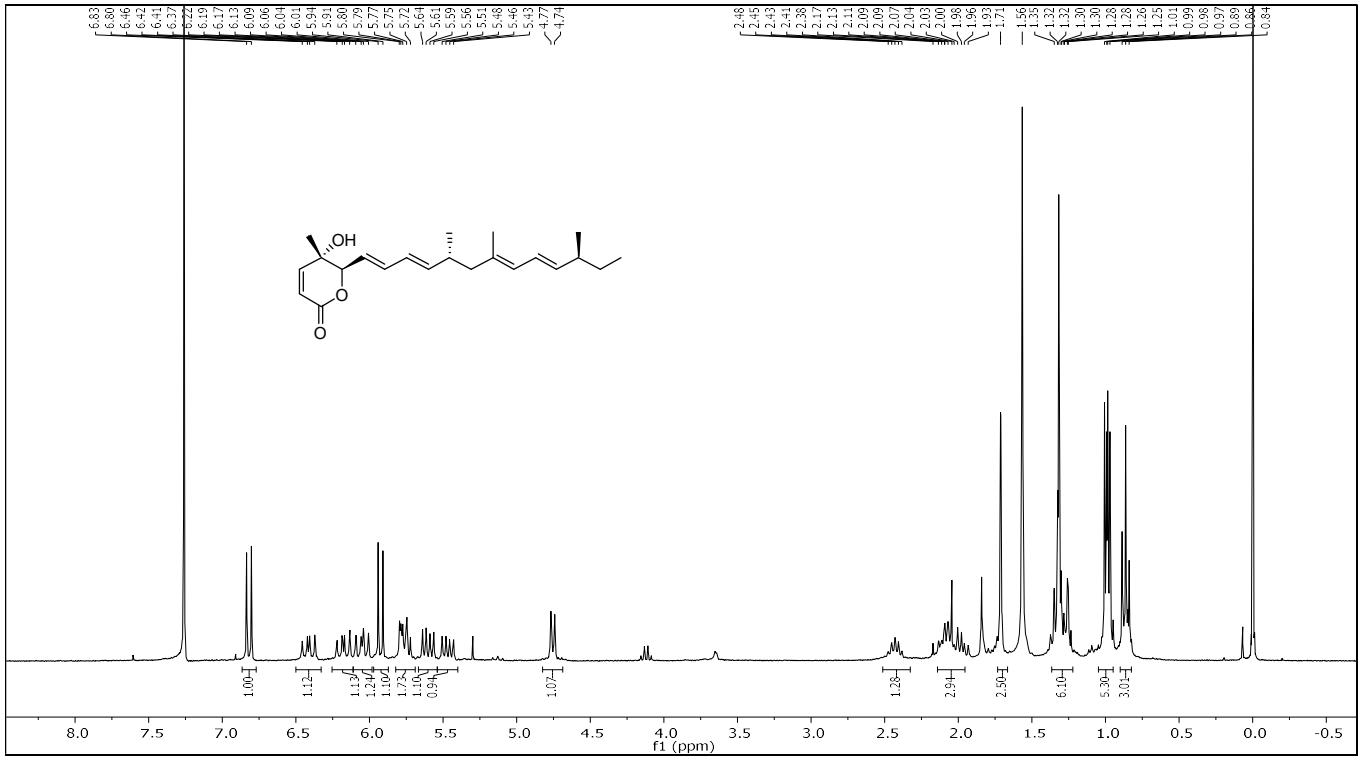
^{1}H-NMR spectrum of compound 30 (300 MHz, $CDCl_3$):



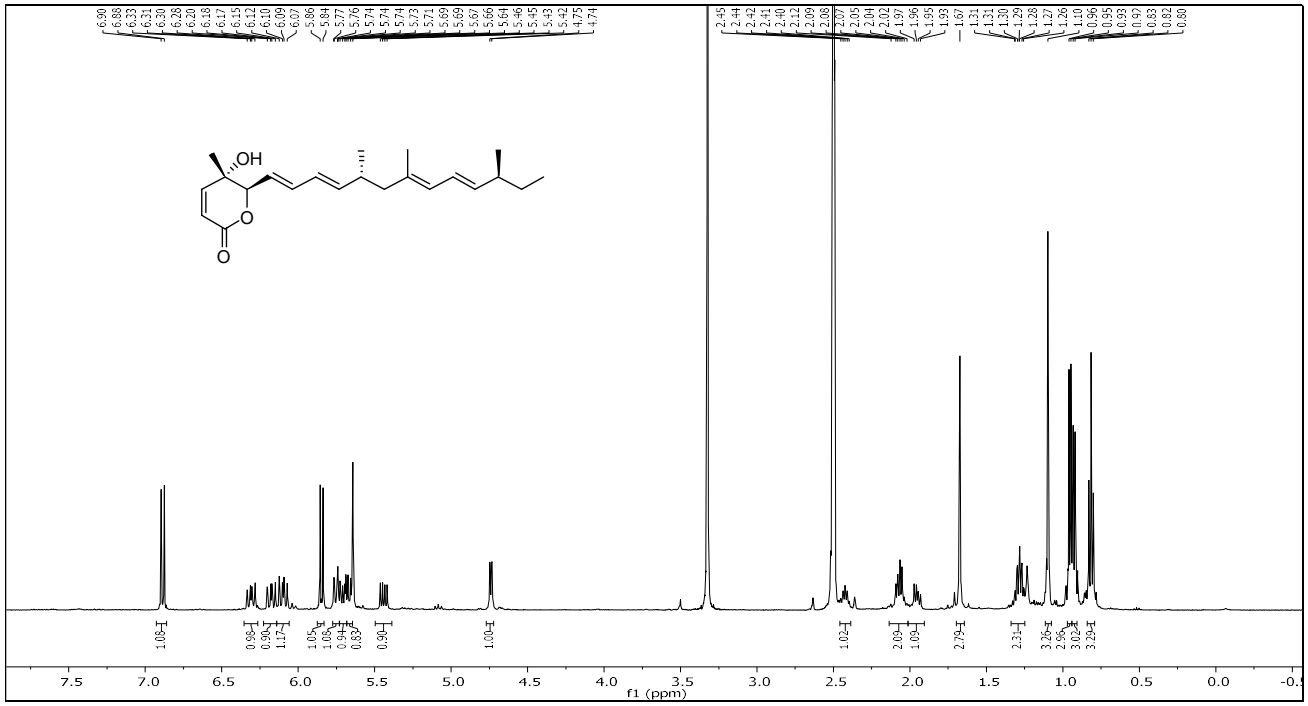
^{13}C-NMR spectrum of compound 30 (75 MHz, $CDCl_3$):



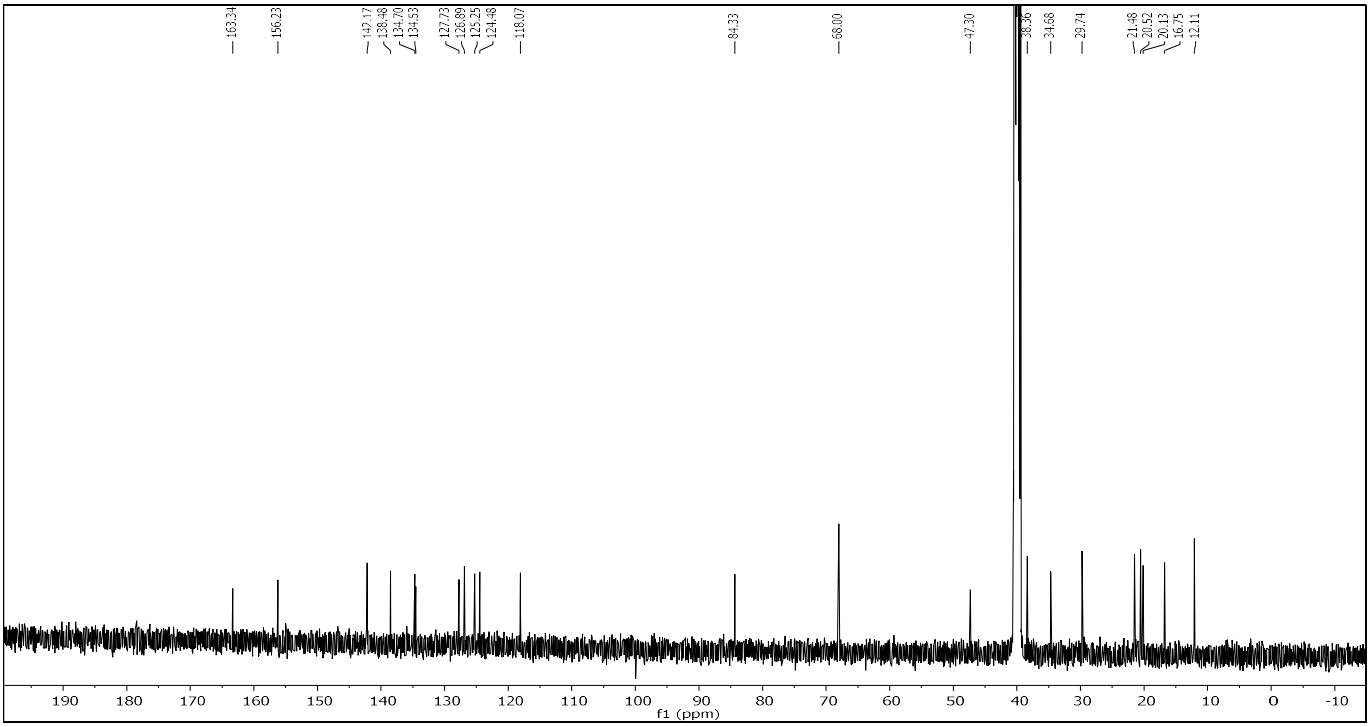
^{1}H-NMR spectrum of compound 5 (300 MHz, $CDCl_3$):



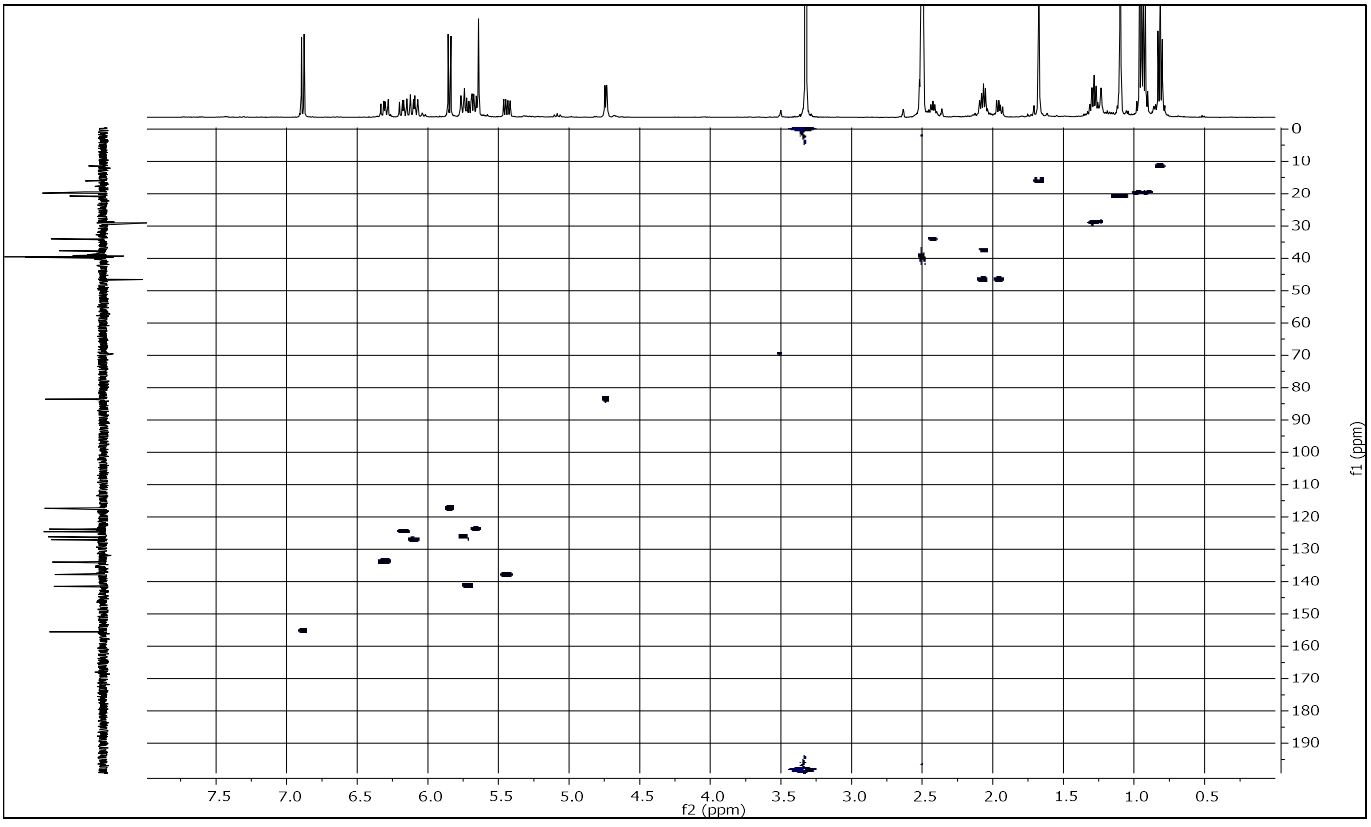
^{1}H-NMR spectrum of compound 5 (500 MHz, DMSO-d_6):



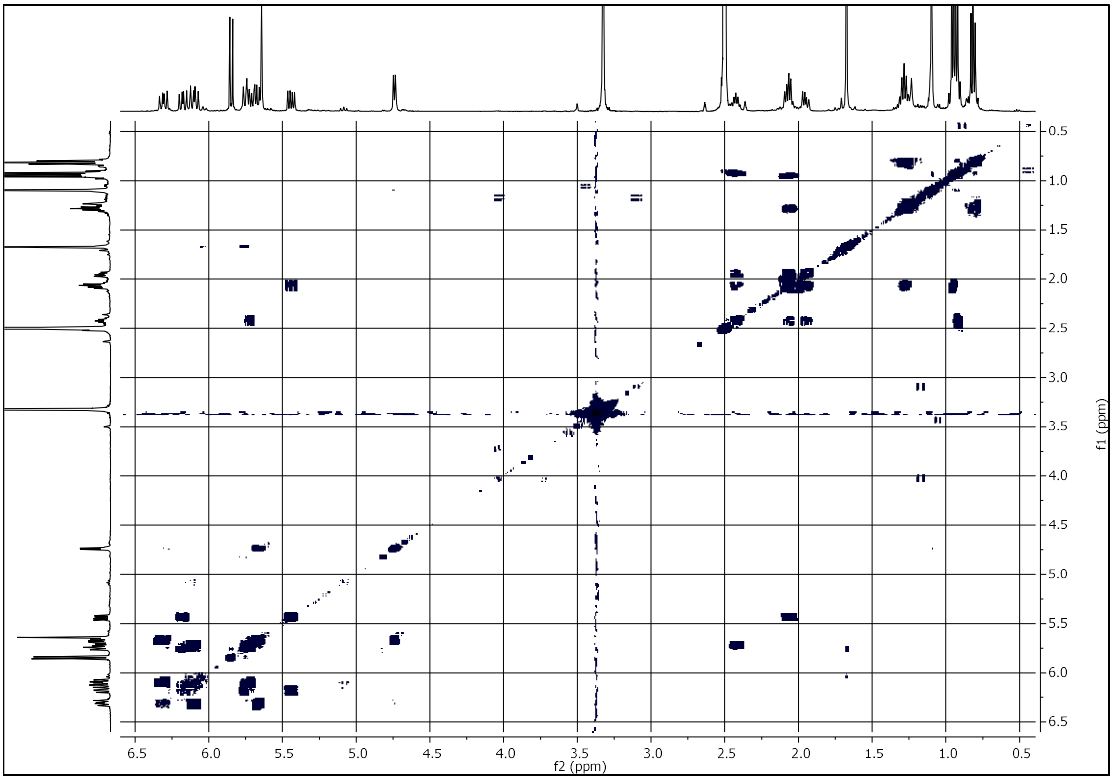
^{13}C-NMR spectrum of compound 5 (125 MHz, DMSO-d_6):



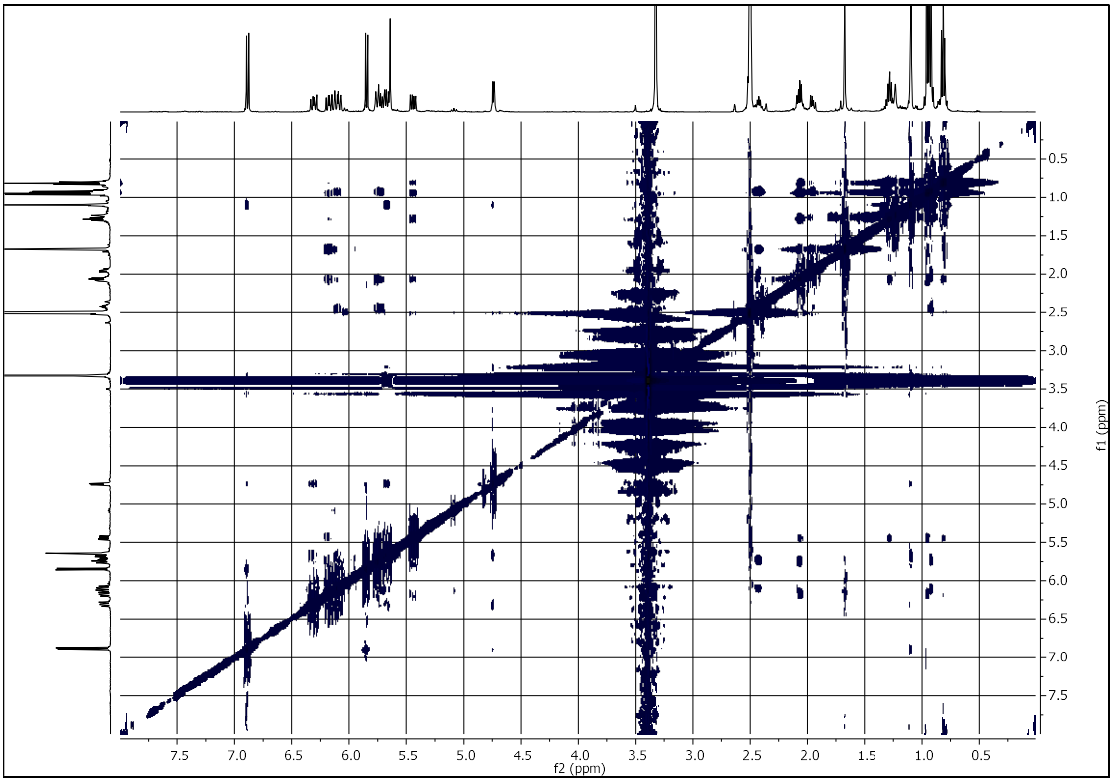
HSQC spectrum of compound 5 (500 MHz, DMSO-d_6):



COSY spectrum of compound 5 (400 MHz, DMSO-d_6):



NOESY spectrum of compound 5 (500 MHz, DMSO-d_6):



HRMS spectrum of compound 5: