Supporting Information

Asymmetric total synthesis of paecilomycin C through intramolecular nucleophilic opening of an epoxide

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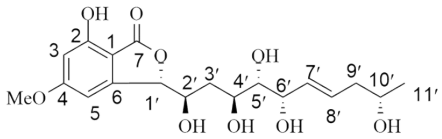
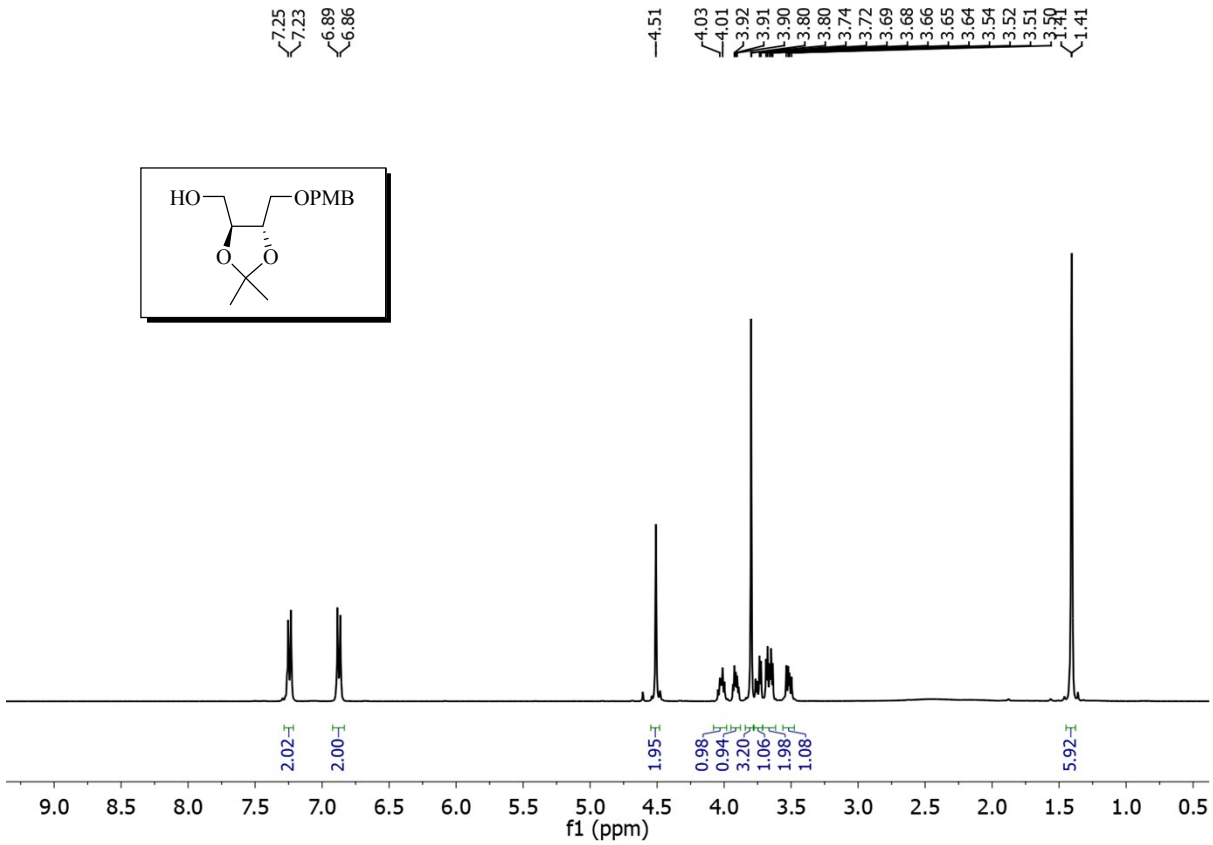
Table SI-1: NMR comparison table of natural and synthetic paecilomycin C (in Pyridine d5)



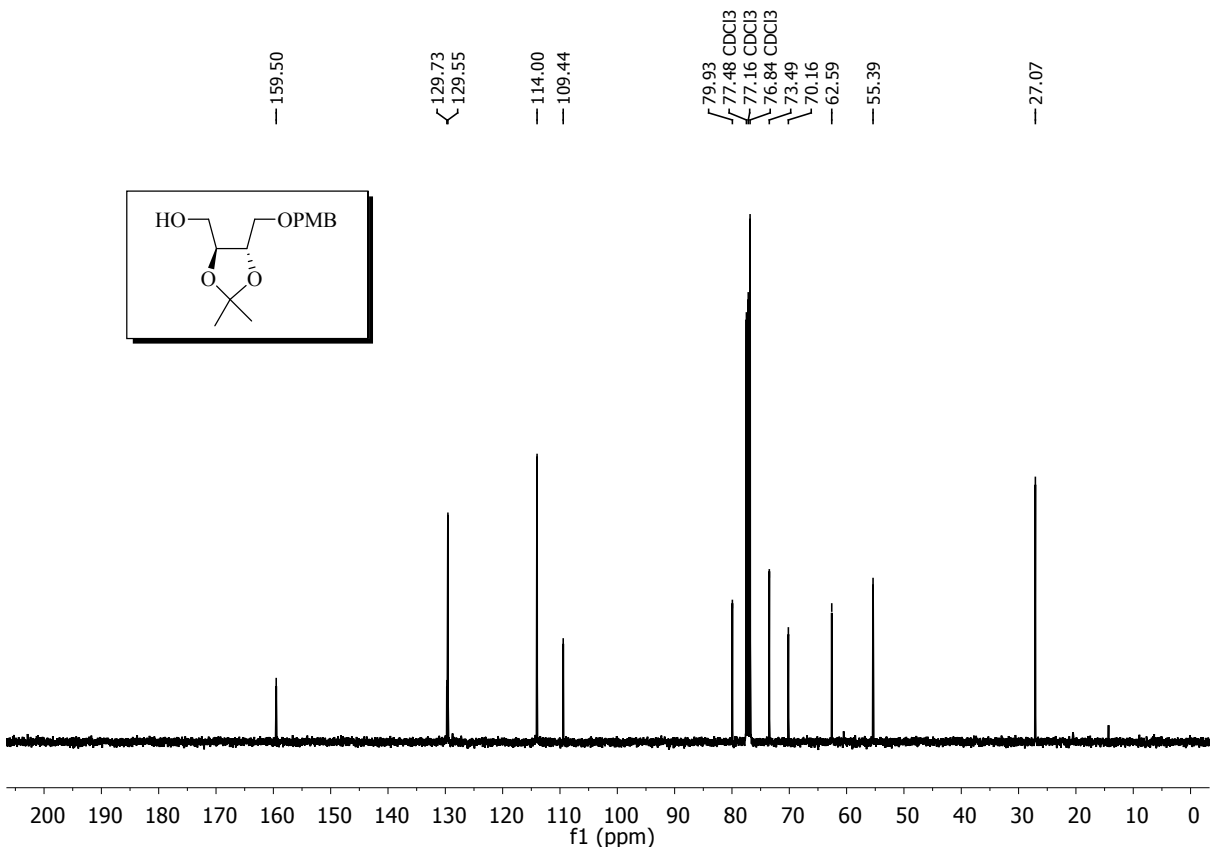
Paecilomycin C

Position	Reported ^{1}H δ (ppm); J (Hz)	Observed ^{1}H δ (ppm); J (Hz)	$\Delta\delta$ (ppm)	Reported ^{13}C δ (ppm)	Observed ^{13}C δ (ppm)	$\Delta\delta$ (ppm)
1				107.3	107.3	0.0
2				159.6	159.3	0.3
3	6.71 (br s)	6.70, (br s)	0.01	103.0	103.0	0.0
4				166.6	166.6	0.0
5	7.00 (br s)	7.00, (br s)	0.0	101.0	101.0	0.0
6				152.3	152.3	0.0
7				169.9	169.8	0.1
1'	5.74 (d, 4.3)	5.73 (d, 4.6)	0.01	83.4	83.4	0.0
2'	4.83 (dt, 8.8,4.3)	4.82 (dt, 8.8, 4.3)	0.01	72.1	72.2	0.1
3'	2.5 (m), 2.84 (dt,13.8, 3.2)	2.5 (m), 2.84 (dt, 13.8, 3.2)	0.0	37.0	37.0	0.0
4'	4.74 (td, 8.2,3.2)	4.74, (td, 8.1, 3.1)	0.0	71.6	71.7	0.1
5'	4.08 (m)	4.06 (m)	0.02	78.2	78.2	0.0
6'	5.05 (br s)	5.03 (br s)	0.02	72.7	72.7	0.0
7'	6.2 (m)	6.2 (m)	0.0	134.8	134.7	0.1
8'	6.2 (m)	6.2 (m)	0.0	128.8	128.8	0.0
9'	2.5 (m), 2.38 (dt,12.3, 5.4)	2.5 (m), 2.38 (dt,12.3, 5.4)	0.0	43.4	43.4	0.0
10'	4.08 (m)	4.08 (m)	0.0	67.2	67.2	0.0
11'	1.30 (d, 6.3)	1.30 (d, 6.1)	0.0	23.8	23.7	0.1
4-OMe	3.64 (s)	3.64 (s)	0.0	55.8	55.7	0.1

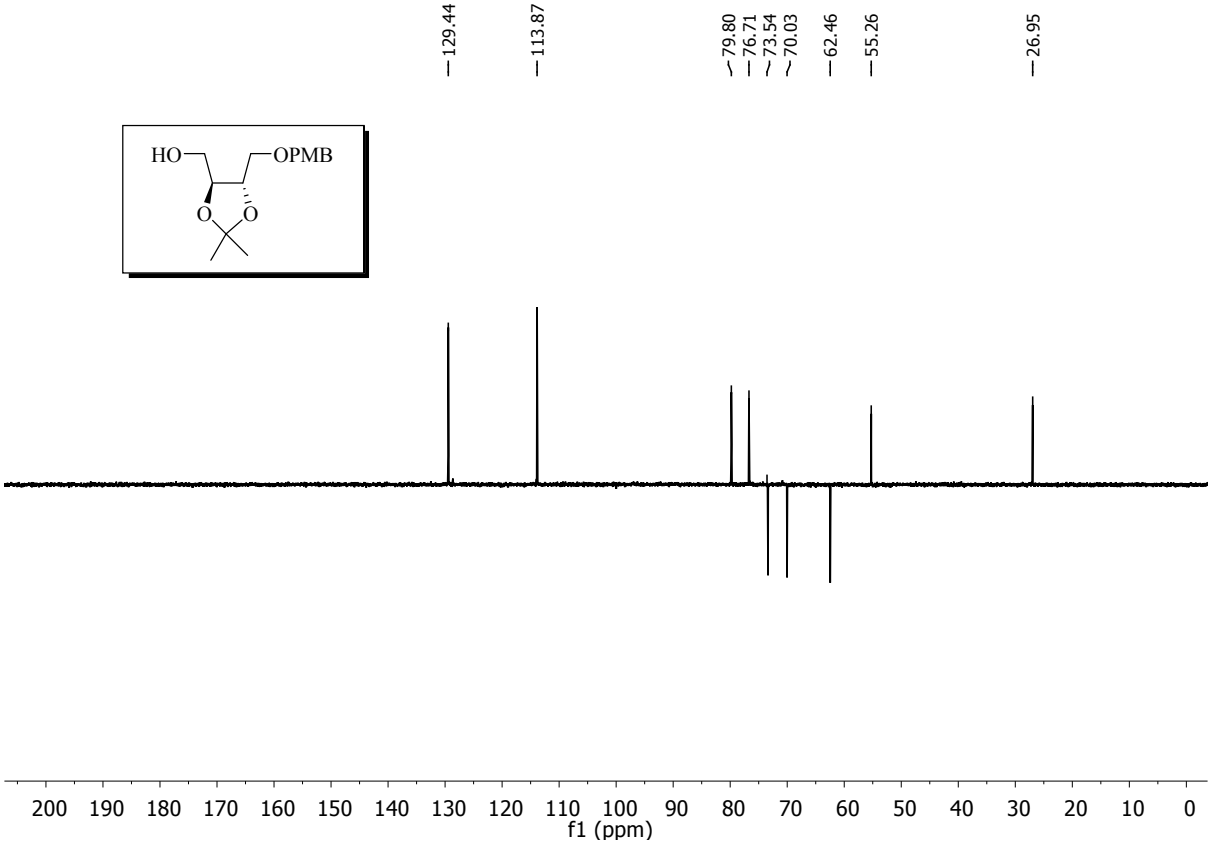
^{1}H NMR of compound 18 (400 MHz, $CDCl_3$)



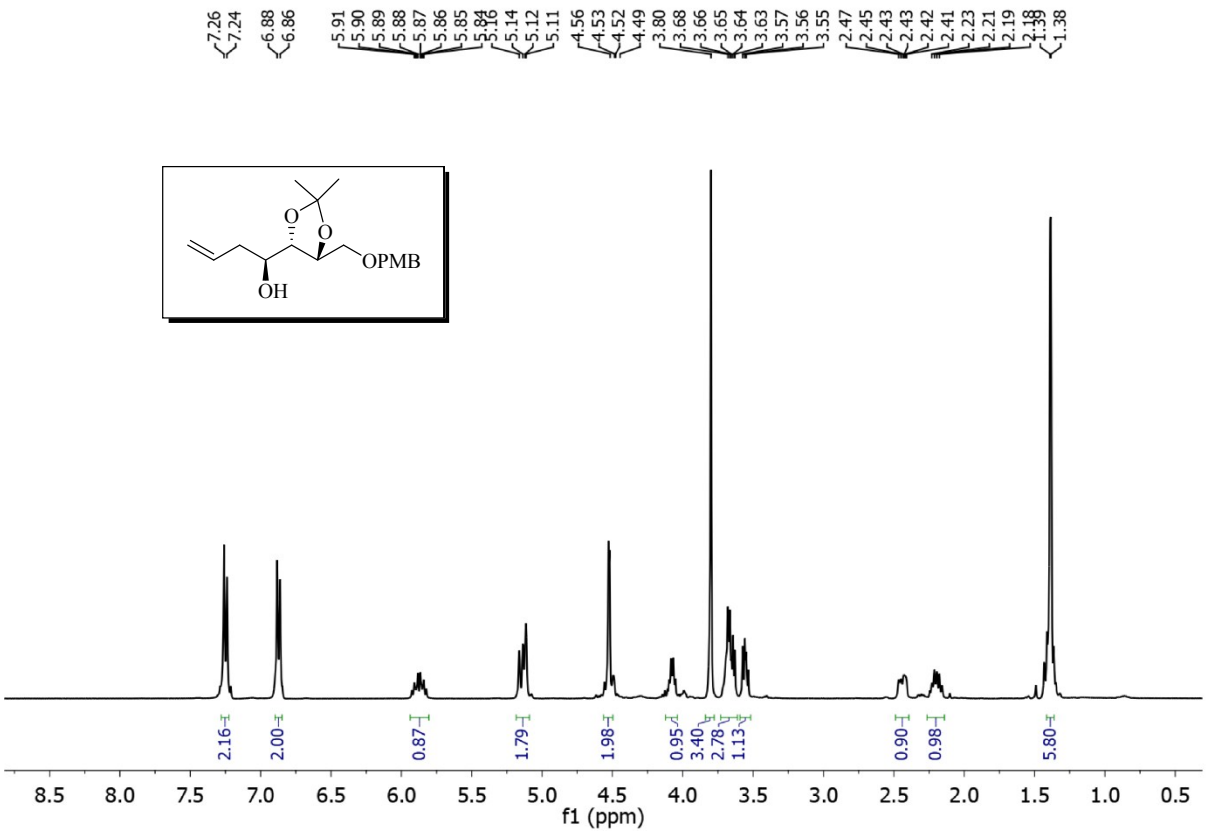
^{13}C NMR of compound 18 (100 MHz, $CDCl_3$



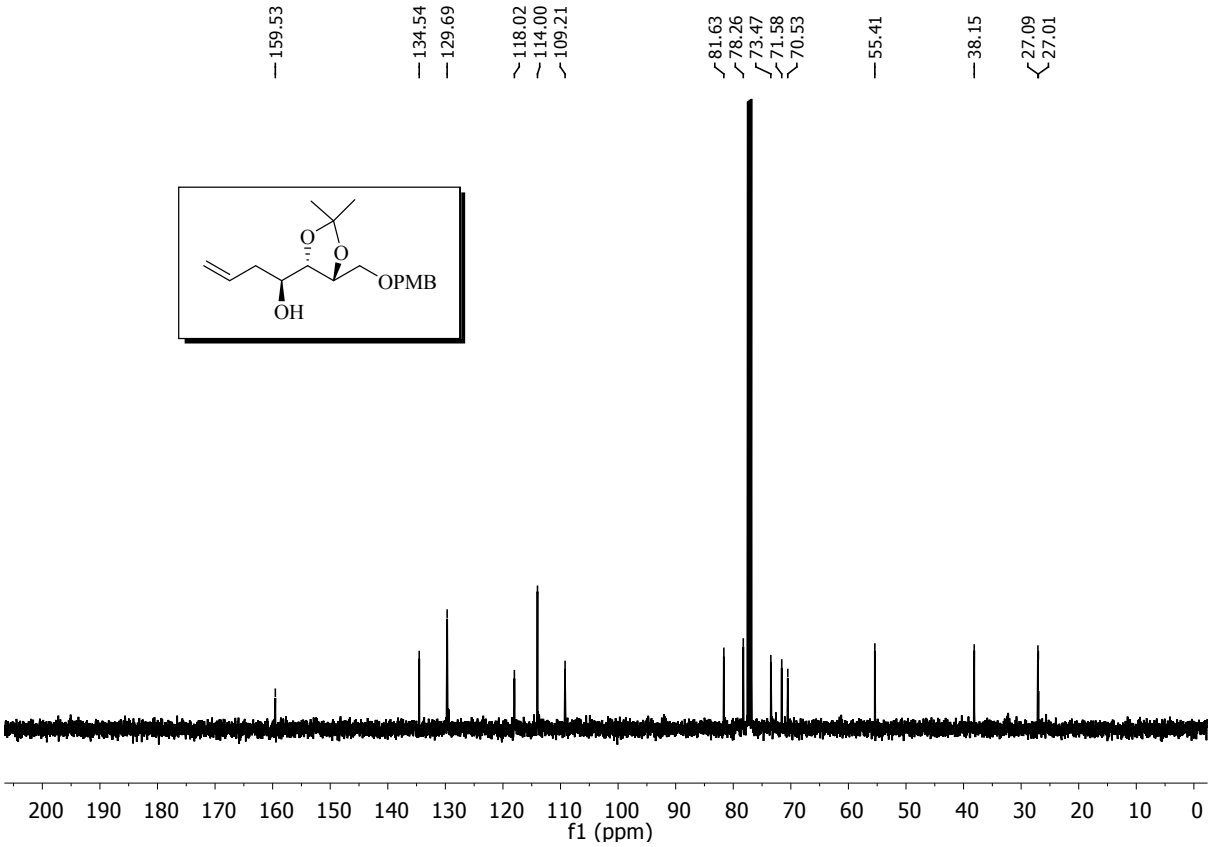
DEPT-135 of compound 18 (100 MHz, $CDCl_3$)



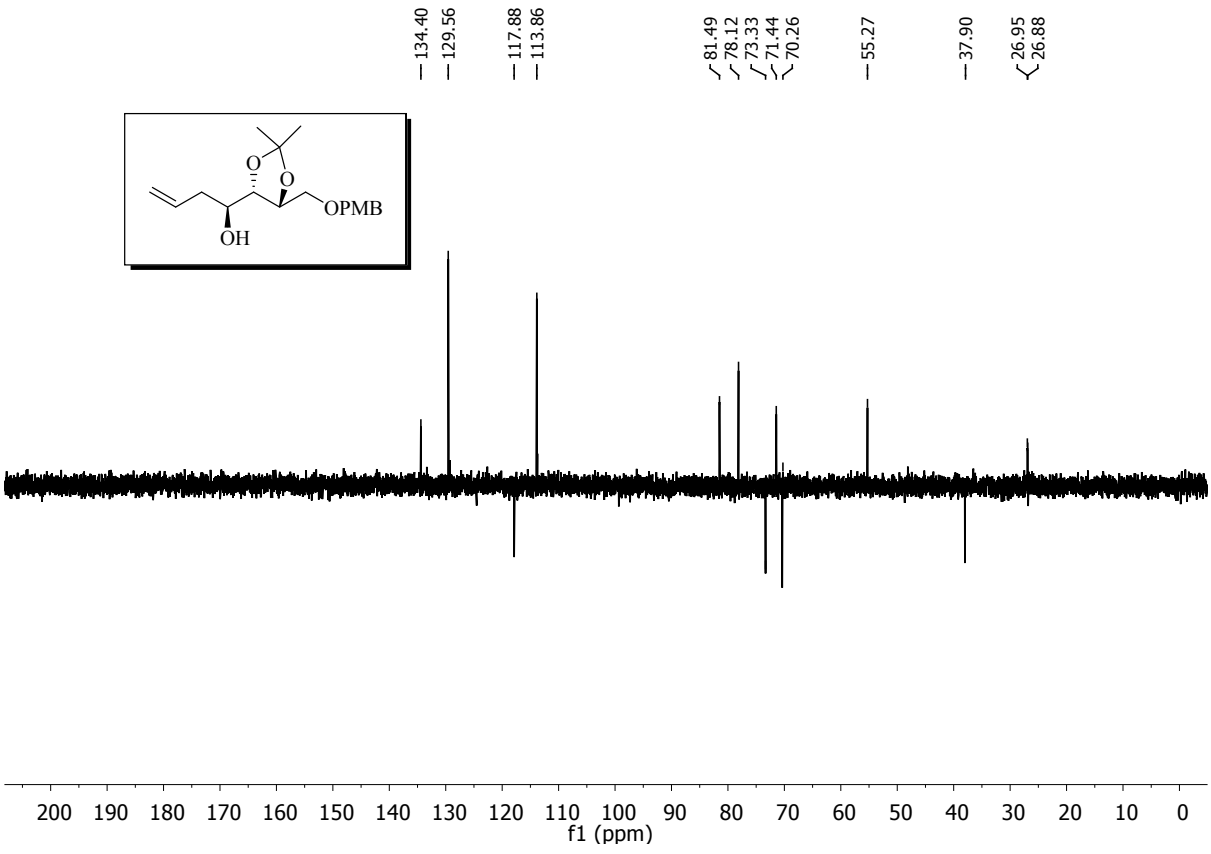
^{1}H NMR of compound 15 (400 MHz, $CDCl_3$)



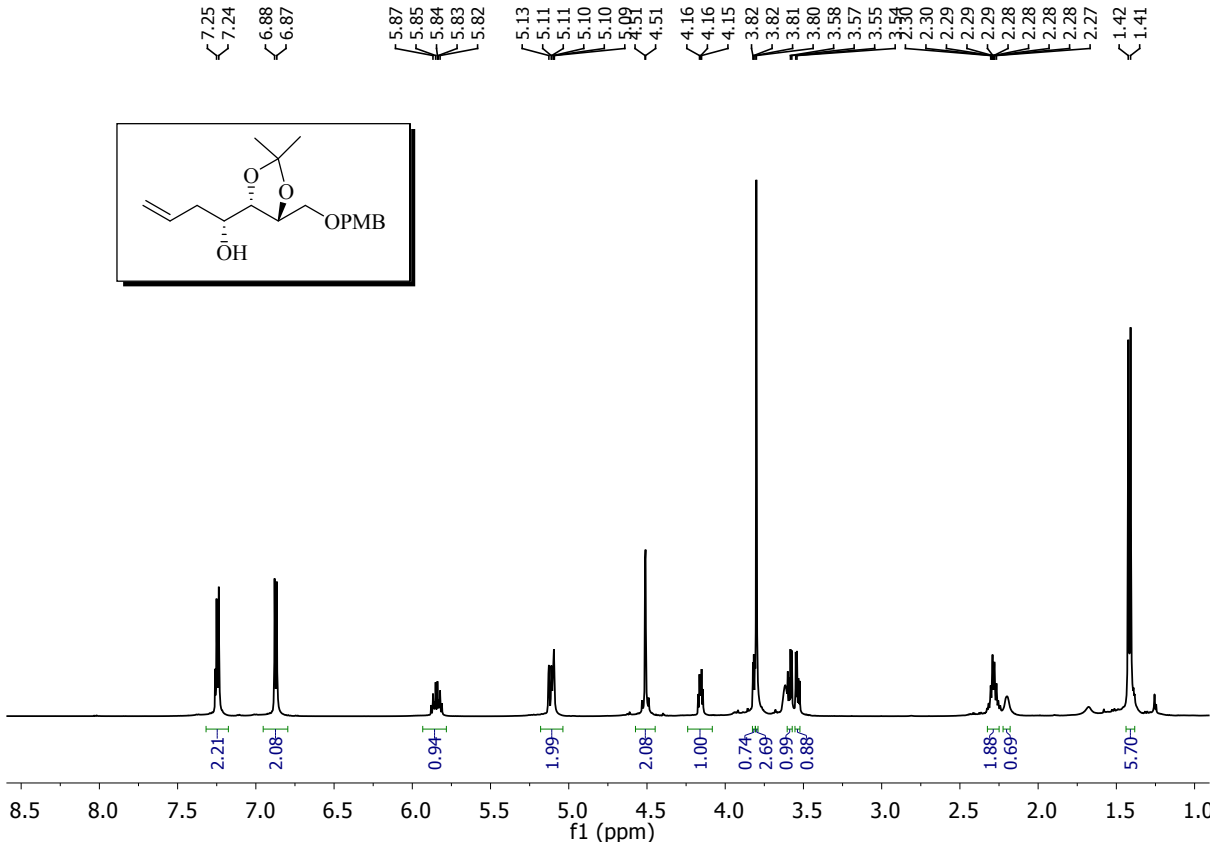
^{13}C NMR of compound 15 (100 MHz, $CDCl_3$)



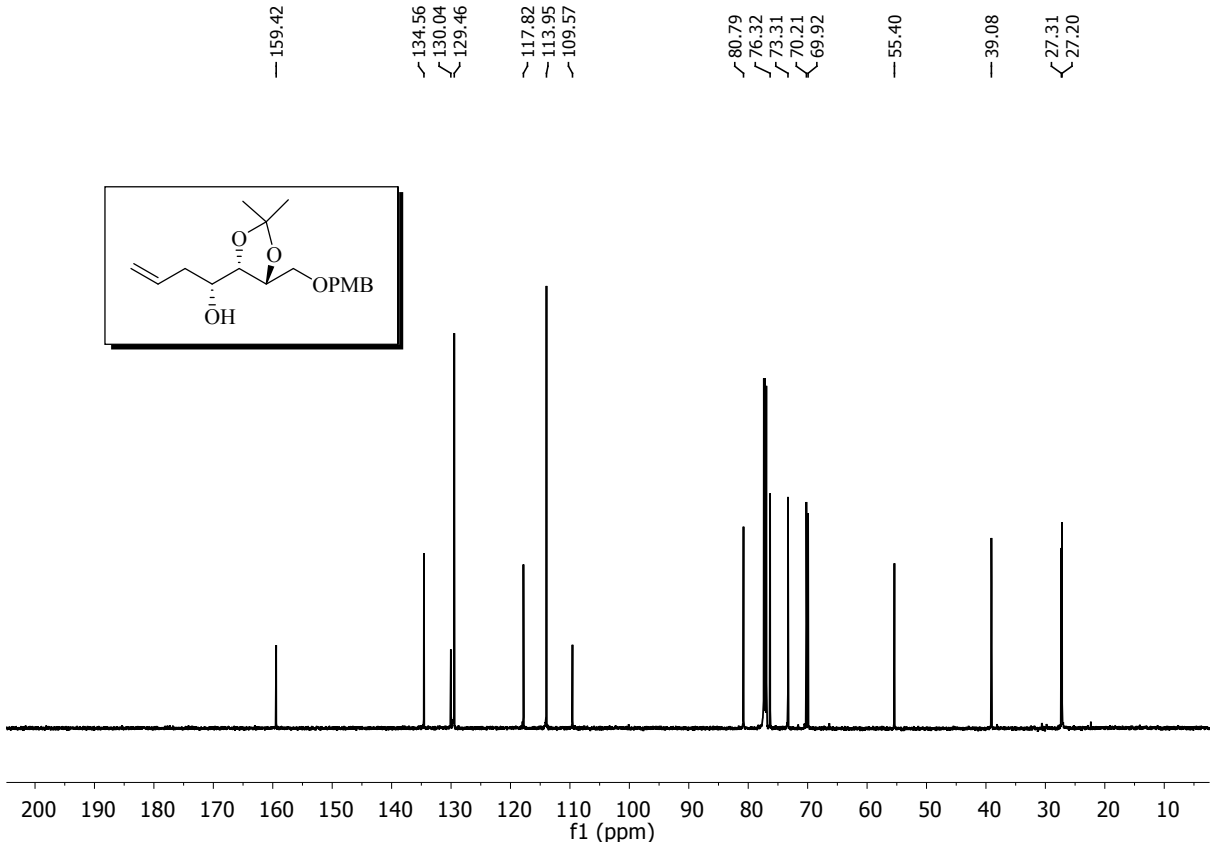
DEPT-135 of compound 15 (100 MHz, $CDCl_3$)



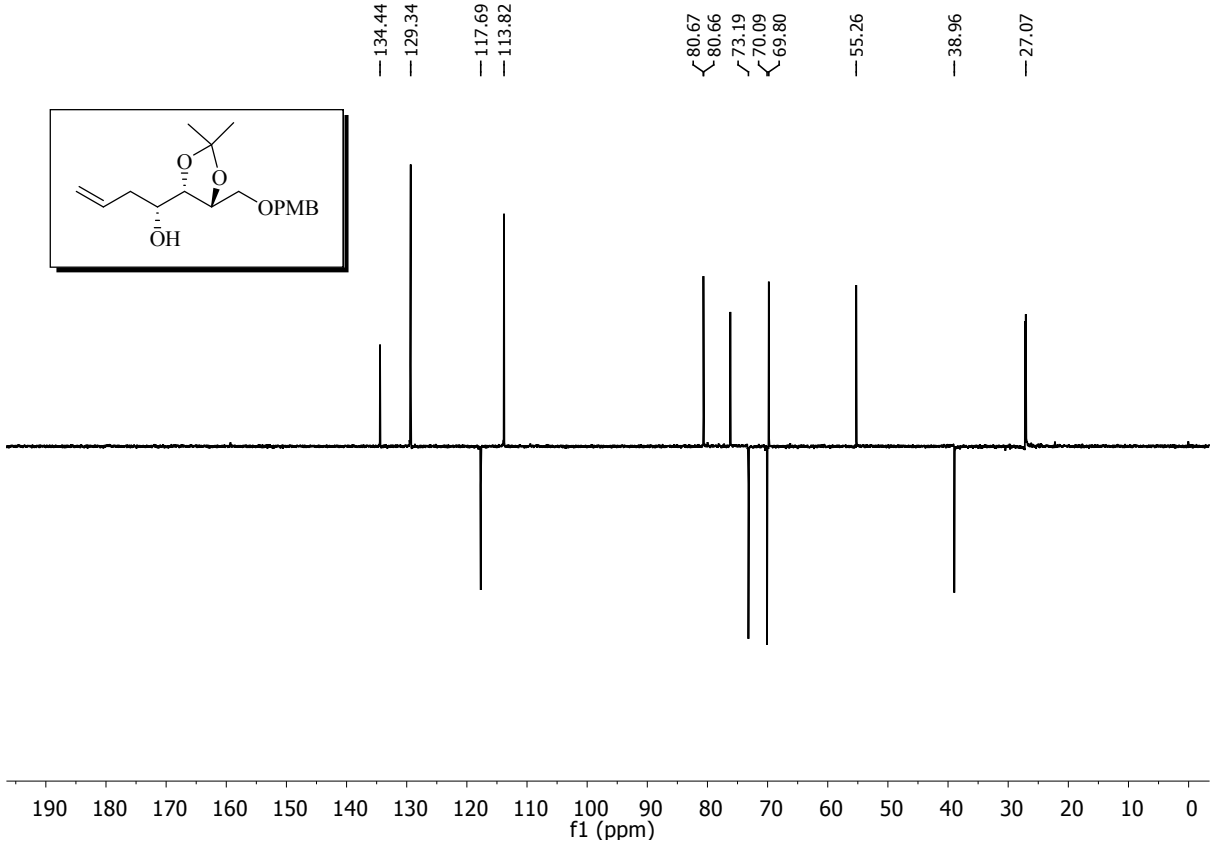
^{1}H NMR of compound 20 (600 MHz, $CDCl_3$)



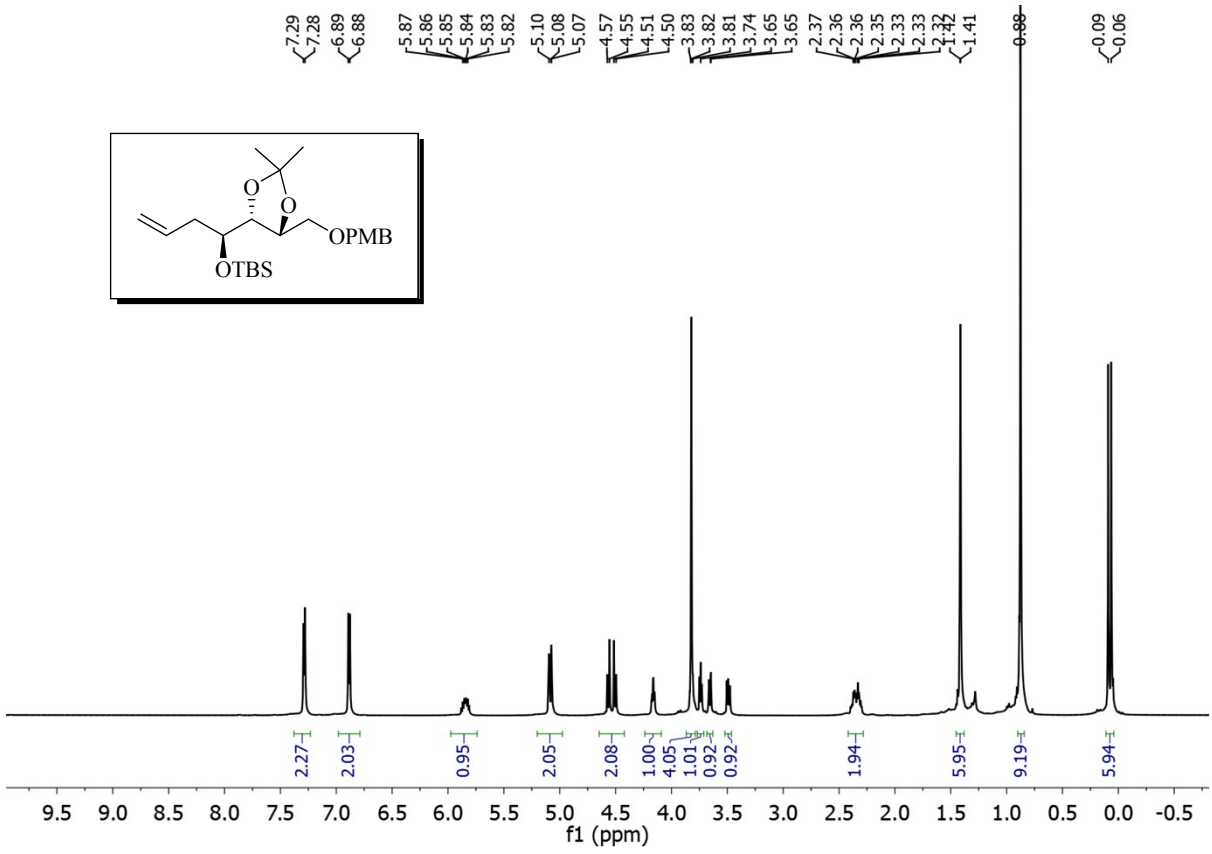
^{13}C NMR of compound 20 (150 MHz, $CDCl_3$)



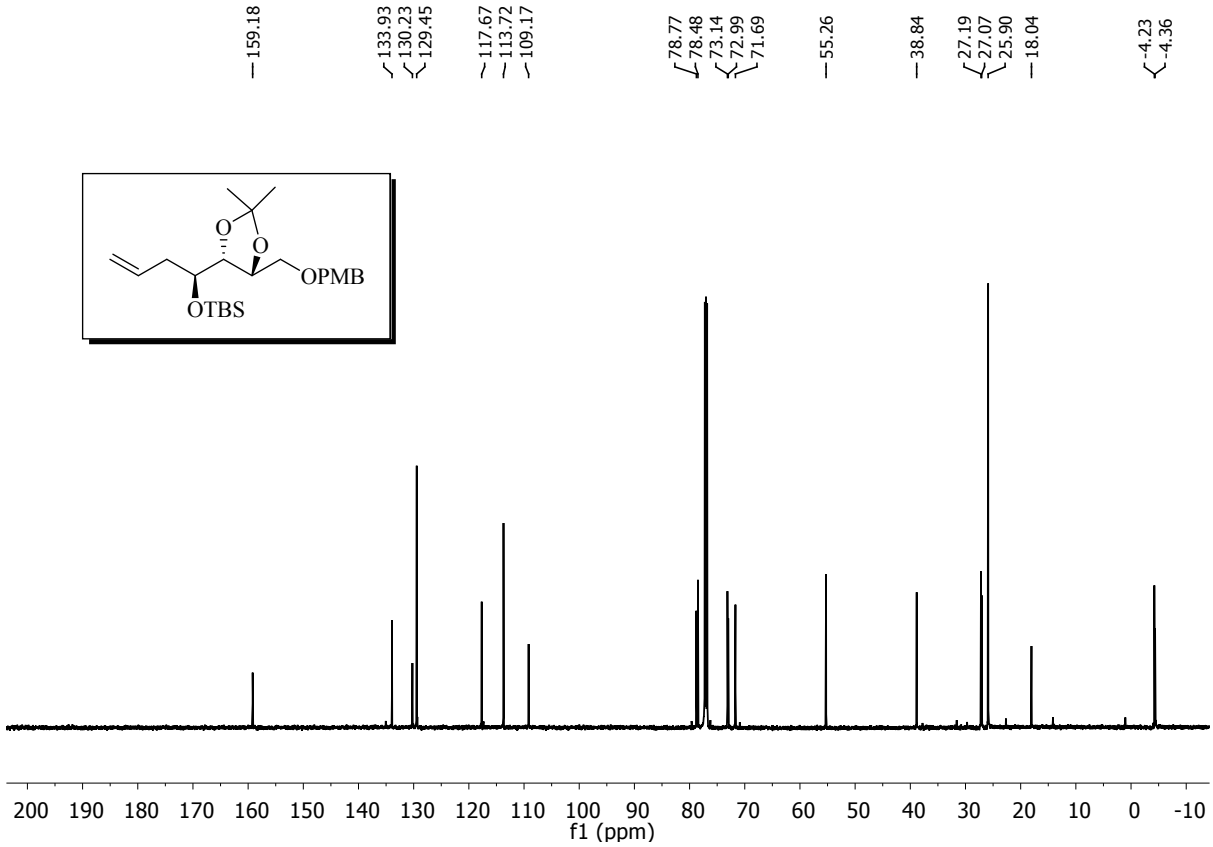
DEPT-135 of compound 20 (150 MHz, $CDCl_3$)



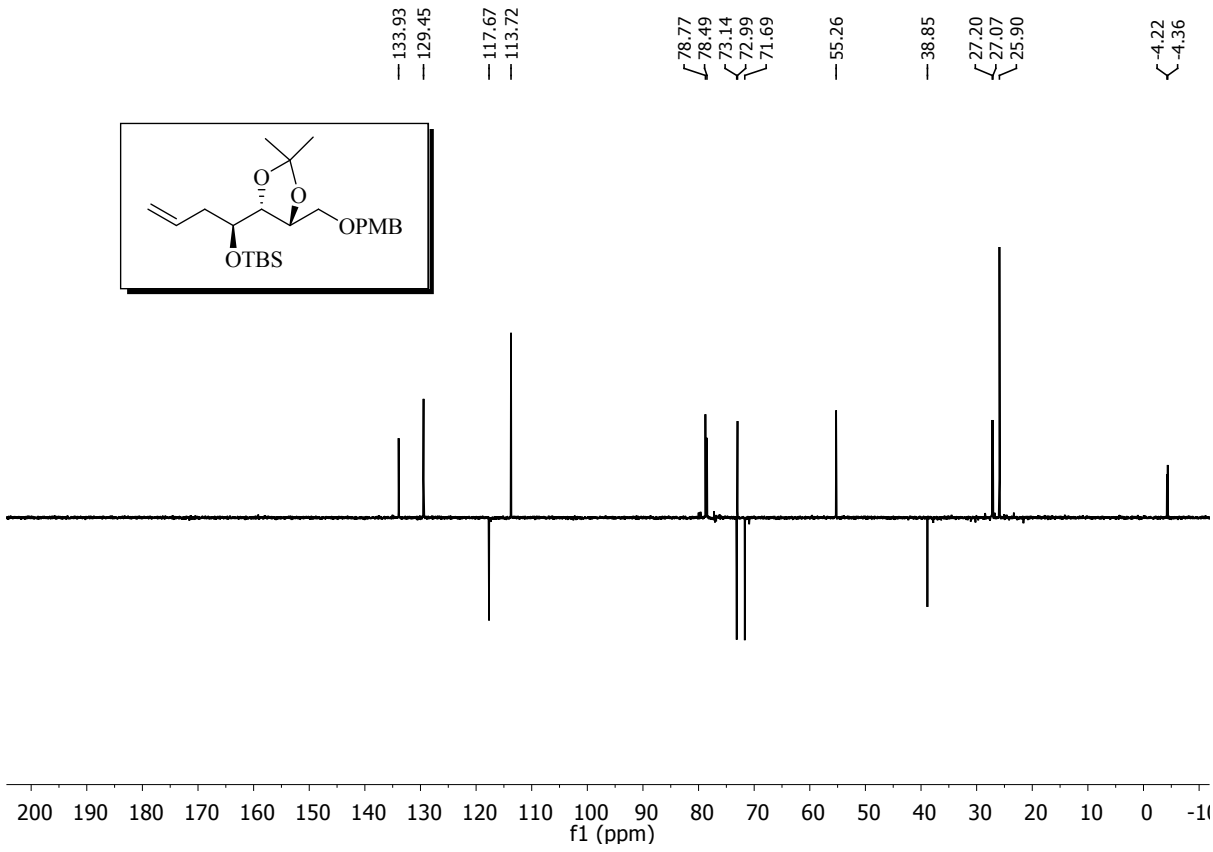
^{1}H NMR of compound 21 (600 MHz, $CDCl_3$)



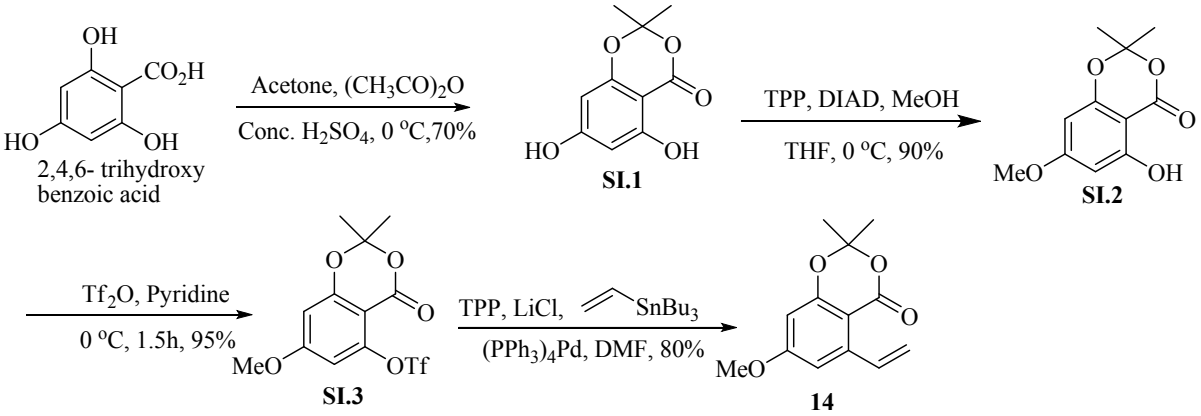
^{13}C NMR of compound 21 (150 MHz, $CDCl_3$)



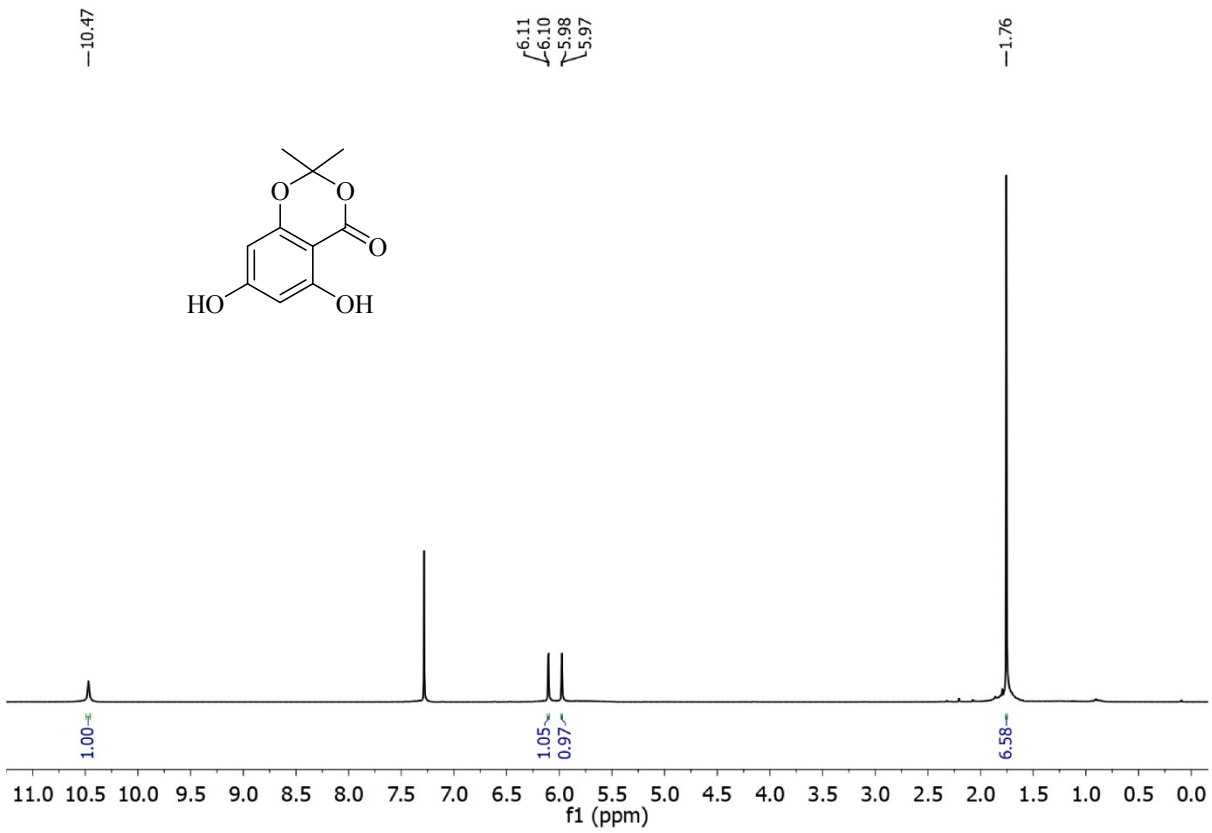
DEPT-135 of compound 21 (150 MHz, $CDCl_3$)



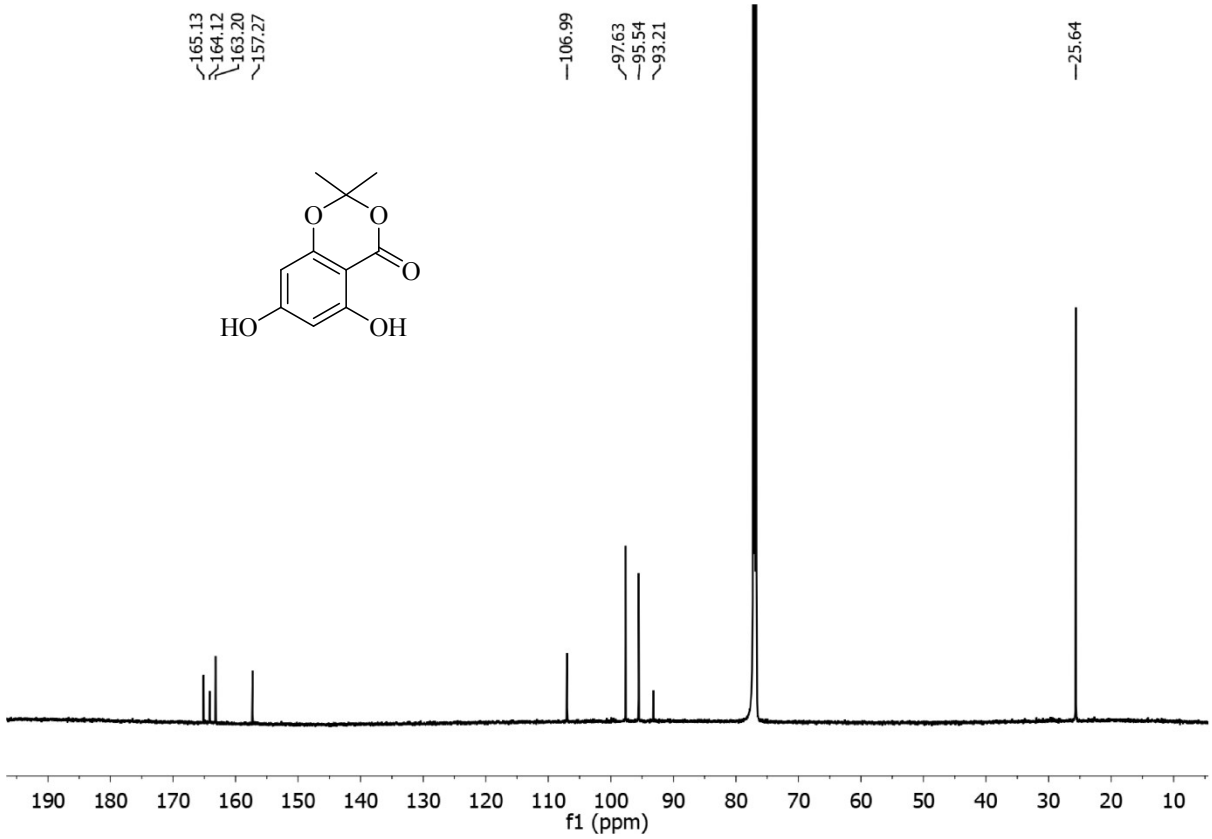
Synthetic route for the preparation of compound 14



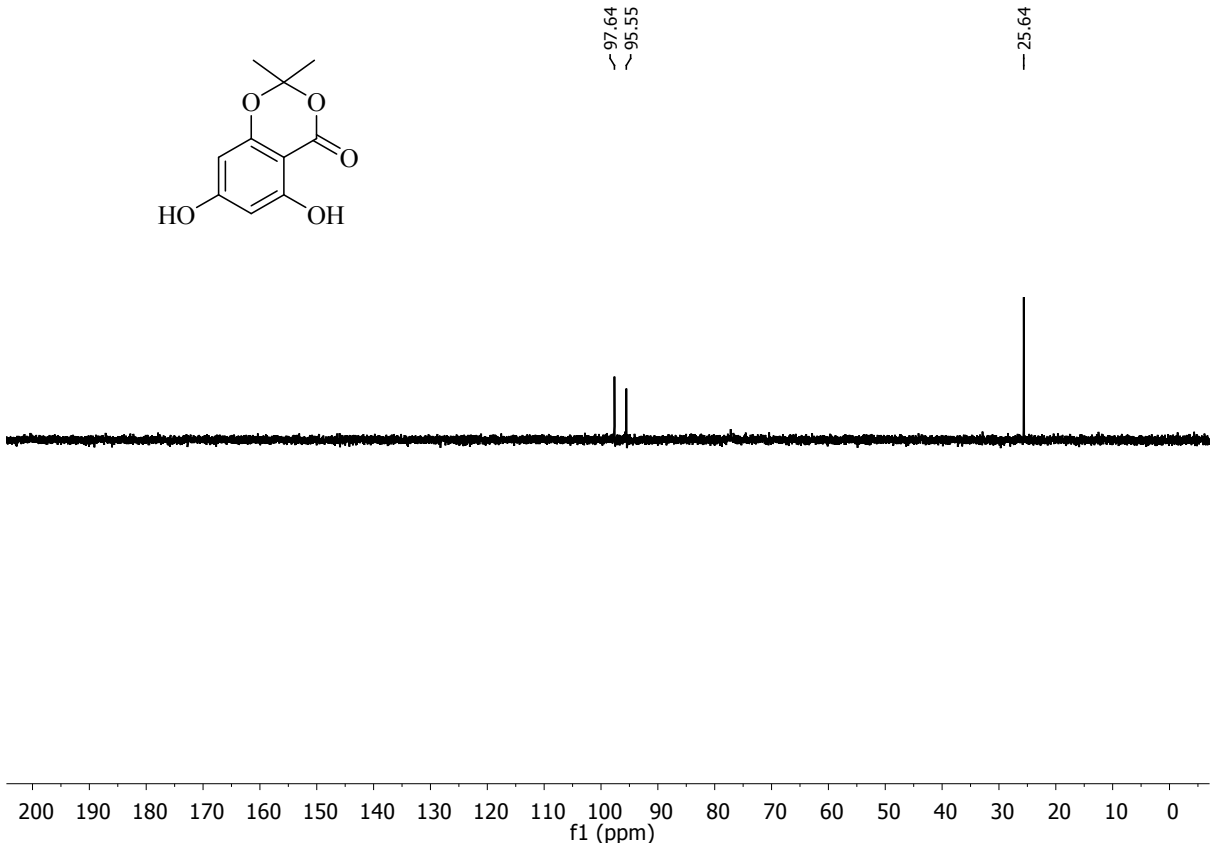
^{1}H NMR of compound SI.1 (600 MHz, $CDCl_3$)



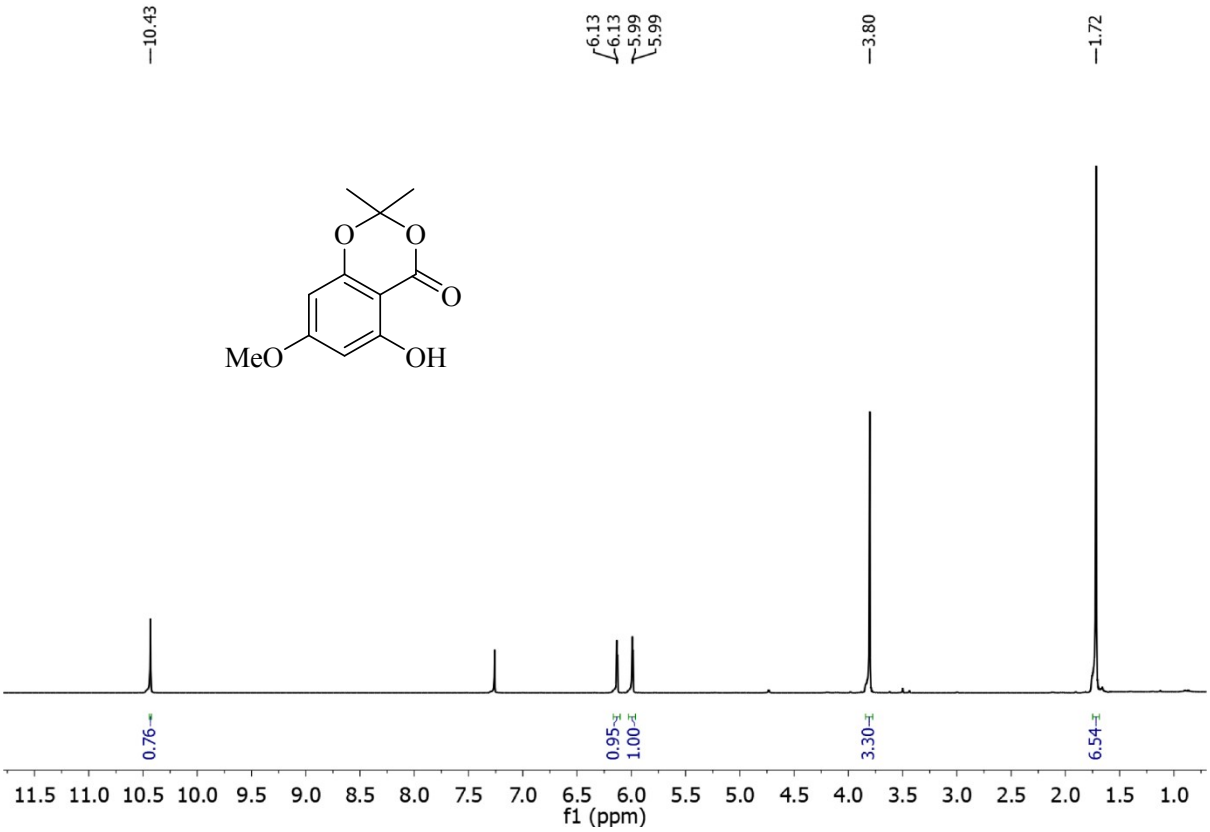
^{13}C NMR of compound SI.1 (150 MHz, $CDCl_3$)



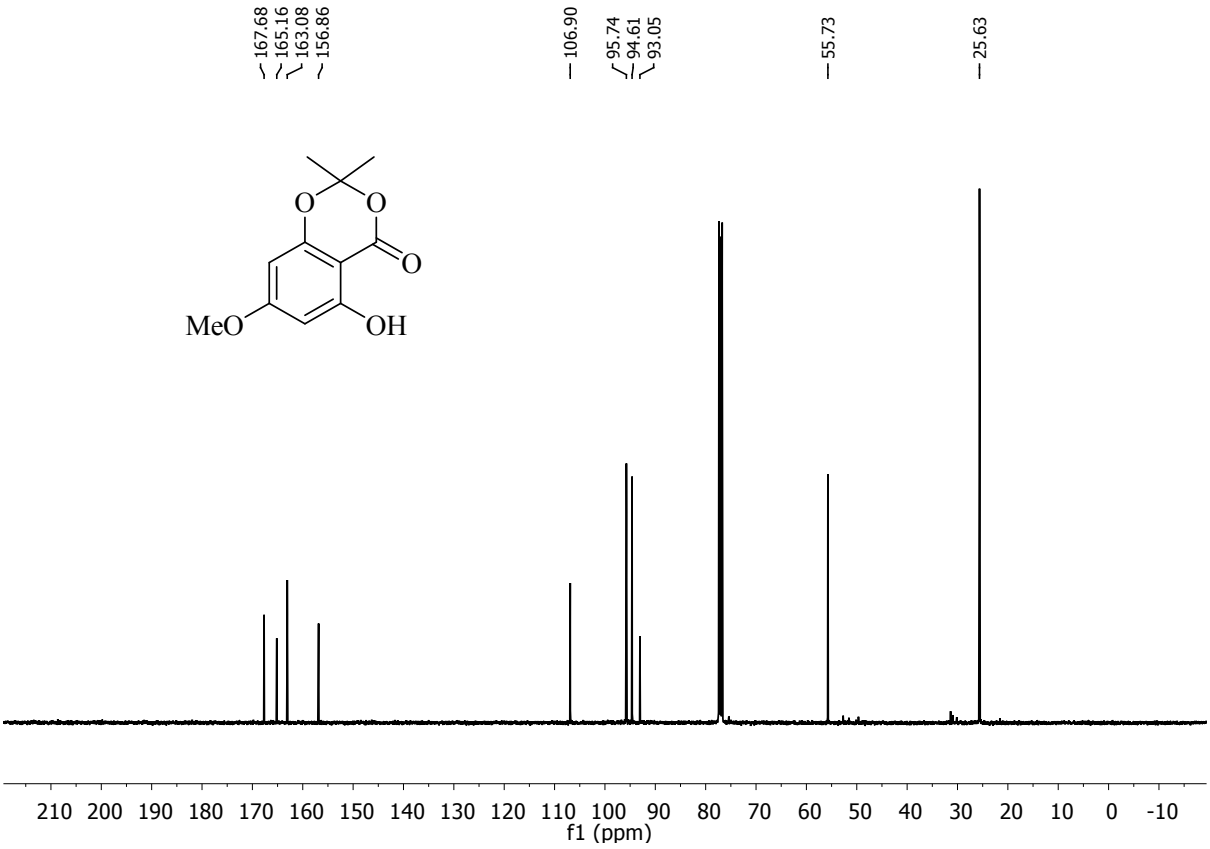
DEPT-135 of compound SI.1 (150 MHz, $CDCl_3$)



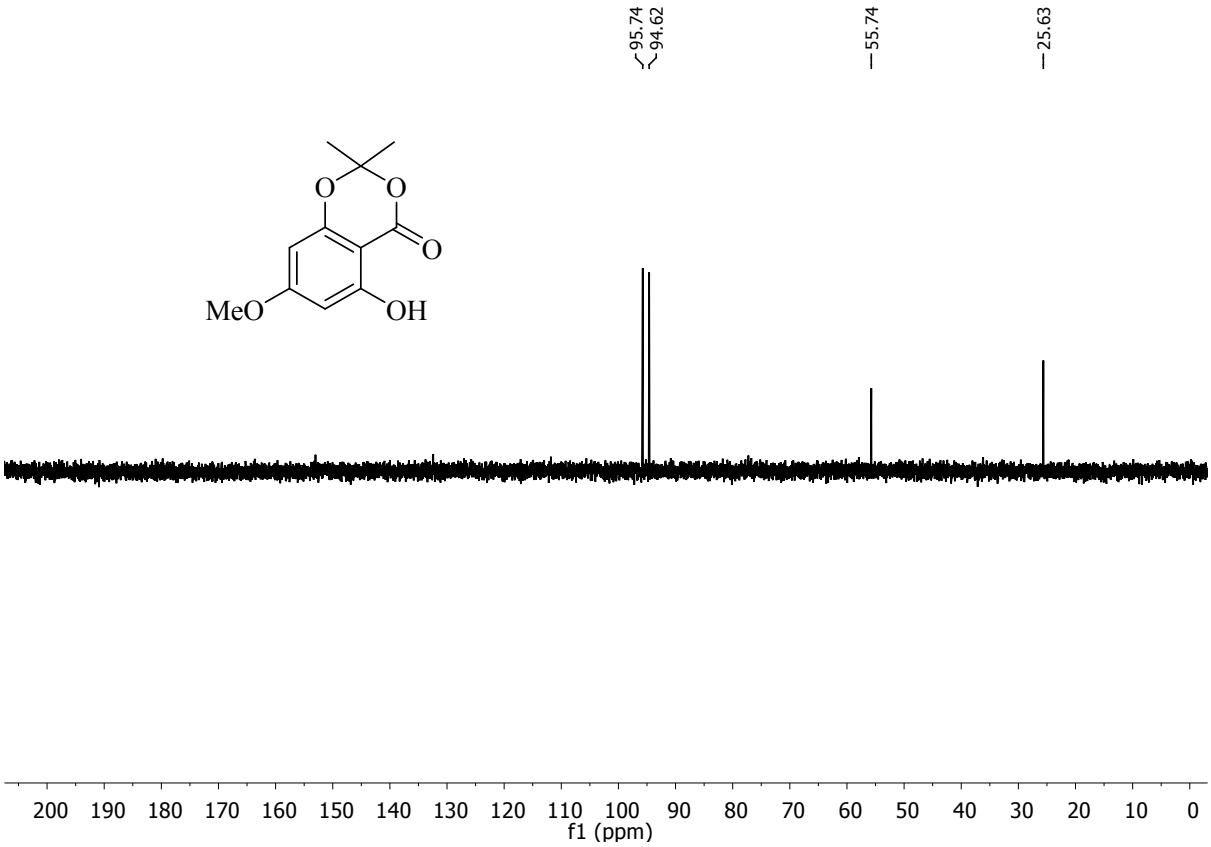
^{1}H NMR of compound SI.2 (400 MHz, $CDCl_3$)



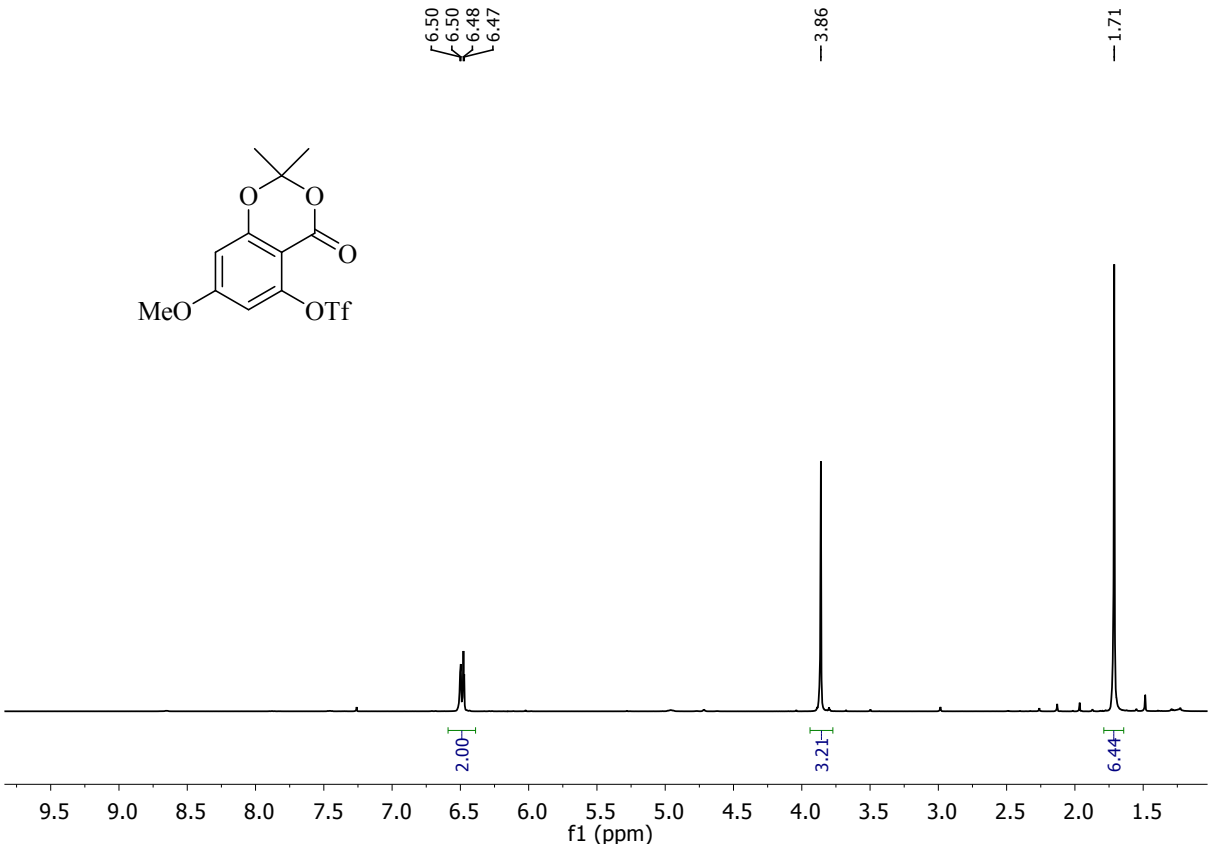
^{13}C NMR of compound SI.2 (100 MHz, $CDCl_3$)



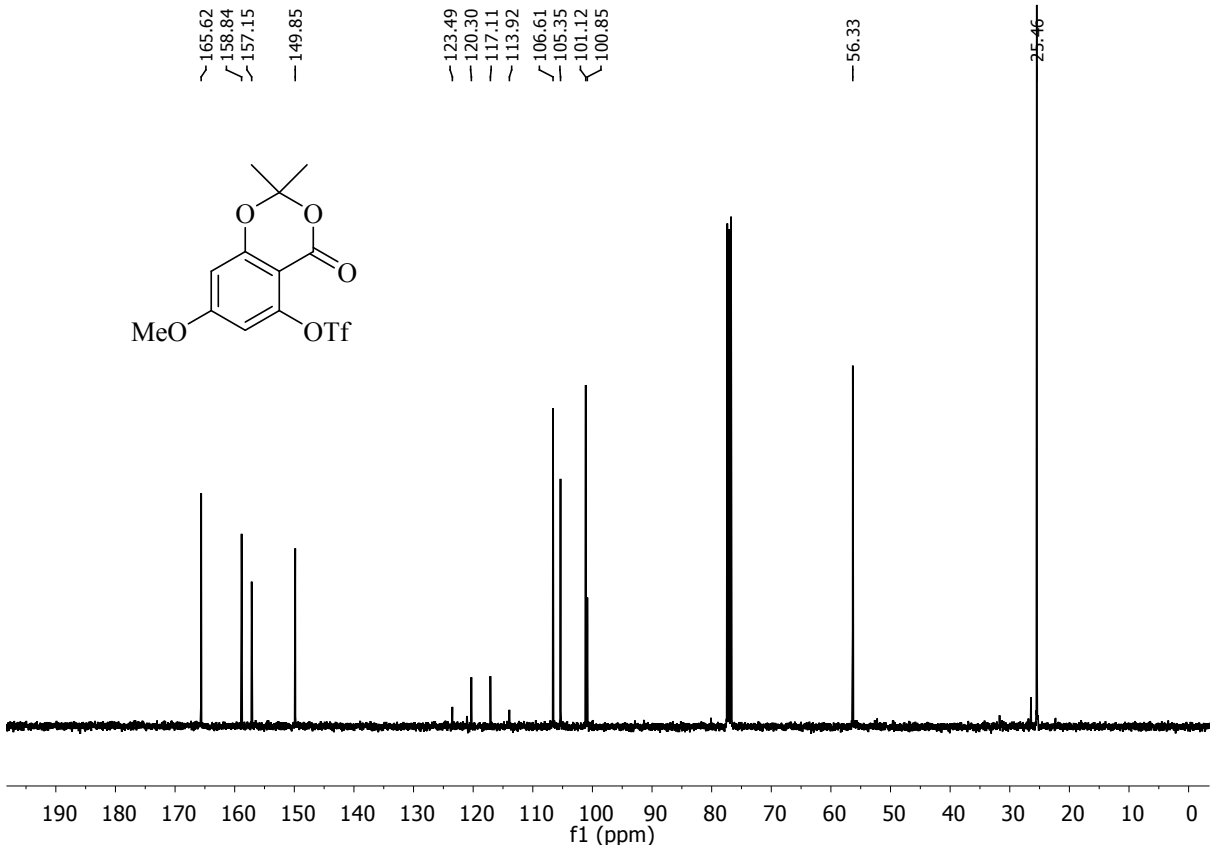
DEPT-135 of compound SI.2 (100 MHz, $CDCl_3$)



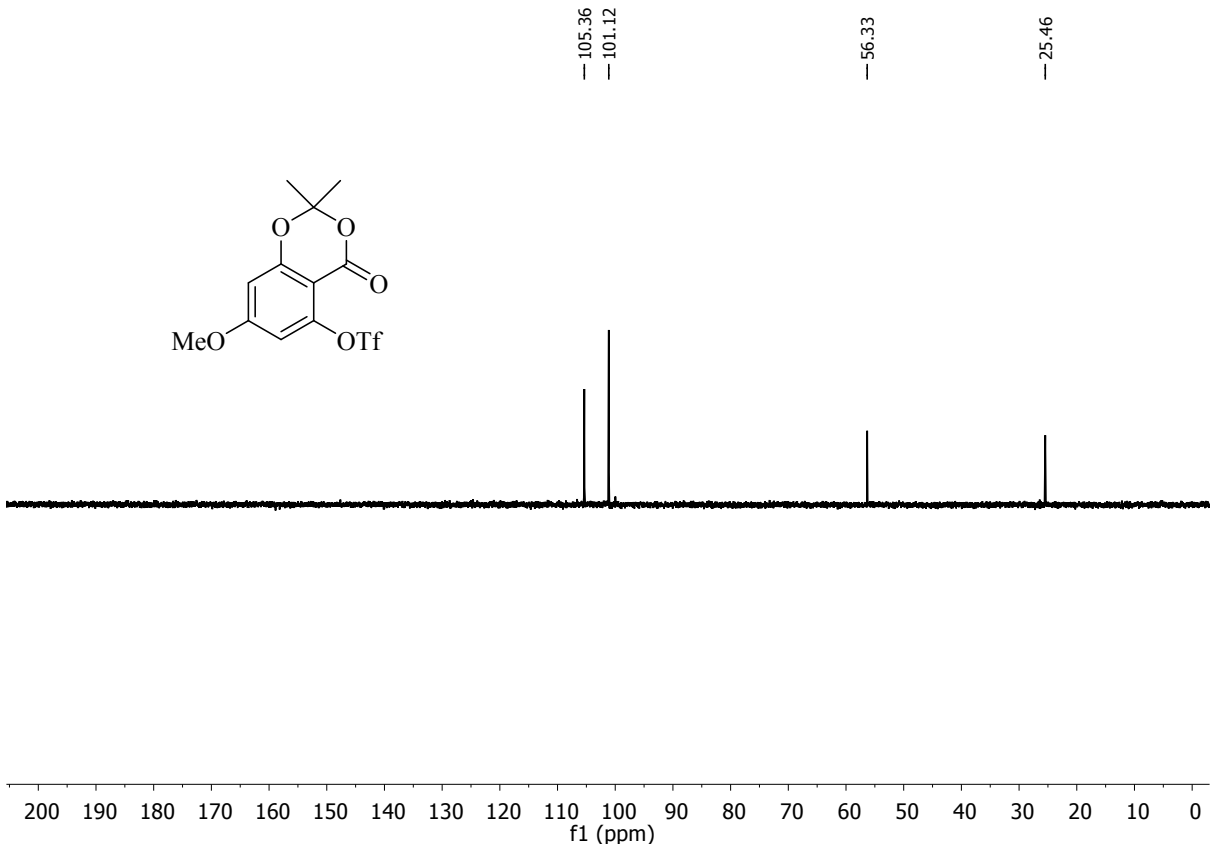
^{1}H NMR of compound SI.3 (400 MHz, $CDCl_3$)



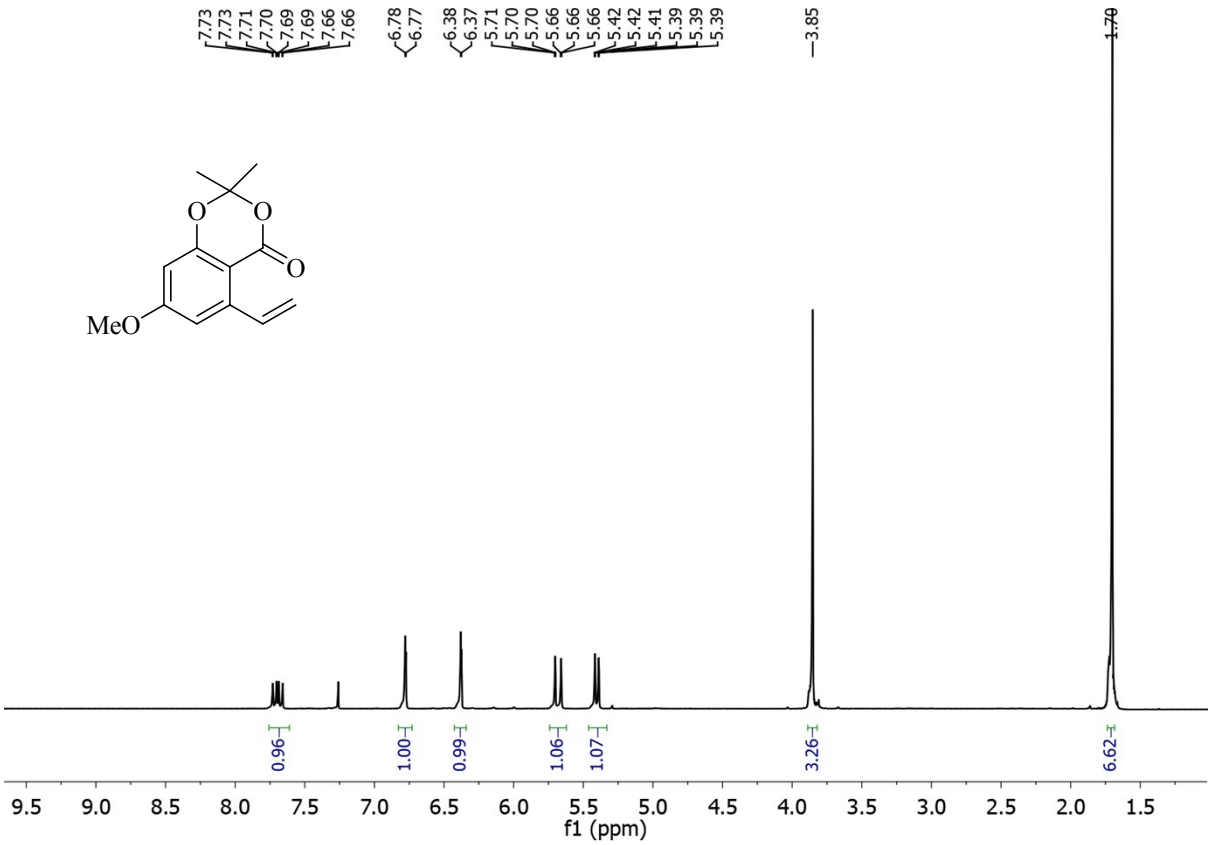
^{13}C NMR of compound SI.3 (100 MHz, $CDCl_3$)



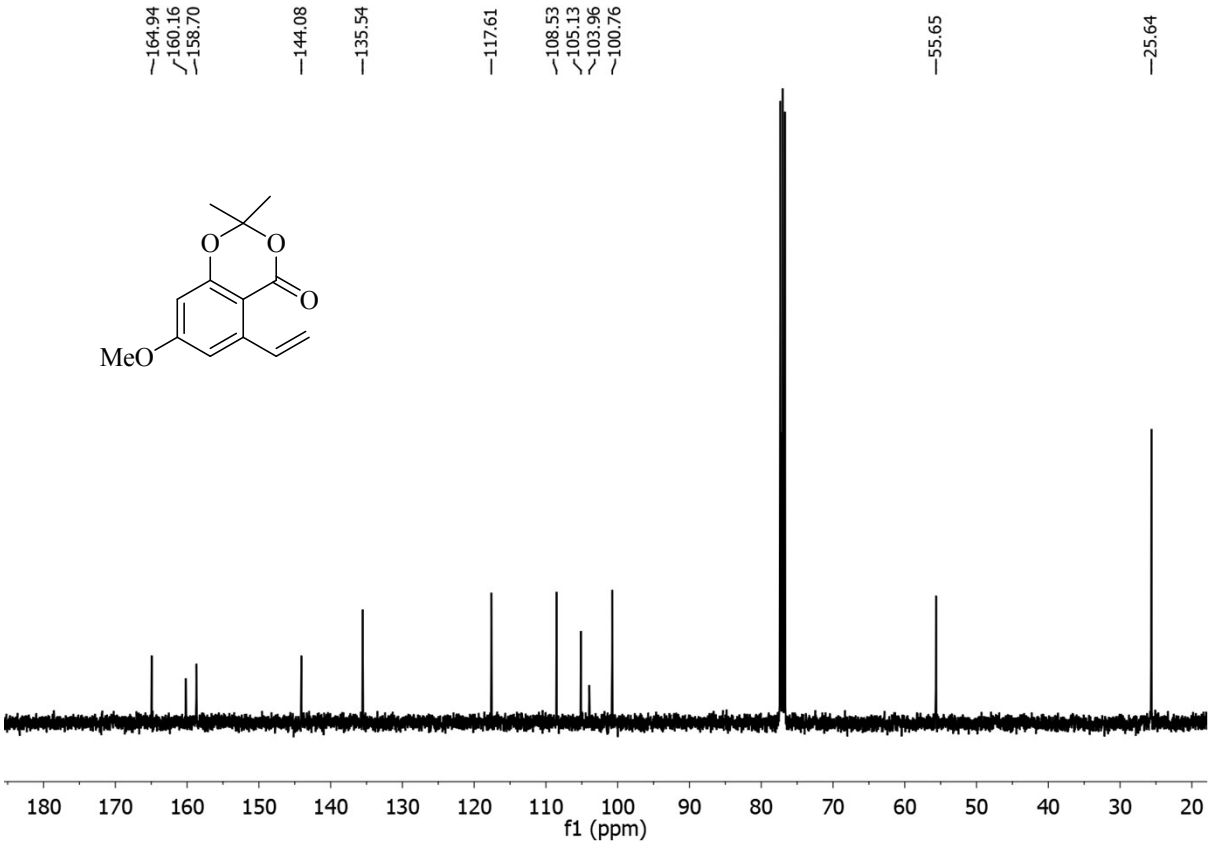
DEPT-135 of compound SI.3 (100 MHz, $CDCl_3$)



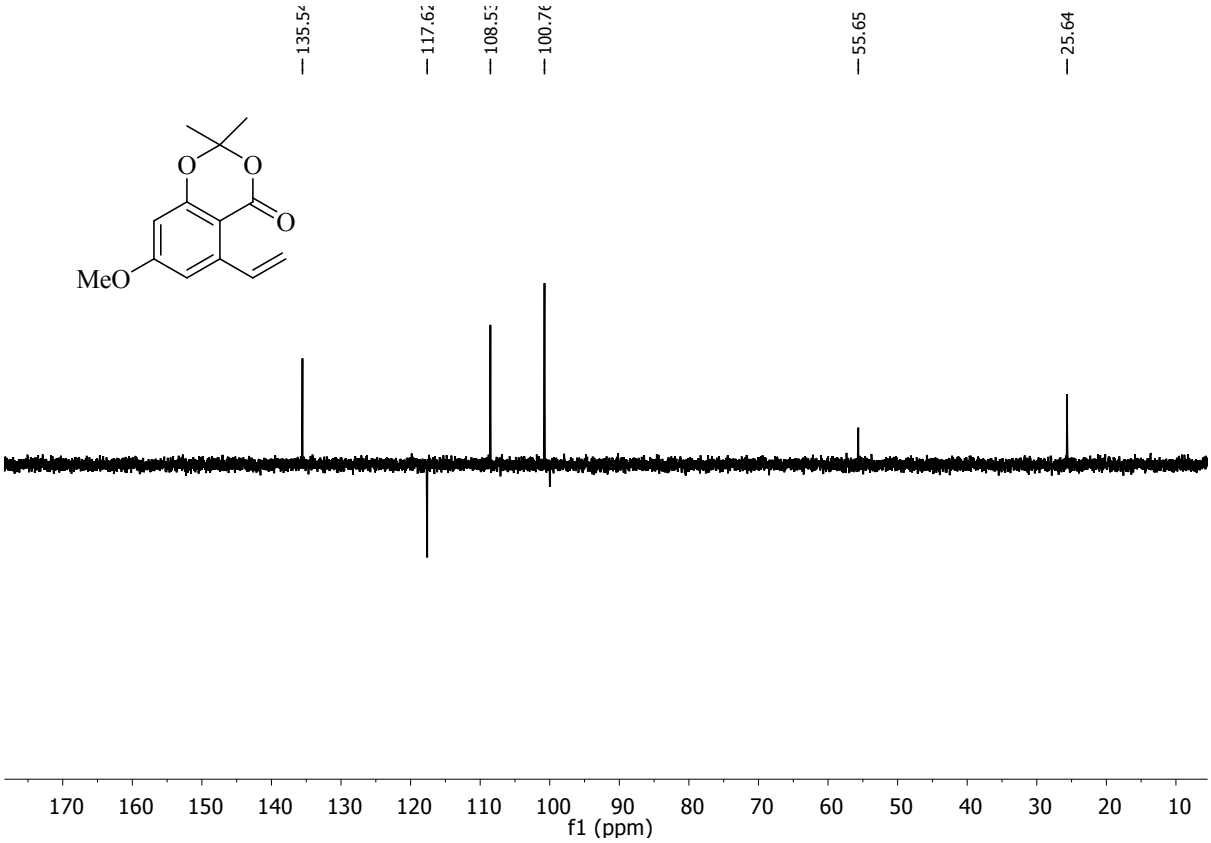
^{1}H NMR of compound 14 (400 MHz, $CDCl_3$)



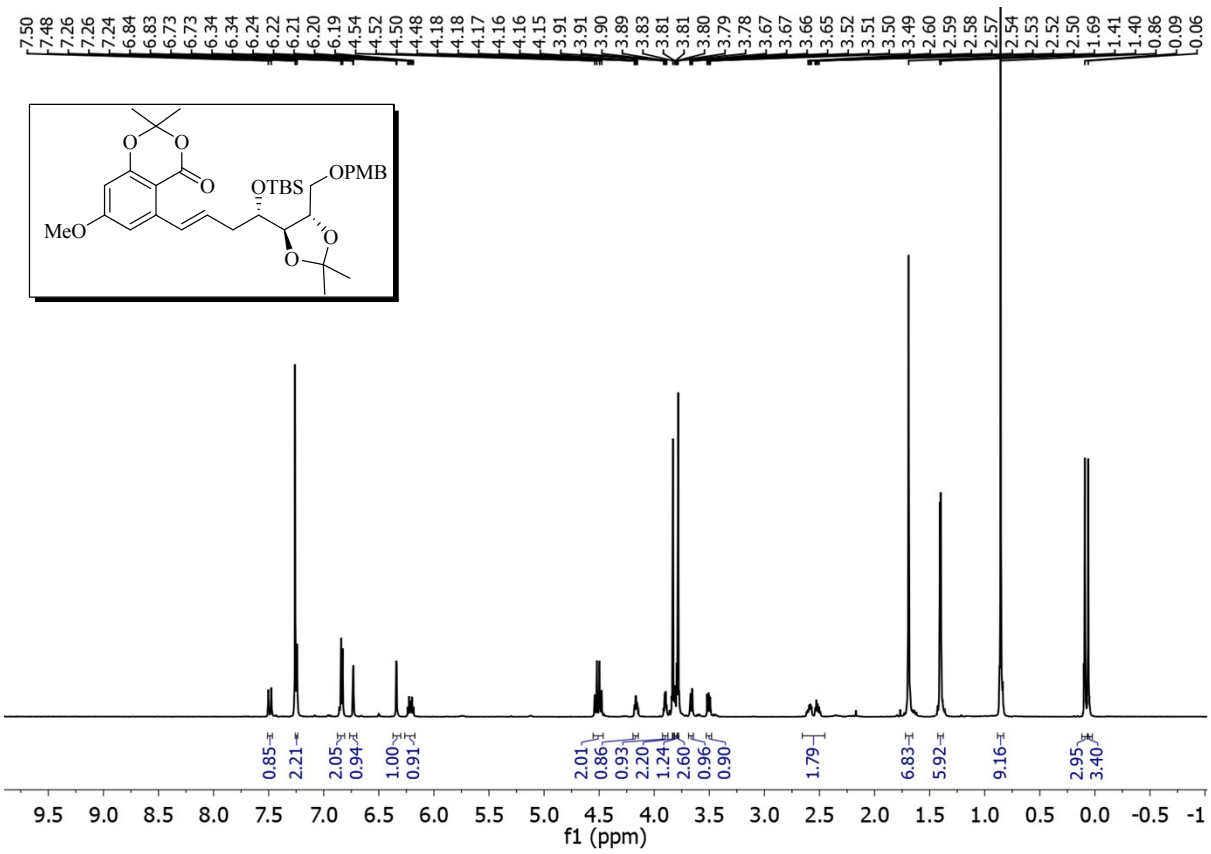
^{13}C NMR of compound 14 (100 MHz, $CDCl_3$)



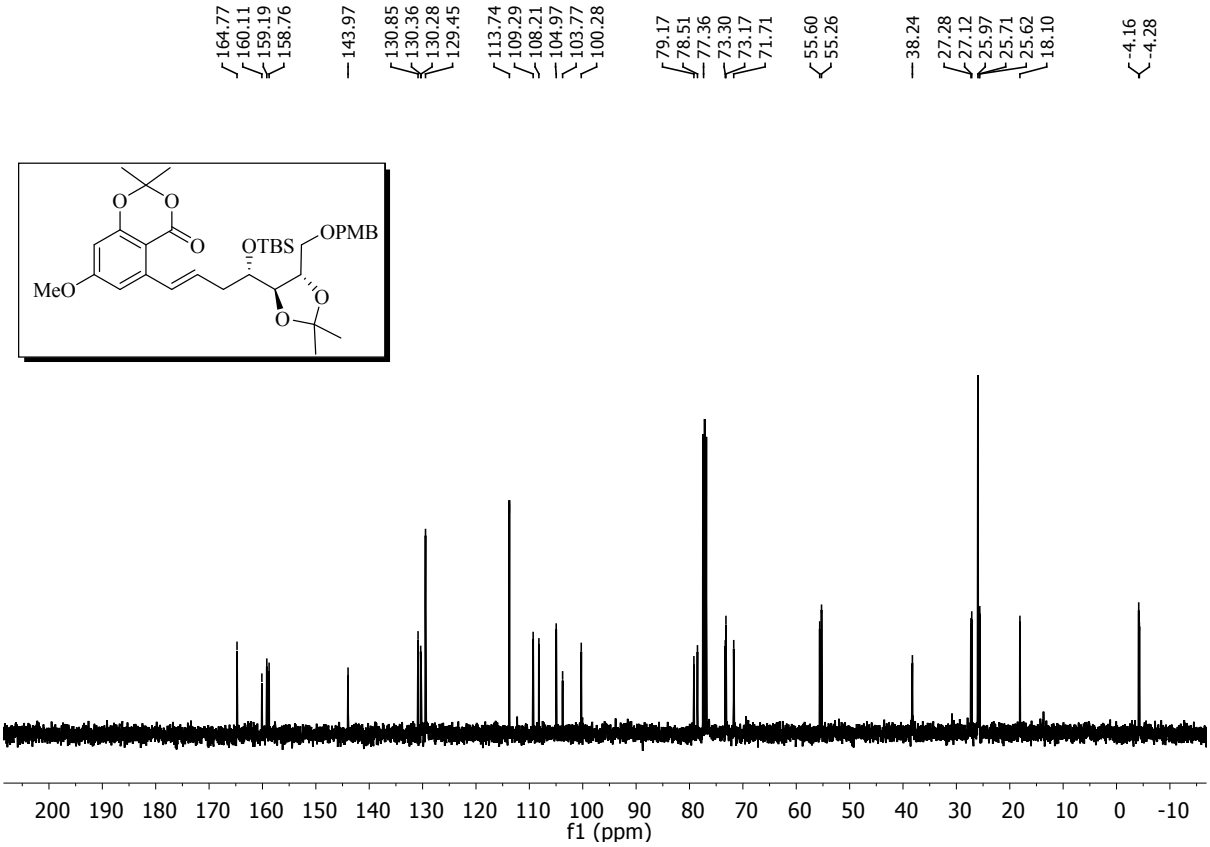
DEPT-135 of compound 14 (100 MHz, $CDCl_3$)



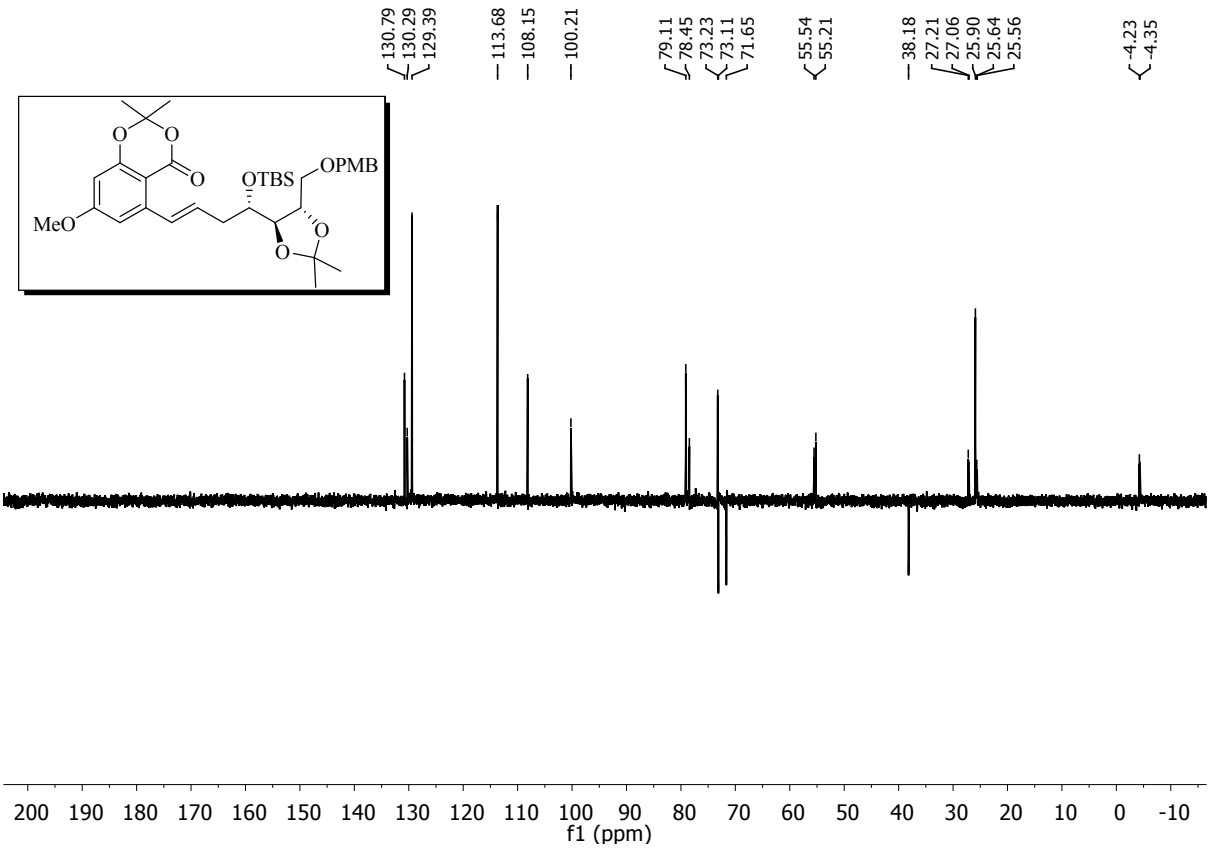
^{1}H NMR of compound 22 (600 MHz, $CDCl_3$)



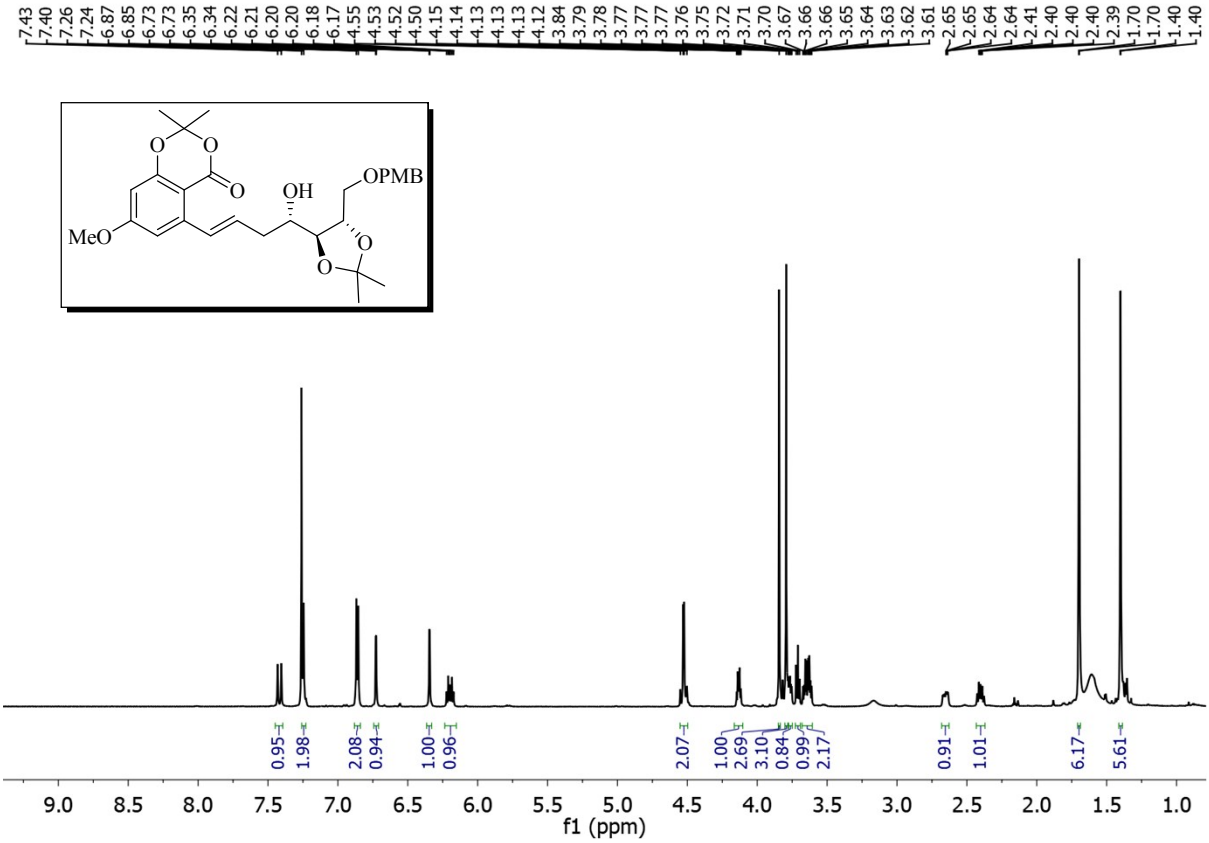
^{13}C NMR of compound 22 (100 MHz, $CDCl_3$)



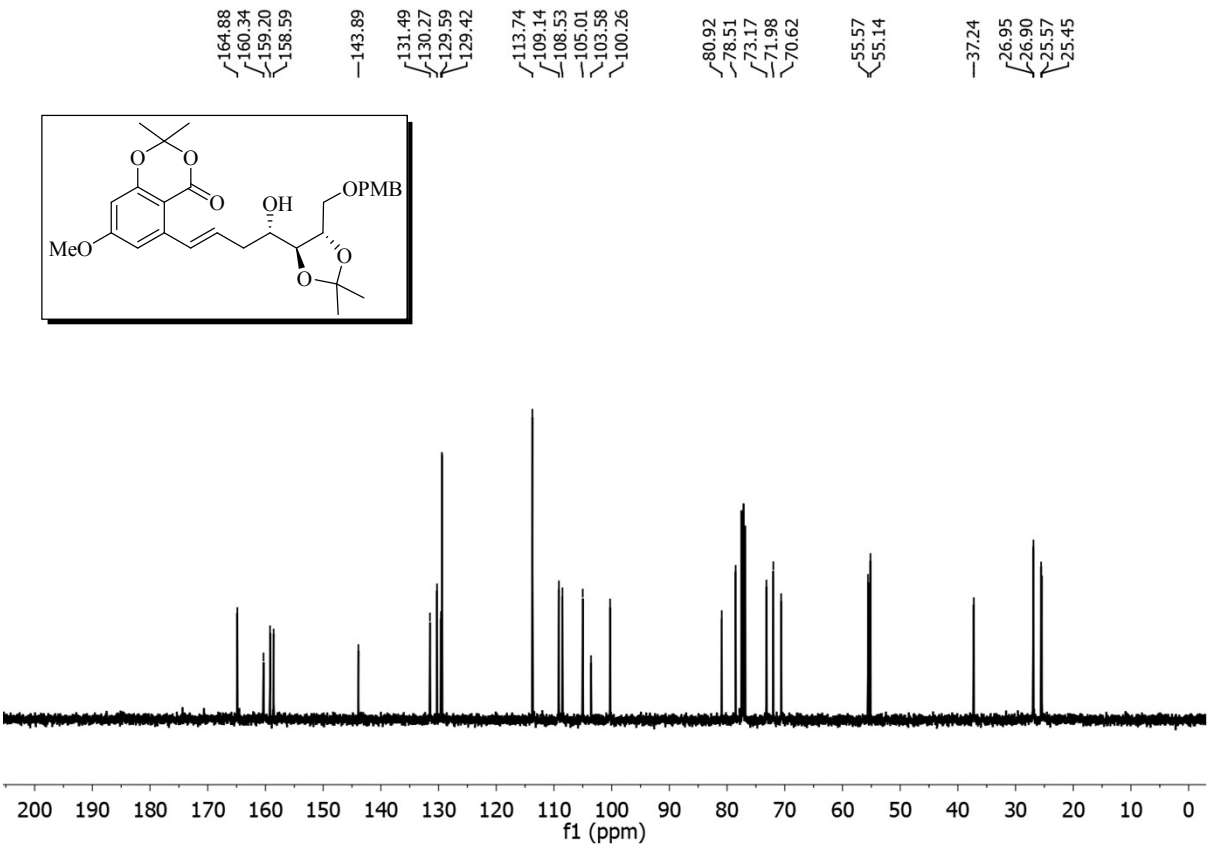
DEPT-135 of compound 22 (100 MHz, $CDCl_3$)



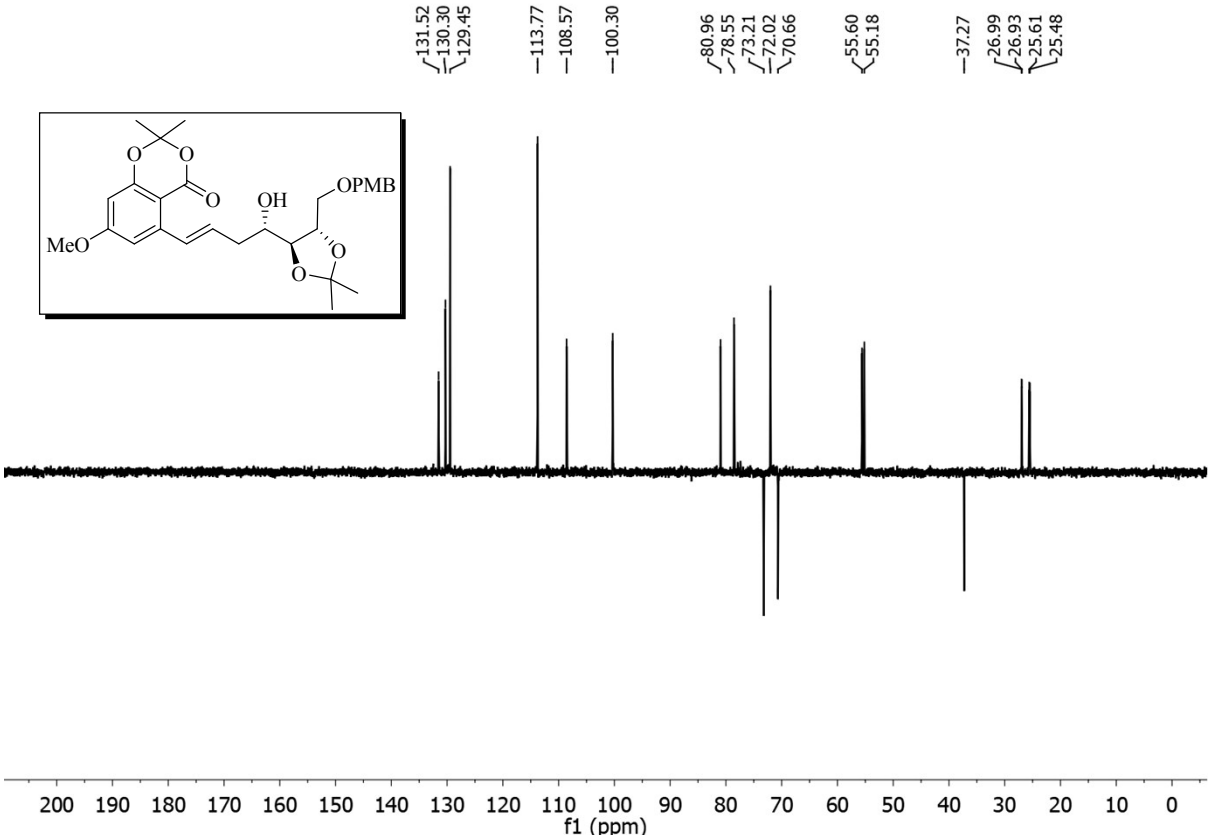
^{1}H NMR of compound 13 (600 MHz, $CDCl_3$)



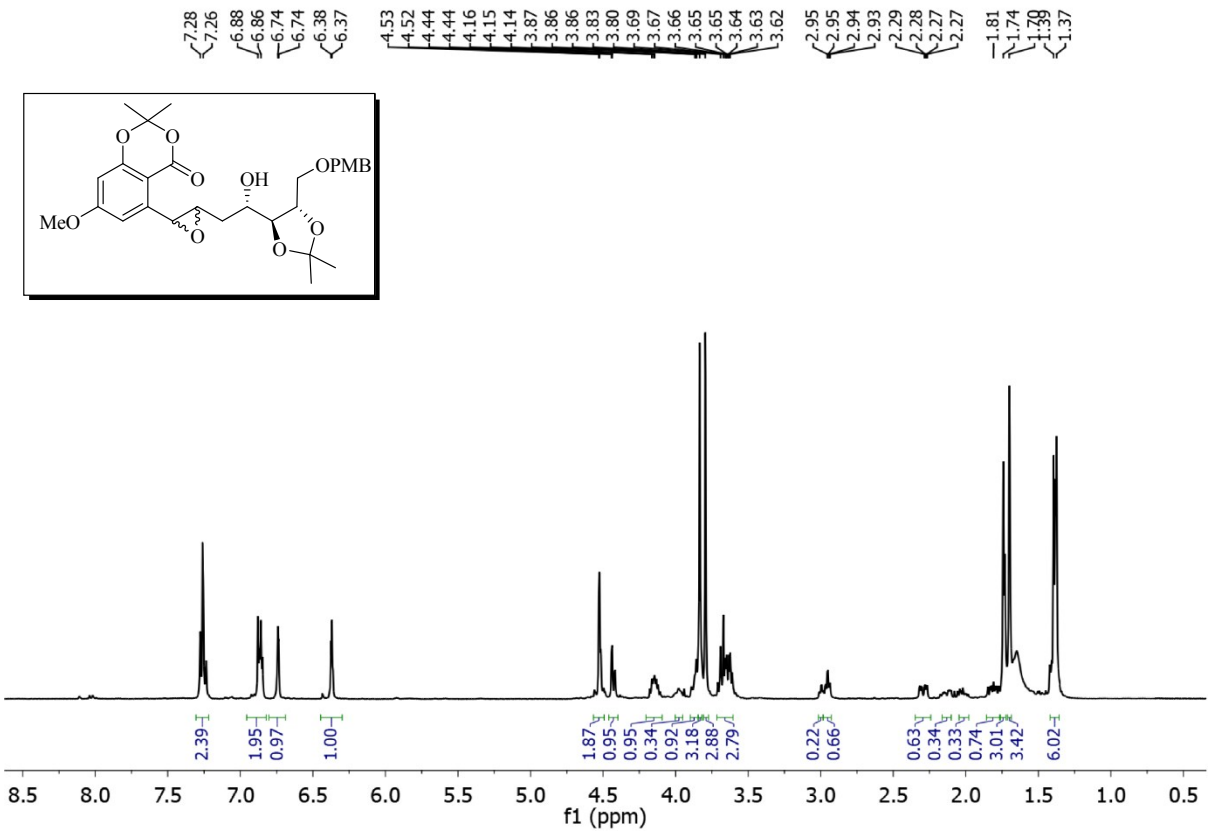
^{13}C NMR of compound 13 (100 MHz, $CDCl_3$)



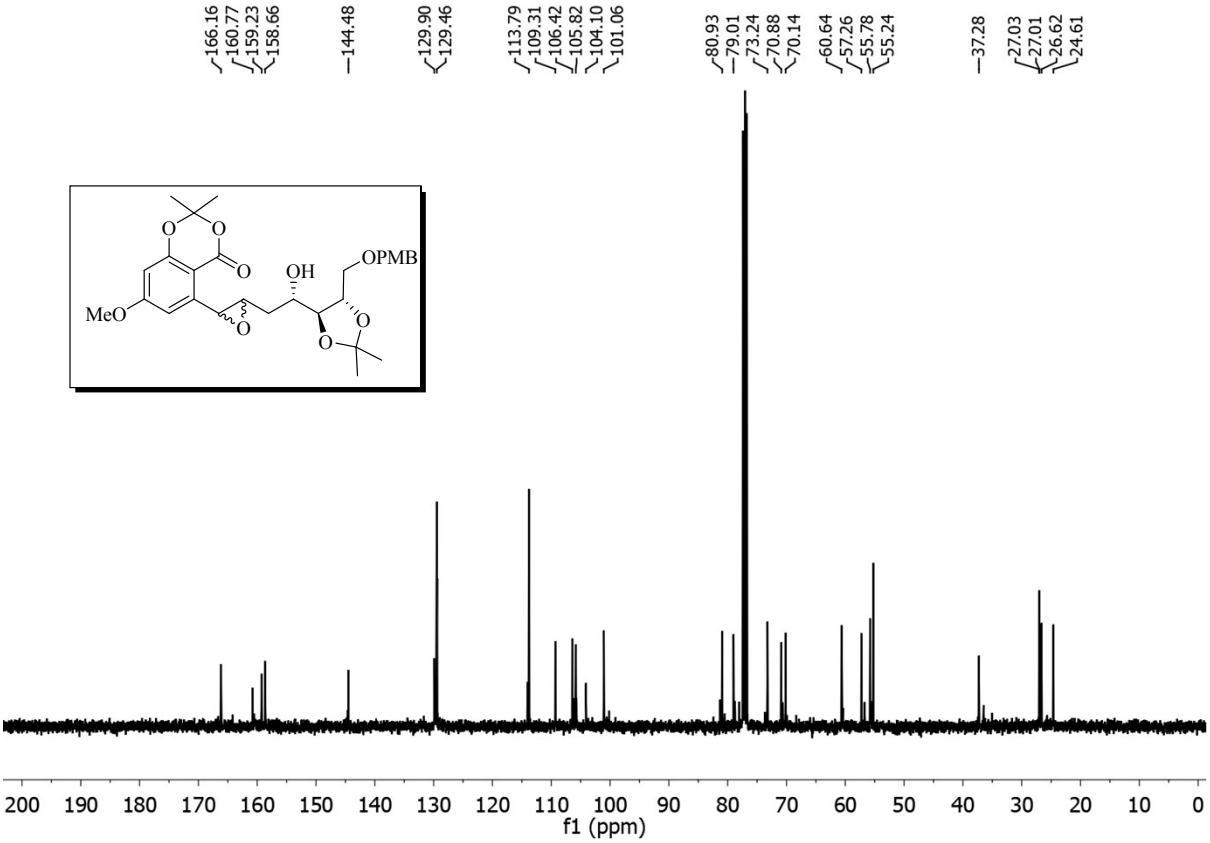
DEPT-135 of compound 13 (100 MHz, $CDCl_3$)



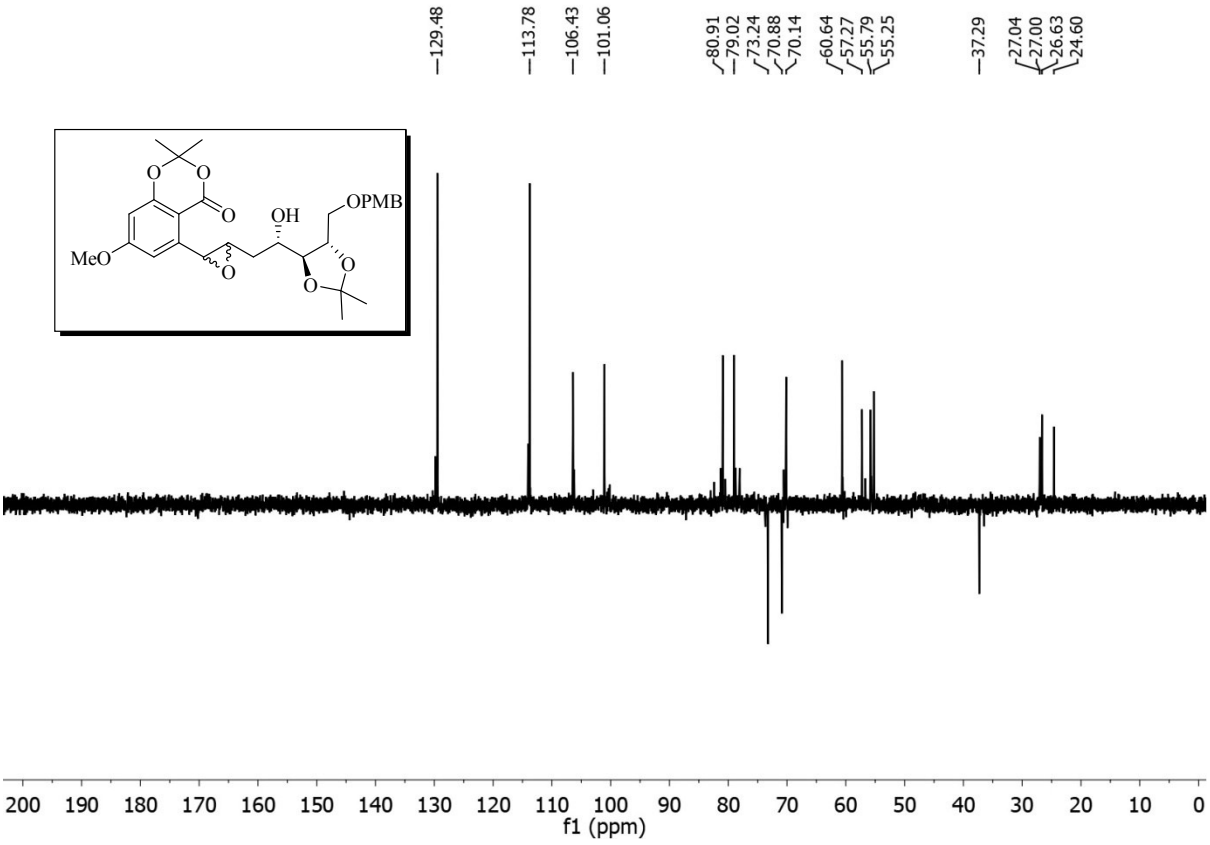
^{1}H NMR of mixture of 23 & 24 (400 MHz, $CDCl_3$)



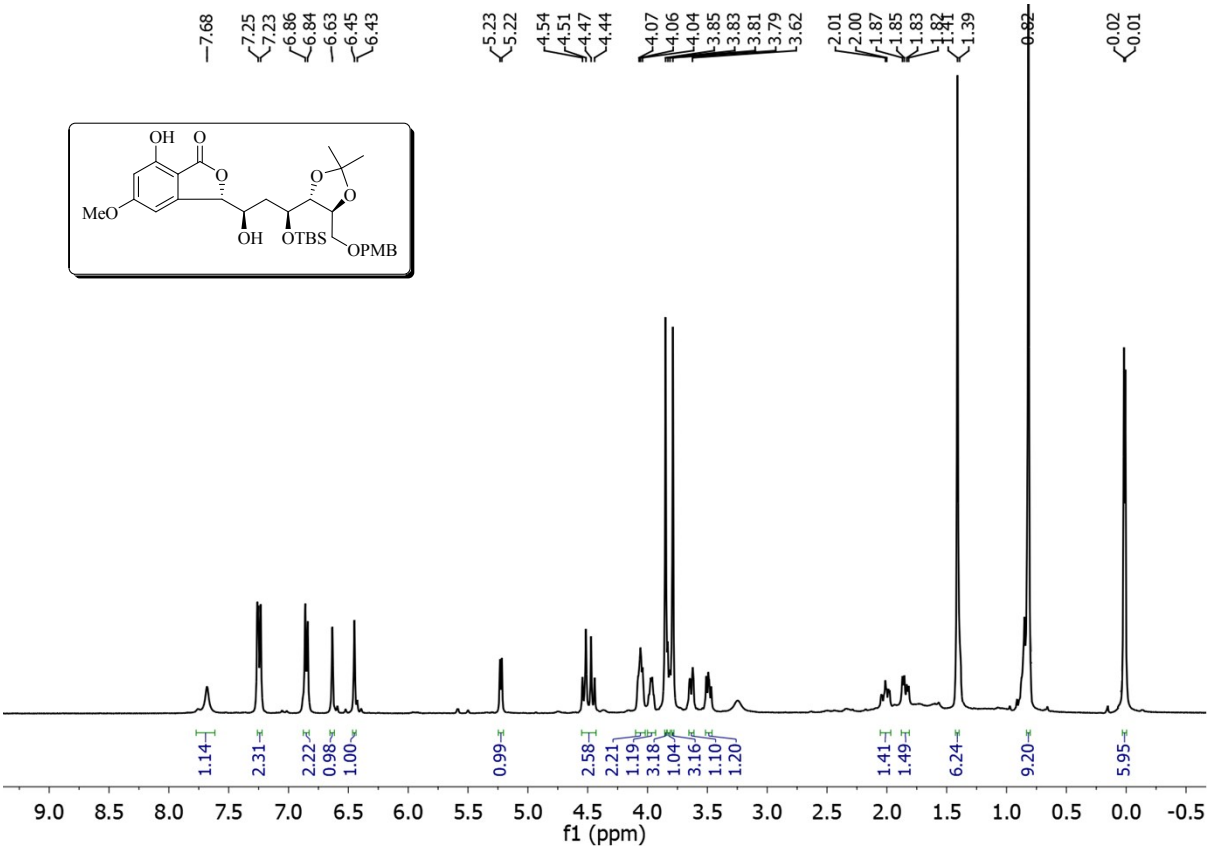
^{13}C NMR of mixture of 23 & 24 (100 MHz, $CDCl_3$)



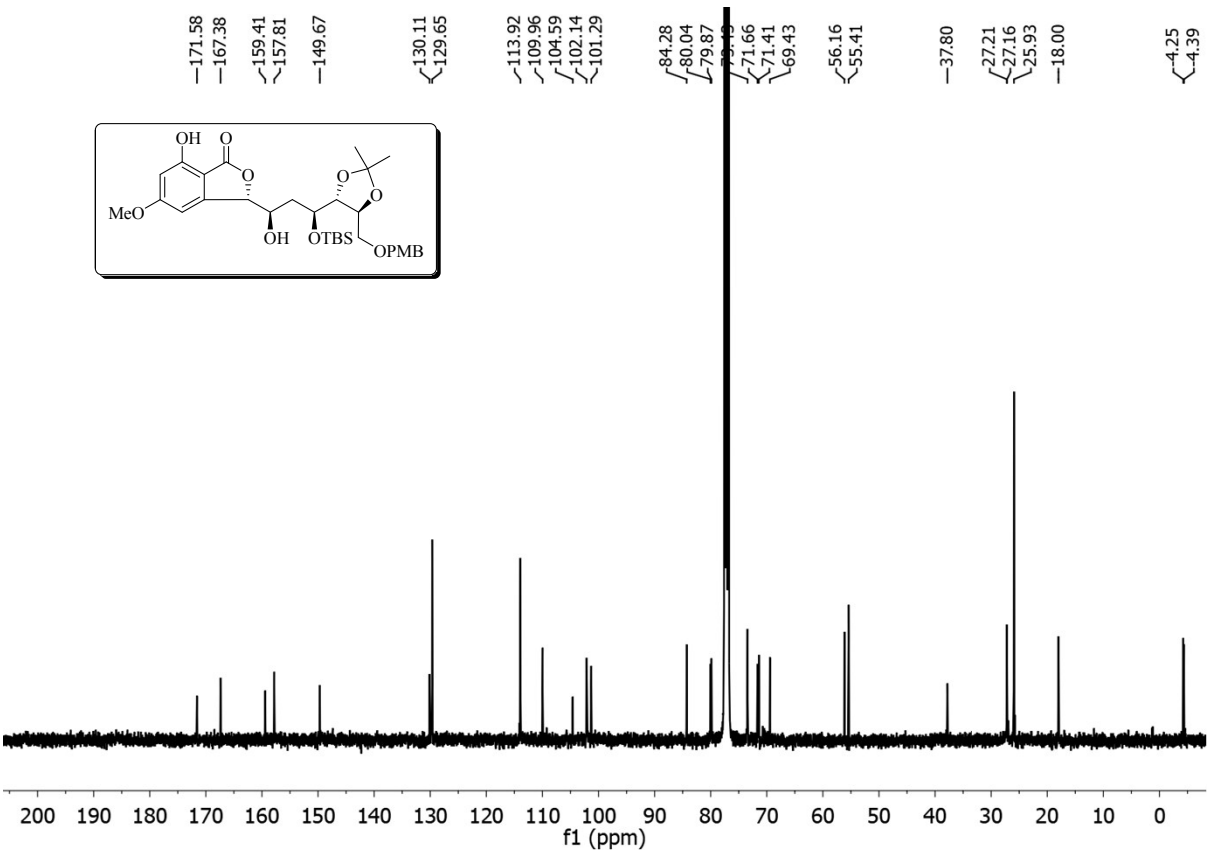
DEPT-135 of mixture of 23 & 24 (100 MHz, $CDCl_3$)



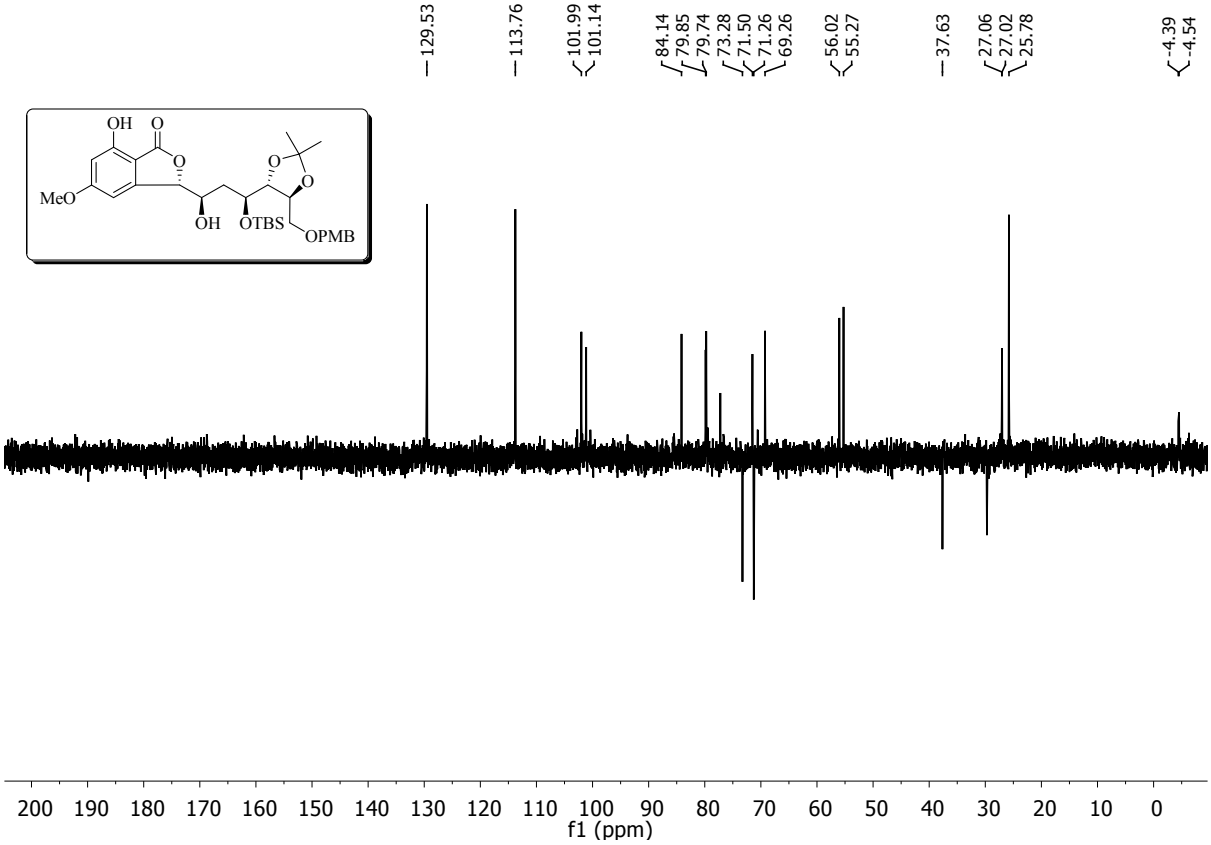
^{1}H NMR of compound 25 (400 MHz, $CDCl_3$)



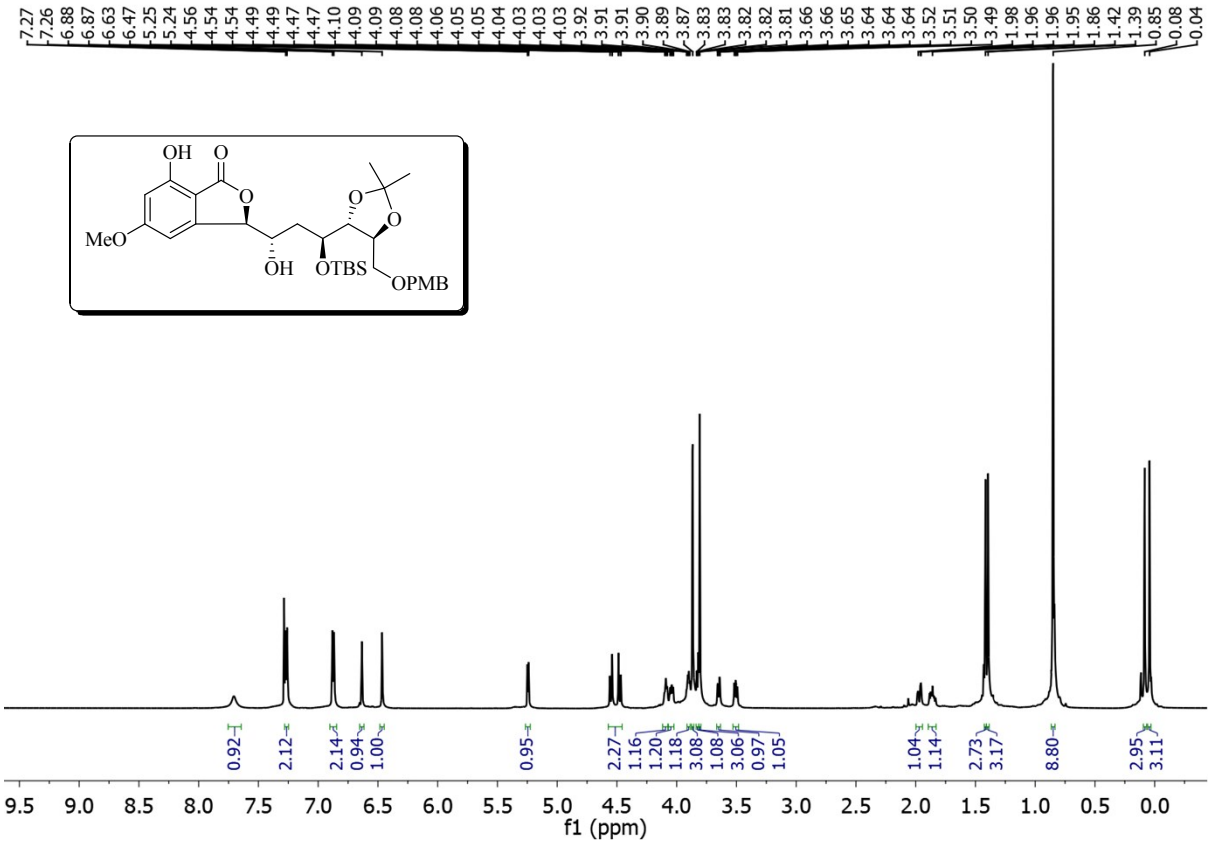
^{13}C NMR of compound 25 (100 MHz, $CDCl_3$)



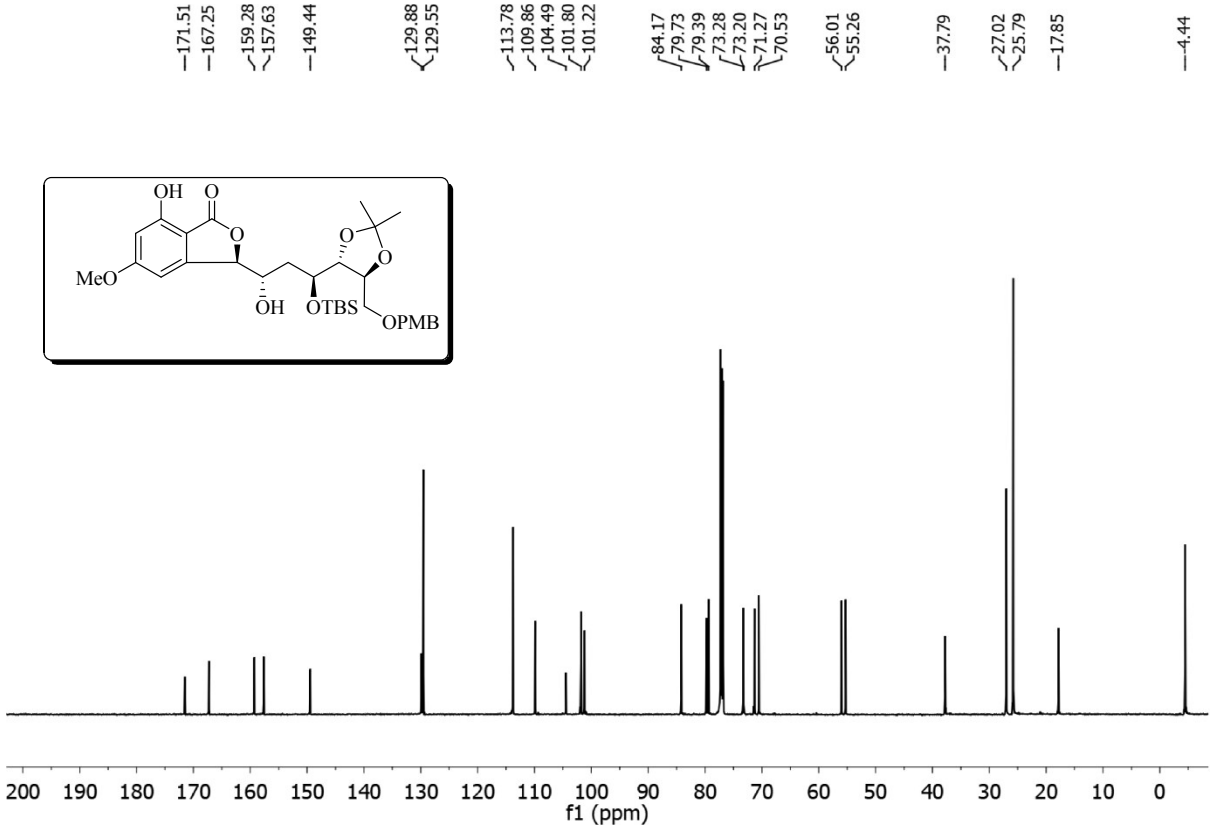
DEPT-135 of compound 25 (100 MHz, $CDCl_3$)



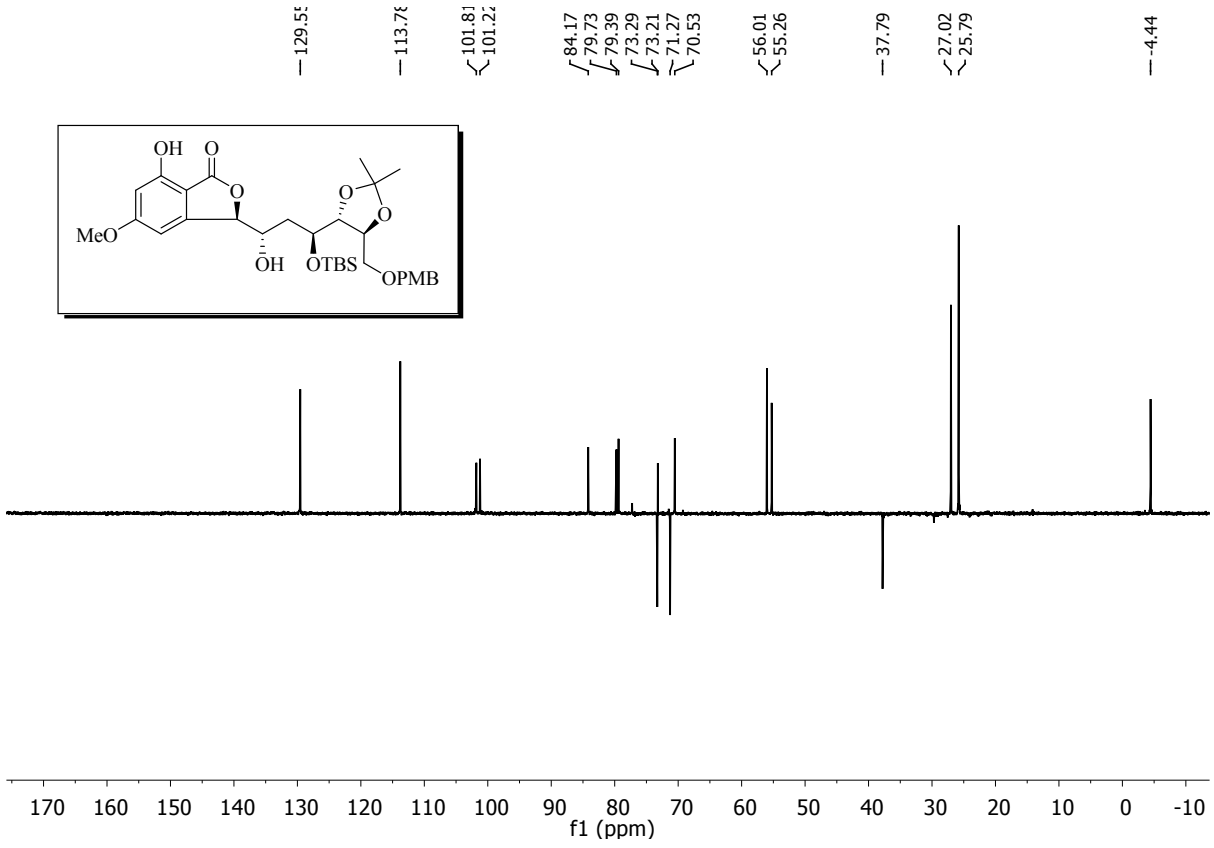
^{1}H NMR of compound 26 (600 MHz, $CDCl_3$)



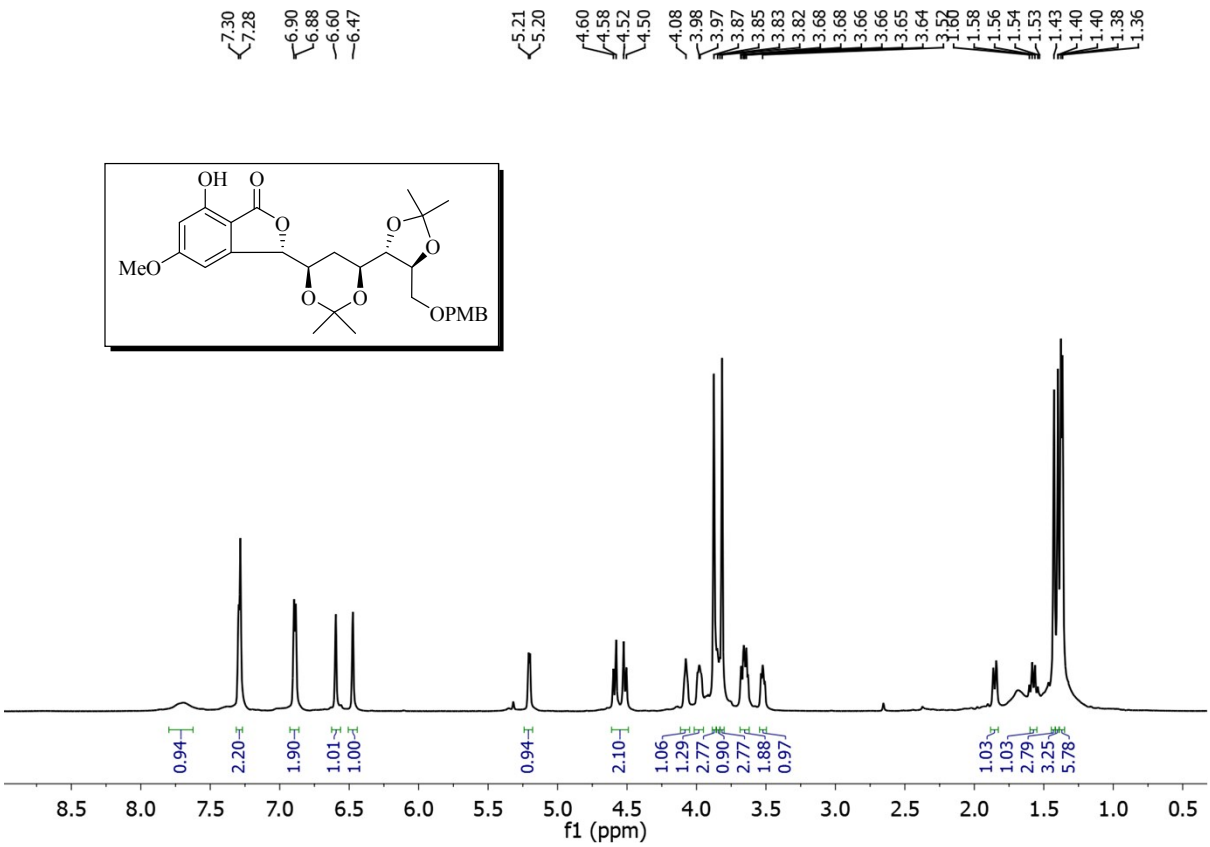
^{13}C NMR of compound 26 (150 MHz, $CDCl_3$)



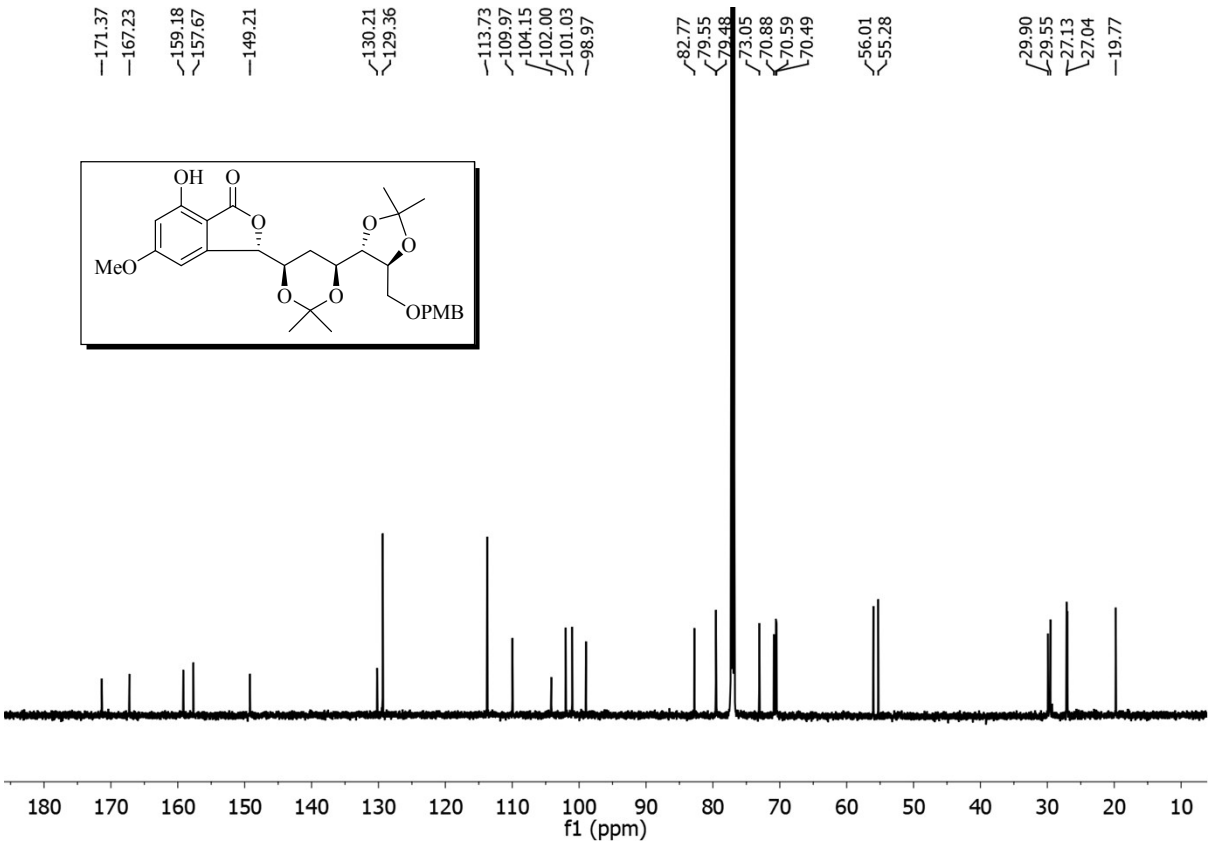
DEPT-135 of compound 26 (150 MHz, $CDCl_3$)



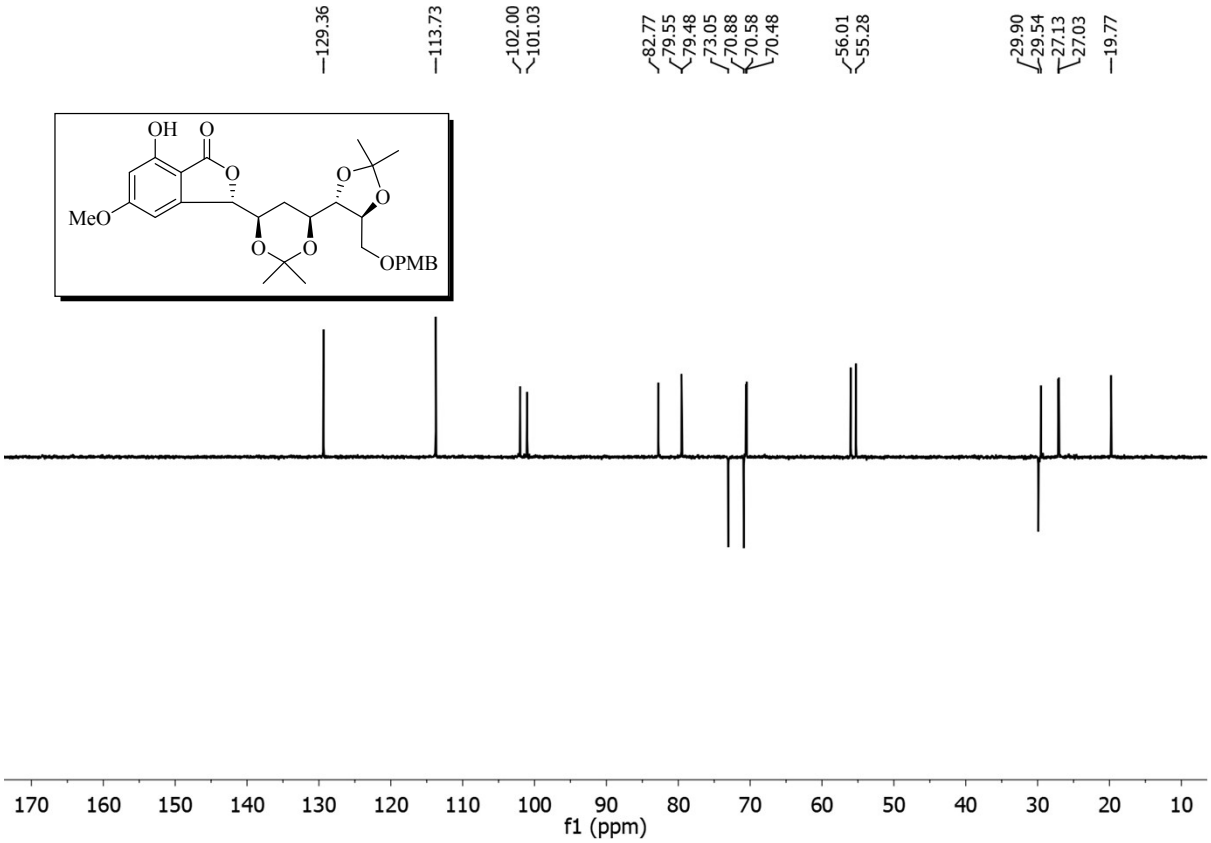
^{1}H NMR of compound 27 (600 MHz, $CDCl_3$)



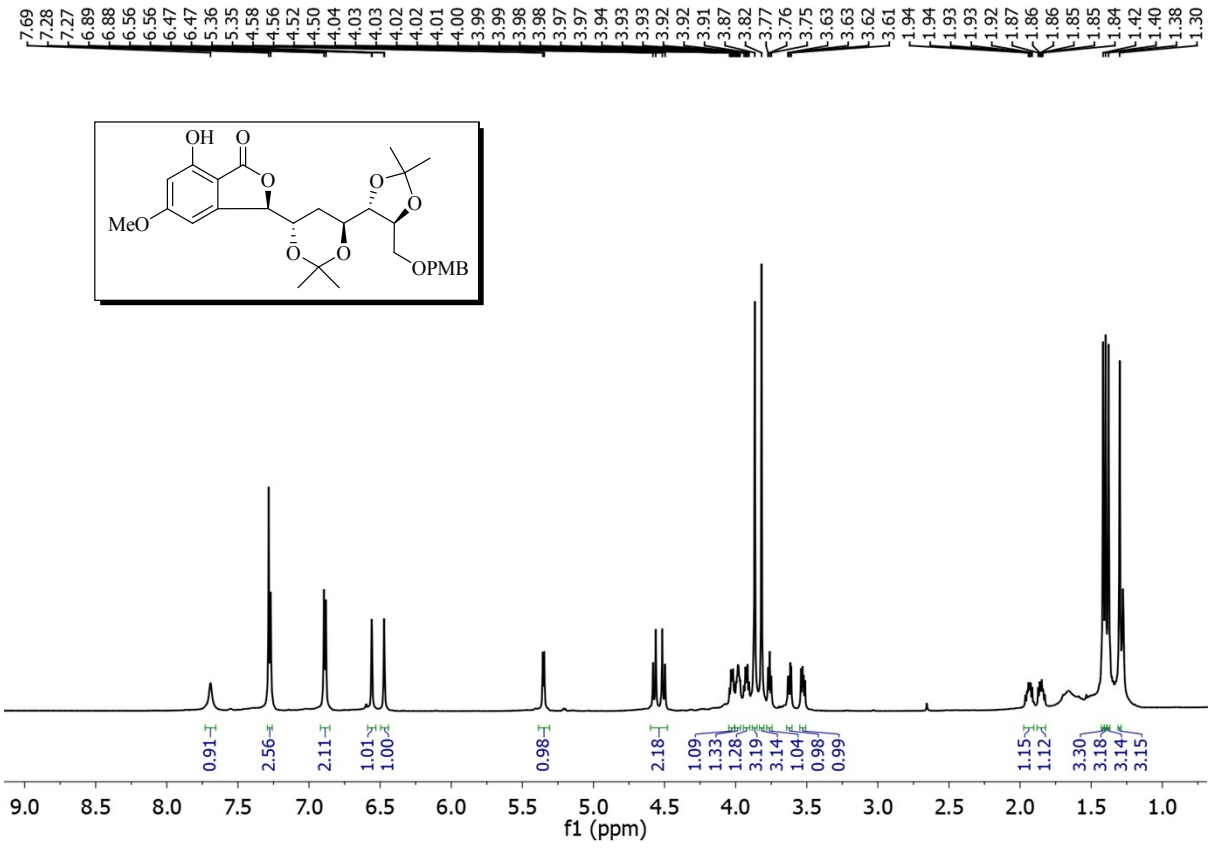
^{13}C NMR of compound 27 (100 MHz, $CDCl_3$)



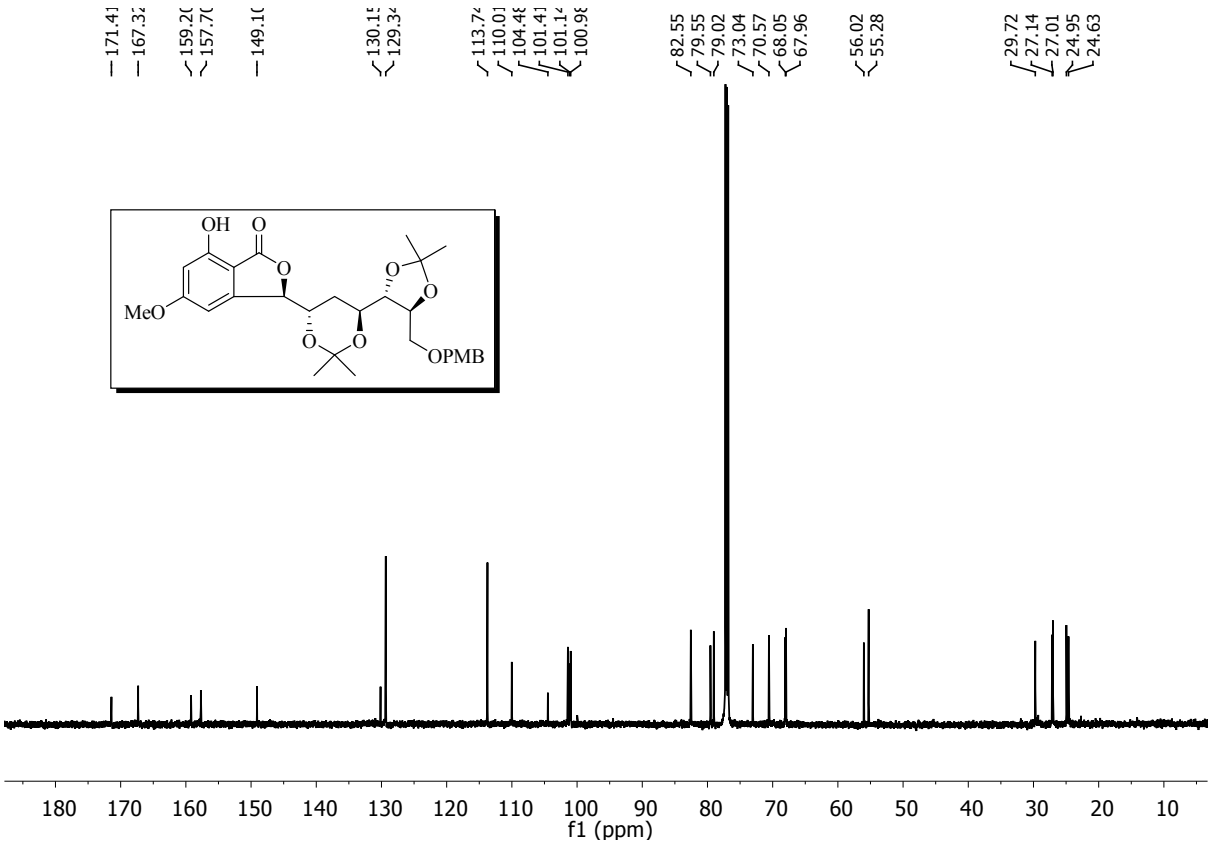
DEPT-135 of compound 27 (100 MHz, $CDCl_3$)



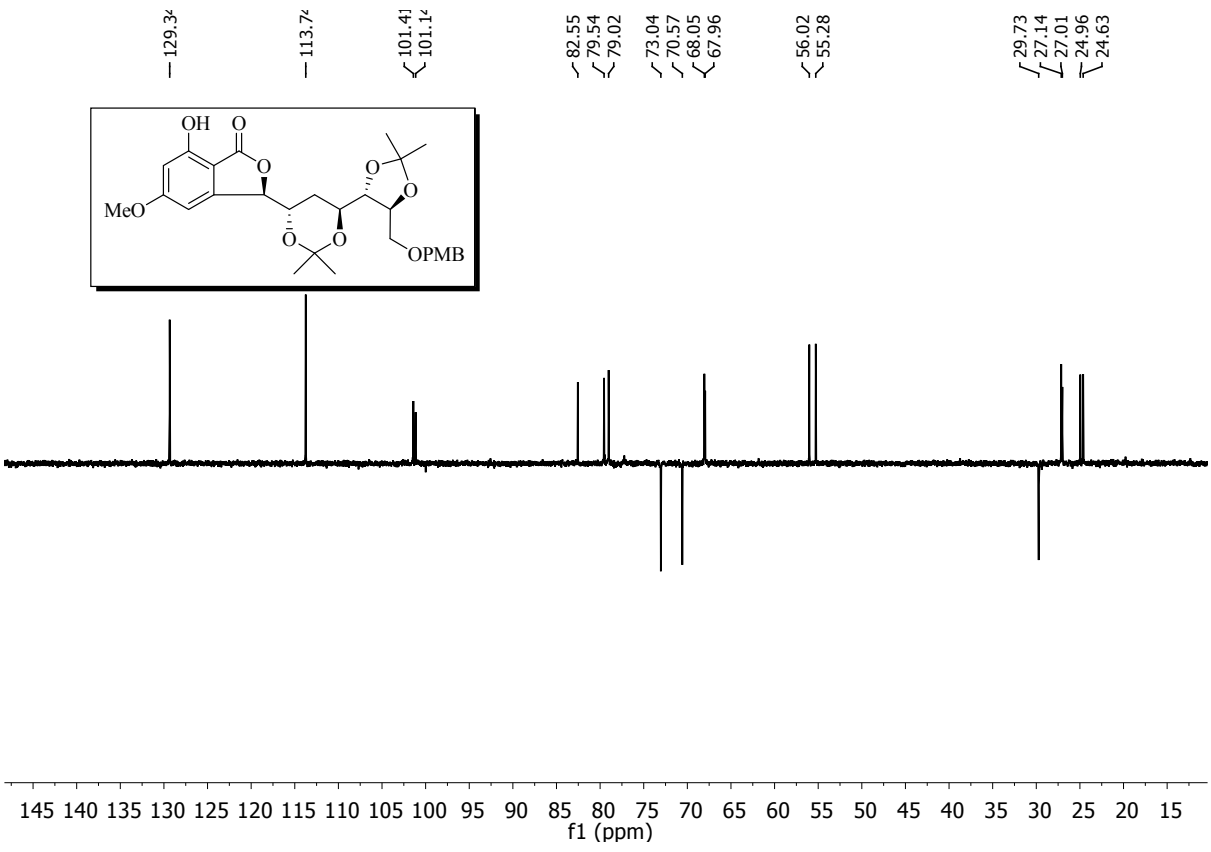
^{1}H NMR of compound 28 (600 MHz, $CDCl_3$)



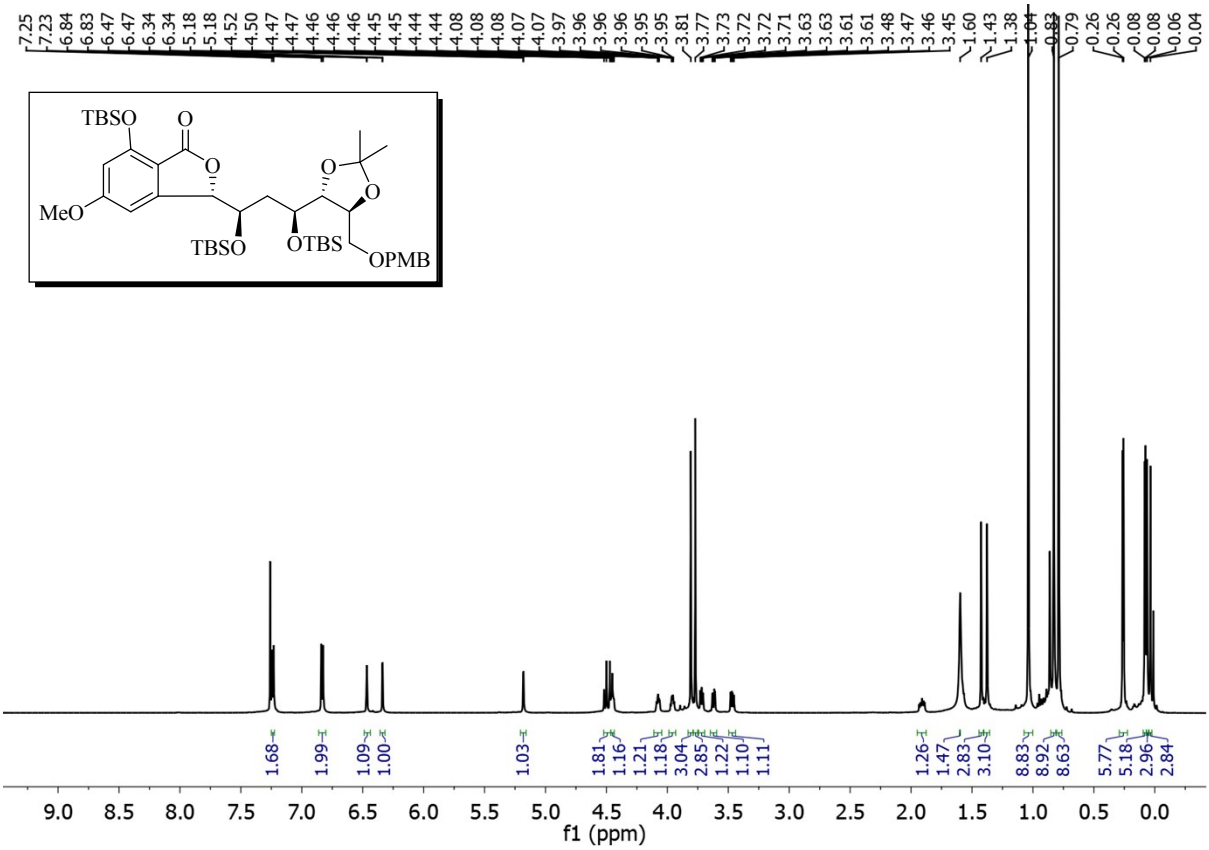
^{13}C NMR of compound 28 (100 MHz, $CDCl_3$)



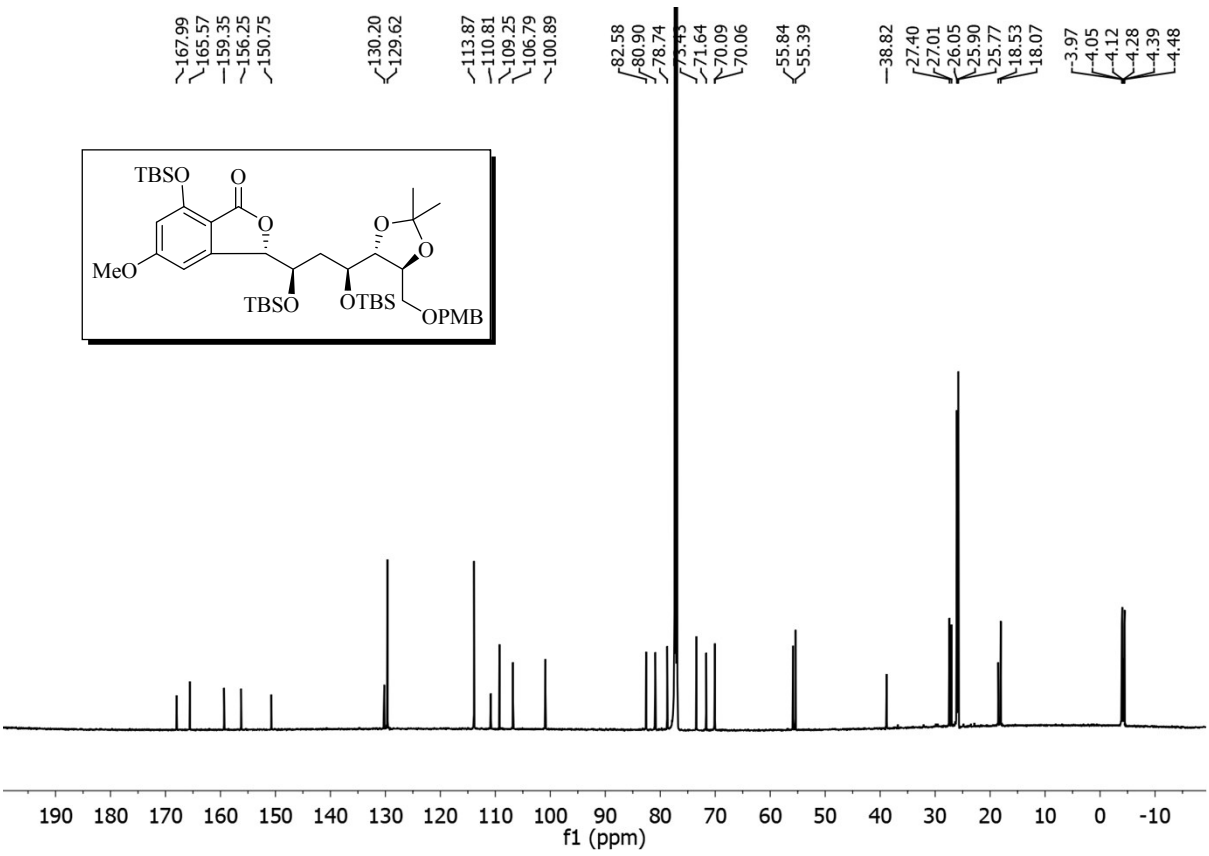
DEPT-135 of compound 28 (100 MHz, $CDCl_3$)



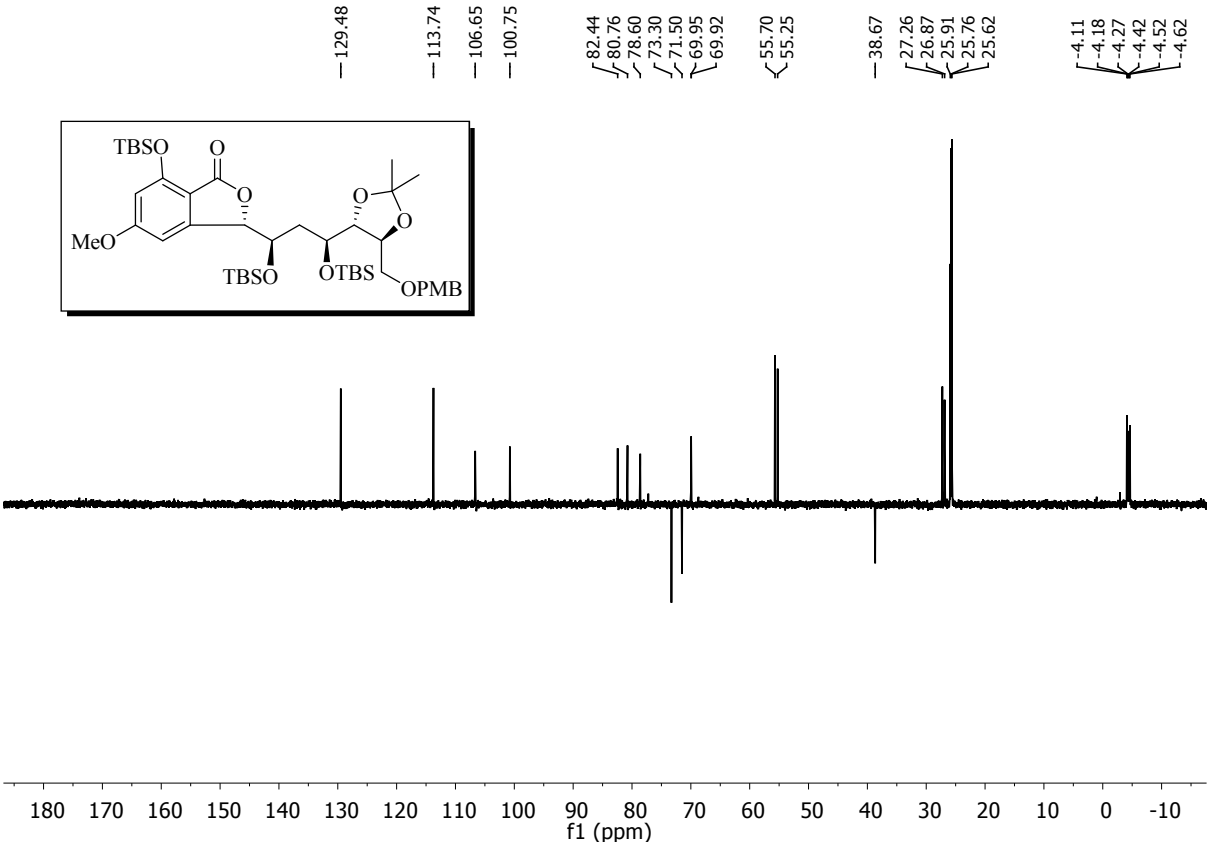
^{1}H NMR of compound 29 (600 MHz, $CDCl_3$)



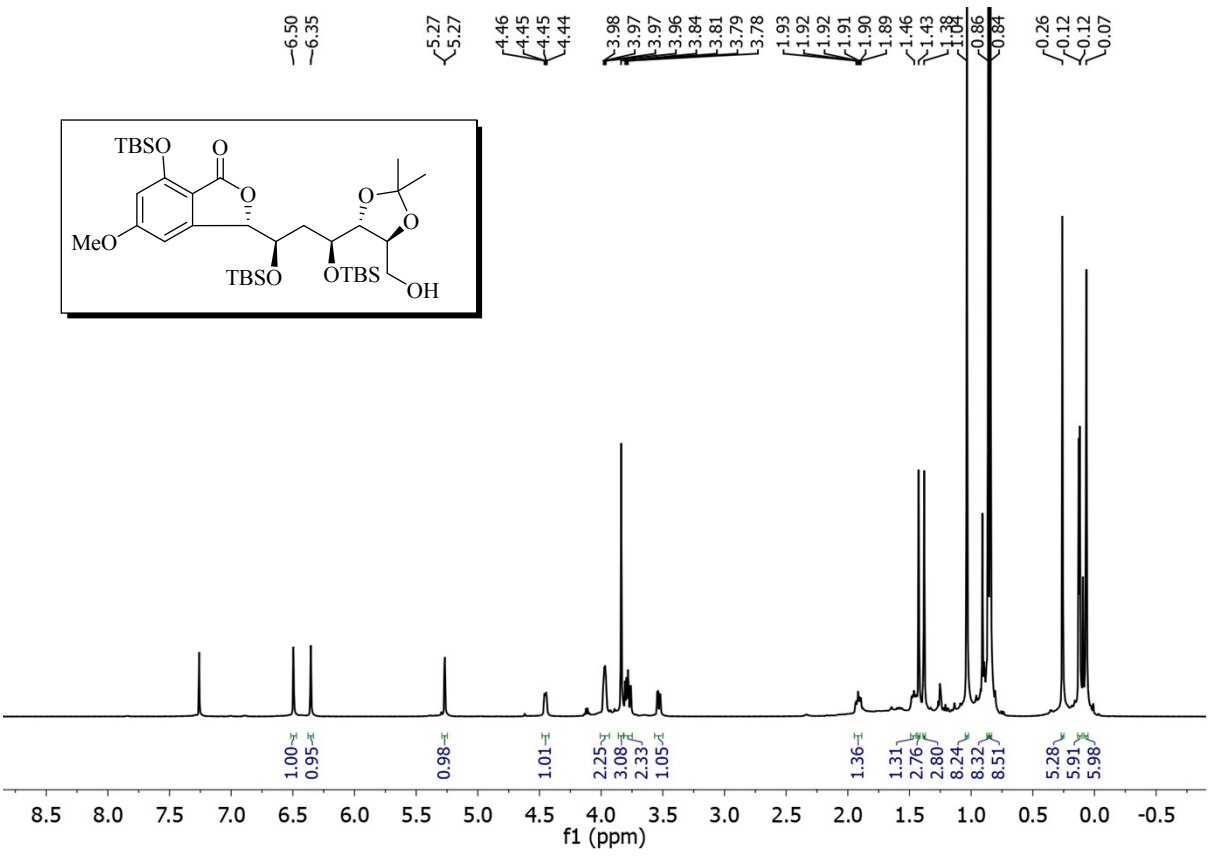
^{13}C NMR of compound 29 (150 MHz, $CDCl_3$)



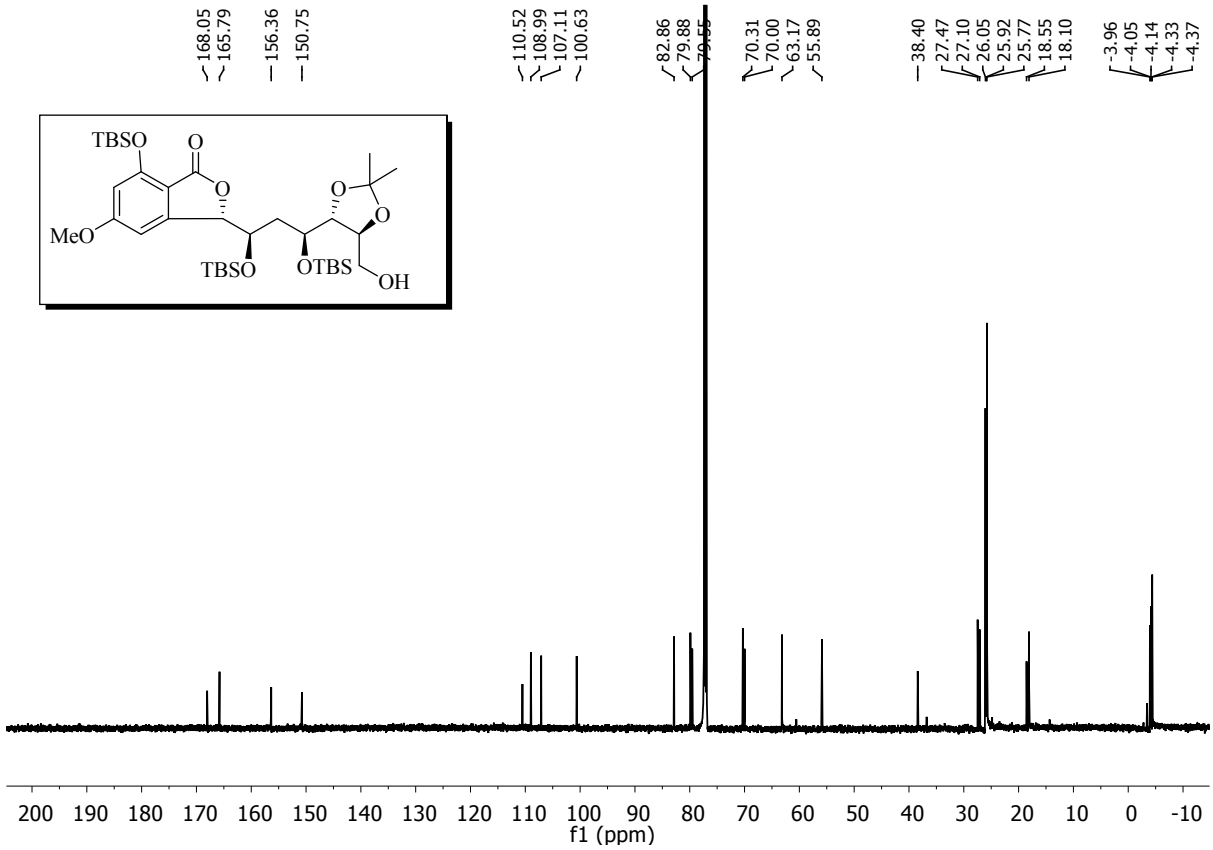
DEPT-135 of compound 29 (150 MHz, $CDCl_3$)



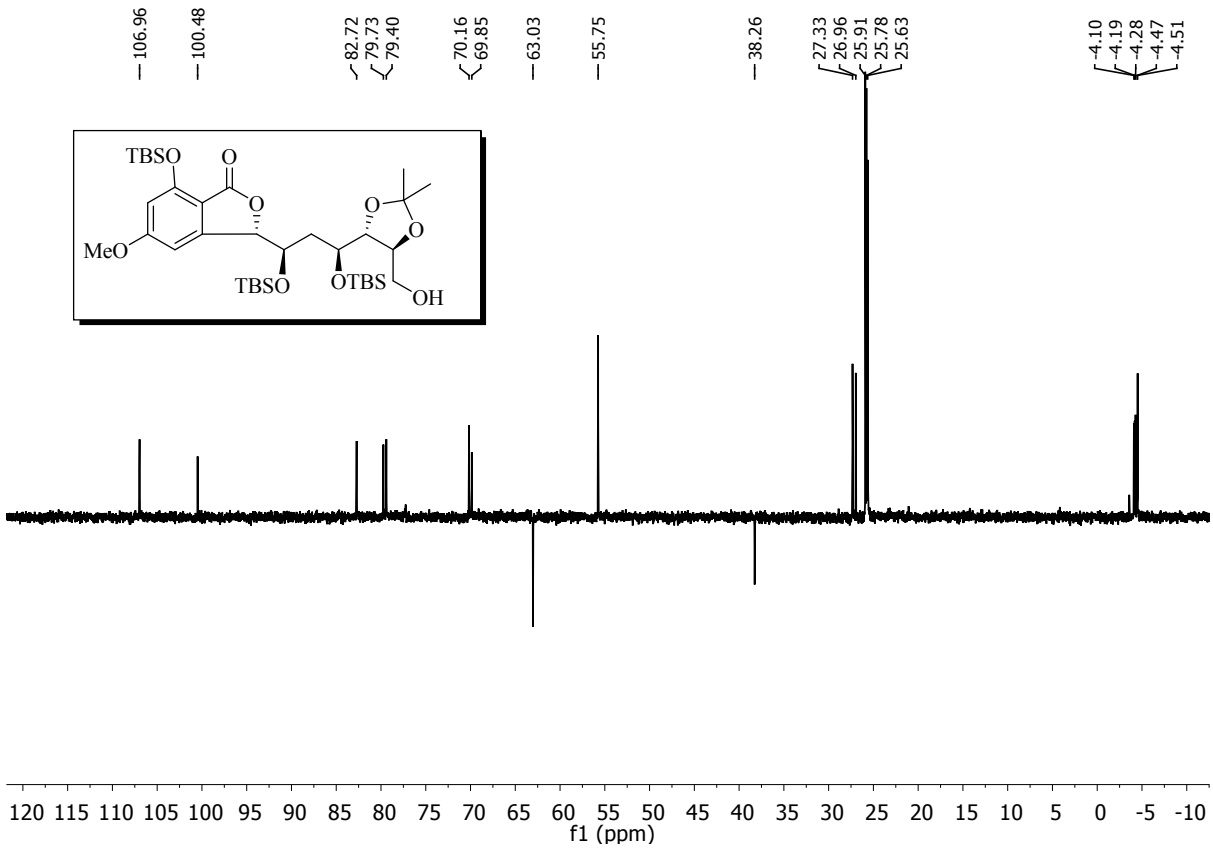
^{1}H NMR of compound 30 (600 MHz, $CDCl_3$)



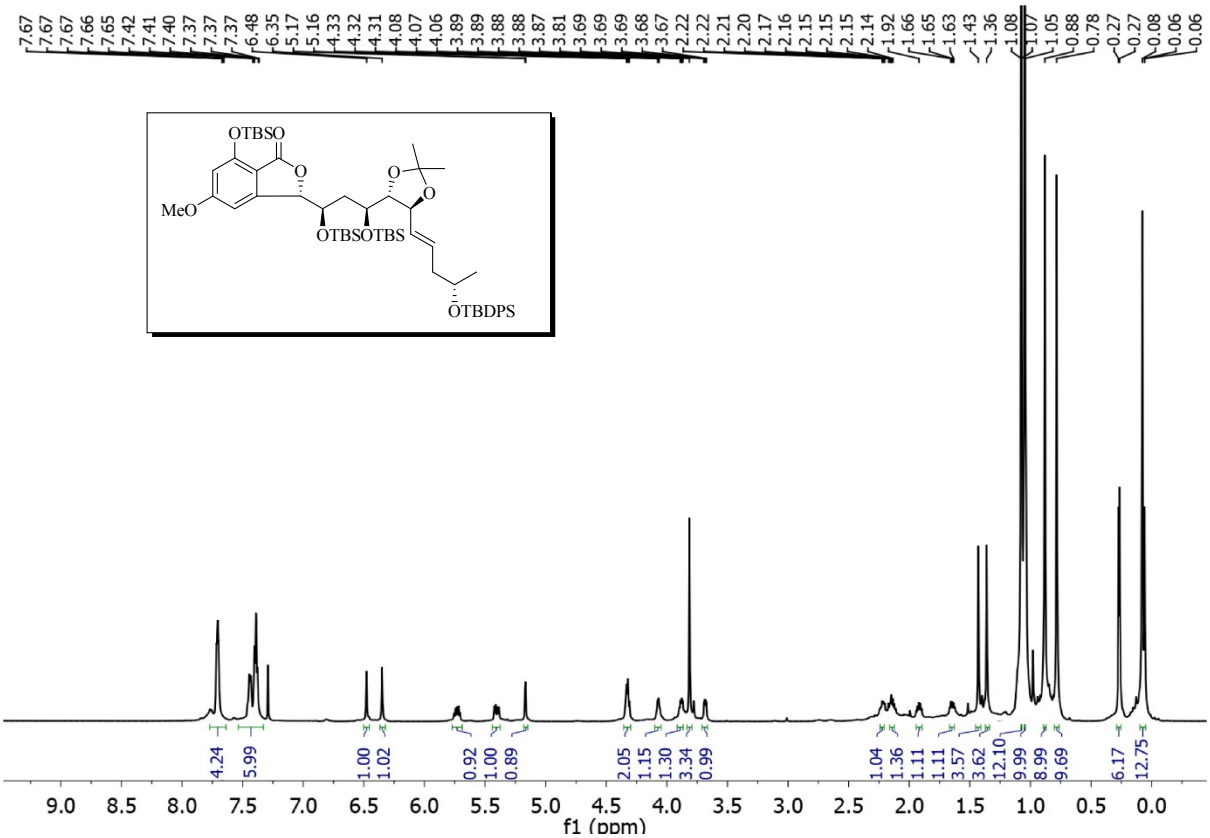
^{13}C NMR of compound 30 (150 MHz, $CDCl_3$)



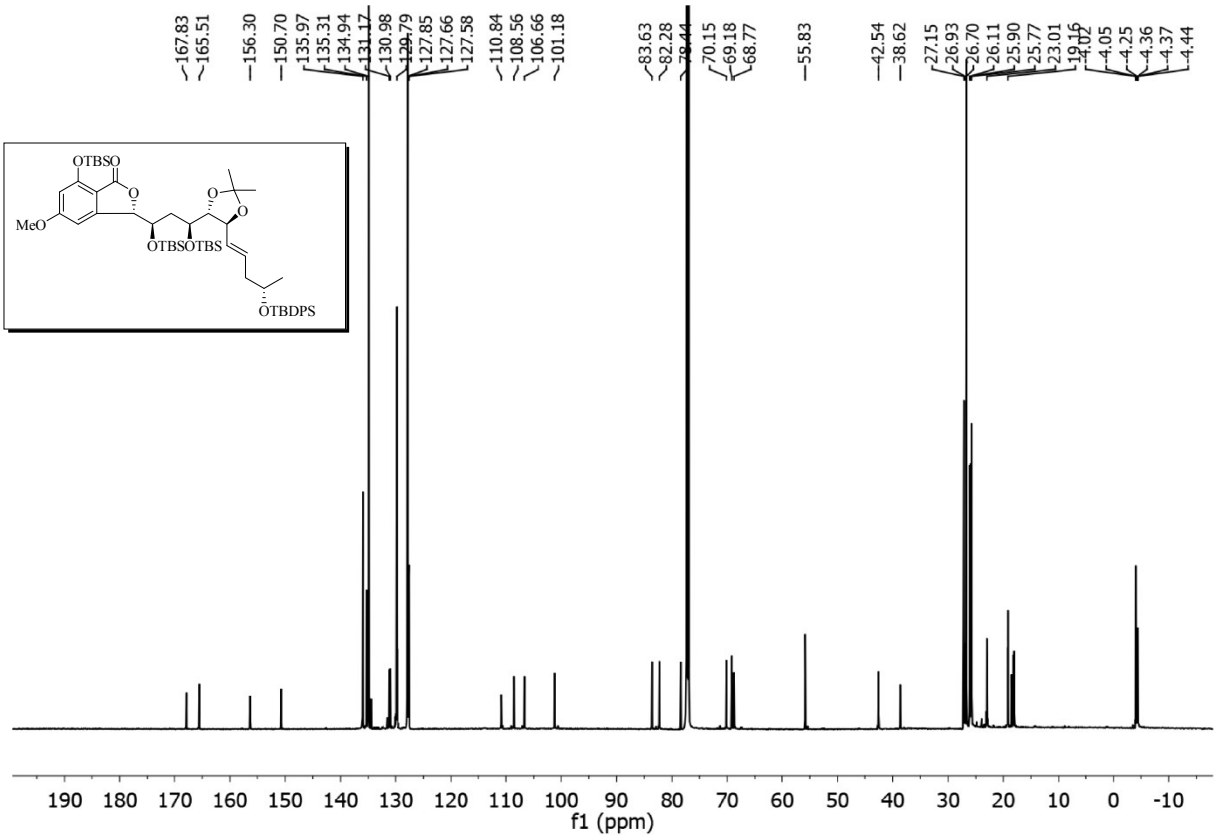
DEPT-135 of compound 30 (150 MHz, $CDCl_3$)



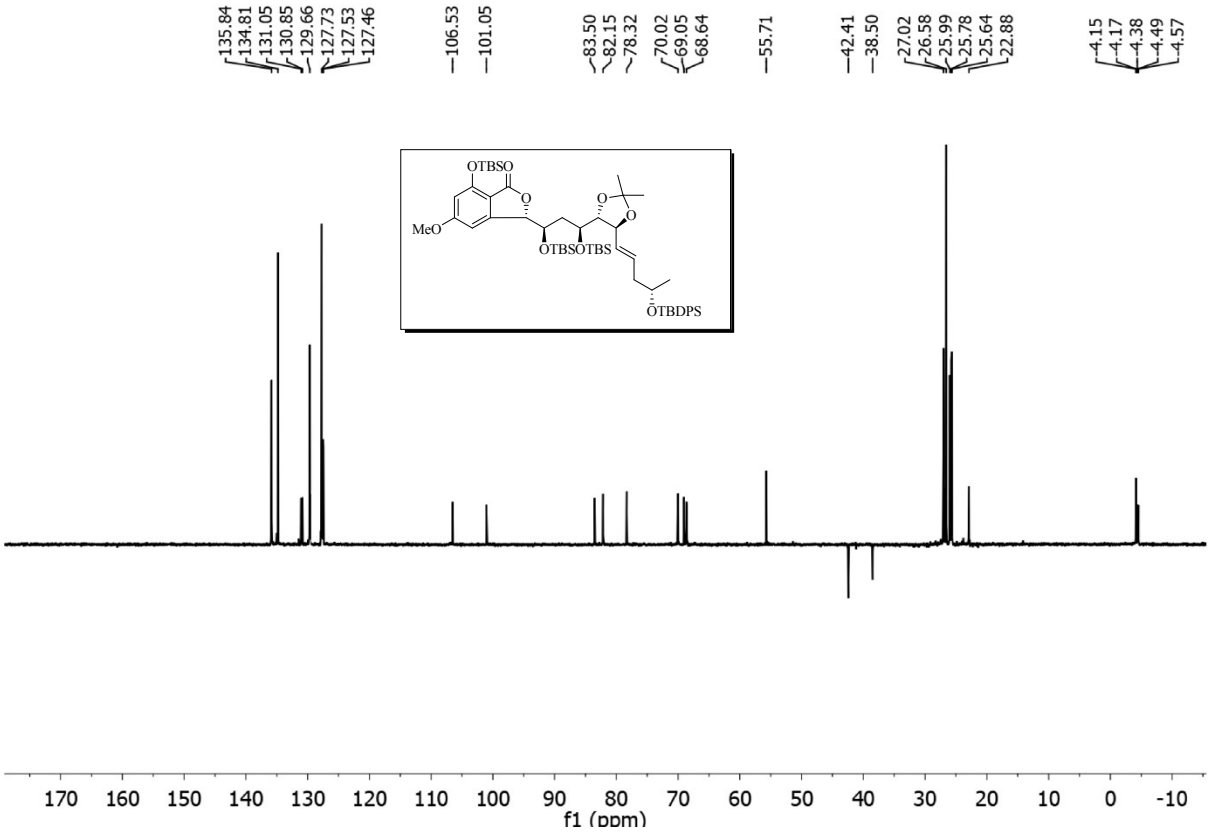
^{1}H NMR of compound 31 (600 MHz, $CDCl_3$)



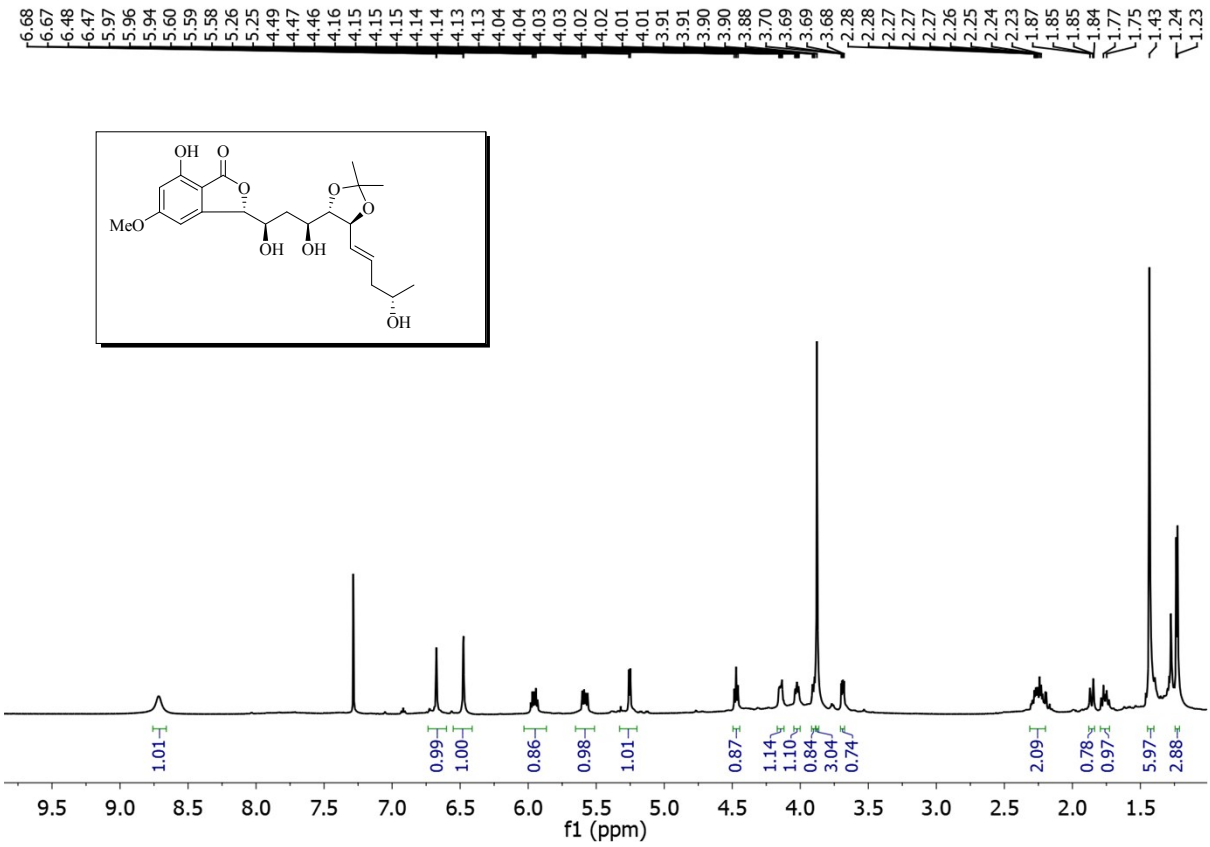
^{13}C NMR of compound 31 (150 MHz, $CDCl_3$)



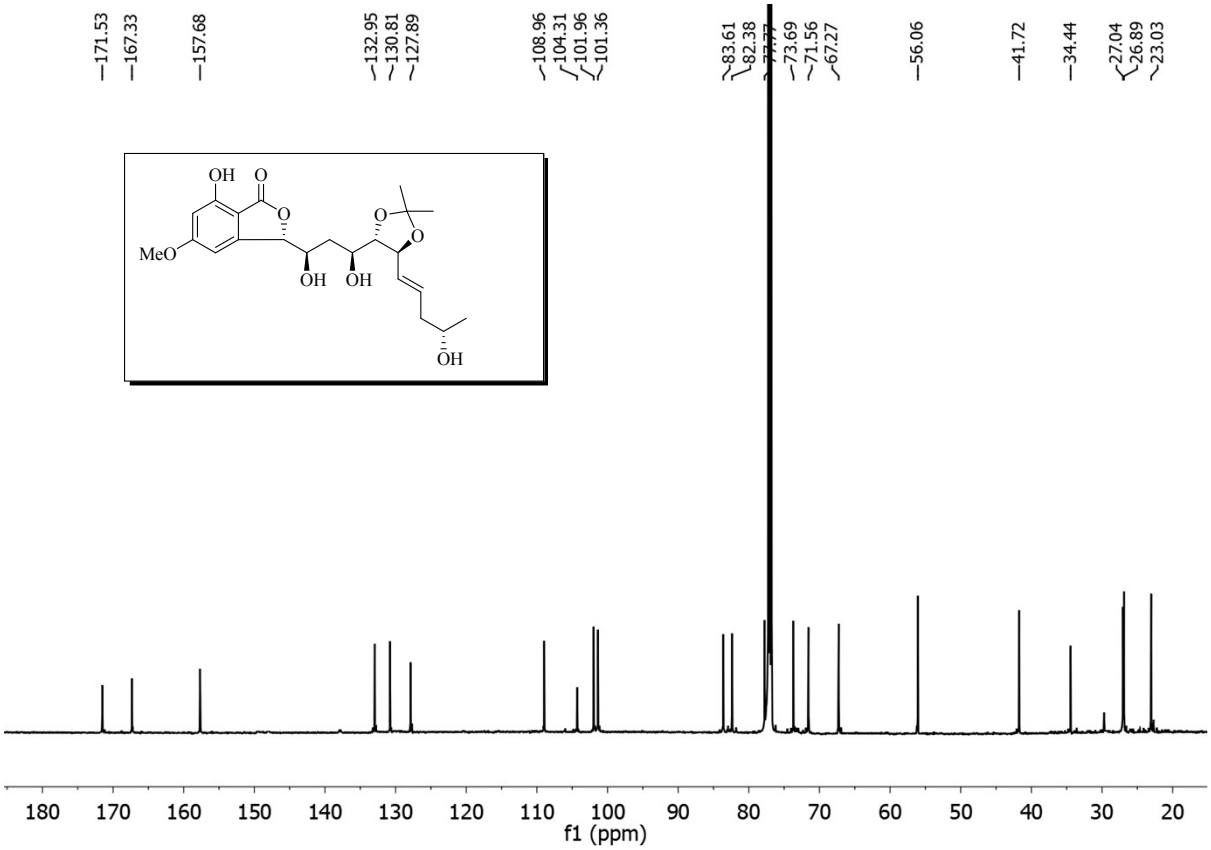
DEPT-135 of compound 31 (150 MHz, $CDCl_3$)



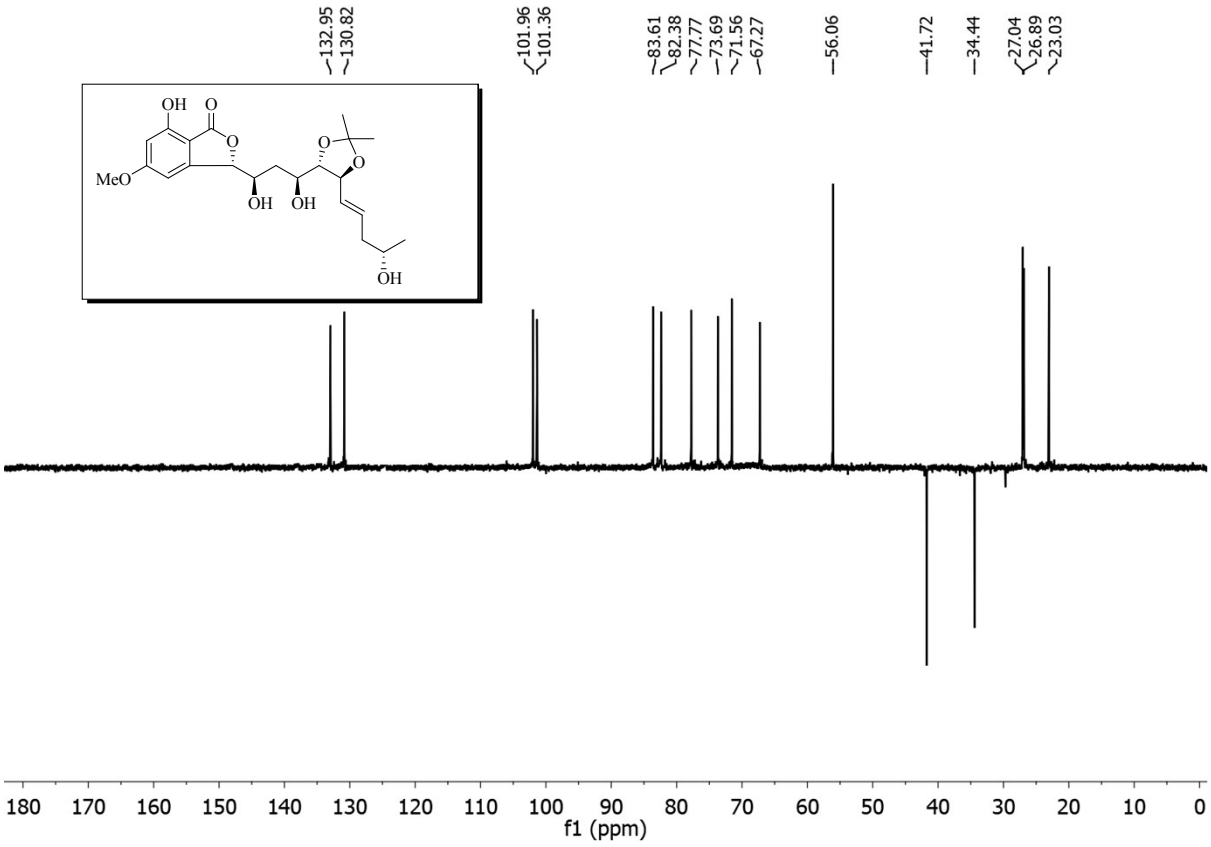
^{1}H NMR of compound 32 (600 MHz, $CDCl_3$)



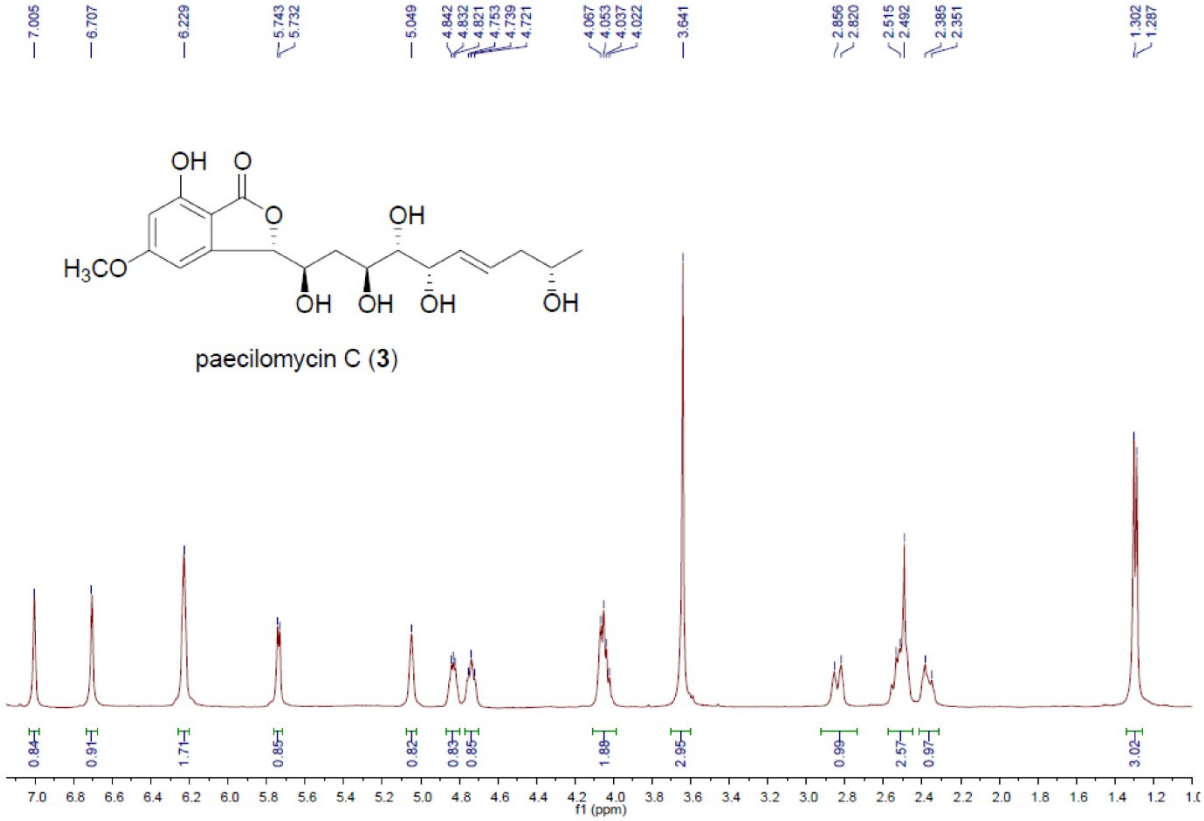
^{13}C NMR of compound 32 (150 MHz, $CDCl_3$)



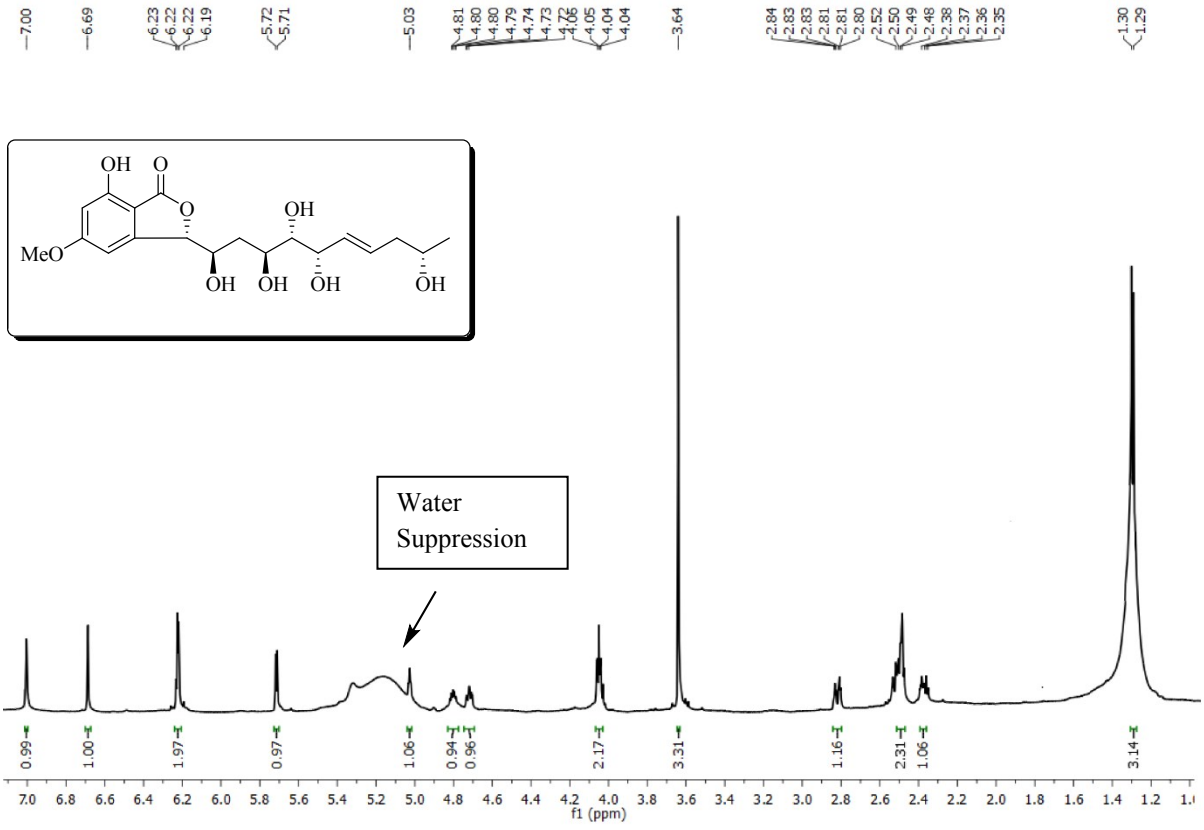
DEPT-135 of compound 32 (150 MHz, $CDCl_3$)



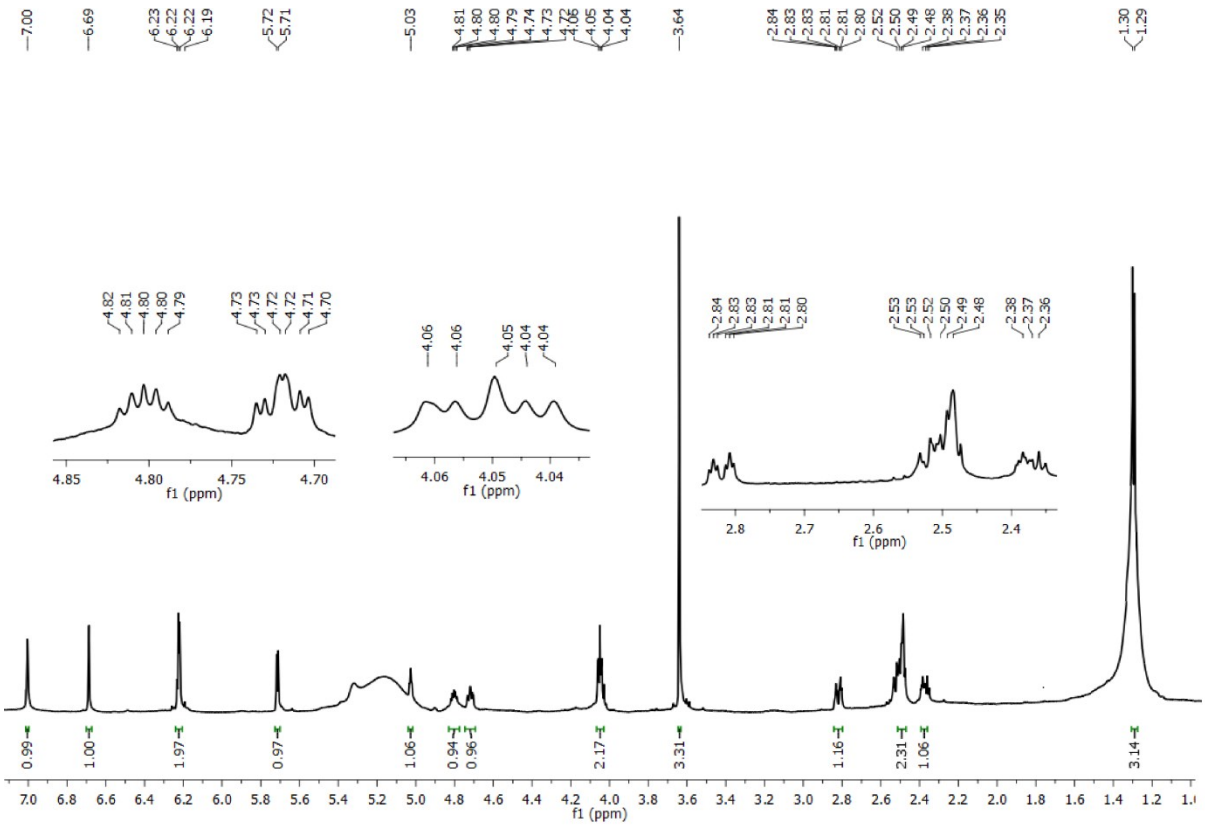
^{1}H NMR of natural Paecilomycin C



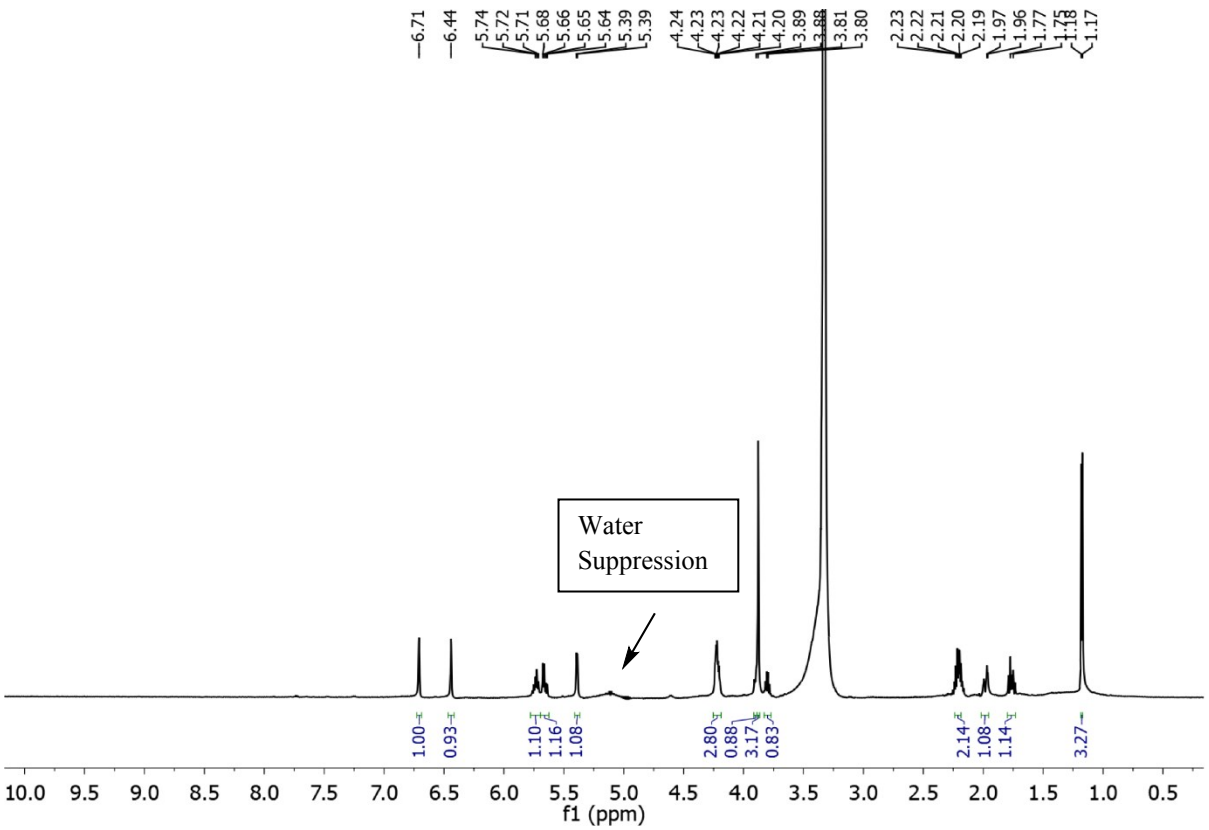
^{1}H NMR of synthetic Paecilomycin C (600 MHz, Pyridine d_5, Water suppression)



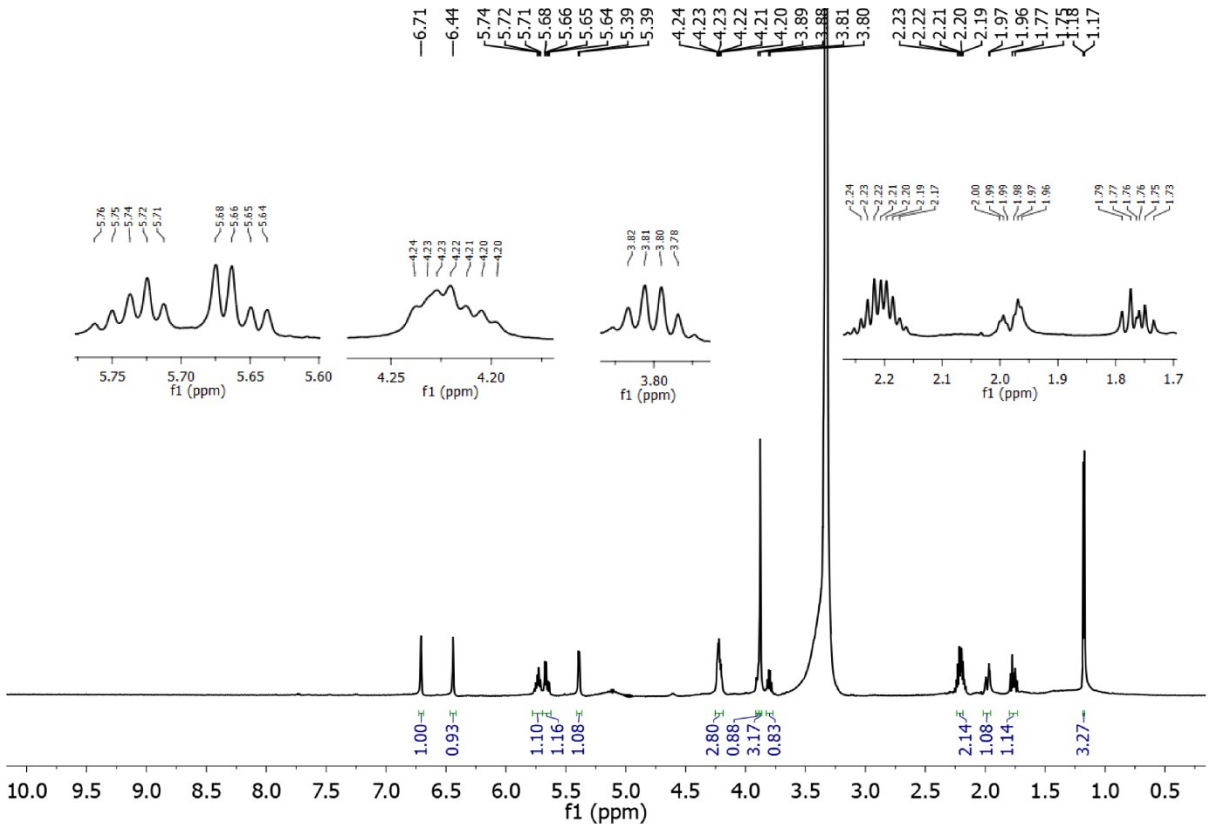
^{1}H NMR of Paecilomycin C (600 MHz, Pyridine d_5, Expanded key region)



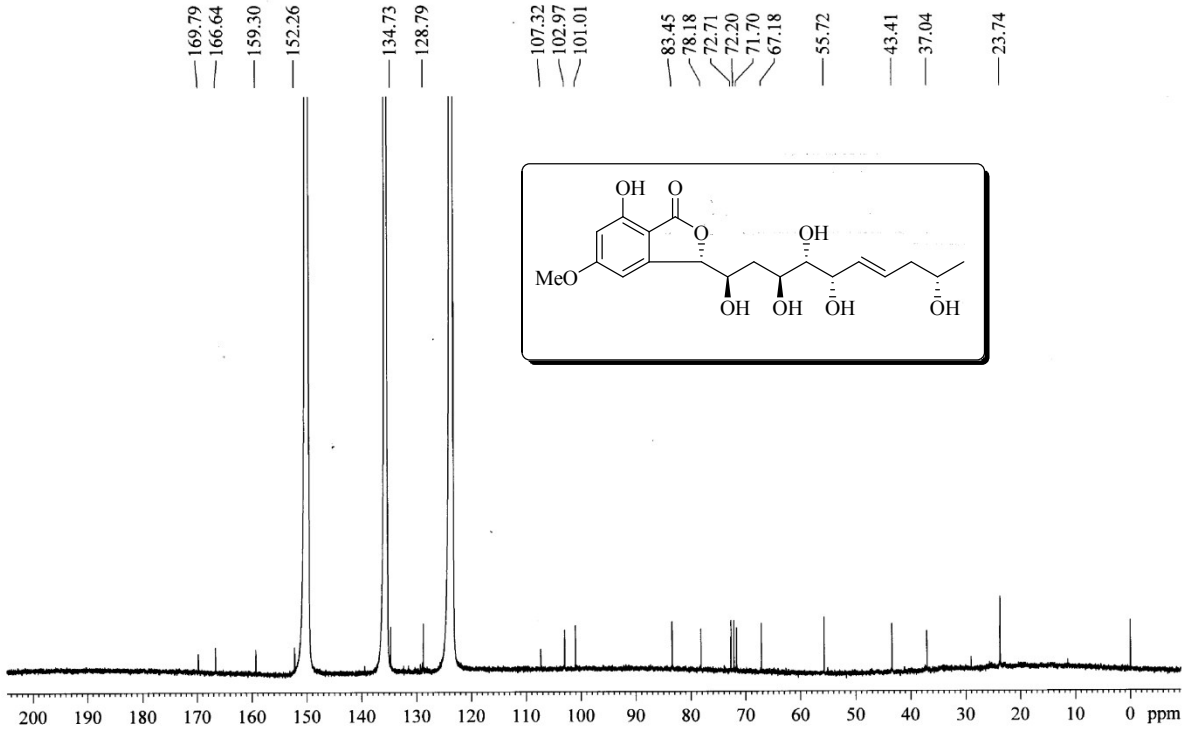
^{1}H NMR of Paecilomycin C (600 MHz, CD_3OD, Water suppression)



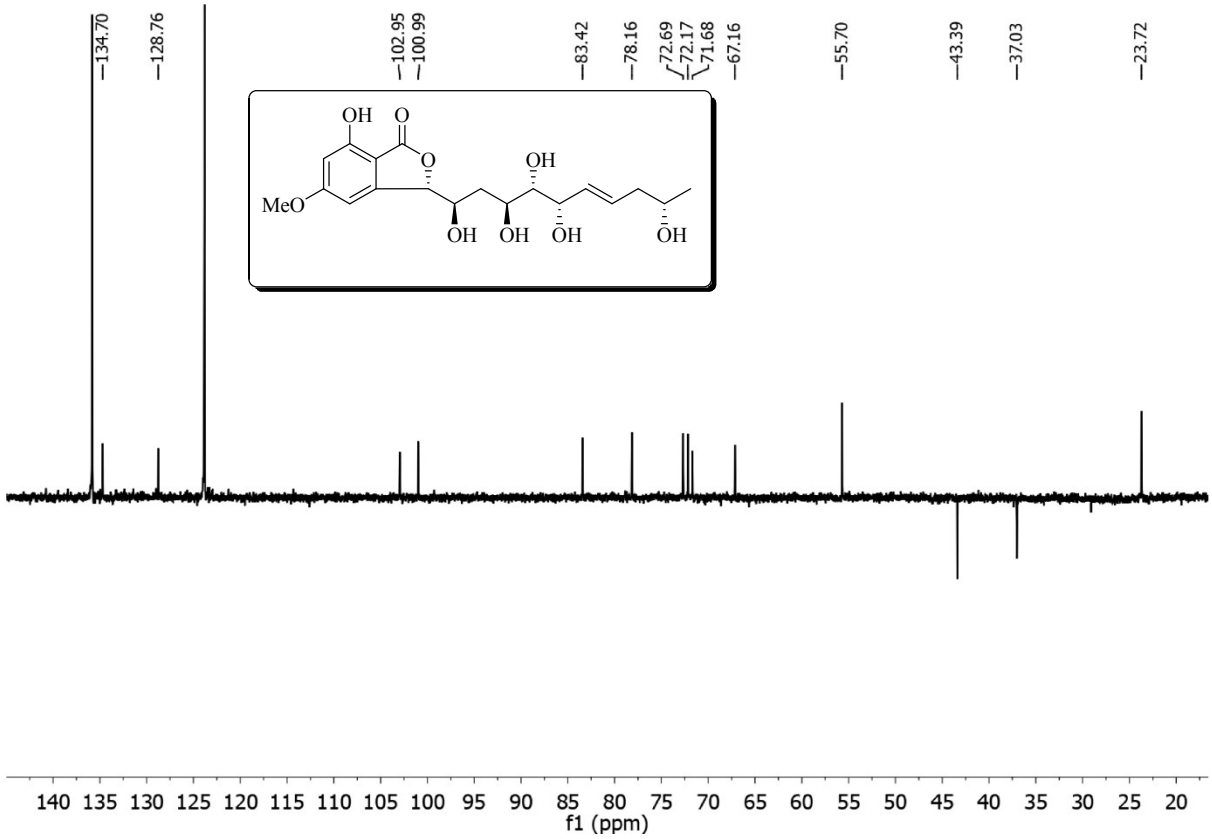
^{1}H NMR of Paecilomycin C (600 MHz, CD_3OD, Expanded key region)



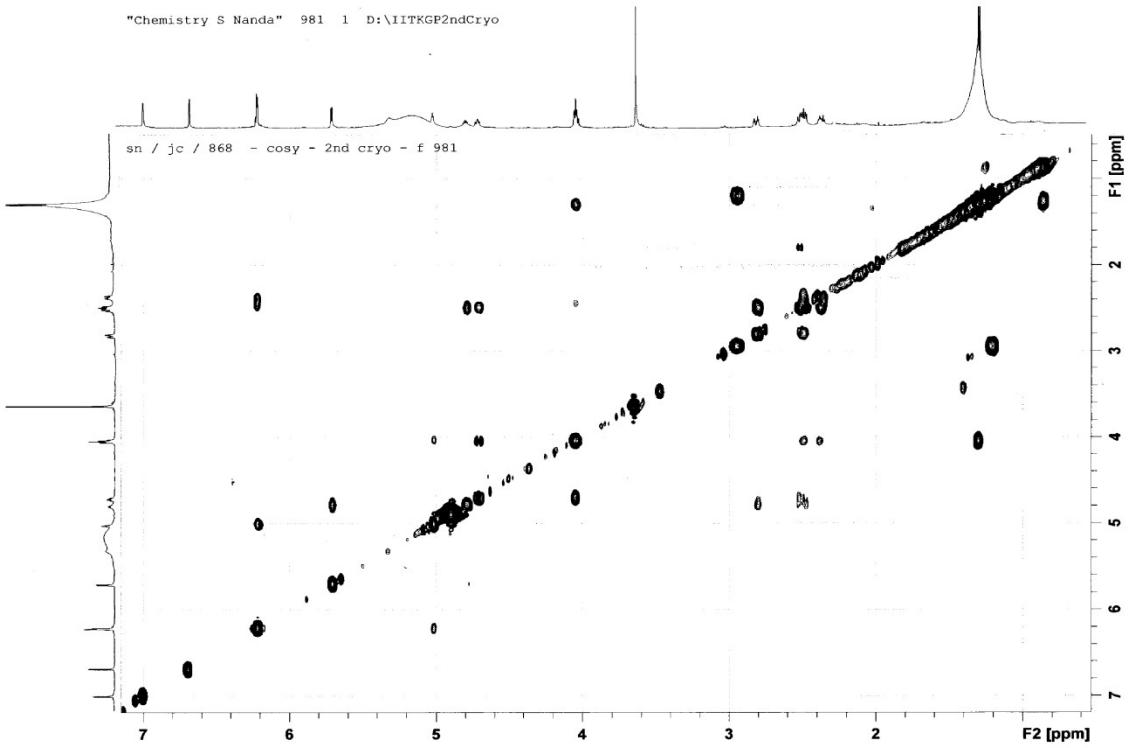
^{13}C NMR of Paecilomycin C (150 MHz, Pyridine d_5)



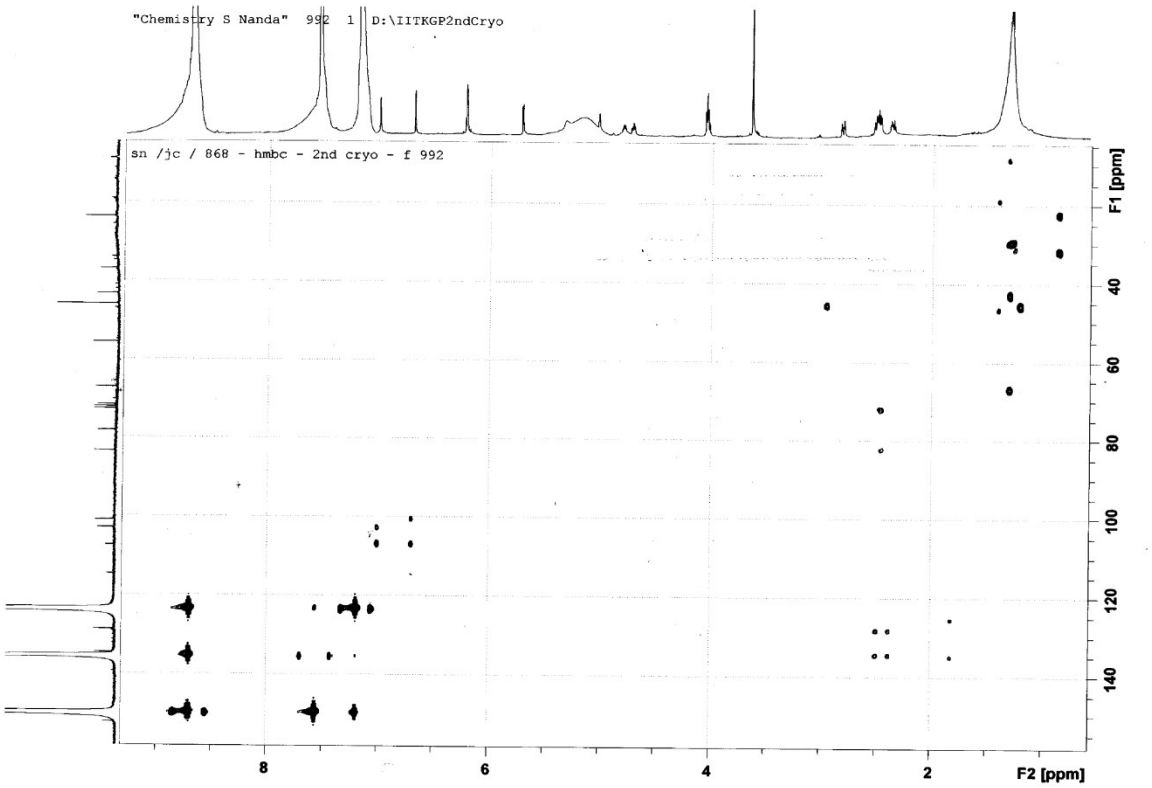
DEPT-135 of Paecilomycin C (150 MHz, Pyridine d_5)

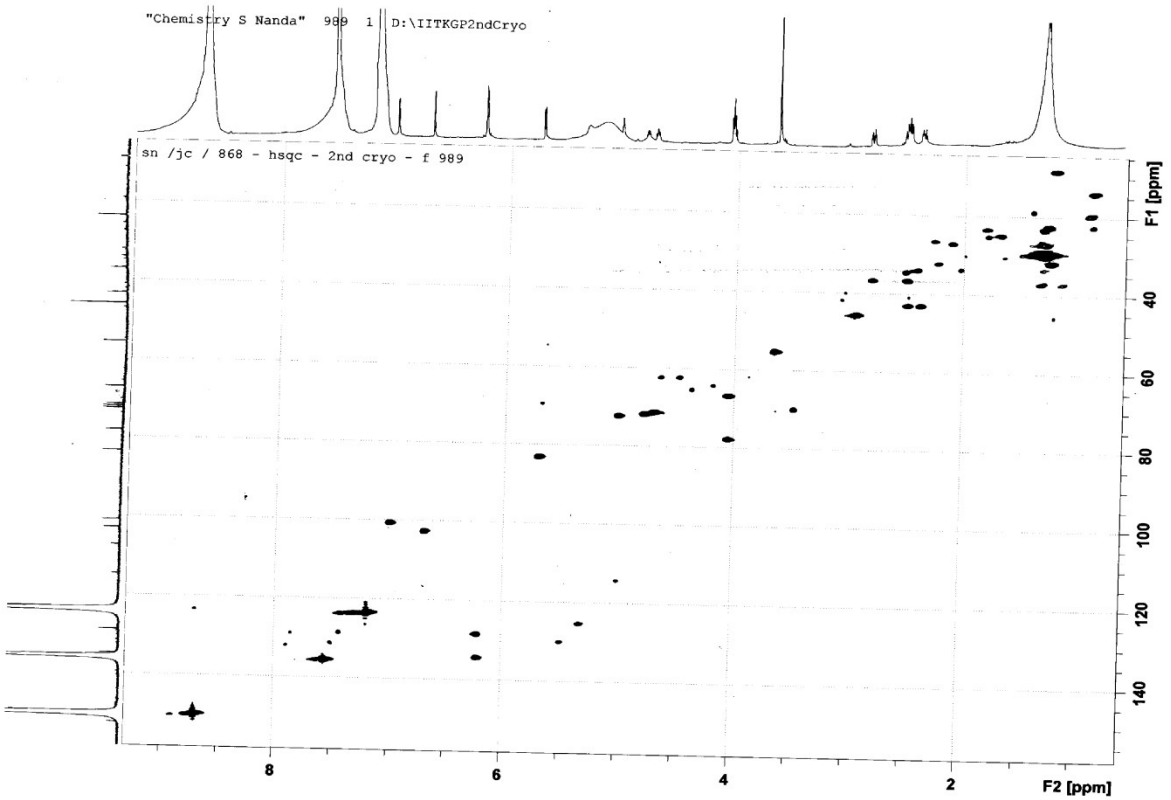


H^1-H^1 COSY of Paecilomycin C (600 MHz, Pyridine d_5)



HMBC & HSQC of Paecilomycin C (Pyridine d_5)

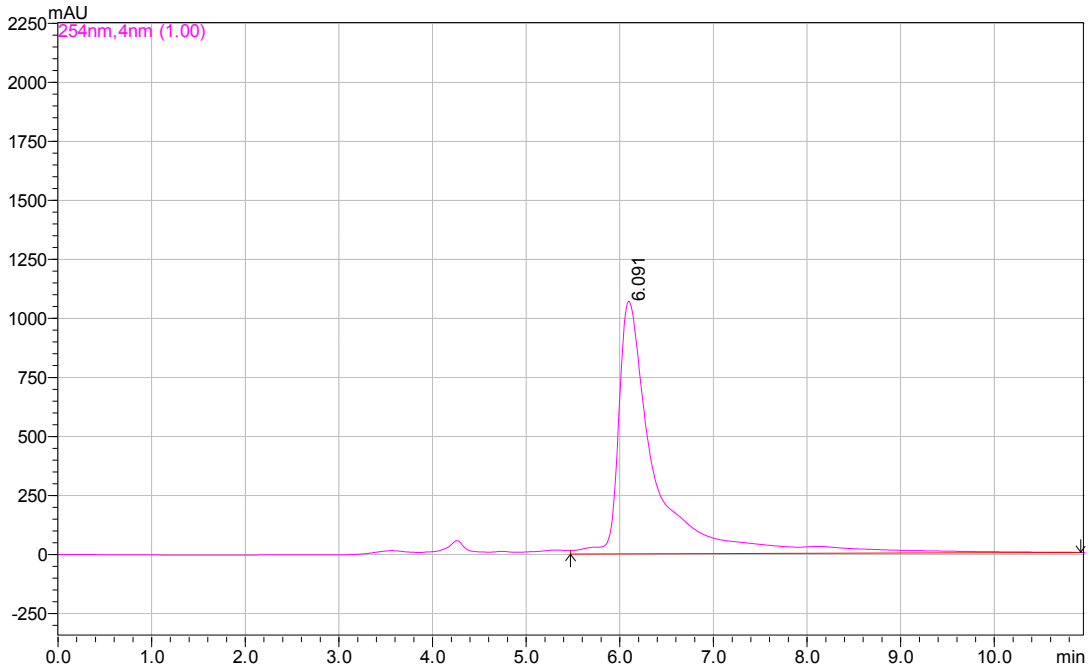




Sample name: Paecilomycin C

Column: Chiralpak IA; Flow rate: 1.0 ml/min

Mobile phase: 6:4; hexane:IPA, Sample injection volume: 5µL



Ret time	Conc	area	Height	Area (%)
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