

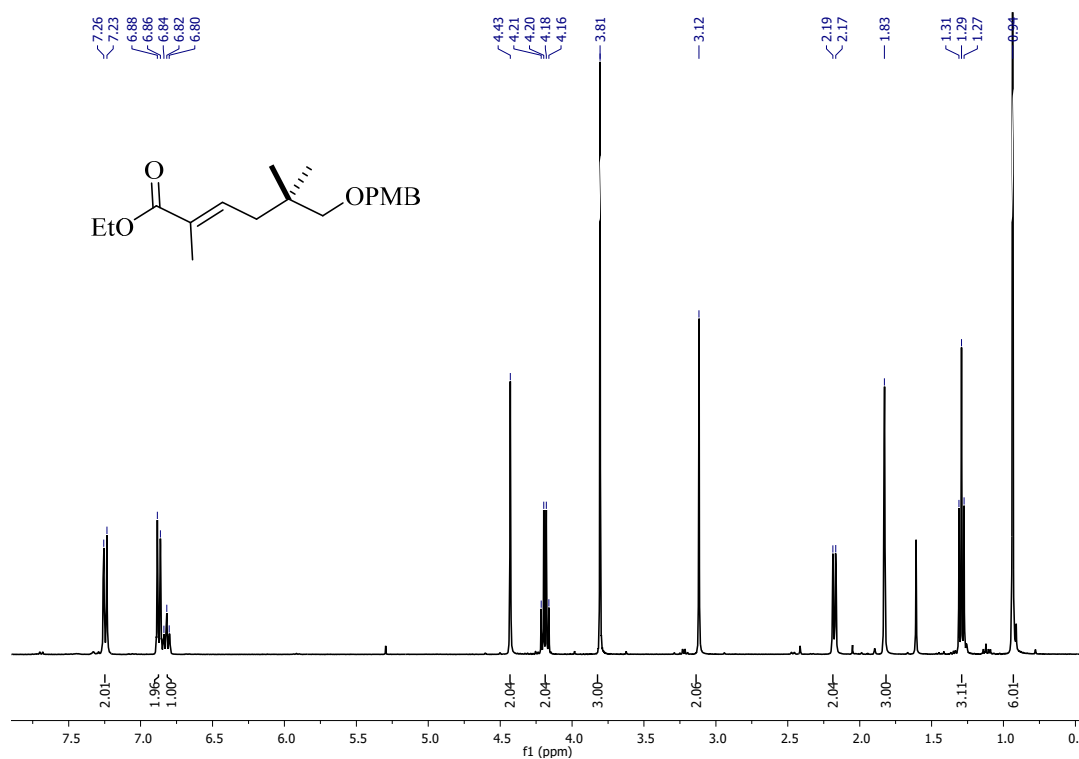
**Synthetic studies towards naturally occurring sesquiterpene capillosanane V:
Construction of fully functionalized cycloheptane core through intramolecular
Reformatsky reaction**

Rasmita Barik, Jayanta Das, and Samik Nanda*

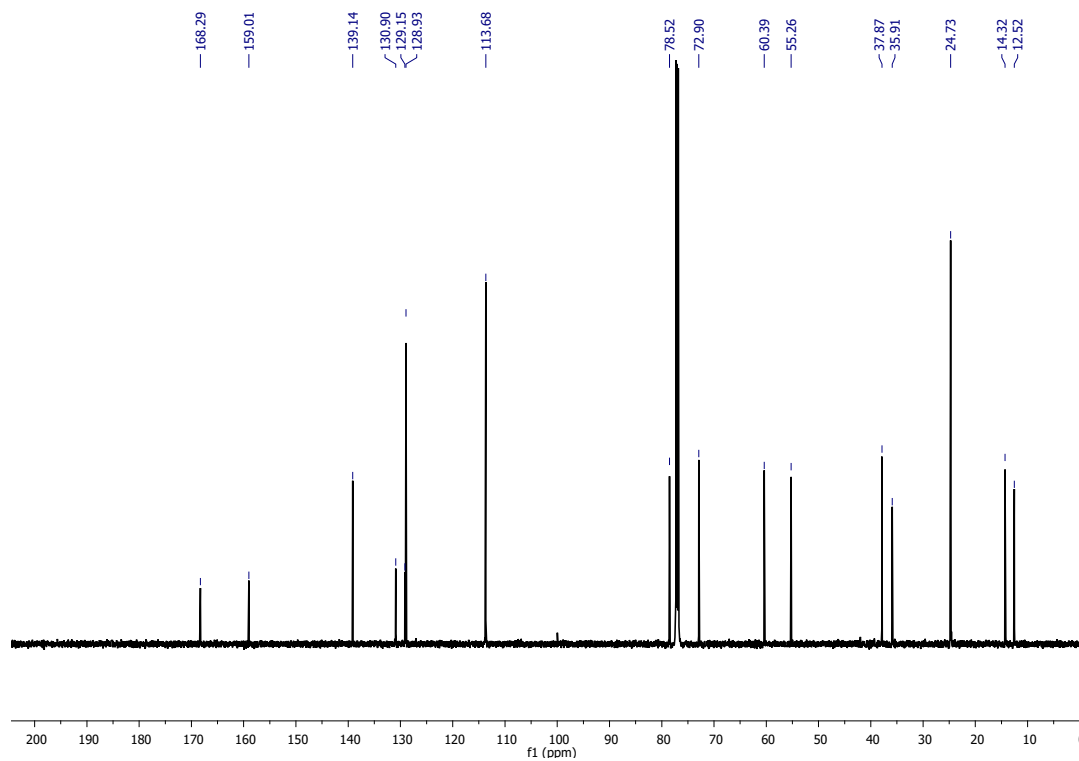
Supporting Information

Content	Page no
^1H , ^{13}C $\{^1\text{H}\}$ and DEPT-135 NMR data for synthesized compounds	2-22
HPLC chromatogram of 18	23-24

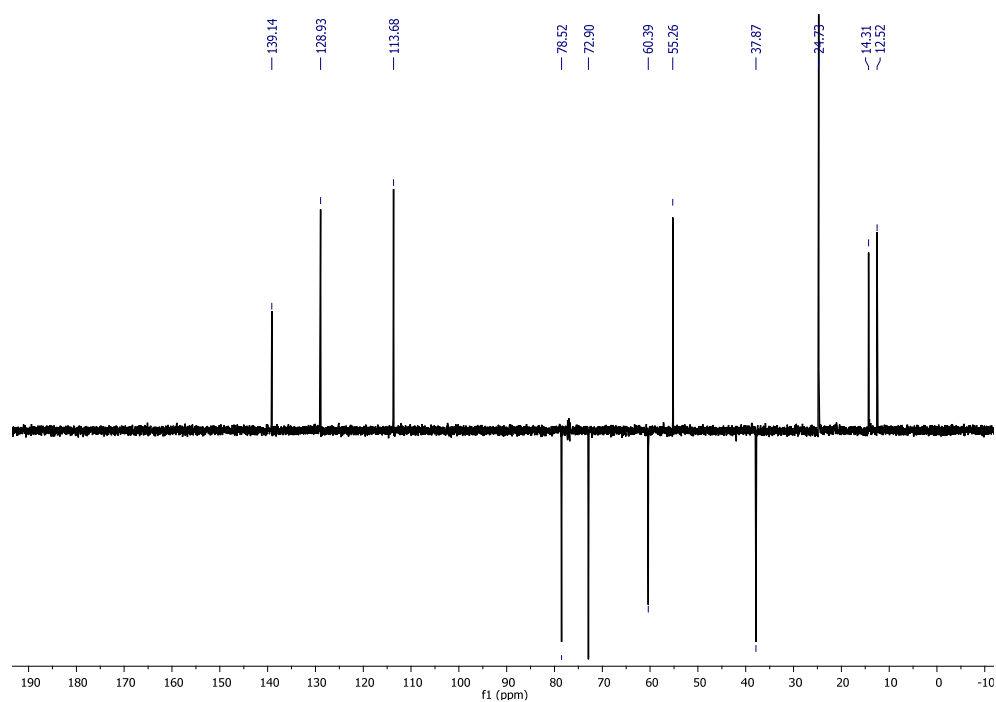
^1H NMR of **16** (400 MHz, CDCl_3)



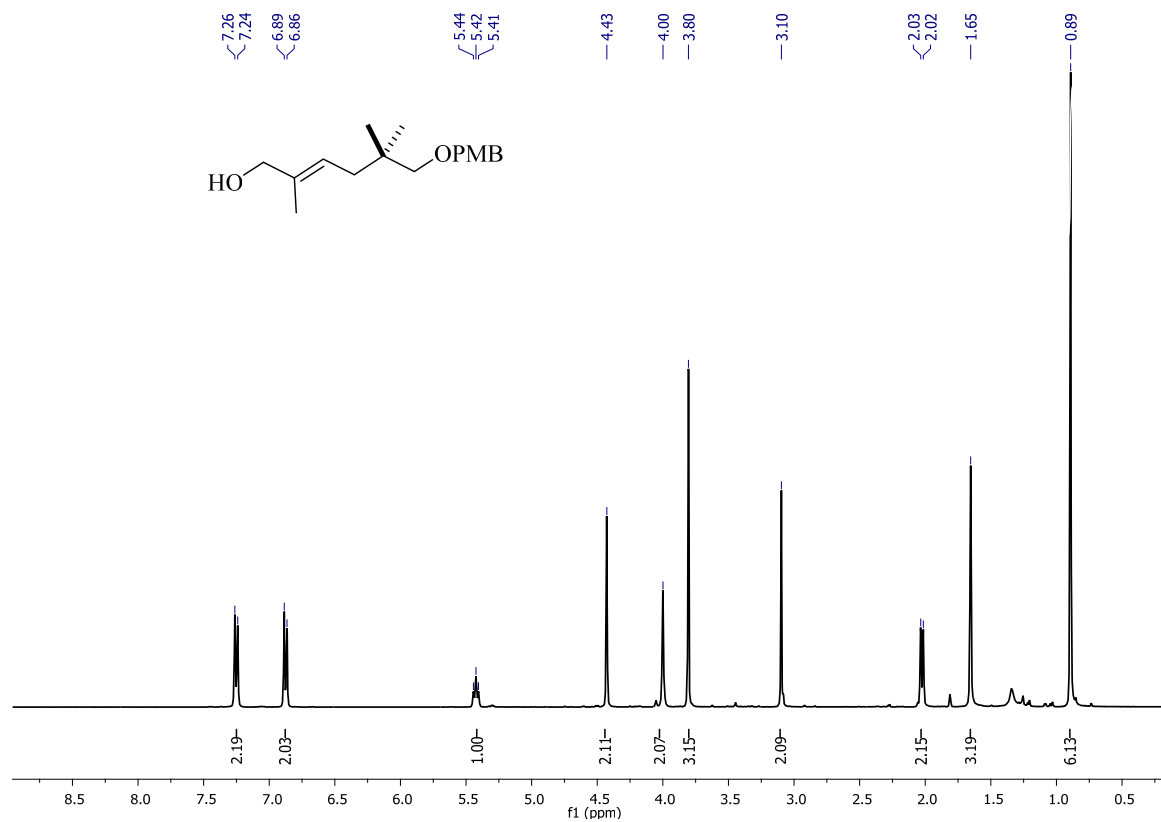
^{13}C NMR of **16** (400 MHz, CDCl_3)



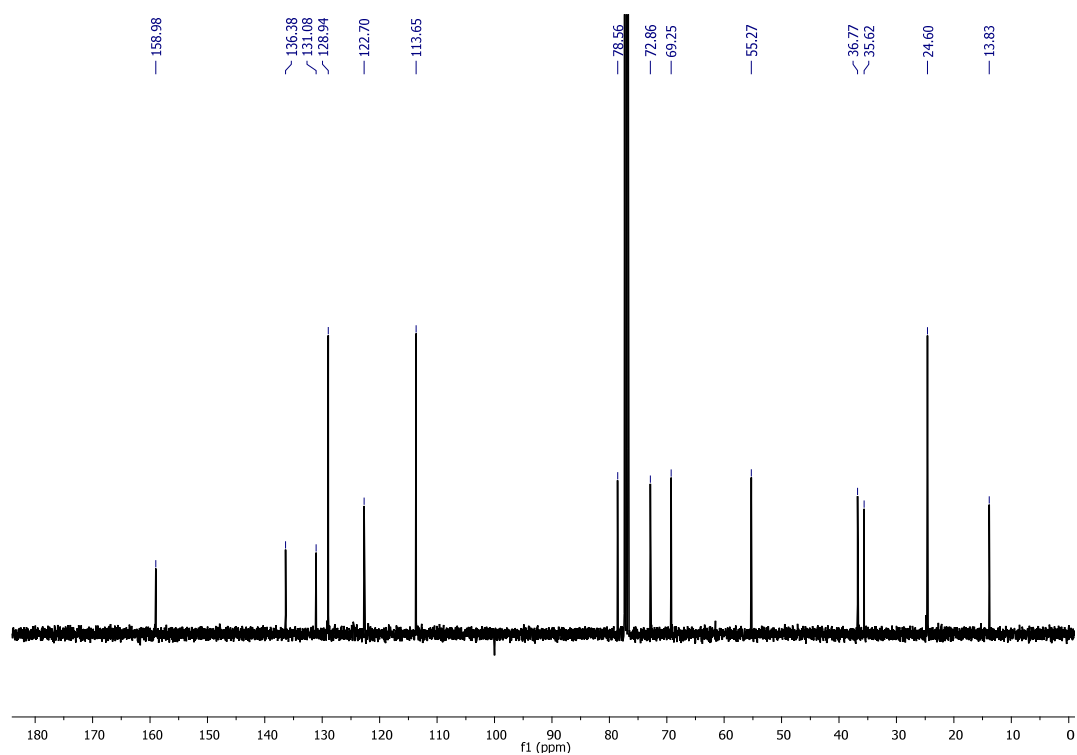
^{13}C -DEPT NMR of **16** (400 MHz, CDCl_3)



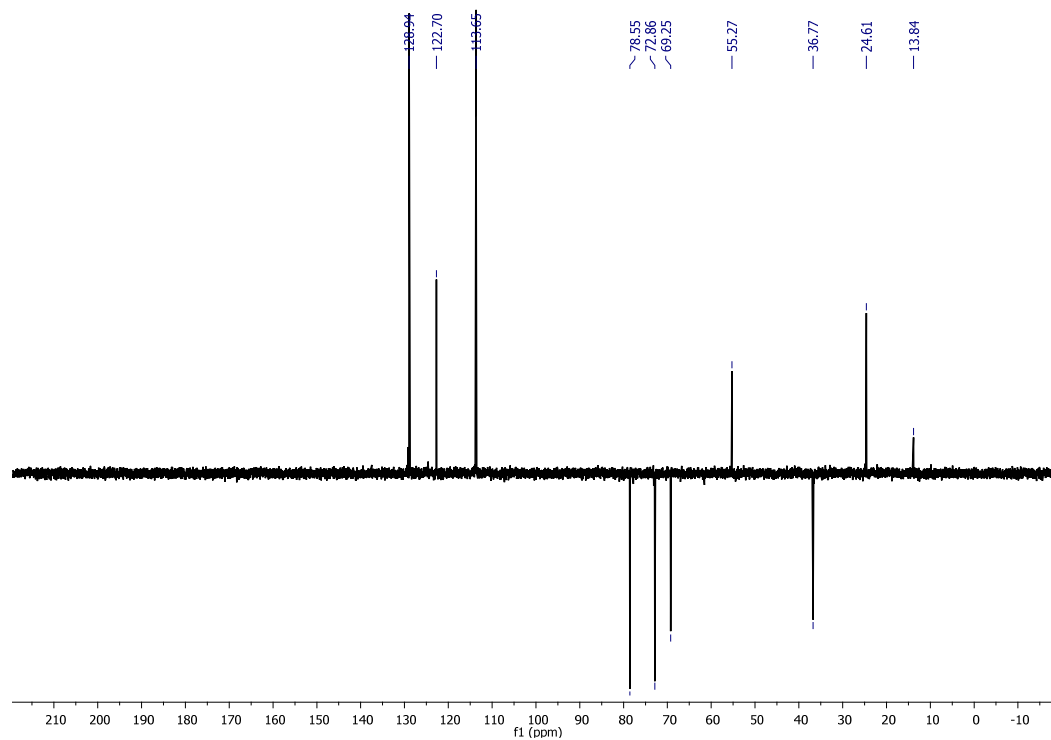
^1H NMR of **17** (400 MHz, CDCl_3)



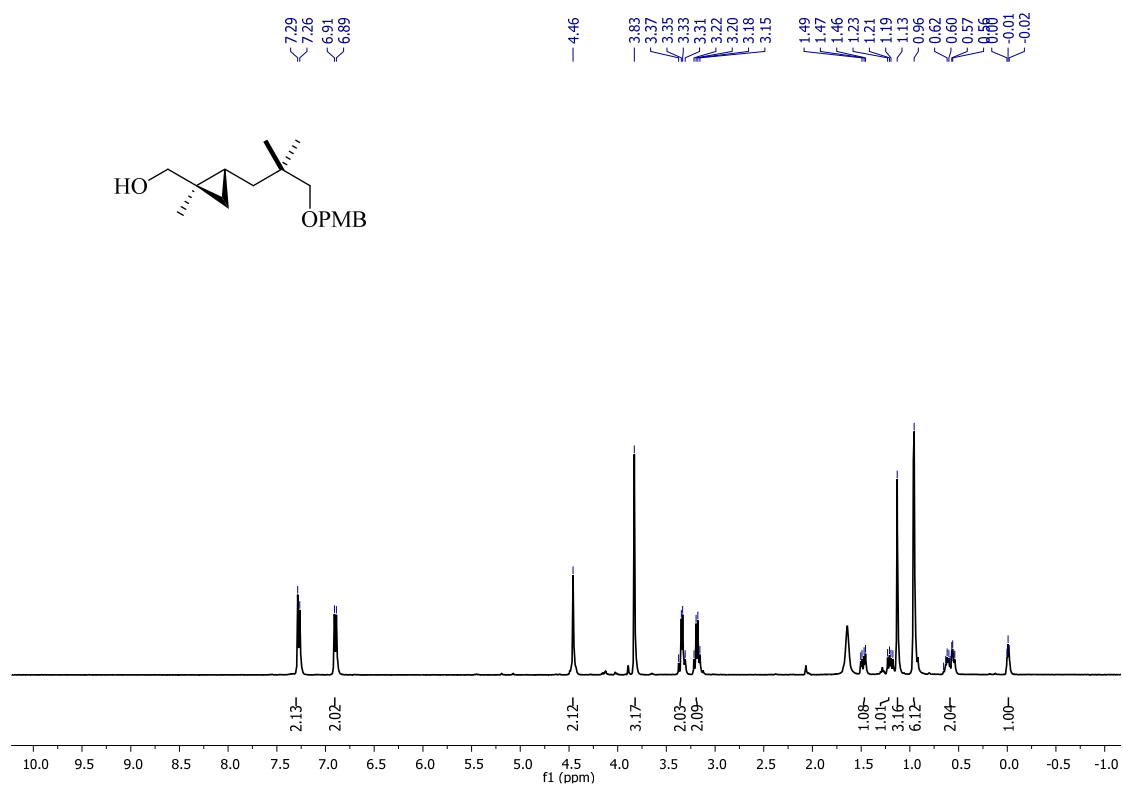
^{13}C NMR of **17** (100 MHz, CDCl_3)



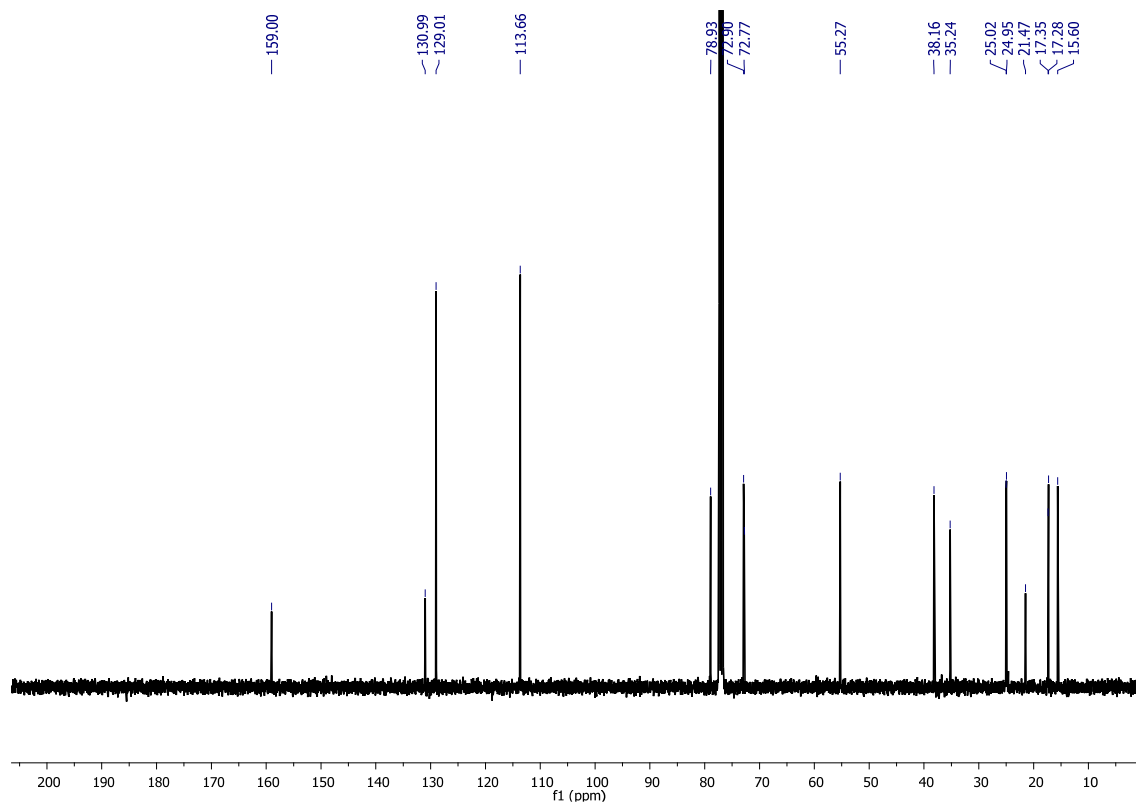
^{13}C -DEPT NMR of **17** (100 MHz, CDCl_3)



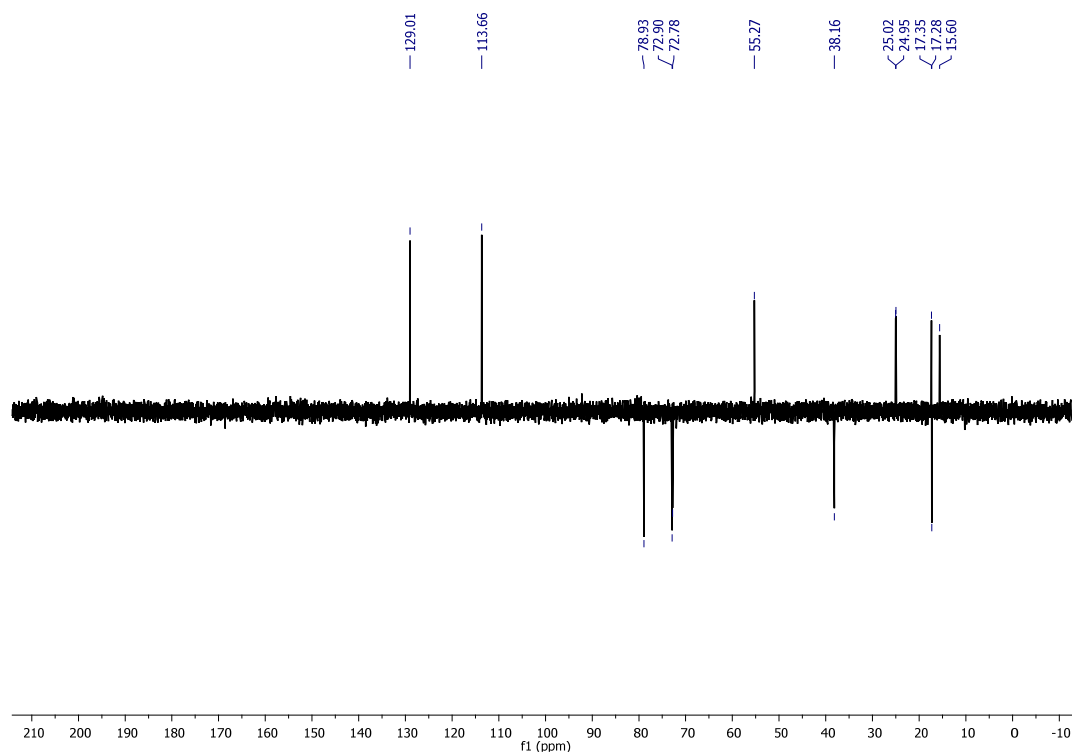
^1H NMR of **18** (400 MHz, CDCl_3)



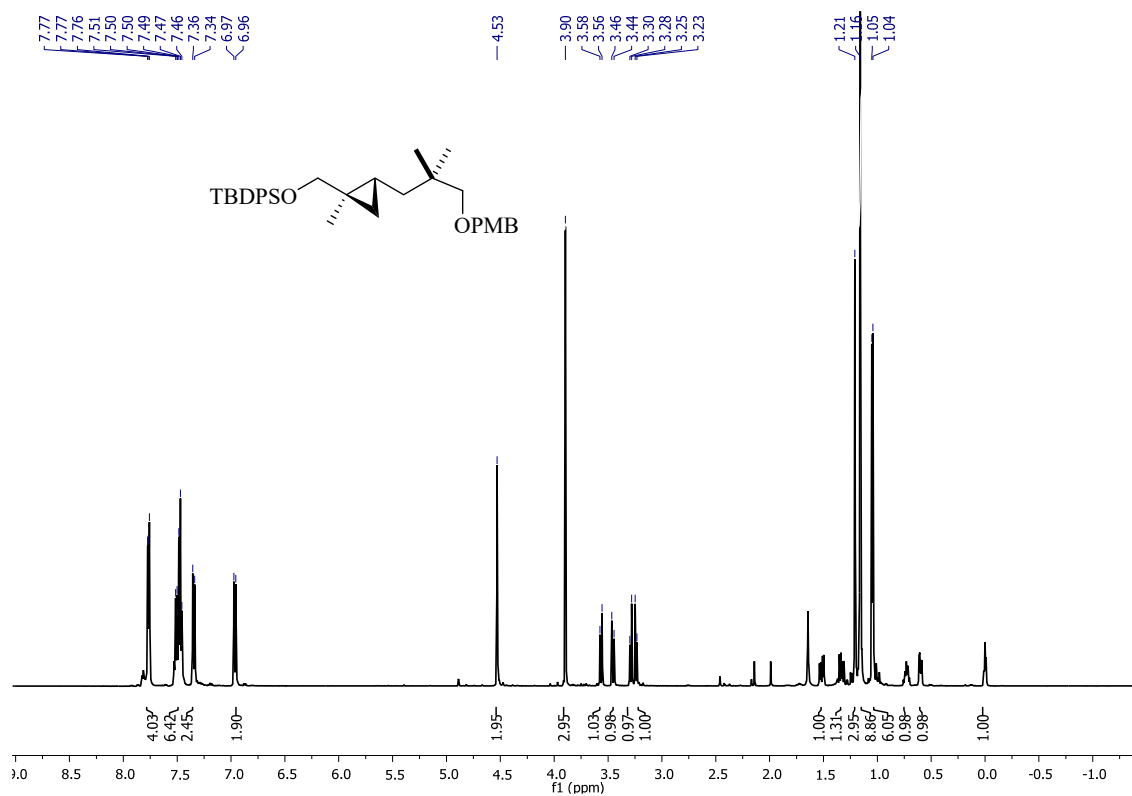
^{13}C NMR of **18** (100 MHz, CDCl_3)



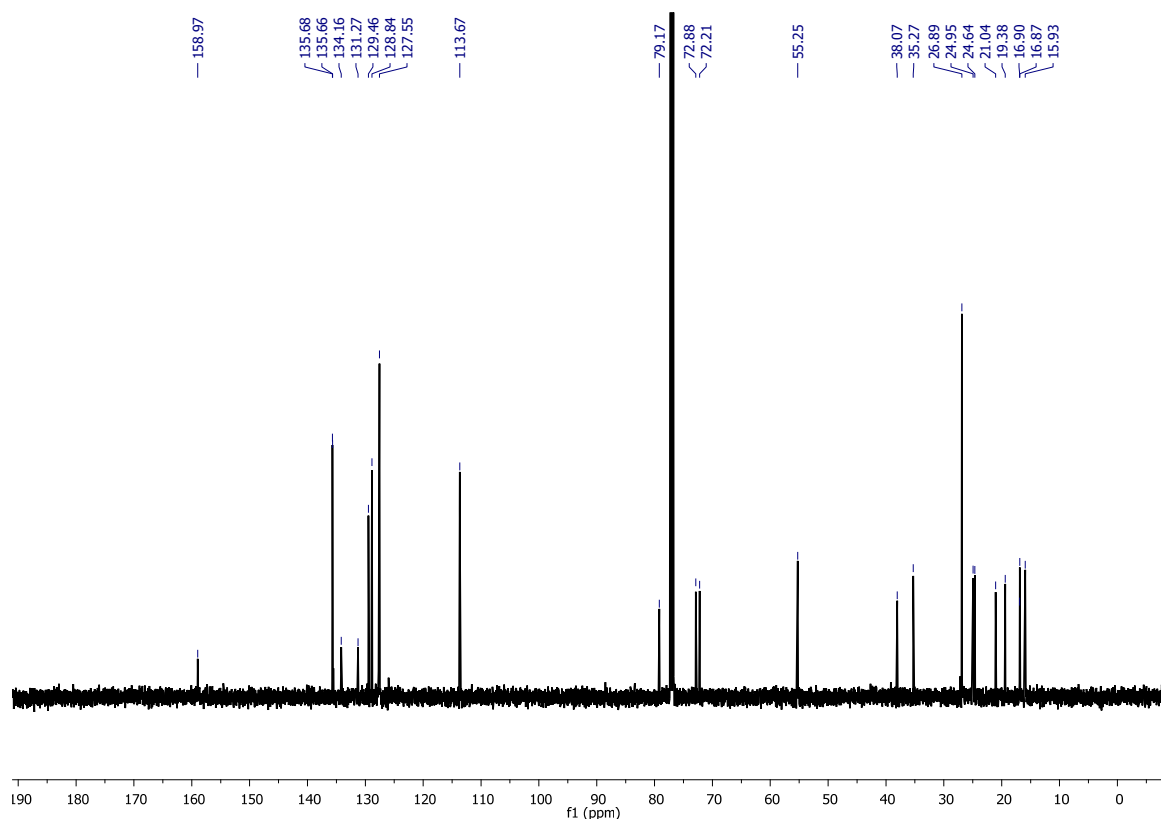
^{13}C -DEPT NMR of **18** (100 MHz, CDCl_3)



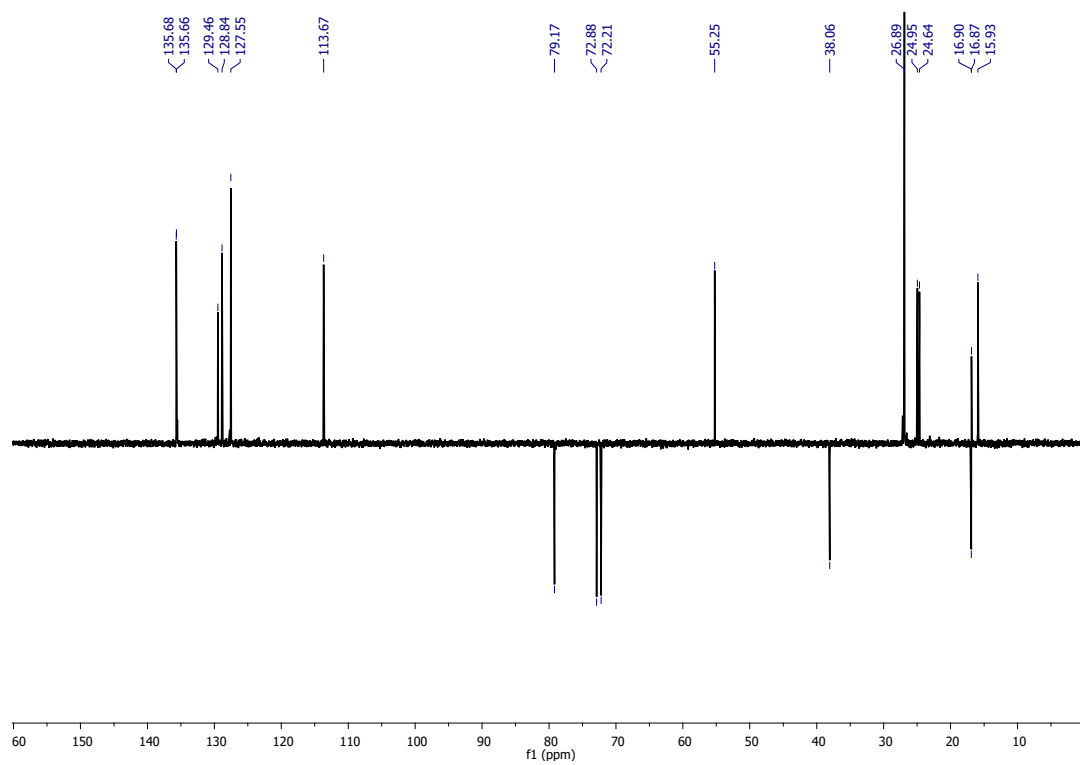
^1H NMR of **19** (400 MHz, CDCl_3)



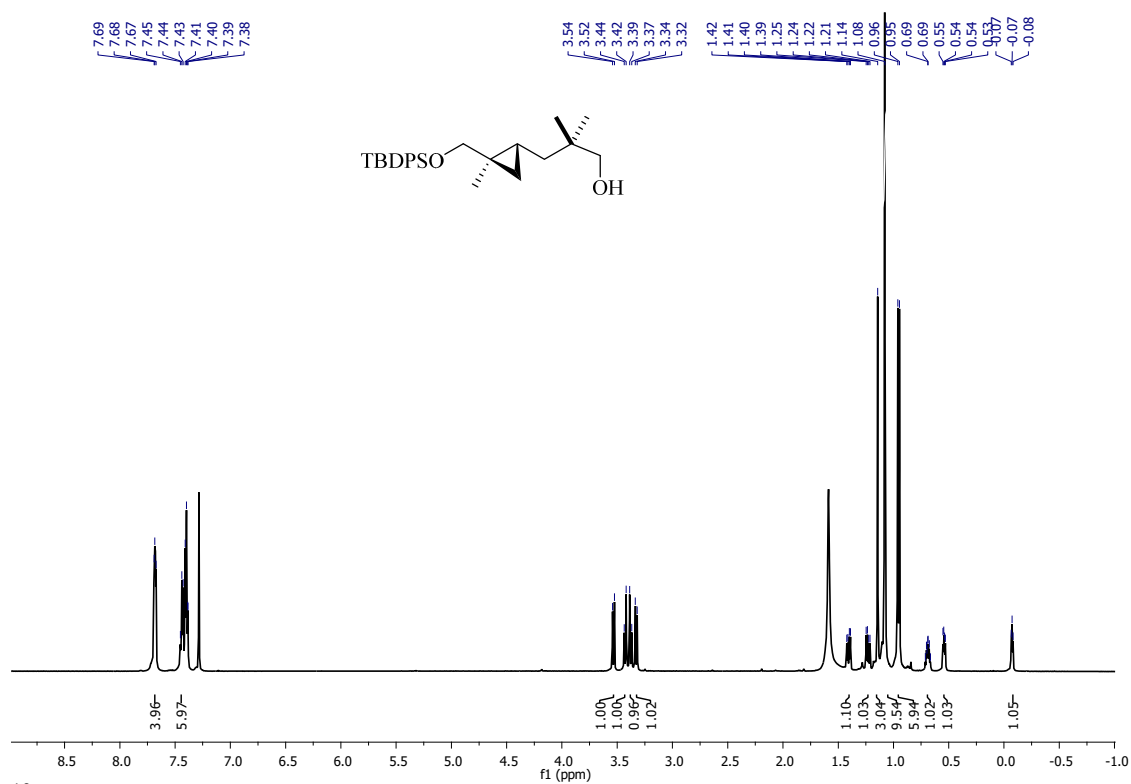
^{13}C NMR of **19** (100 MHz, CDCl_3)



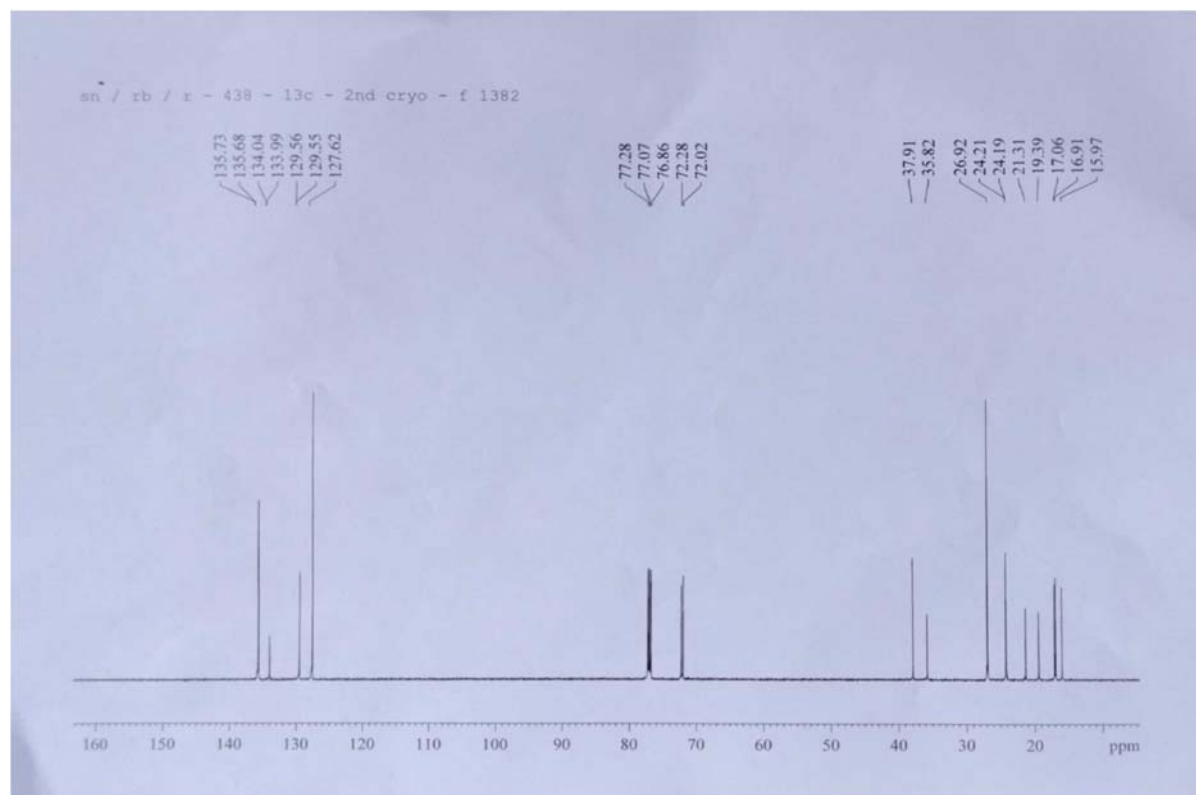
^{13}C -DEPT NMR of **19** (100 MHz, CDCl_3)



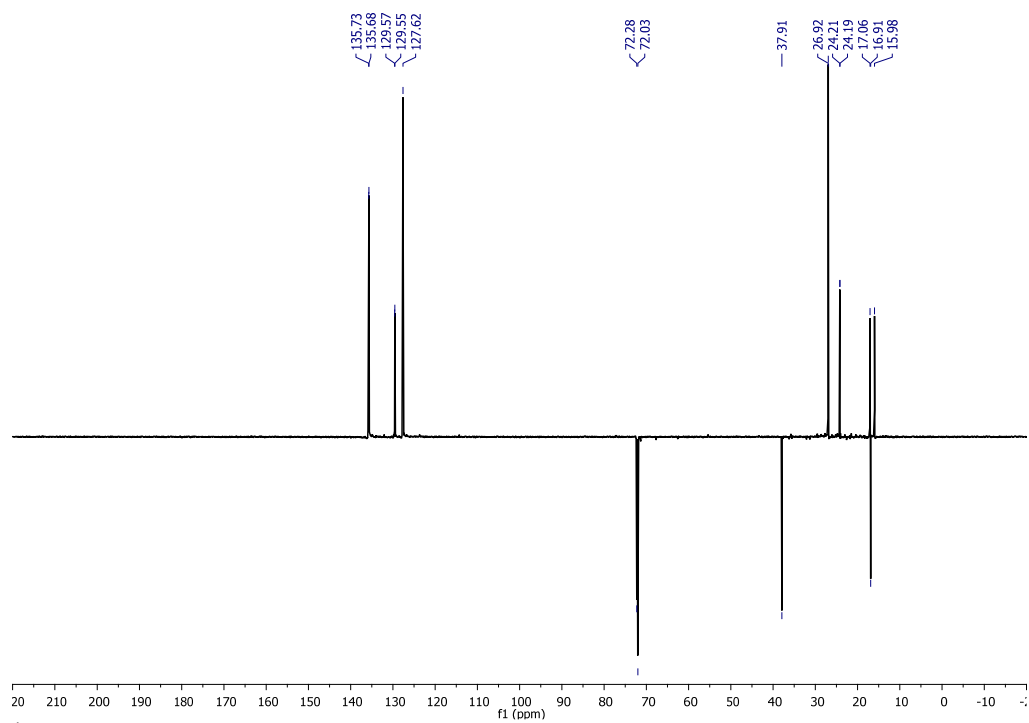
^1H NMR of **20** (600 MHz, CDCl_3)



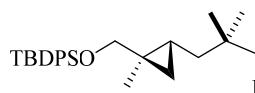
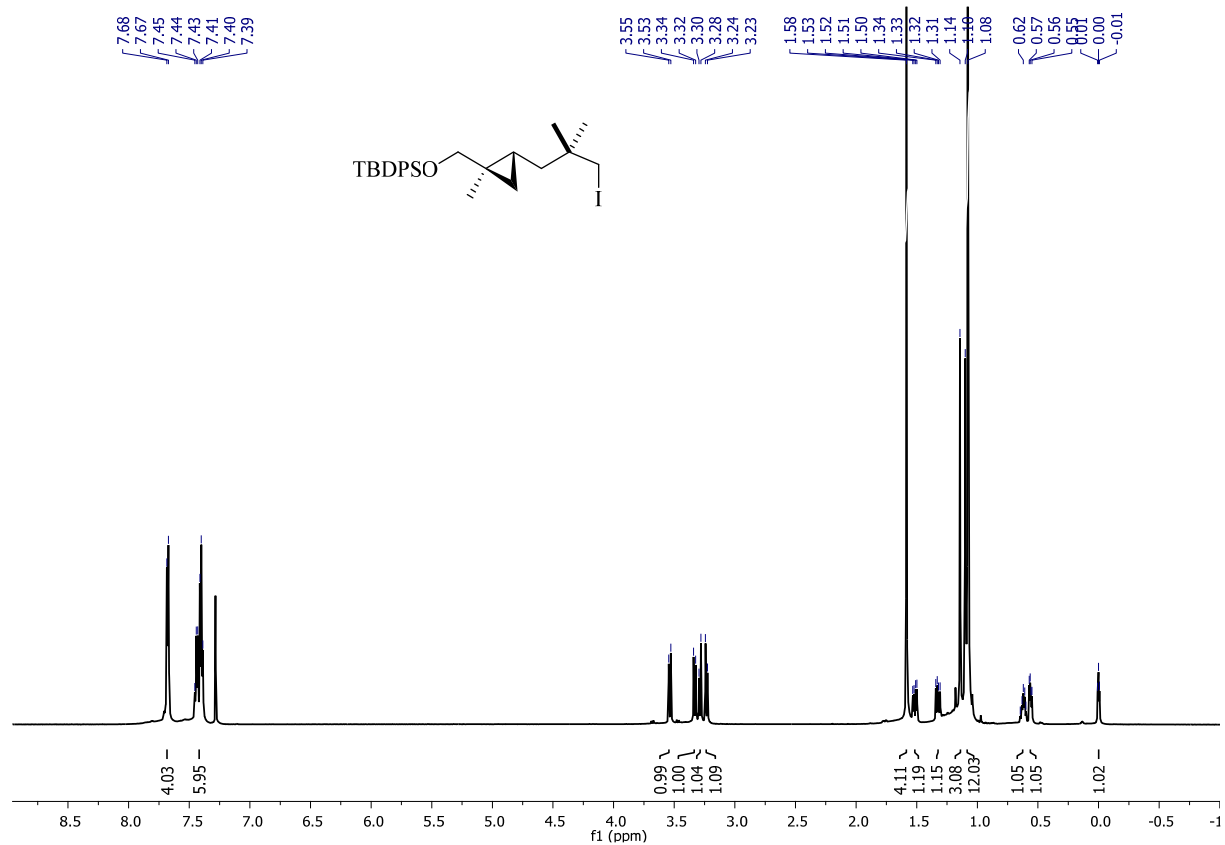
^{13}C NMR of **20** (150 MHz, CDCl_3)



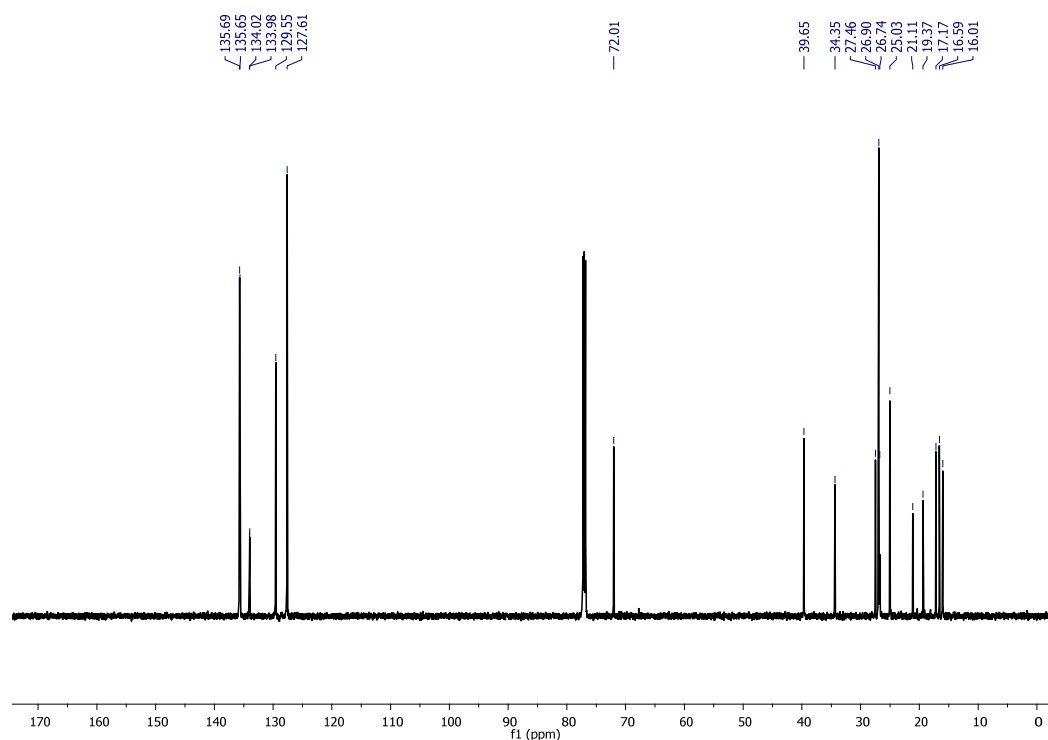
^{13}C -DEPT NMR of **20** (150 MHz, CDCl_3)



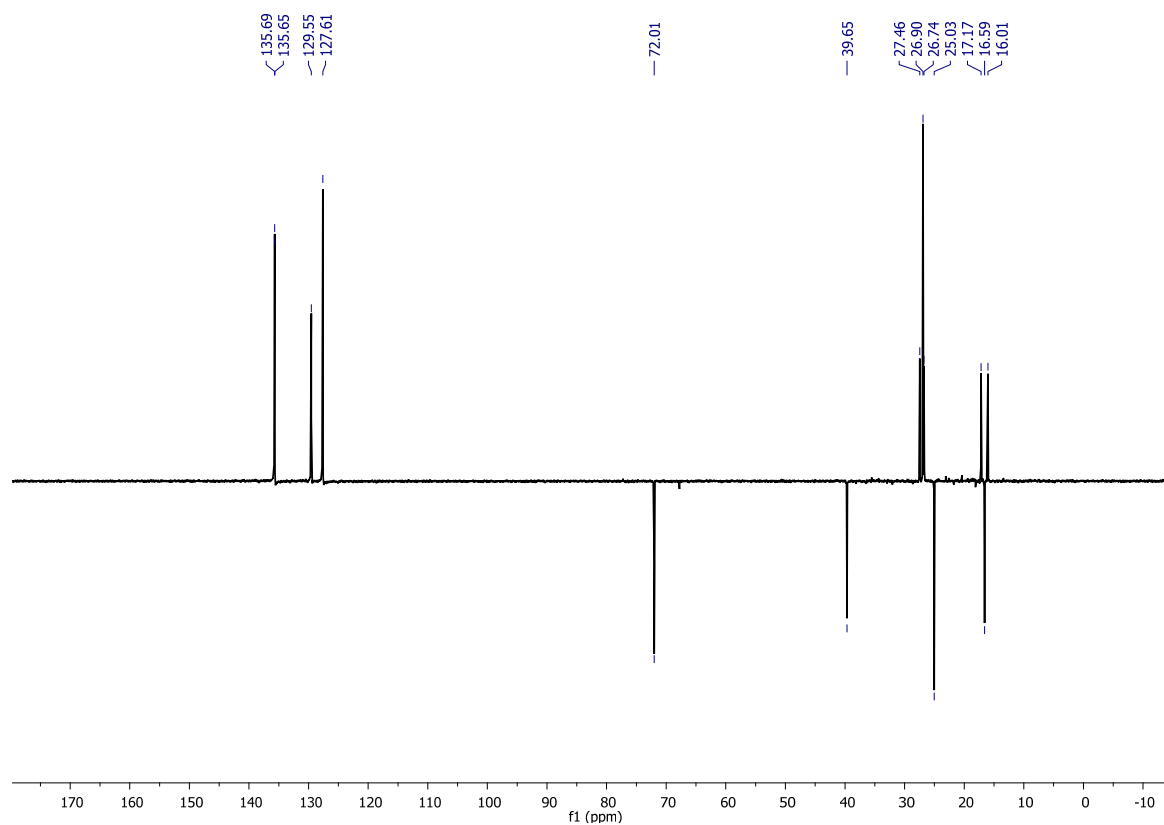
^1H NMR of **21** (600 MHz, CDCl_3)



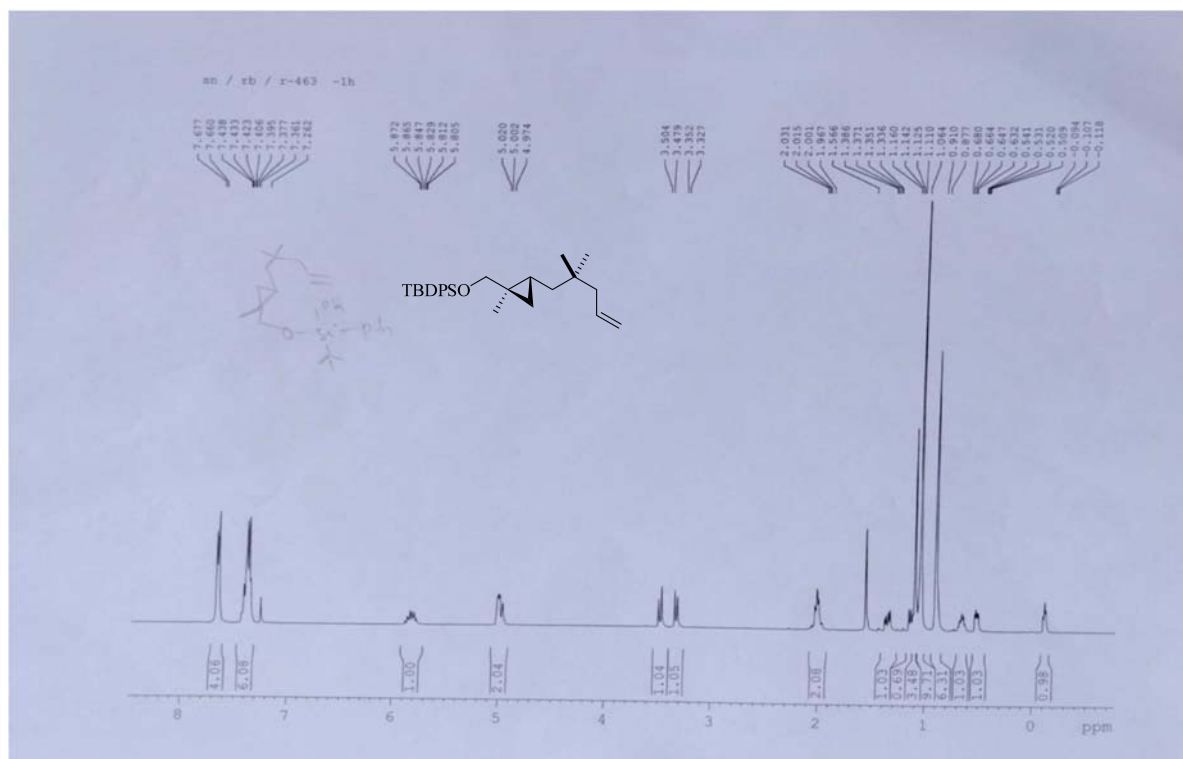
^{13}C NMR of **21** (150 MHz, CDCl_3)



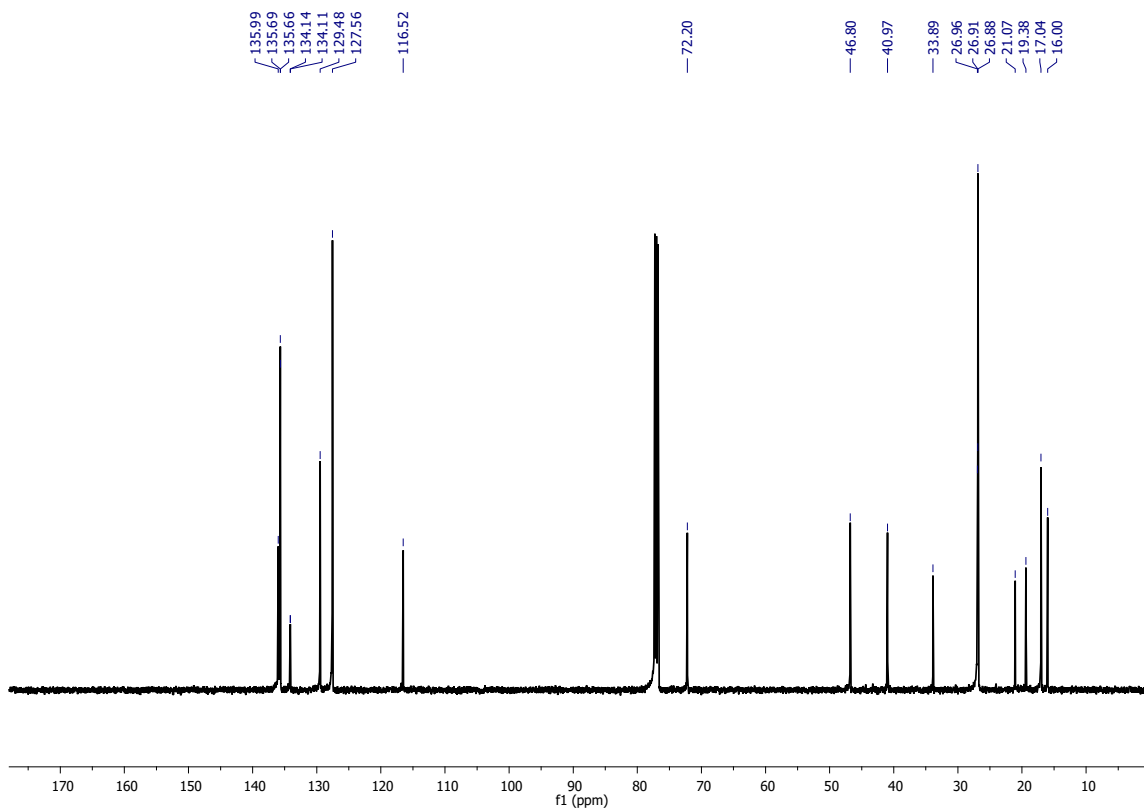
^{13}C -DEPT NMR of **21** (100 MHz, CDCl_3)



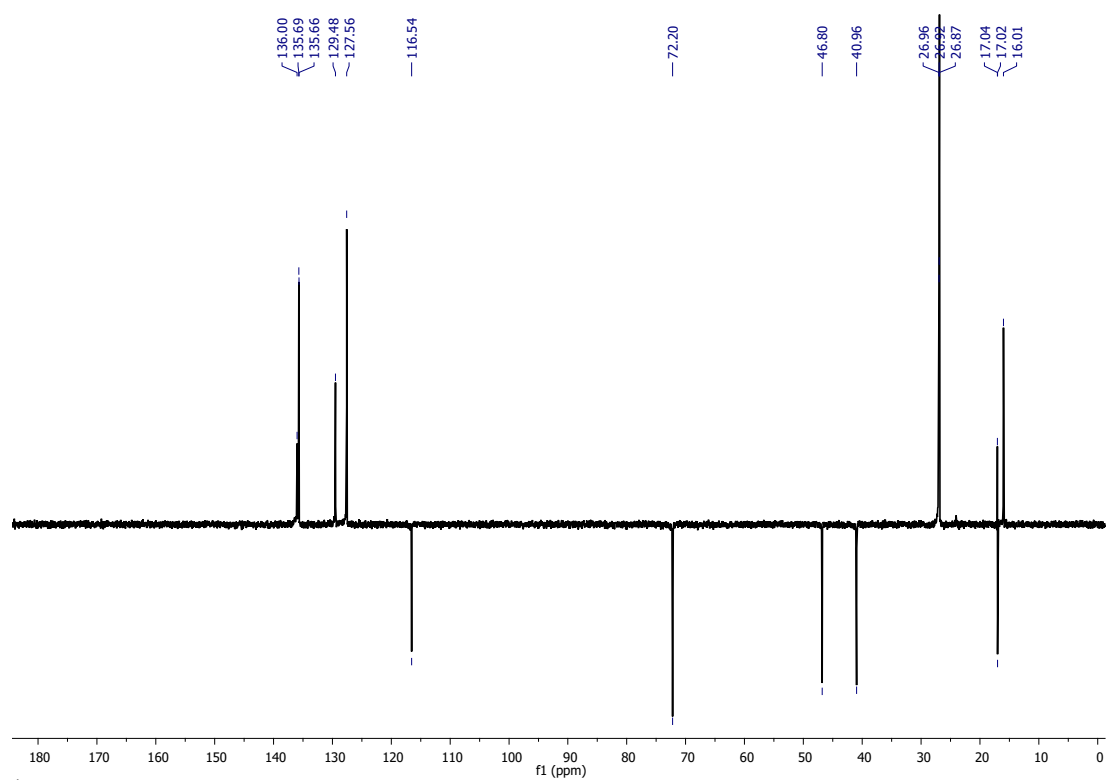
^1H NMR of **22** (400 MHz, CDCl_3)



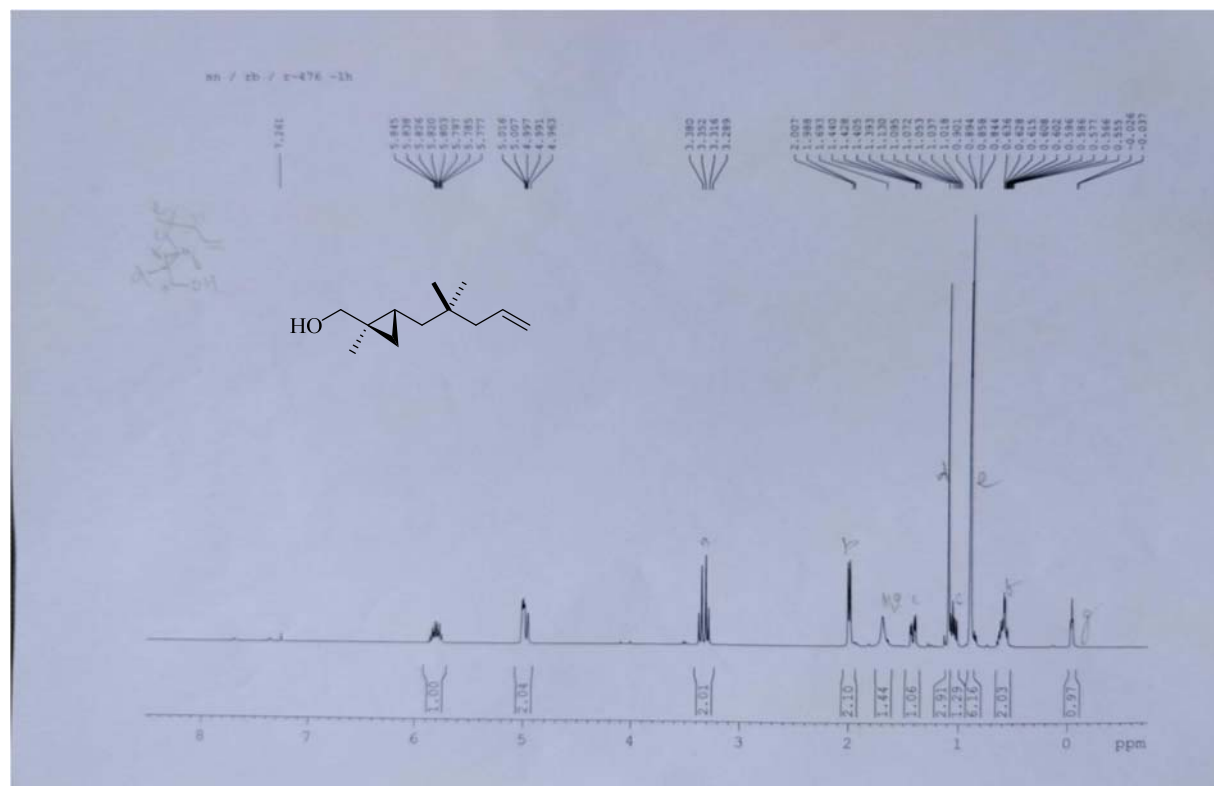
^{13}C NMR of **22** (100 MHz, CDCl_3)



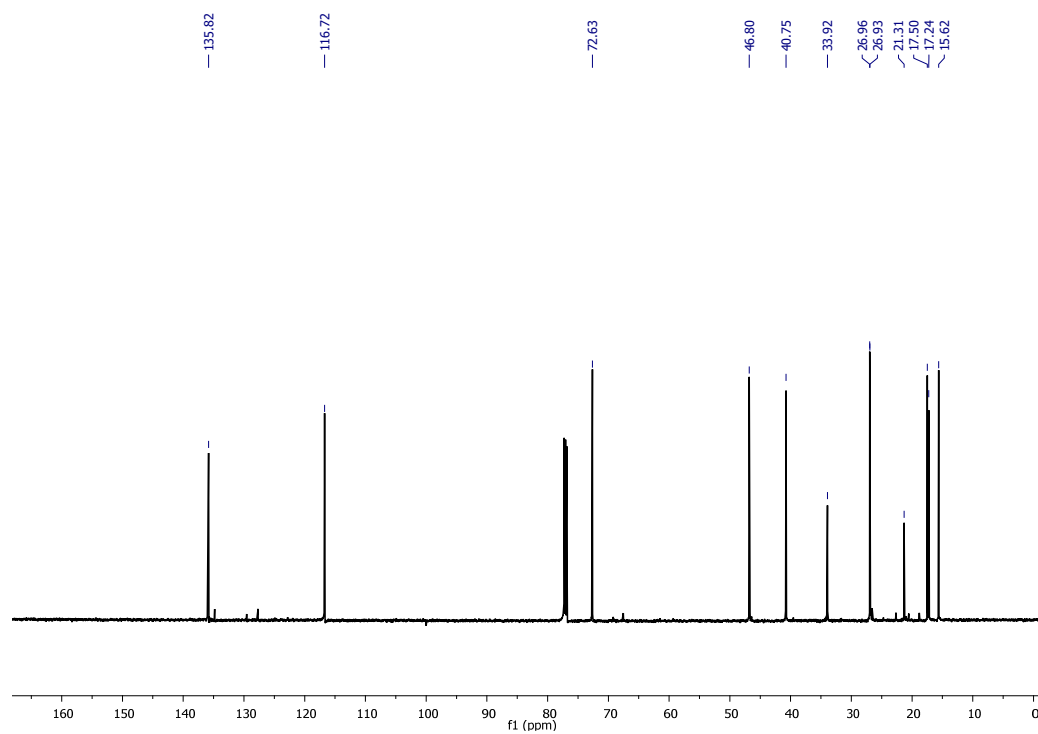
^{13}C DEPT NMR of **22** (100 MHz, CDCl_3)



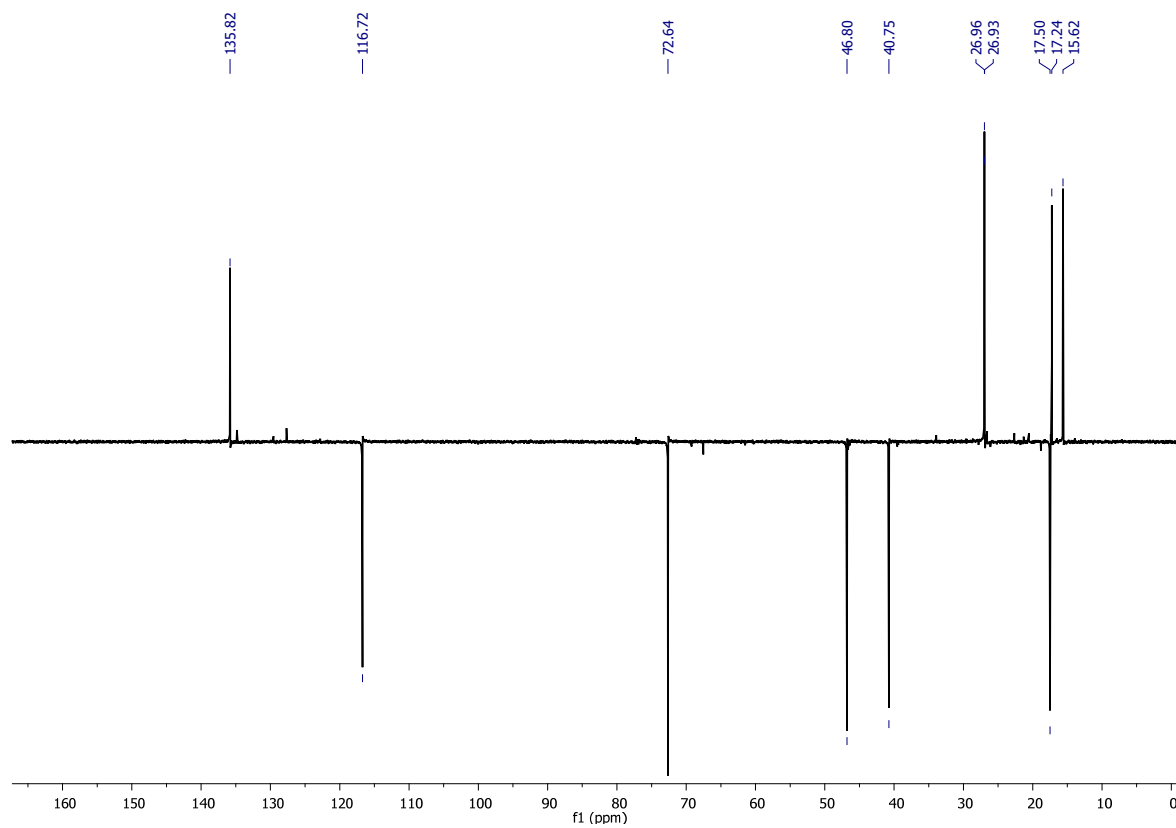
^1H NMR of **23** (100 MHz, CDCl_3)



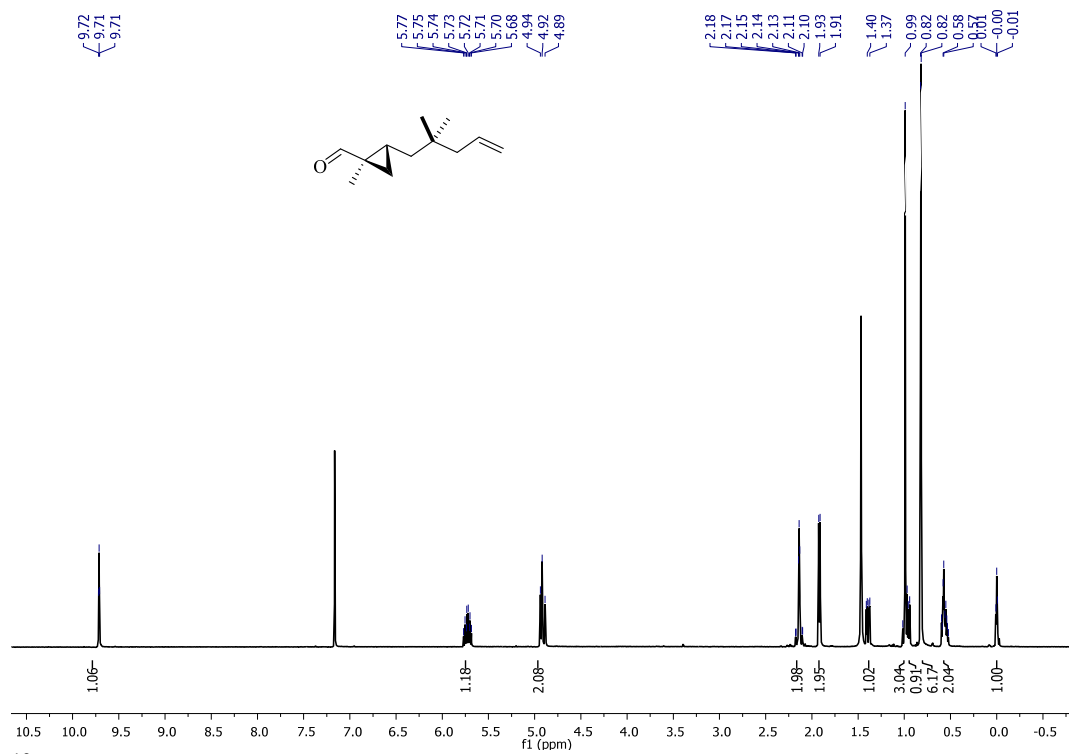
^{13}C NMR of **23** (100 MHz, CDCl_3)



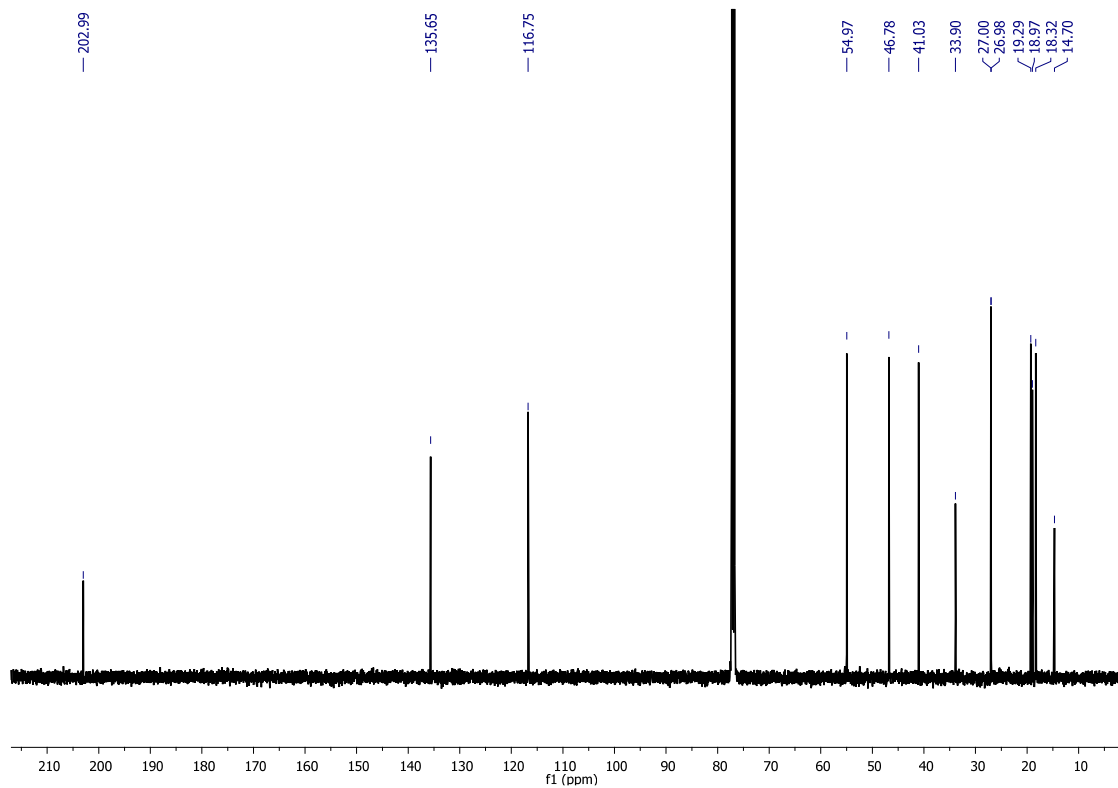
^{13}C DEPT NMR of **23** (100 MHz, CDCl_3)



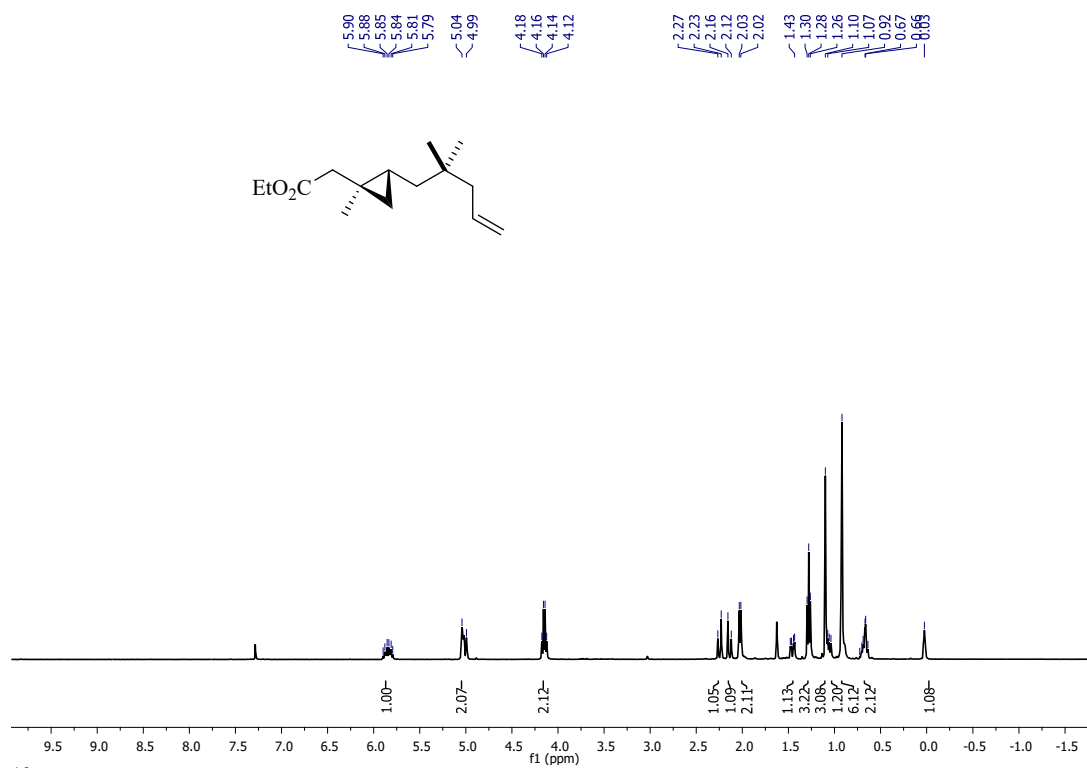
^1H NMR of **14** (500 MHz, CDCl_3)



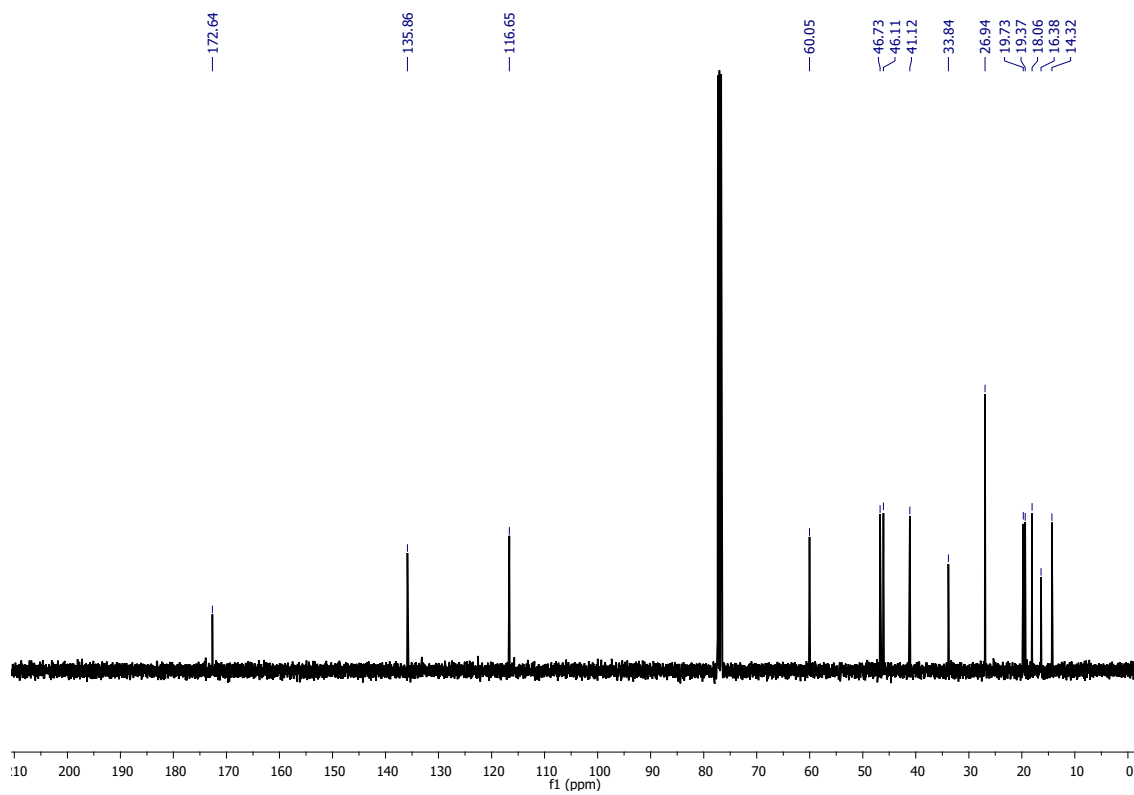
^{13}C NMR of **14** (125 MHz, CDCl_3)



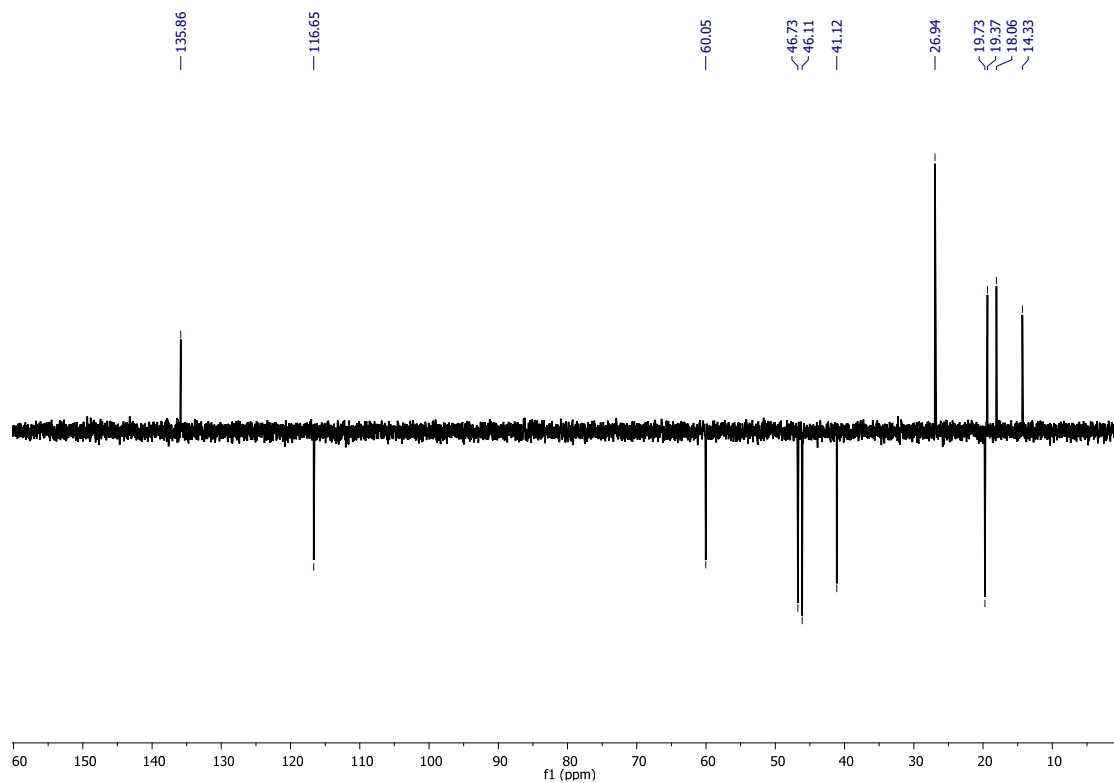
^1H NMR of **12** (100 MHz, CDCl_3)



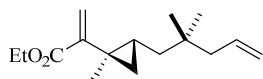
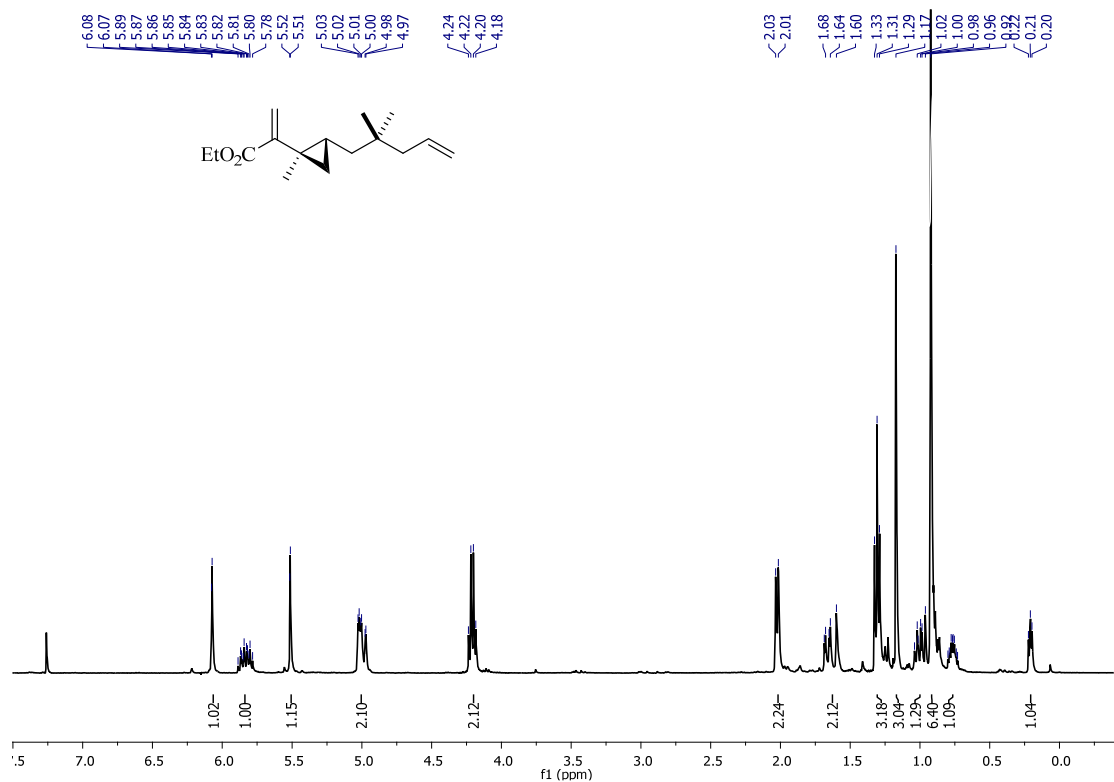
^{13}C NMR of **12** (100 MHz, CDCl_3)



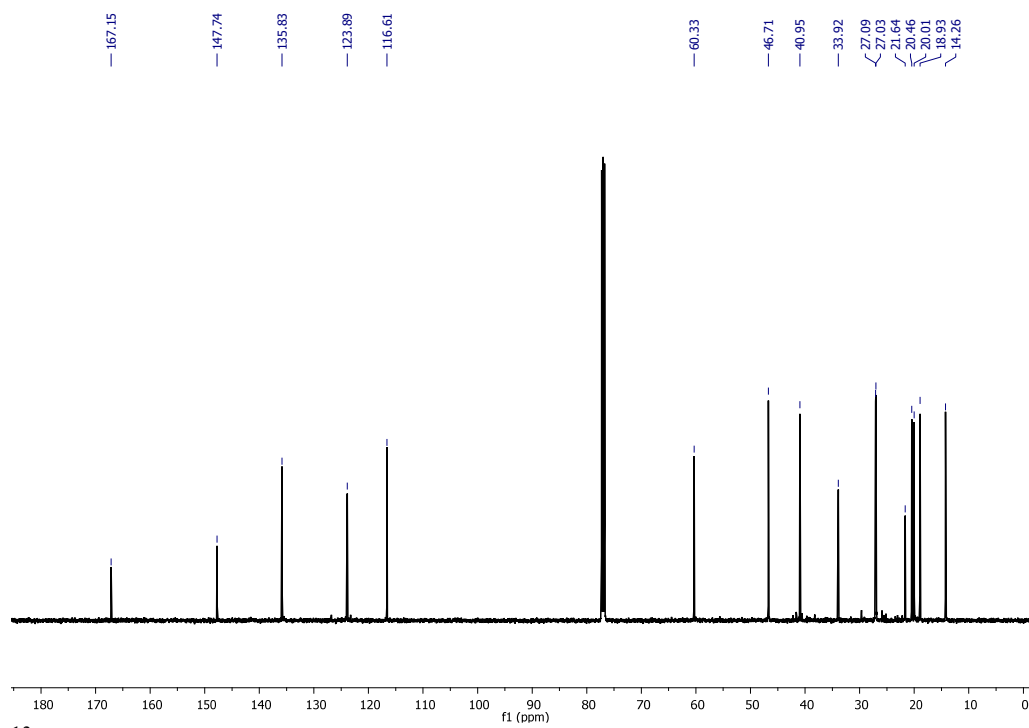
^{13}C DEPT NMR of **12** (100 MHz, CDCl_3)



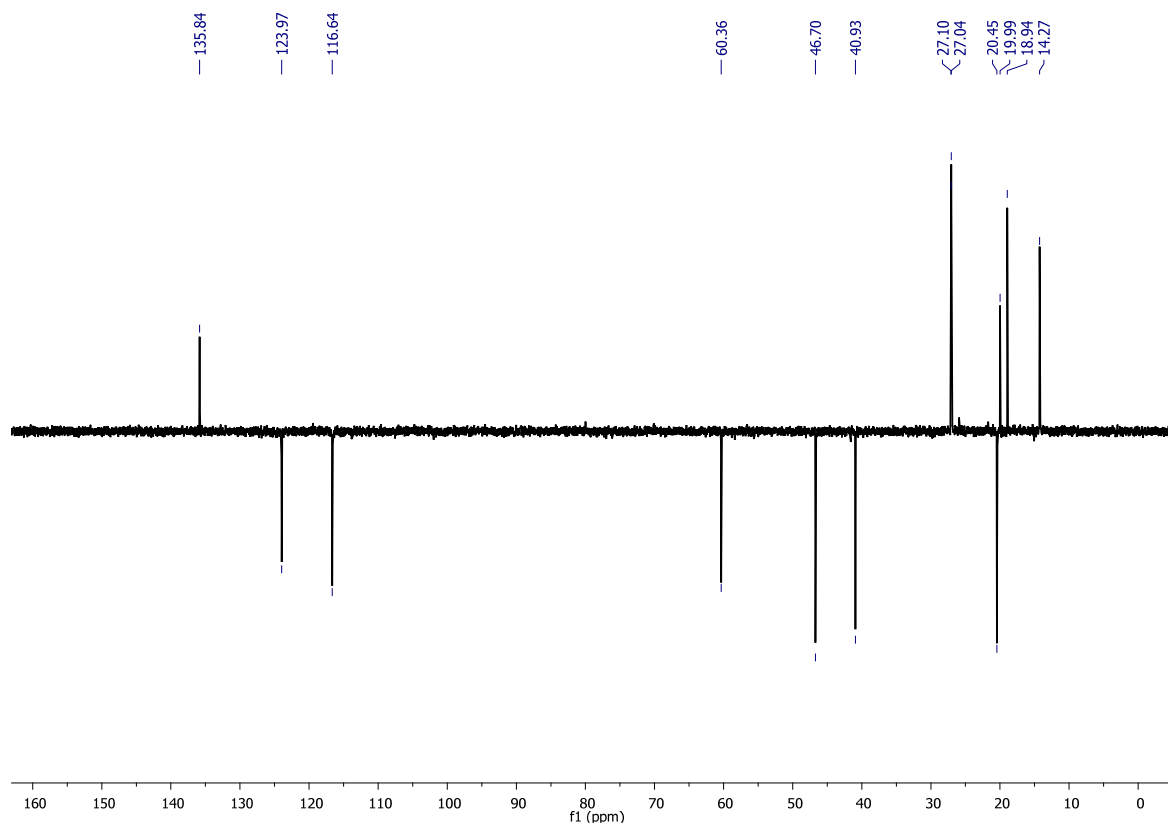
^1H NMR of **11** (100 MHz, CDCl_3)



^{13}C NMR of **11** (100 MHz, CDCl_3)



^{13}C DEPT NMR of **11** (100 MHz, CDCl_3)



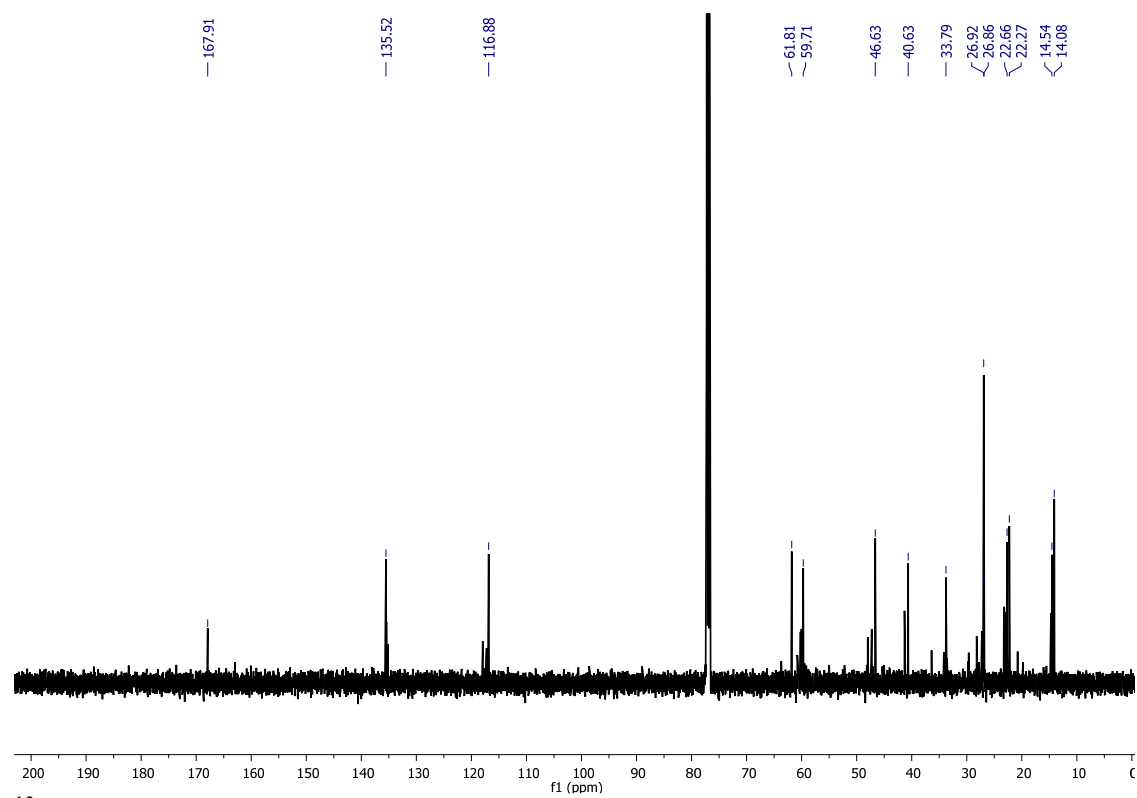
[illegible]

Chemical structure: CCOC(=O)[C@H]1[C@H](Br)[C@H](C)C[C@H]1C=C

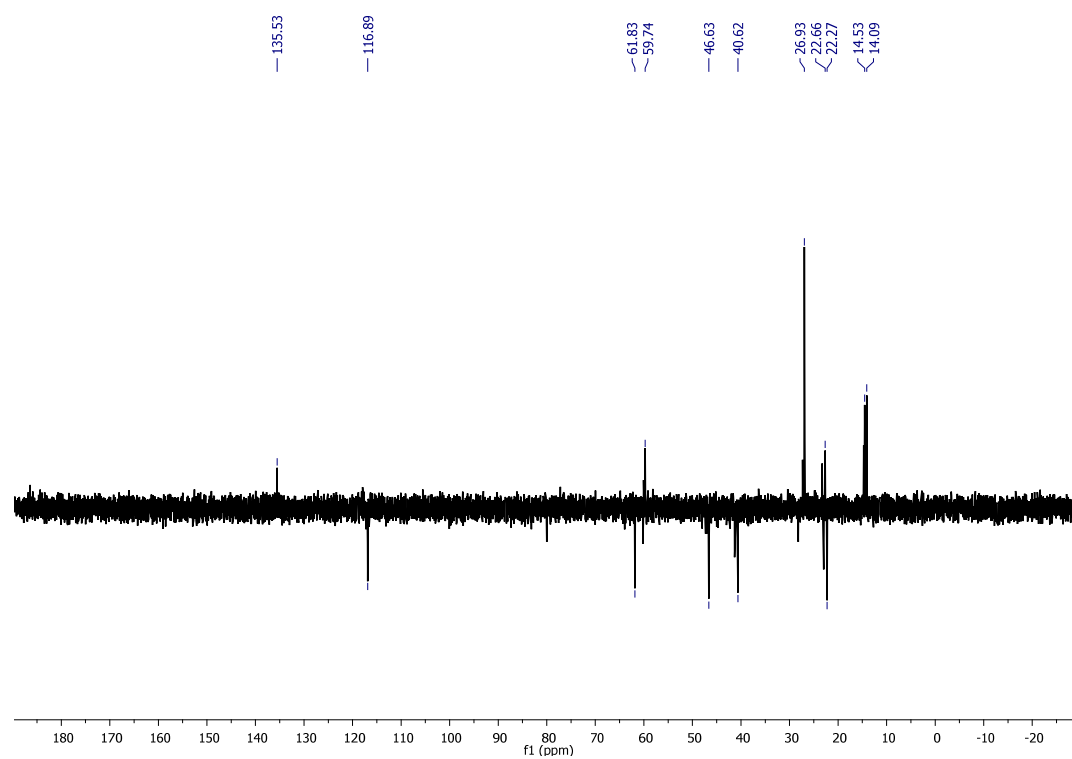
¹H NMR spectrum (CDCl₃) showing peaks from 0.6 to 5.7 ppm. The x-axis is labeled f1 (ppm) and the y-axis is labeled intensity. Integration values are provided below the baseline.

Chemical Shift (ppm)	Integration
7.1 (s, 1H)	-
5.6 (d, 1H)	1.00
4.8 (d, 2H)	2.04
4.0 (d, 2H)	2.02
3.6 (d, 2H)	1.00
1.8 (d, 2H)	2.31
1.0 - 1.4 (m, 10H)	3.19, 0.98, 3.20, 1.12, 6.19, 1.15, 1.23, 1.16

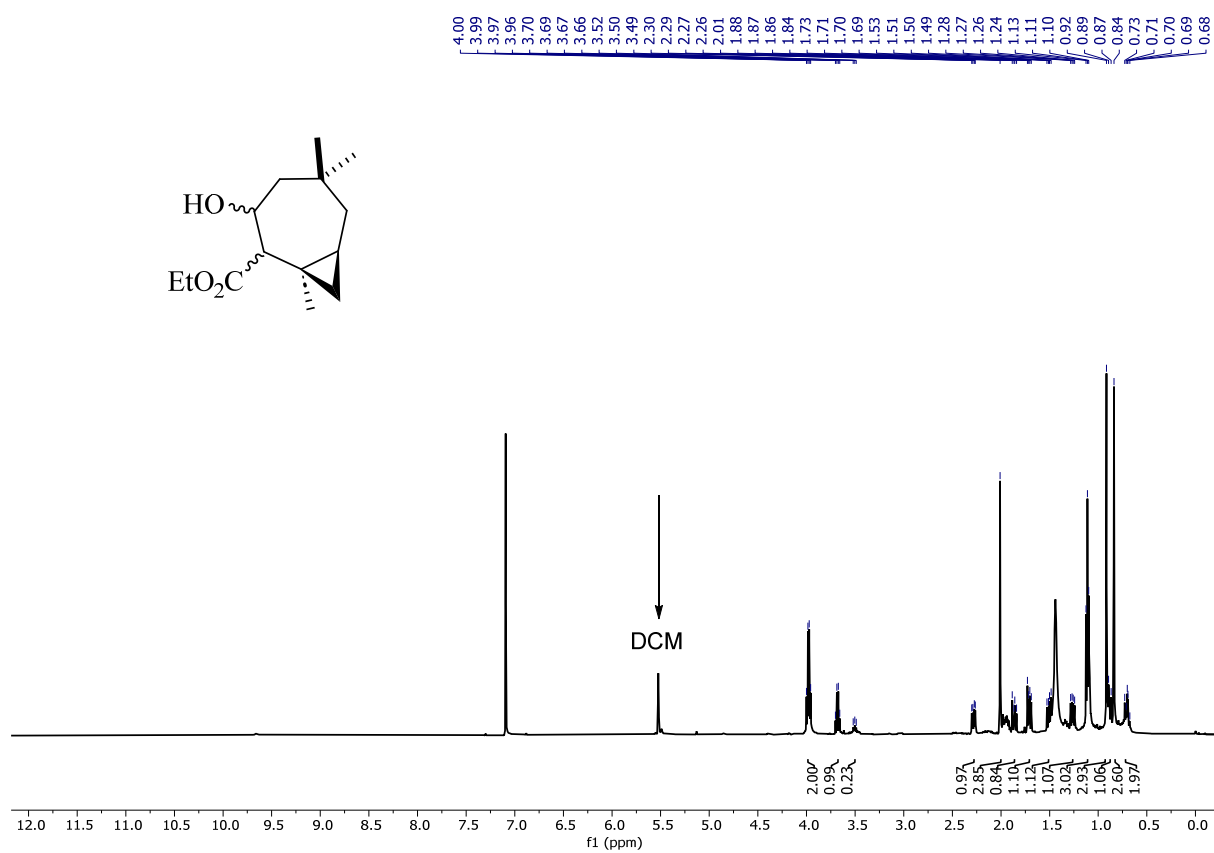
^{13}C NMR of **26** (100 MHz, CDCl_3)



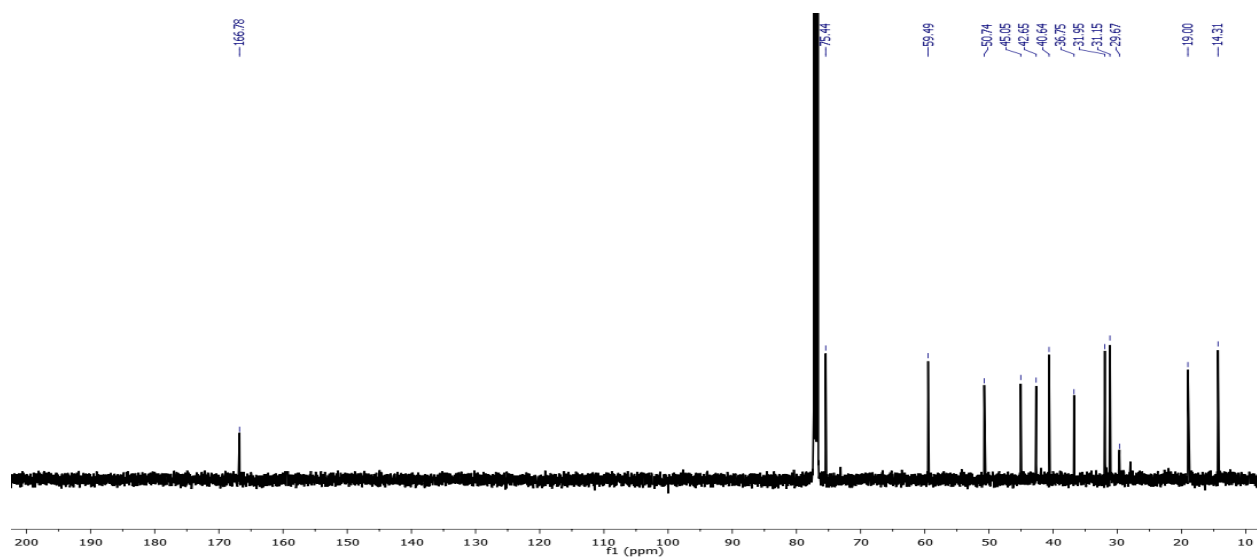
^{13}C DEPT NMR of **26** (100 MHz, CDCl_3)



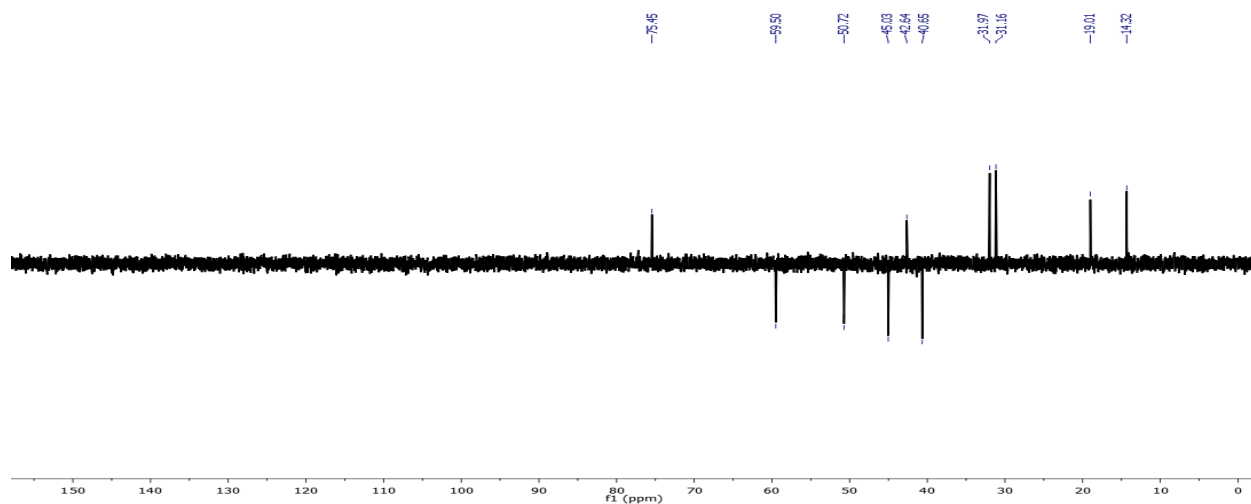
^1H NMR of **28a** and **28b** (500 MHz, CDCl_3)



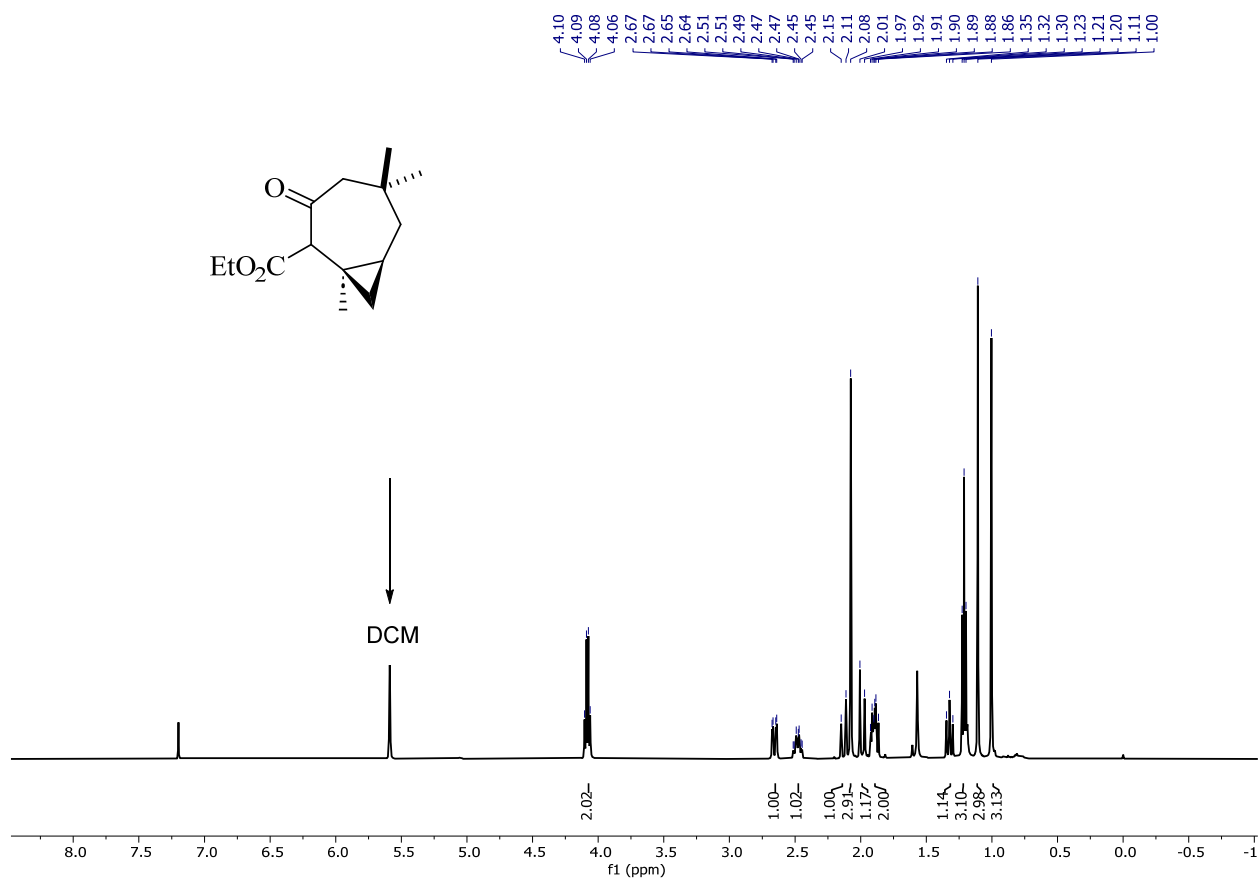
^{13}C NMR of **28a** and **28b** (125 MHz, CDCl_3)



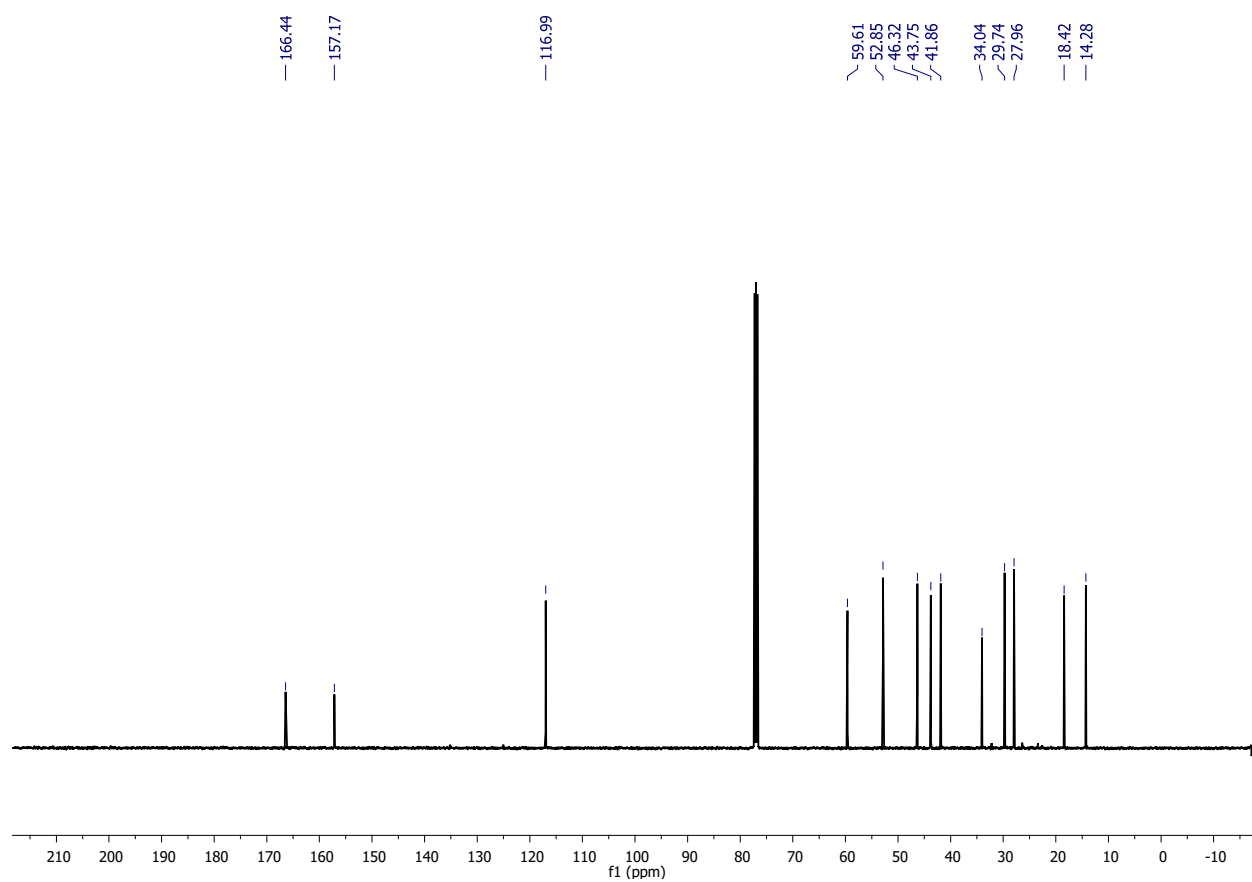
^{13}C DEPT NMR of **28a** and **28b** (100 MHz, CDCl_3)



^1H NMR of **9** (100 MHz, CDCl_3)



^{13}C NMR of **9** (100 MHz, CDCl_3)



HPLC chromatogram of racemic benzoate of **18** (column: OJ-H, hexane:2-propanol = 19:1, flow rate: 1ml/min)

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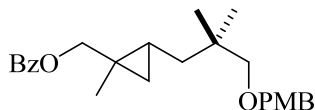
Racemic cyclopropanation benzoate C:\lab-solutions\data\copillo\racemic.lcd

Sample name: Racemic benzoate cyclopropane

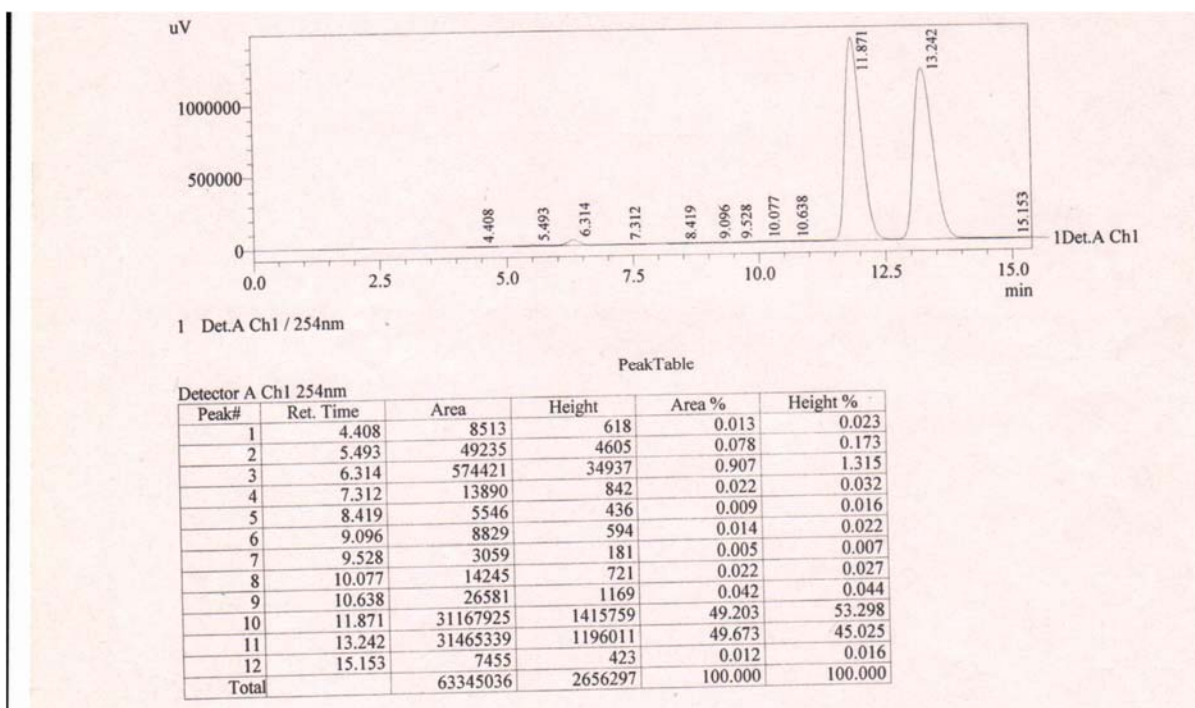
Injection volume: 5µl

Data acquired: 01/1/2024 6:15 PM

Data processed: 01/1/2024 7:00 PM



Racemic cyclopropanation benzoate C:\lab-solutions\data\copillo\racemic.lcd



HPLC chromatogram of chiral benzoate of **18** (column: OJ-H, hexane:2-propanol = 19:1, flow rate: 1ml/min)

Department of Chemistry, IIT-Kharagpur

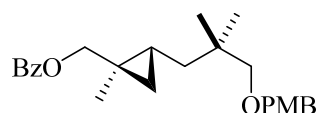
Chiral cyclopropanation benzoate C:\lab-solutions\data\copillo\chiral.lcd

Sample name: Chiral benzoate cyclopropane

Injection volume: 5µl

Data acquired: 01/1/2024 6:40 PM

Data processed: 01/1/2024 7:30 PM



Chiral cyclopropanation benzoate C:\lab-solutions\data\copillo\chiral.lcd

