

Total Synthesis and Biological Evaluation of the Natural Product (–)-Cyclonerodiol, a New Inhibitor of IL-4 Signaling

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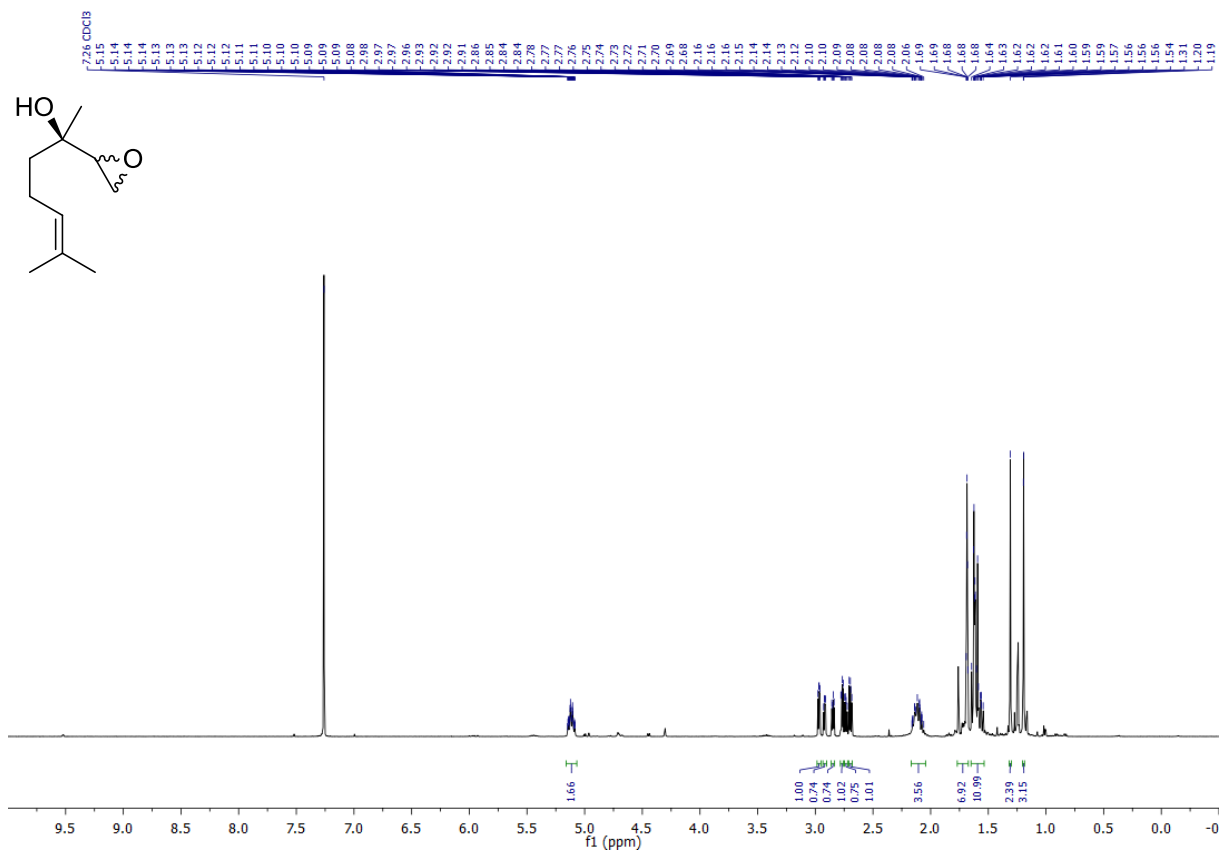
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[†]: authors contributed equally to this work.

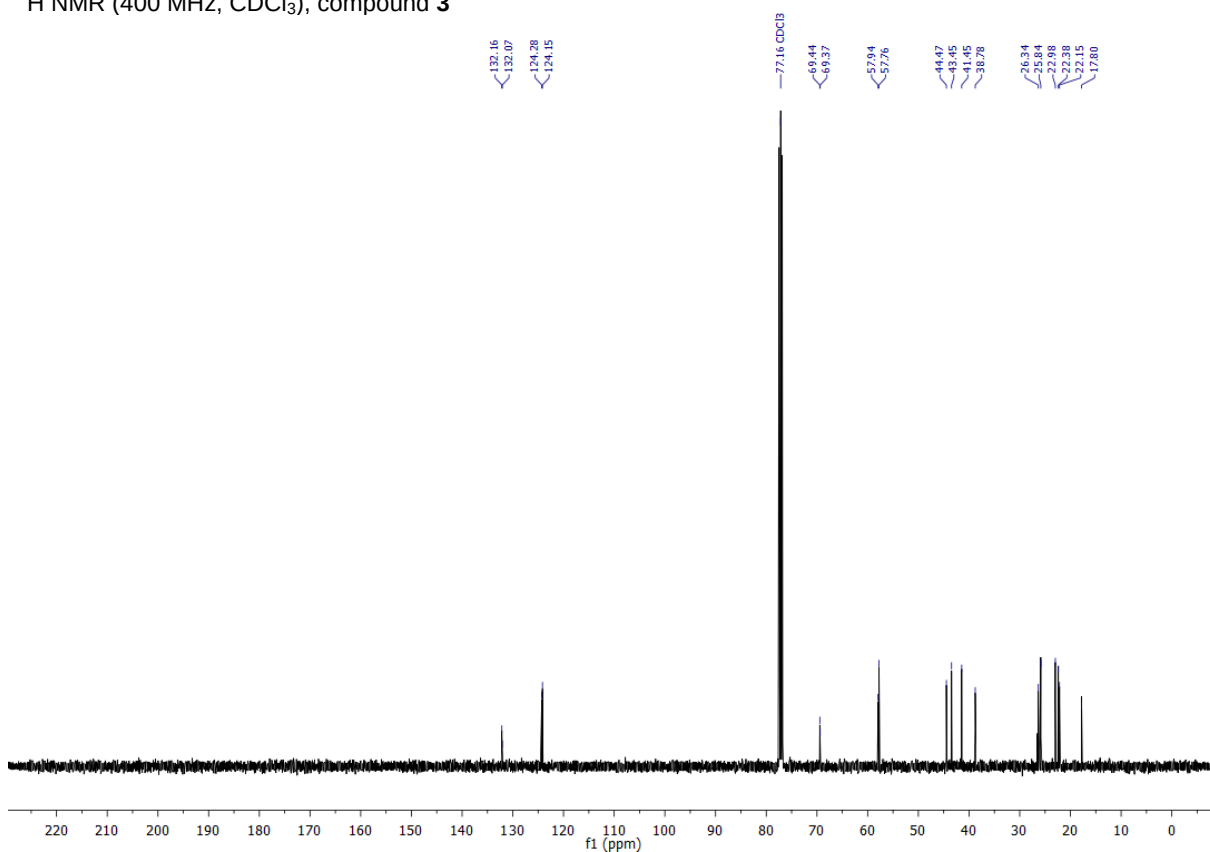
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I. ¹H and ¹³CNMR Spectra

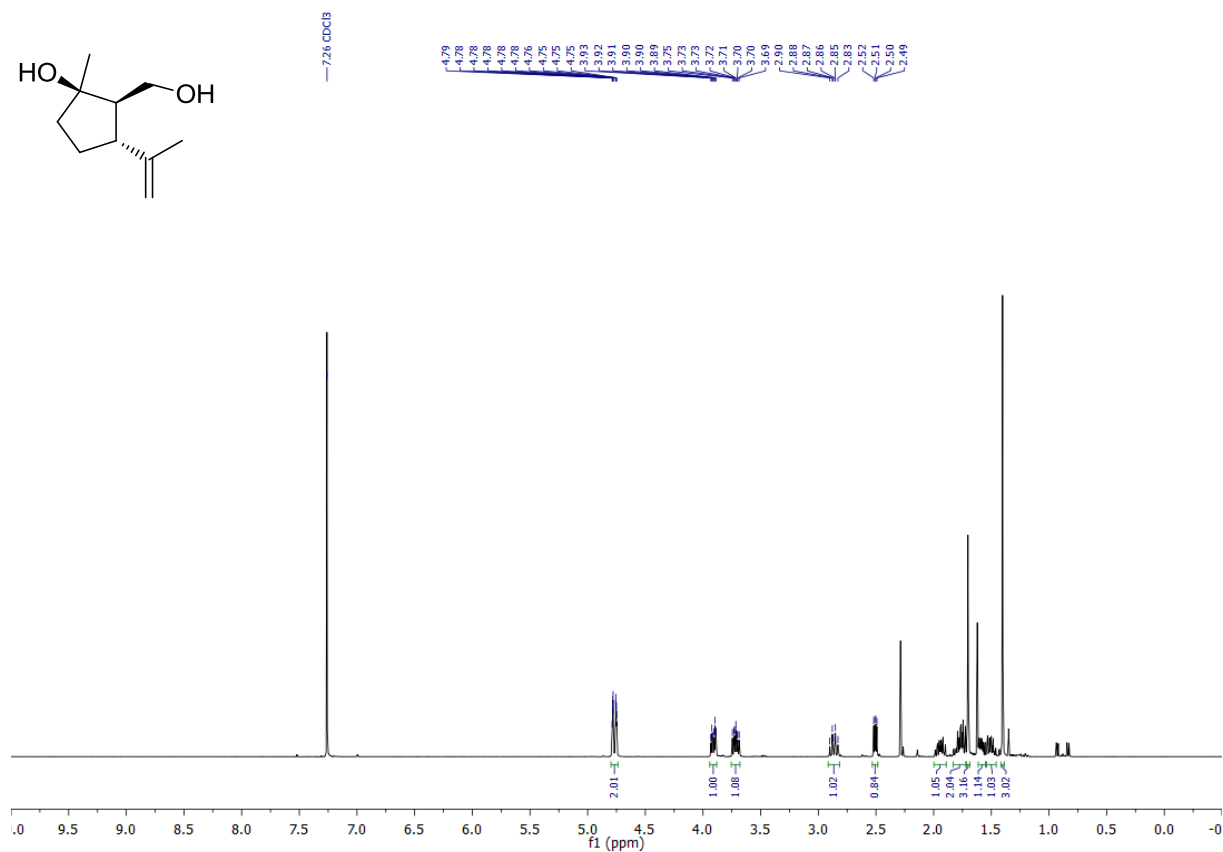
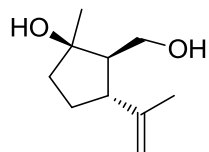
I) ^1H and ^{13}C NMR Spectra of compounds



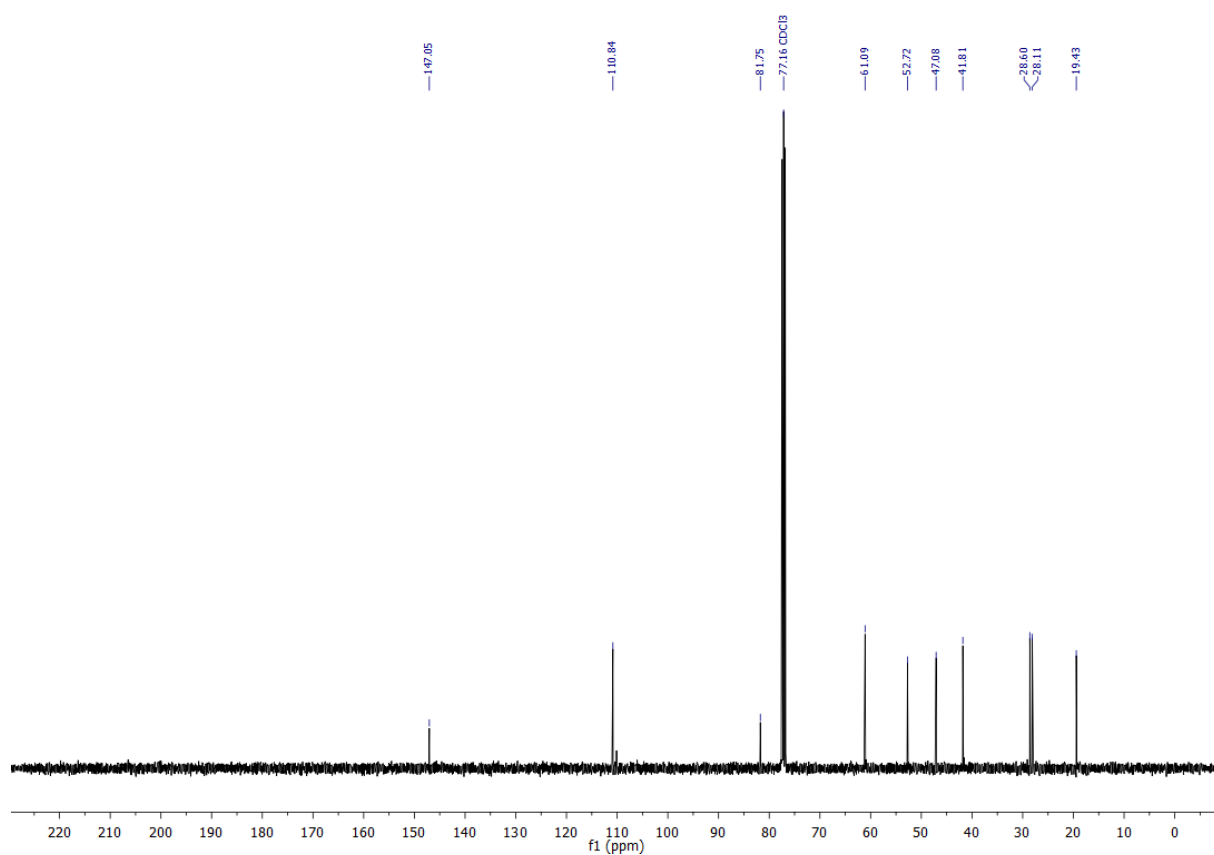
^1H NMR (400 MHz, CDCl_3), compound 3



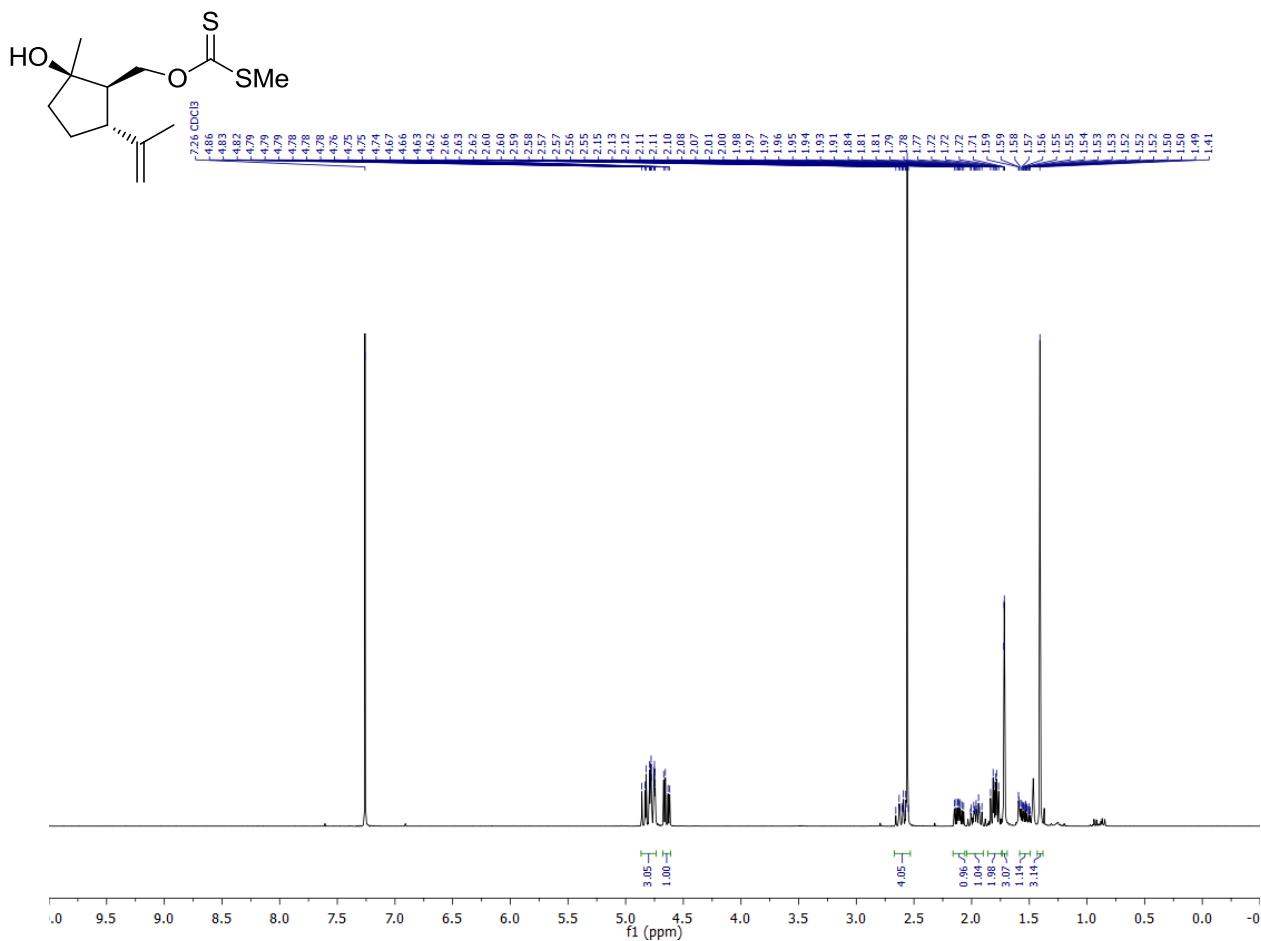
^{13}C NMR (100.6 MHz, CDCl_3), compound 3



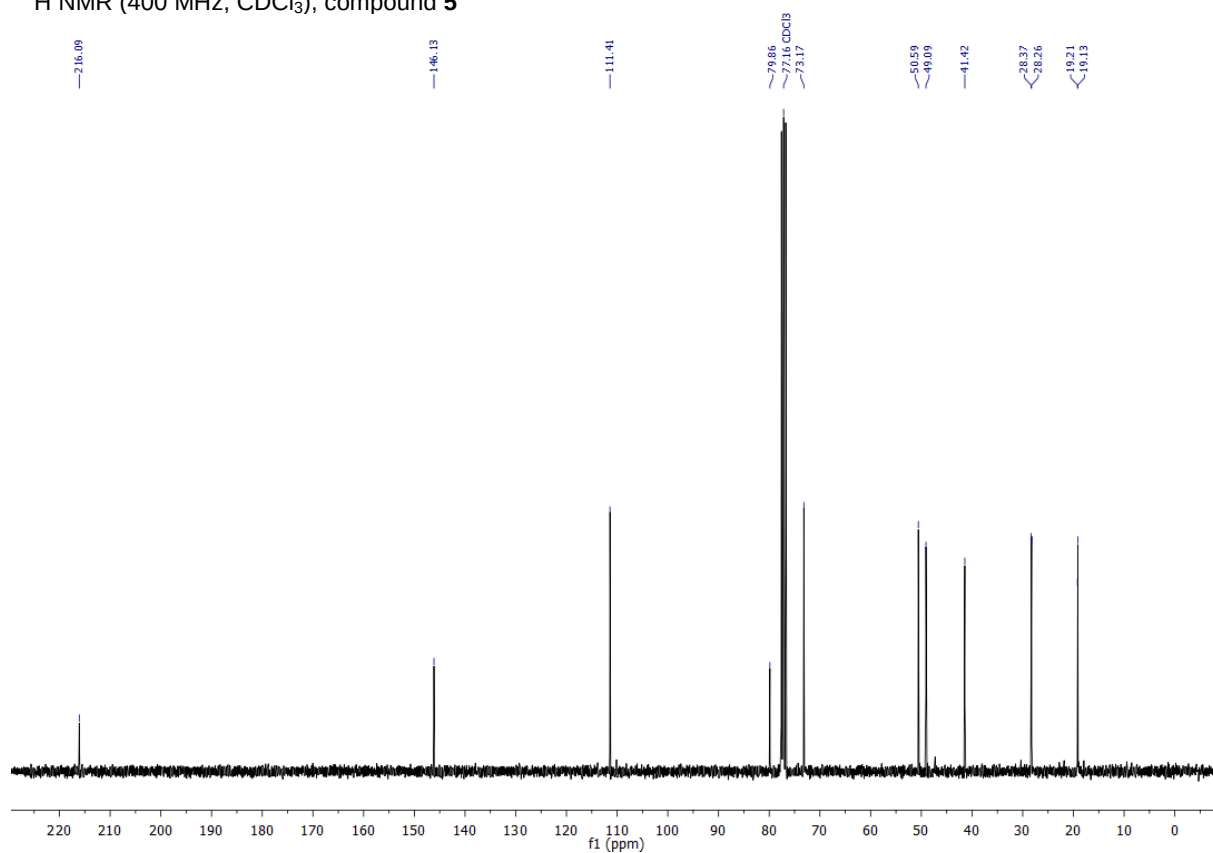
¹H NMR (400 MHz, CDCl₃), compound 4



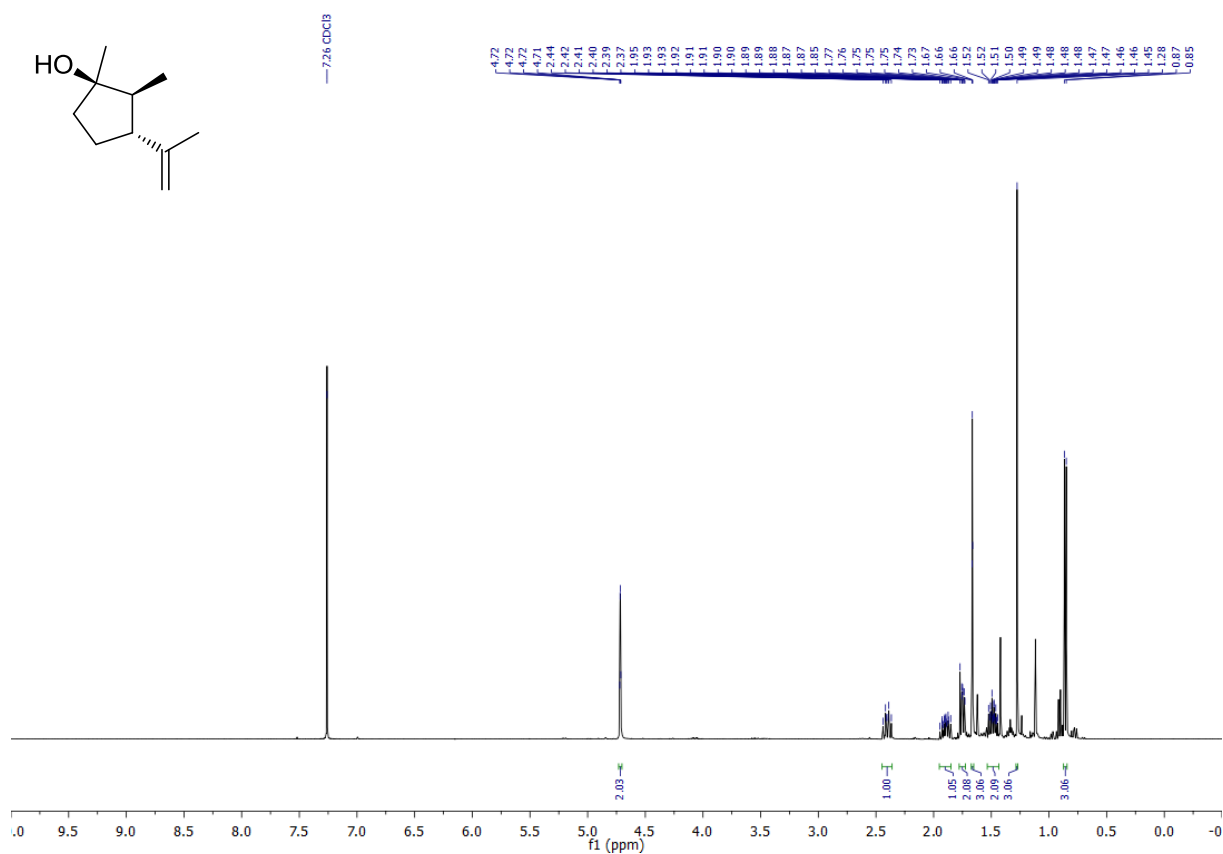
¹³C NMR (100.6 MHz, CDCl₃), compound 4



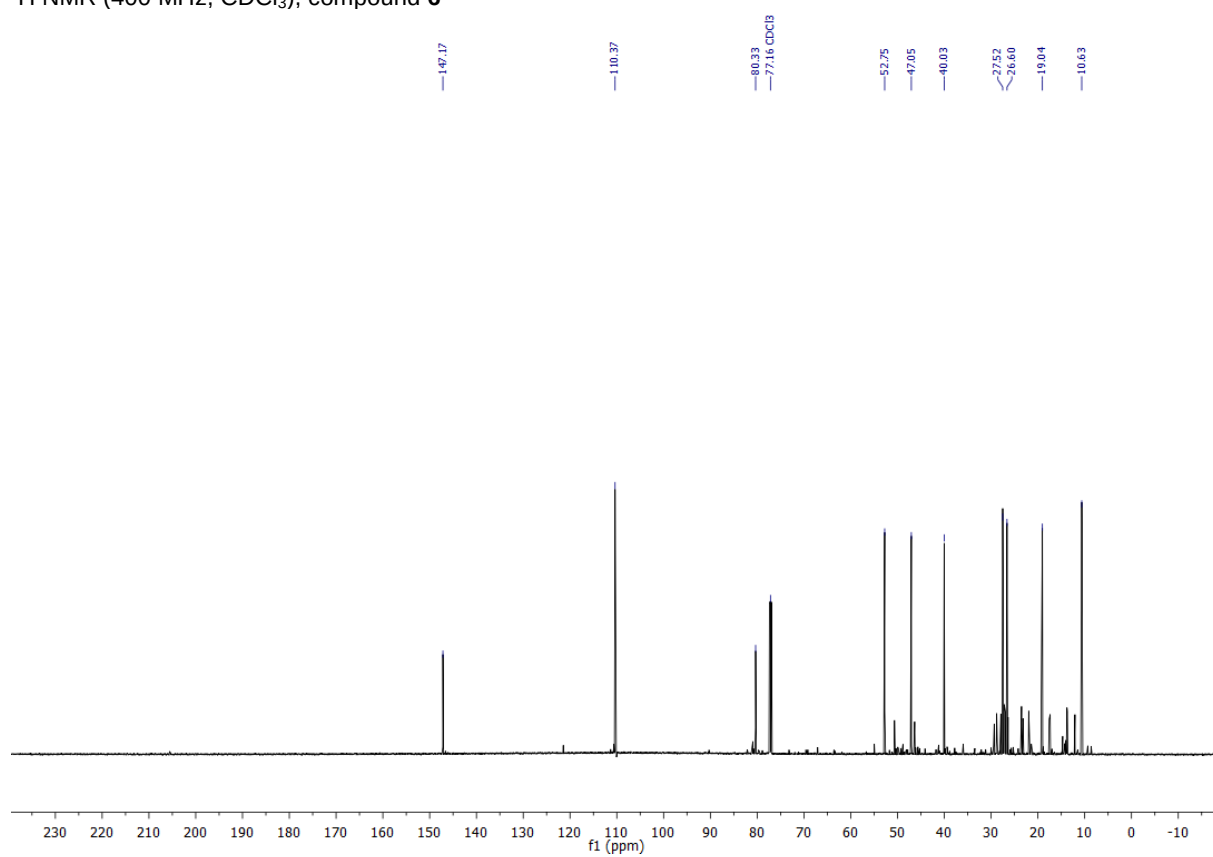
¹H NMR (400 MHz, CDCl₃), compound 5



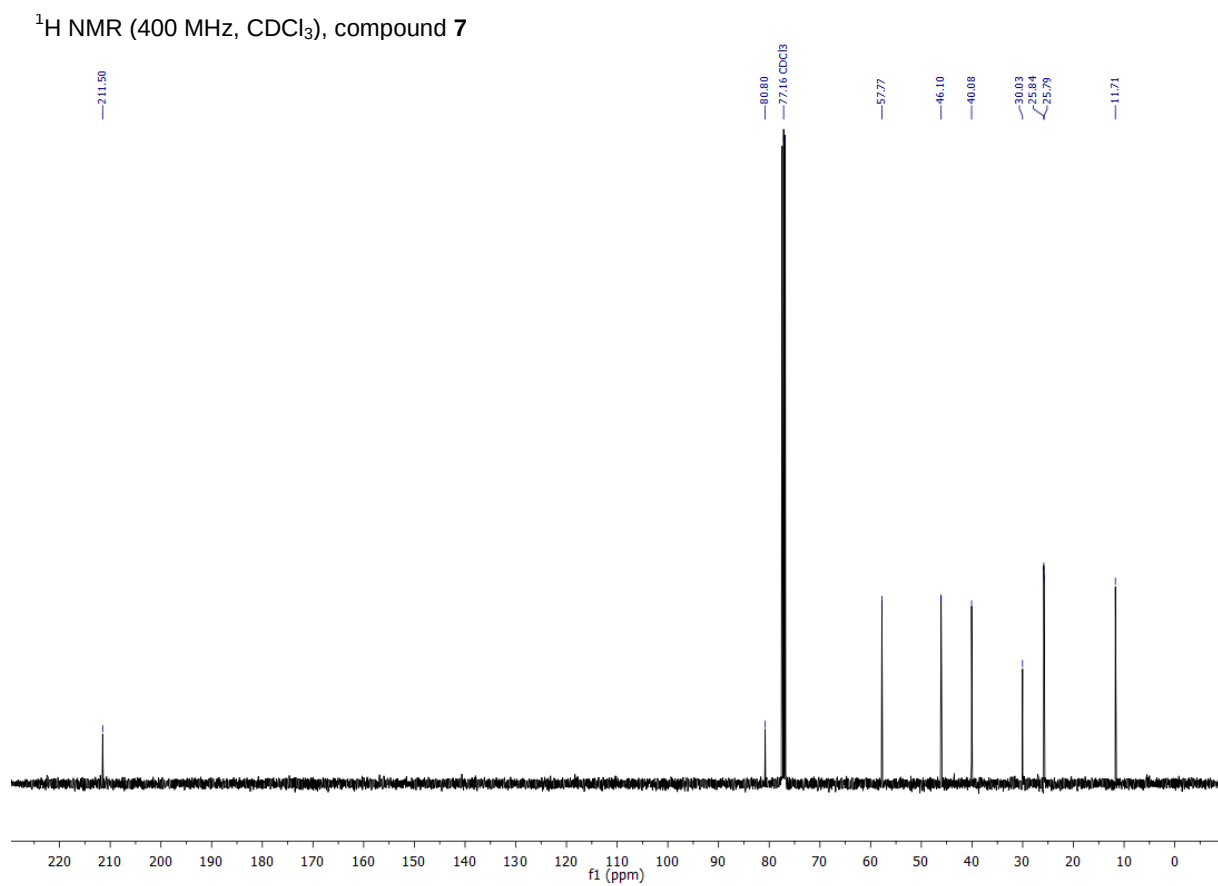
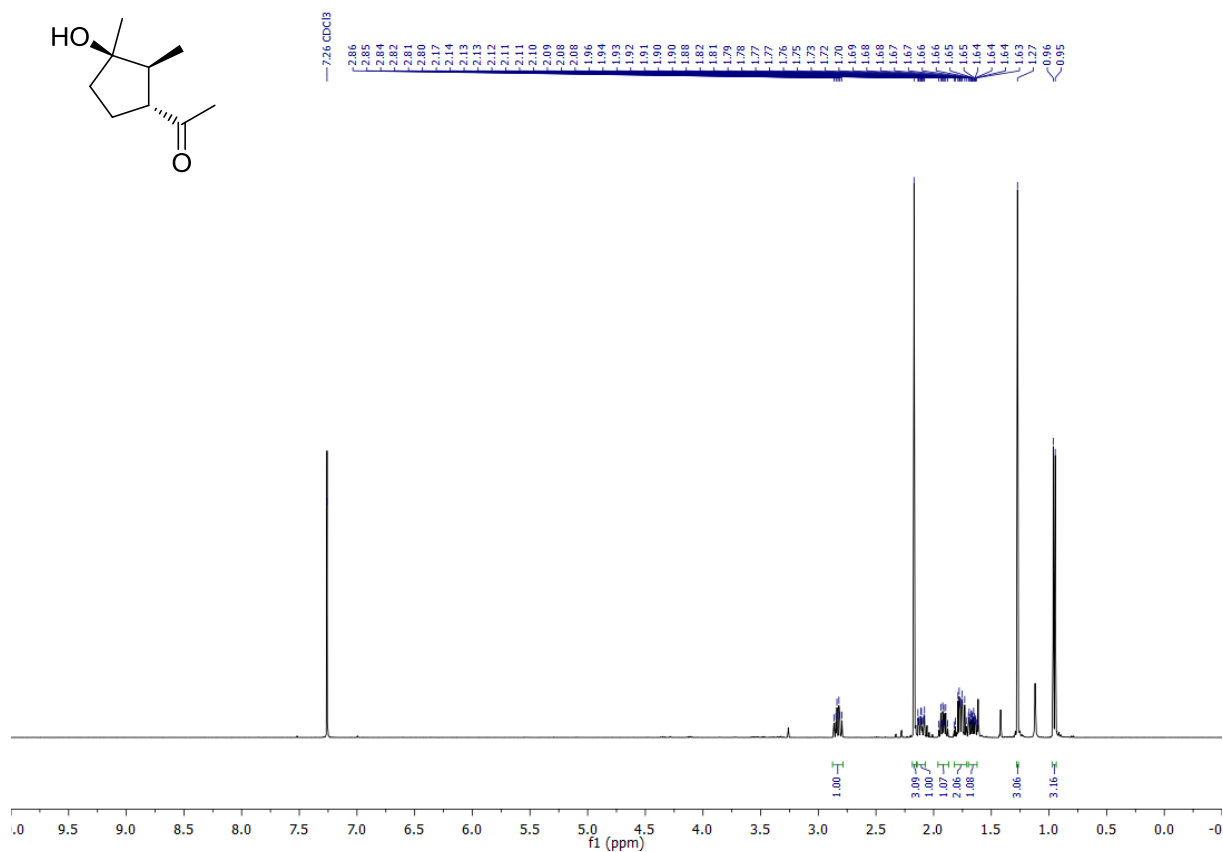
¹³C NMR (100.6 MHz, CDCl₃), compound 5

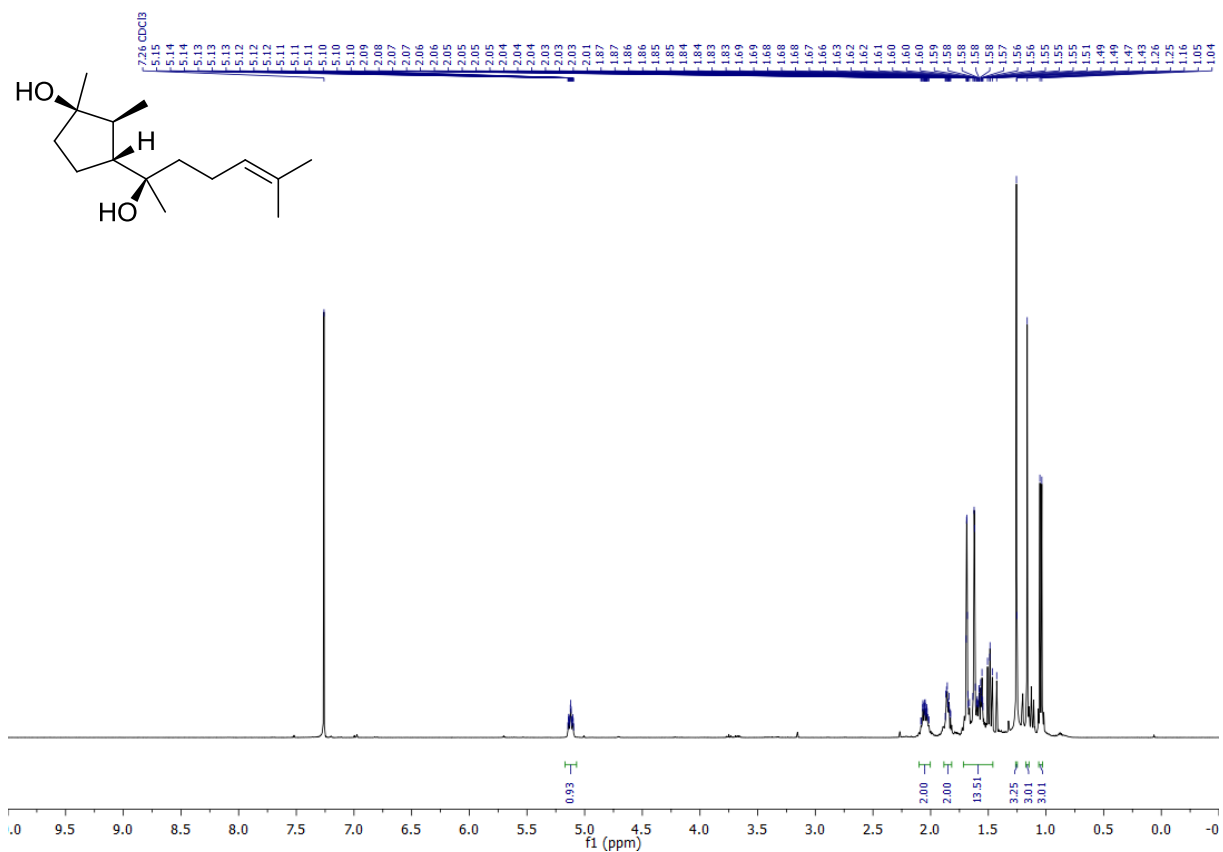


¹H NMR (400 MHz, CDCl₃), compound 6

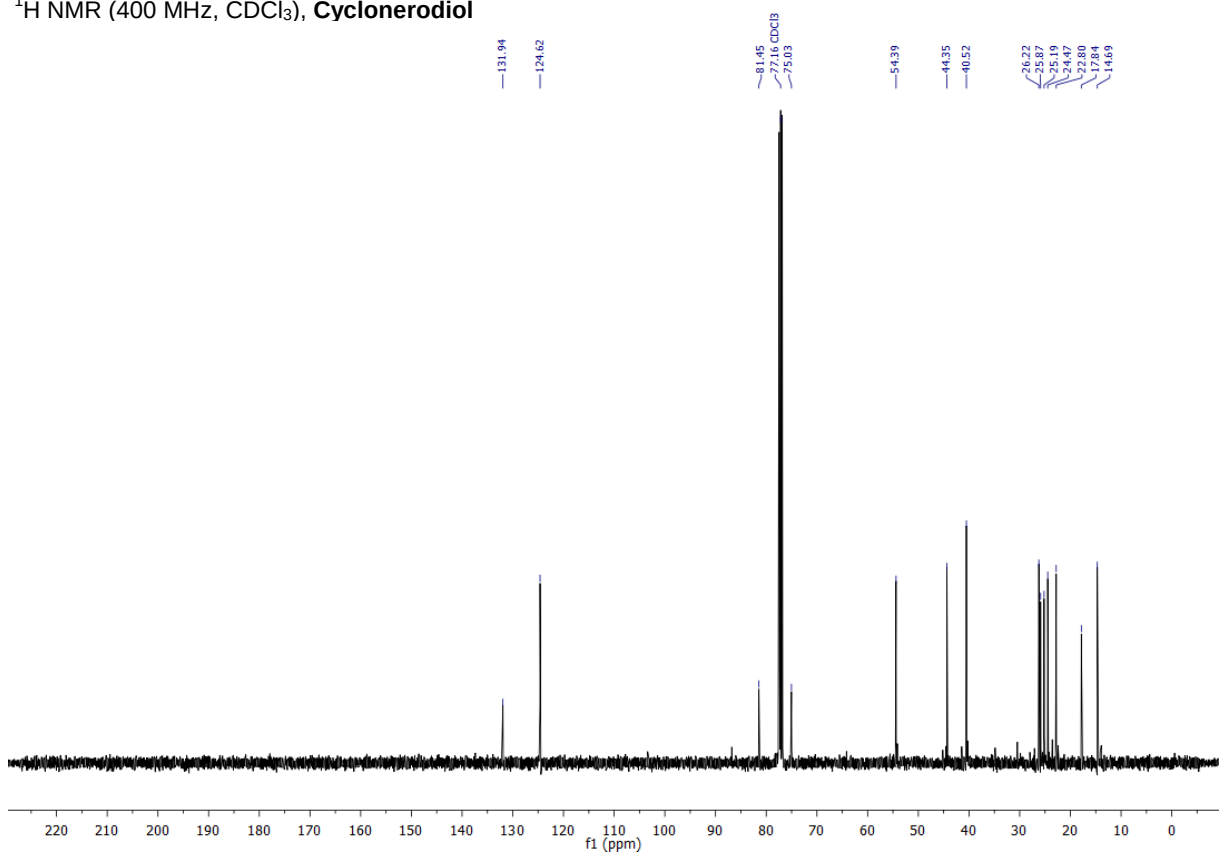


¹³C NMR (100.6 MHz, CDCl₃), compound 6





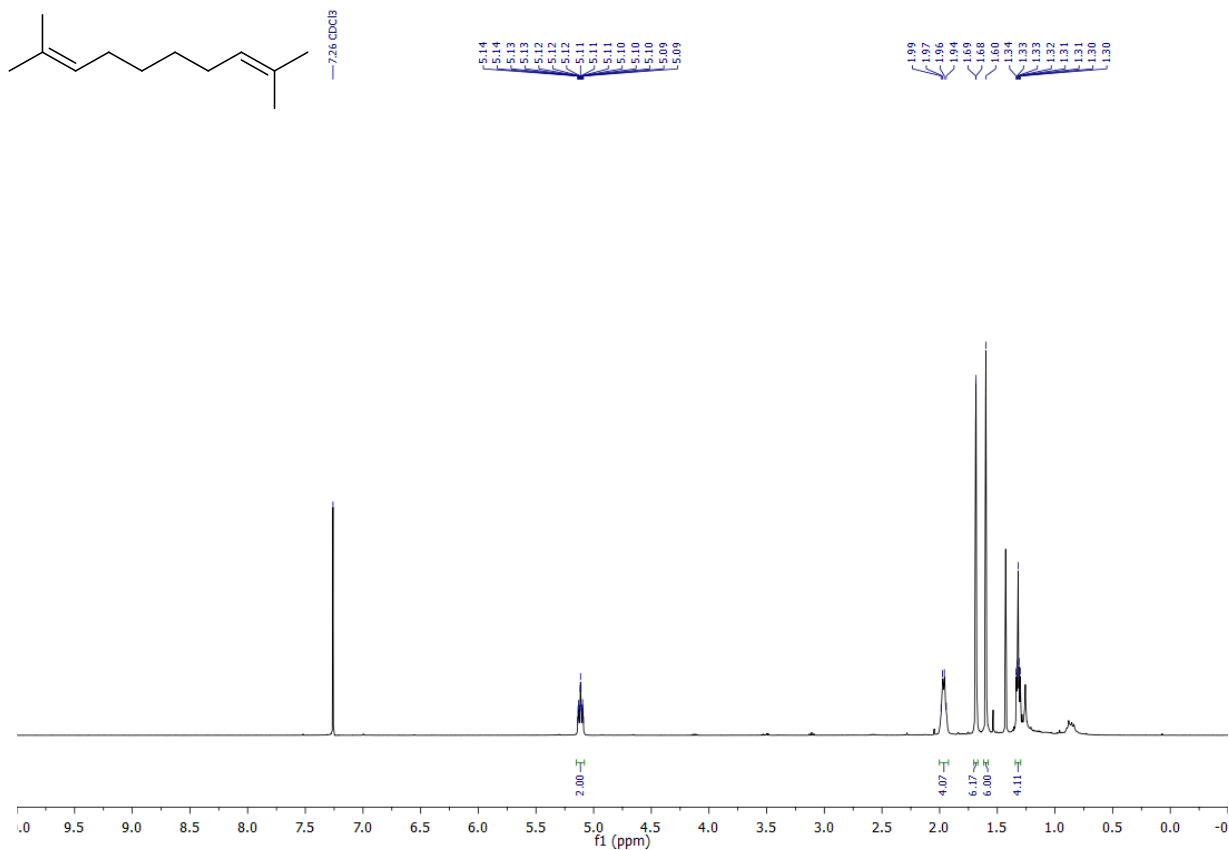
¹H NMR (400 MHz, CDCl₃), Cyclonerodiol



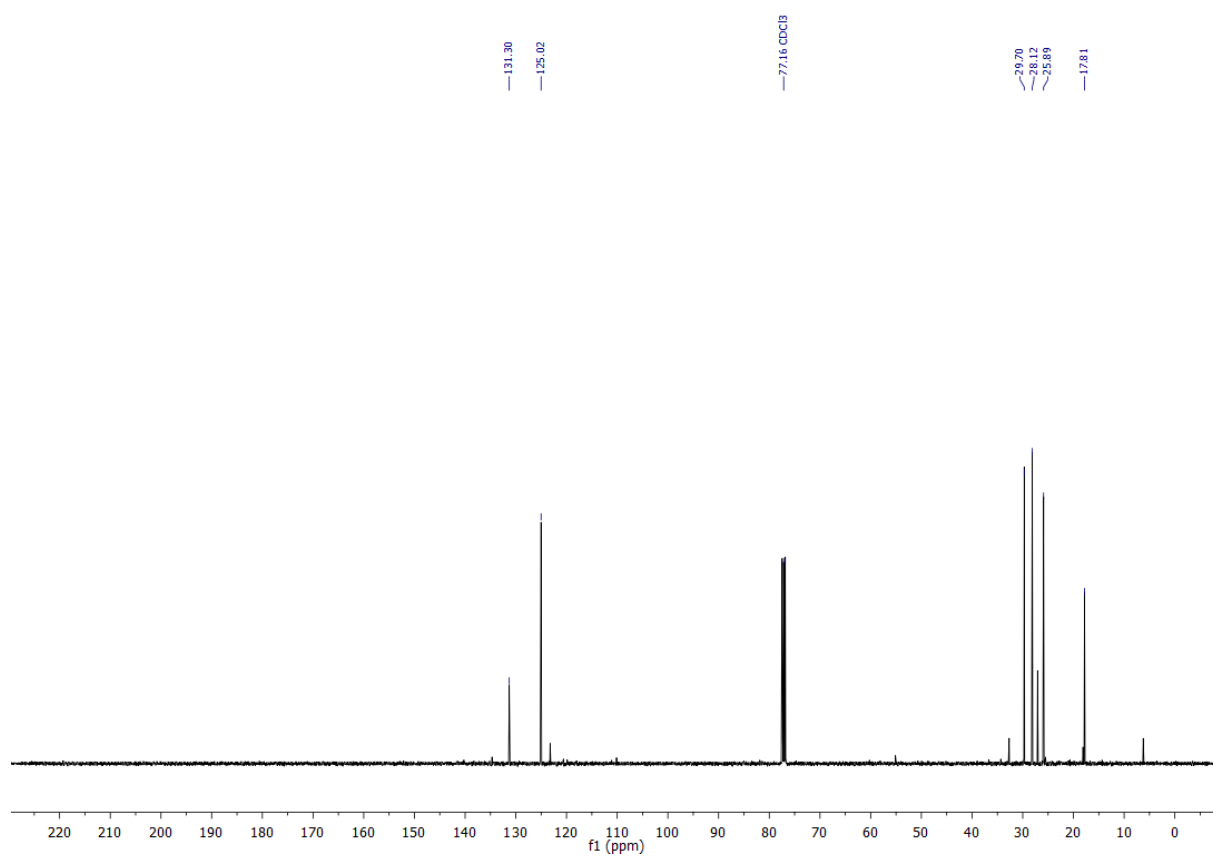
¹³C NMR (100.6 MHz, CDCl₃), Cyclonerodiol

Table of the compared NMR shifts in methanol:

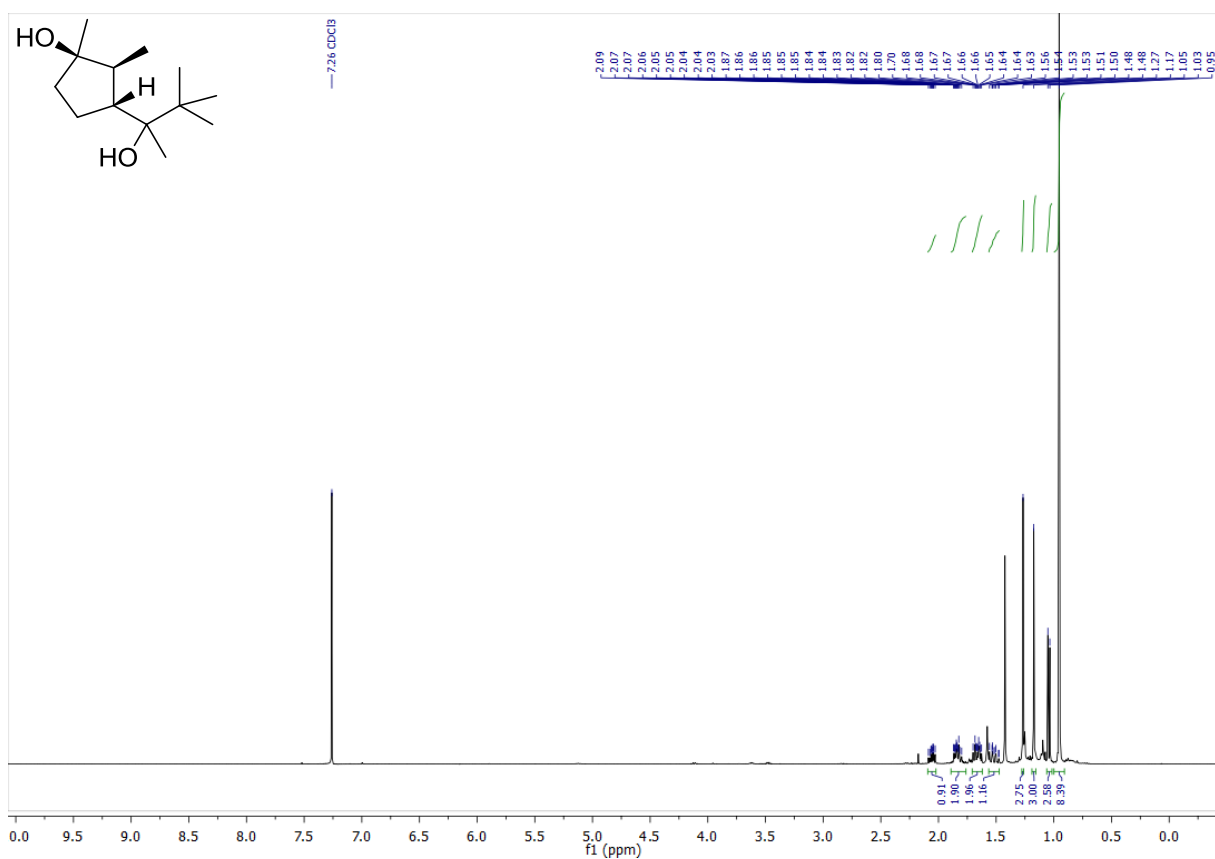
carbon	¹³ C Lit	¹ H Lit	¹³ C synthetic 1	¹ H synthetic 1	¹³ C minor diastereomer	¹ H minor diastereomer
C2-Me	15.45	1.01	15.4	1.05	15.1	1.05
2	45.11	1.59	45.4	1.73–1.45	45.6	1.73–1.45
1	81.82	-	82.0	-	81.9	-
5	41.26	1.64	41.4	1.73–1.45	41.2	1.73–1.45
		1.49				
4	25.01	1.78	25.1	1.90–1.82; 1.73–1.45	23.4	1.90–1.82; 1.73–1.45
		1.60				
3	55.11	1.82	55.3	1.90–1.82	55.5	1.90–1.82
2'	75.33	-	75.5	-	75.8	-
3'	41.88	1.43	42.1	1.73–1.45	42.5	1.73–1.45
4'	23.58	2.02	23.7	2.12–2.02		2.12–2.02
5'	125.82	5.12	125.9	5.16–5.10	126.0	5.16–5.10
6'	131.64	-	132.0	-	132.0	-
7'	26.06	1.67	25.9	1.61	25.9	1.61
C1-Me	26.25	1.21	26.1	1.27	26.1	1.27
1'	24.79	1.12	24.7	1.17	23.3	1.17
8'	17.87	1.61	17.7	1.67	17.7	1.67



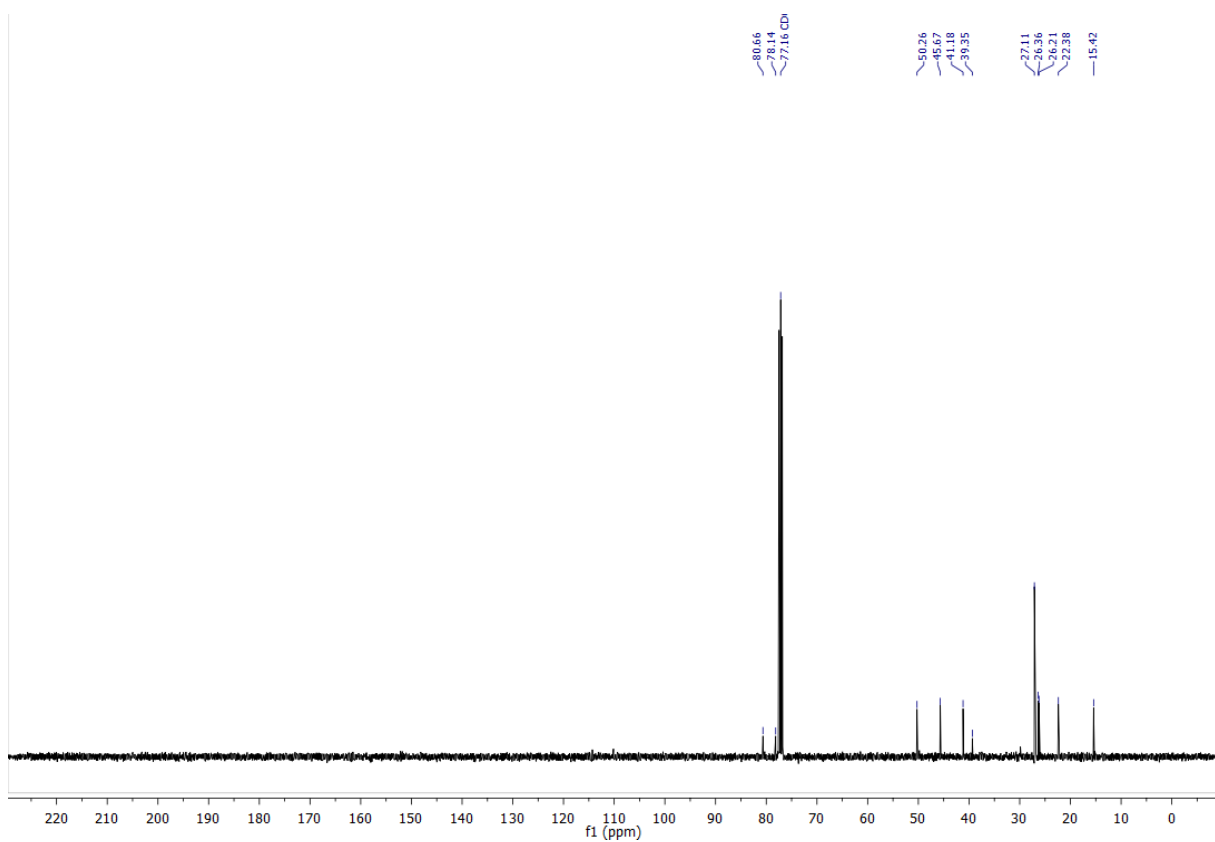
¹H NMR (400 MHz, CDCl₃), 2,9-dimethyldeca-2,8-diene



¹³C NMR (100.6 MHz, CDCl₃), 2,9-dimethyldeca-2,8-diene



¹H NMR (400 MHz, CDCl₃), (1*R*,2*S*,3*R*)-3-(2-hydroxy-3,3-dimethylbutan-2-yl)-1,2-dimethylcyclopentanol



¹³C NMR (100.6 MHz, CDCl₃), (1*R*,2*S*,3*R*)-3-(2-hydroxy-3,3-dimethylbutan-2-yl)-1,2-dimethylcyclopentanol