

Supporting Information

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New Diterpenes Isolated from the Colombian Caribbean Soft Coral *Pseudoplexaura flagellosa* and their Cytotoxic Properties

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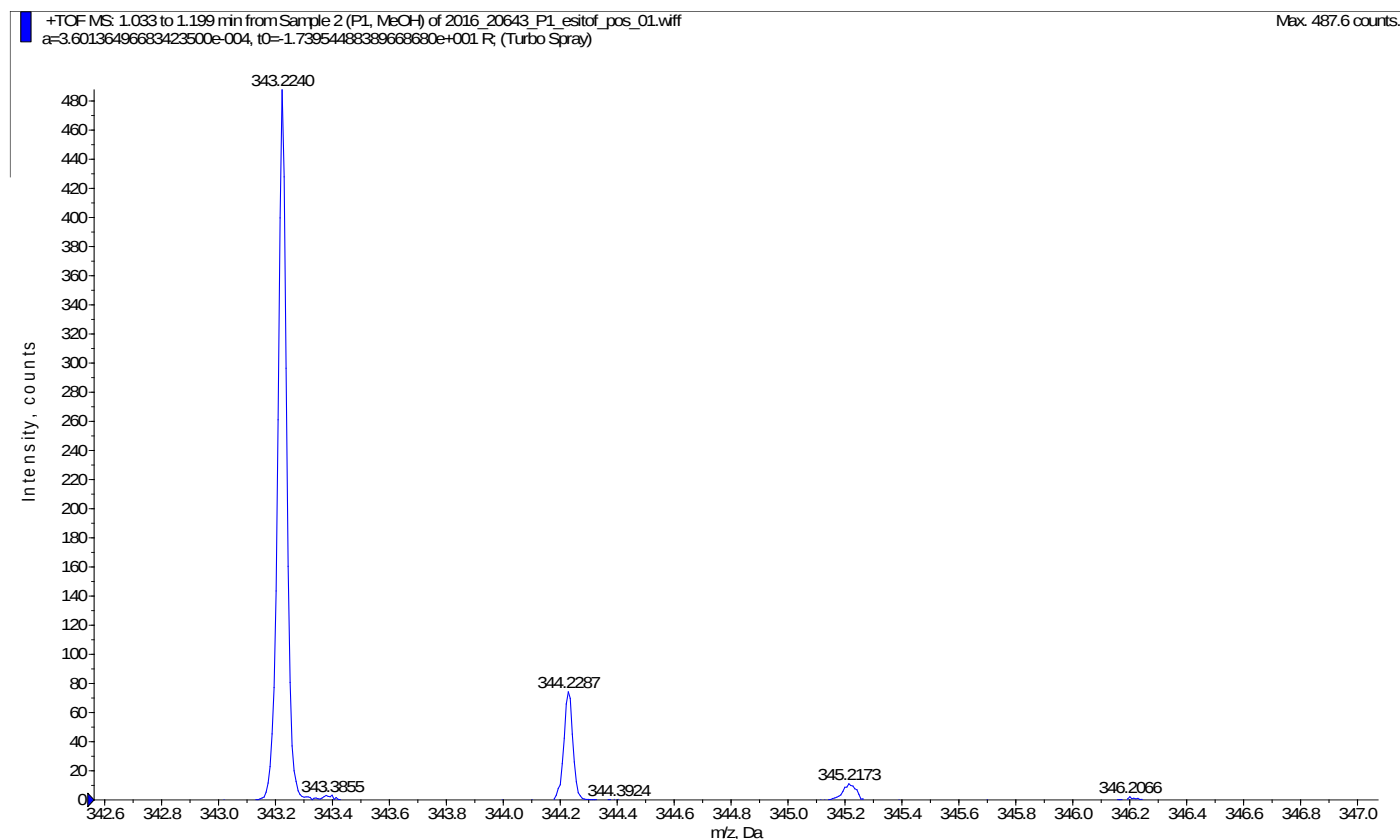
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Table of Contents	Page
Figure S1: HRESI-MS Spectrum of Compound 1	2
Figure S2: ¹ H NMR Spectrum of Compound 1	3
Figure S3: APT ¹³ C NMR Spectrum of Compound 1	3
Figure S4: ¹ H- ¹ H COSY experiment of Compound 1	4
Figure S5: HRESI-MS Spectrum of Compound 2	5
Figure S6: ¹ H NMR Spectrum of Compound 2	6
Figure S7: APT ¹³ C NMR Spectrum of Compound 2	6
Figure S8: ¹ H- ¹ H NOESY experiment of Compound 2	7
Figure S9: HRESI-MS Spectrum of Compound 3	8
Figure S10: ¹ H NMR Spectrum of Compound 3	9
Figure S11: HRESI-MS Spectrum of Compound 4	10
Figure S12: ¹ H NMR Spectrum of Compound 4	11
Figure S13: ¹ H NMR Spectrum of R-MPA ester of Compound 2	11
Figure S14: ¹ H NMR Spectrum of S-MPA ester of Compound 2	12
Figure S15: Table of Chemical Shifts Differences of R and S-MPA Esters of 2	12
Figure S16: ¹ H NMR Spectrum of Compound 5	13
Figure S17: ¹ H NMR Spectrum of Compound 6	13
Figure S18: ¹ H NMR Spectrum of Compound 7	14

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<i>m/z</i> experimental	343.2240			
Formula	<i>m/z</i> theoretical	Erro, mDa	Erro,ppm	
C₂₀ H₃₂ O₃ Na	343.2243	-0.3663	-1.0672	4.5
C₂₂ H₃₁ O₃	343.2267	-2.7715	-8.0751	7.5

Figure S1: HRESI-MS Spectrum of Compound 1

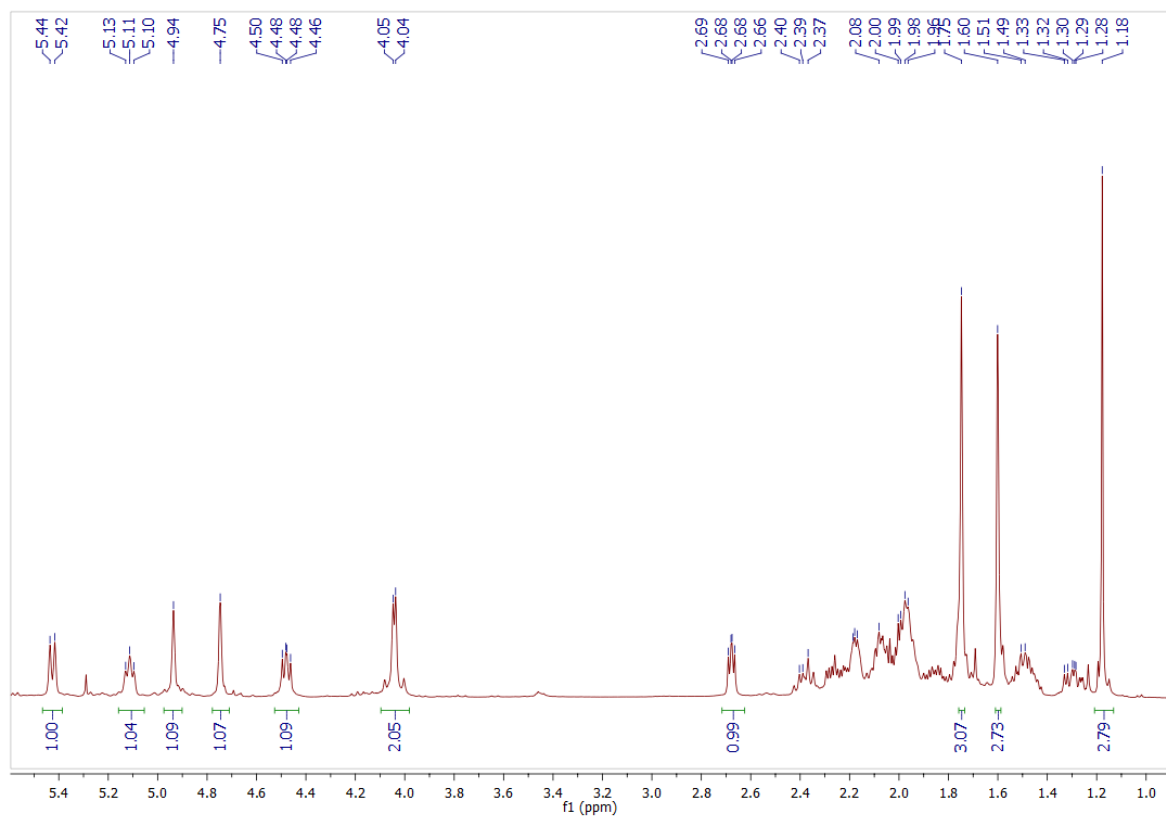


Figure S2: ^1H NMR Spectrum of Compound 1

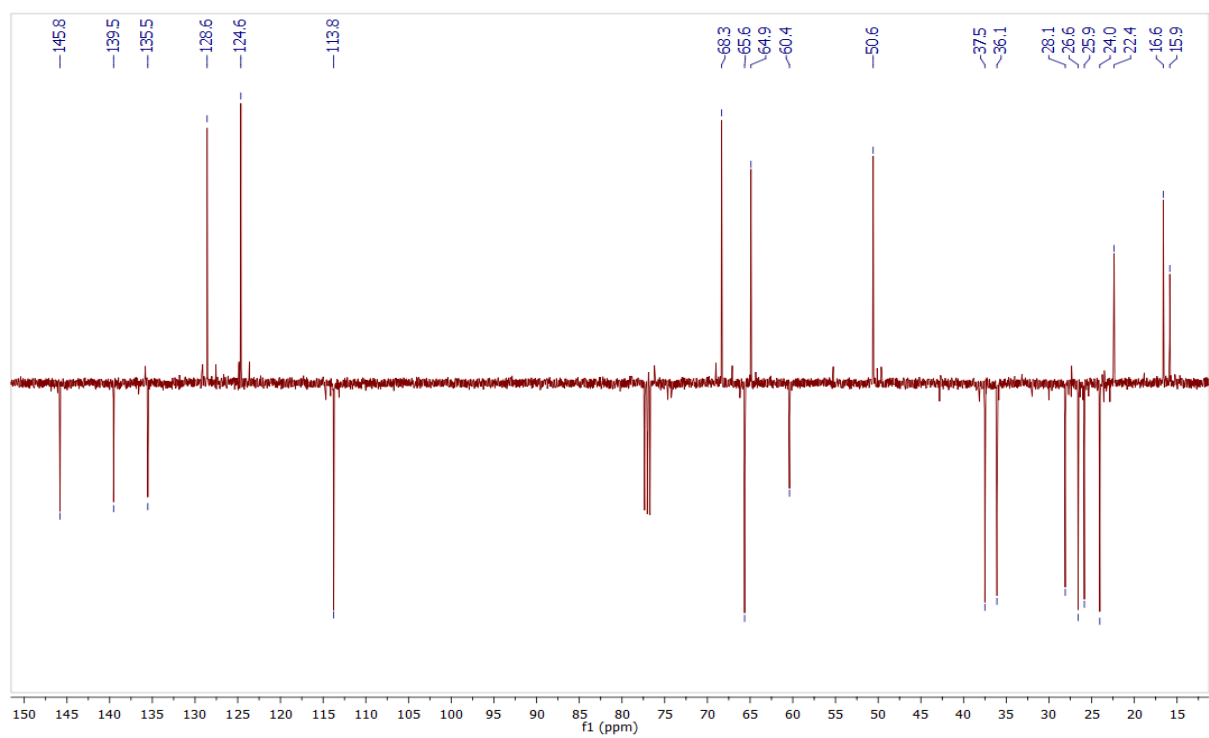


Figure S3: APT ^{13}C NMR Spectrum of Compound 1

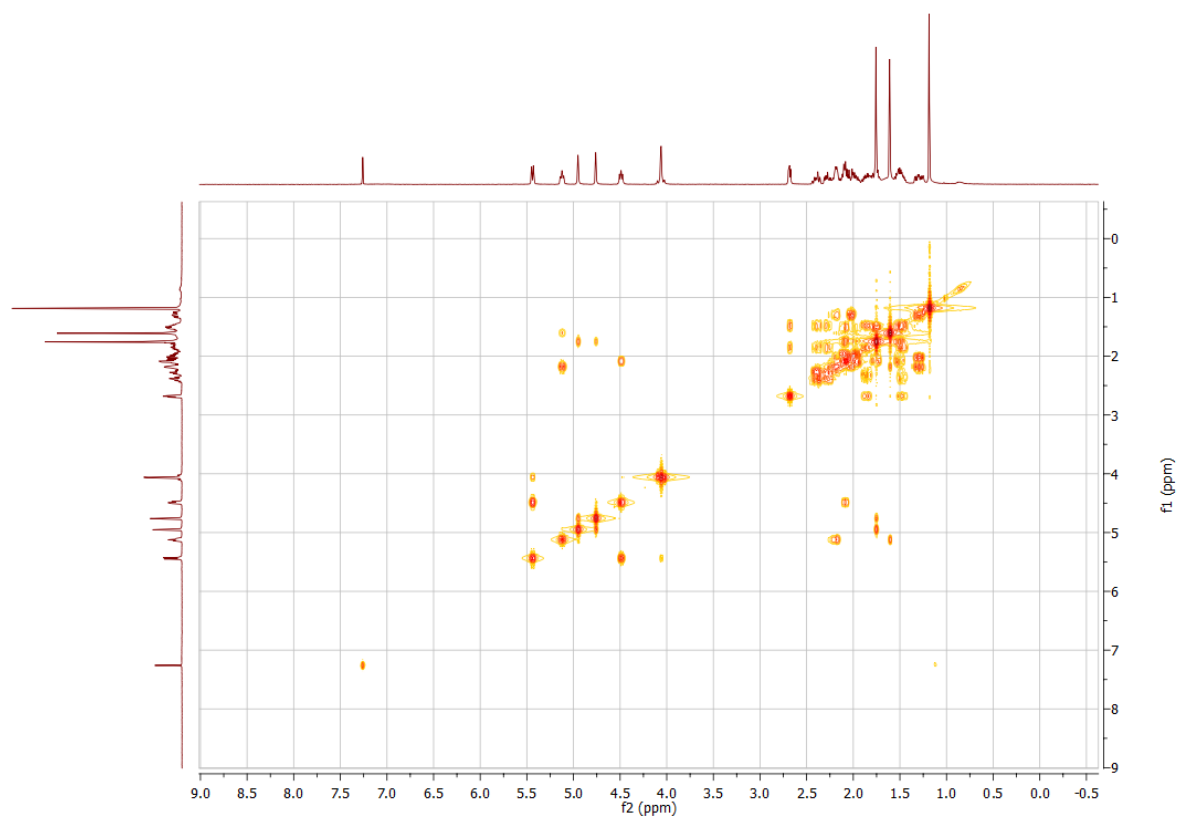
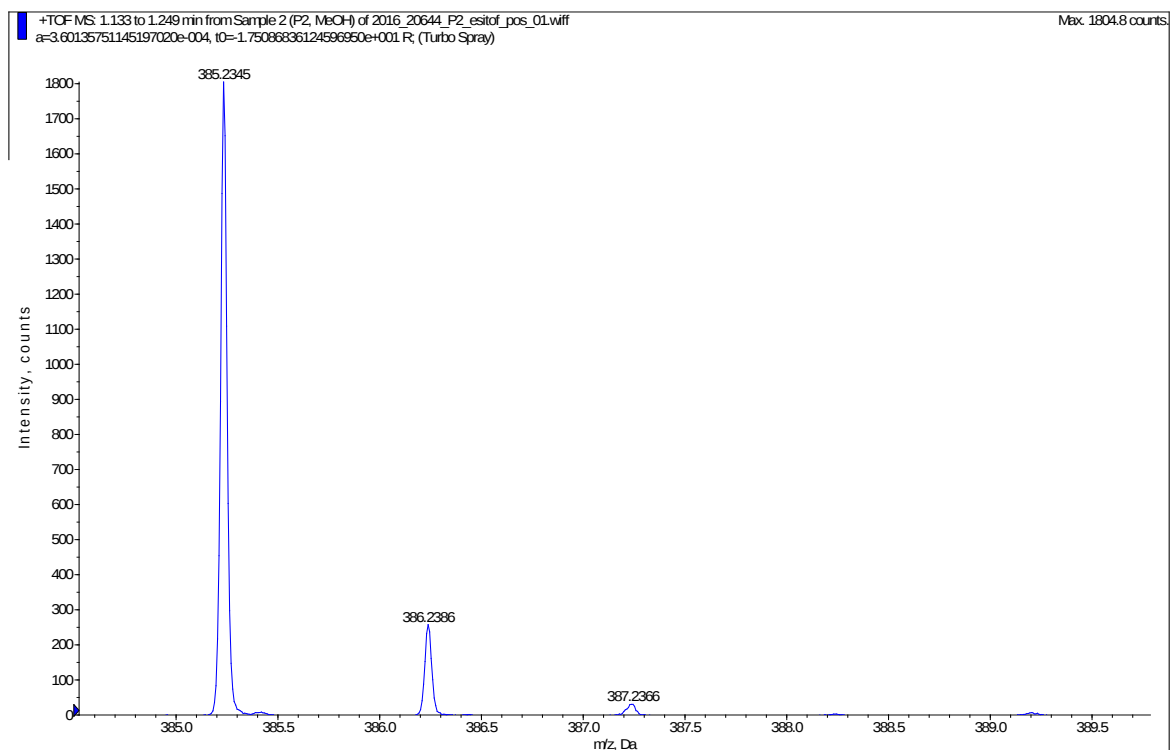


Figure S4: ^1H - ^1H COSY experiment of Compound **1**



<i>m/z</i> experimental	385.2345			
Formula	<i>m/z</i> theoretical	Erro, mDa	Erro, ppm	
C₂₂ H₃₄ O₄ Na	385.2349	-0.431	-1.1189	5.5
C₂₄ H₃₃ O₄	385.2373	-2.8363	-7.3625	8.5

Figure S5: HRESI-MS Spectrum of Compound 2

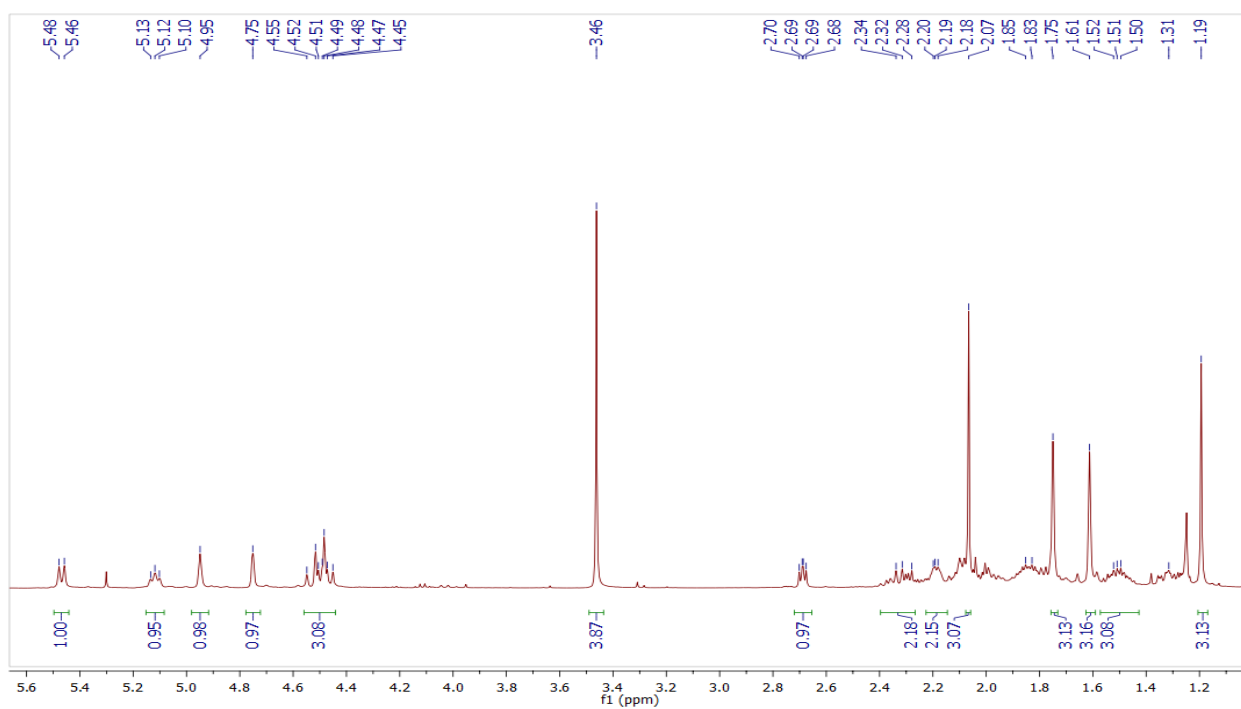


Figure S6: ¹H NMR Spectrum of Compound 2

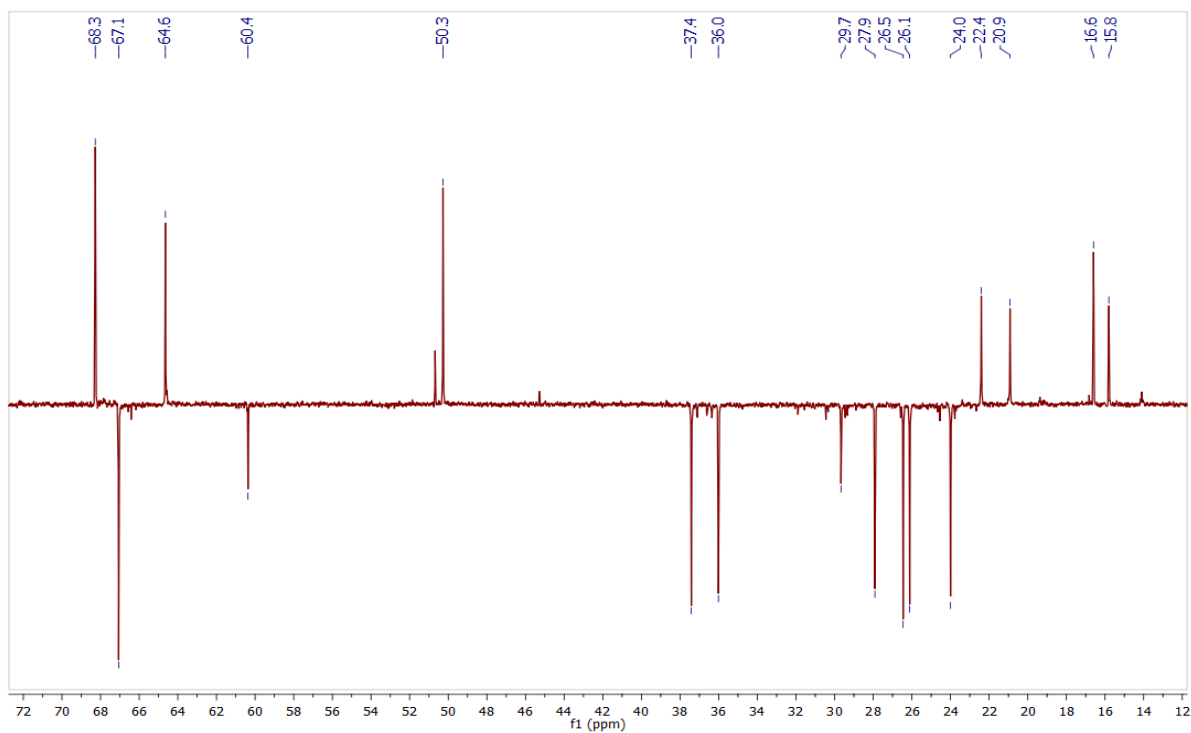


Figure S7: APT ¹³C NMR Spectrum of Compound 2

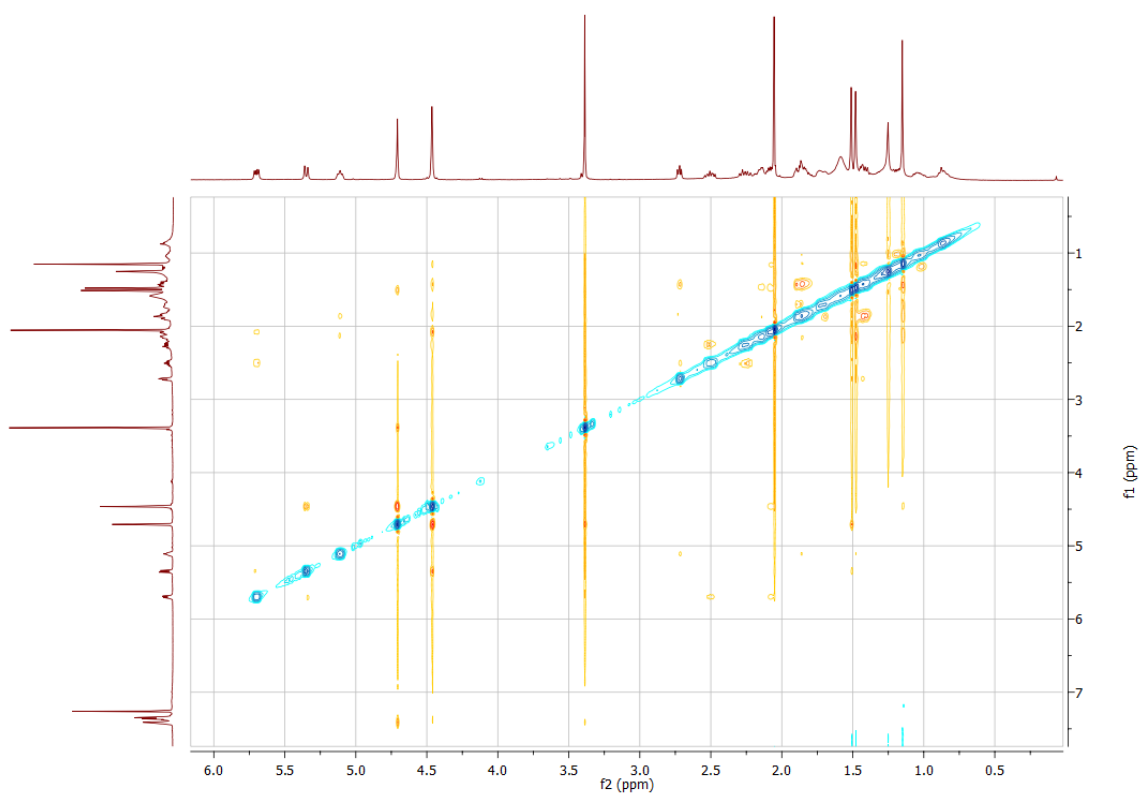
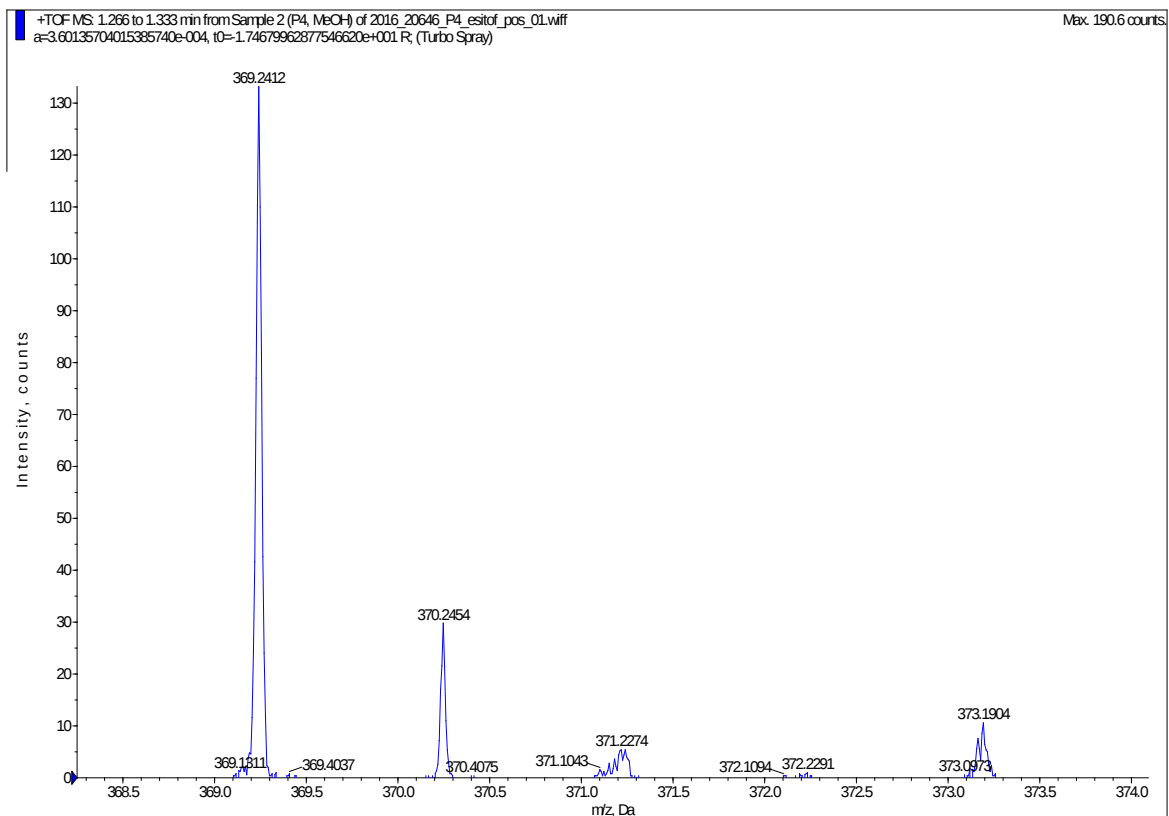


Figure S8: ^1H - ^1H NOESY experiment of Compound 2



<i>m/z</i> experimental	369.2412			
Formula	<i>m/z</i> theoretical	Erro, mDa	Erro, ppm	
C₂₂ H₃₄ O₃ Na	369.2400	1.1835	3.2054	5.5
C₂₄ H₃₃ O₃	369.2424	-1.2216	-3.3085	8.5

Figure S9: HRESI-MS Spectrum of Compound 3

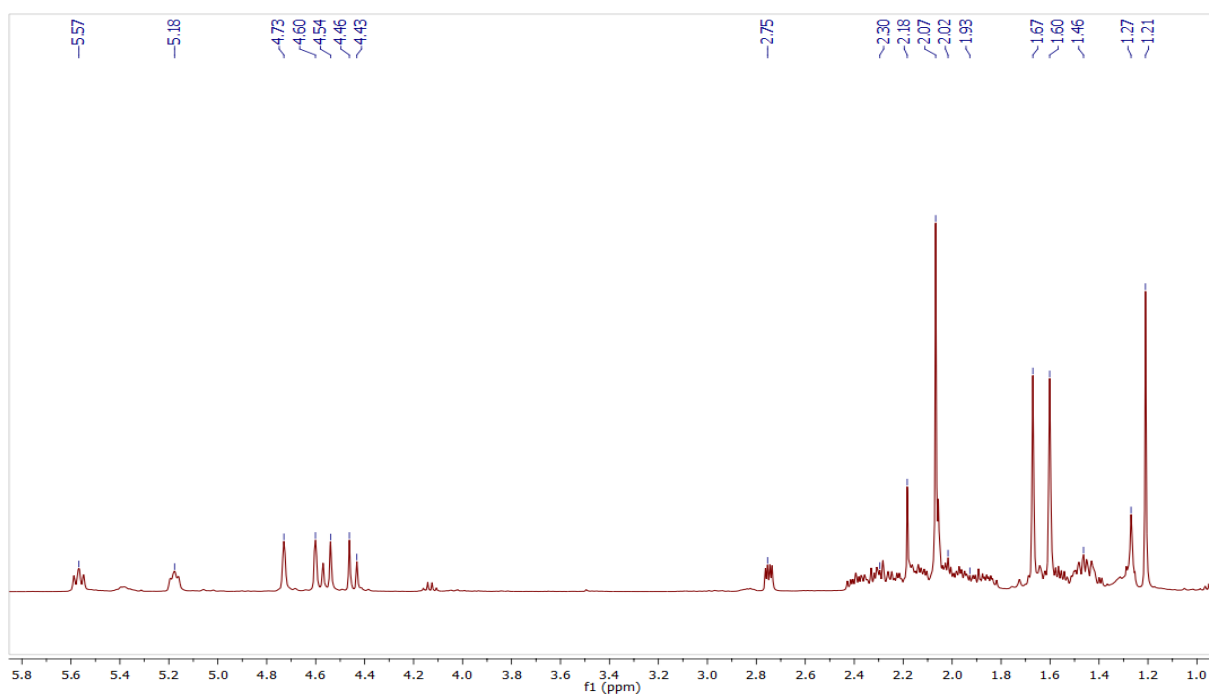
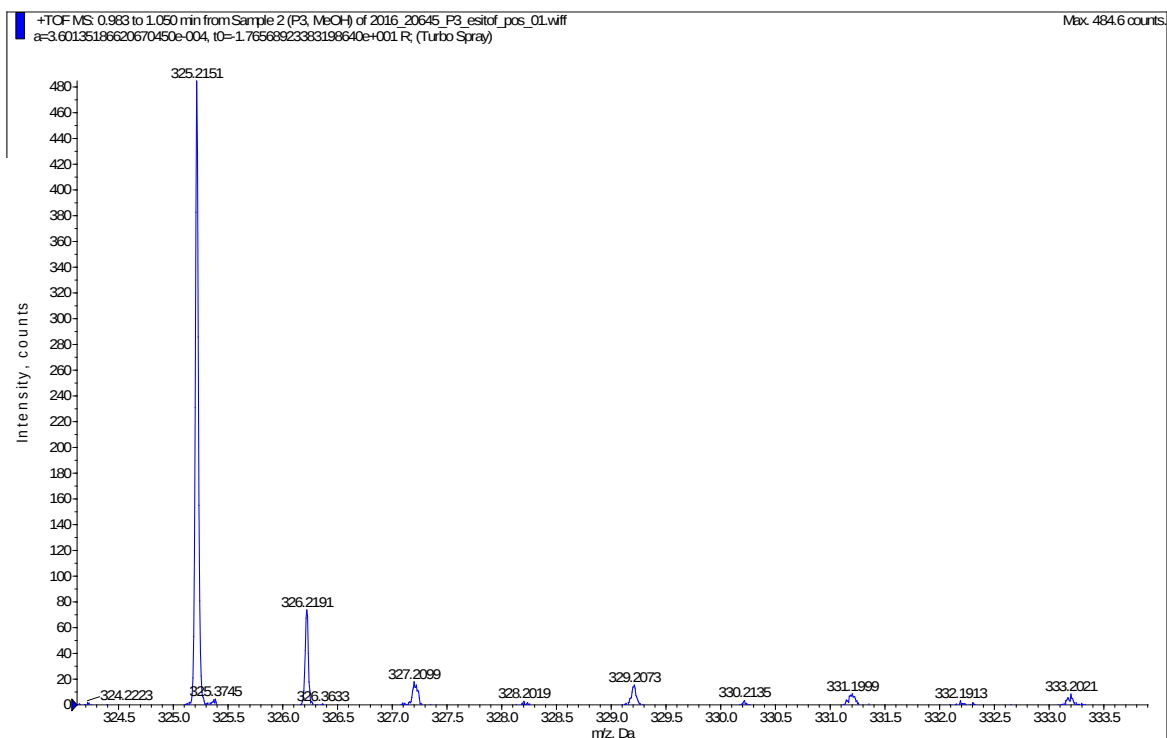


Figure S10: ^1H NMR Spectrum of Compound 3



<i>m/z</i> experimental	325.2151			
Formula	<i>m/z</i> theoretical	Erro, mDa	Erro,ppm	
C₂₂ H₂₉ O₂	325.2162	-1.1068	-3.4034	8.5
C₂₀ H₃₀ O₂ Na	325.2138	1.2983	3.9924	5.5

Figure S11: HRESI-MS Spectrum of Compound 4

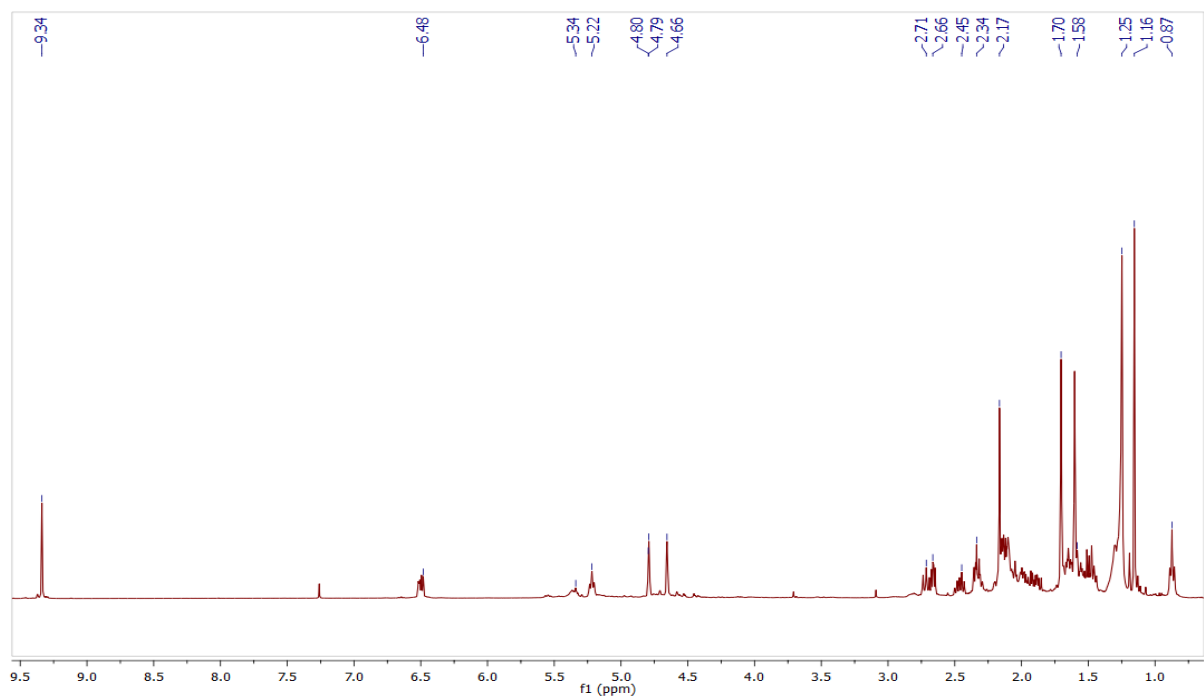


Figure S12: ^1H NMR Spectrum of Compound 4

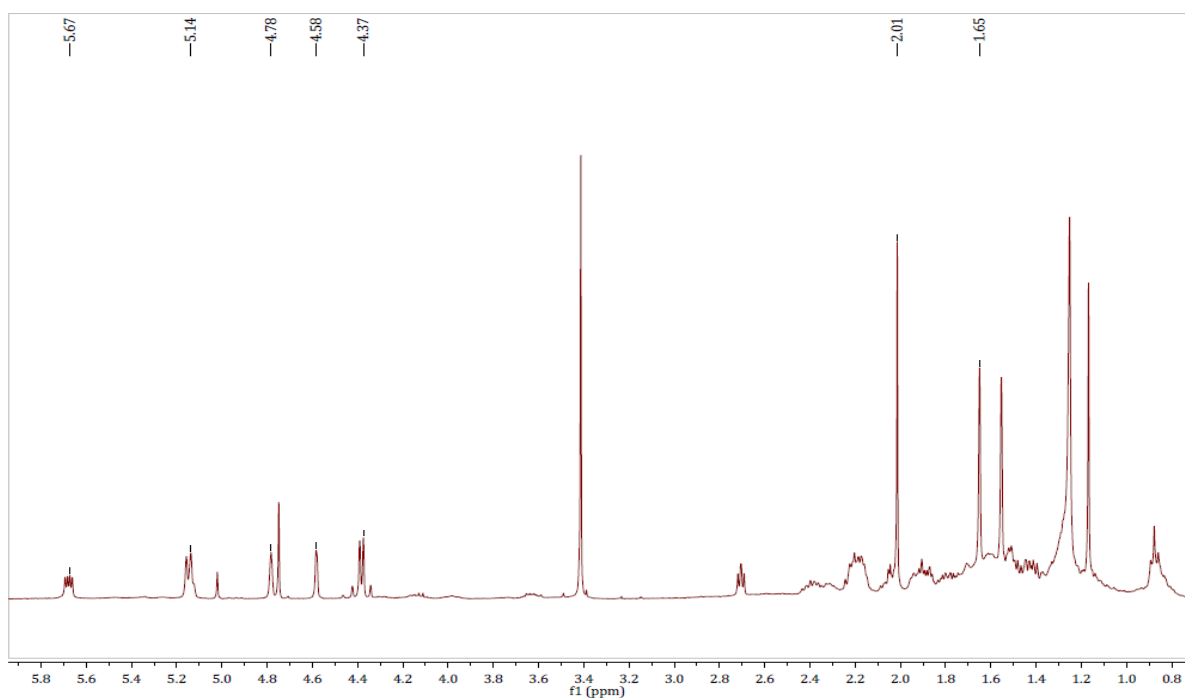


Figure S13: ^1H NMR Spectrum of *R*-MPA ester of Compound 2

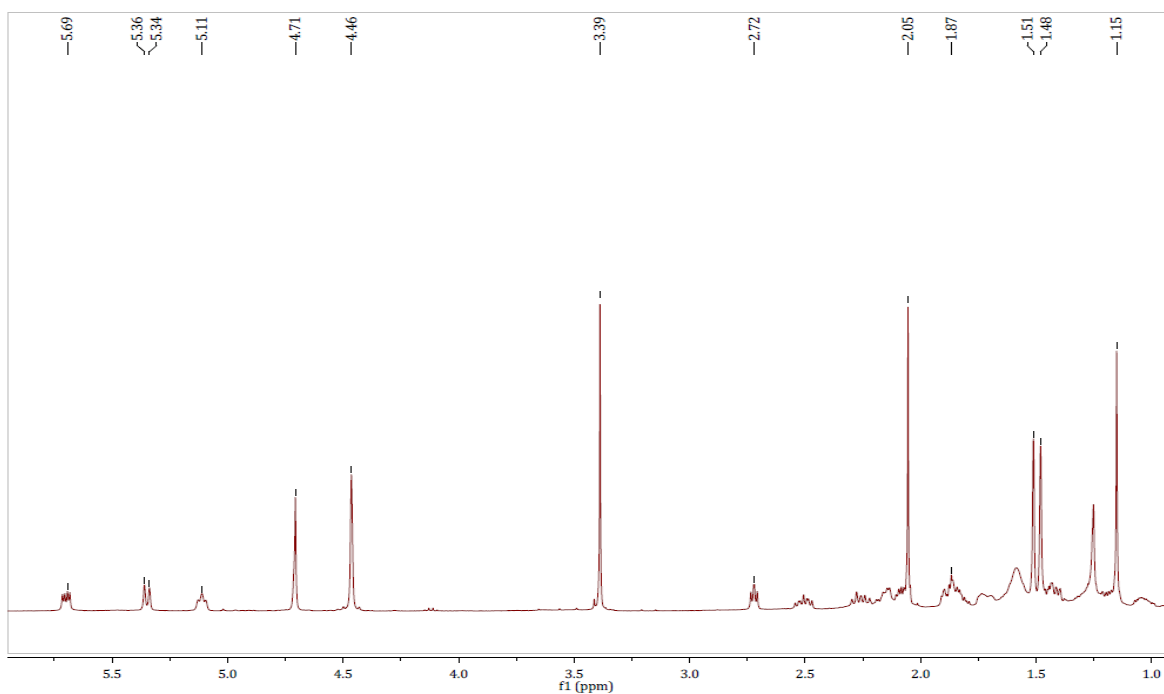


Figure S14: ^1H NMR Spectrum of S-MPA ester of Compound 2

no.	δ_{H} 2S	δ_{H} 2R	$\Delta\delta_{\text{RS}}$
H-2			
H-3	5.34, d, $J=8.6$	5.14, d, $J=7.9$	-0.20
H-11	5.11, t, $J=6.5$	5.13, m	+0.02
H-16	1.51, s	1.65, s	+0.14
H-17	4.71, s	4.78, s	+0.07
H-17'	4.46, s	4.58, s	+0.12
H-18	4.46, s	4.37, s	-0.09
H-19	1.25, s	1.17, s	-0.08
H-20	1.48, s	1.55, s	+0.07

Figure S15: Table of Chemical Shifts Differences of R and S-MPA Esters of 2

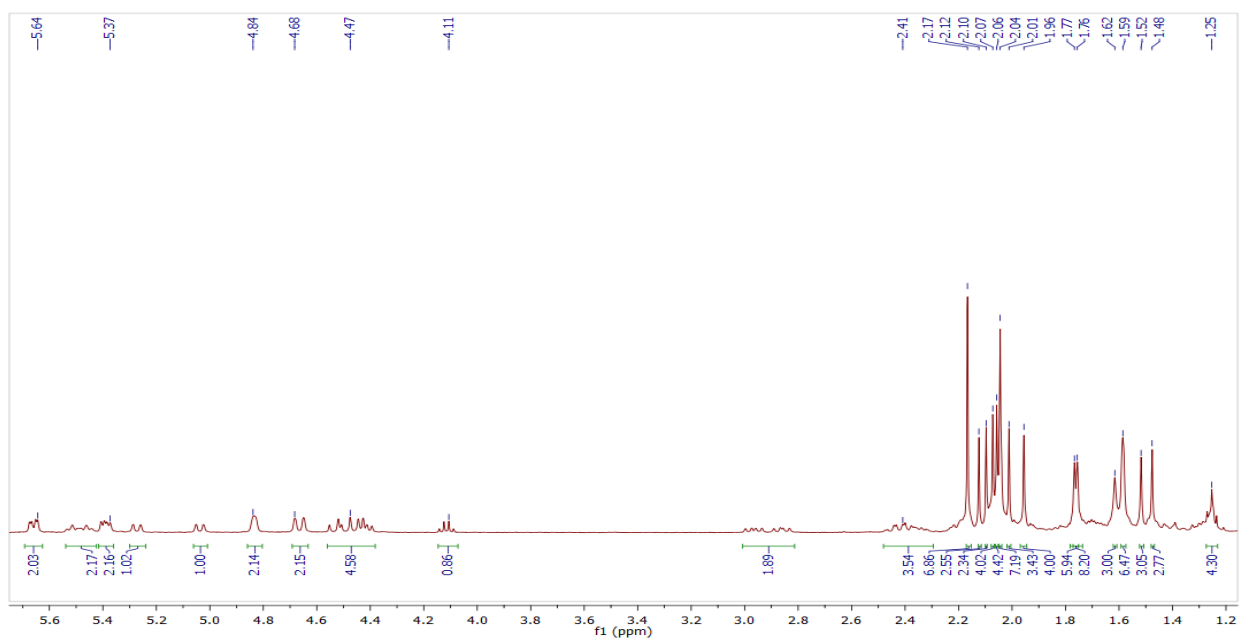


Figure S16: ¹H NMR Spectrum of Compound 5

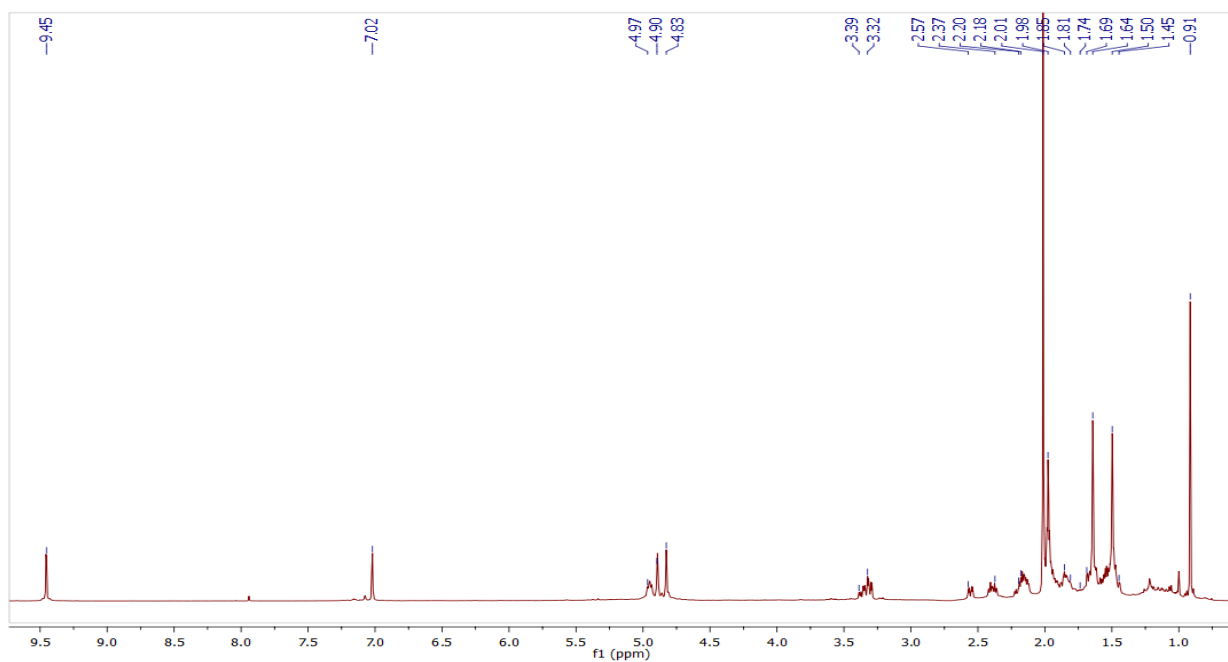


Figure S17: ¹H NMR Spectrum of Compound 6

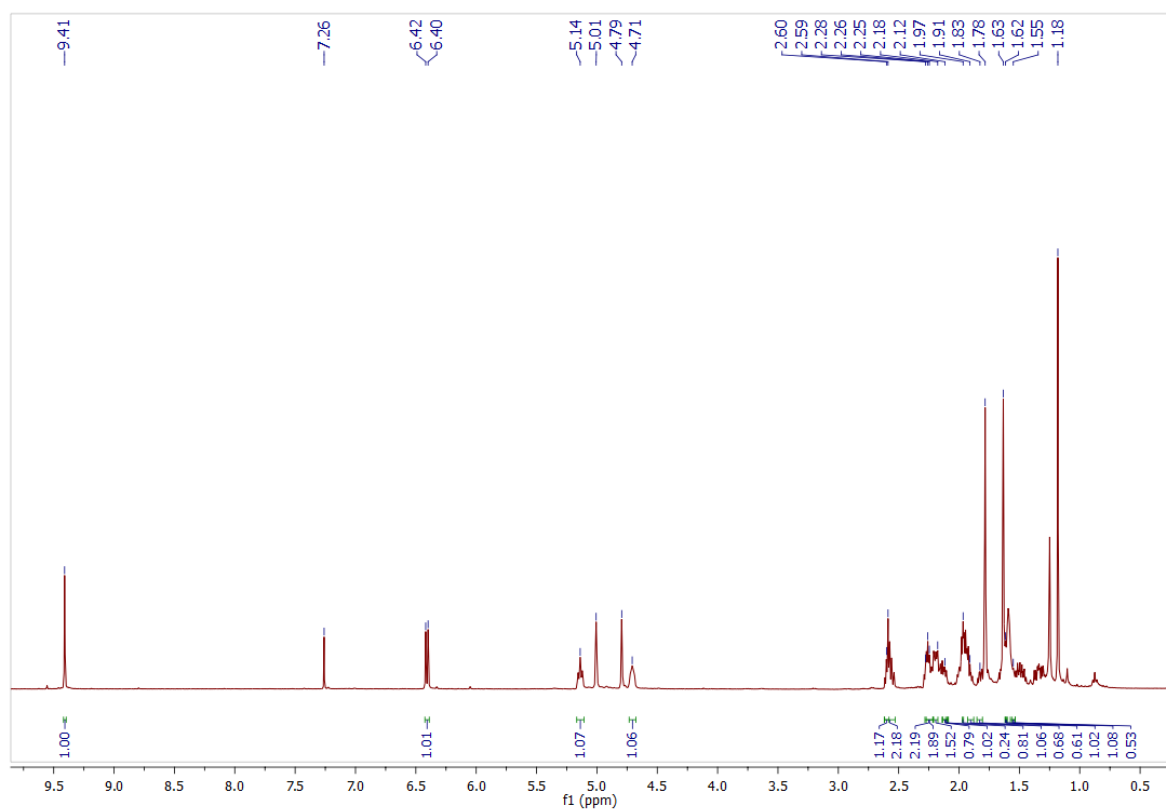


Figure S18: ^1H NMR Spectrum of Compound 7