

Anti-inflammatory Butenolides from marine-derived *Streptomyces* sp 13G036

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Table S1: Comparison of Chemical Shifts in ^{13}C NMR data and Specific Rotation of Synthesized Butenolides with **4** and **7**.

No	synthetic 4 <i>S</i> ,10 <i>S</i> ,11 <i>R</i>	synthetic 4 <i>S</i> ,10 <i>R</i> ,11 <i>S</i>	4	synthetic 4 <i>S</i> ,10 <i>S</i> ,11 <i>S</i>	synthetic 4 <i>S</i> ,10 <i>R</i> ,11 <i>R</i>	7
1	173.19	173.19	173.13	173.17	173.15	173.20
2	121.55	121.54	121.59	121.58	121.57	121.60
3	126.30	156.30	156.22	156.26	156.23	156.20
4	83.41	83.41	83.39	83.39	83.38	83.40
5	33.16	33.15	33.19	33.17	33.16	33.21
6	24.97	24.95	24.97	24.97	24.97	25.00
7	29.60	29.60	29.63	29.61	29.60	29.65
8	26.99	26.98	27.01	27.13	27.12	27.16
9	32.35	32.34	32.36	32.42	32.42	32.48
10	39.99	39.97	40.01	39.69	39.67	39.73
11	71.72	71.70	71.74	71.33	71.31	71.34
12	19.51	19.49	19.54	20.27	20.26	20.32
13	14.58	14.57	14.61	14.11	14.11	14.15
	4 <i>S</i> ,10 <i>S</i> ,11 <i>R</i>	4 <i>S</i> ,10 <i>R</i> ,11 <i>S</i>	4	4 <i>S</i> ,10 <i>S</i> ,11 <i>S</i>	4 <i>S</i> ,10 <i>R</i> ,11 <i>R</i>	7
Specific rotation	+42.9	+70.9	+65.8	+33.6	+64.3	+35.6

Same symbol means same configurations.



Figure S1: The picture of *Streptomyces* sp 13G036.

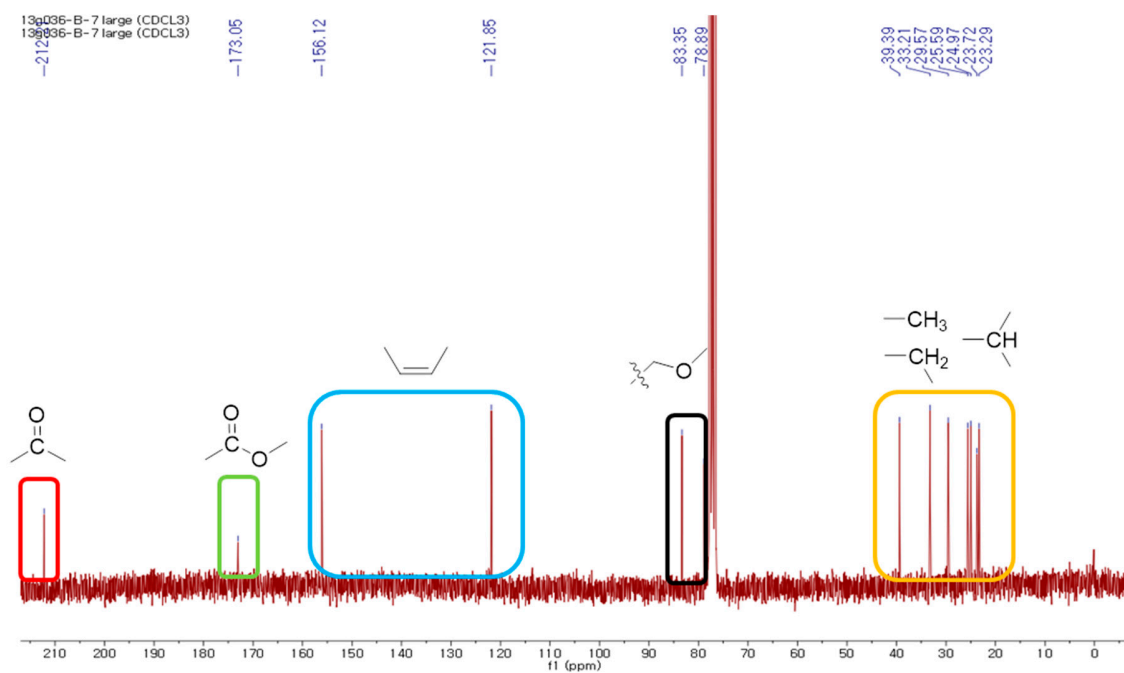


Figure S2: The assignment of functional group of compound **1**.

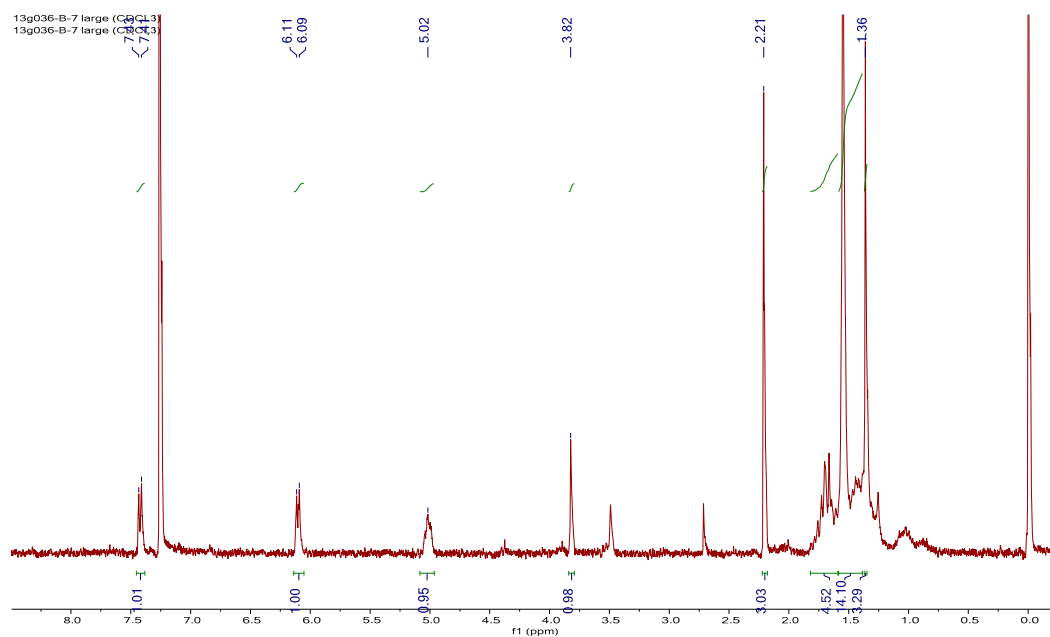


Figure S3: ¹H NMR Spectrum of Compound **1** (CDCl₃, 250 MHz)

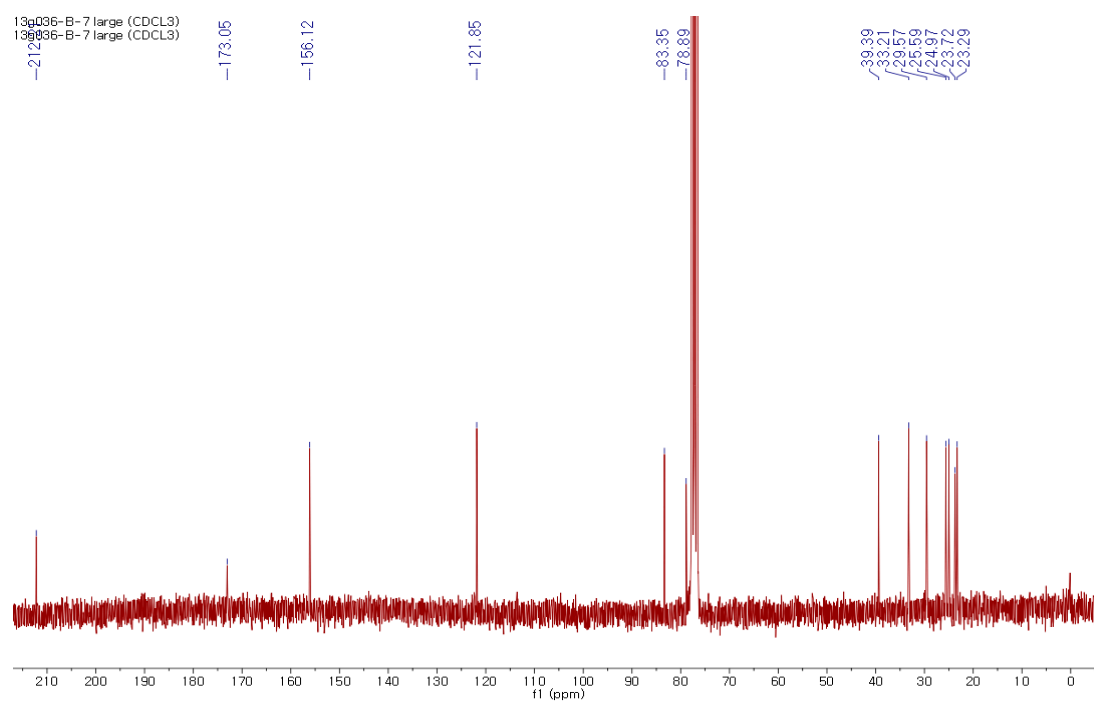


Figure S4: ¹³C NMR Spectrum of Compound **1** (CDCl₃, 62.5 MHz)

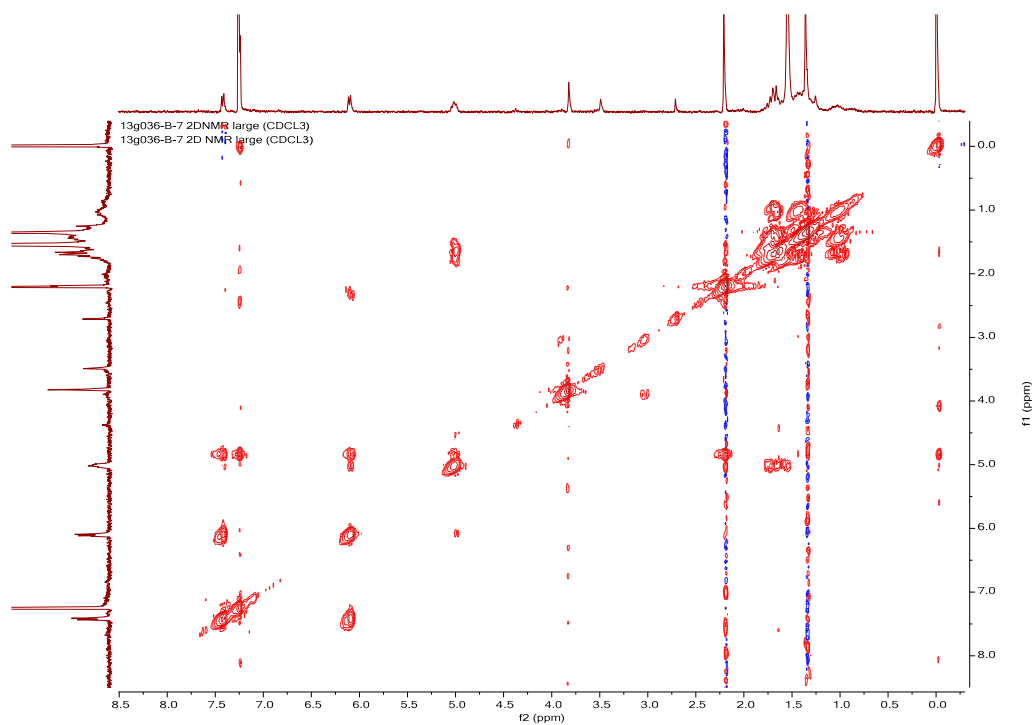


Figure S5: COSY Spectrum of Compound **1** (CDCl₃, 250 MHz)

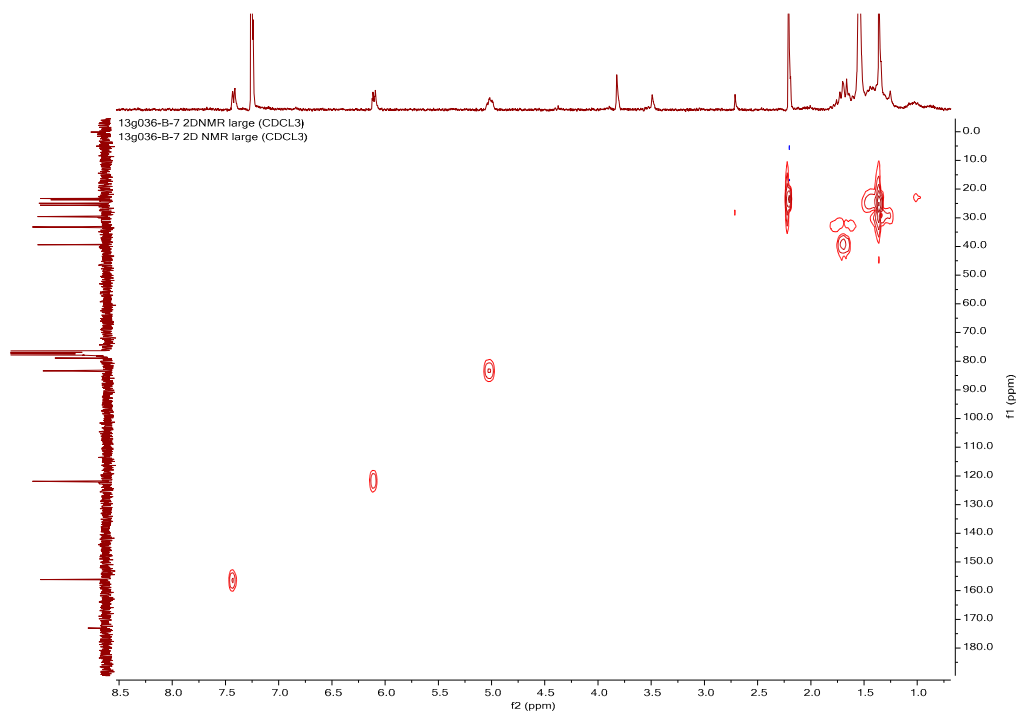


Figure S6: HMBC Spectrum of Compound **1** (CDCl₃, 250 MHz)

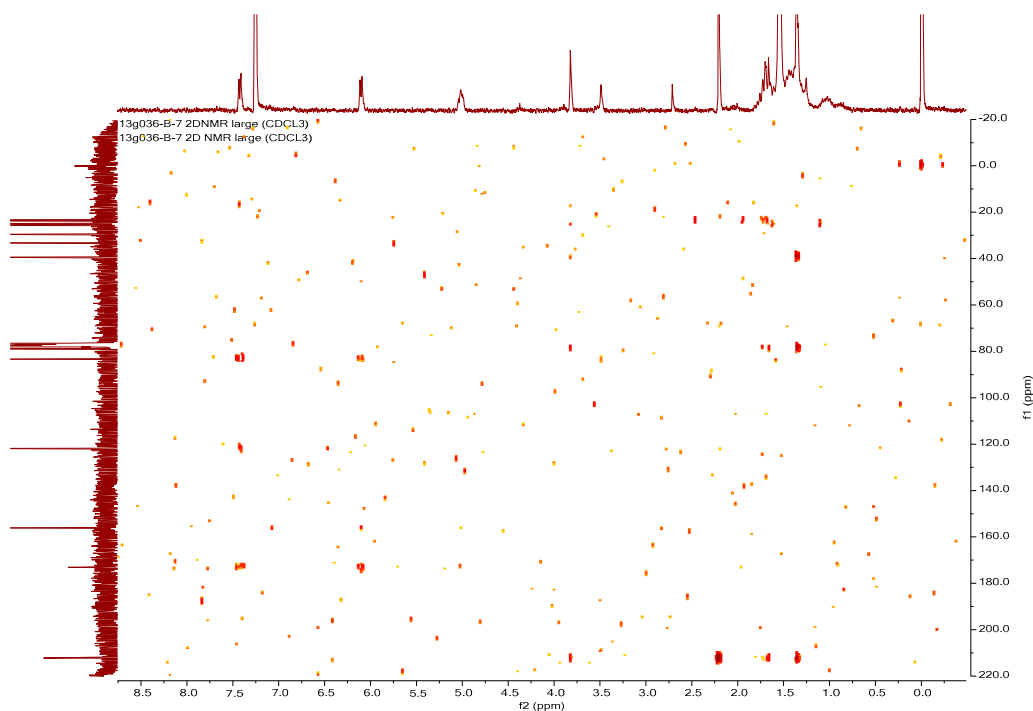


Figure S7: HMBC Spectrum of Compound **1** (CDCl₃, 250 MHz)

[Elemental Composition]
 Data : FAB-R084
 Sample: 13G036-B-'/
 Note : m-NBA
 Inlet : Direct
 RT : 0.18 min
 Elements : C 100/0, H 100/0, N 10/0, O 10/0
 Mass Tolerance : 20ppm, 5mmu if m/z < 250, 10mmu if m/z > 500
 Unsaturation (U.S.) : -0.5 - 50.0

Date : 19-Jul-2018 11:23

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[Theoretical Ion Distribution]
 Molecular Formula : C13 H21 O4
 (m/z 241.1440, MW 241.3073, U.S. 3.5)
 Base Peak : 241.1440, Averaged MW : 241.3050(a), 241.3058(w)

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m/z	INT.
241.1440	100.0000 *****
242.1473	14.6114 *****
243.1496	1.7889 *
244.1522	0.1577
245.1547	0.0114
246.1572	0.0007

Figure S8: HR-FAB-MS Data of Compound **1**

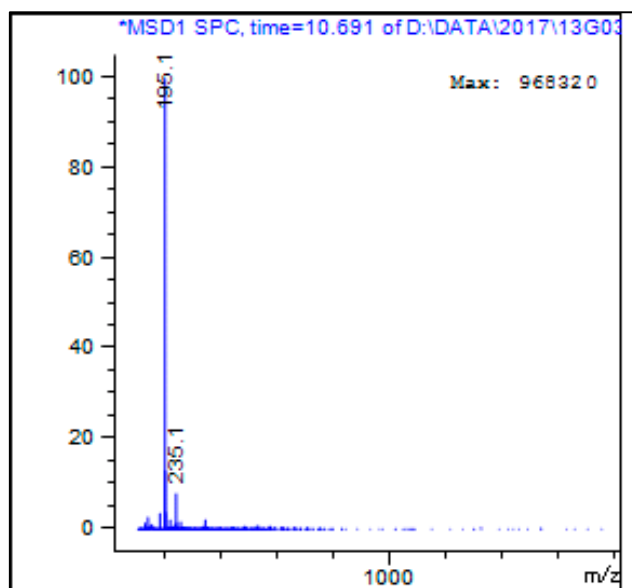


Figure S9: LR-ESI-MS Data of Compound **2**

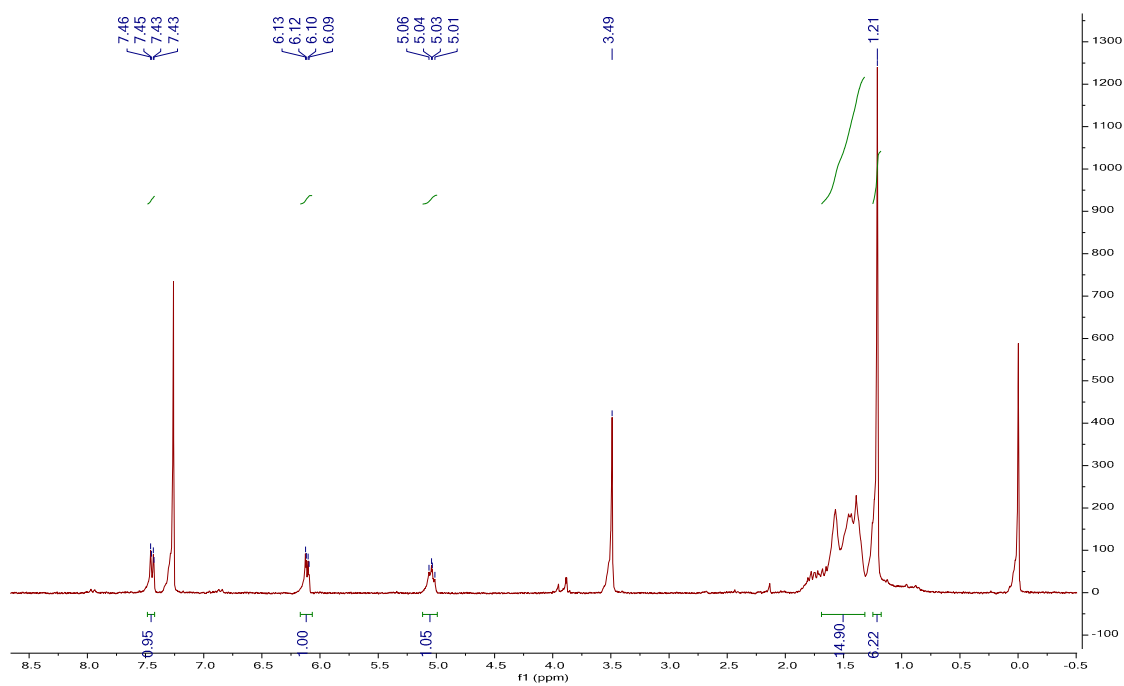


Figure S10: ^1H NMR Spectrum of Compound **2** (CDCl_3 , 250 MHz)

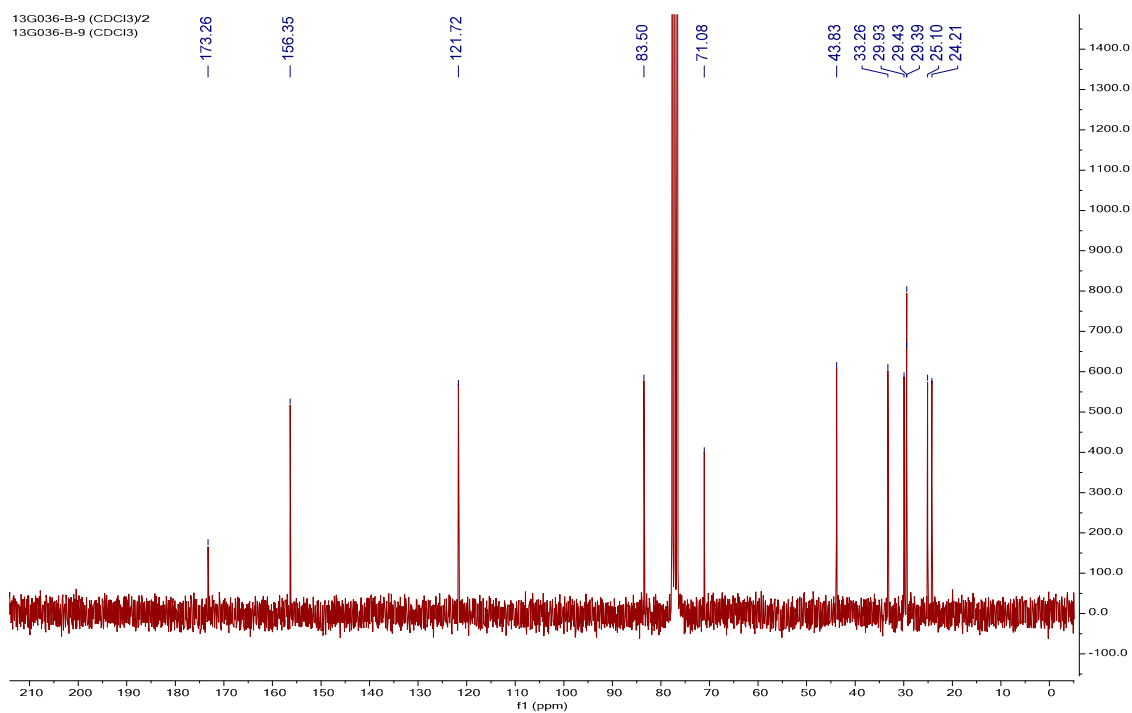


Figure S11: ¹³C NMR Spectrum of Compound **2** (CDCl₃, 62.5 MHz)

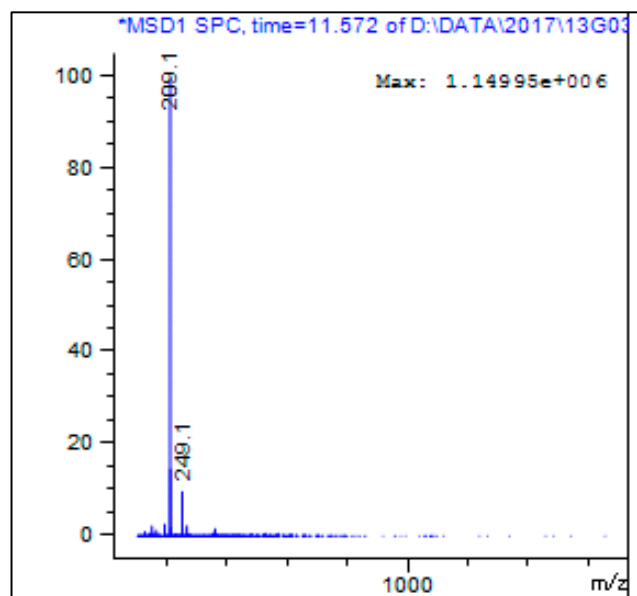


Figure S12: LR-ESI-MS Data of Compound **3**

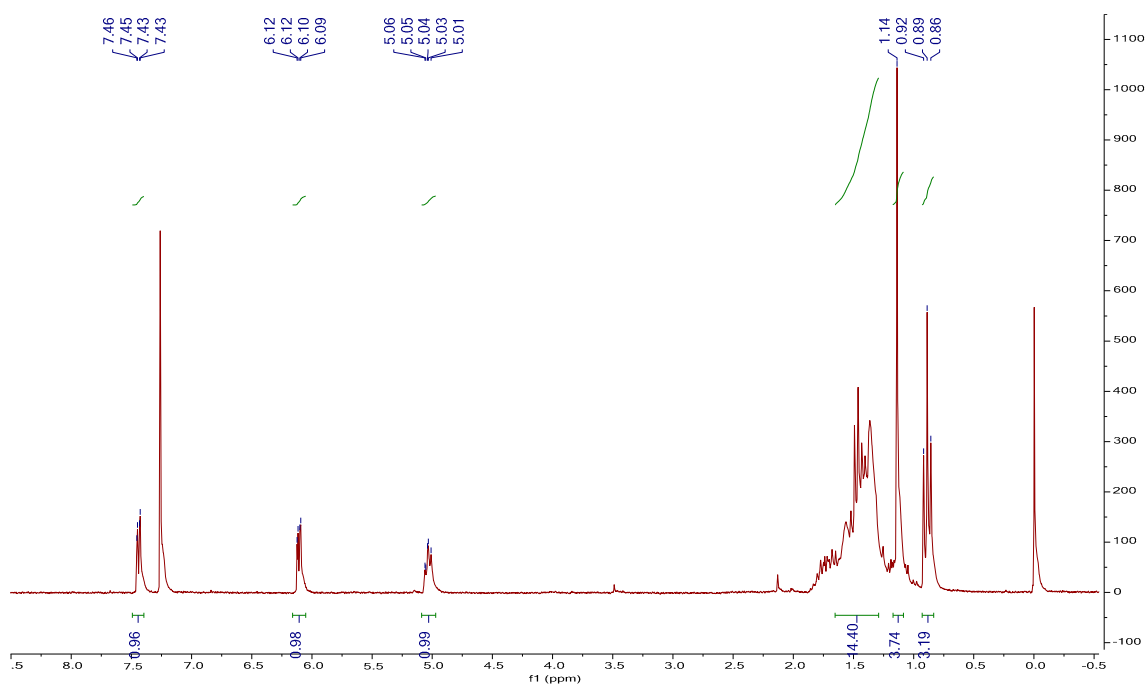


Figure S13: ¹H NMR Spectrum of Compound **3** (CDCl₃, 250 MHz)

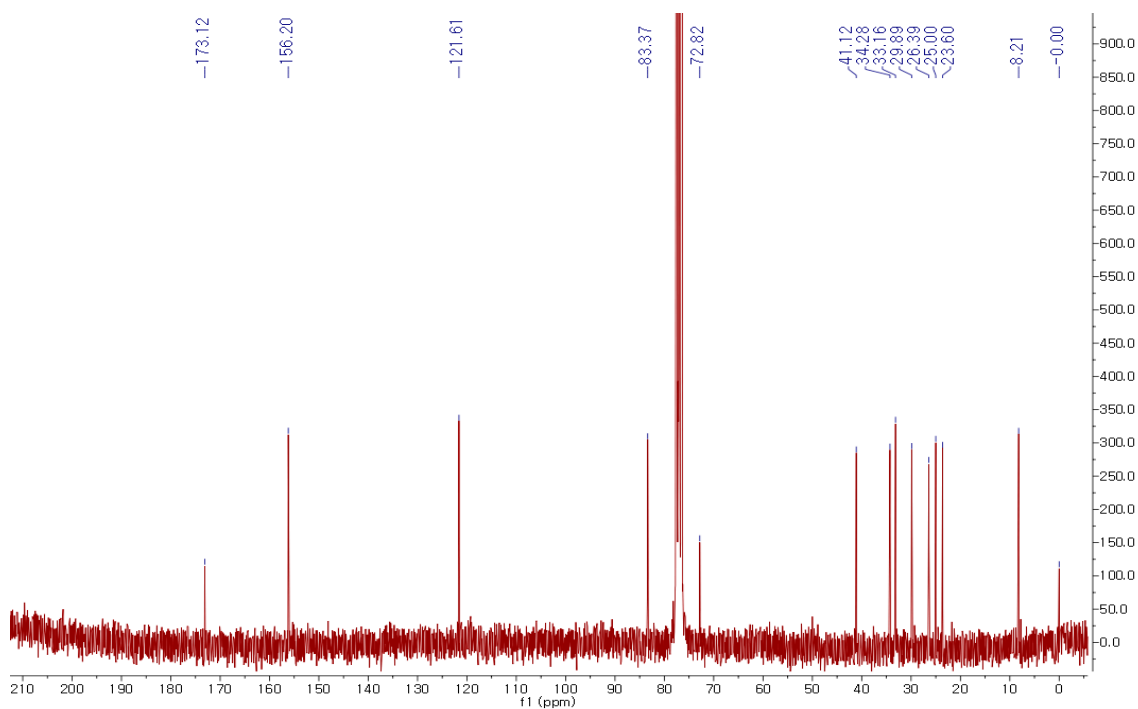


Figure S14: ¹³C NMR Spectrum of Compound **3** (CDCl₃, 62.5 MHz)

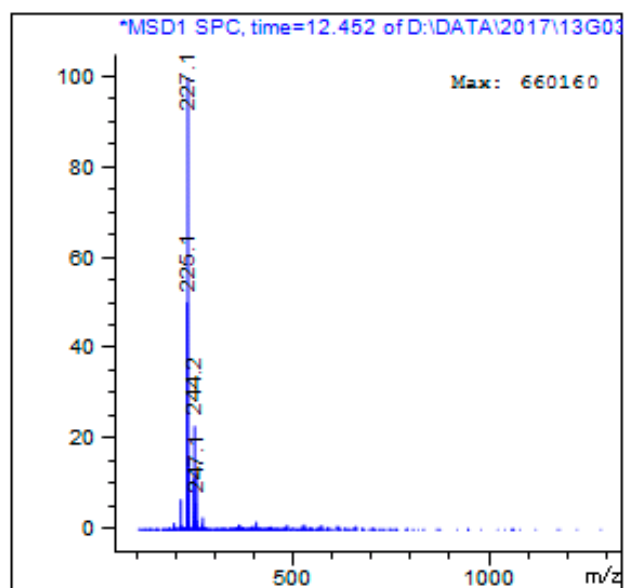


Figure S15: LR-ESI-MS Data of Compound **4**

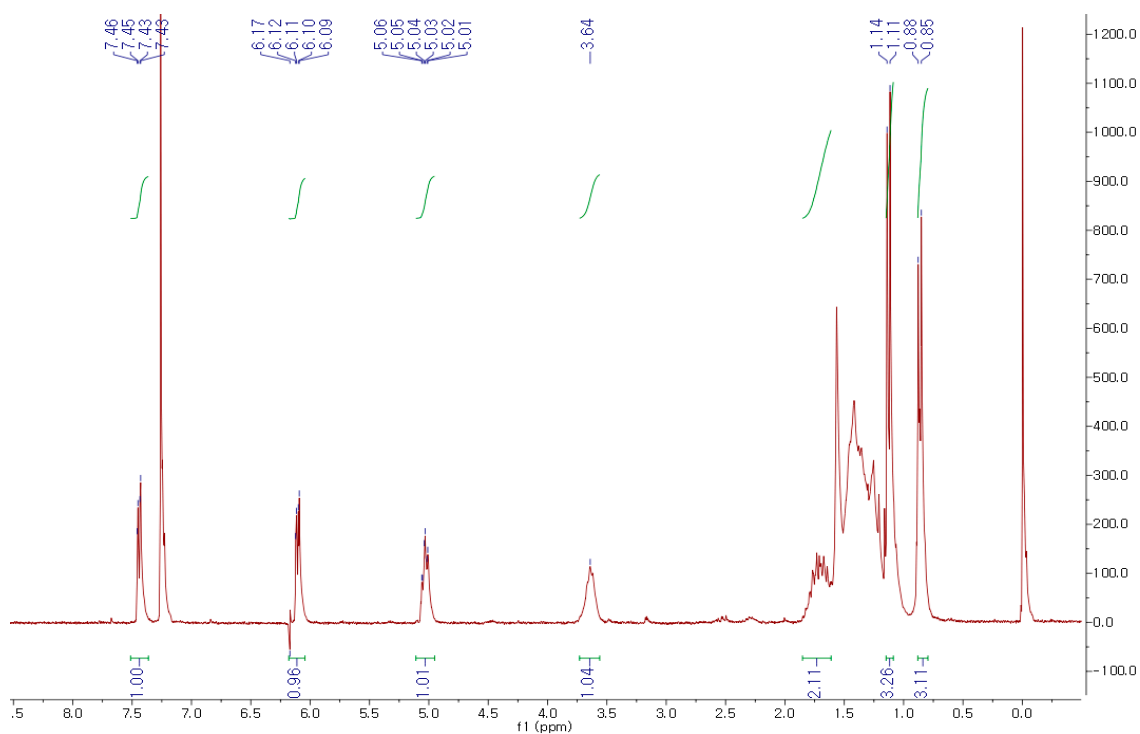


Figure S16: ¹H NMR Spectrum of Compound **4** (CDCl₃, 250 MHz)

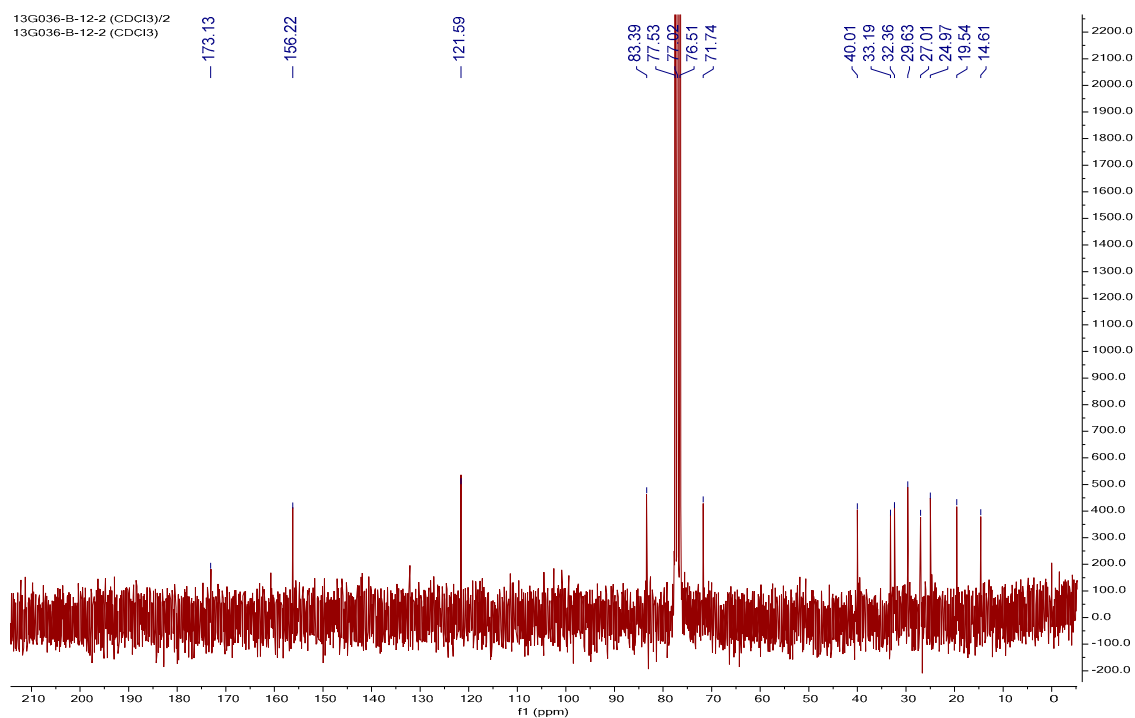


Figure S17: ^{13}C NMR Spectrum of Compound **4** (CDCl_3 , 62.5 MHz)

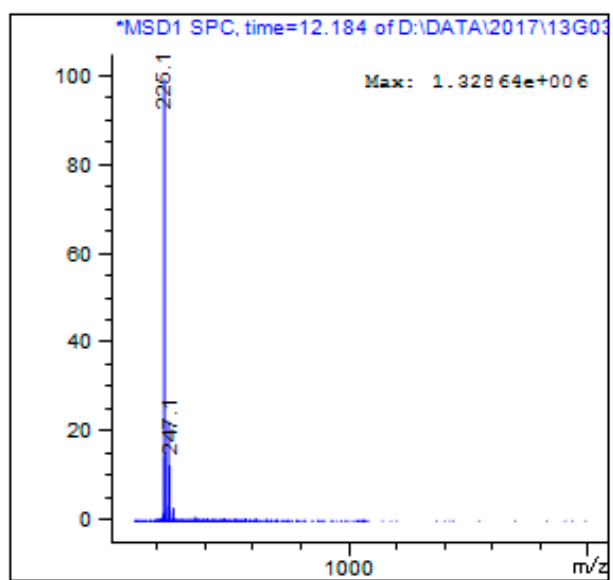


Figure S18: LR-ESI-MS Data of Compound **5**

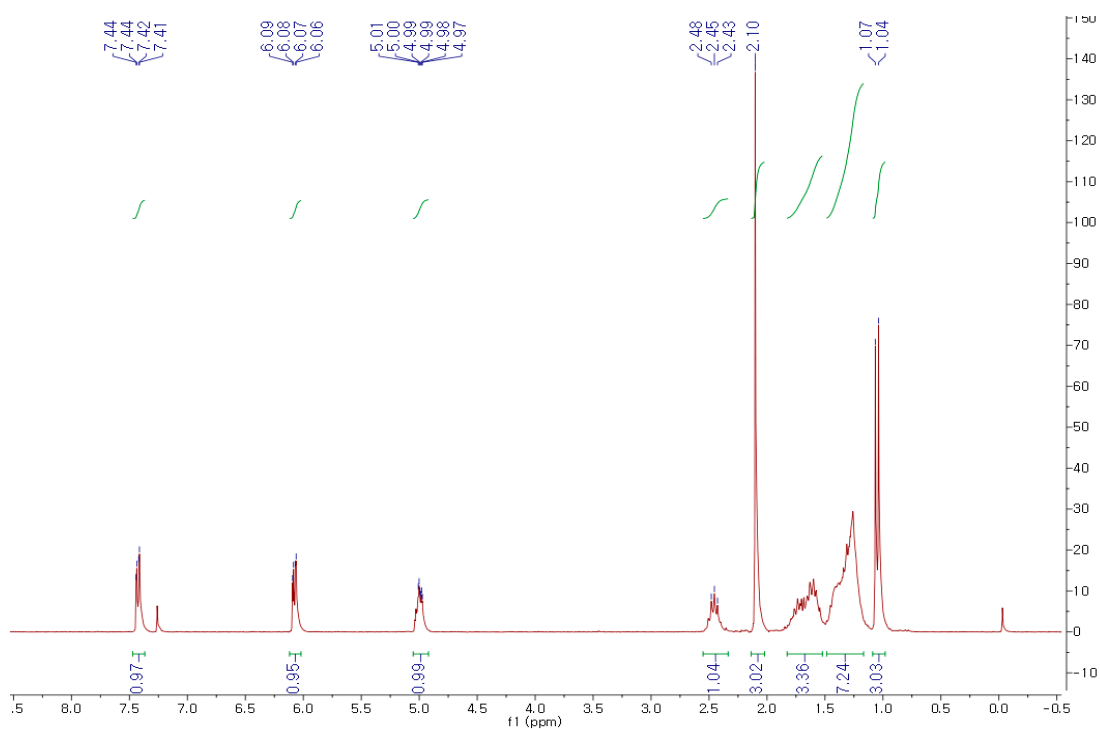


Figure S19: ¹H NMR Spectrum of Compound **5** (CDCl₃, 250 MHz)

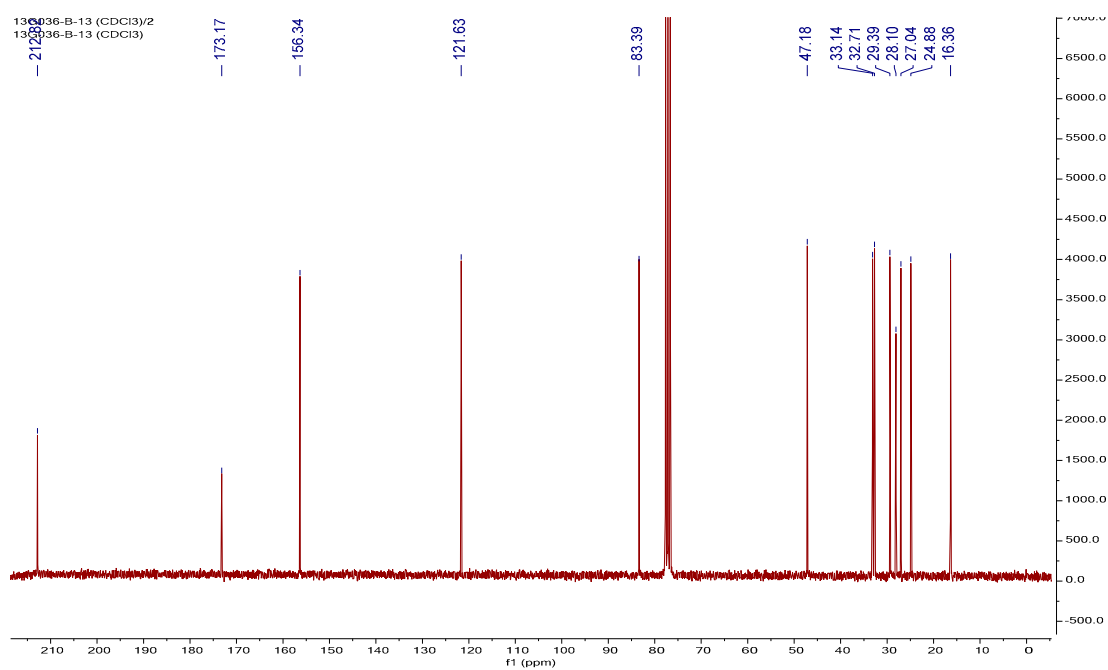


Figure S20: ¹³C NMR Spectrum of Compound **5** (CDCl₃, 62.5 MHz)

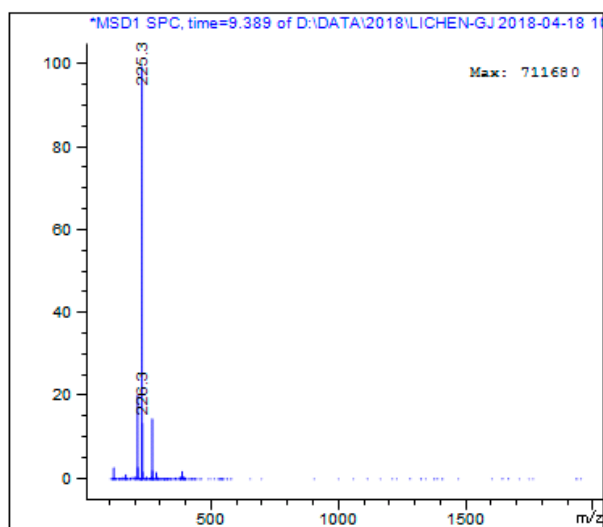


Figure S21: LR-ESI-MS Data of Compound **6**

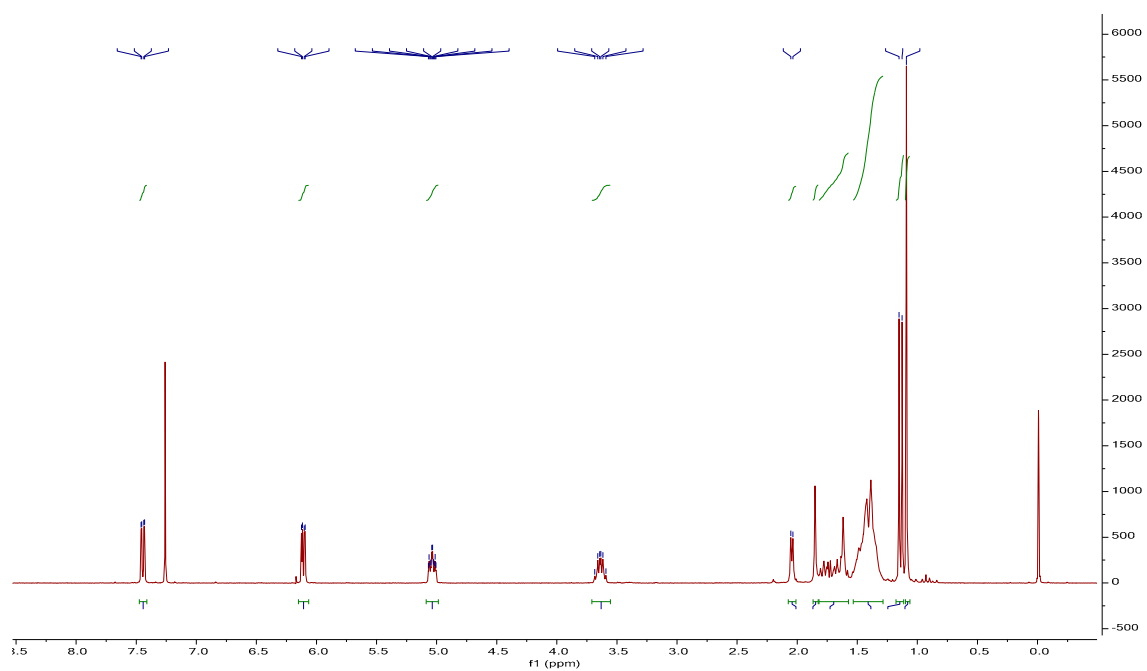


Figure S22: ¹H NMR Spectrum of Compound **6** (CDCl₃, 250 MHz)

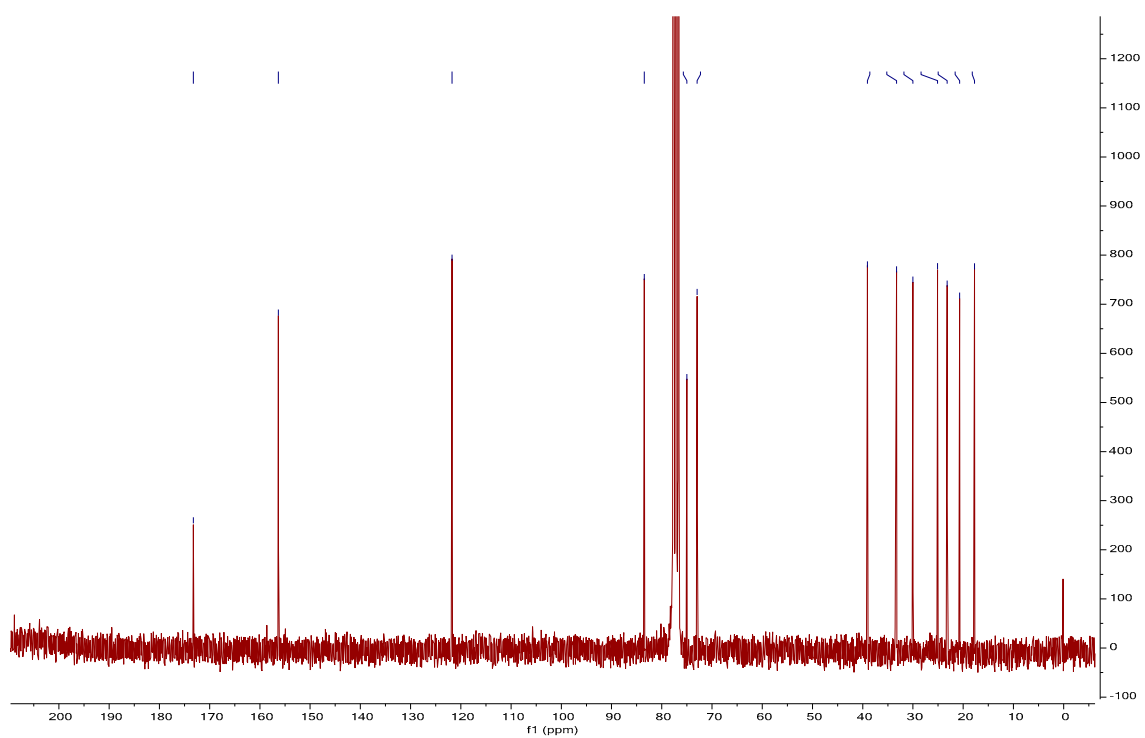


Figure S23: ^{13}C NMR Spectrum of Compound **6** (CDCl_3 , 62.5 MHz)

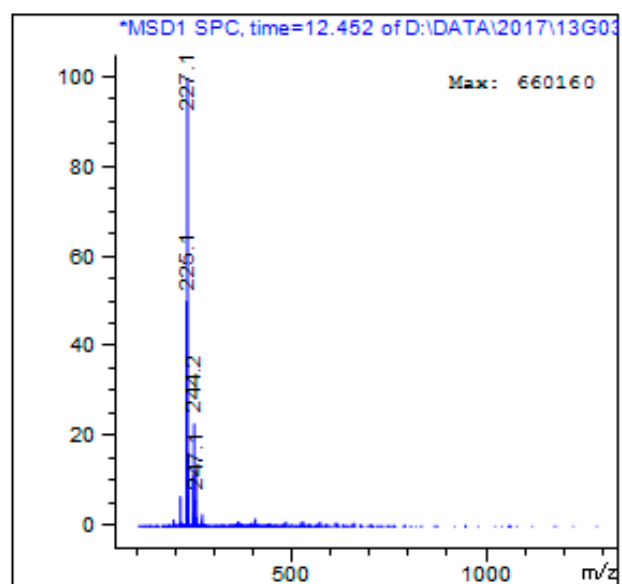


Figure S24: LR-ESI-MS data of Compound **7**

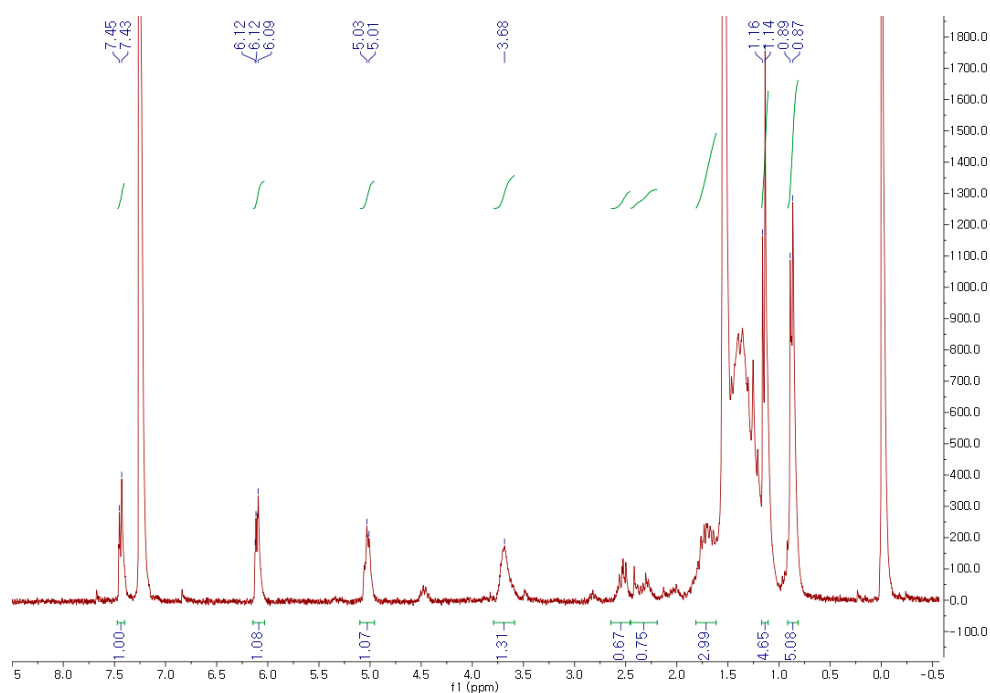


Figure S25: ¹H NMR Spectrum of Compound 7 (CDCl₃, 250 MHz)

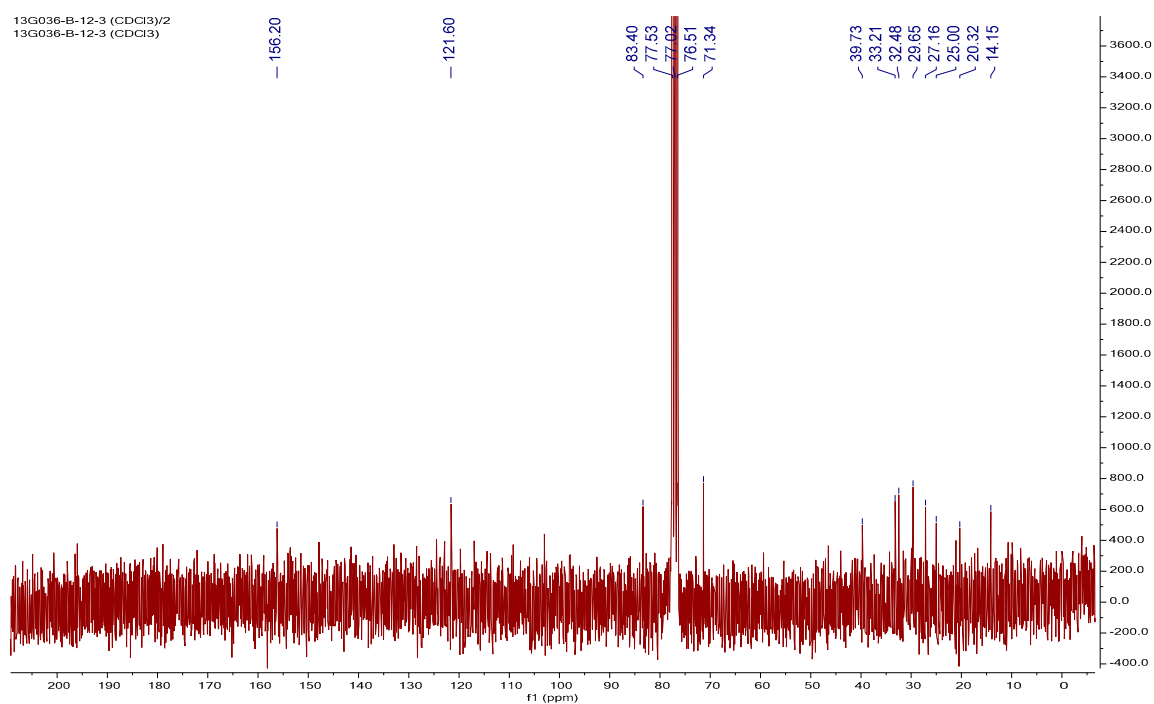


Figure S26: ¹³C NMR Spectrum of Compound 7 (CDCl₃, 62.5 MHz)