

# Supplementary Information

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Instrument: MAT 95XP(Thermo)  
D:\DATA-HR\14\101502-5b-5-1-c1

10/15/2014 11:04:18 AM

5B-5-1

101502-5b-5-1-c1 #8 RT: 0.25 AV: 1 NL: 2.02E3  
T: + c EI Full ms [ 370.50-382.50]

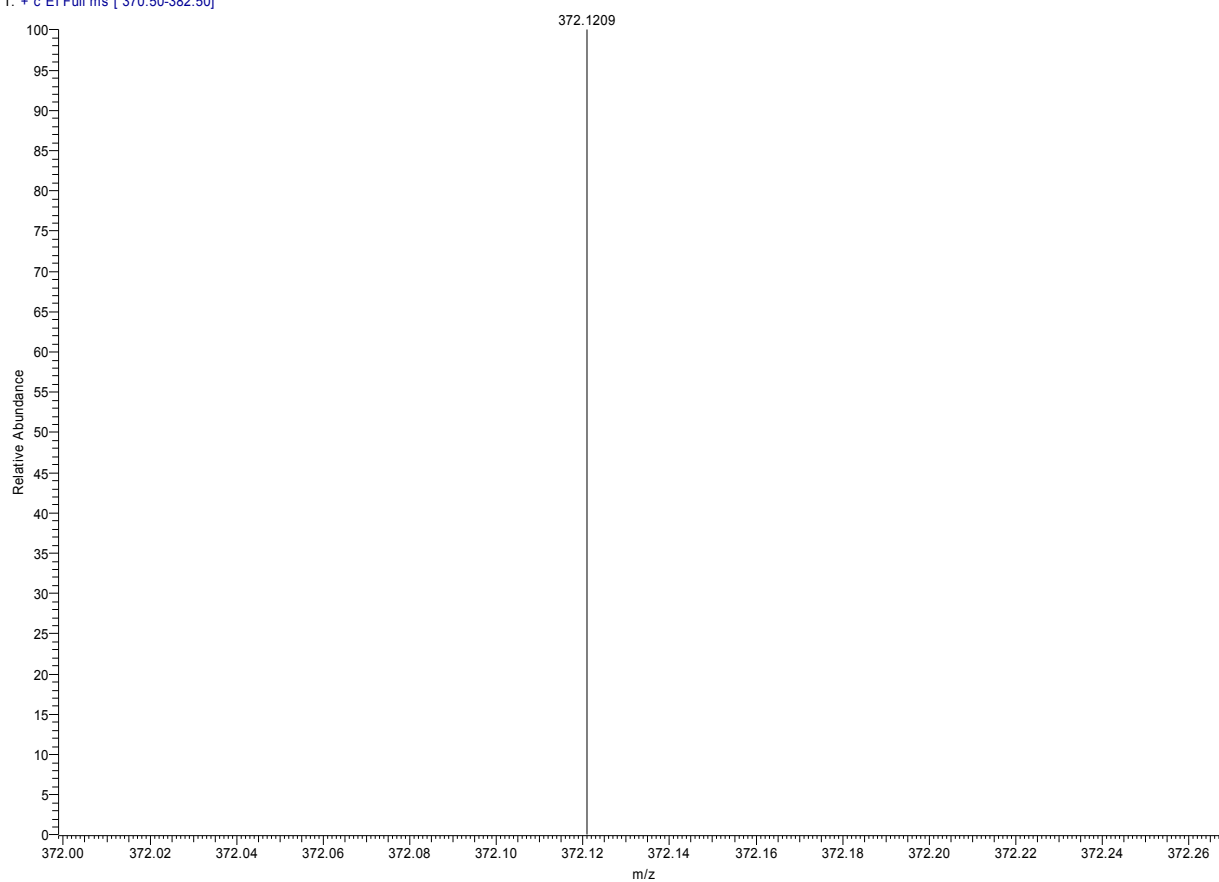


Figure S1. HREIMS spectrum of Compound 1.

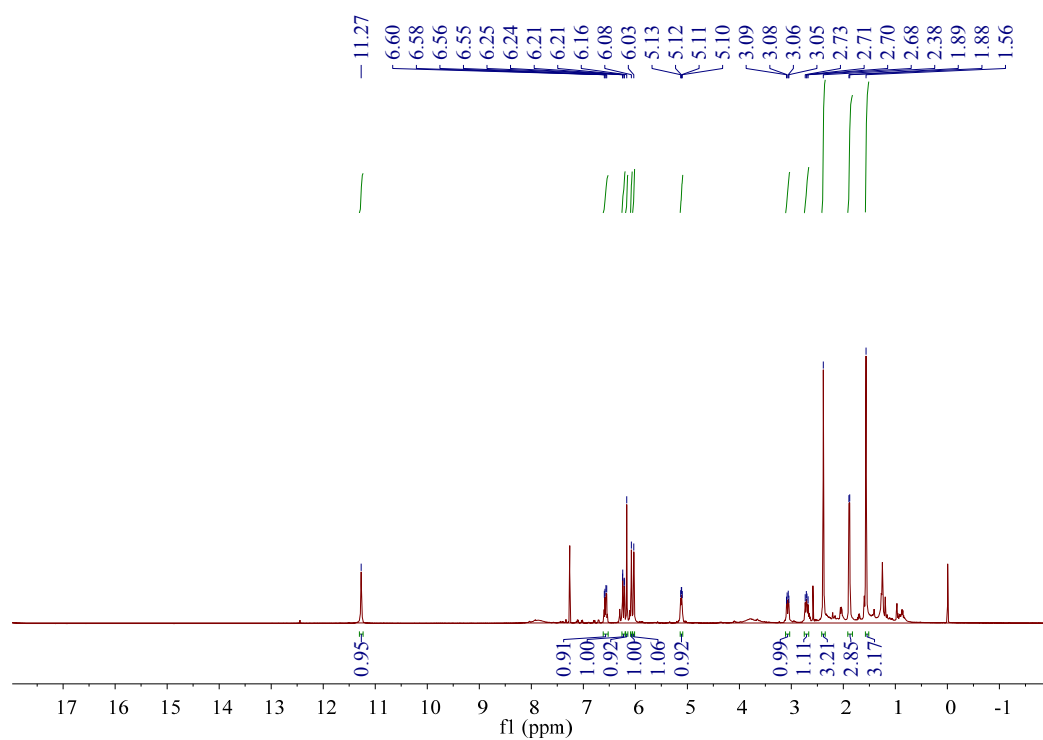
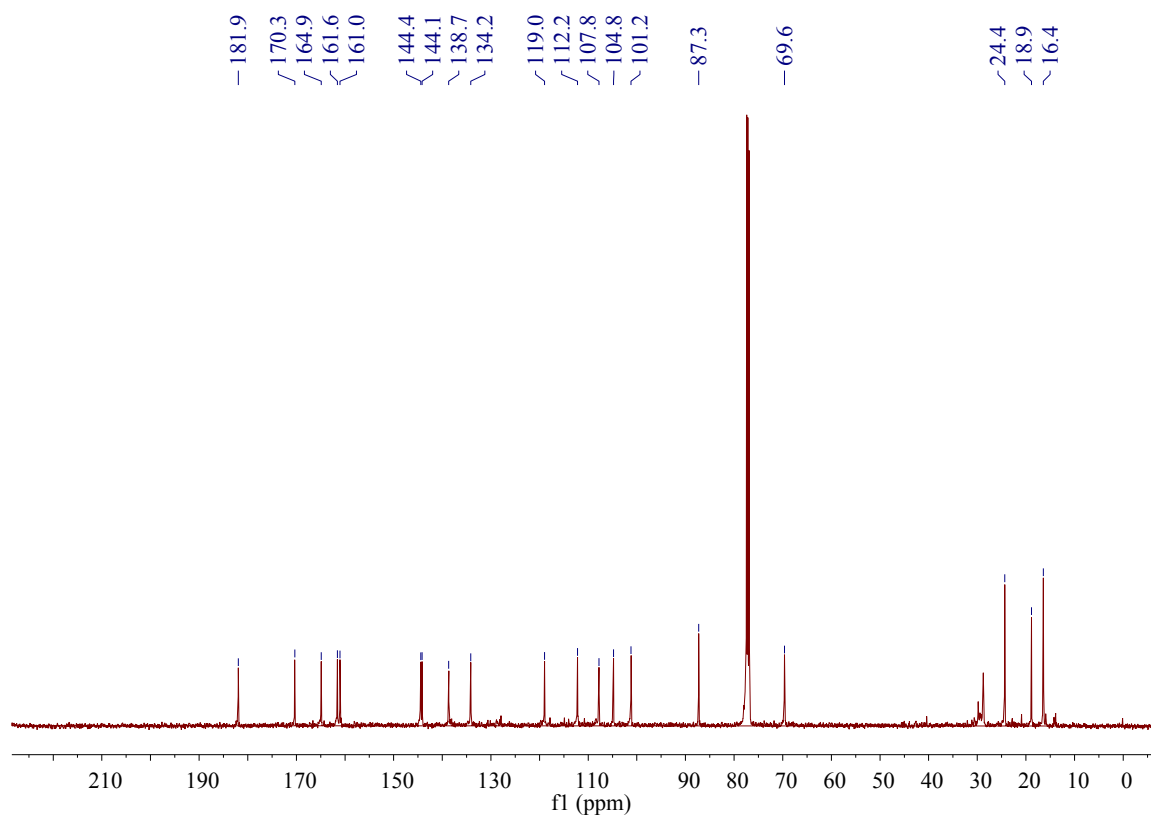
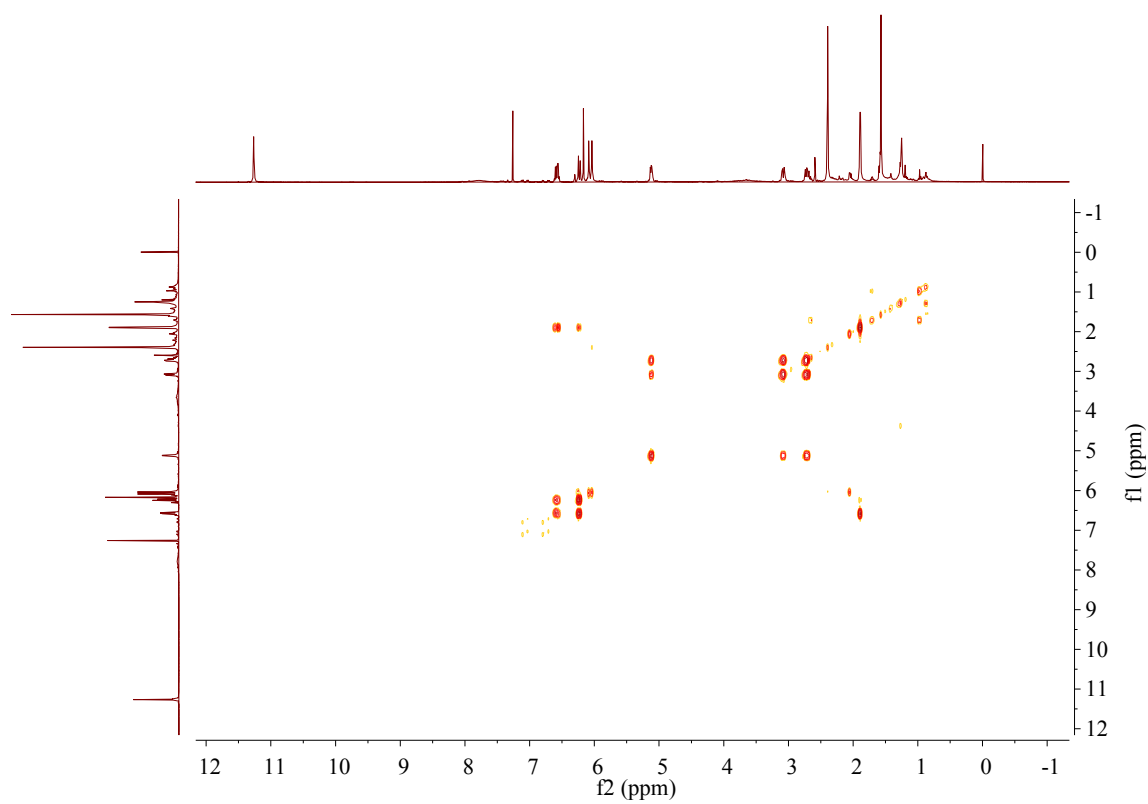


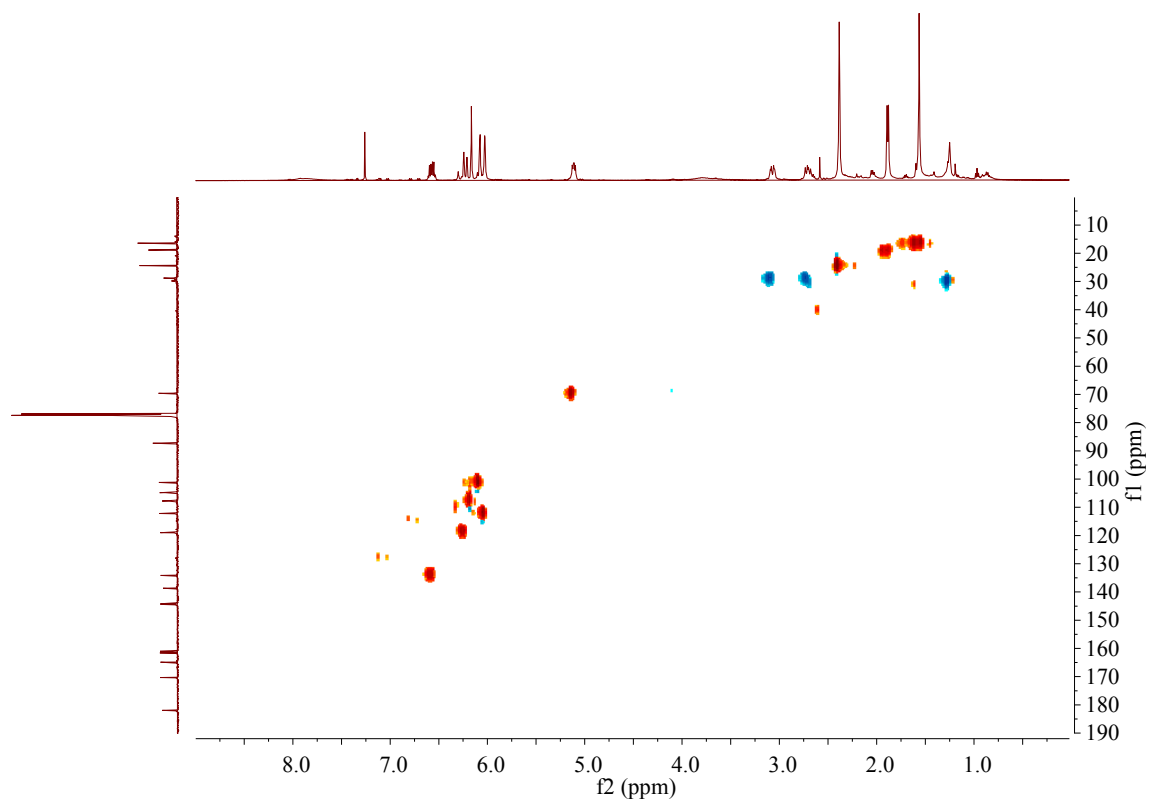
Figure S2. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of Compound 1.



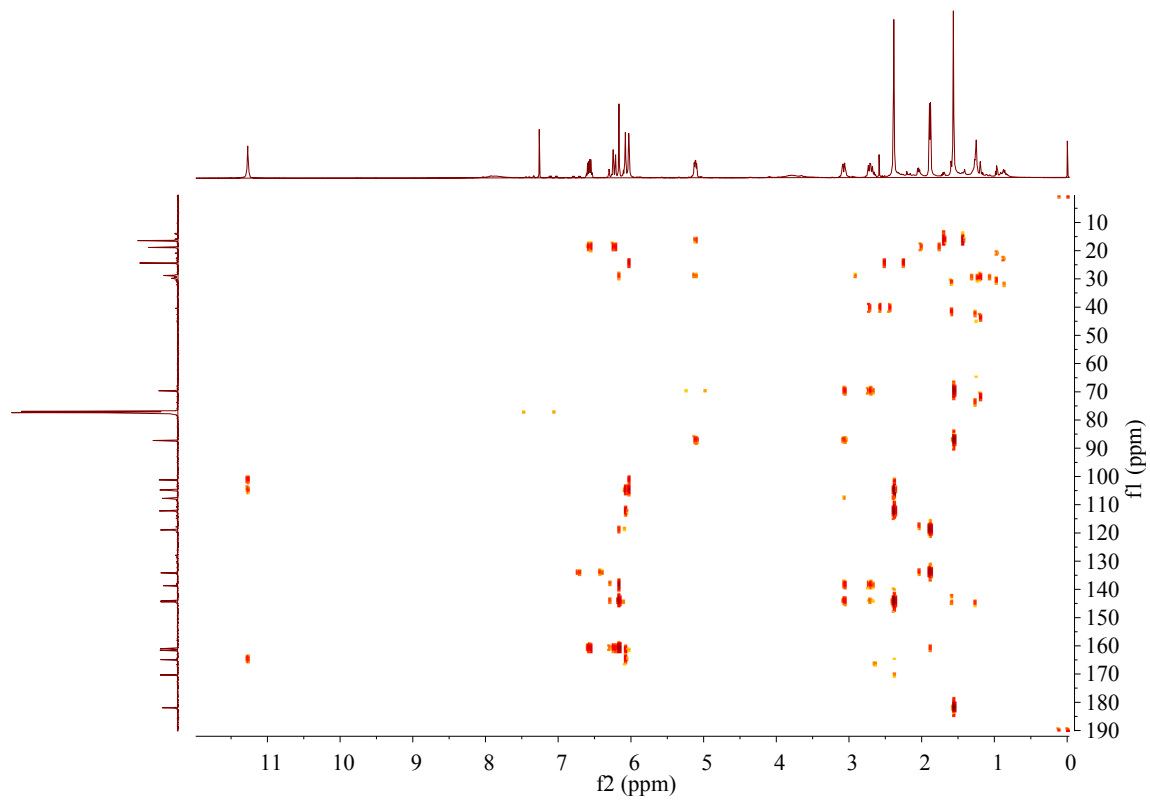
**Figure S3.** <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) spectrum of Compound 1.



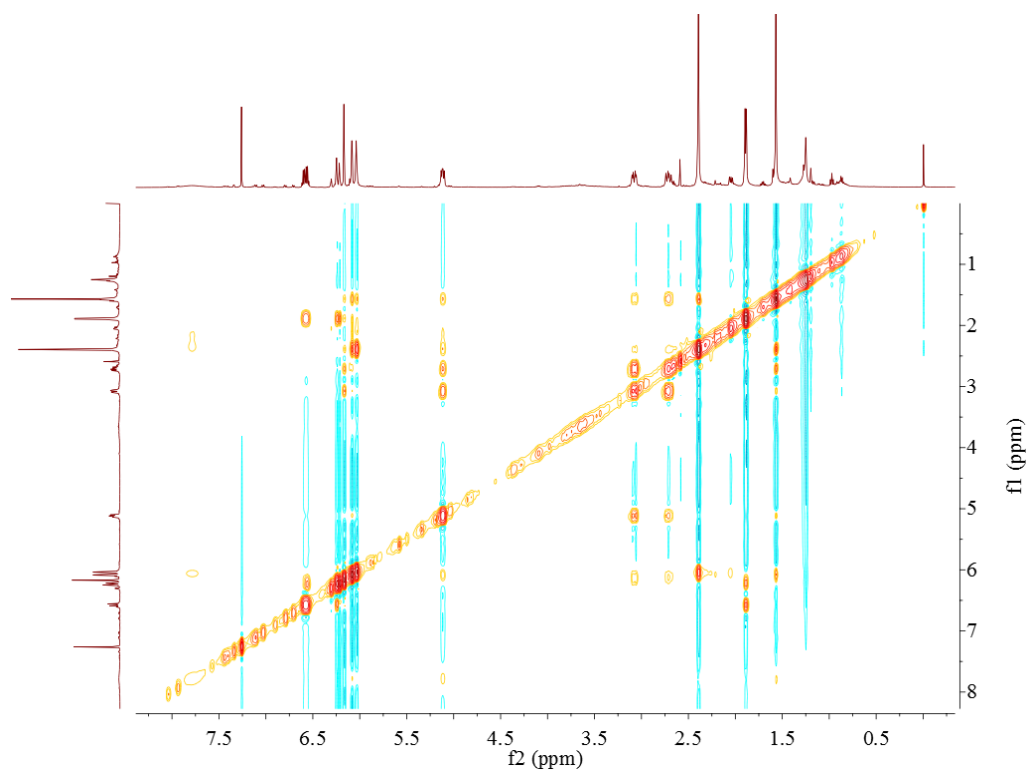
**Figure S4.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of Compound 1.



**Figure S5.** HSQC spectrum of Compound 1.



**Figure S6.** HMBC spectrum of Compound 1.



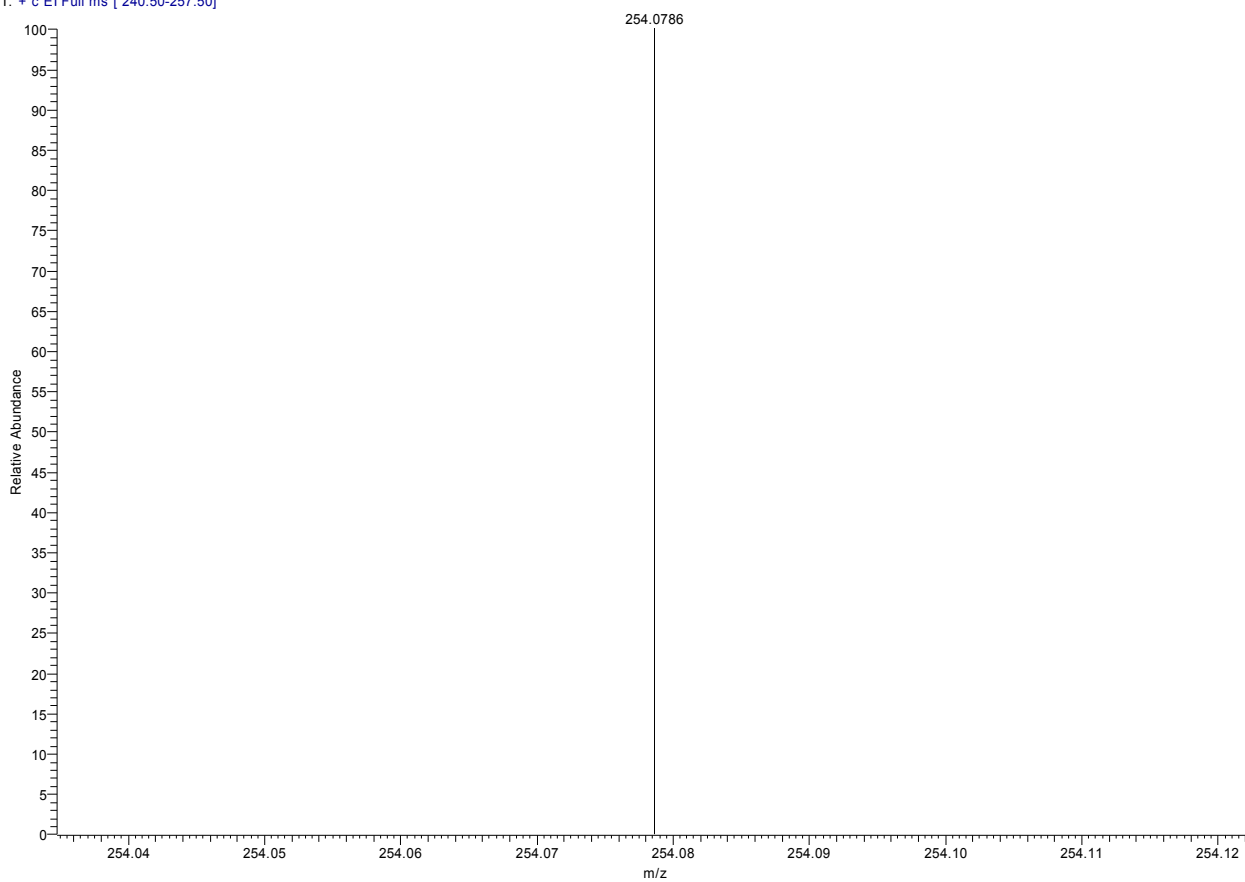
**Figure S7.** NOESY spectrum of Compound 1.

Instrument: MAT 95XP (Thermo)  
D:\DATA-HR\15\011901-hy9-5-1-c1

1/19/2015 10:18:20 AM

HY9-5-1

011901-hy9-5-1-c1 #3 RT: 0.12 AV: 1 NL: 1.67E4  
T: + e EI Full ms [ 240.50-257.50]



**Figure S8.** HREIMS spectrum of Compound 2.

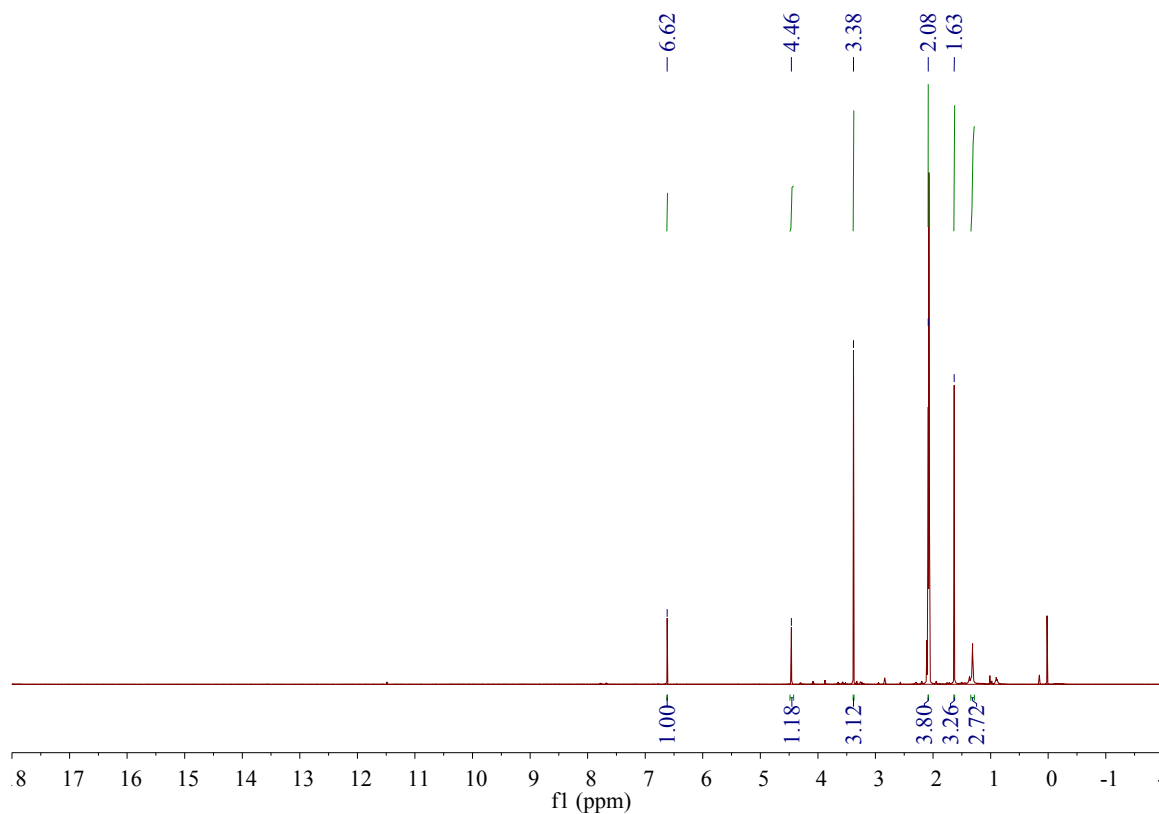


Figure S9. <sup>1</sup>H NMR (500 MHz, acetone-*d*<sub>6</sub>) spectrum of Compound 2.

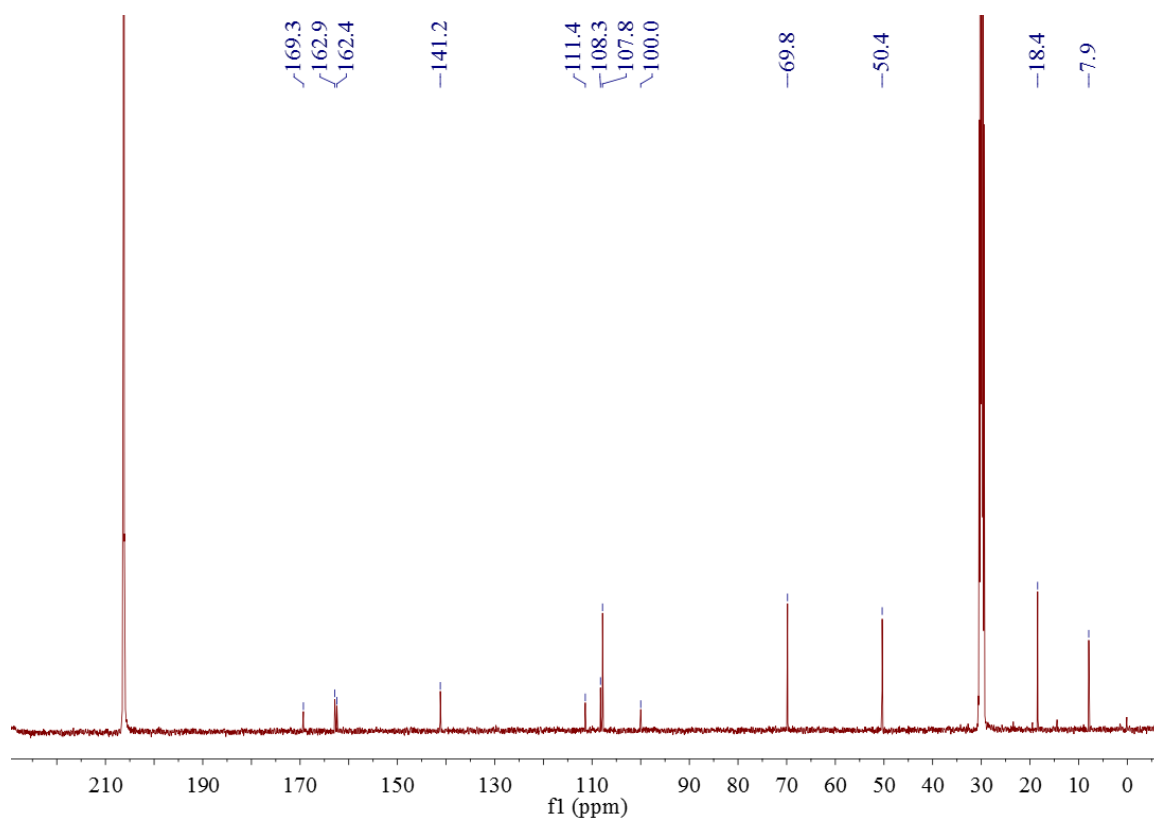


Figure S10. <sup>13</sup>C NMR (125 MHz, acetone-*d*<sub>6</sub>) spectrum of Compound 2.

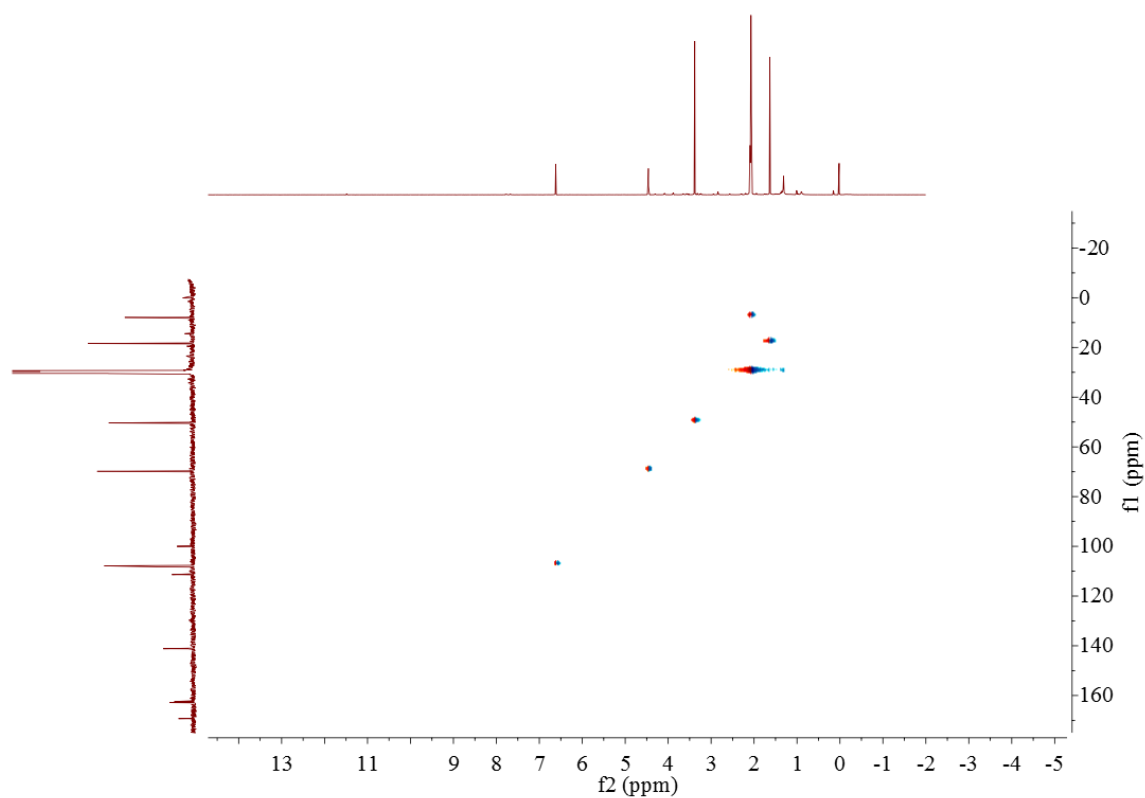


Figure S11. HSQC spectrum of Compound 2.

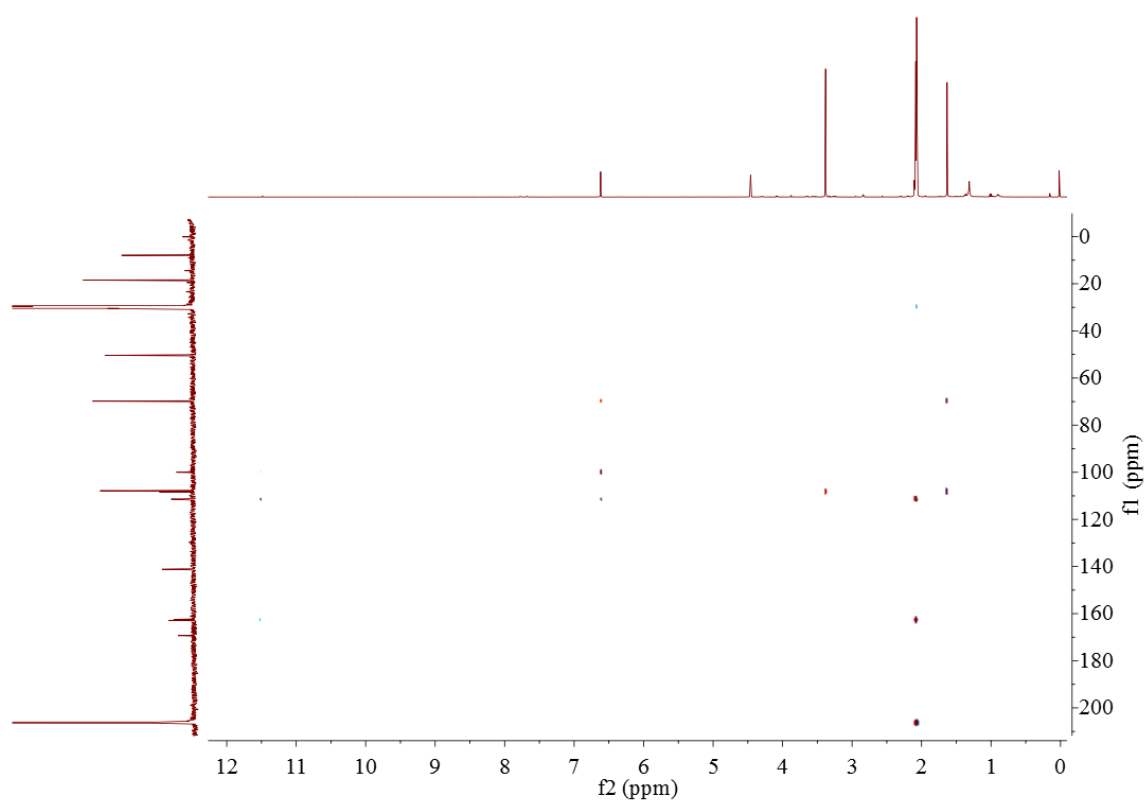
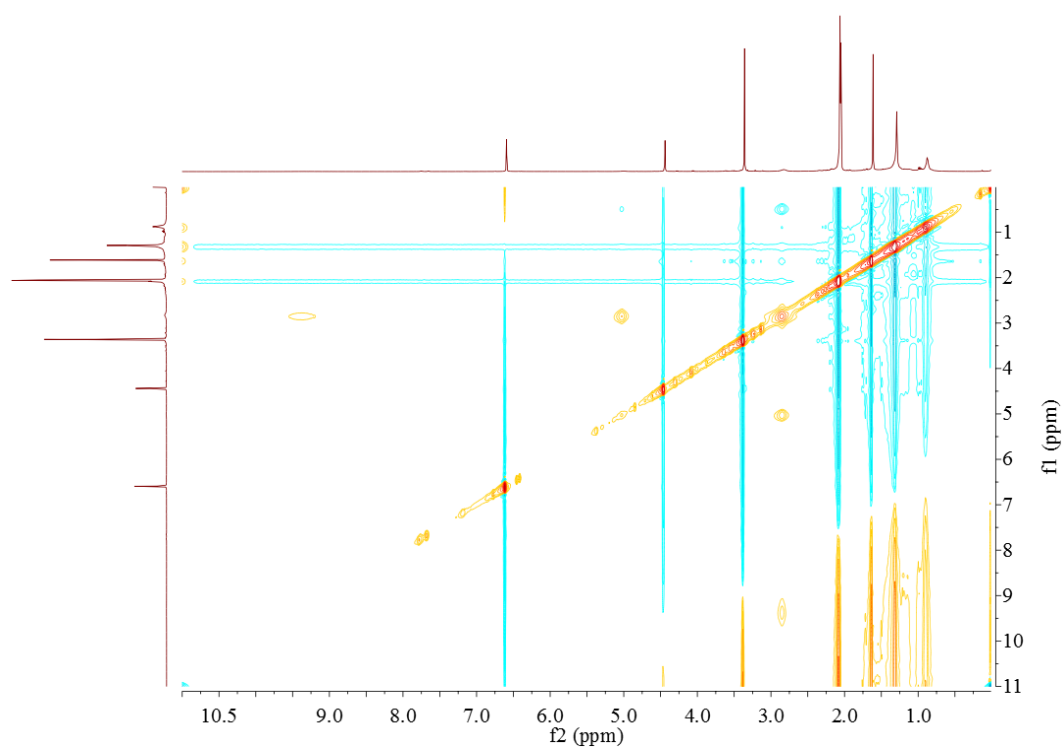


Figure S12. HMBC spectrum of Compound 2.



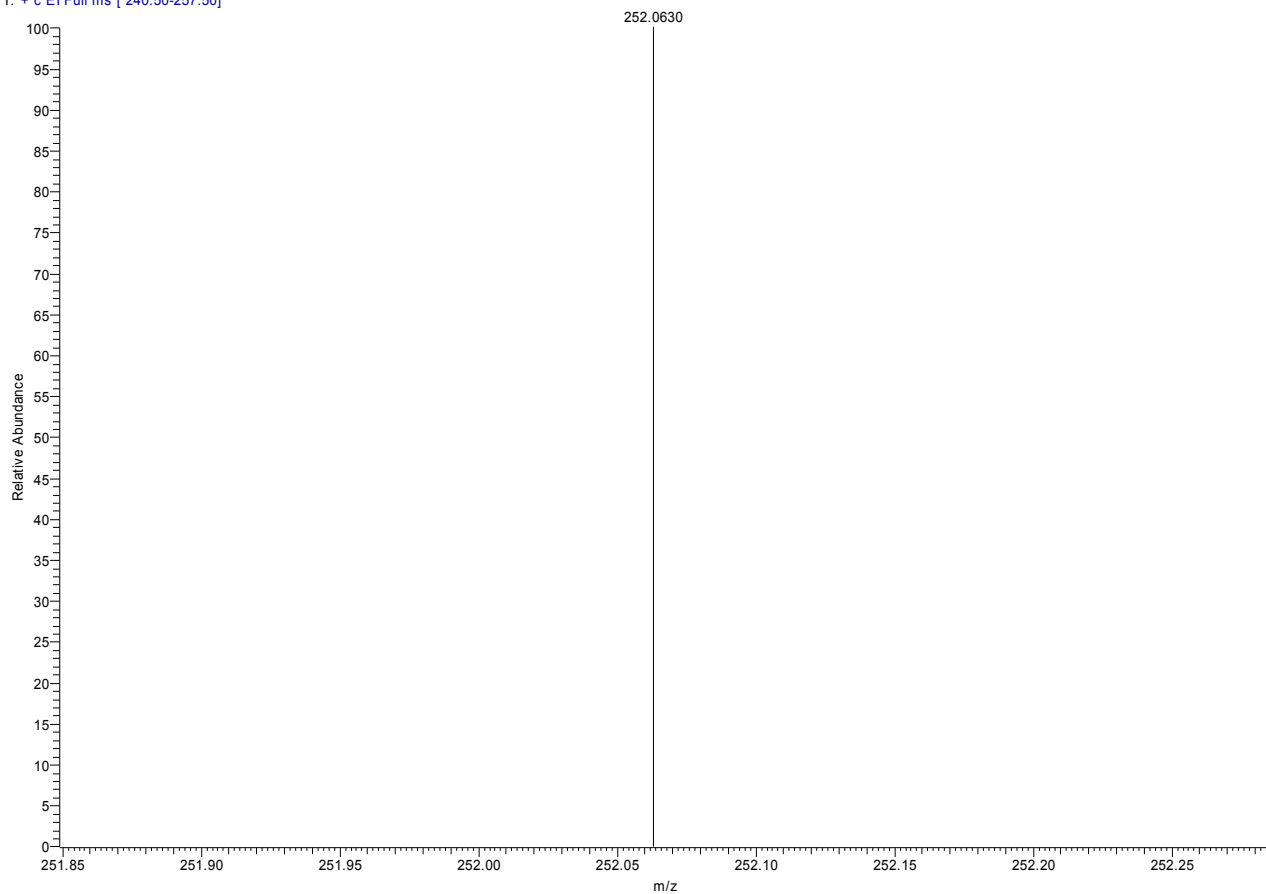
**Figure S13.** NOESY spectrum of Compound 2.

Instrument: MAT 95XP (Thermo)  
D:\DATA-HR\15\011902-hy9-3-1-1-c1

1/19/2015 10:25:06 AM

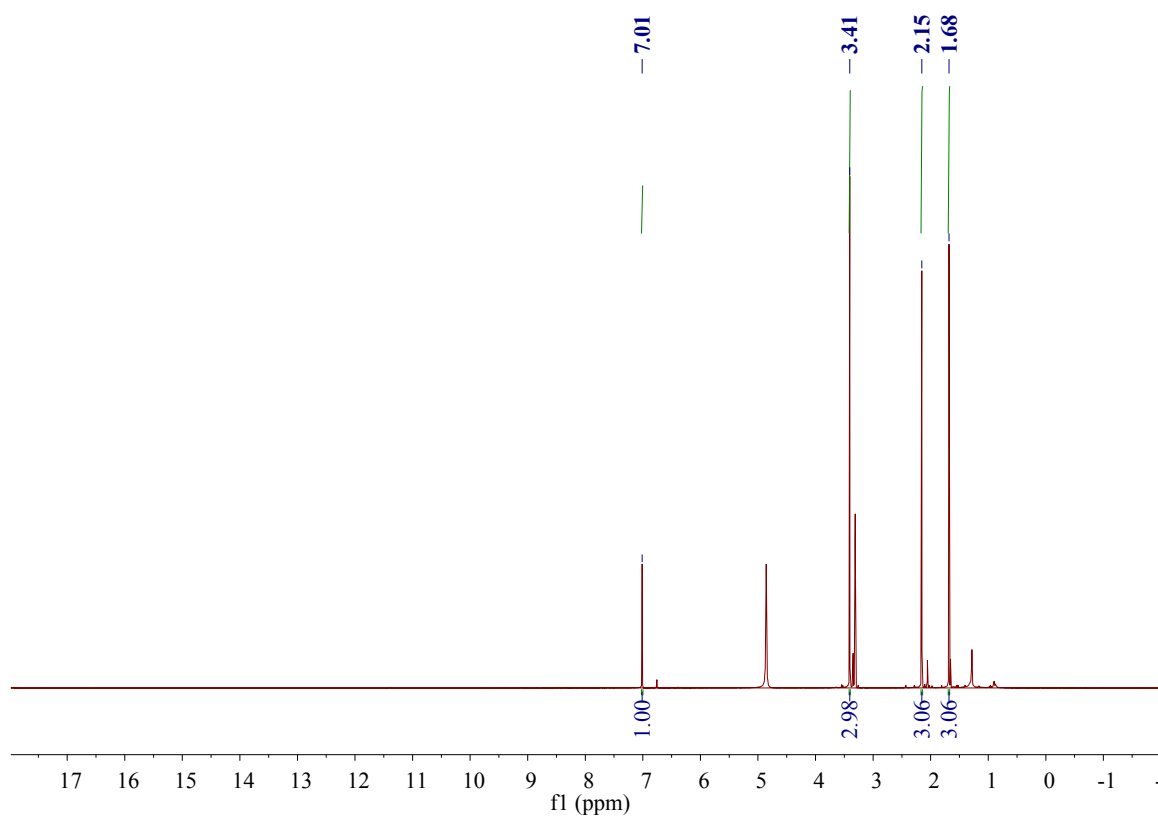
HY9-3-1-1

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T: + c EI Full ms [ 240.50-257.50]

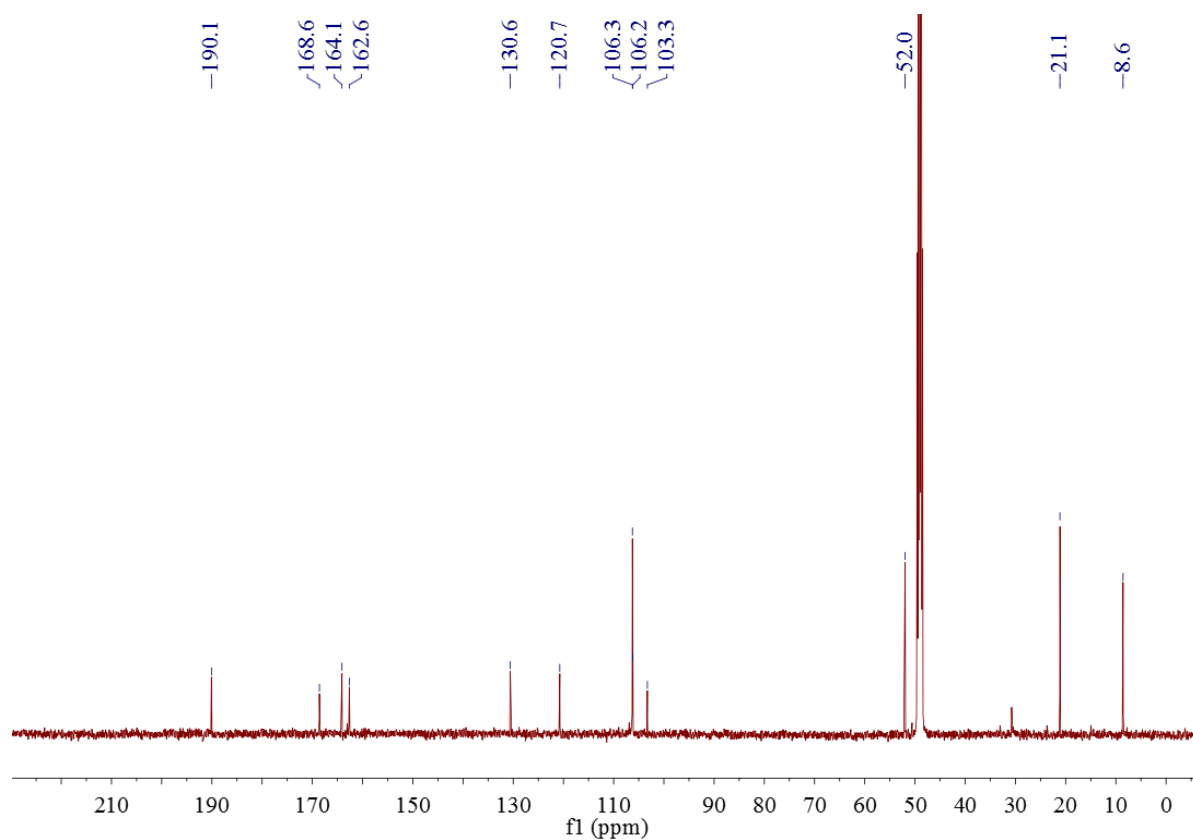


**Figure S14.** HREIMS spectrum of Compound 3.

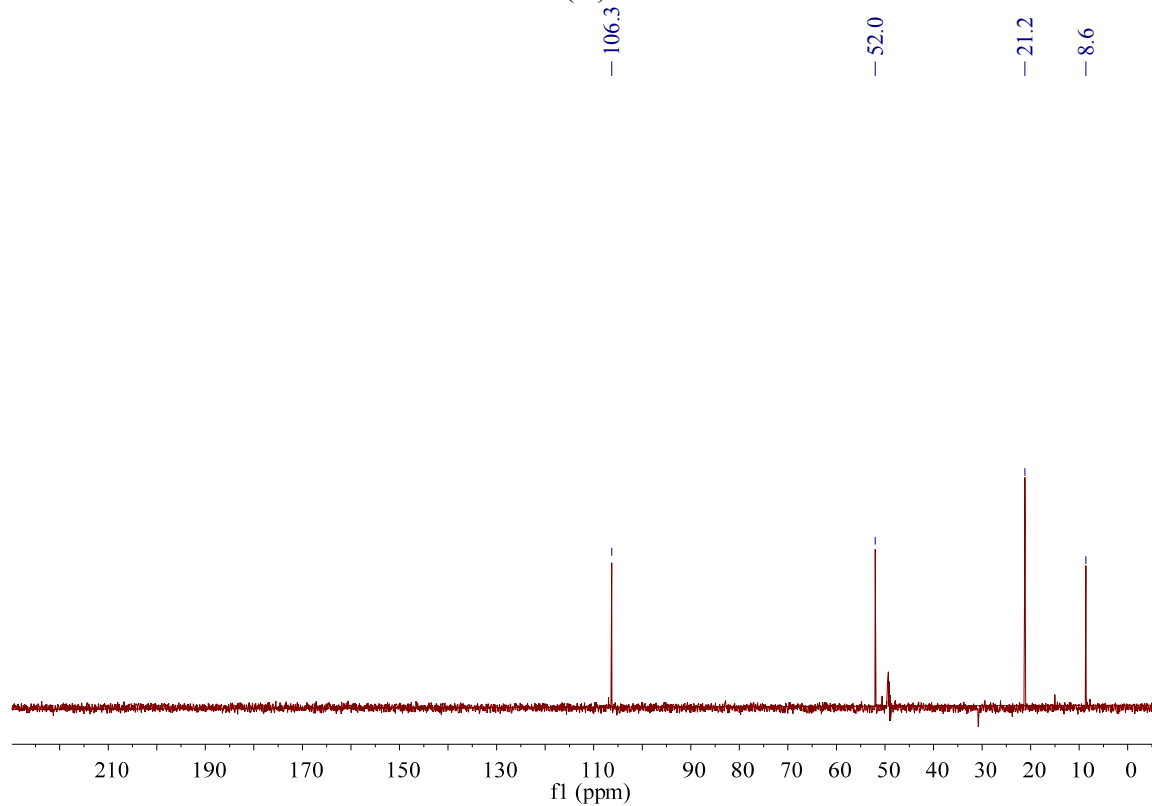




**Figure S15.**  $^1\text{H}$  NMR (500 MHz, Methanol- $d_4$ ) spectrum of Compound 3.

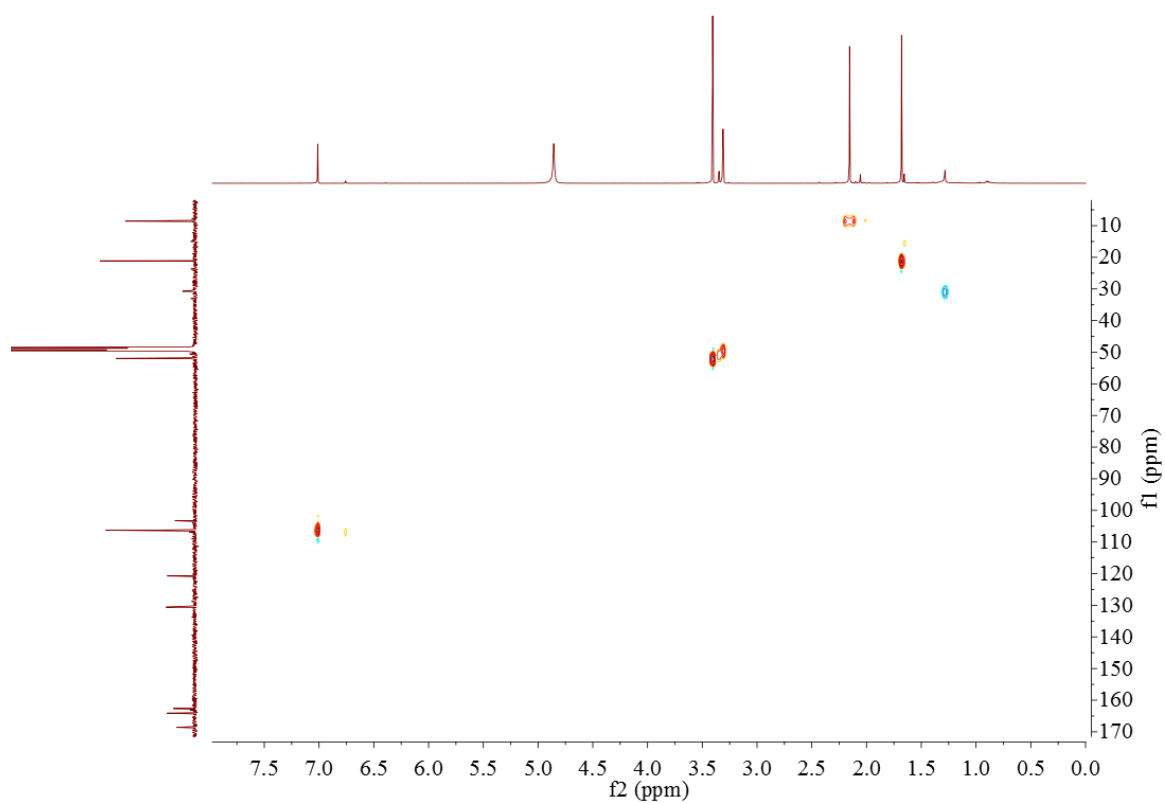


(A)

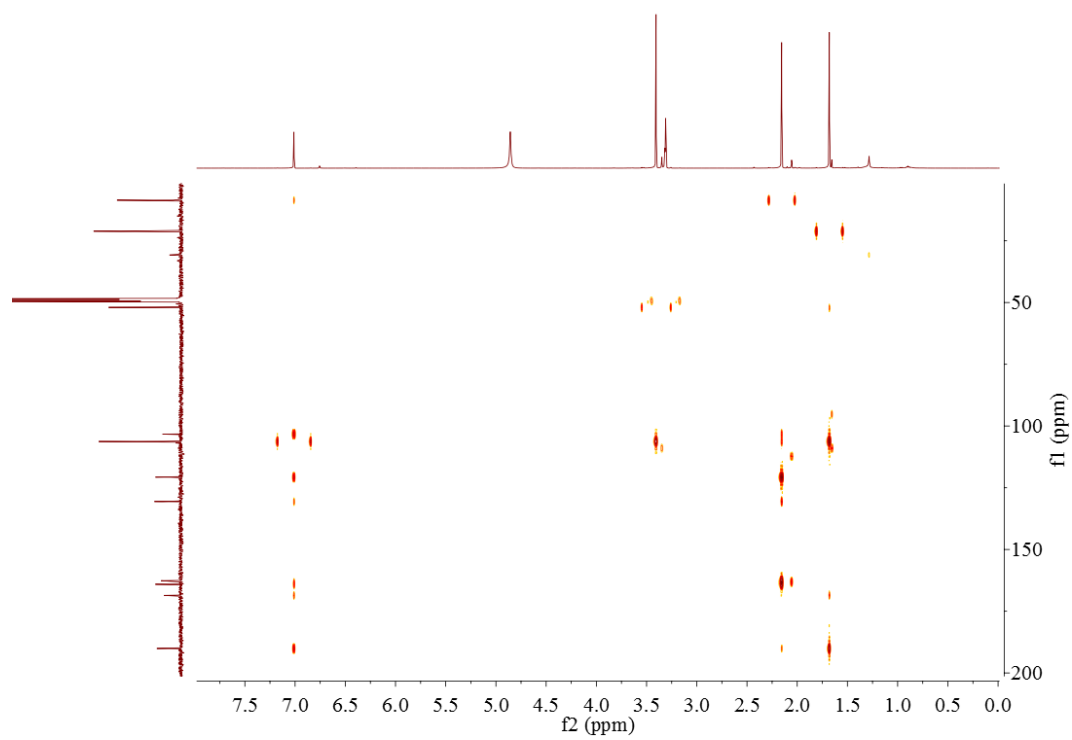


(B)

**Figure S16.**  $^{13}\text{C}$  NMR (125 MHz, Methanol- $d_4$ ) (A) and DEPT spectra of Compound **3** (B).



**Figure S17.** HSQC spectrum of Compound 3.



**Figure S18.** HMBC spectrum of Compound 3.

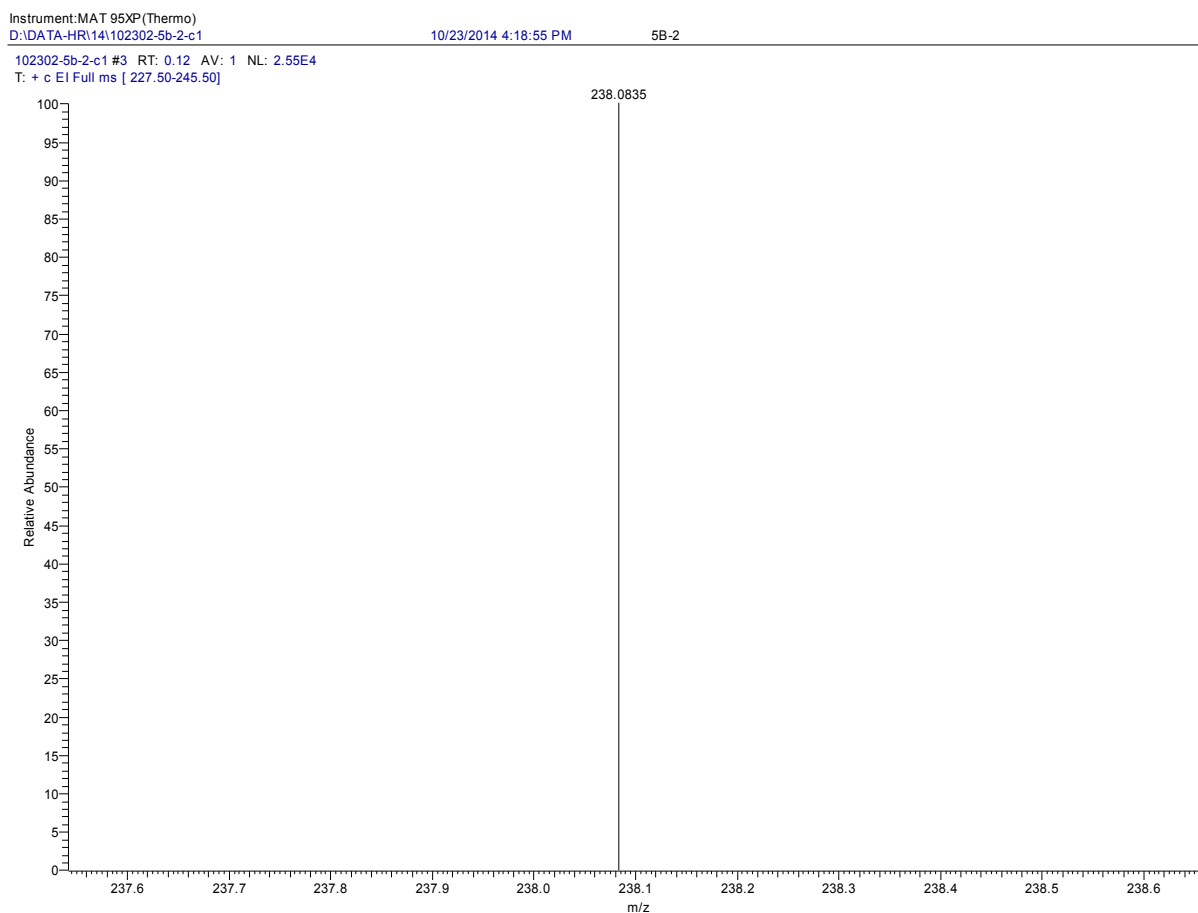


Figure S19. HREIMS spectrum of Compound 4.

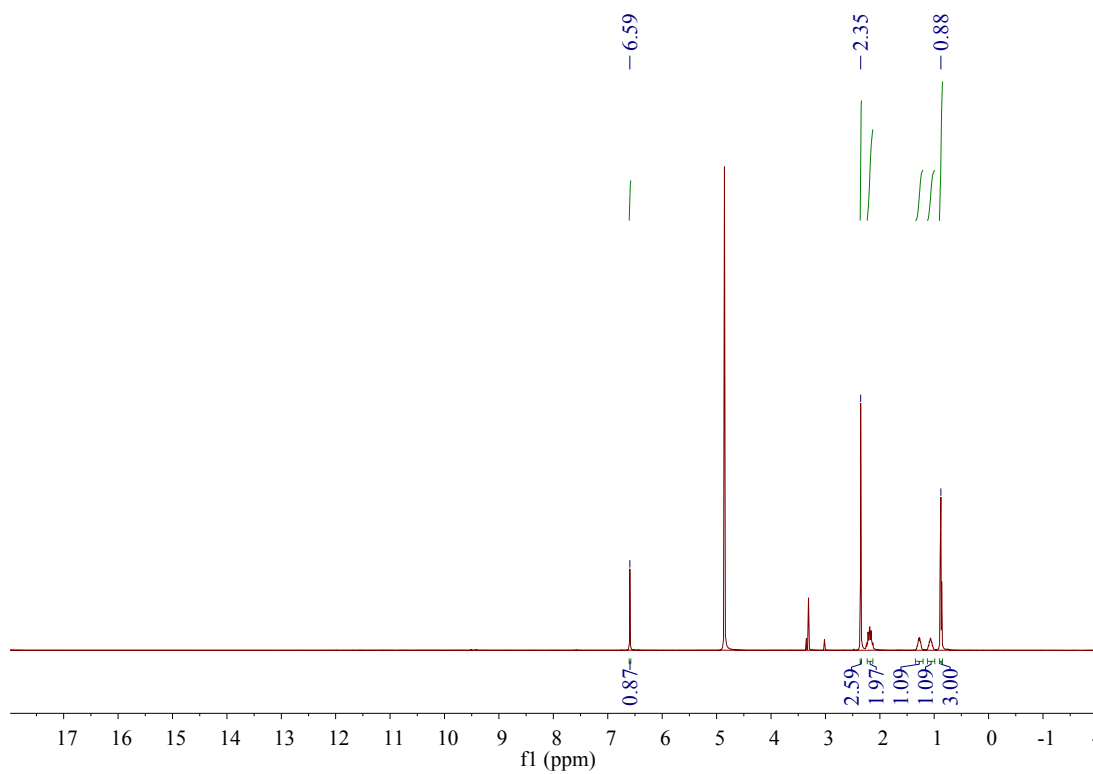
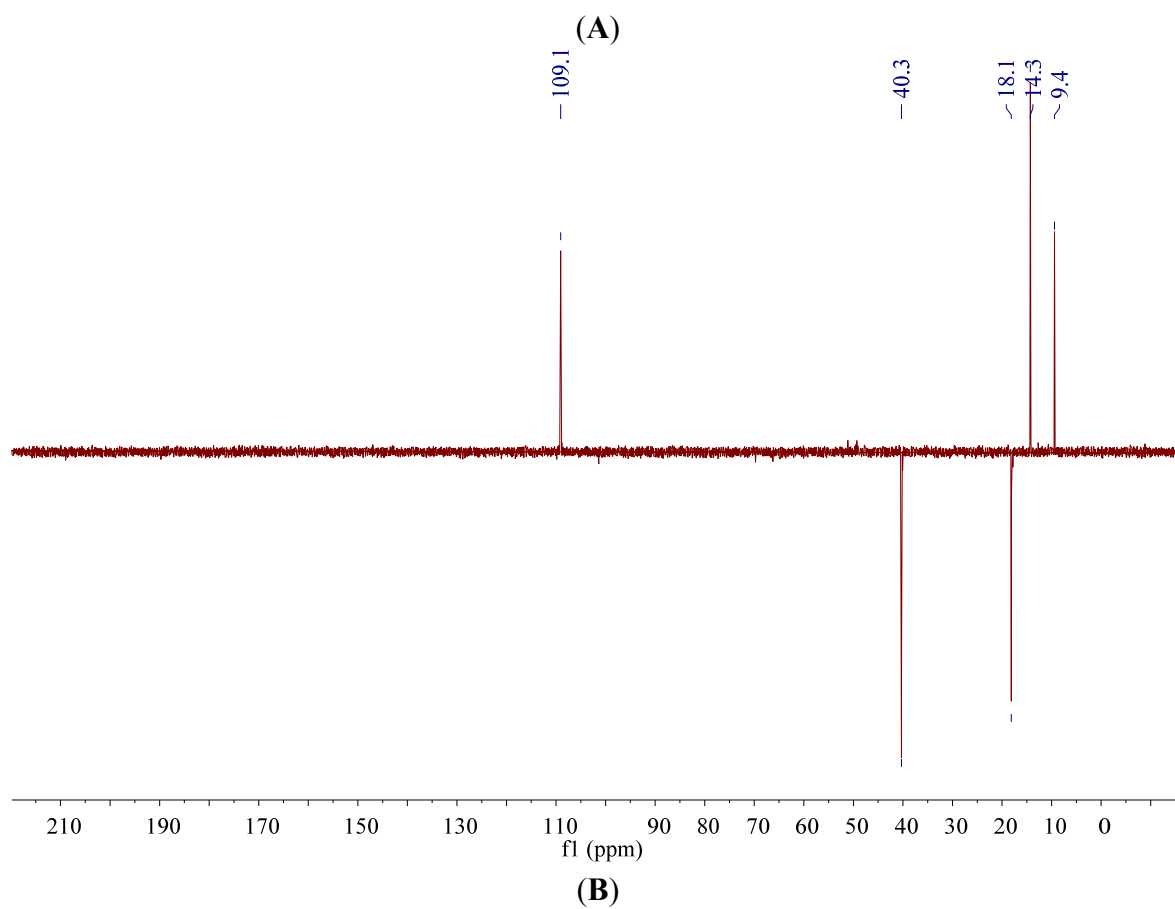
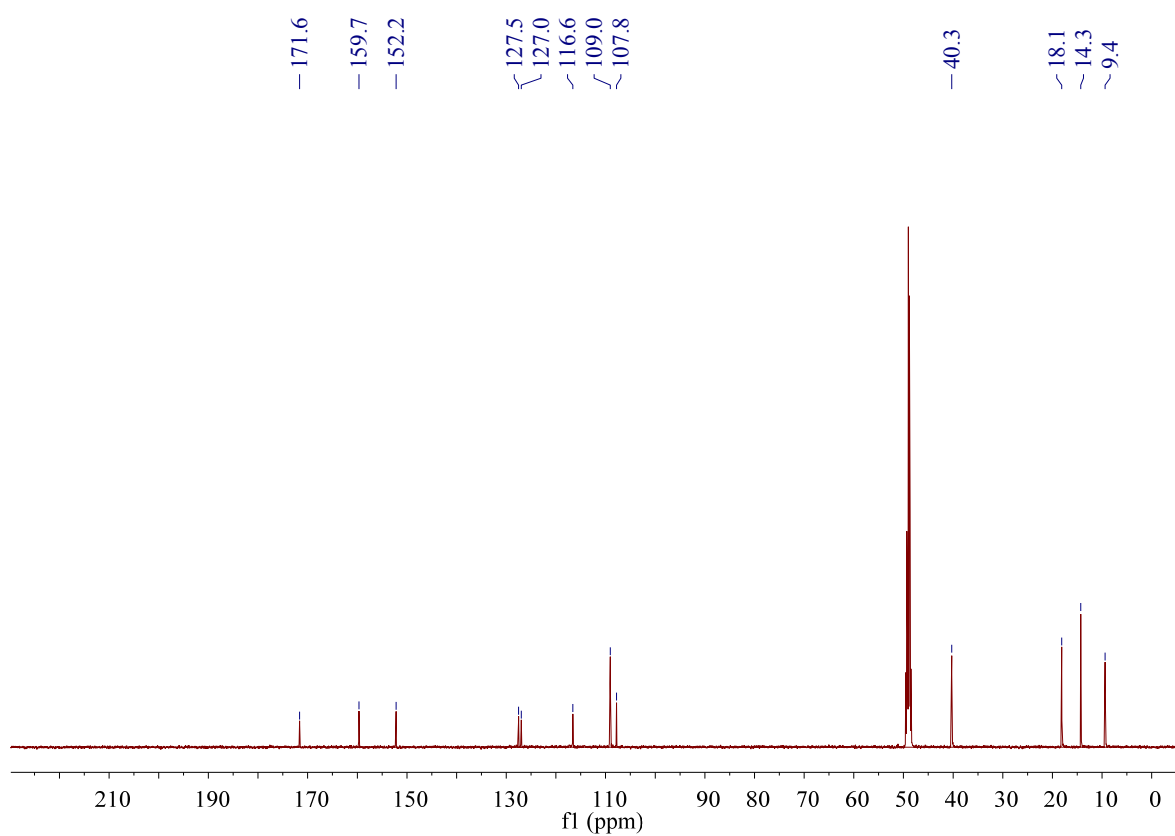
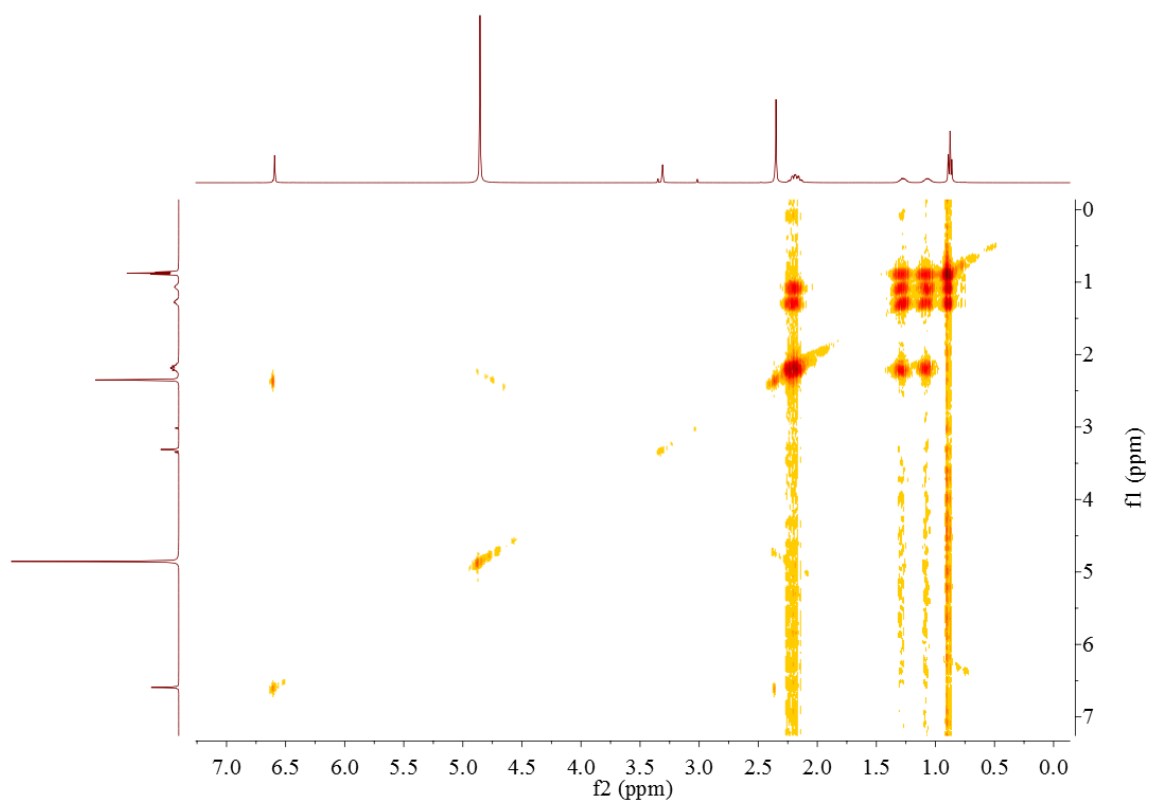


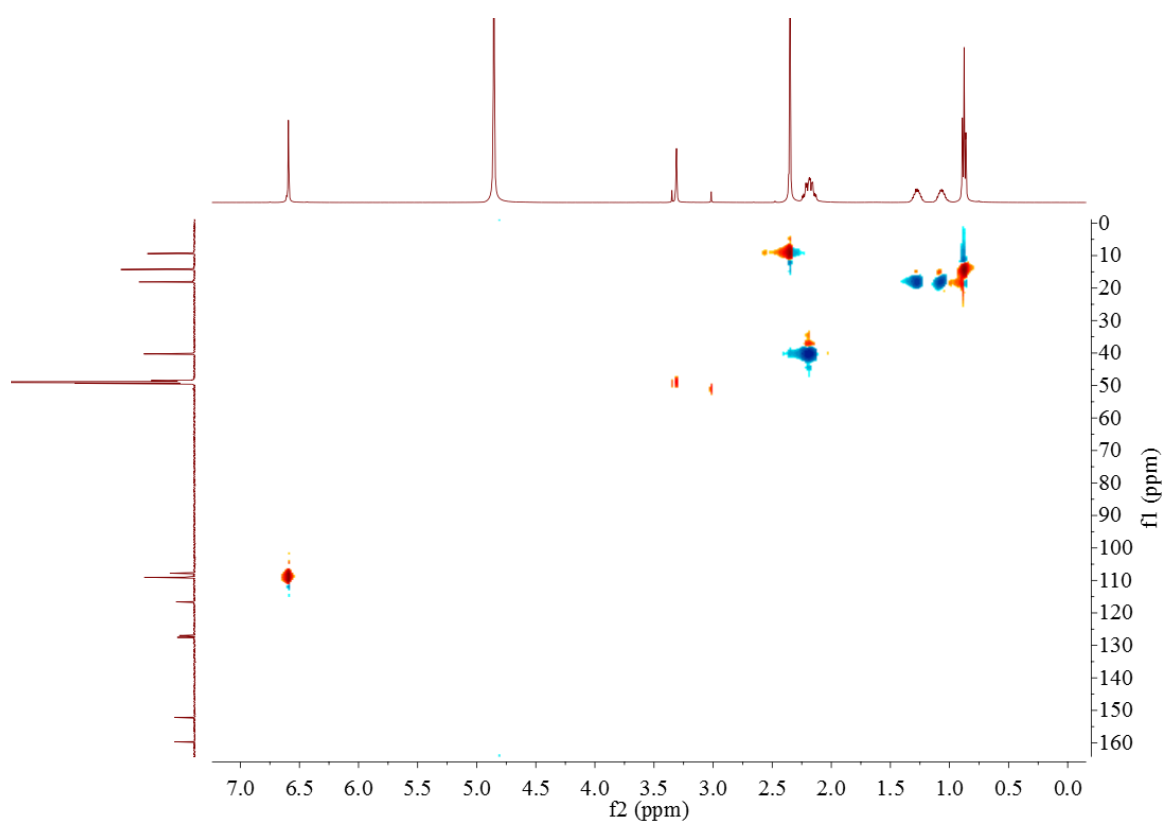
Figure S20. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of Compound 4.



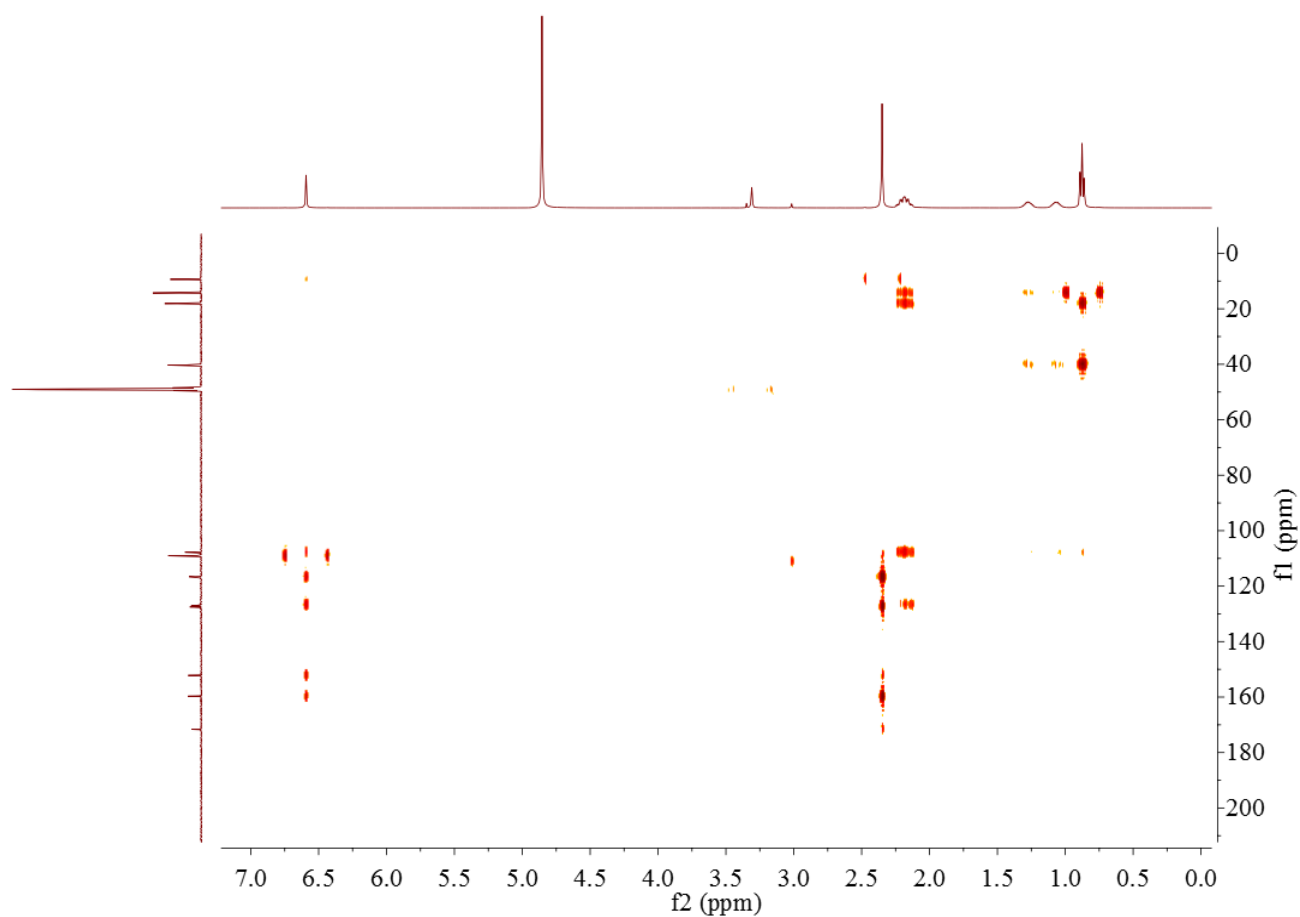
**Figure S21.**  $^{13}\text{C}$  NMR (125 MHz, Methanol- $d_4$ ) (A) and DEPT spectra of Compound **4** (B).



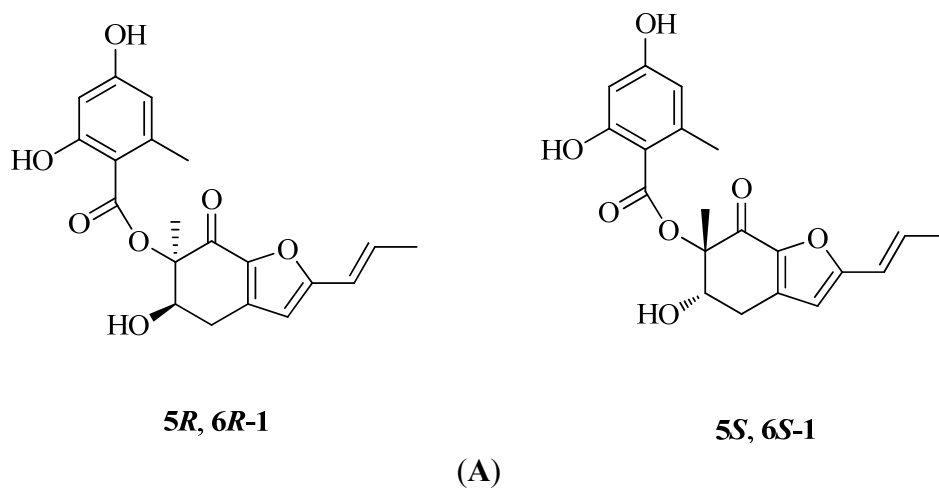
**Figure S22.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of Compound 4.



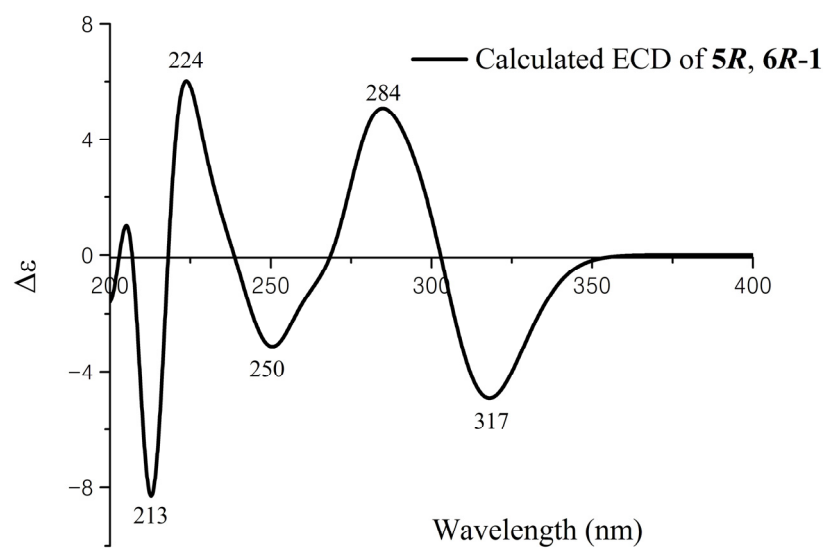
**Figure S23.** HSQC spectrum of Compound 4.



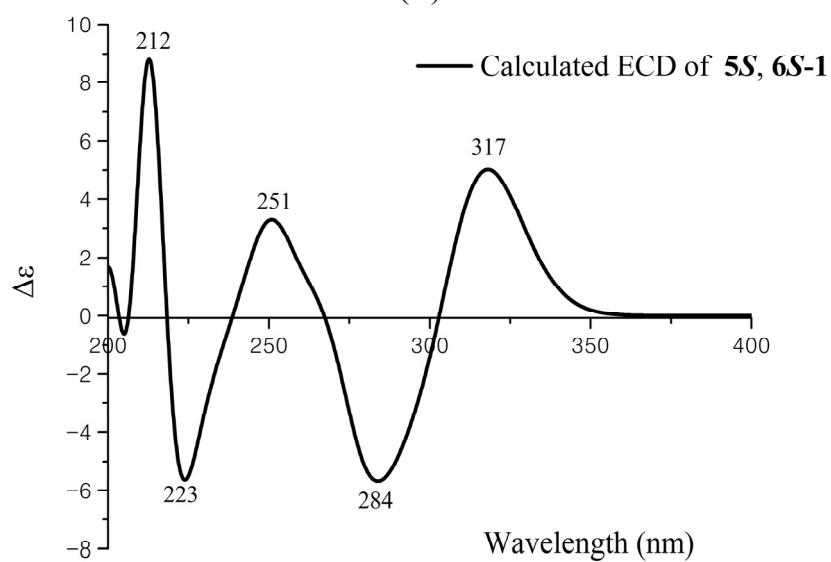
**Figure S24.** HMBC spectrum of Compound 4.



**Figure S25.** Cont.



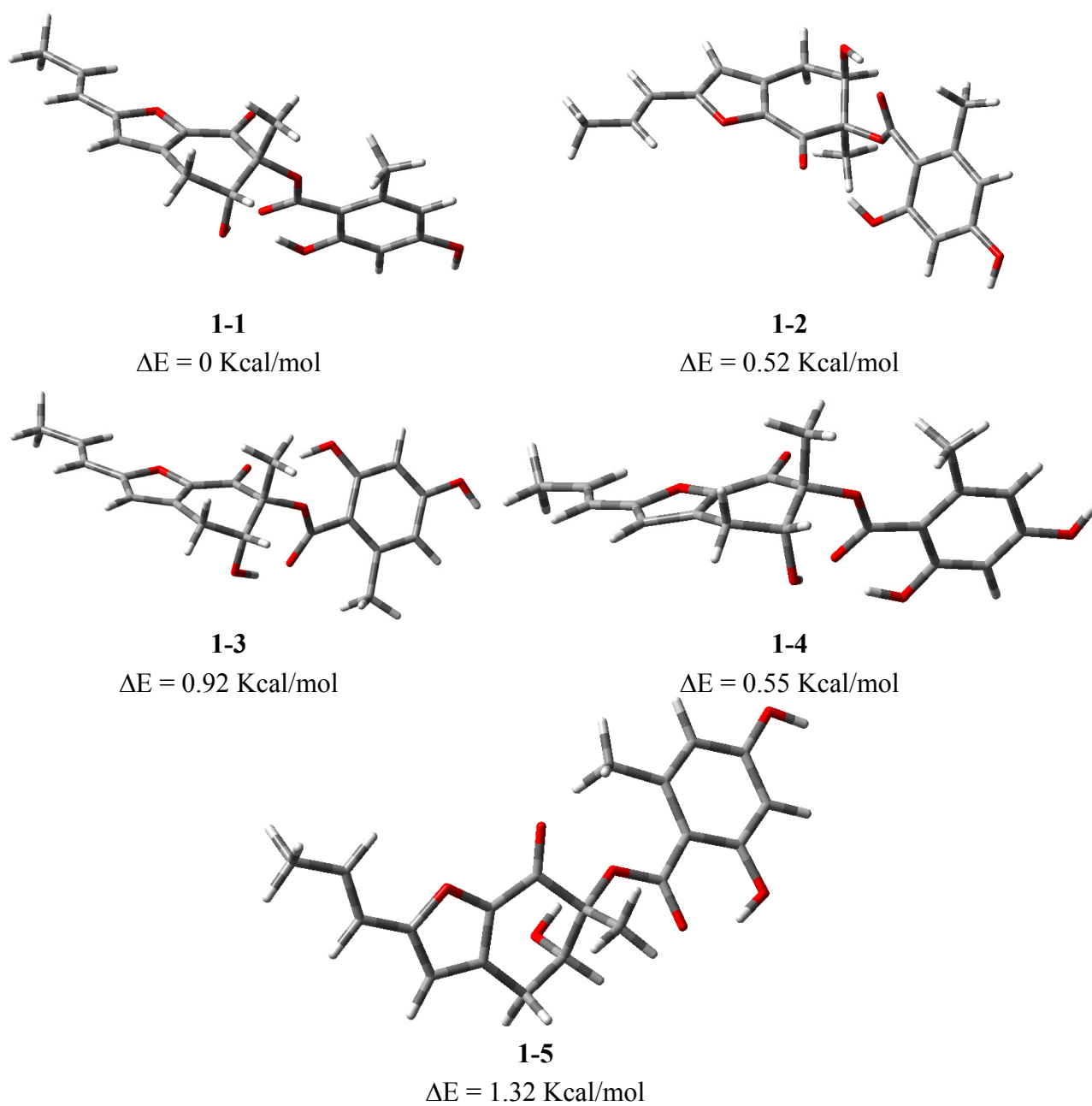
(B)



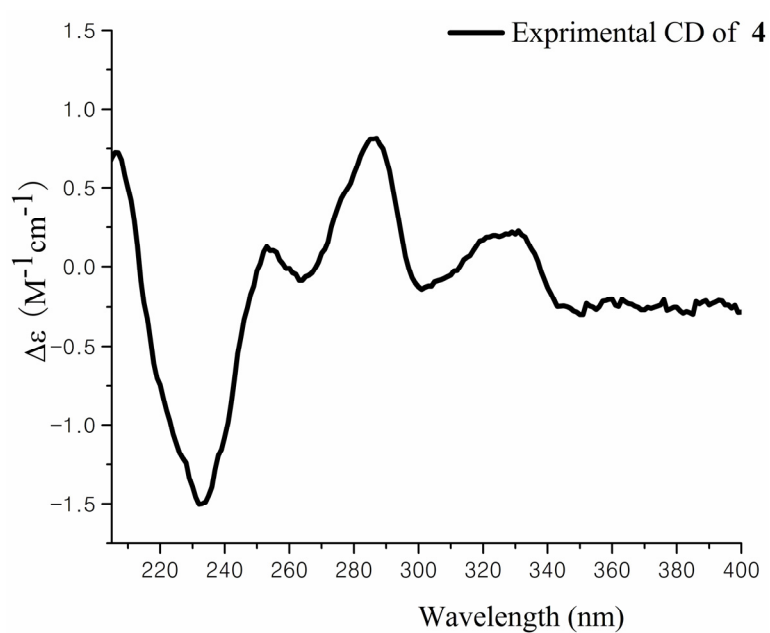
(C)

**Figure S25.** The structures (A) and calculated ECD spectra of the two isomers of **5R,6R-1** (B) and **5S,6S-1** (C).





**Figure S26.** DFT-optimized low-energy structures (1-1–1-5) for 5*R*,6*R*.



**Figure S27.** CD spectrum of Compound 4.

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