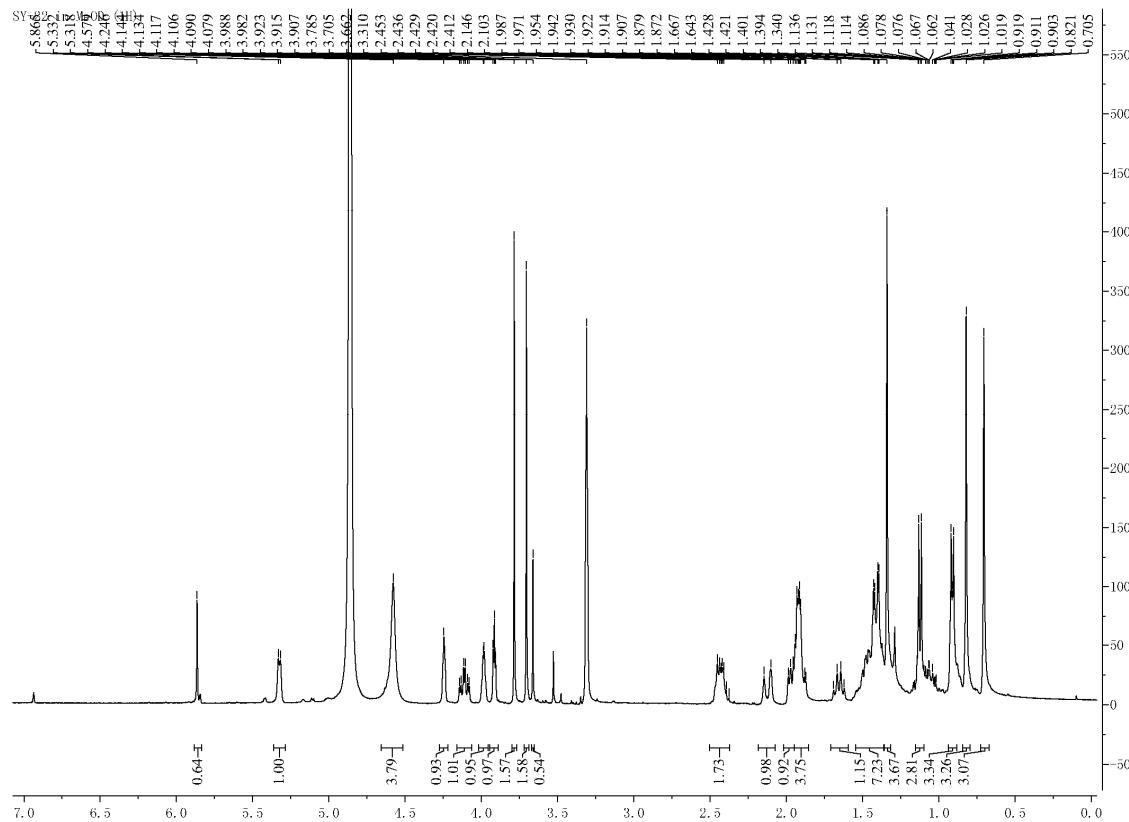
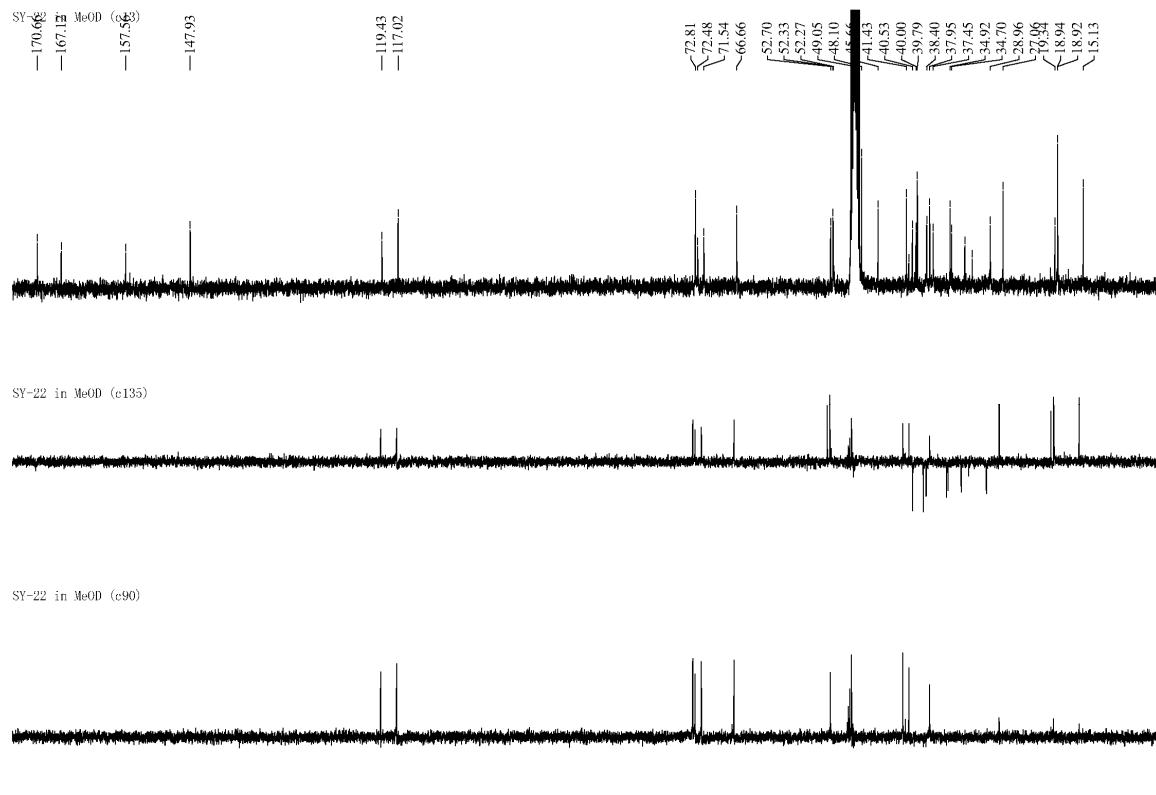


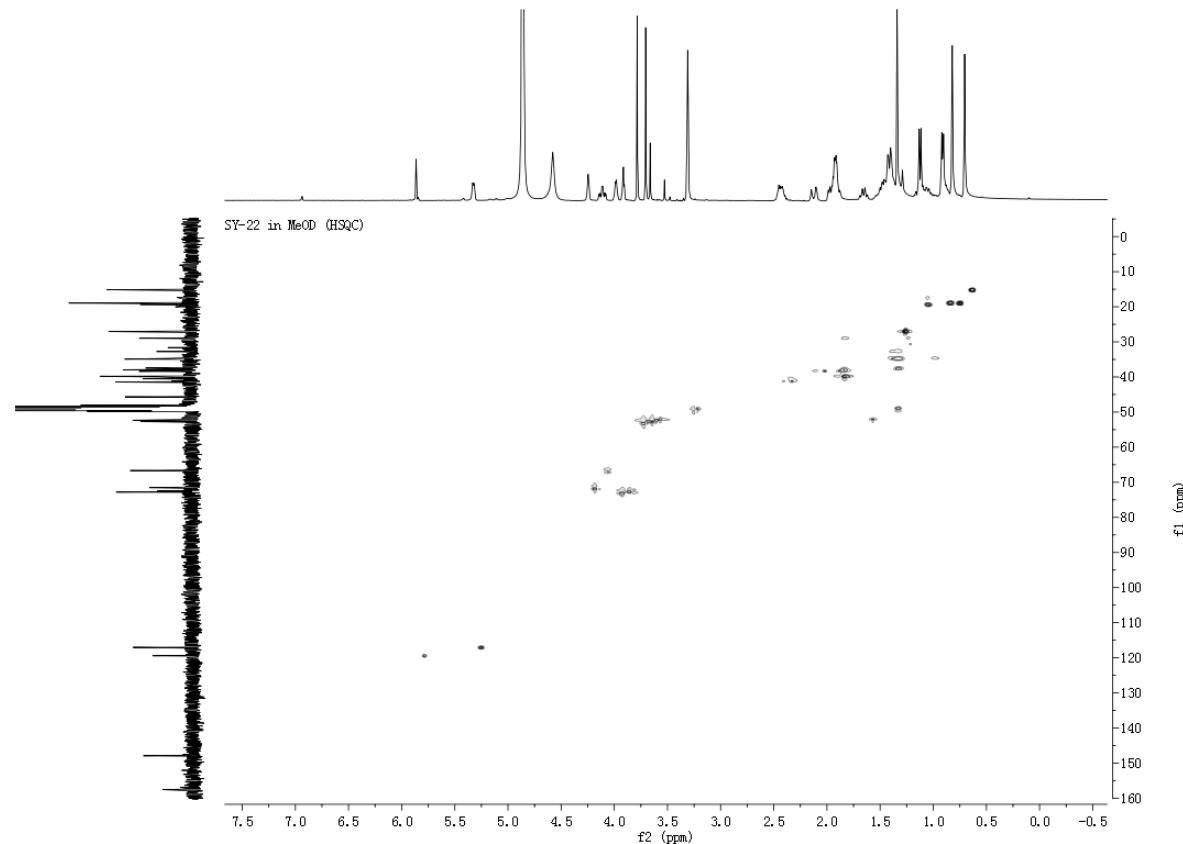
# Supplementary Materials: Topsensterols A–C, Cytotoxic Polyhydroxylated Sterol Derivatives from a Marine Sponge *Topsentia* sp.

Min Chen, Xu-Dong Wu, Qing Zhao and Chang-Yun Wang

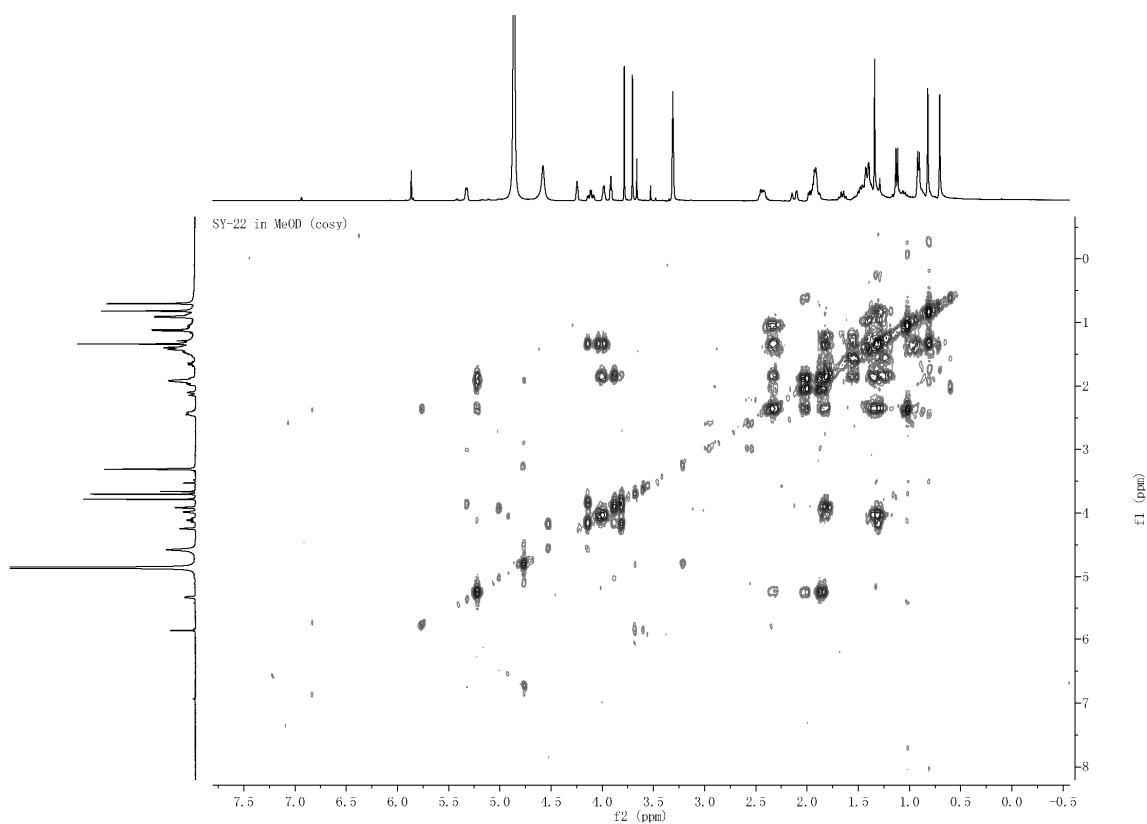
## List of Supplementary Materials

- Figure S1.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**  
**Figure S2.**  $^{13}\text{C}$  NMR and DEPT (100 MHz,  $\text{CD}_3\text{OD}$ ) spectra of compound **1**  
**Figure S3.** HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **1**  
**Figure S4.**  $^1\text{H}$ – $^1\text{H}$  COSY ( $\text{CD}_3\text{OD}$ ) spectrum of compound **1**  
**Figure S5.** HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **1**  
**Figure S6.** NOESY ( $\text{CD}_3\text{OD}$ ) spectrum of compound **1**  
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**Figure S14.** HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **2**  
**Figure S15.** NOESY ( $\text{CD}_3\text{OD}$ ) spectrum of compound **2**  
**Figure S16.** HRESIMS spectrum of compound **2**  
**Figure S17.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **3**  
**Figure S18.**  $^{13}\text{C}$  NMR and DEPT (100 MHz,  $\text{CD}_3\text{OD}$ ) spectra of compound **3**  
**Figure S19.** HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **3**  
**Figure S20.**  $^1\text{H}$ – $^1\text{H}$  COSY ( $\text{CD}_3\text{OD}$ ) spectrum of compound **3**  
**Figure S21.** HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **3**  
**Figure S22.** HRESIMS spectrum of compound **3**

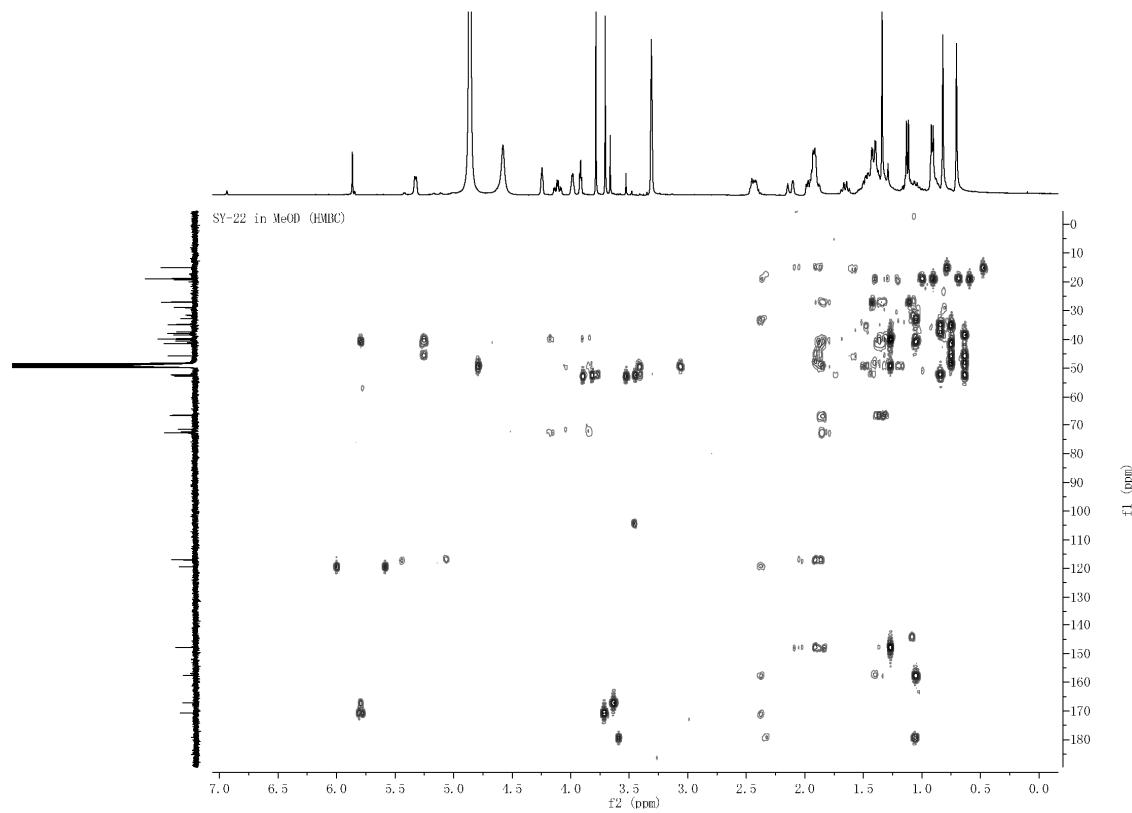
Figure S1.  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 1.Figure S2.  $^{13}\text{C}$  NMR and DEPT (100 MHz,  $\text{CD}_3\text{OD}$ ) spectra of compound 1.



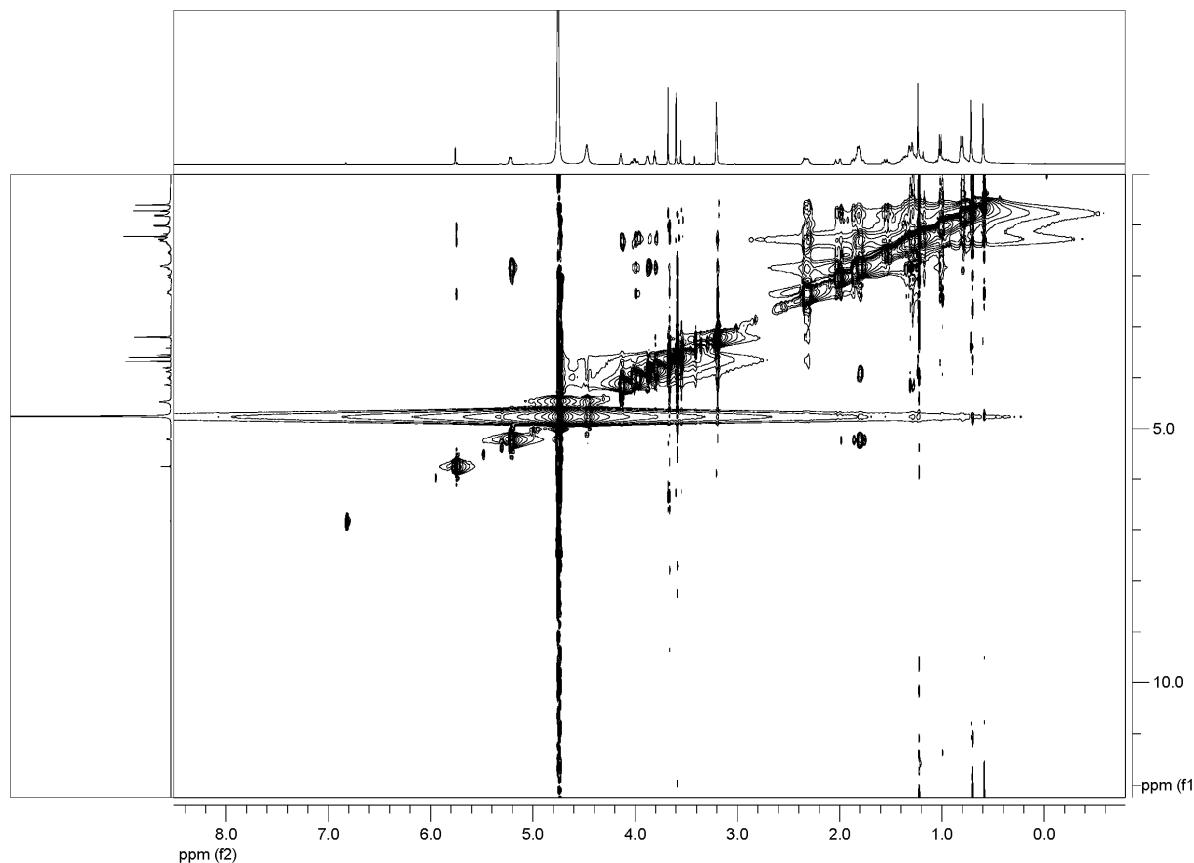
**Figure S3.** HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of compound 1.



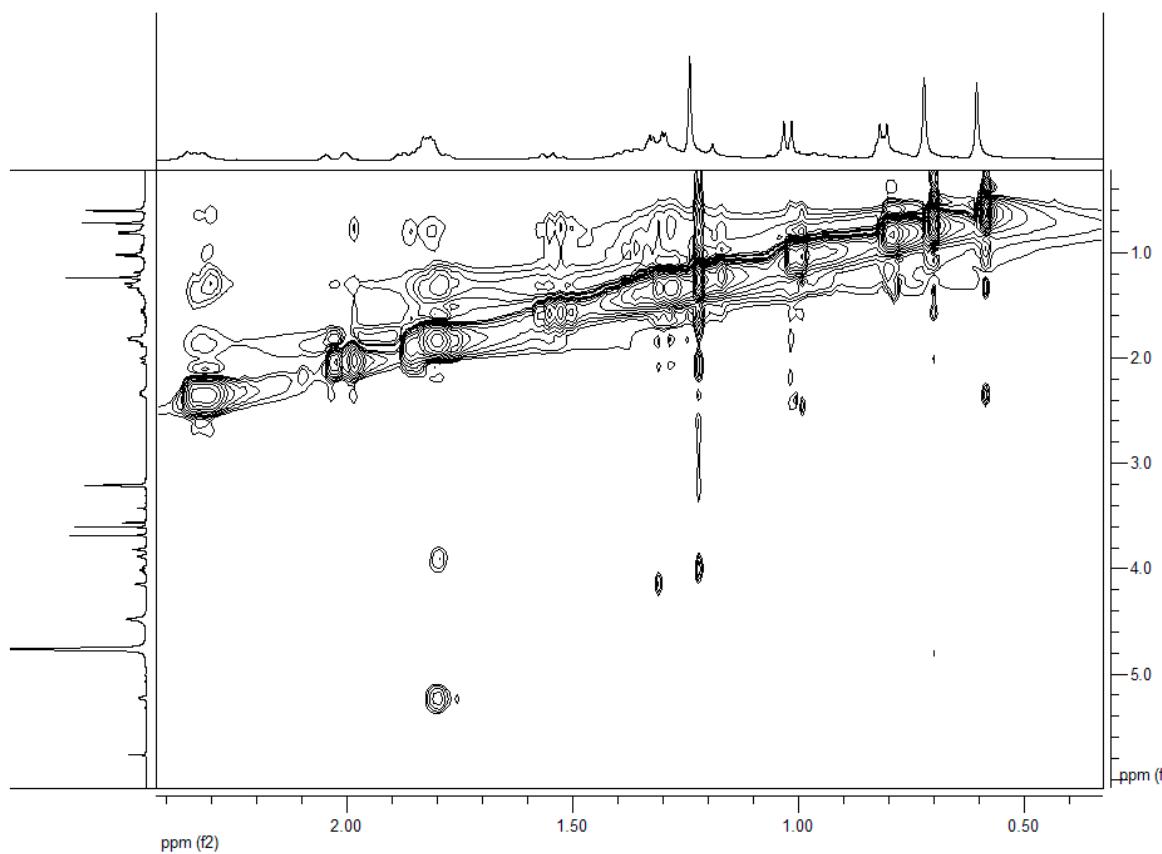
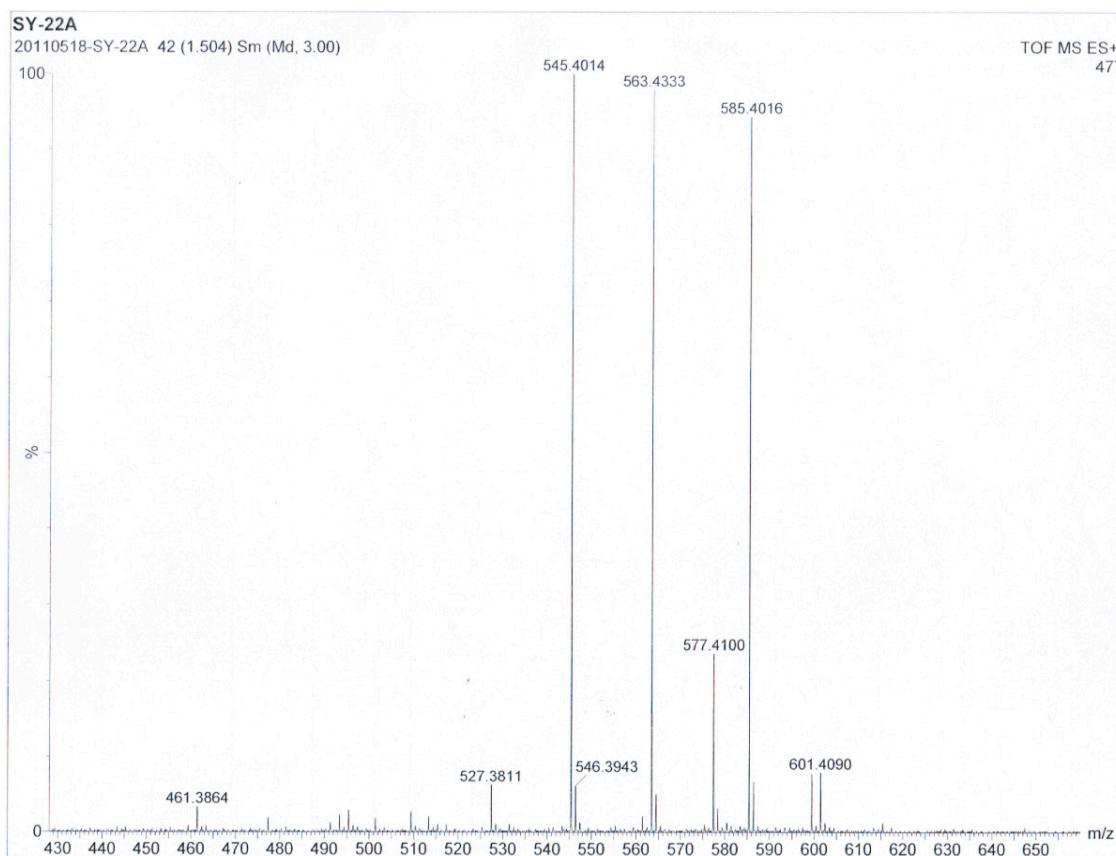
**Figure S4.**  $^1\text{H}$ - $^1\text{H}$  COSY ( $\text{CD}_3\text{OD}$ ) spectrum of compound 1.



**Figure S5.** HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of compound 1.



**Figure S6.** NOESY ( $\text{CD}_3\text{OD}$ ) spectrum of compound 1.

**Figure S7.** Partial NOESY ( $\text{CD}_3\text{OD}$ ) spectrum of compound **1**.**Figure S8.** ESIMS spectrum of compound **1**.

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 19 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

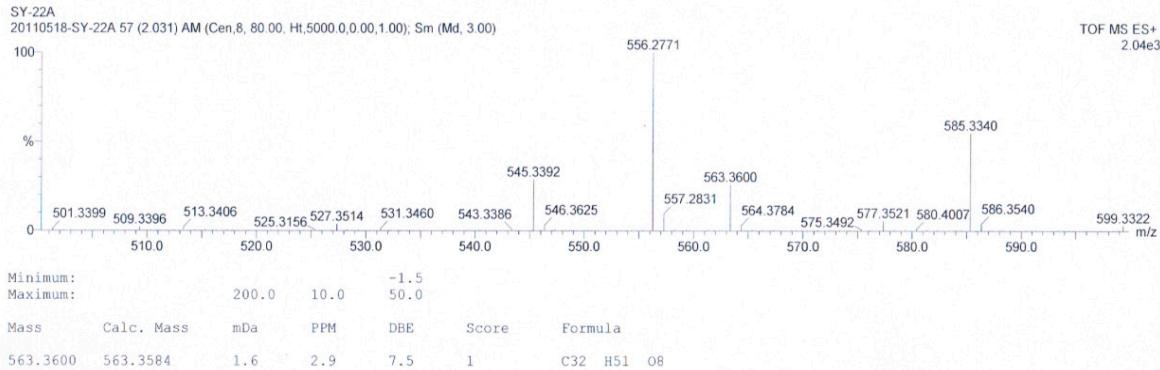
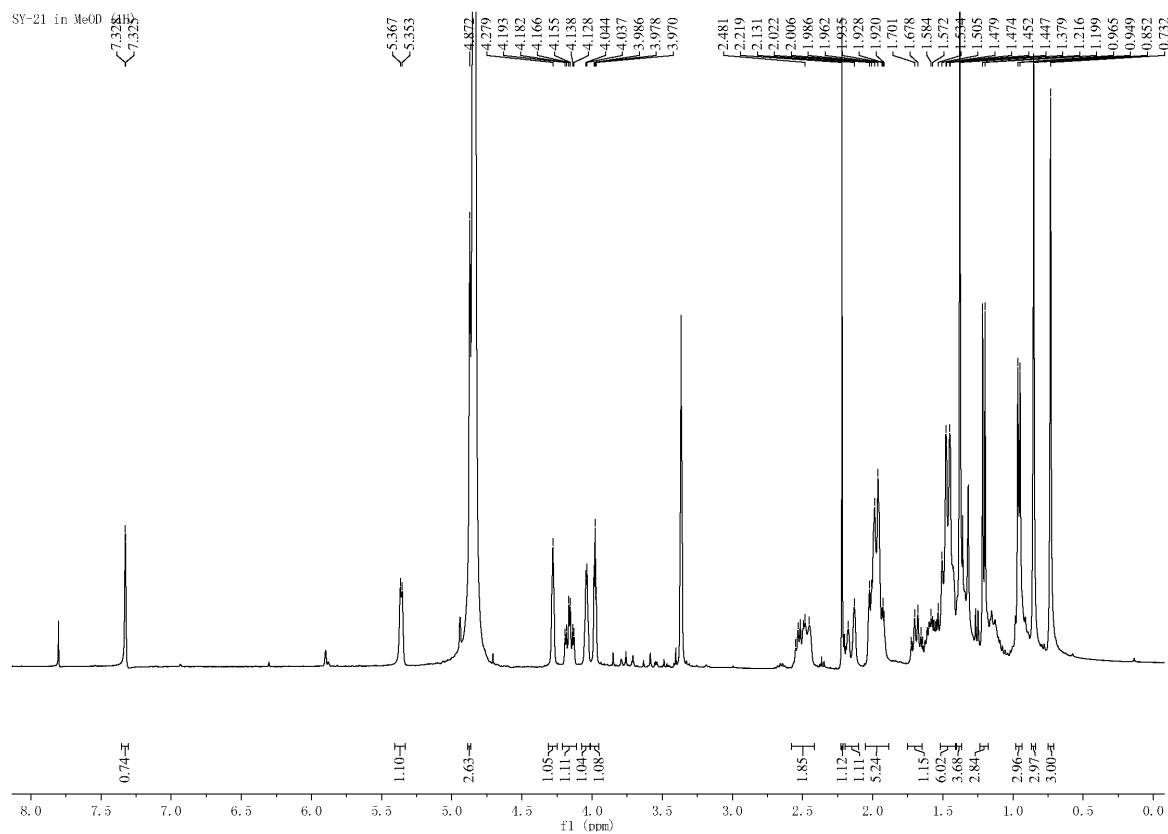
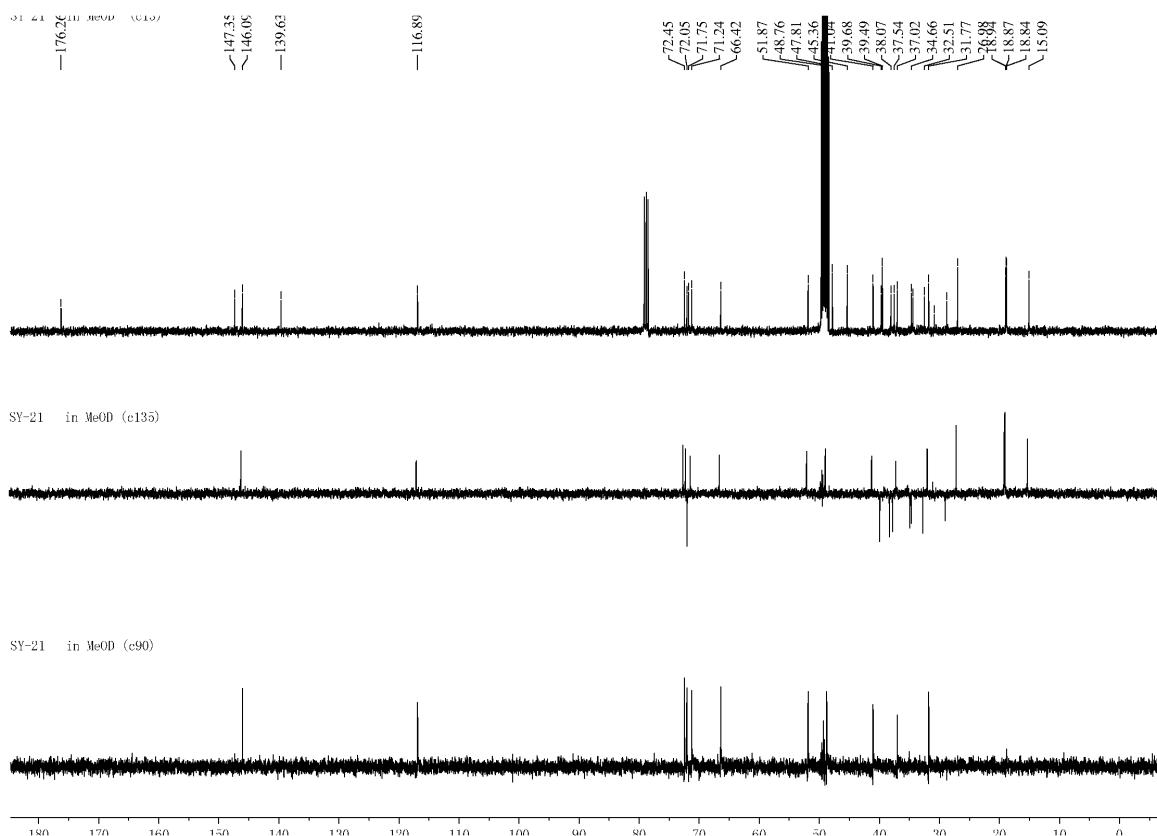
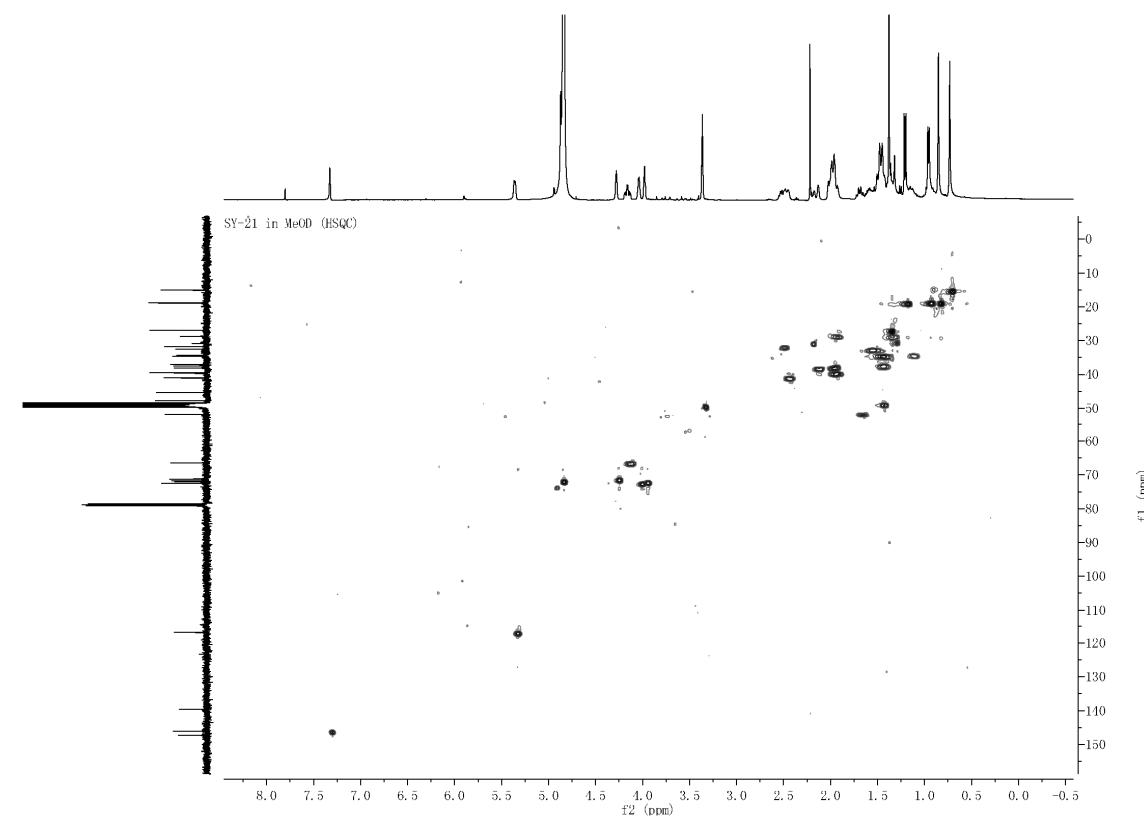


Figure S9. HRESIMS spectrum of compound 1.

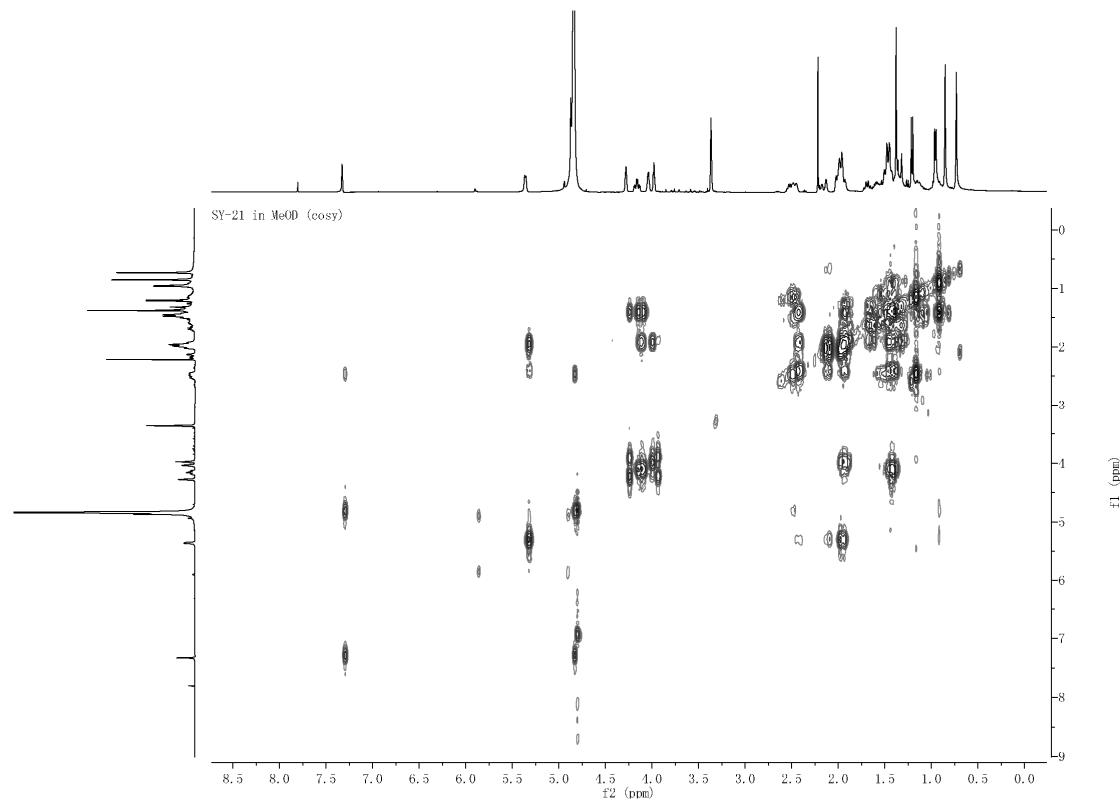
Figure S10.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2.



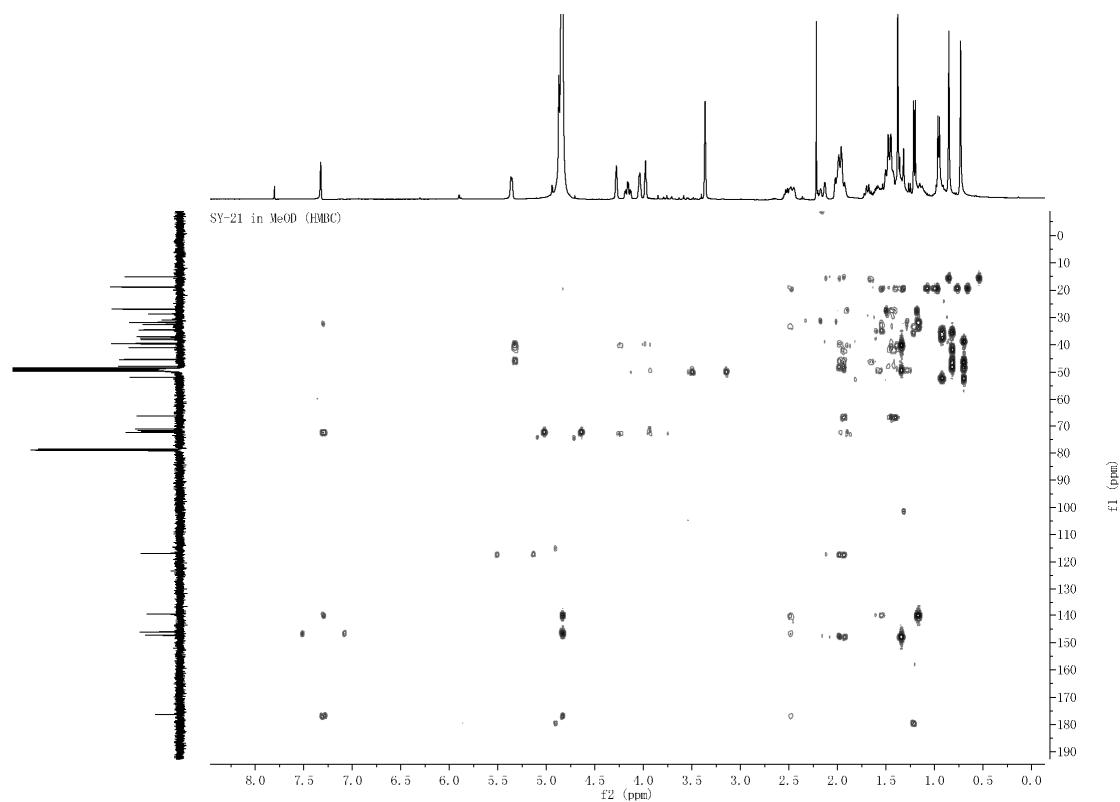
**Figure S11.**  $^{13}\text{C}$  NMR and DEPT (100 MHz,  $\text{CD}_3\text{OD}$ ) spectra of compound 2.



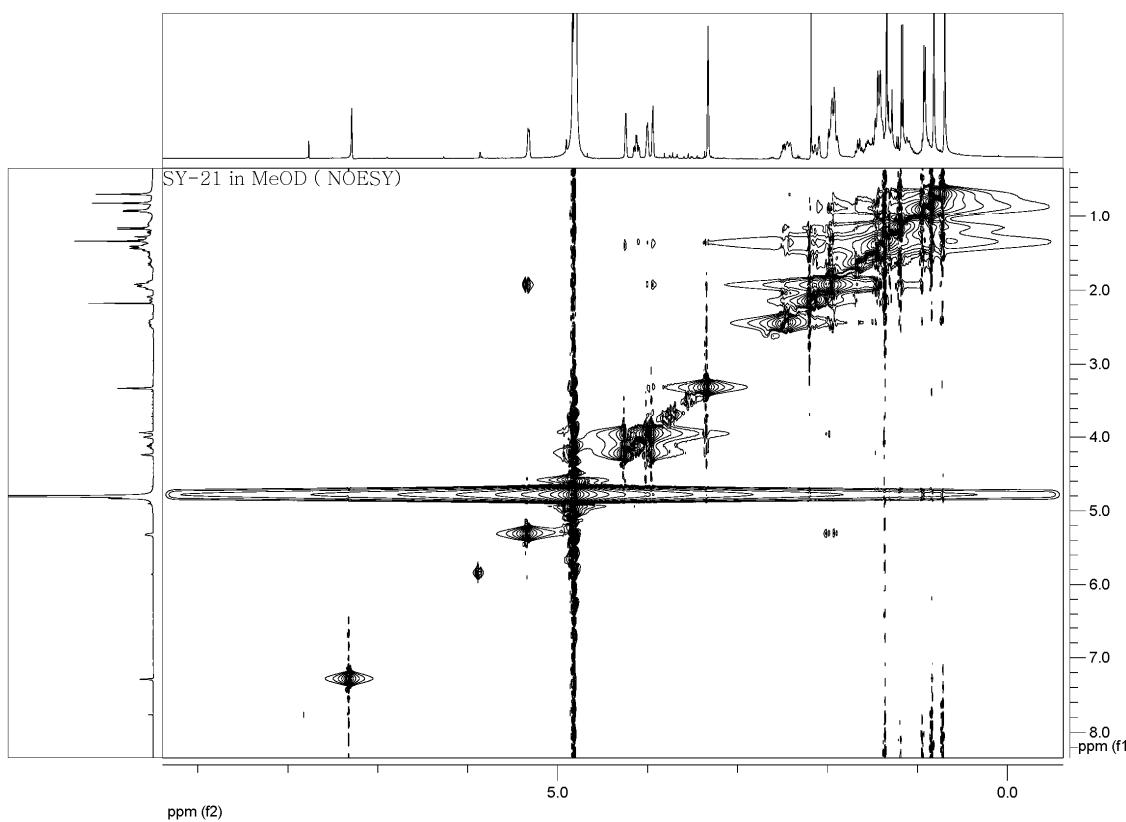
**Figure S12.** HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of compound 2.



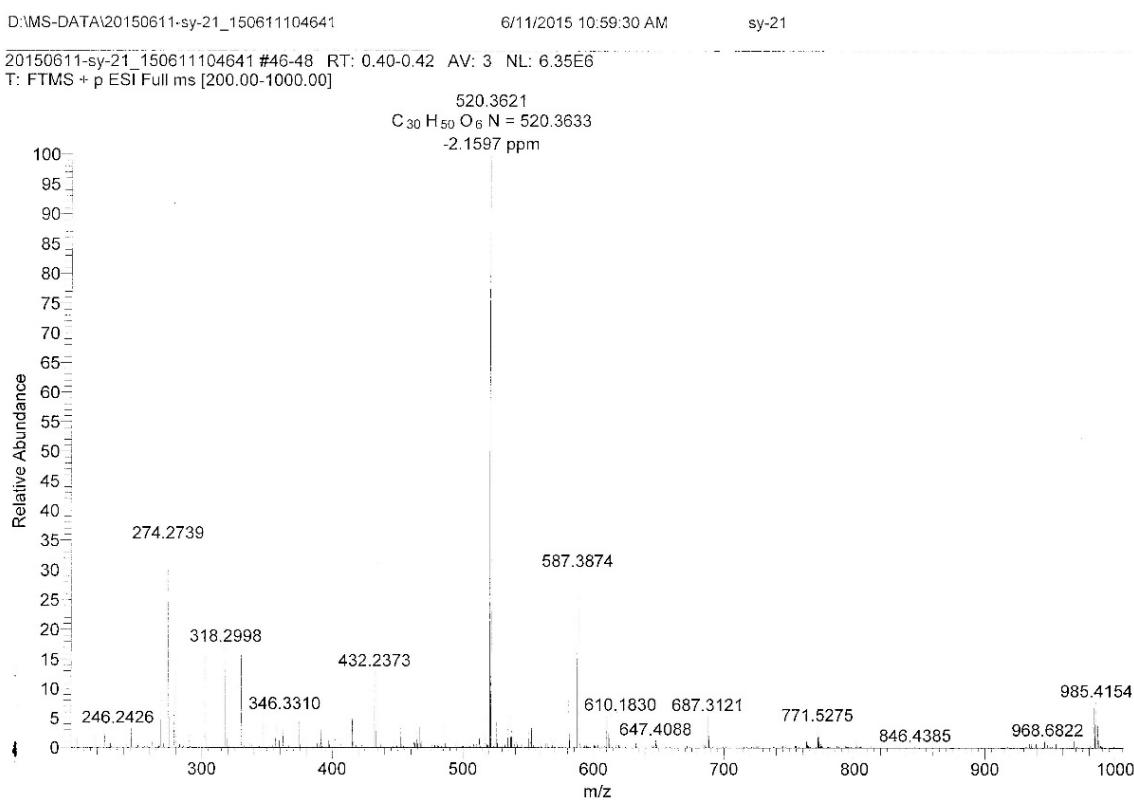
**Figure S13.** <sup>1</sup>H-<sup>1</sup>H COSY ( $\text{CD}_3\text{OD}$ ) spectrum of compound **2**.



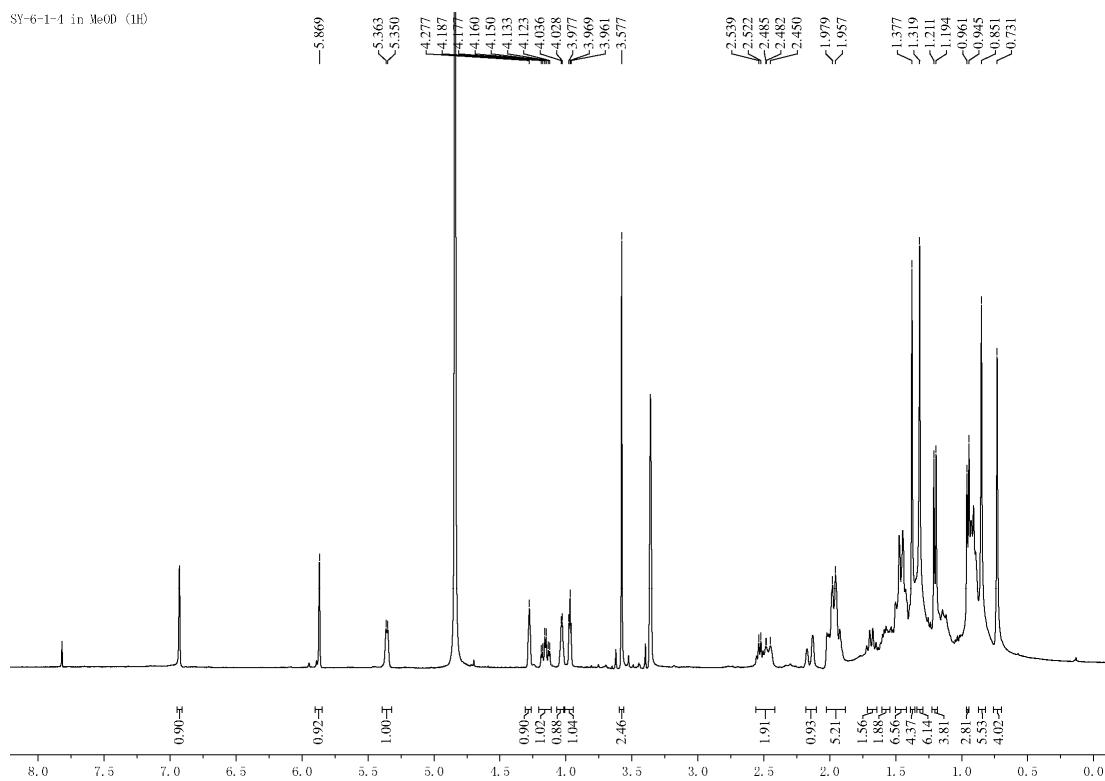
**Figure S14.** HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **2**.



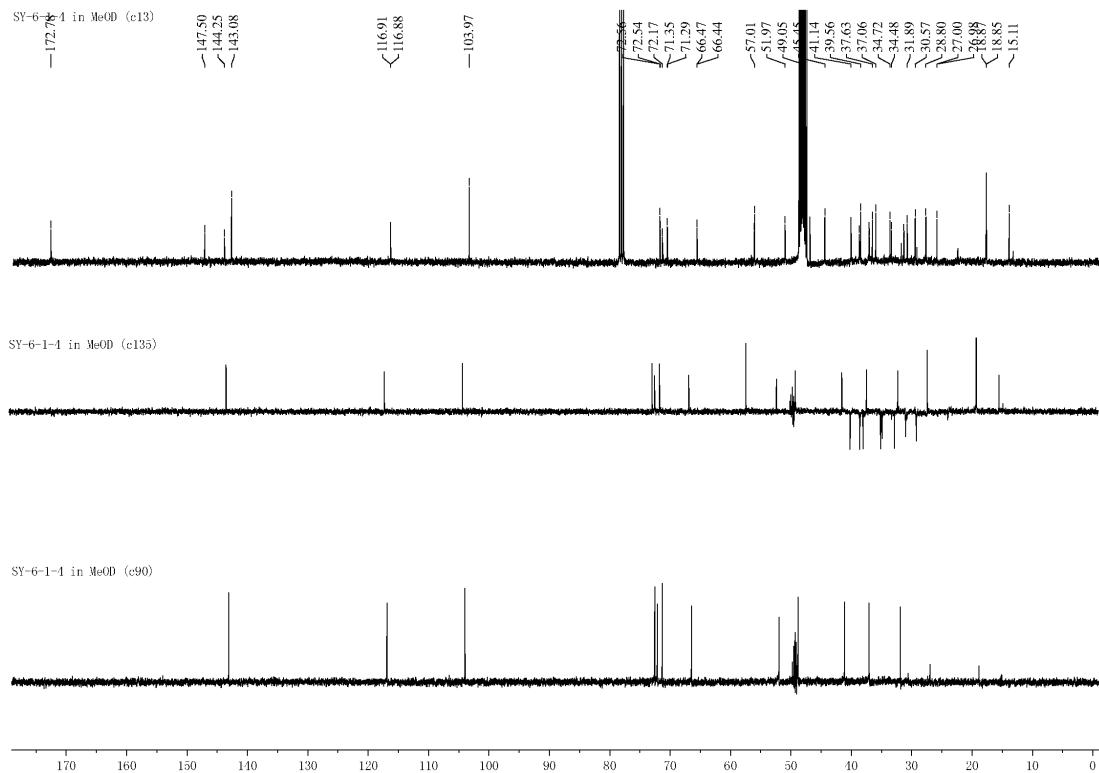
**Figure S15.** NOESY ( $\text{CD}_3\text{OD}$ ) spectrum of compound 2.



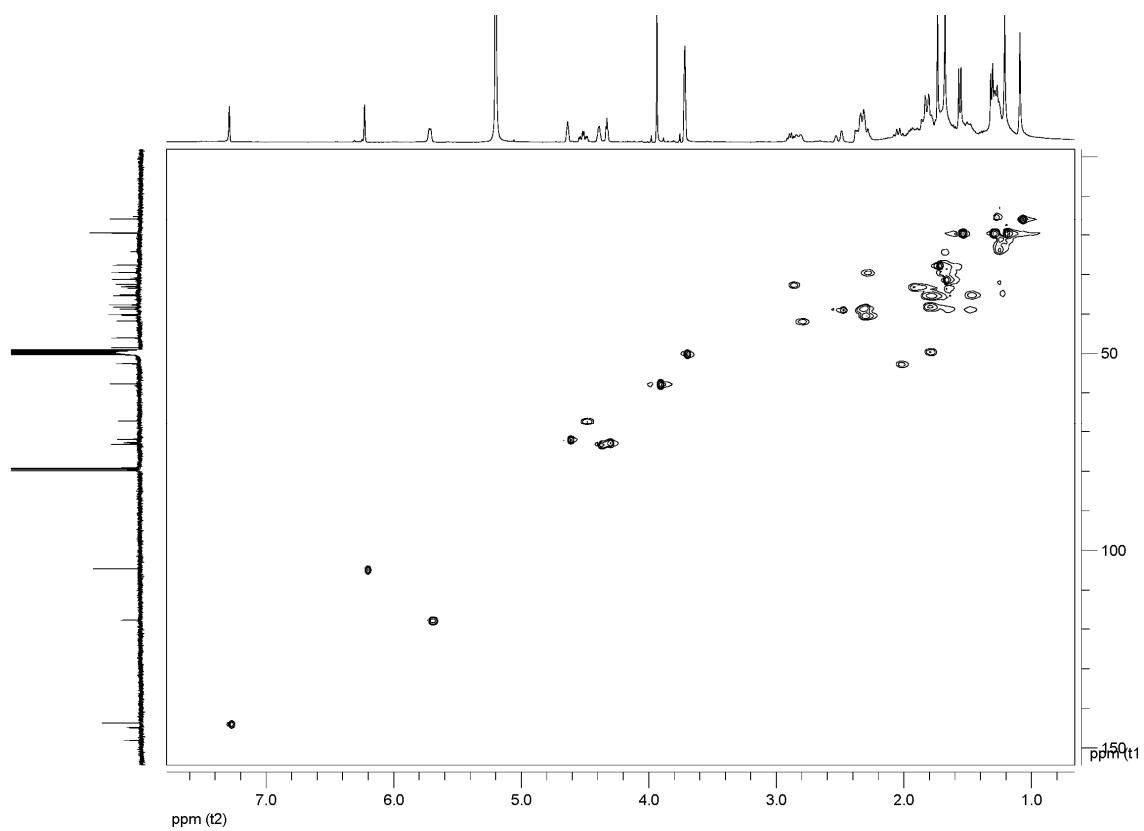
**Figure S16.** HRESIMS spectrum of compound 2.



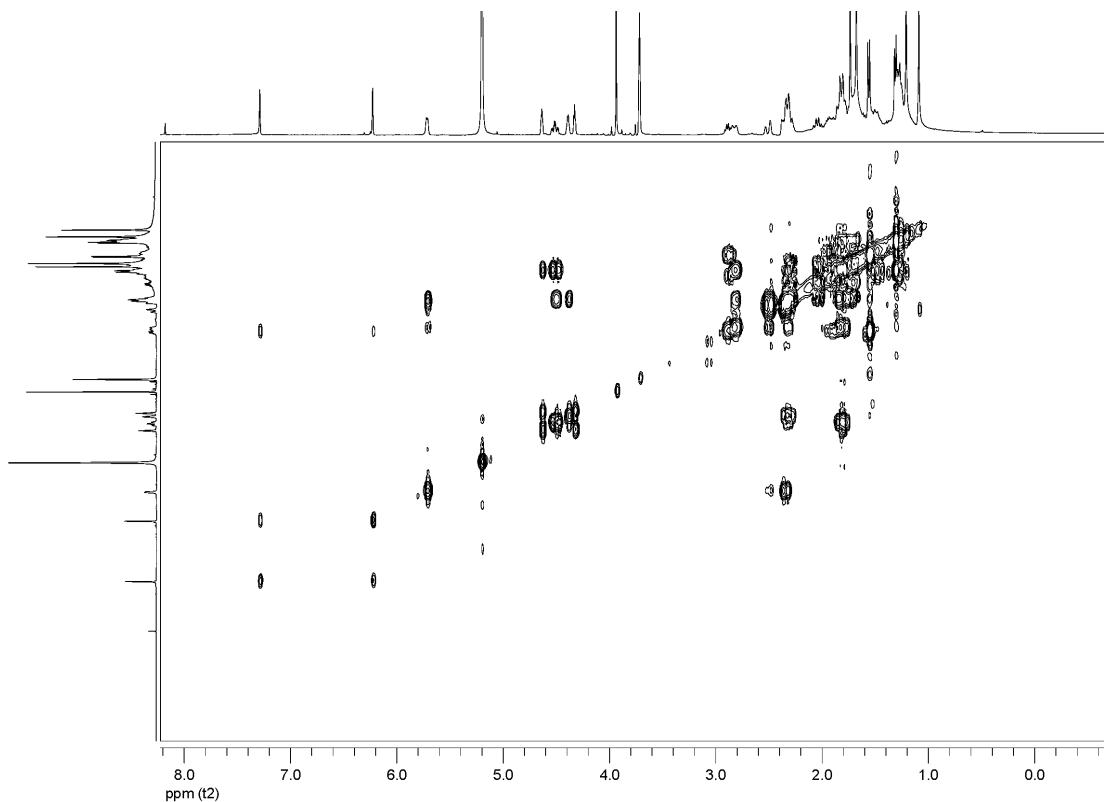
**Figure S17.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 3.



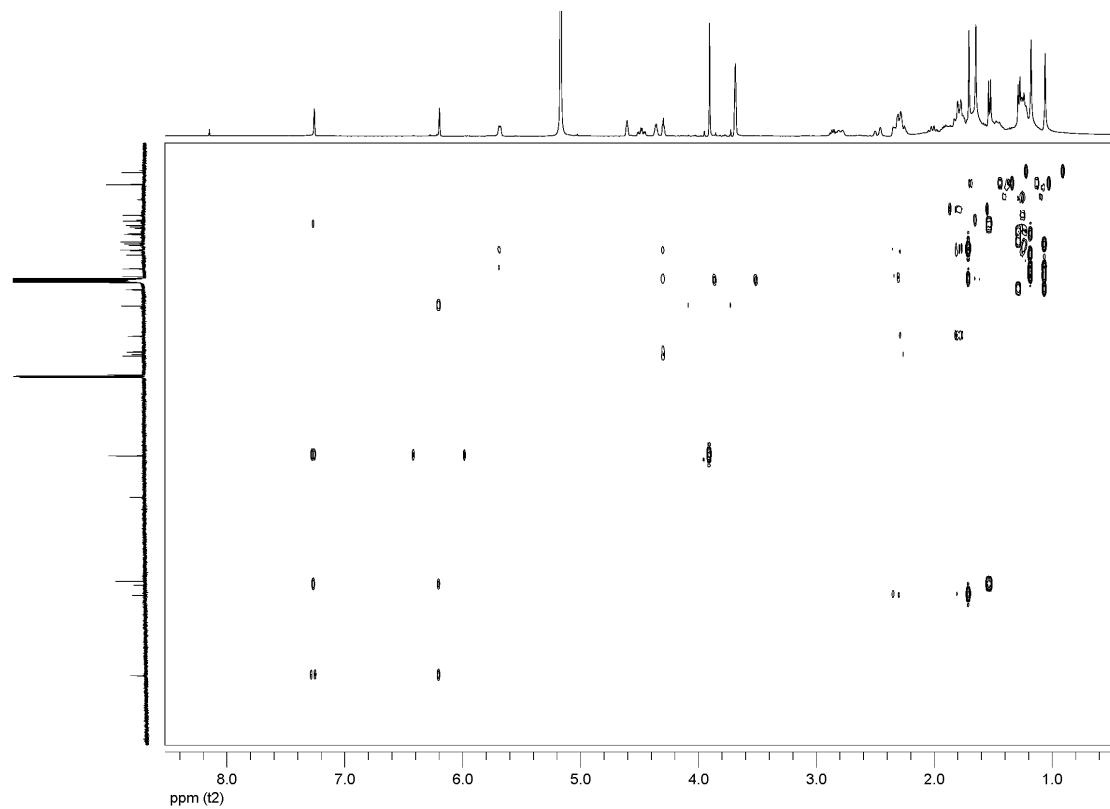
**Figure S18.**  $^{13}\text{C}$  NMR and DEPT (100 MHz,  $\text{CD}_3\text{OD}$ ) spectra of compound 3.



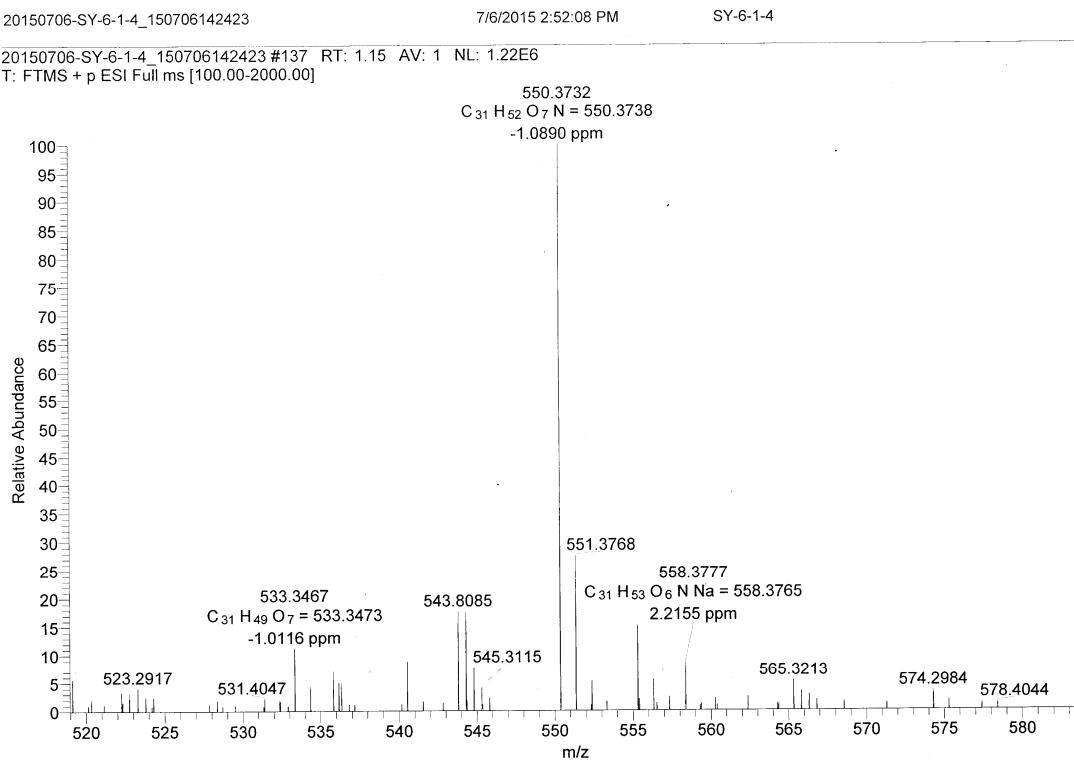
**Figure S19.** HSQC ( $\text{CD}_3\text{OD}$ ) spectrum of compound 3.



**Figure S20.**  $^1\text{H}$ - $^1\text{H}$  COSY ( $\text{CD}_3\text{OD}$ ) spectrum of compound 3.



**Figure S21.** HMBC ( $\text{CD}_3\text{OD}$ ) spectrum of compound 3.



**Figure S22.** HRESIMS spectrum of compound 3.