# Supplementary Materials: Austalides S-U, New Meroterpenoids from the Sponge-Derived Fungus *Aspergillus aureolatus* HDN14-107

**Jixing Peng, Xiaomin Zhang, Wei Wang, Tianjiao Zhu, Qianqun Gu and Dehai Li**

HRESIMS, 1D and 2D NMR data of **1** in $CDCl_3$ (Figures S1–S9);
HRESIMS, 1D and 2D NMR data of **2** in $CDCl_3$ (Figures S10–S17);
HRESIMS, 1D and 2D NMR data of **3** in $CD_3CN$ (Figures S17–S25);
HPLC analysis of the EtOAc extract of *Aspergillus aureolatus* HDN14-107 (Figure S26);
Computational data (Figures S27).

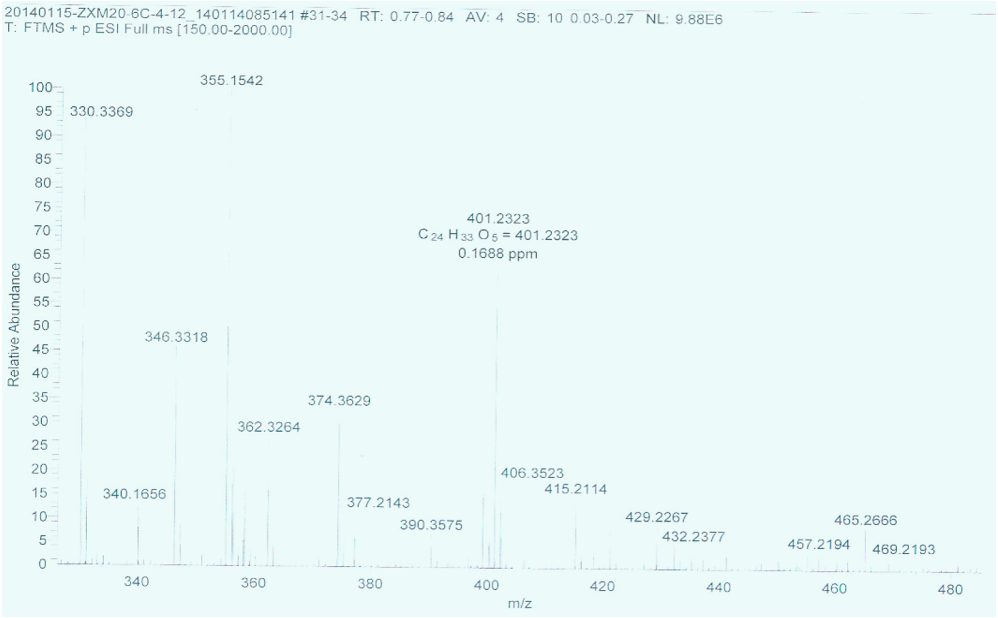



**Figure S1.** HR-ESI-MS of **1**.

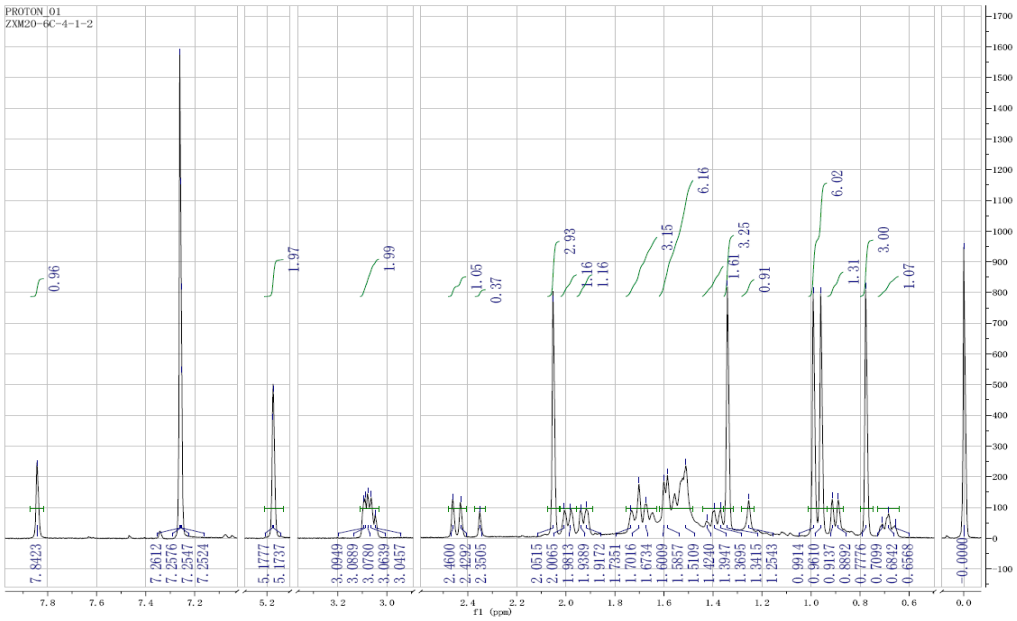



**Figure S2.** $^1$H NMR (500 MHz) spectrum of **1** in $CDCl_3$.

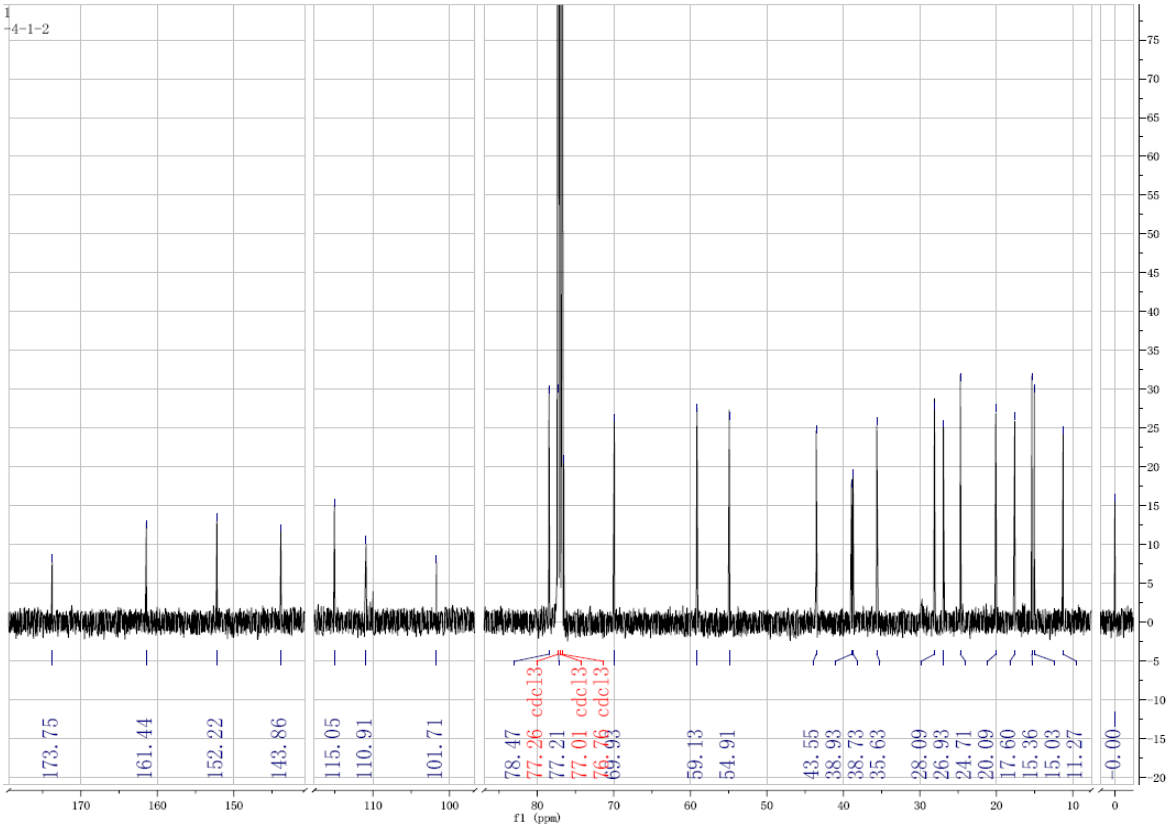



**Figure S3.** $^{13}C$ NMR spectrum of **1** in $CDCl_3$.

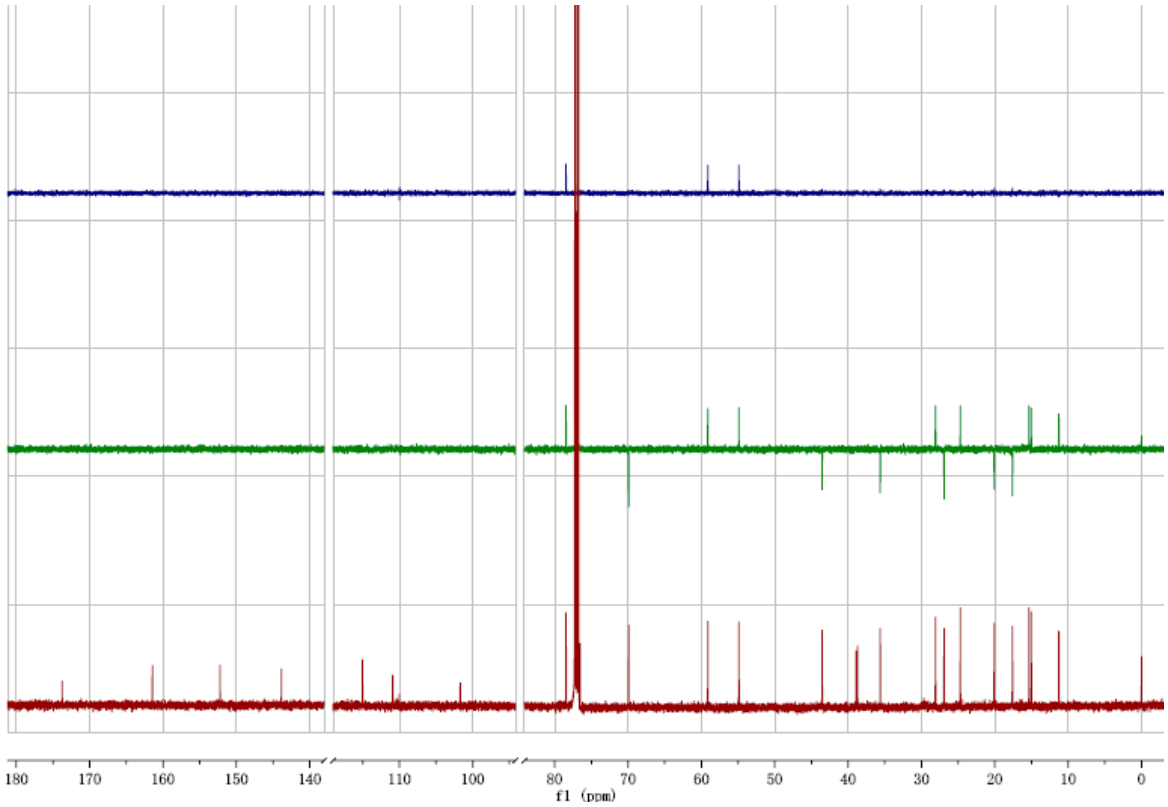



**Figure S4.** DEPT spectrum of **1** in $CDCl_3$.

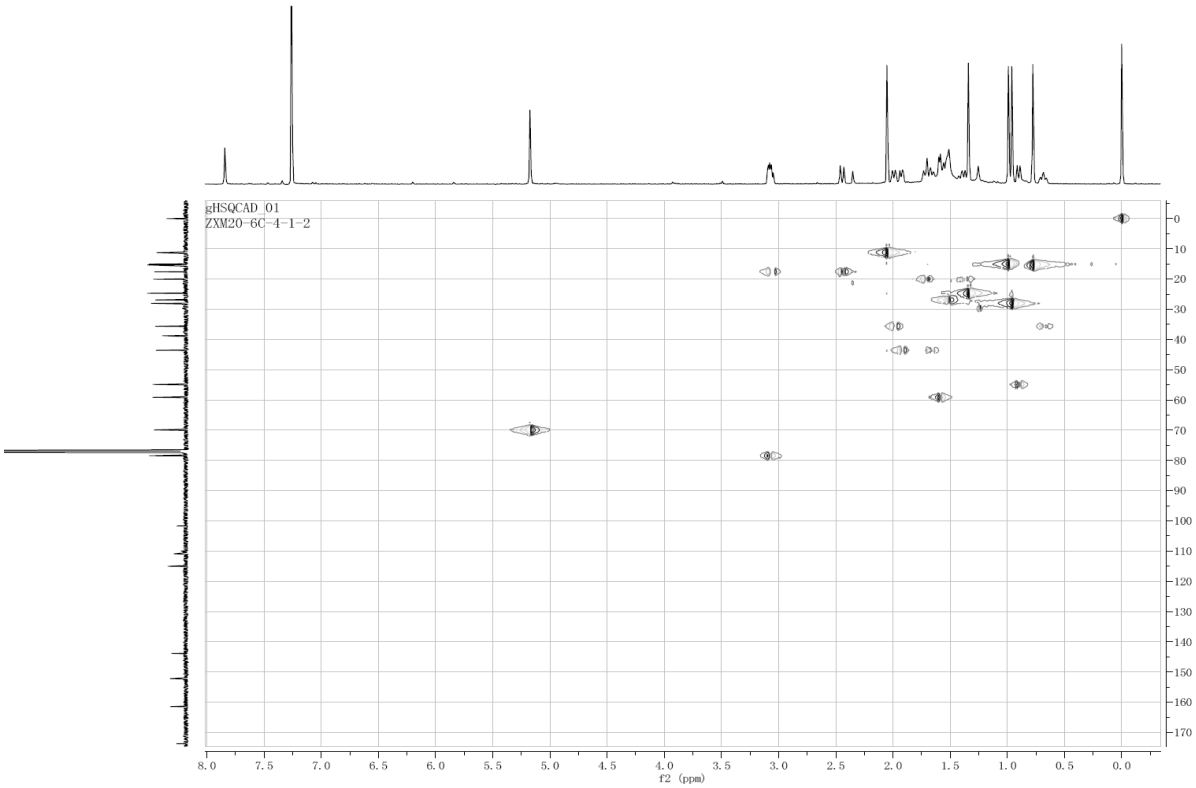



**Figure S5.** HMQC spectrum of **1** in $CDCl_3$.

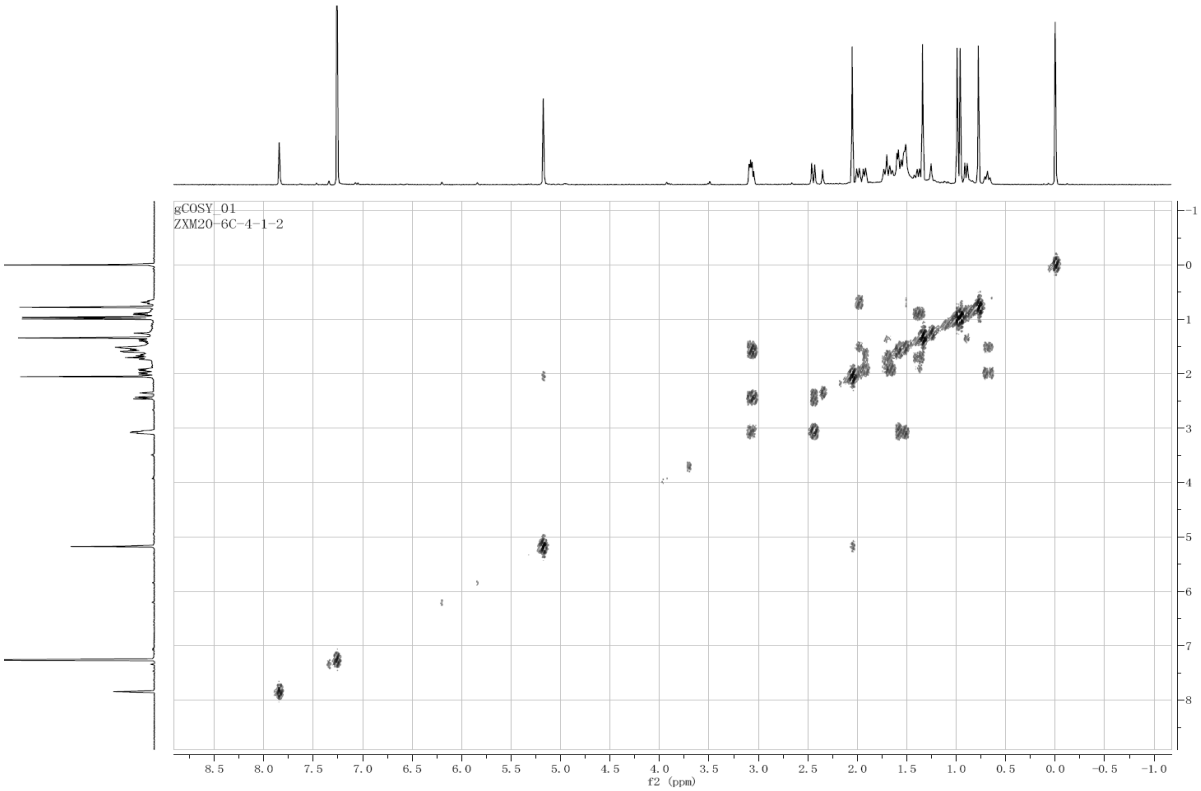



**Figure S6.** COSY spectrum of **1** in $CDCl_3$.

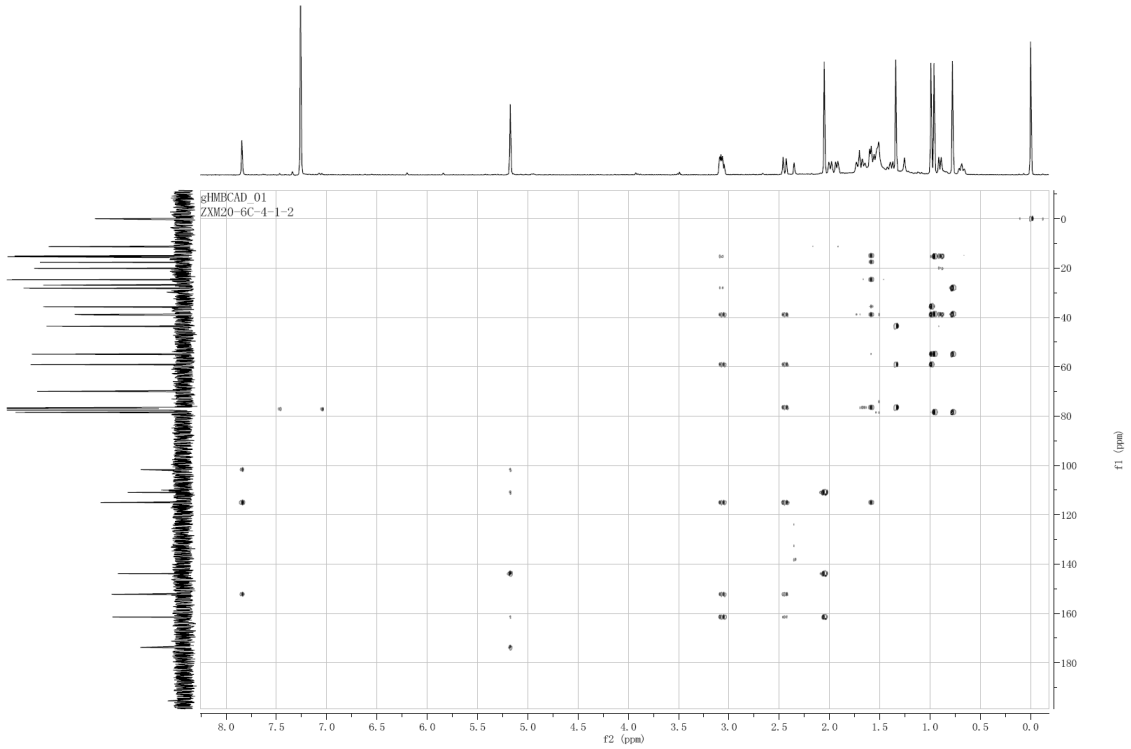



**Figure S7.** HMBC spectrum of **1** in $CDCl_3$.

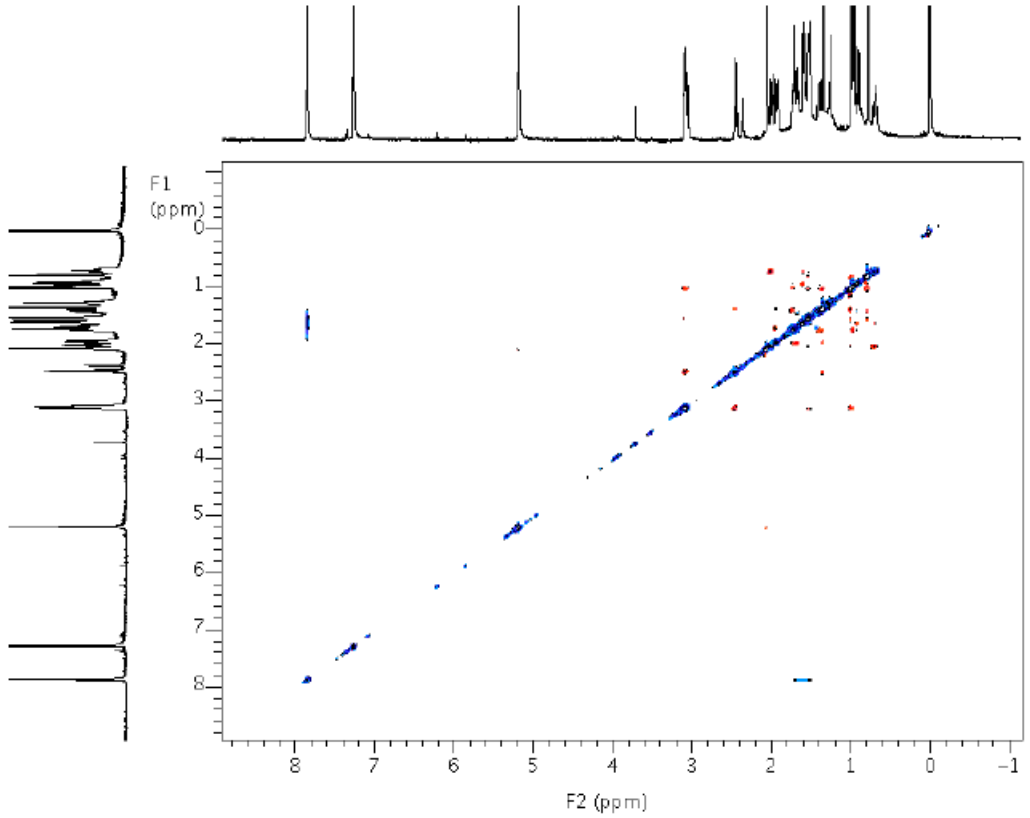



**Figure S8.** NOESY spectrum of **1** in $CDCl_3$.

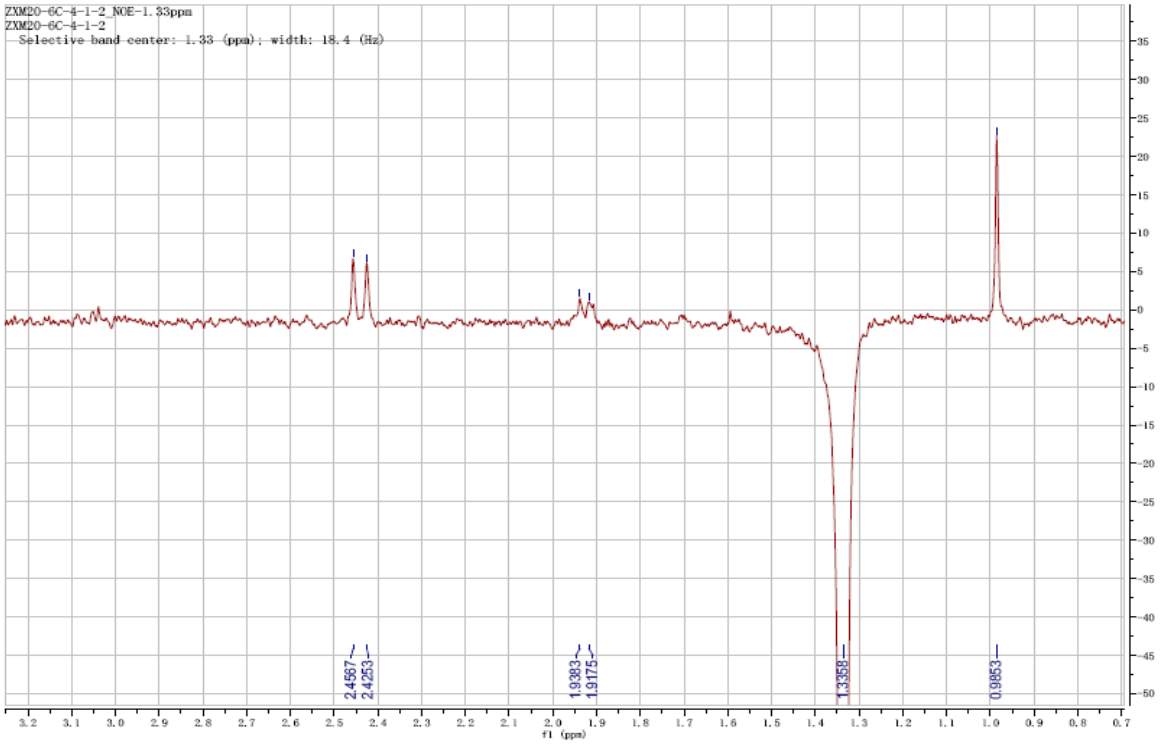



**Figure S9.** NOE spectrum of **1** in $CDCl_3$.

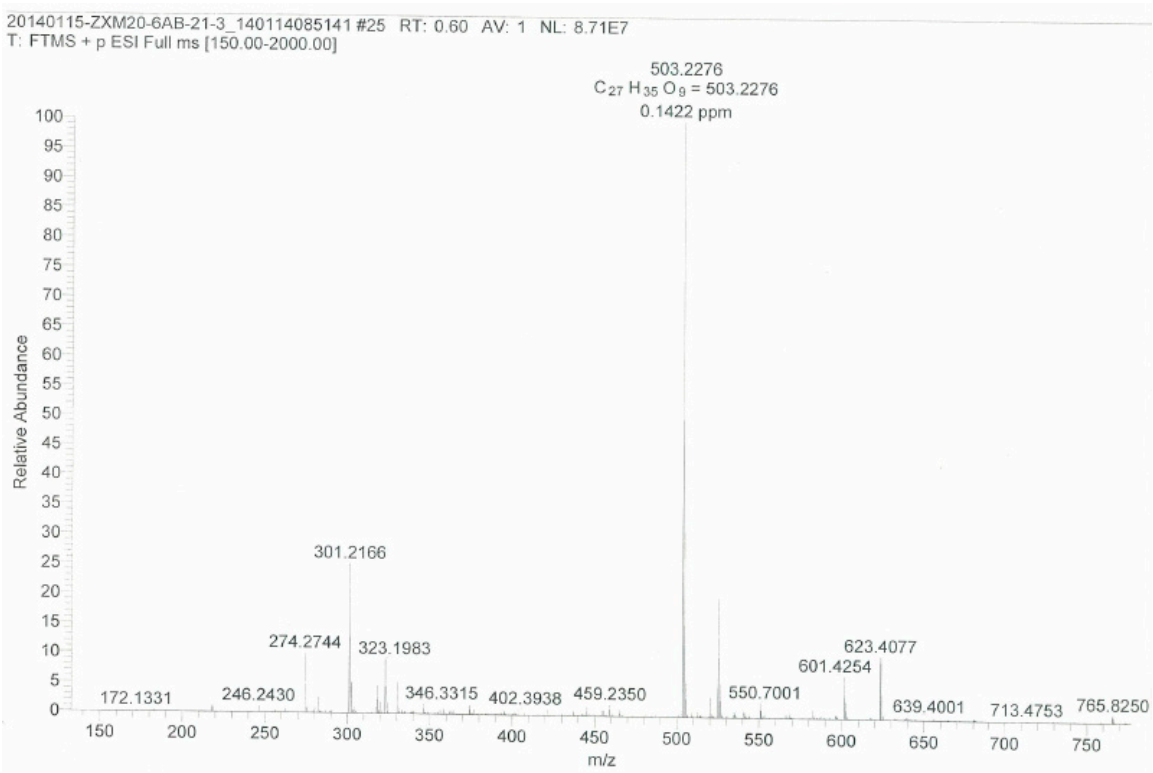



**Figure S10.** HR-ESI-MS of **2**.

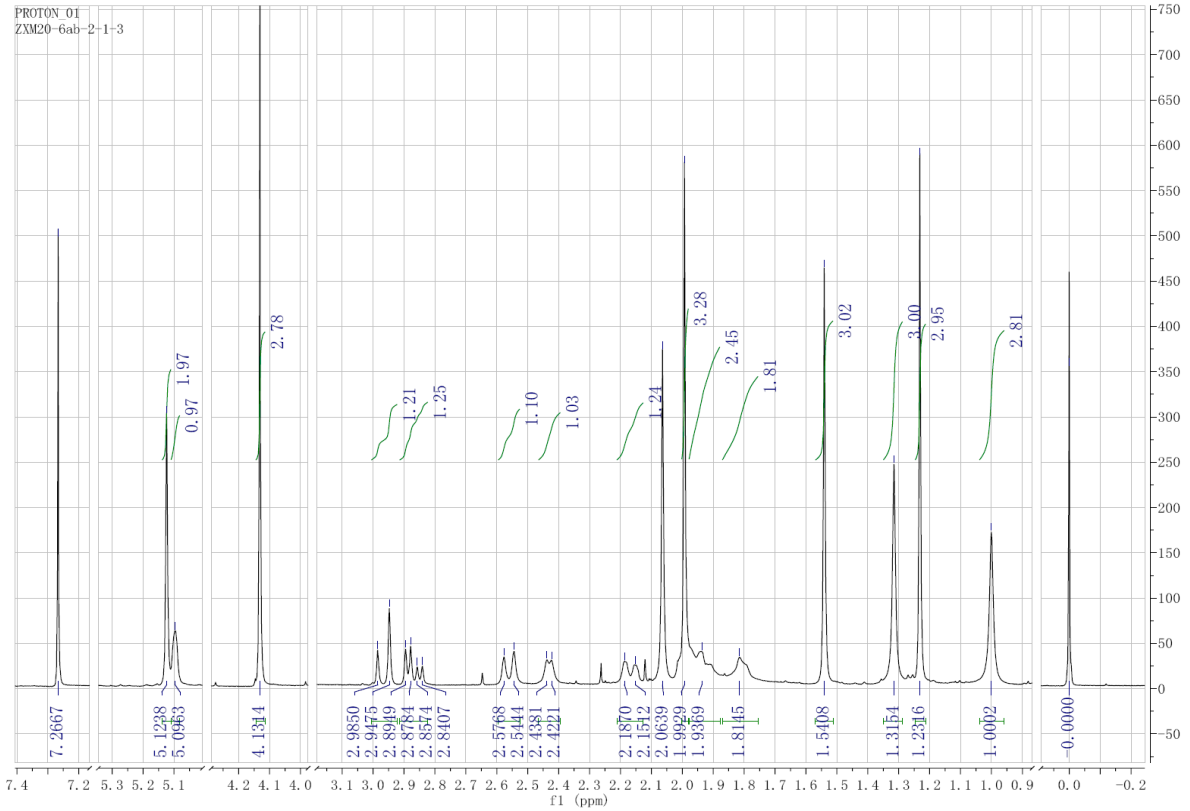



**Figure S11.** $^{1}$H NMR (500 MHz) spectrum of **2** in $CDCl_3$.

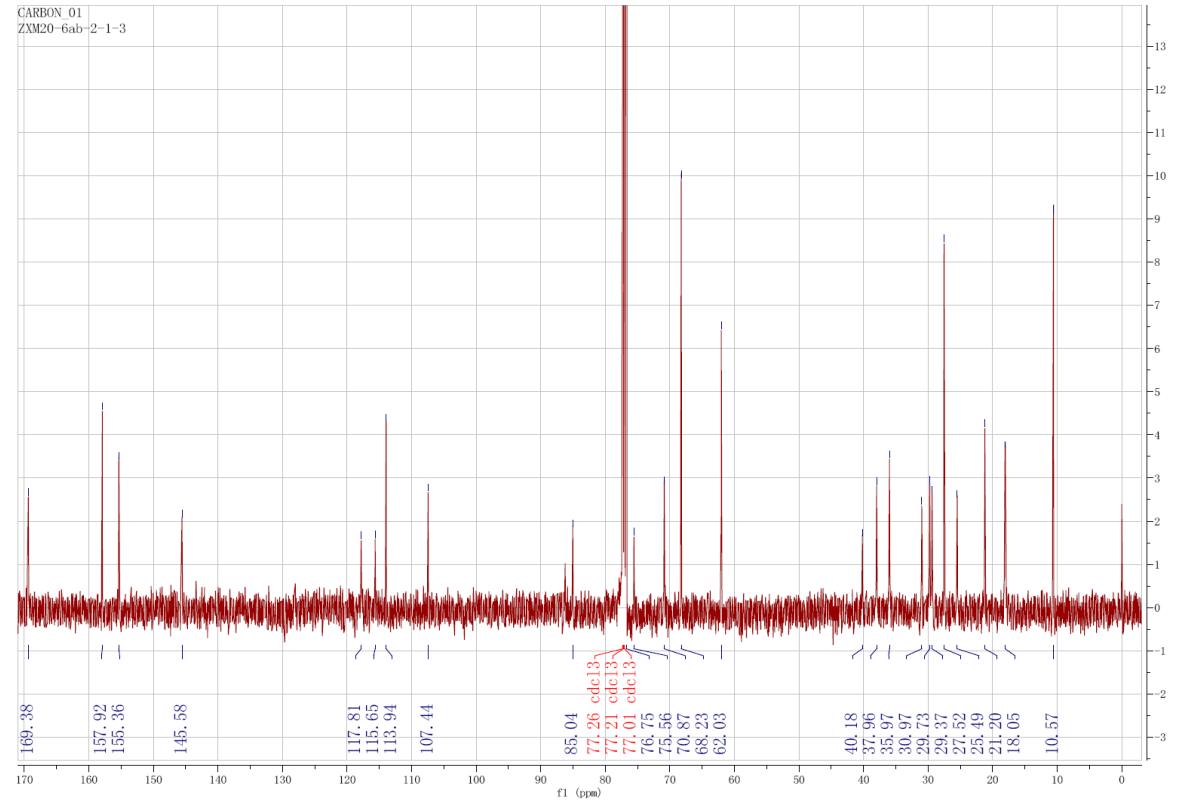



**Figure S12.** $^{13}$C NMR spectrum of **2** in $CDCl_3$.

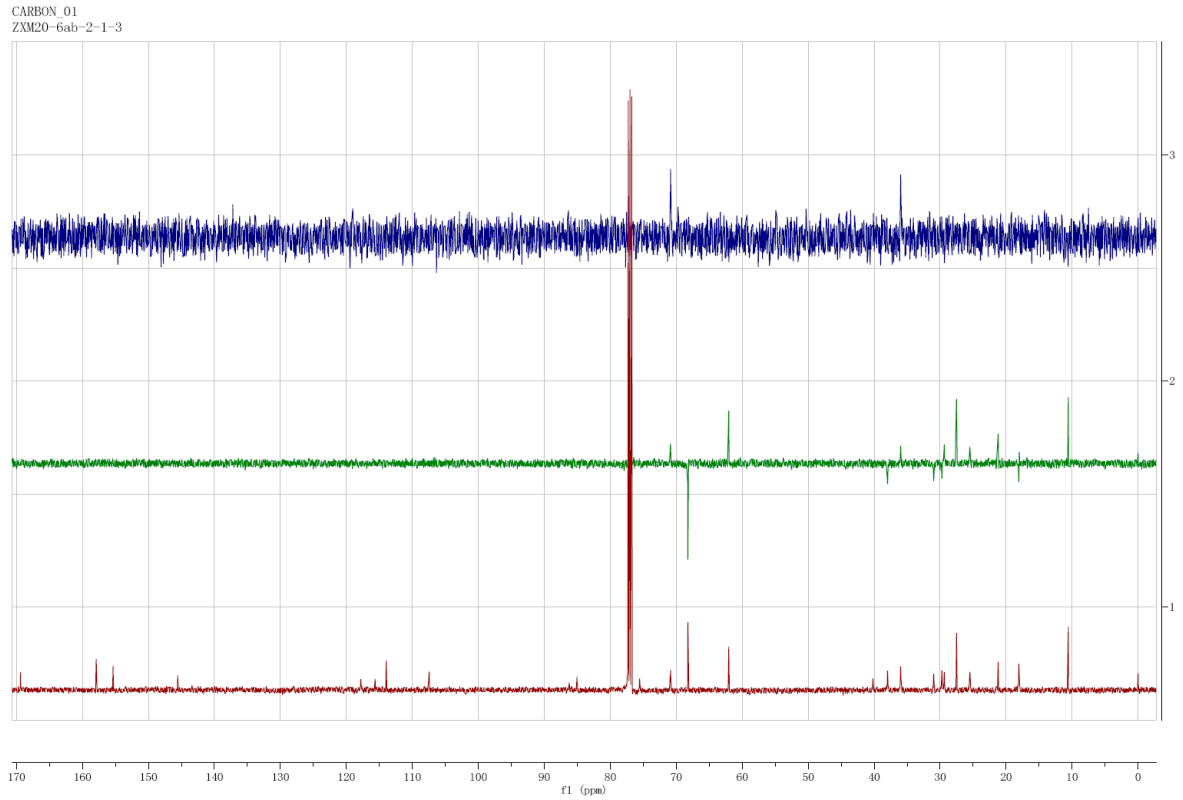



**Figure S13.** DEPT spectrum of **2** in $CDCl_3$.

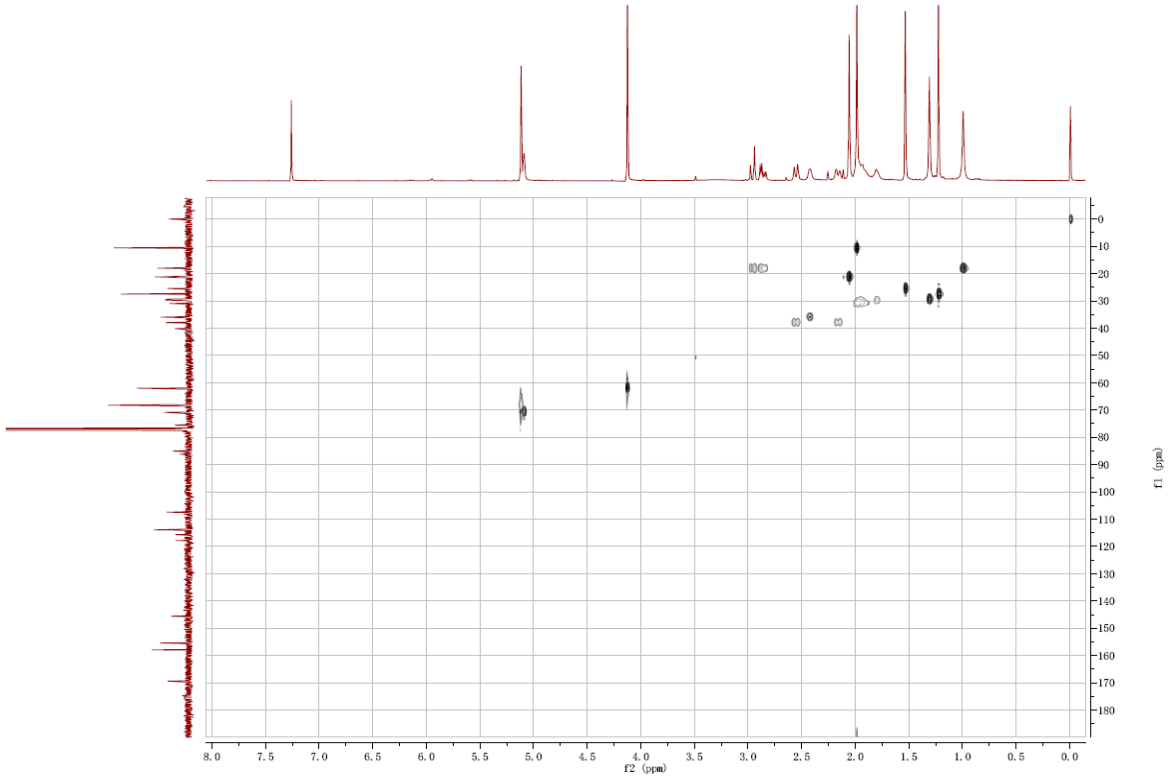



**Figure S14.** HMQC spectrum of **2** in $CDCl_3$.

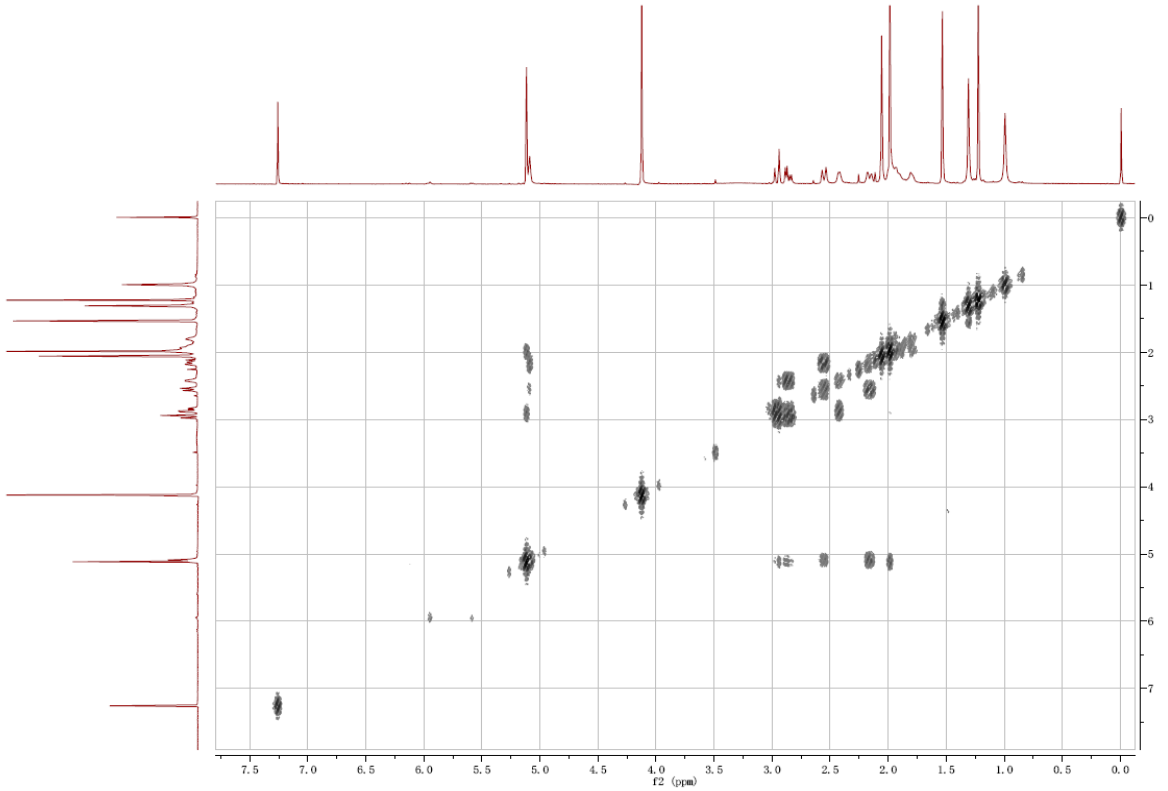



**Figure S15.** COSY spectrum of **2** in $CDCl_3$.

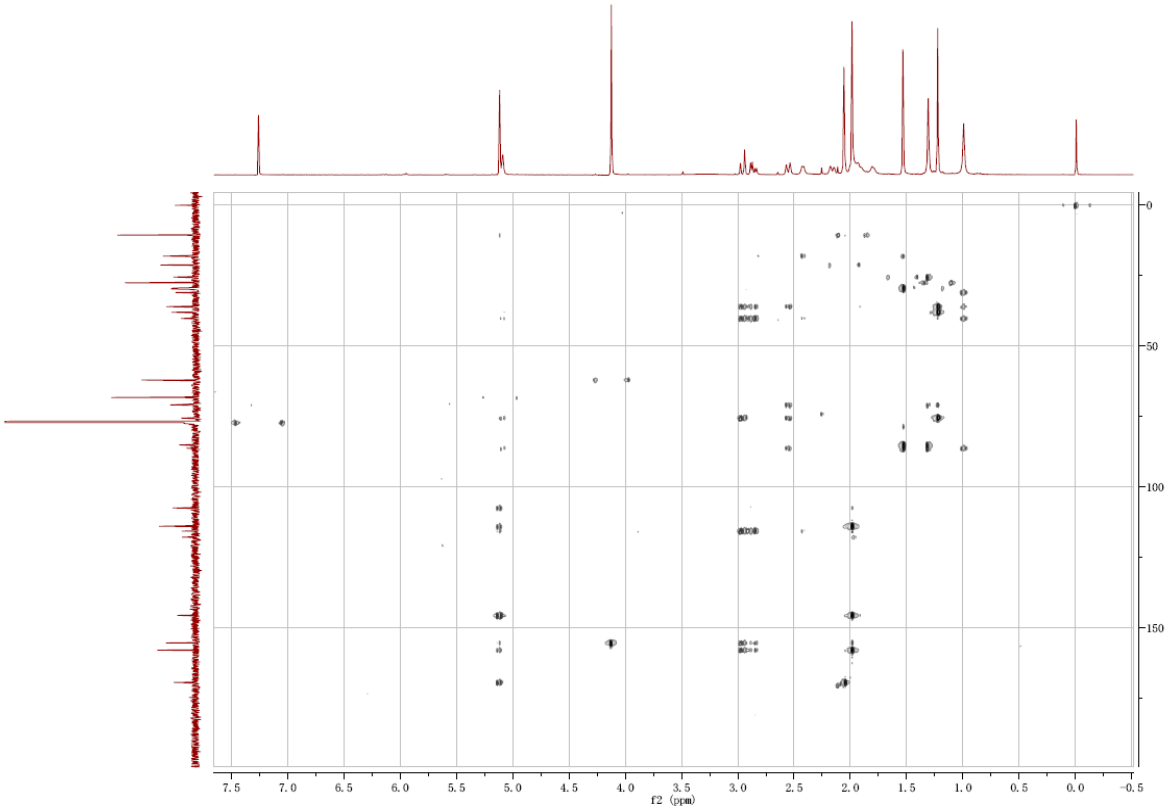
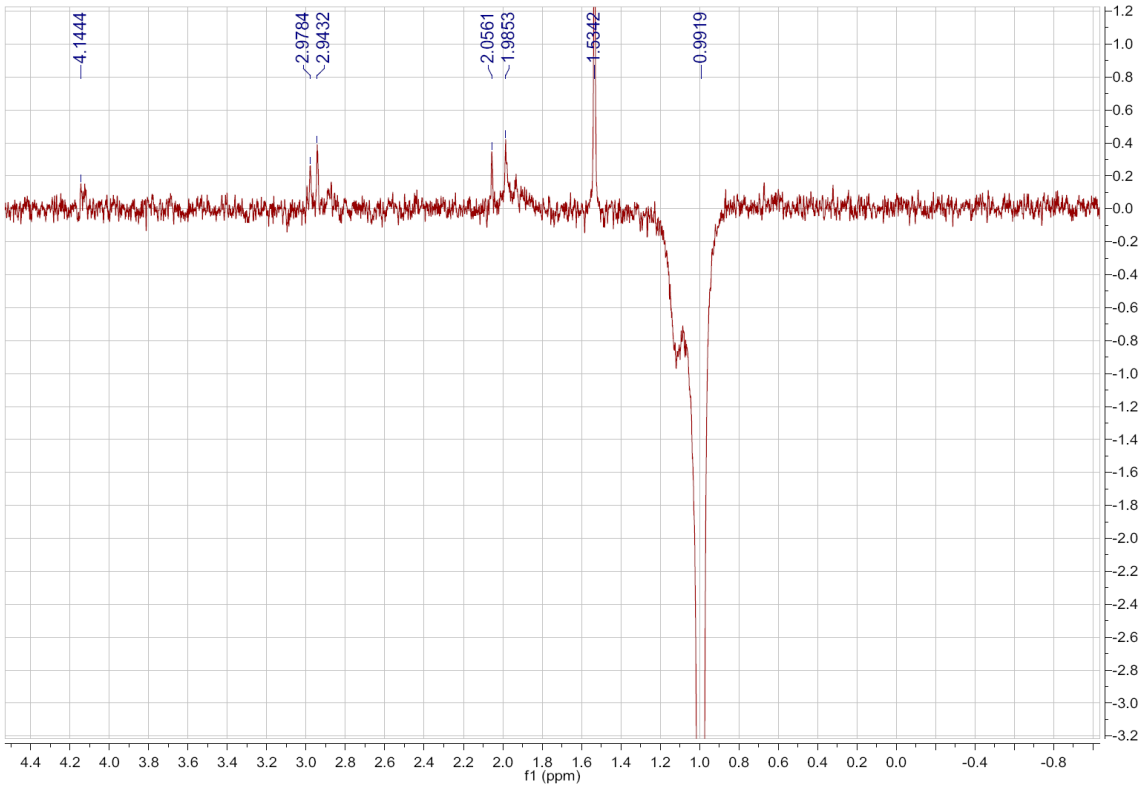
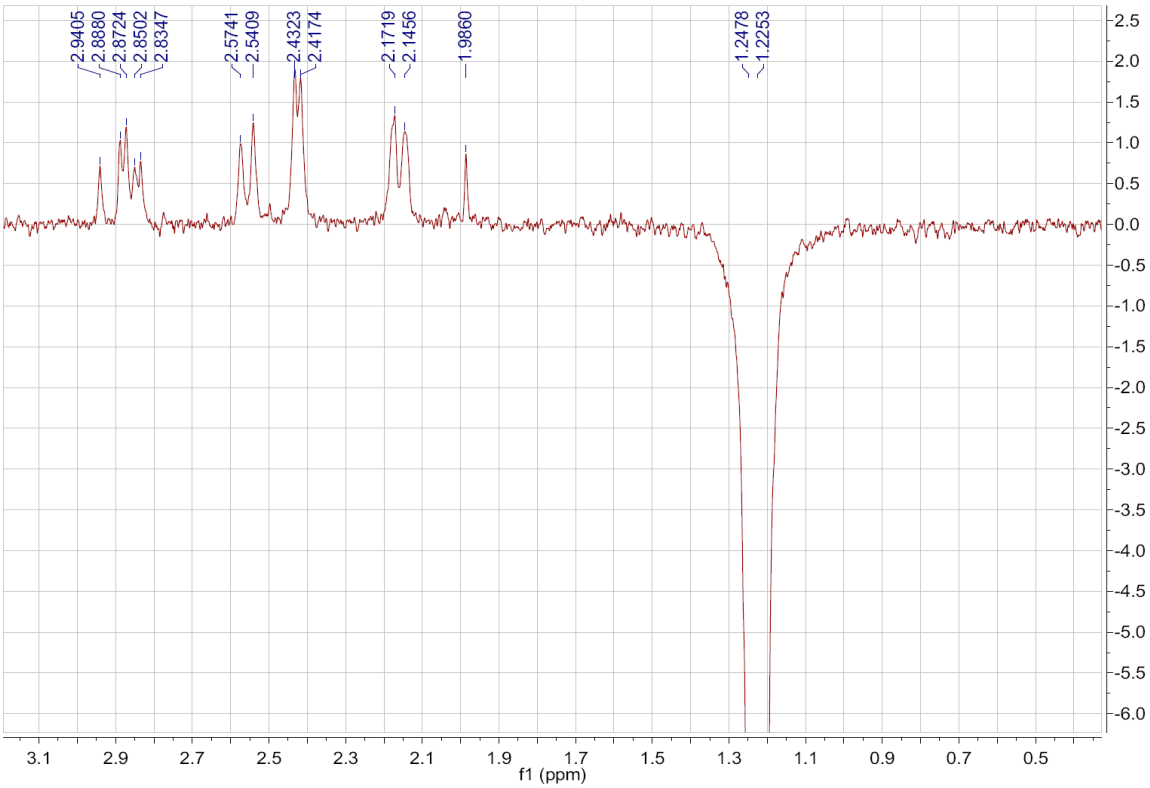



**Figure S16.** HMBC spectrum of **2** in $CDCl_3$.


4.1444
2.9784
2.9432
2.0561
1.9853
1.5342
0.9919
f1 (ppm)


2.9405
2.8880
2.8724
2.8502
2.8347
2.5741
2.5409
2.4323
2.4174
2.1719
2.1456
1.9860
1.2478
1.2253
f1 (ppm)

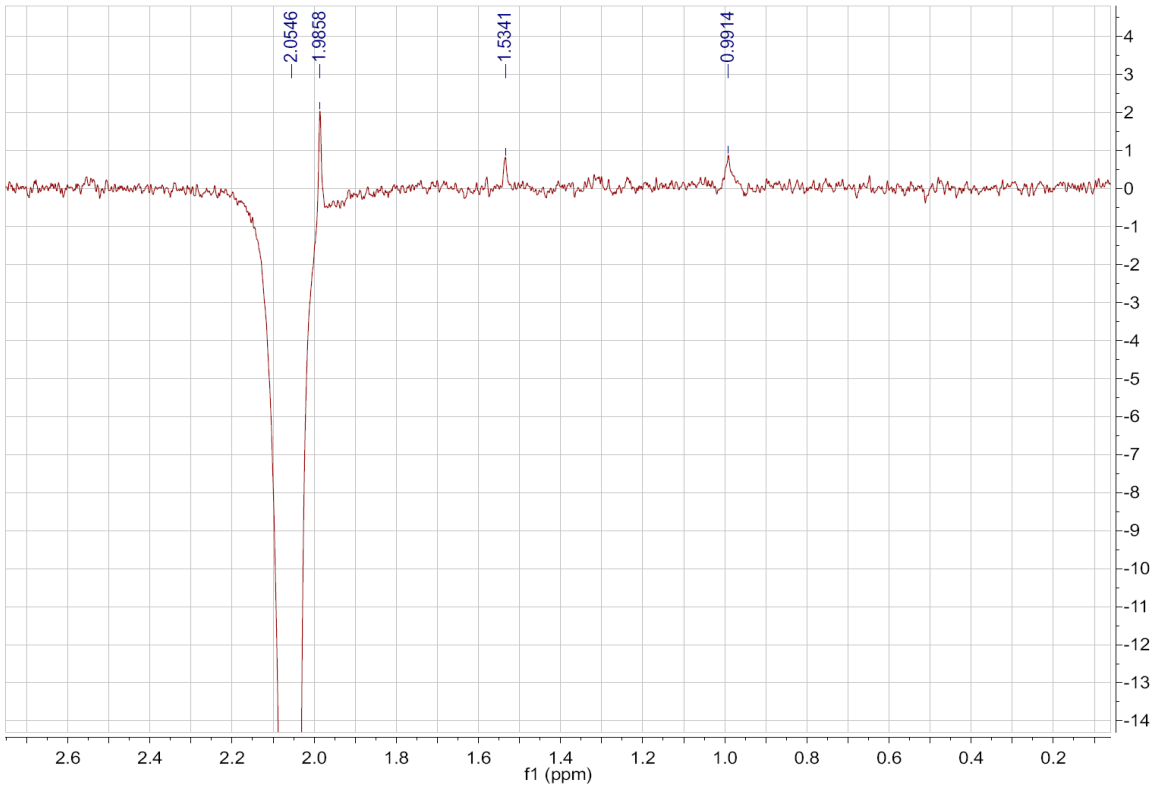



**Figure S17.** NOE spectra of **2** in $CDCl_3$.

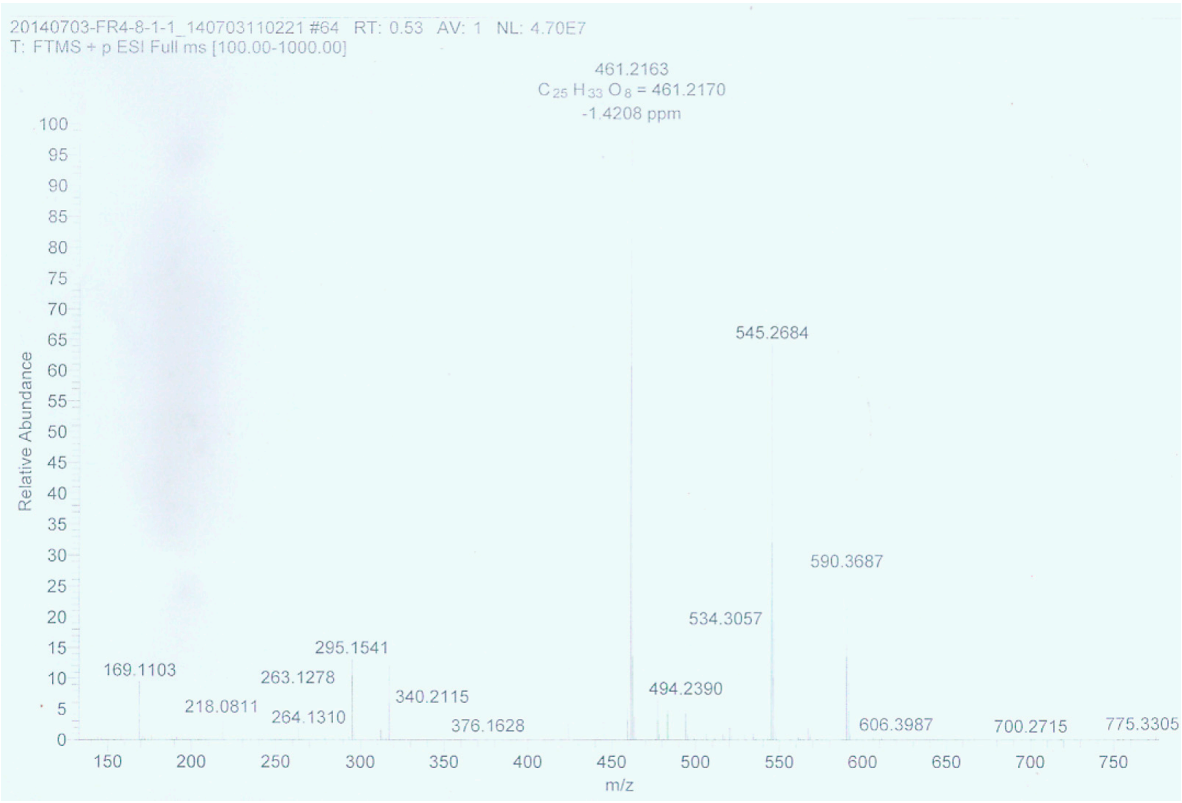



**Figure S18.** HRESIMS of Compound **3**.

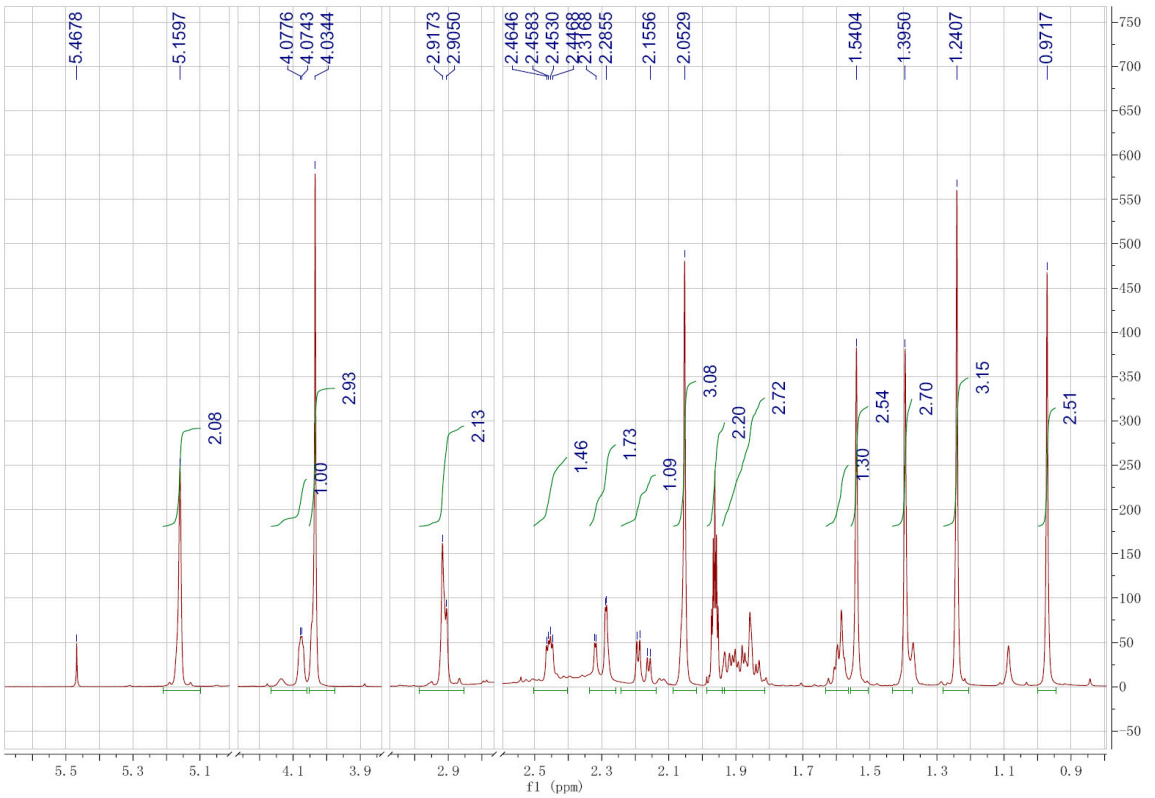



**Figure S19.** $^{1}$H NMR (500 MHz) spectrum of Compound **3** in $CD_3CN$.

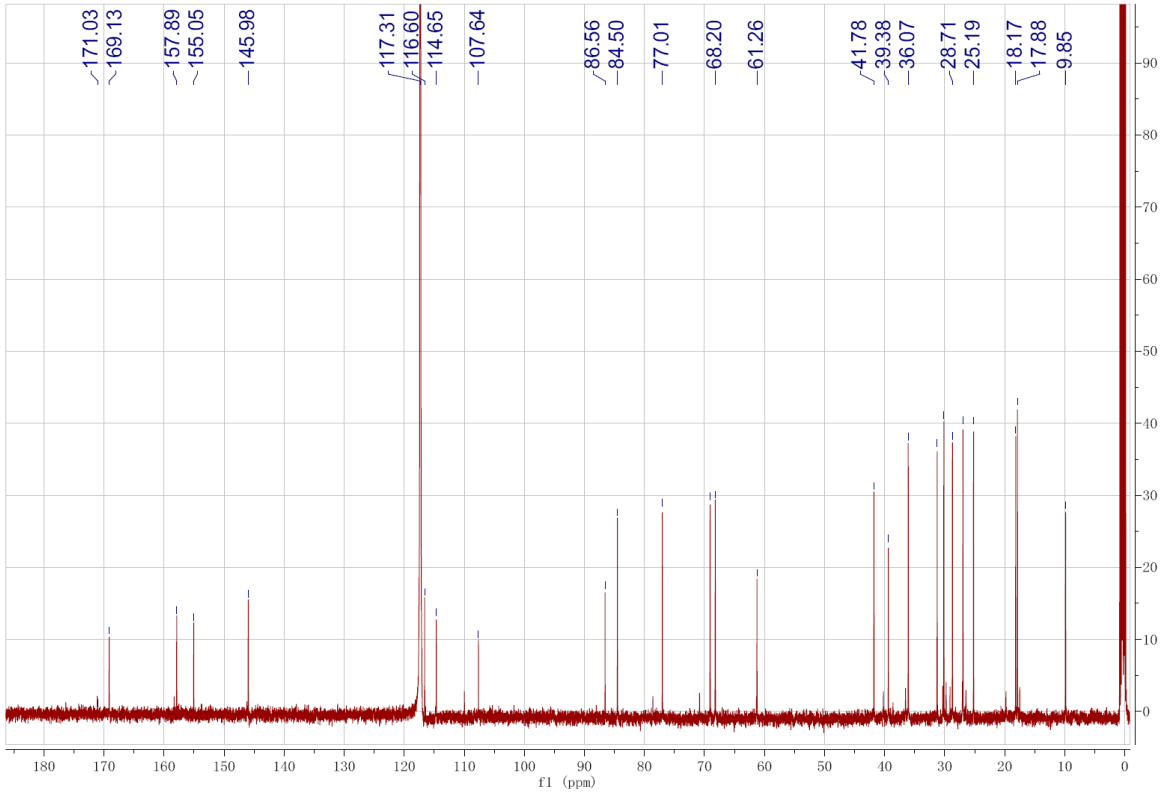



**Figure S20.** $^{13}$C NMR spectrum of Compound **3** in $CD_3CN$.

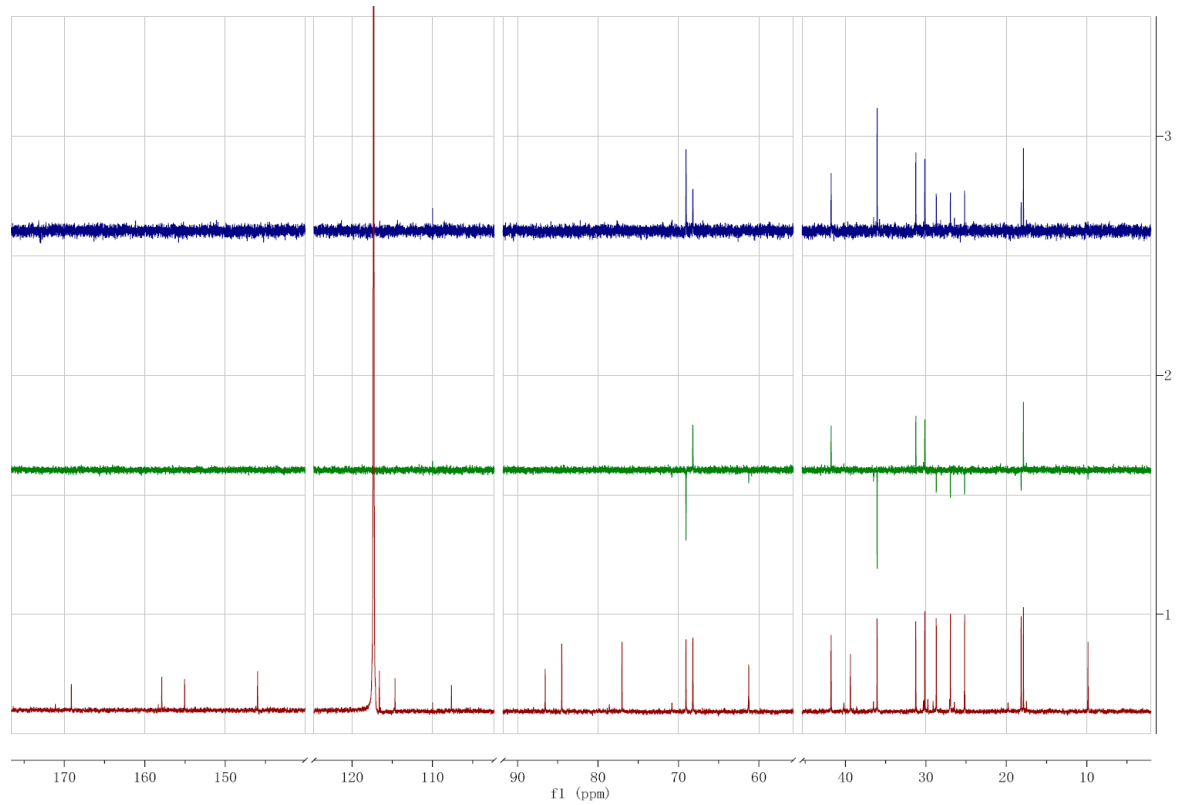



**Figure S21.** DEPT spectrum of Compound **3** in $CD_3CN$.

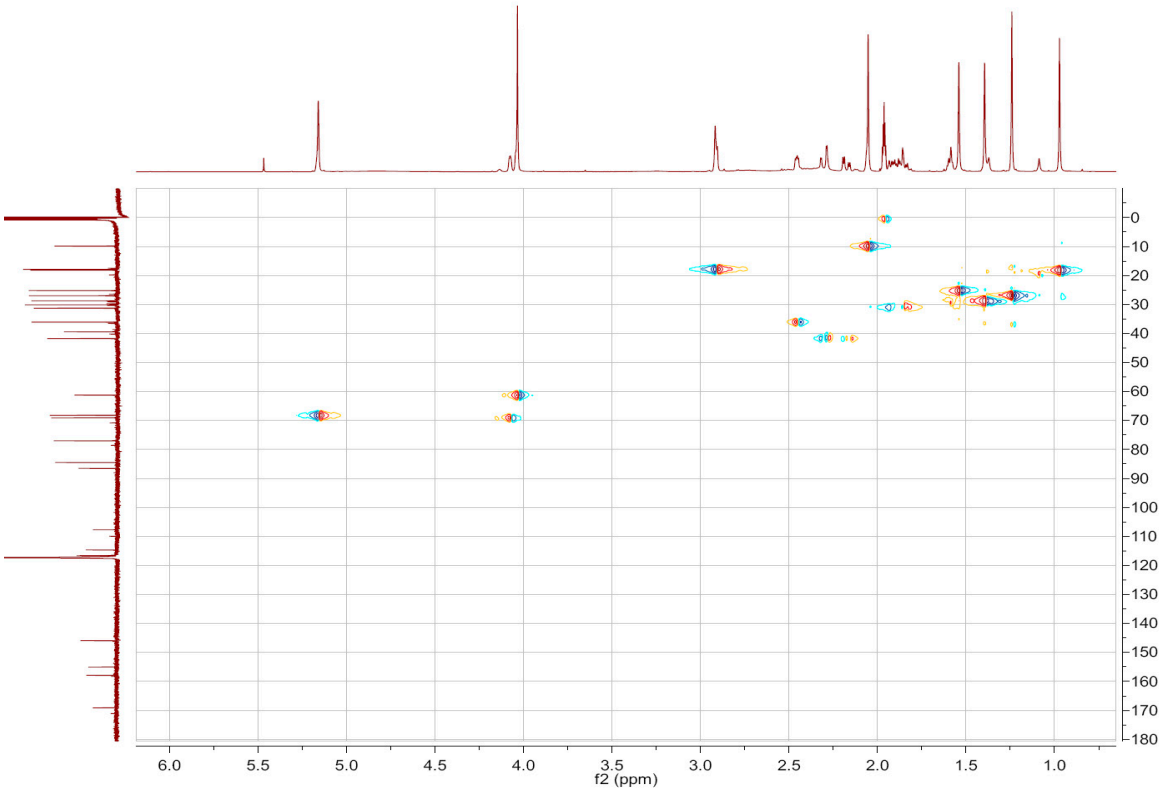



**Figure S22.** HMQC spectrum of Compound **3** in $CD_3CN$.

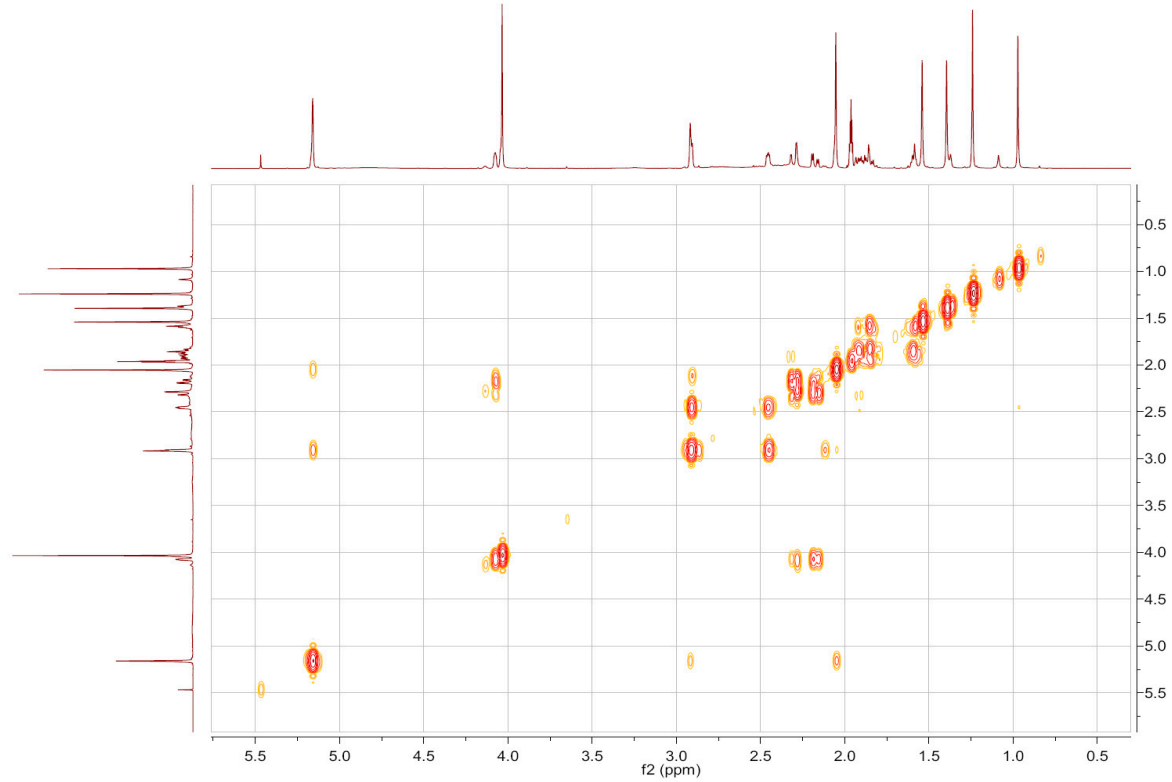



**Figure S23.** $^{1}H$–$^{1}H$ COSY spectrum of Compound **3** in $CD_3CN$.

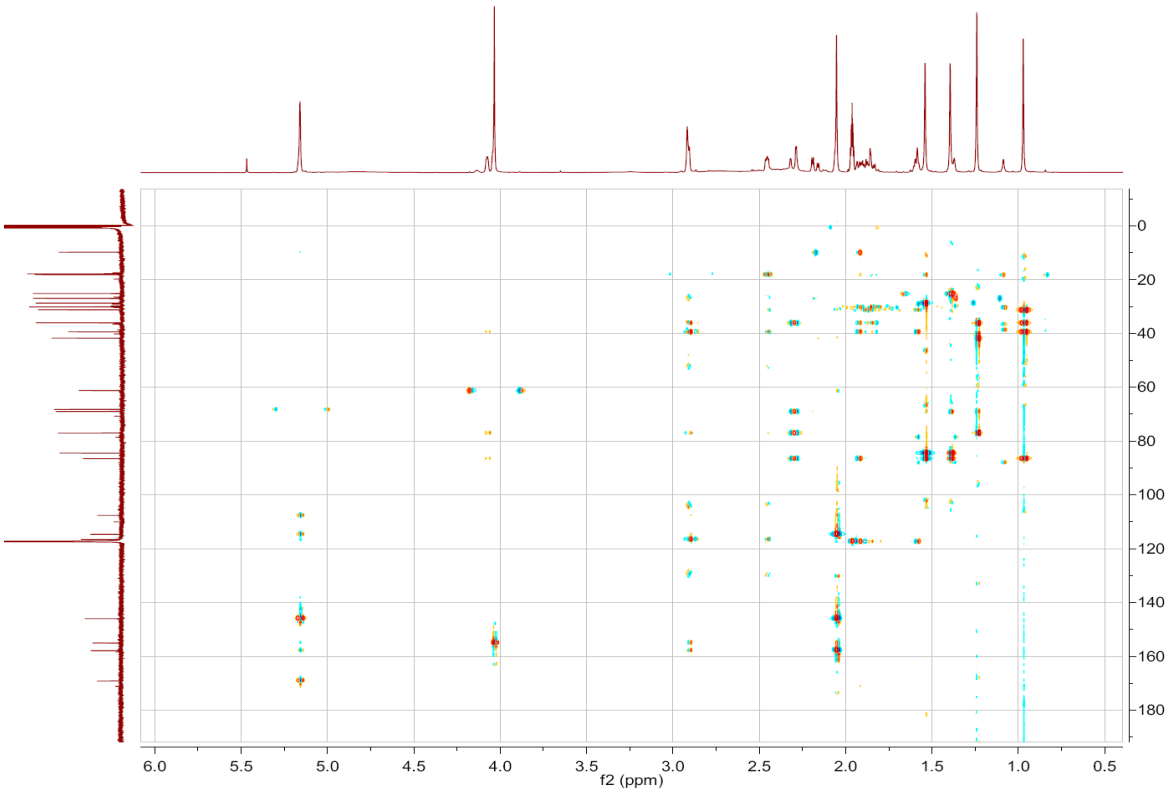
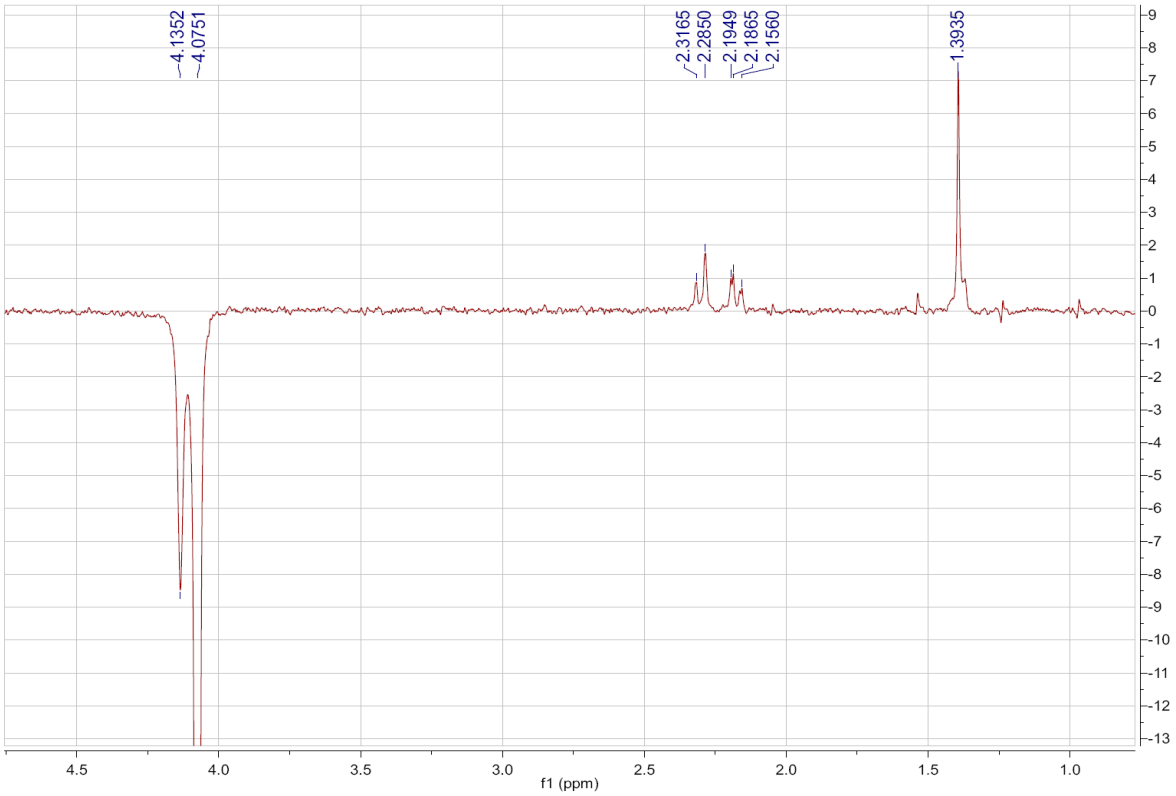
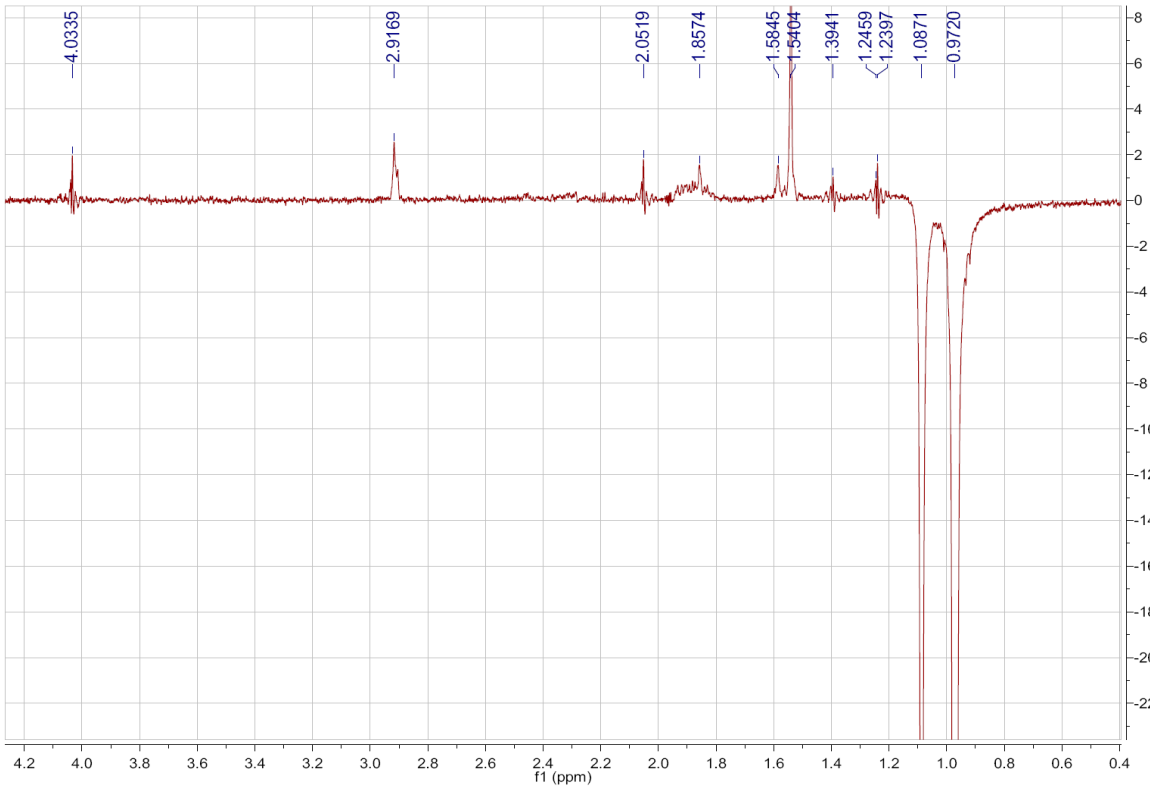



**Figure S24.** HMBC spectrum of Compound **3** in $CD_3CN$.


4.1352
4.0751
2.3165
2.2850
2.1949
2.1865
2.1560
1.3935
f1 (ppm)


4.0335
2.9169
2.0519
1.8574
1.5845
1.5404
1.3941
1.2459
1.2397
1.0871
0.9720
f1 (ppm)

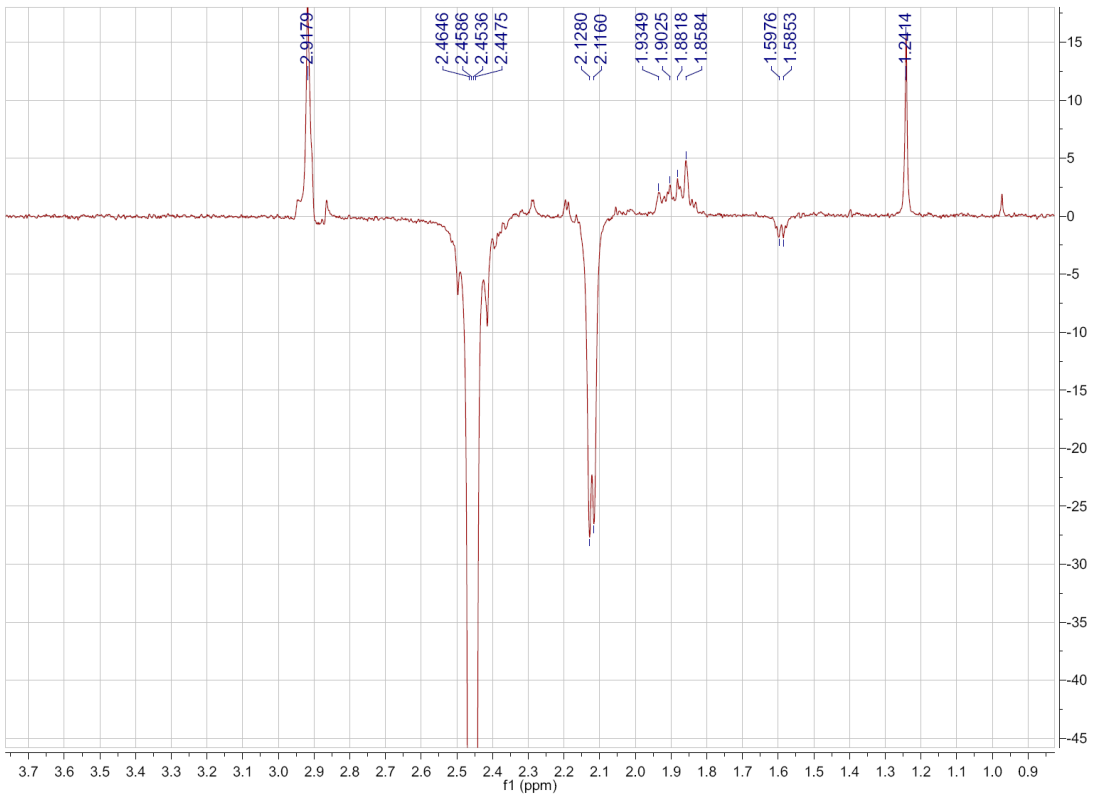



**Figure S25.** NOE spectra of Compound **3** in $CD_3CN$.

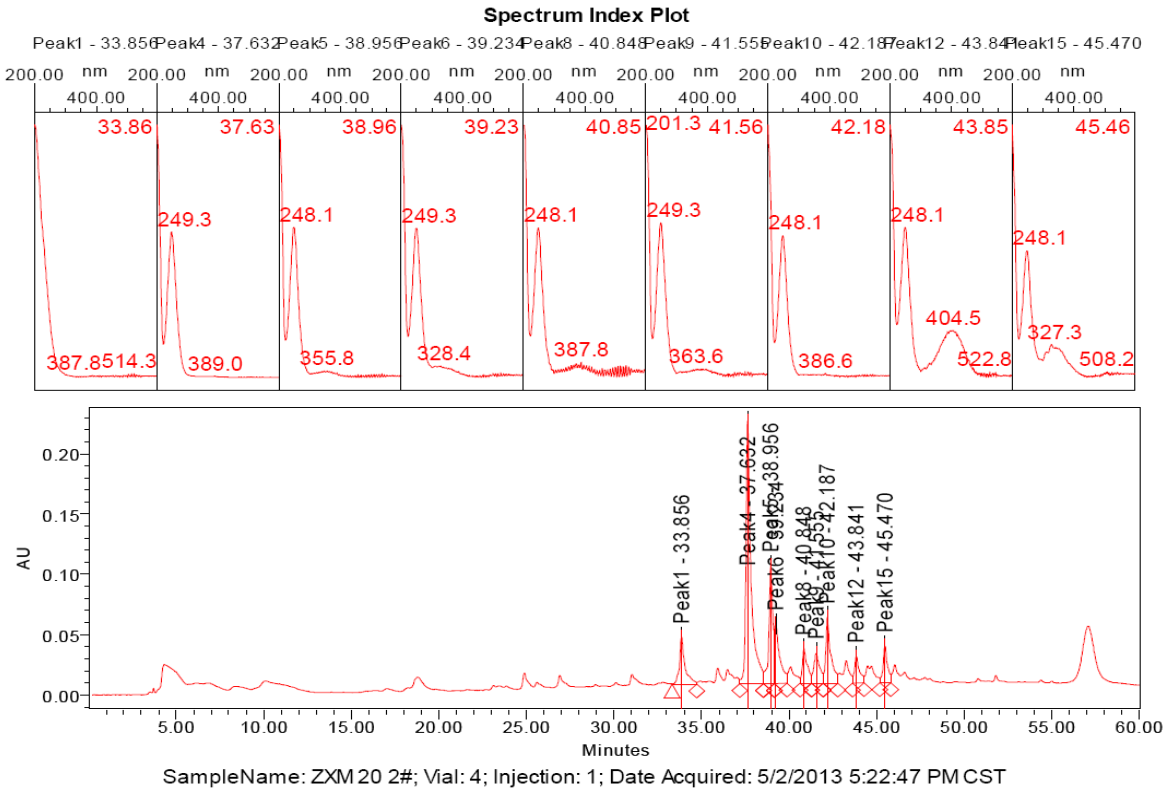



**Figure S26.** HPLC analysis of the EtOAc extract of *Aspergillus aureolatus* HDN14-107.

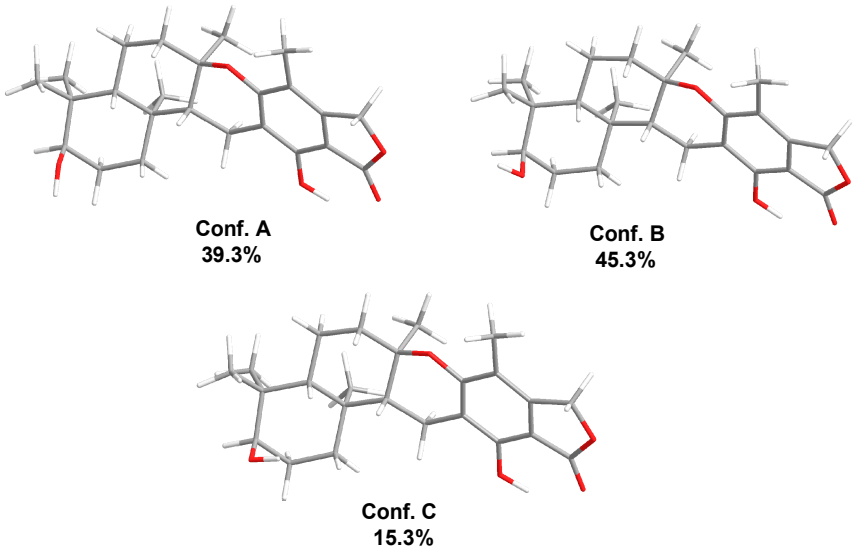



**Figure S27.** DFT-optimized structures for low-energy conformers of (11*R*, 14*R*, 17*R*, 20*S*, 21*R*)-**1** at B3LYP/6-31+G (d) level in acetonitrile (Conformer populations were calculated using the Gibbs free energy and Boltzmann population at 298 K estimated thereof).