

SUPPLEMENTAAL MATERIALS

Four new pterosins from *Pteris cretica* and their cytotoxic activities

Jian Lu, Caiying Peng, Shuang Cheng, Jianqun Liu, Qinge Ma and Jicheng Shu *

Key Laboratory of Modern Preparation of Traditional Chinese Medicines, Ministry of Education, Jiangxi University of Traditional Chinese Medicine, Nanchang, 330004, China;
E-Mail: lujian10120801@sina.com

*Correspondence: 20101042@jxutcm.edu.cn; Tel.: 86-791-7118658.

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Abstract: Phytochemical investigation of the aerial parts of *Pteris cretica* led to isolation and elucidation of nine pterosins, including four new pterosins, creticolacton A (**1**), 13-hydroxyl-2(*R*),3(*R*)-pterosin L (**2**), creticoside A (**3**), spelosin 3-*O*- β -D-glucopyranoside (**4**), together with five known pterosins (**5-9**). Their structures were identified mainly on the basis of 1D and 2D NMR spectral data, ESI-MS and literature comparisons. Compounds **1** and **3** were new type of pterosins with a six membered ring between C-14 and C-15 of positions. The new compounds were tested *in vitro* for their cytotoxic activities against four human tumor cell lines (SH-SY5Y, SGC-7901, HCT-116, Lovo). Results showed that compounds **1** and **2** exhibited cytotoxic activity against HCT-116 cells with IC₅₀ value of 22.4 μ M and 15.8 μ M, respectively.

Keywords: *Pteris cretica* Linn.; pterosins; Cytotoxic activity.

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1. UV, HRESI-MS, ^1H NMR, ^{13}C NMR, HSQC, HMBC, NOESY and CD spectra of 1

Figure S1 UV spectra of 1

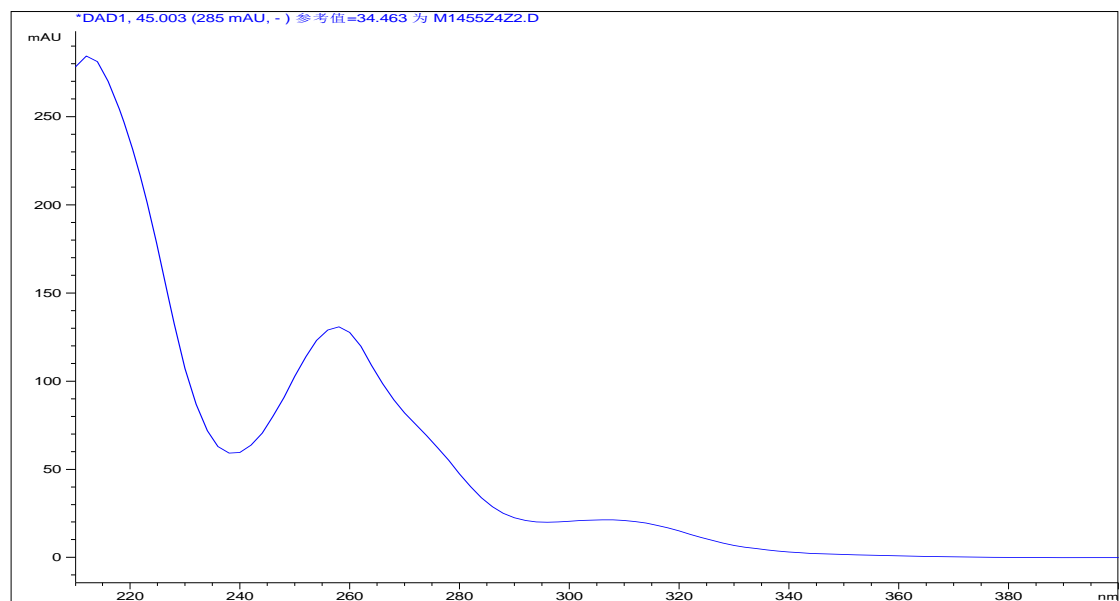


Figure S2 HRESIMS spectra of 1

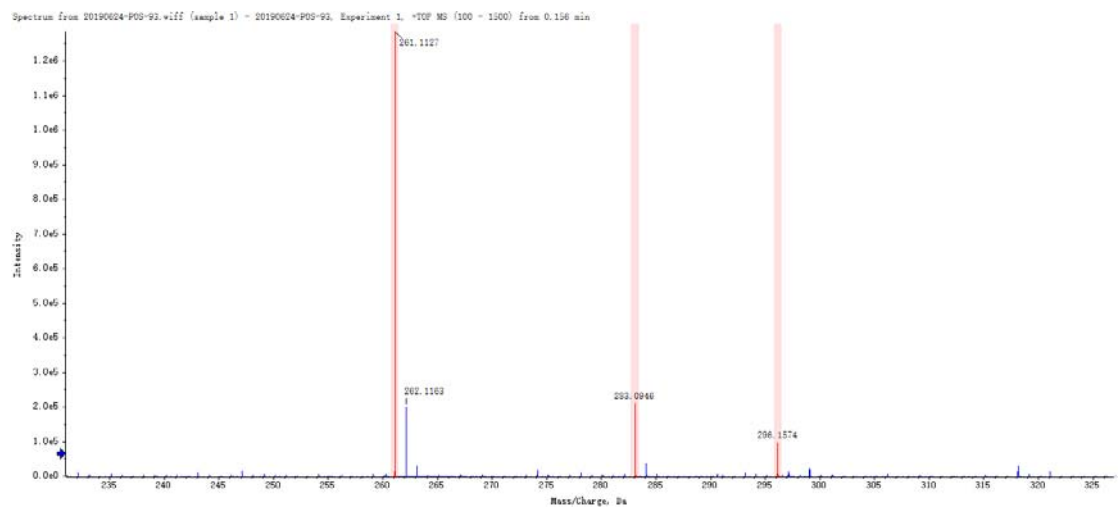


Figure S3 ^1H NMR spectra of 1

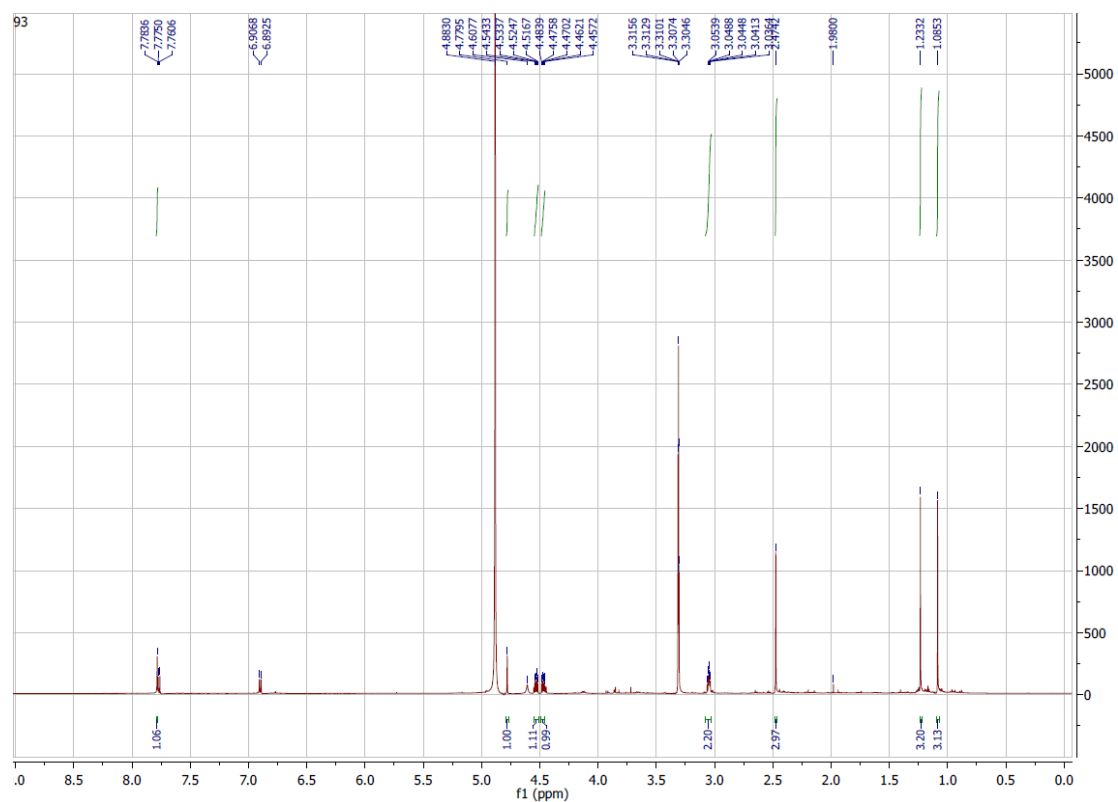


Figure S4 ^{13}C NMR spectra of 1

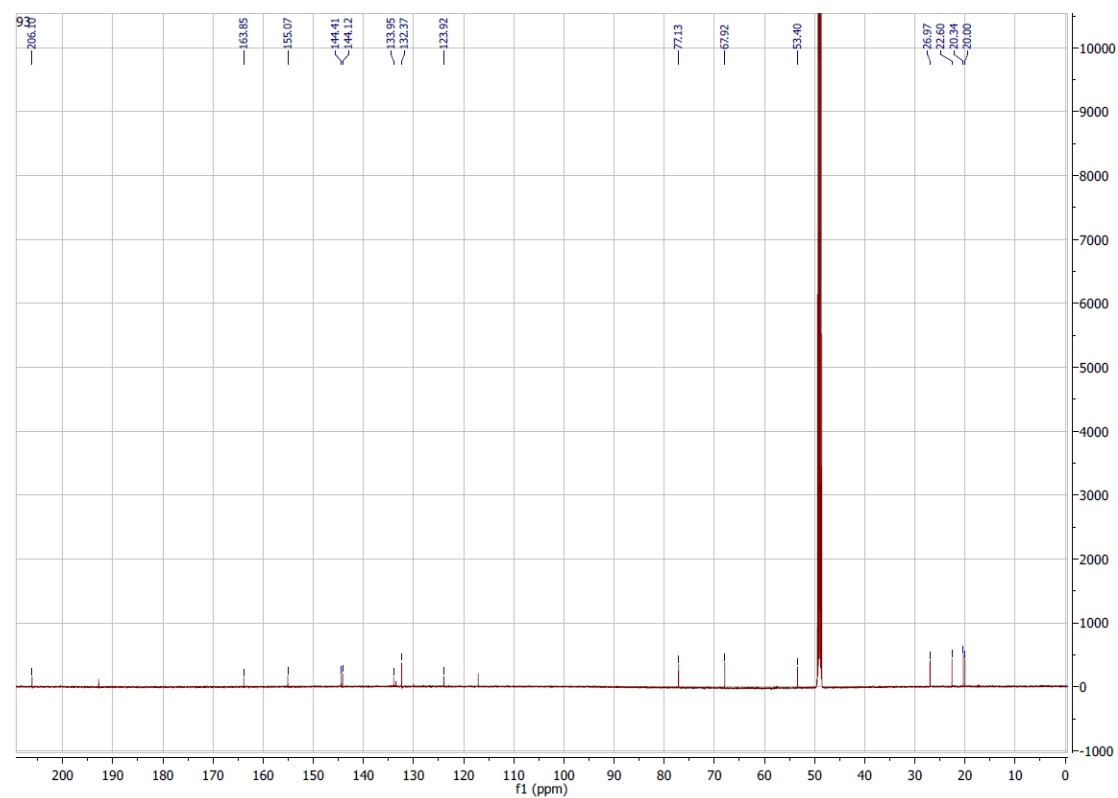


Figure S5 HSQC spectra of **1**

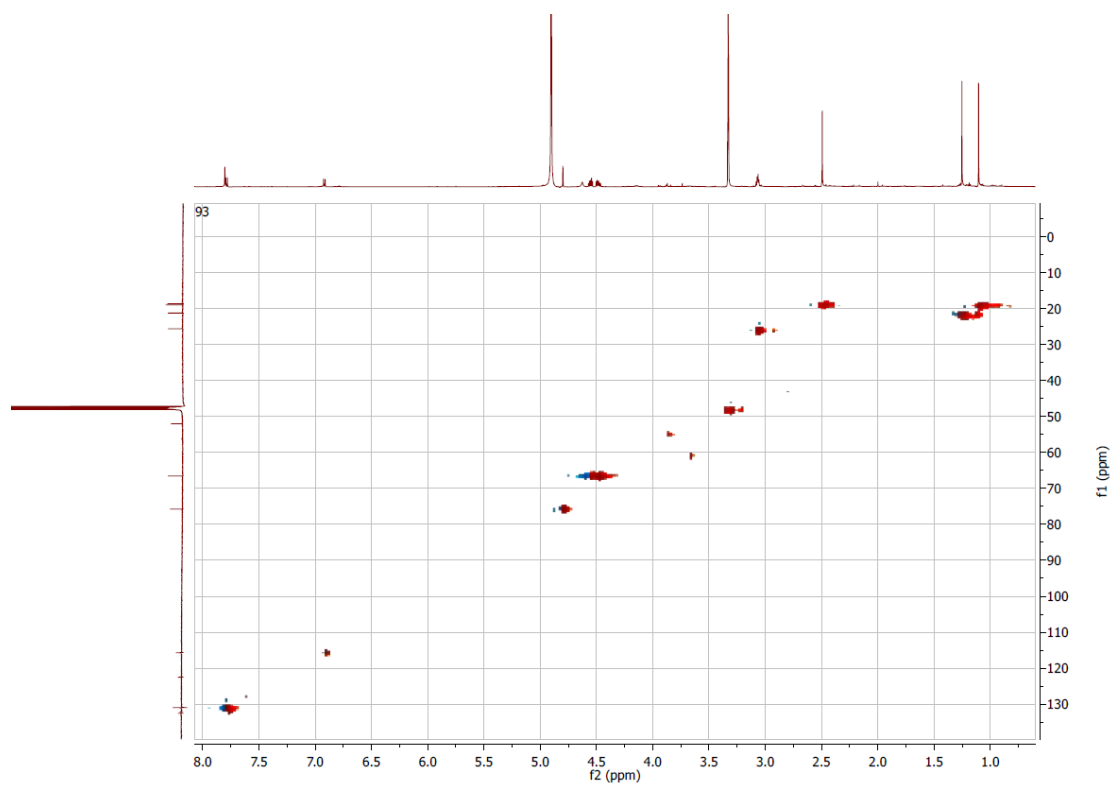


Figure S6 HMBC spectra of **1**

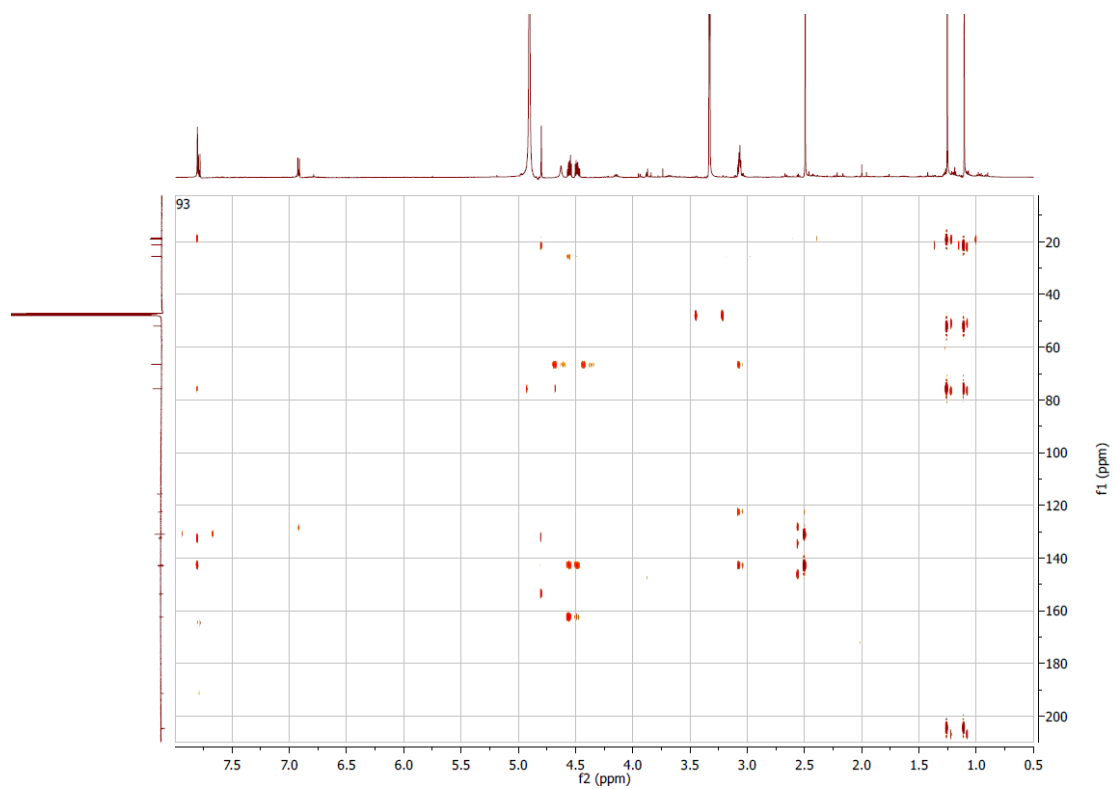


Figure S7 H-H NOESY spectra of 1

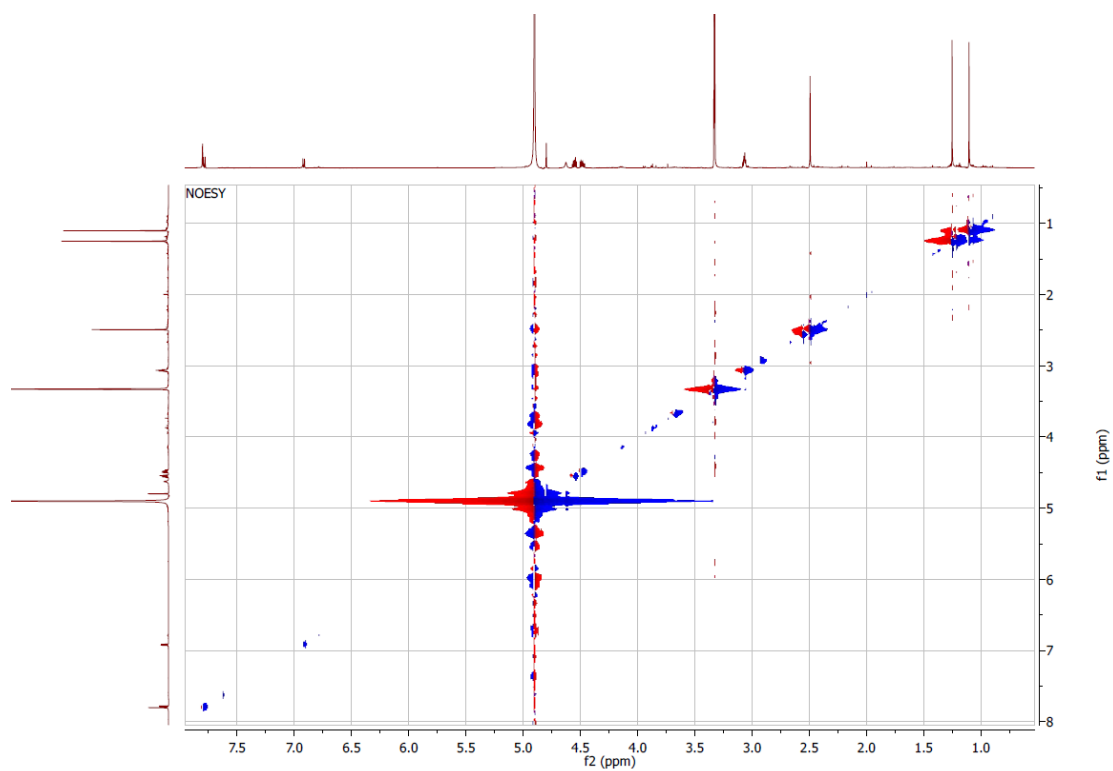
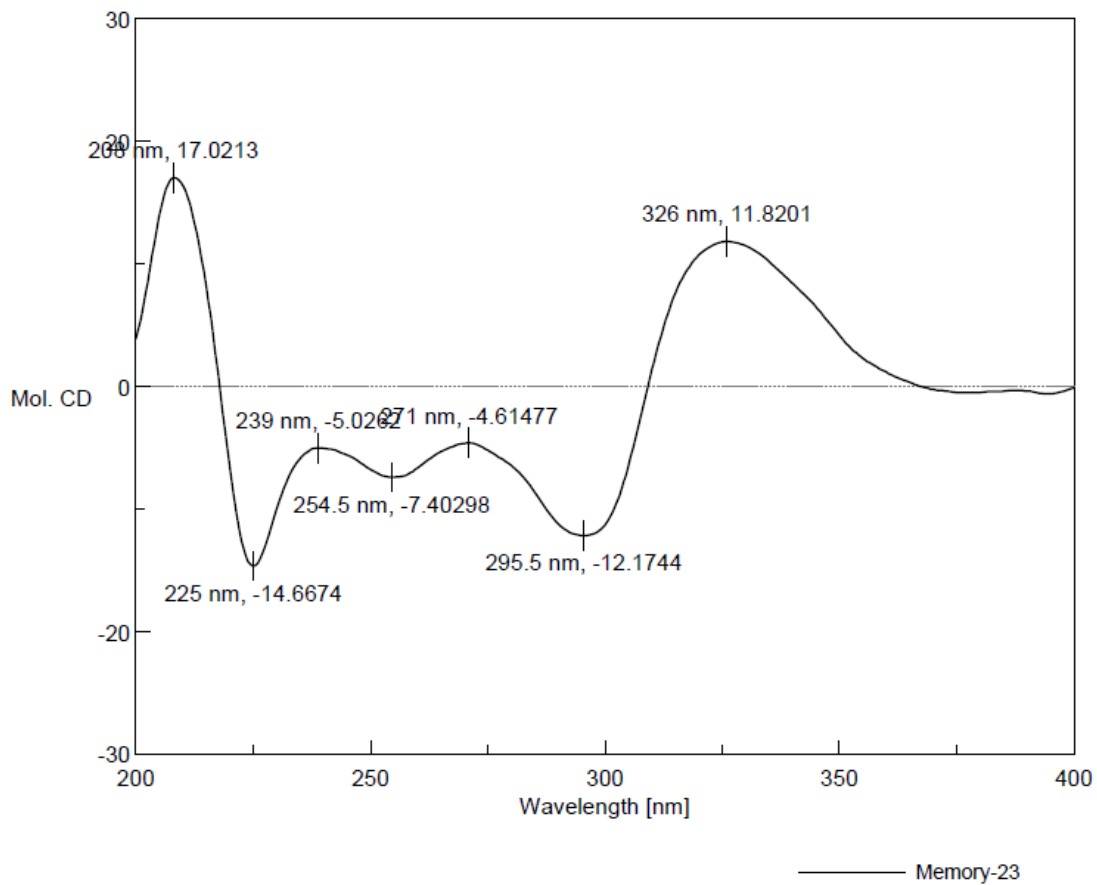


Figure S8 CD spectra of 1



2. UV, HRESI-MS, ^1H NMR, ^{13}C NMR, HSQC, HMBC, NOESY and CD spectra of 2

Figure S9 UV spectra of 2

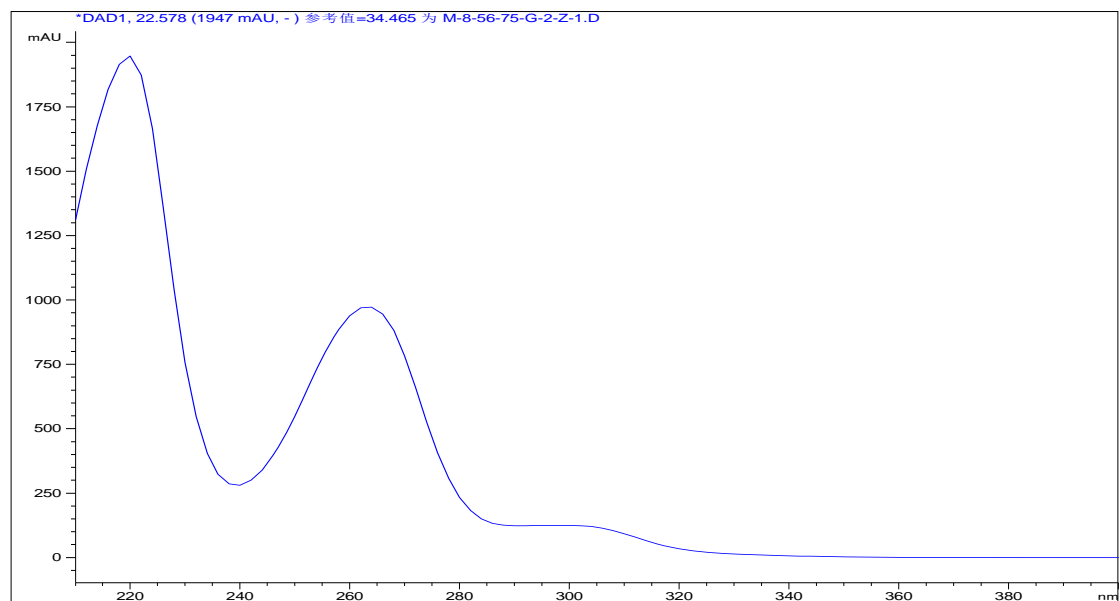


Figure S10 HRESIMS spectra of 2

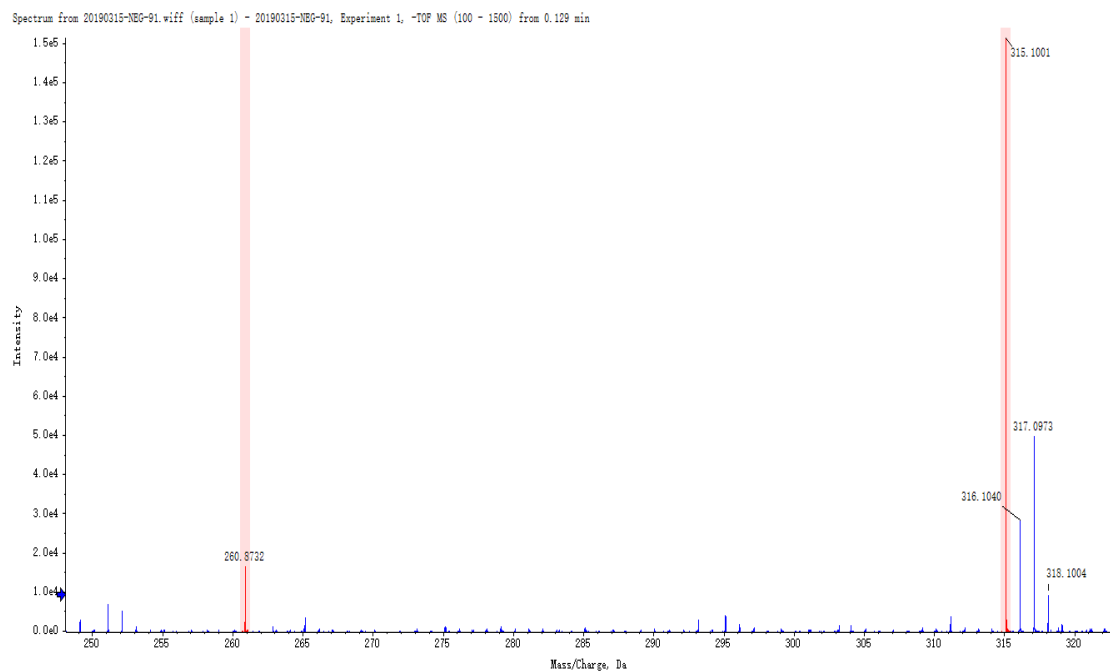


Figure S11 ^1H NMR spectra of 2

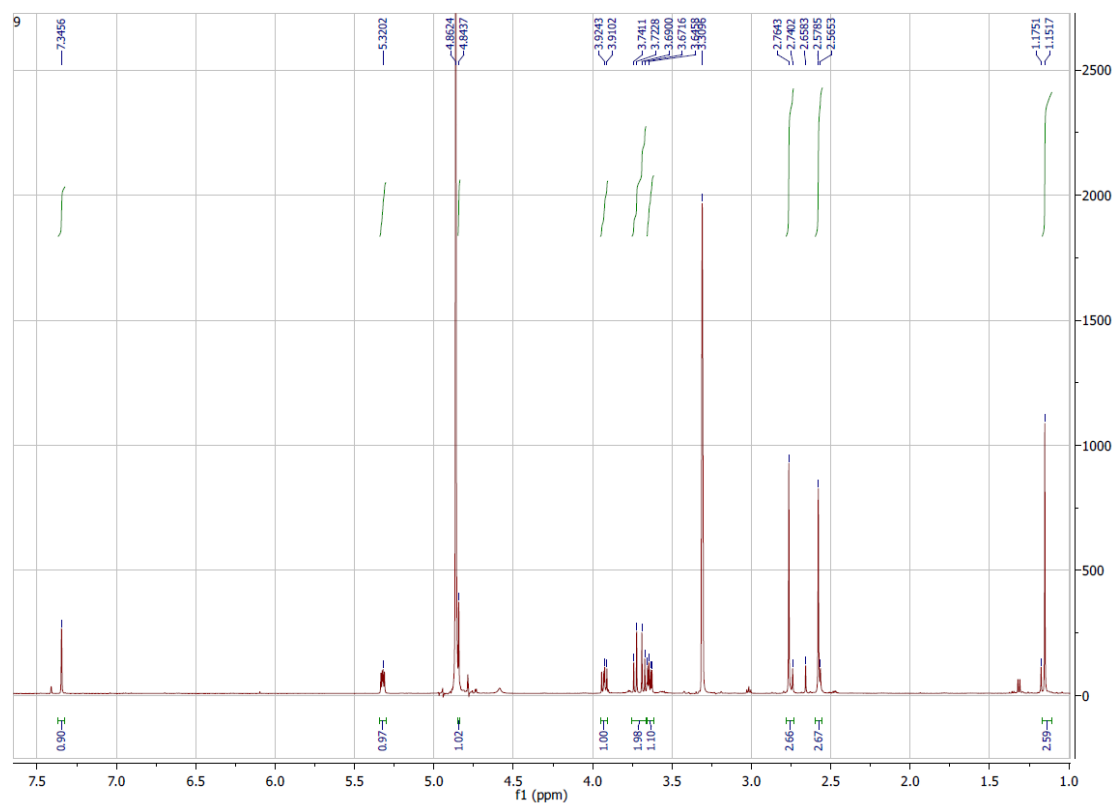


Figure S12 ^{13}C NMR spectra of 2

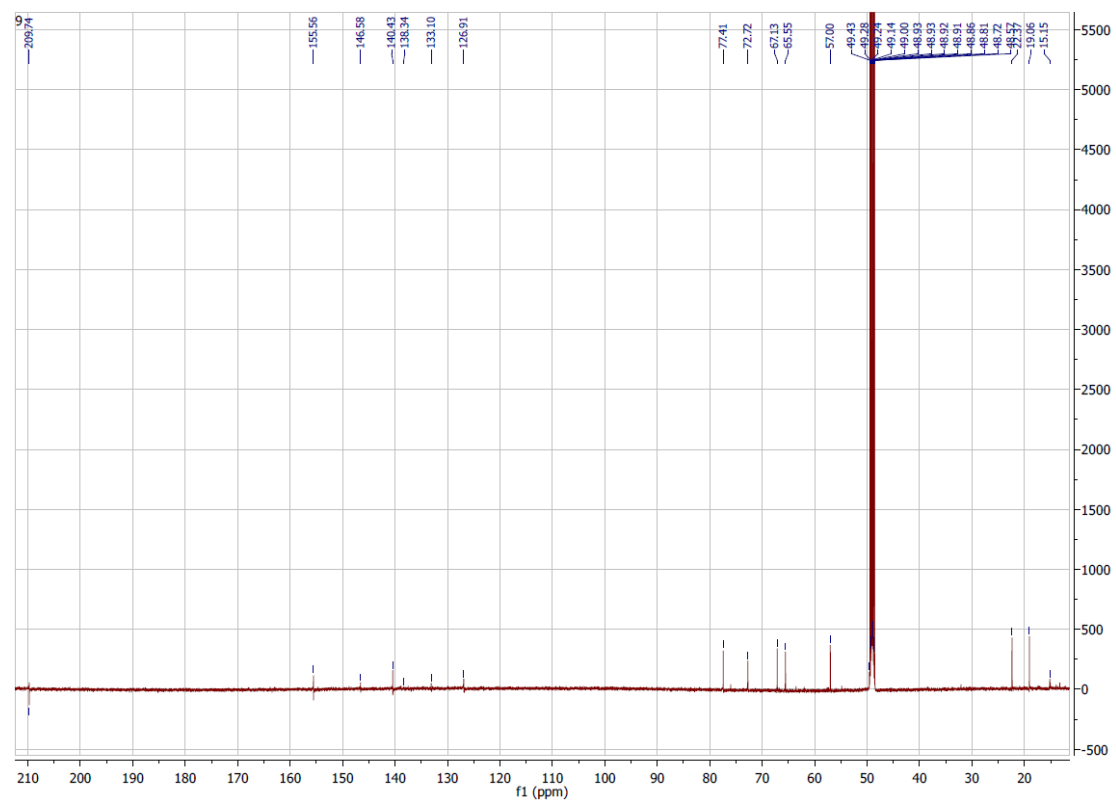


Figure S13 HSQC spectra of 2

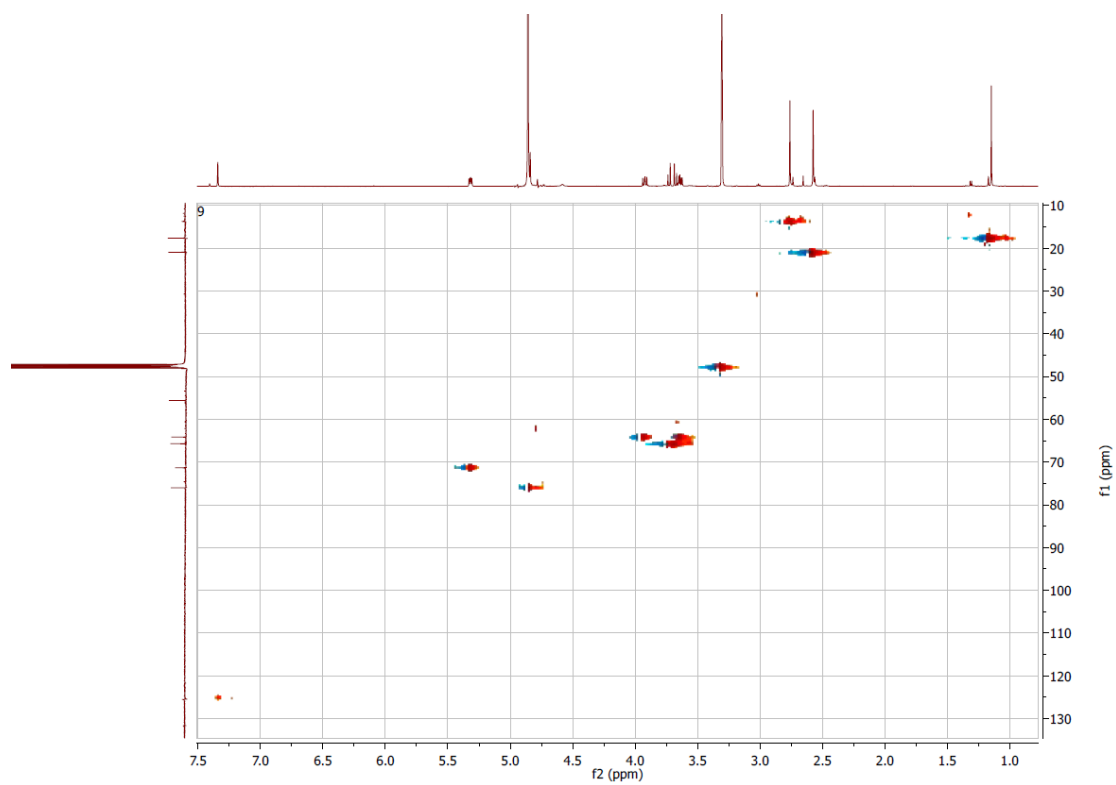


Figure S14 HMBC spectra of 2

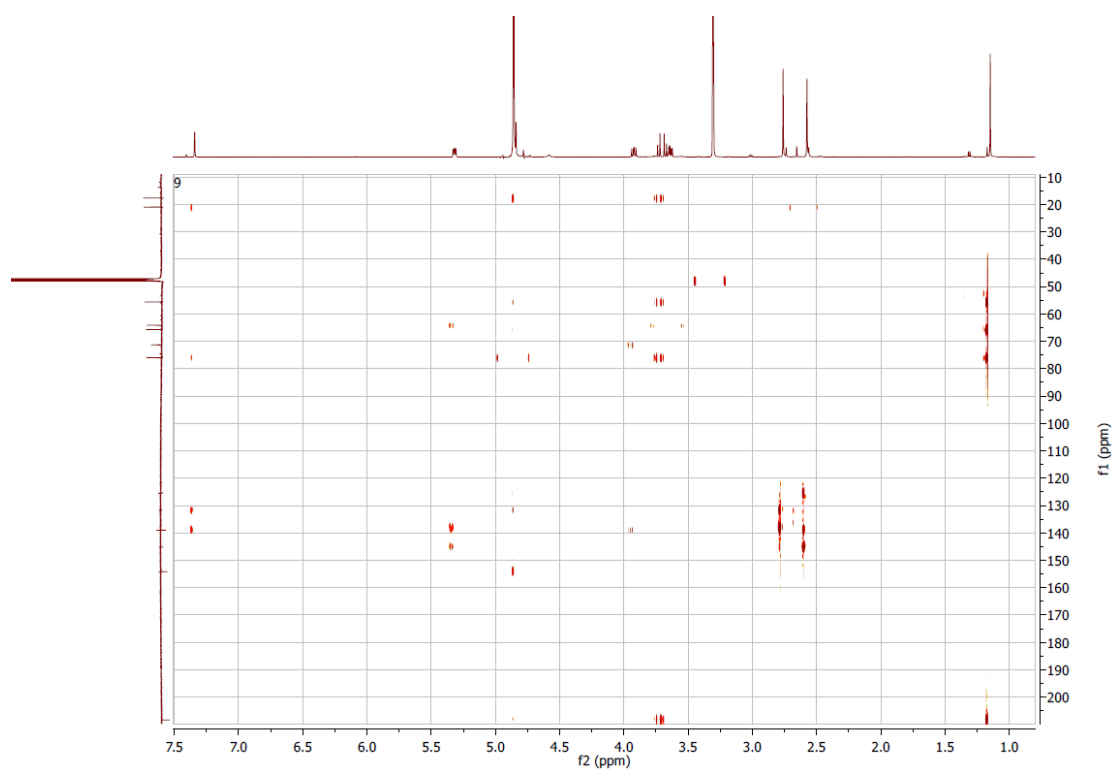


Figure S15 H-H NOESY spectra of 2

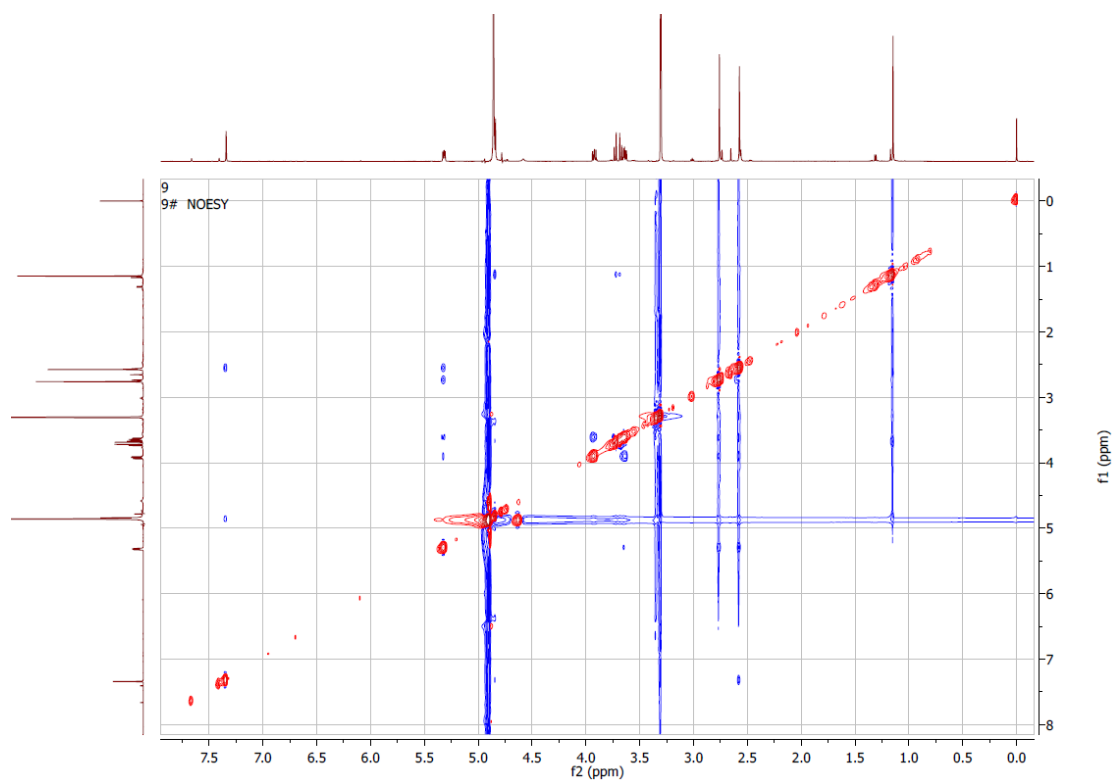
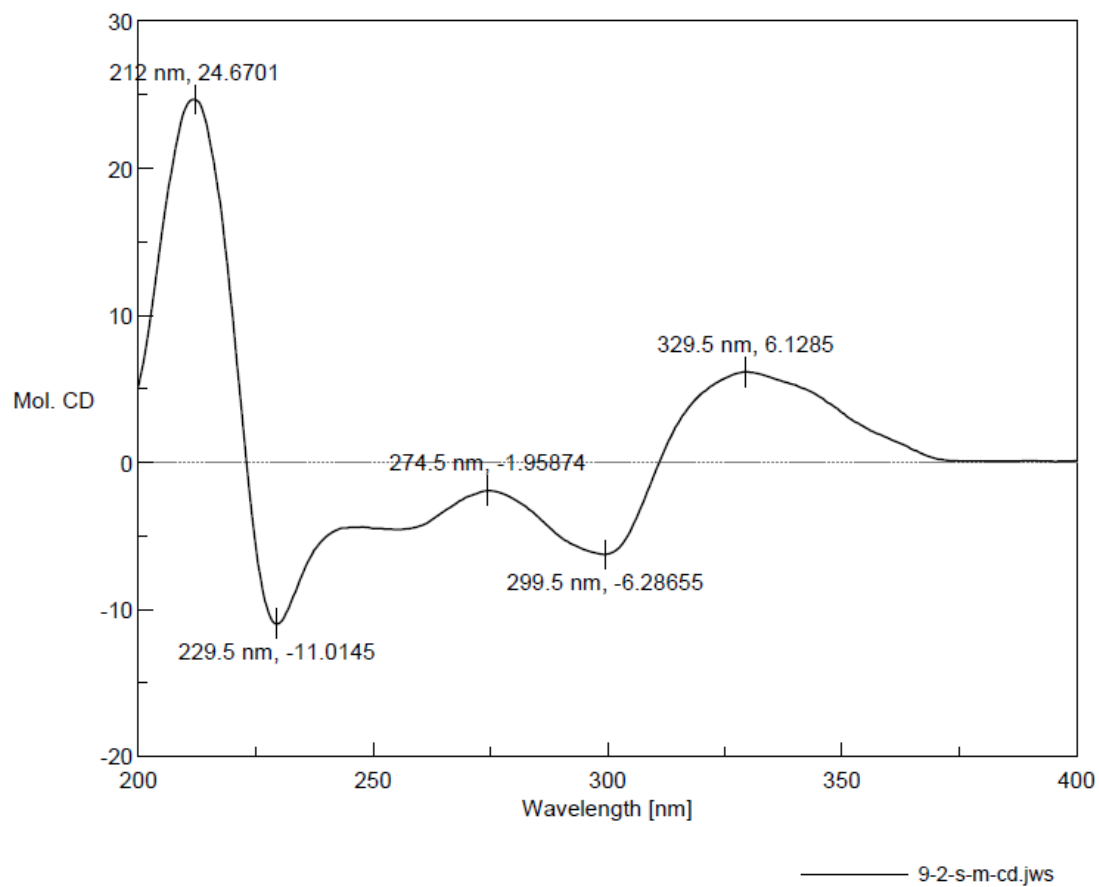


Figure S16 CD spectra of 2



3. UV, HRESI-MS, ^1H NMR, ^{13}C NMR, HSQC, HMBC, NOESY and CD spectra of 3

Figure S17 UV spectra of 3

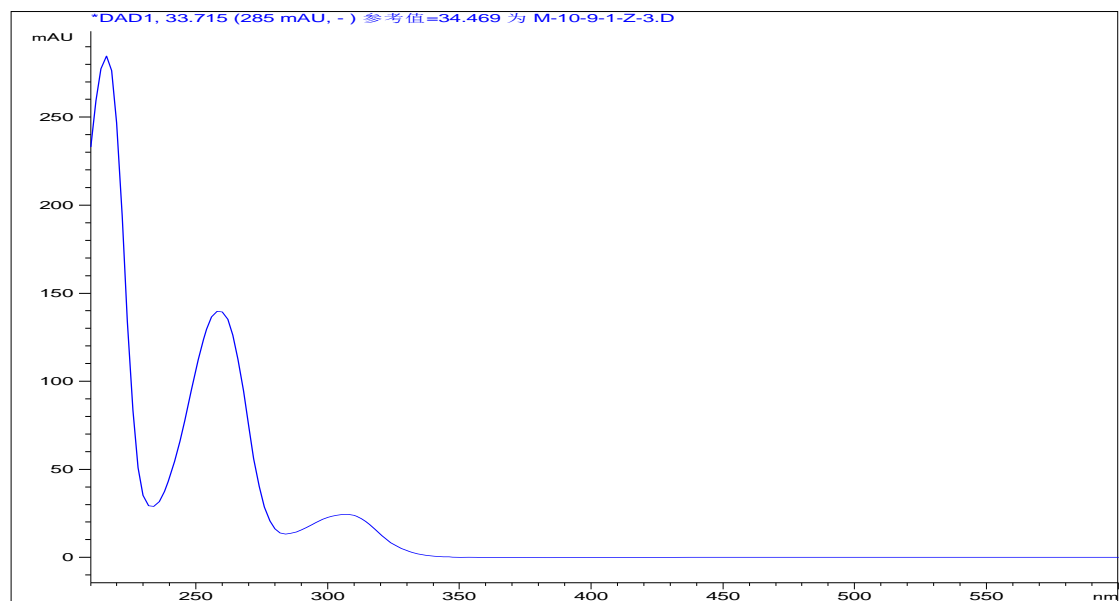


Figure S18 HRESIMS spectra of 3

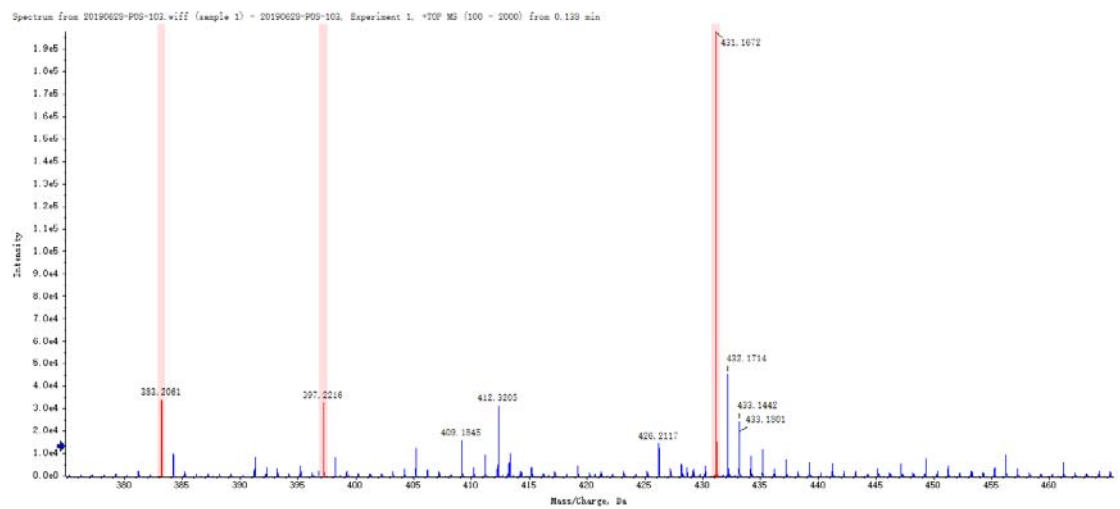


Figure S19 ^1H NMR spectra of 3

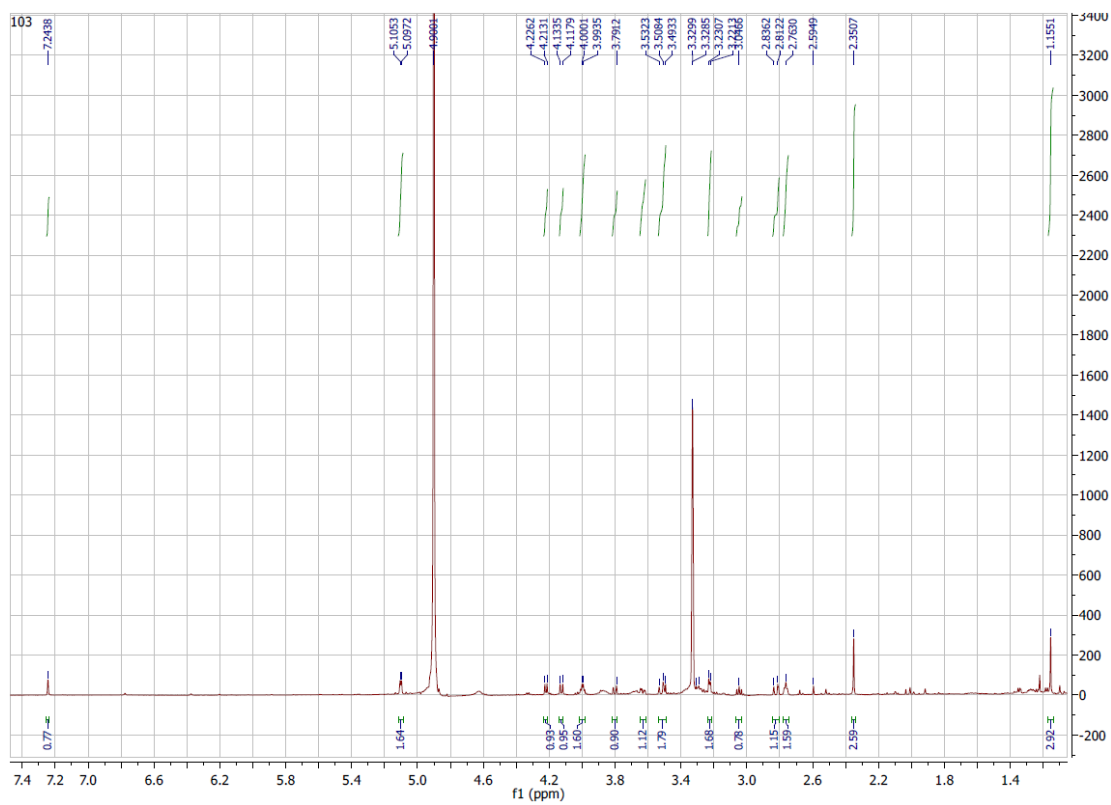


Figure S20 ^{13}C NMR spectra of 3

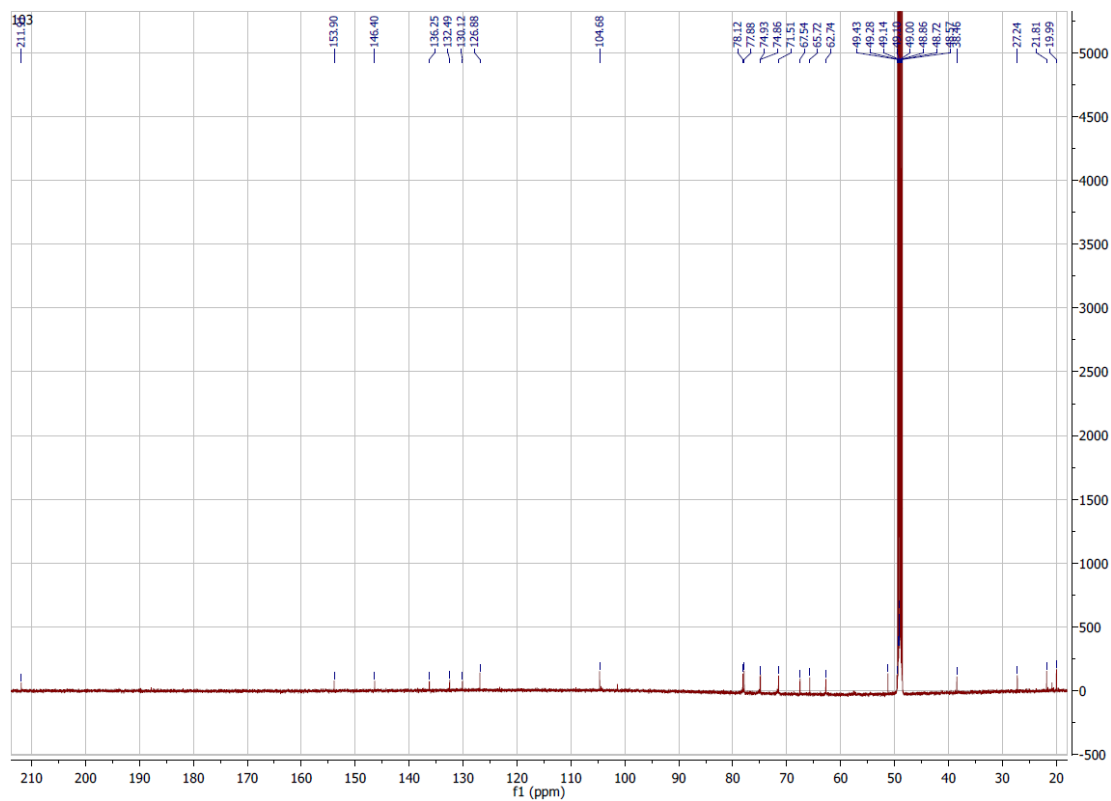


Figure S21 HSQC spectra of 3

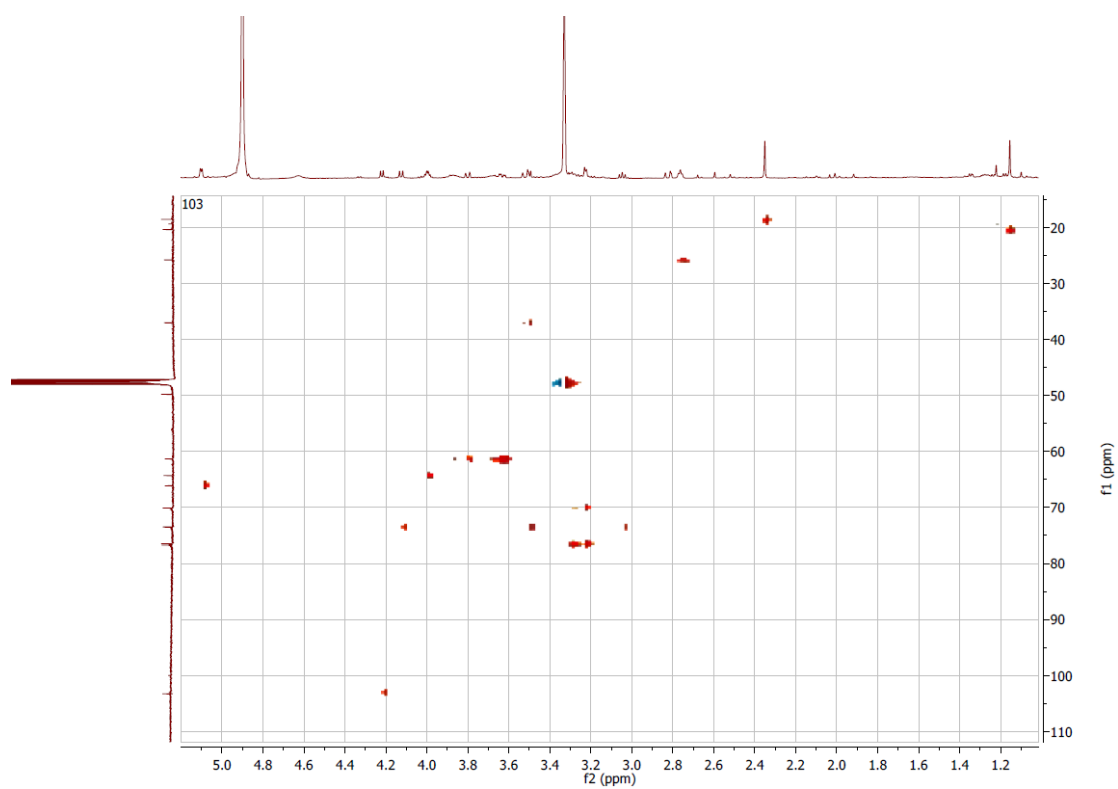


Figure S22 HMBC spectra of 3

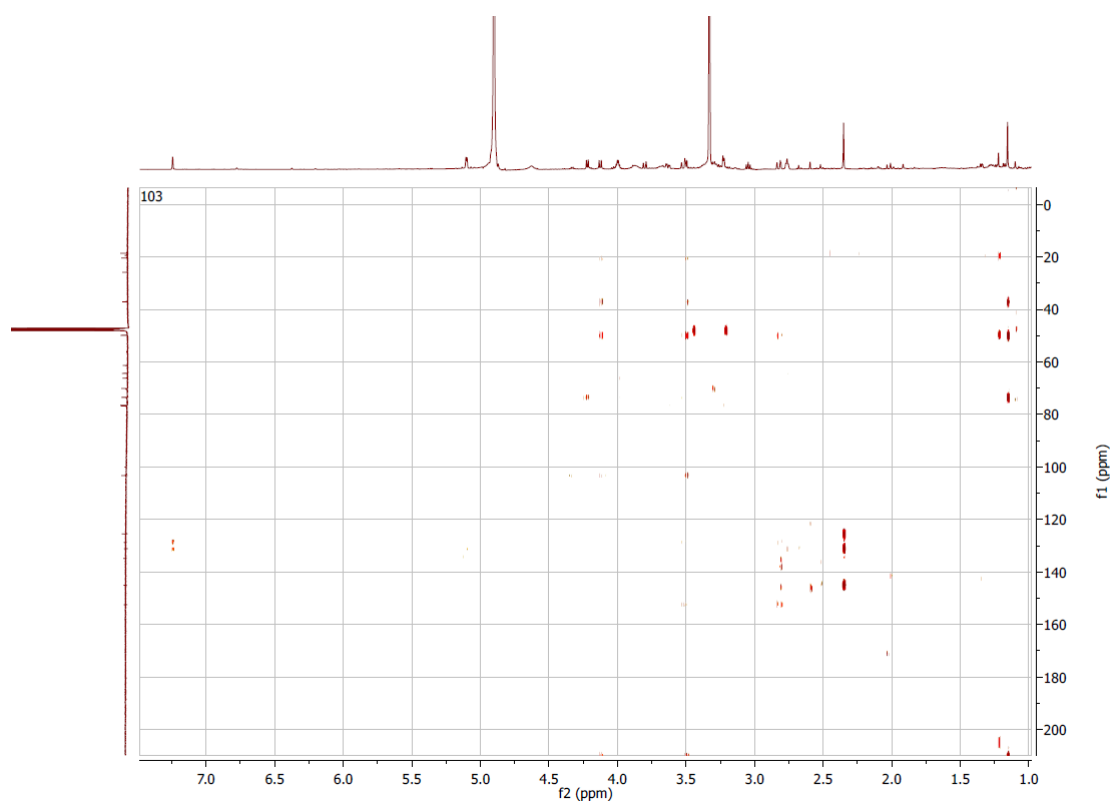


Figure S23 H-H NOESY spectra of 3

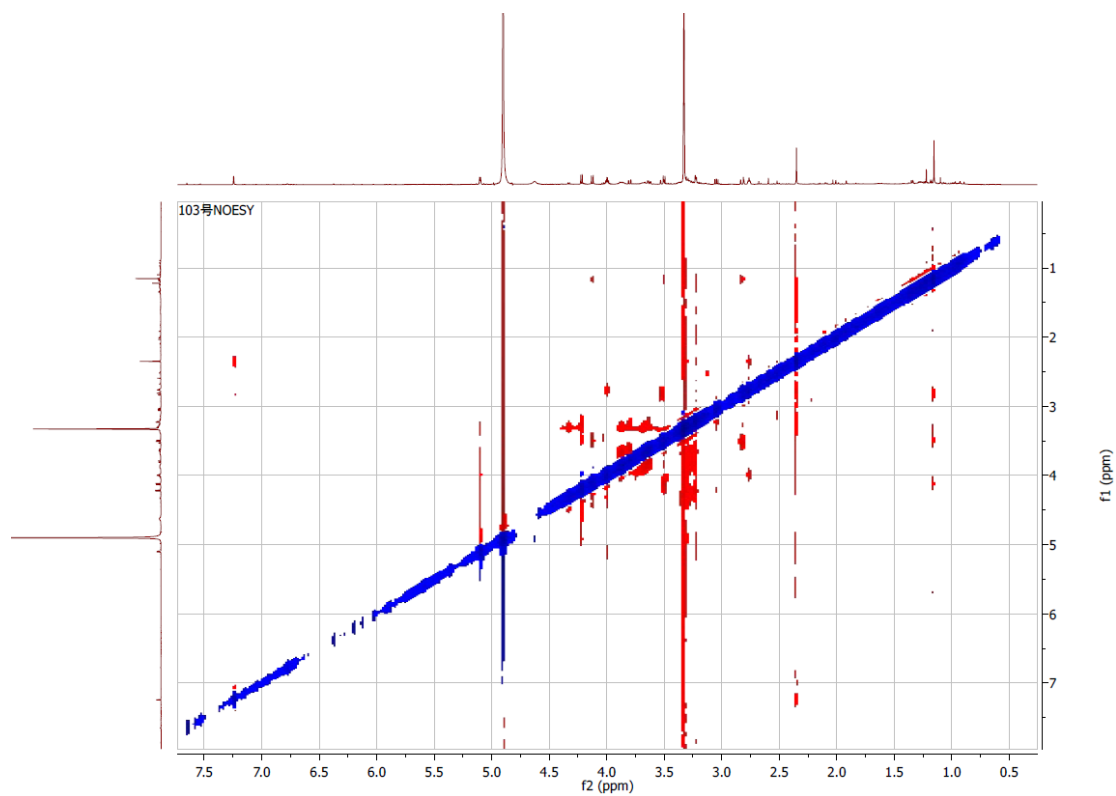
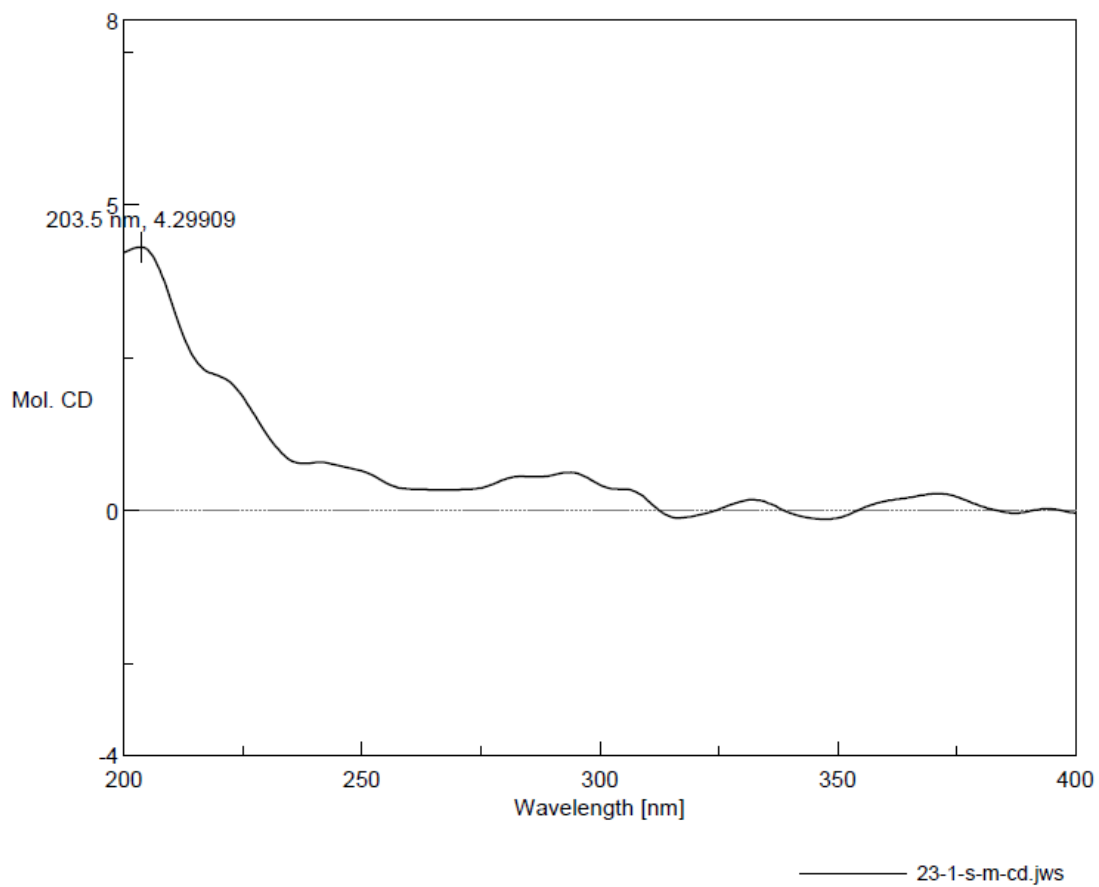


Figure S24 CD spectra of 3



4. UV, HRESI-MS, ^1H NMR, ^{13}C NMR, HSQC, HMBC, NOESY and CD spectra of 4

Figure S25 UV spectra of 4

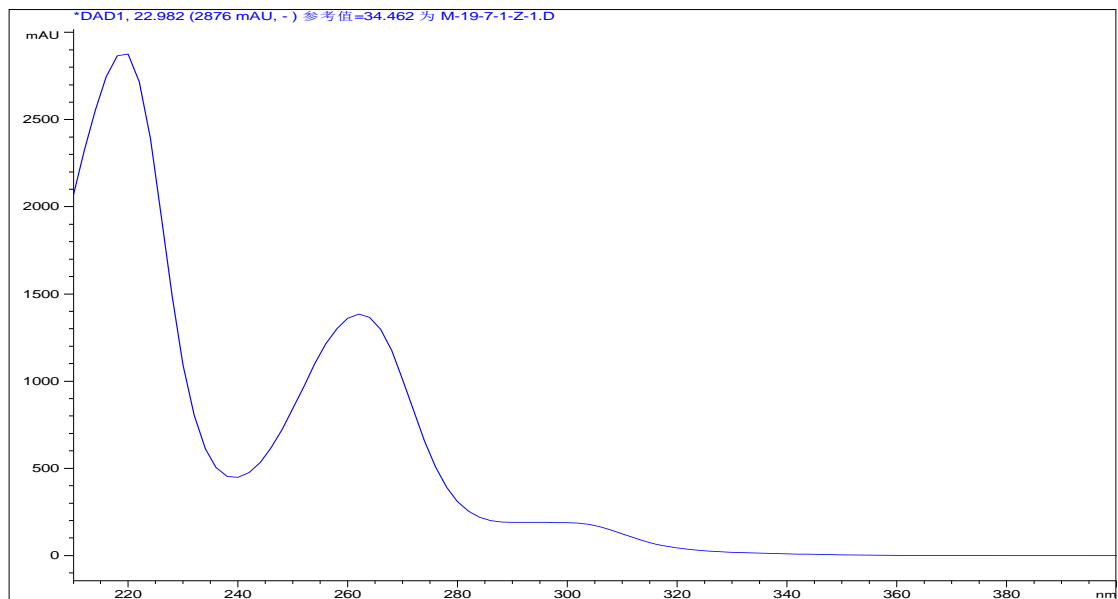


Figure S26 HRESIMS spectra of 4

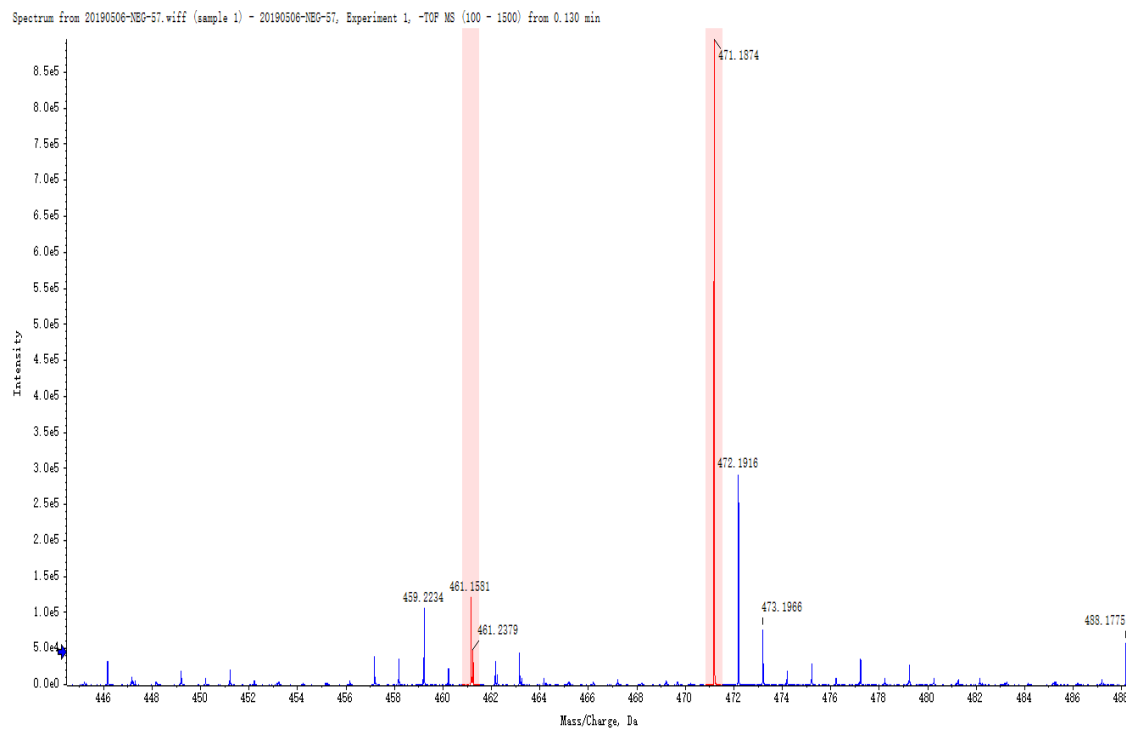


Figure S27 ^1H NMR spectra of 4

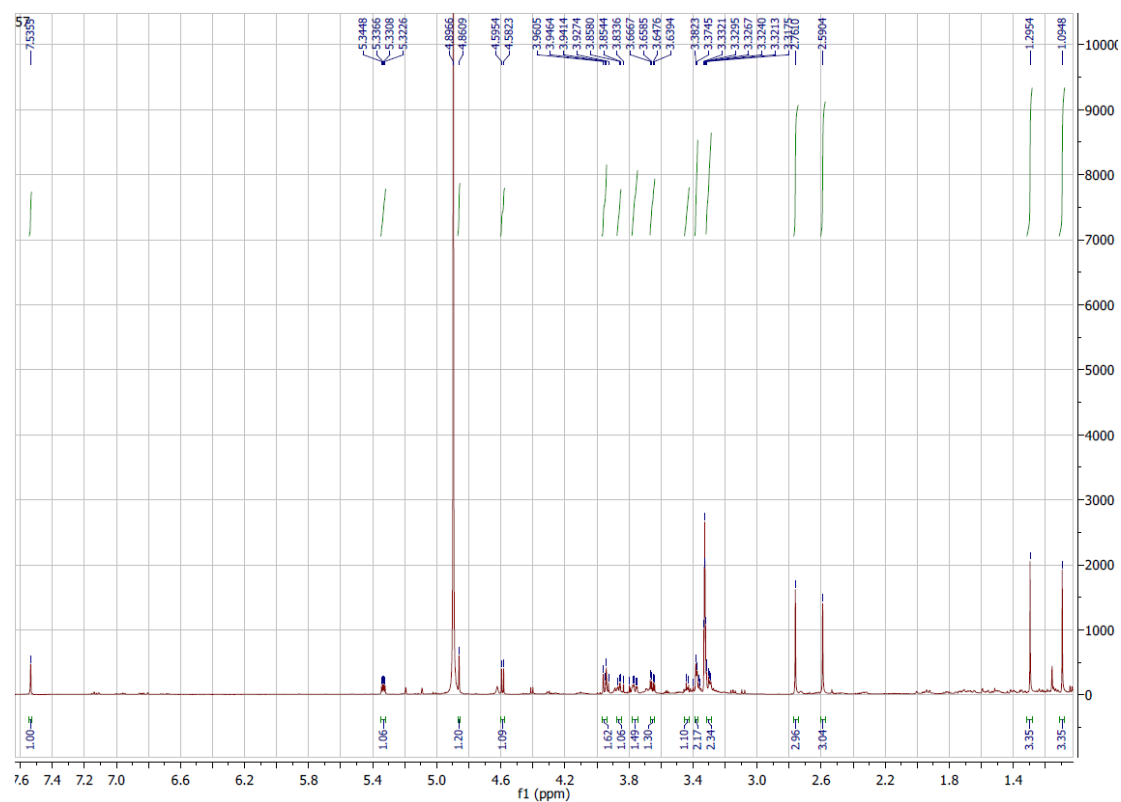


Figure S28 ^{13}C NMR spectra of 4

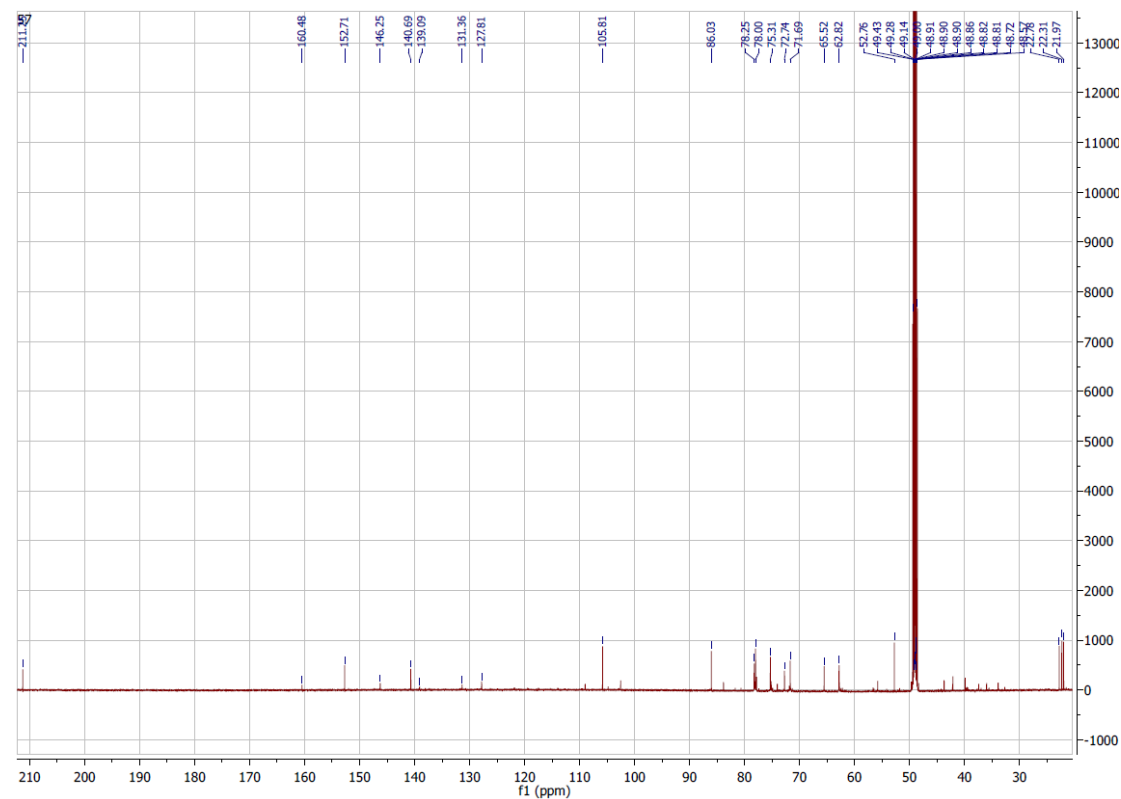


Figure S29 HSQC spectra of 4

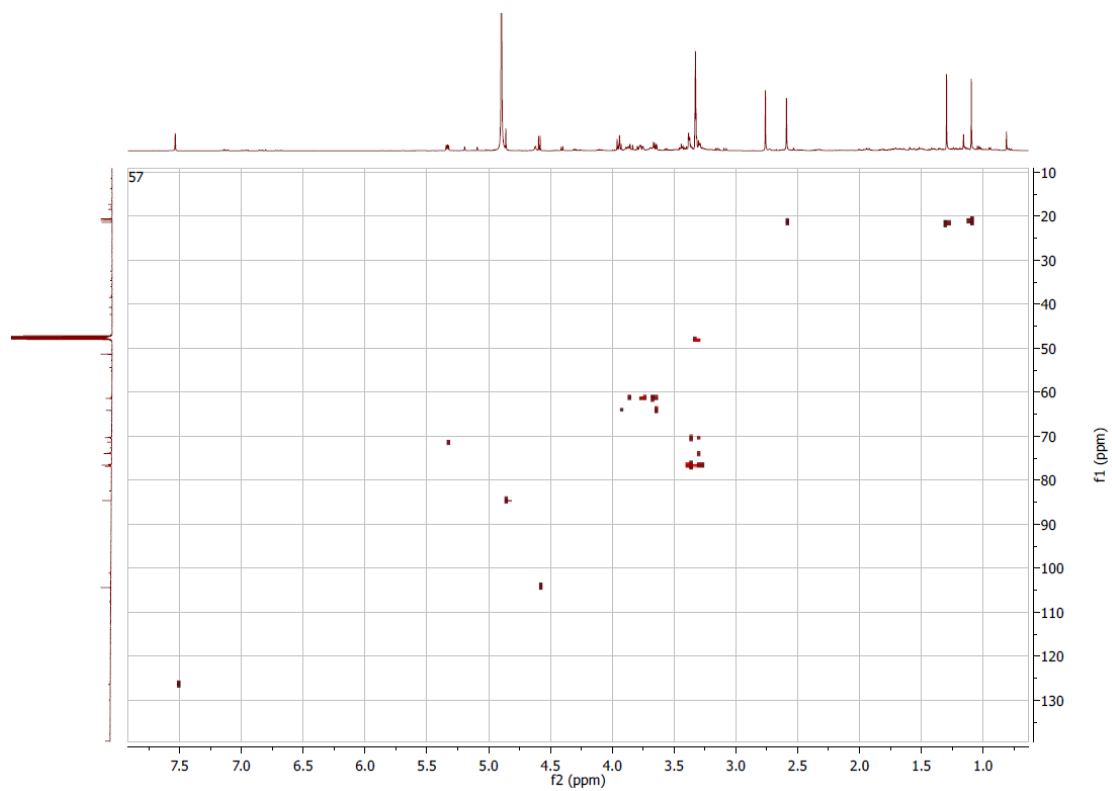


Figure S30 HMBC spectra of 4

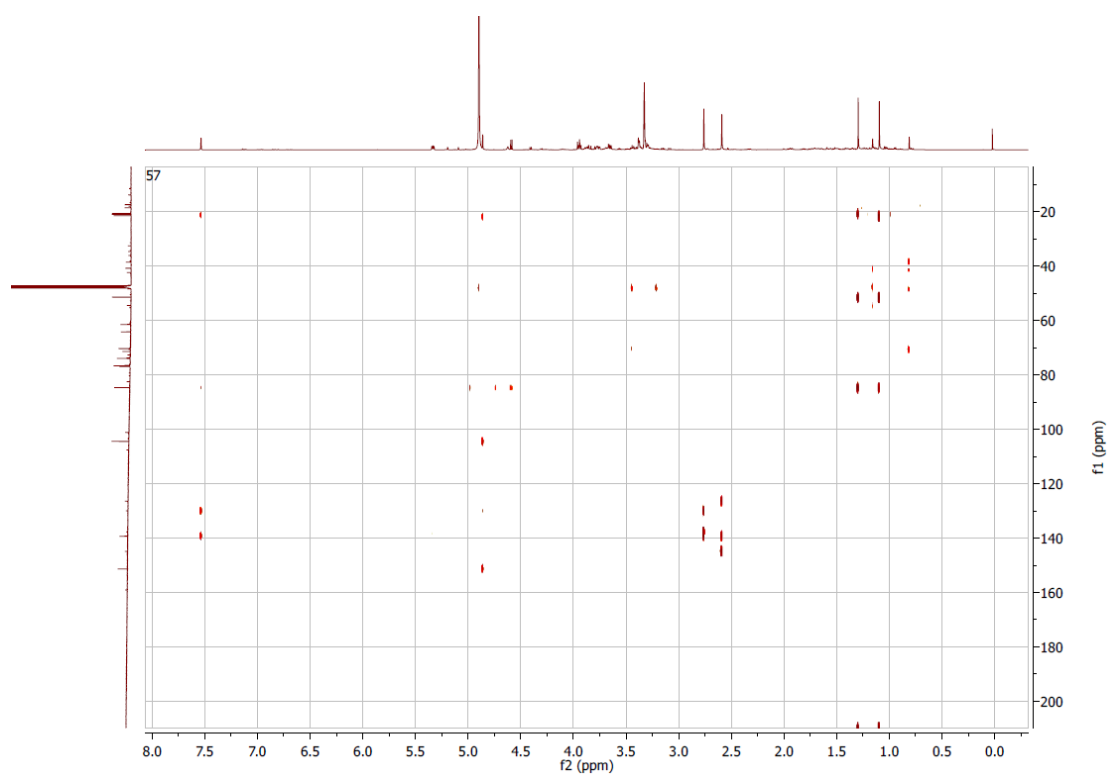


Figure S31 H-H NOESY spectra of 4

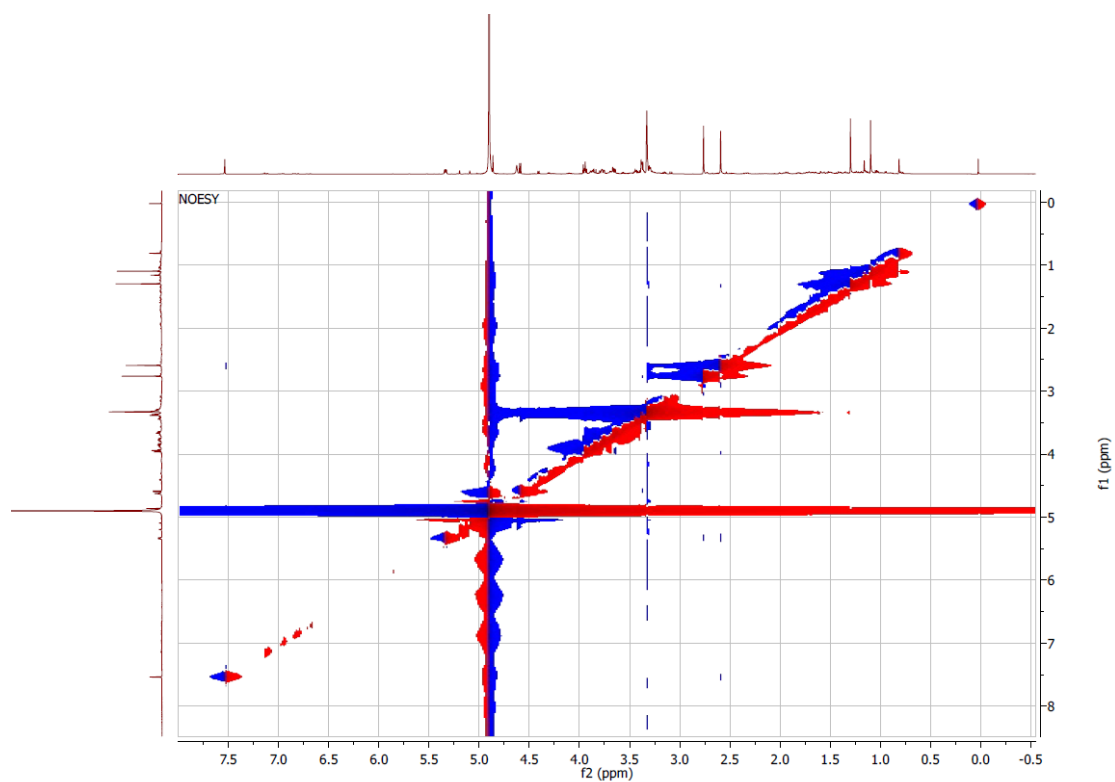


Figure S32 CD spectra of 4

