Bioactive Novel Indole Alkaloids and Steroids from Deep Sea-Derived Fungus *Aspergillus fumigatus* SCSIO 41012

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Abstract: Two new alkaloids, fumigatosides E (**1**) and F (**2**), and a new natural product, 3, 7-diketo-cephalosporin P_1 (**6**) along with five known compounds (**3**–**5**, **7**, **8**) were isolated from deep-sea derived fungal *Aspergillus fumigatus* SCSIO 41012. Their structures were determined by extensive spectroscopic data analysis, including 1D, 2D NMR and MS, and comparison between the calculated and experimental ECD spectra. In addition, all compounds were tested for antibacterial and antifungal inhibitory activities. Compound **1** showed significant antifungal activity against *Fusarium oxysporum* f. sp. *momordicae* with MIC at 1.56 μg/mL. Compound **4** exhibited significant higher activity against *S. aureus* (16339 and 29213) with MIC values of 1.56, and 0.78 μg/mL, respectively, and compound **2** exhibited significant activity against *A. baumanii* ATCC 19606 with MIC value of 6.25 μg/mL.

Keywords: deep sea-derived fungus; *Aspergillus fumigatus* SCSIO 41012; indole alkaloids; steroids; antibacterial activity; antifungal activity

List of supporting information

Figure S25: HMBC spectra of the new compound **3**.

Figure S26: NOESY spectra of the new compound **3.**

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Figure S29: The experimental CD curve of the new compound **3**.

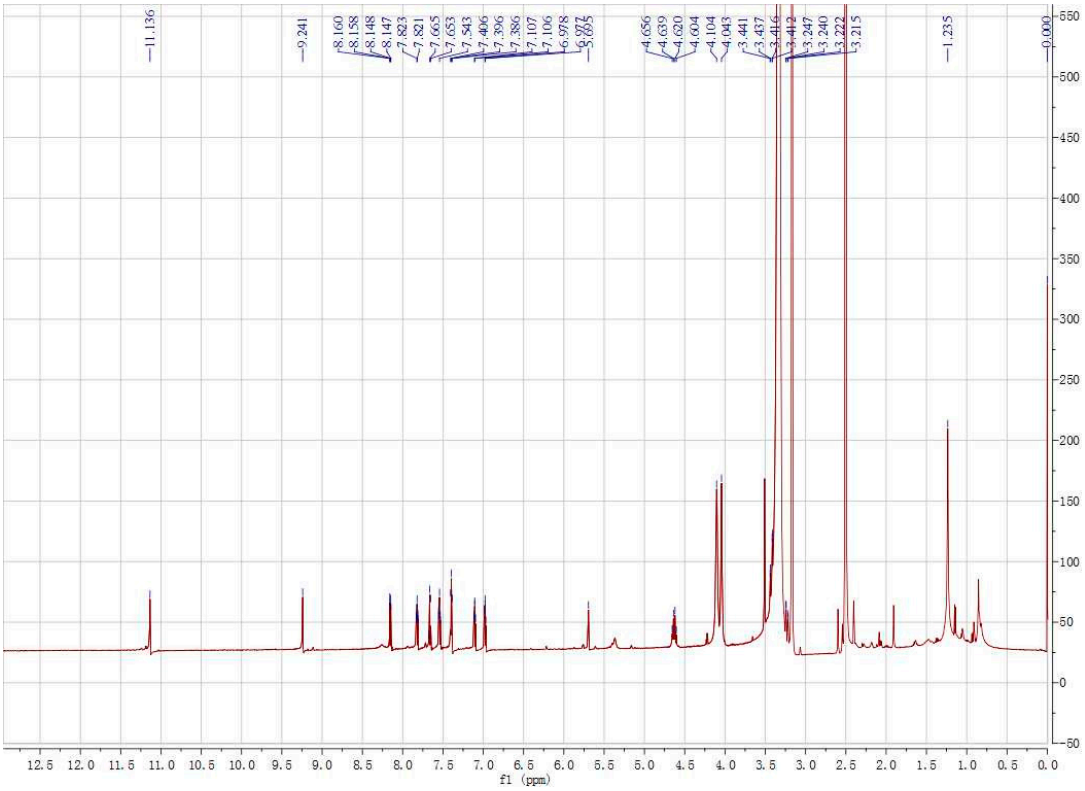

Figure S1. [1]H NMR spectra (700 MHZ, DMSO-*d6*) of the new compound **1**.

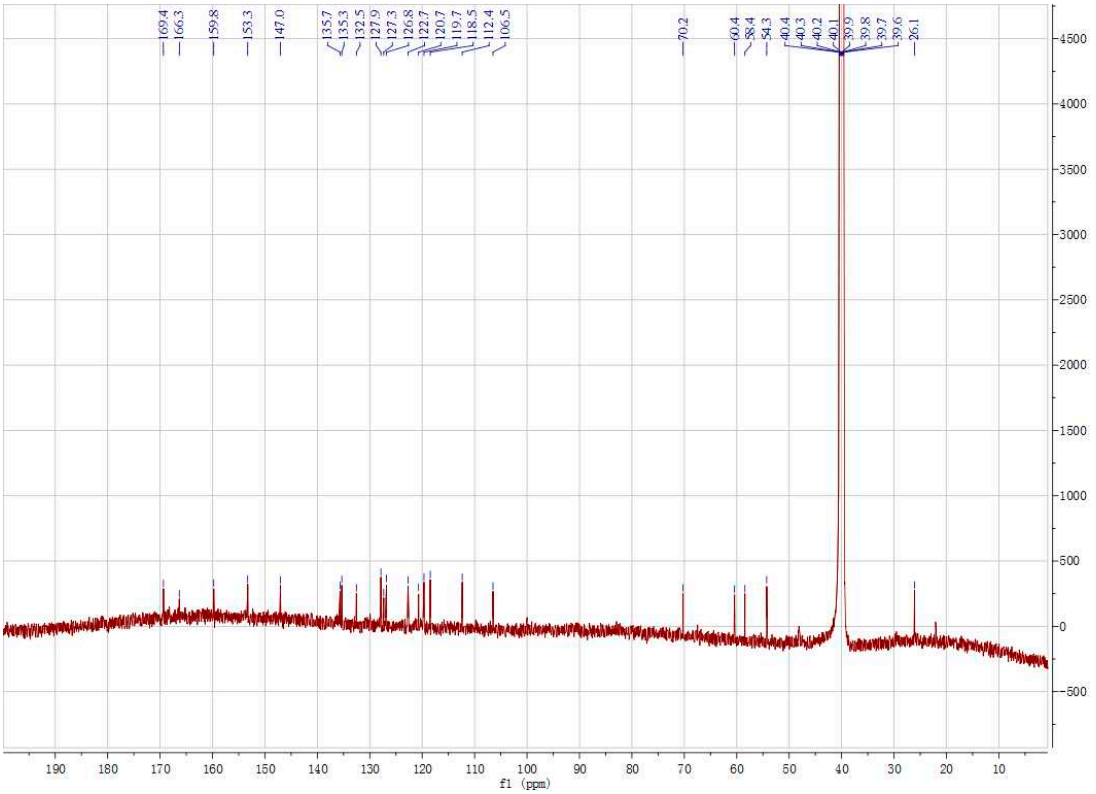

Figure S2. ^{13}C NMR spectra (175 MHZ, DMSO-*d6*) of the new compound **1.**

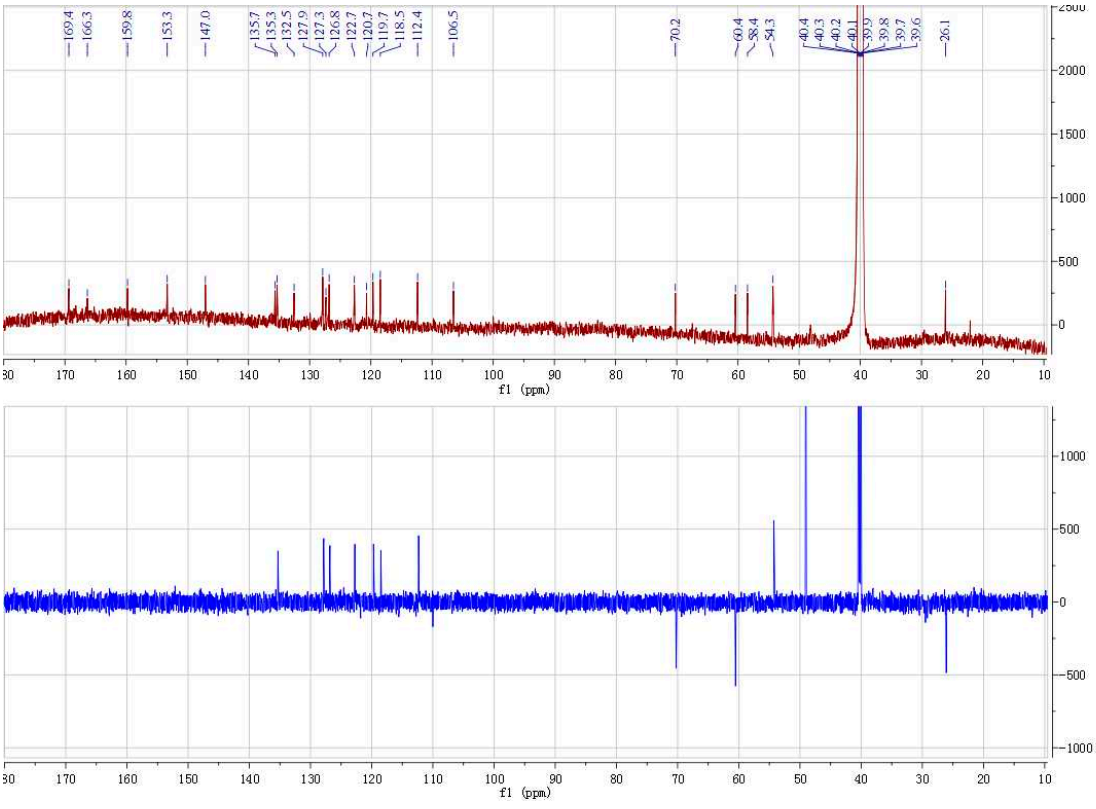

Figure S3. DEPT spectra of the new compound **1.**

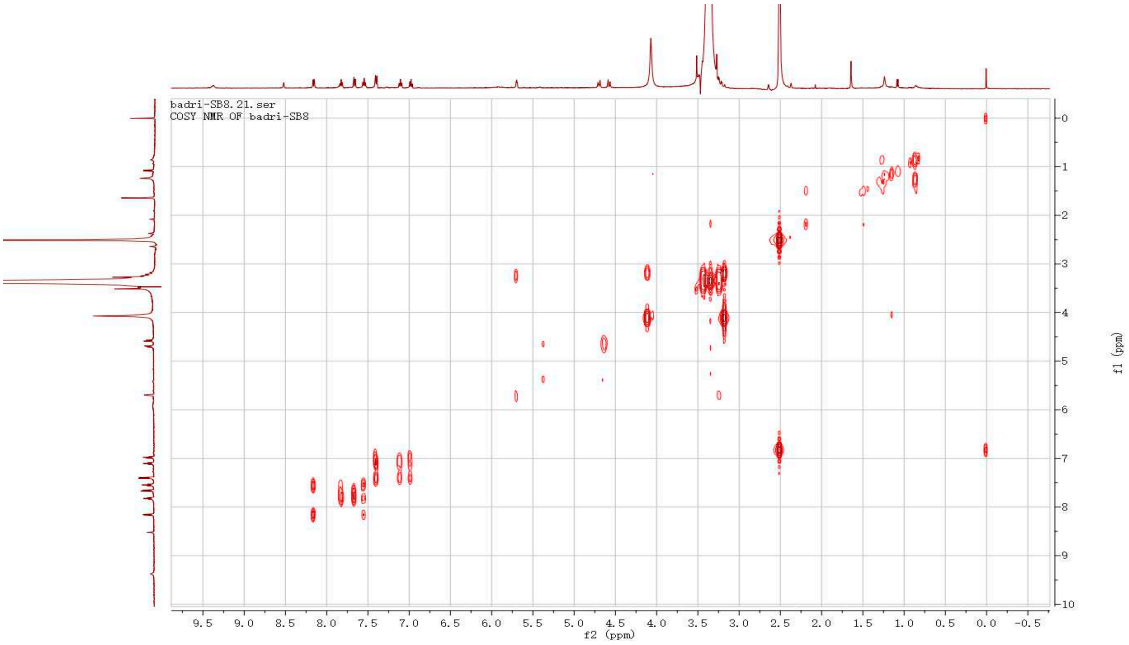

Figure S4. COSY spectra of the new compound **1**.

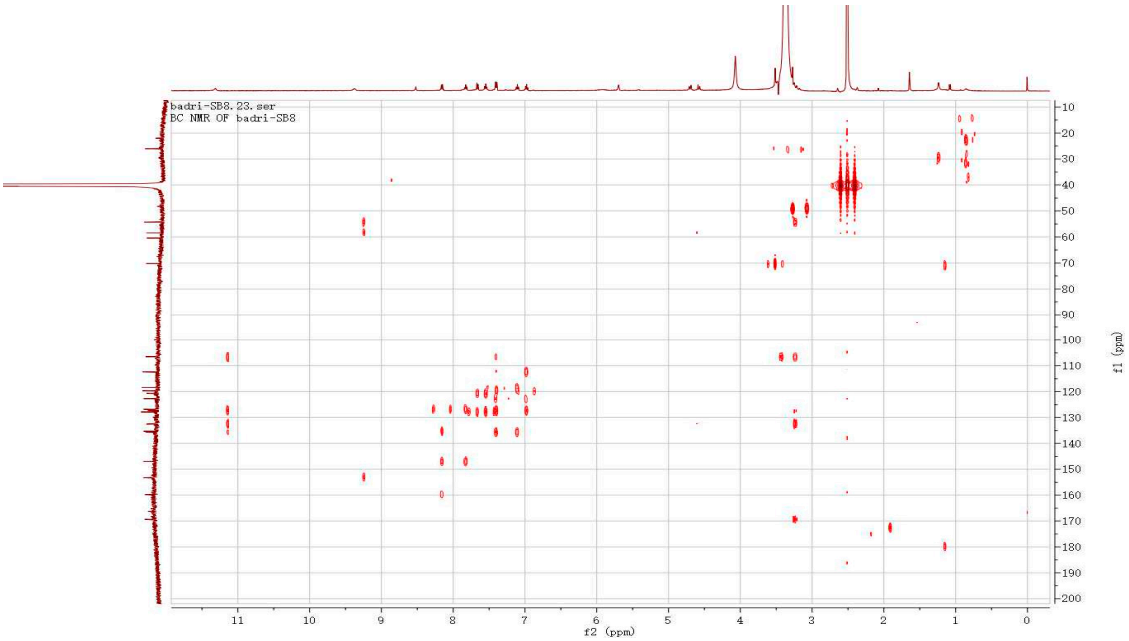

Figure S5. HMBC spectra of the new compound **1.**

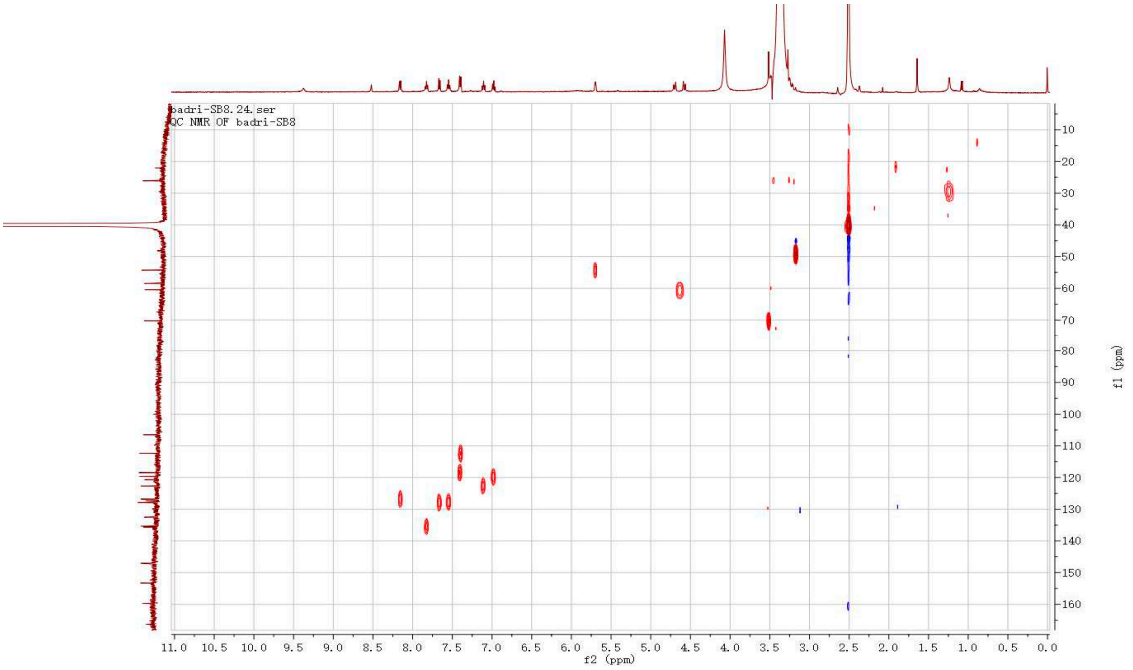

Figure S6. HMQC spectra of the new compound **1**.

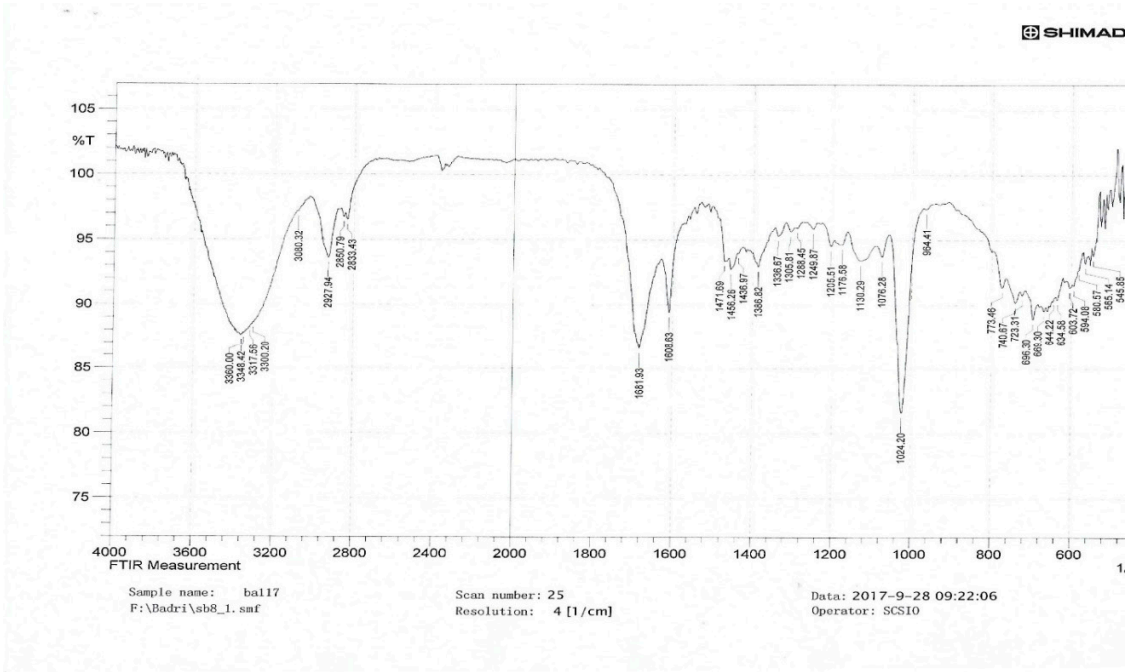

Figure S7. IR spectra of the new compound **1**.

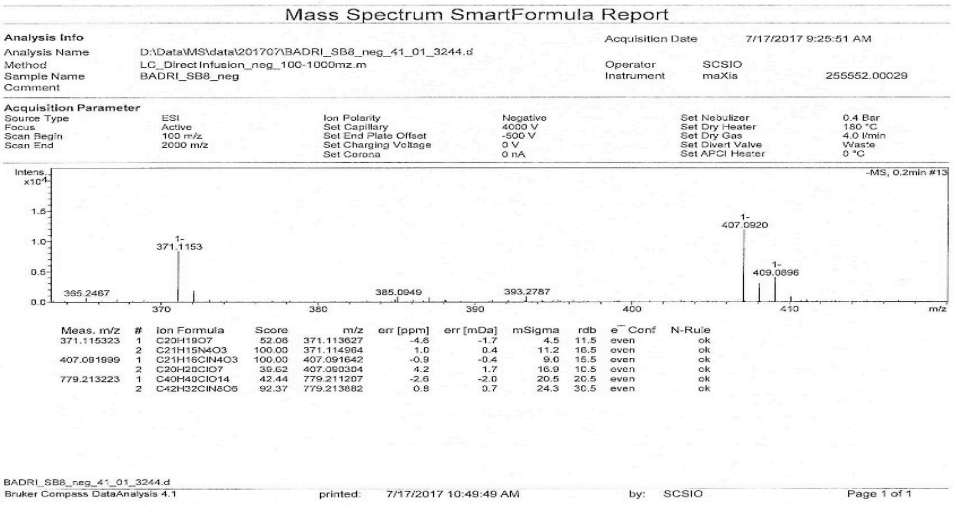

Figure S8. HRESIMS of the new compound **1**.

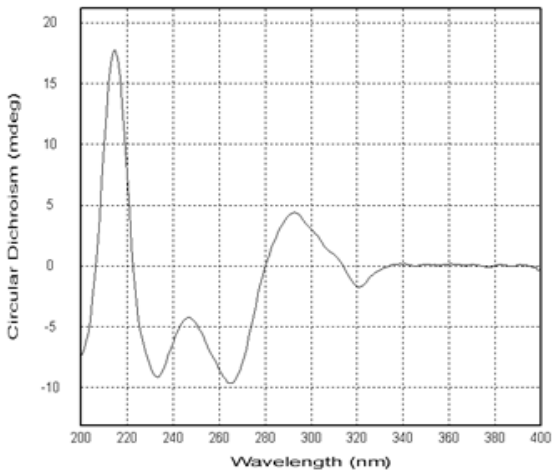

Figure S9. The experimental CD curve of the new compound **1.**

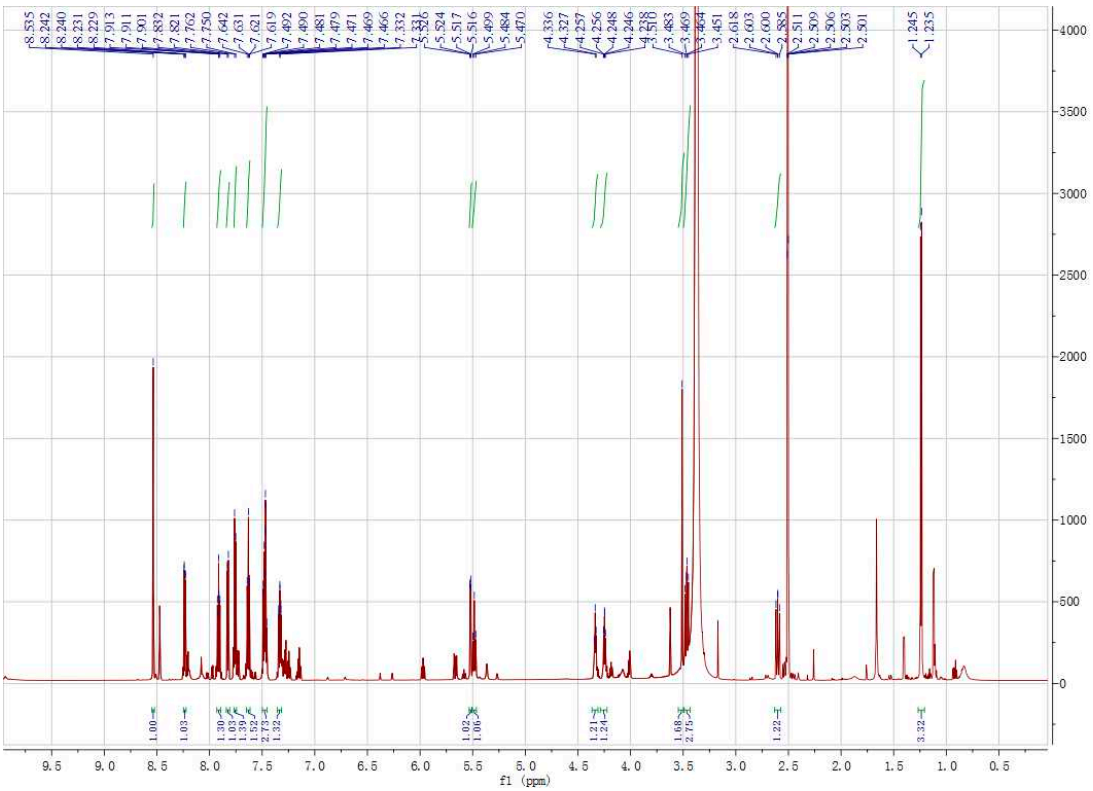

Figure S10. ^{1}H NMR spectra (700 MHZ, DMSO-*d6*) of the new compound **2**.

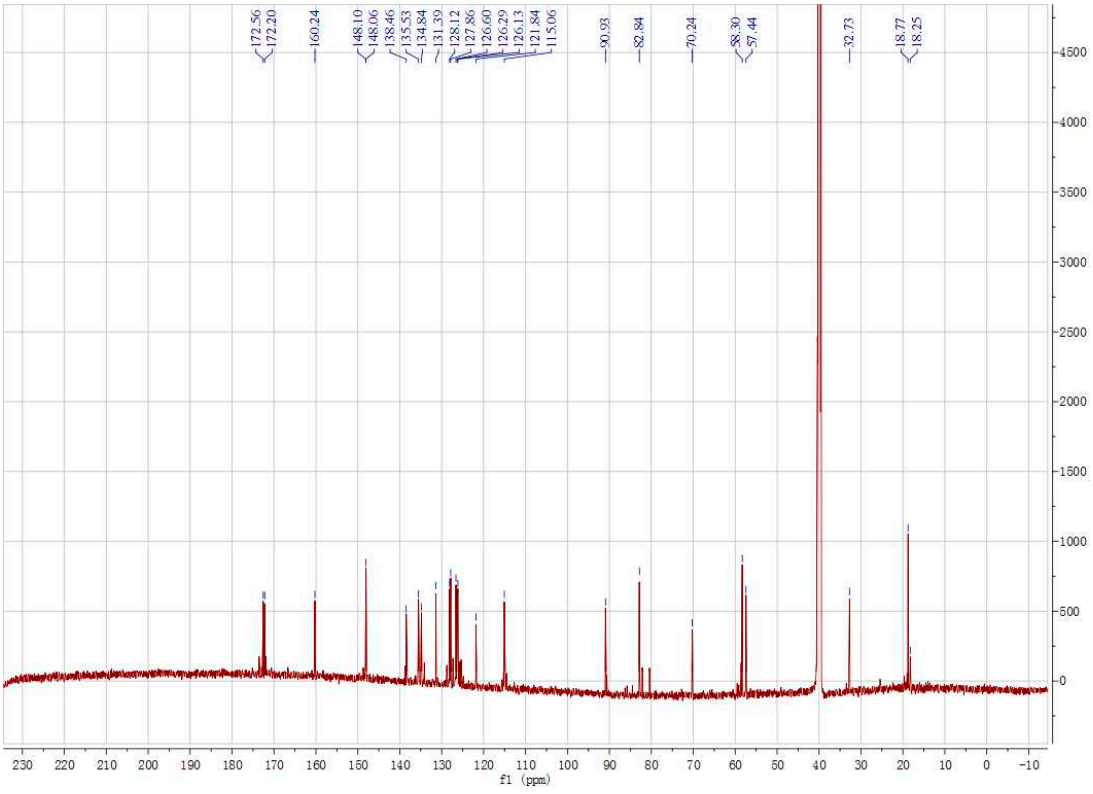

Figure S11. ^{13}C NMR spectra (175 MHZ, DMSO-*d6*) of the new compound **2.**

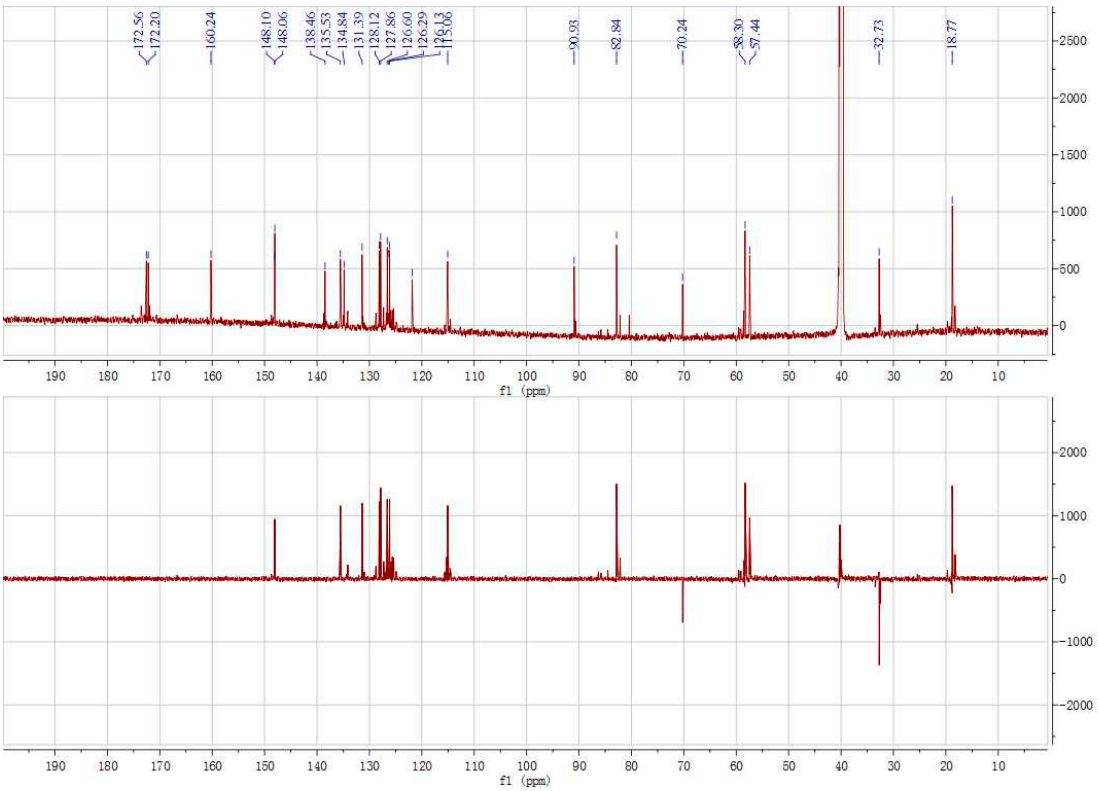

Figure S12. DEPT spectra of the new compound **2.**

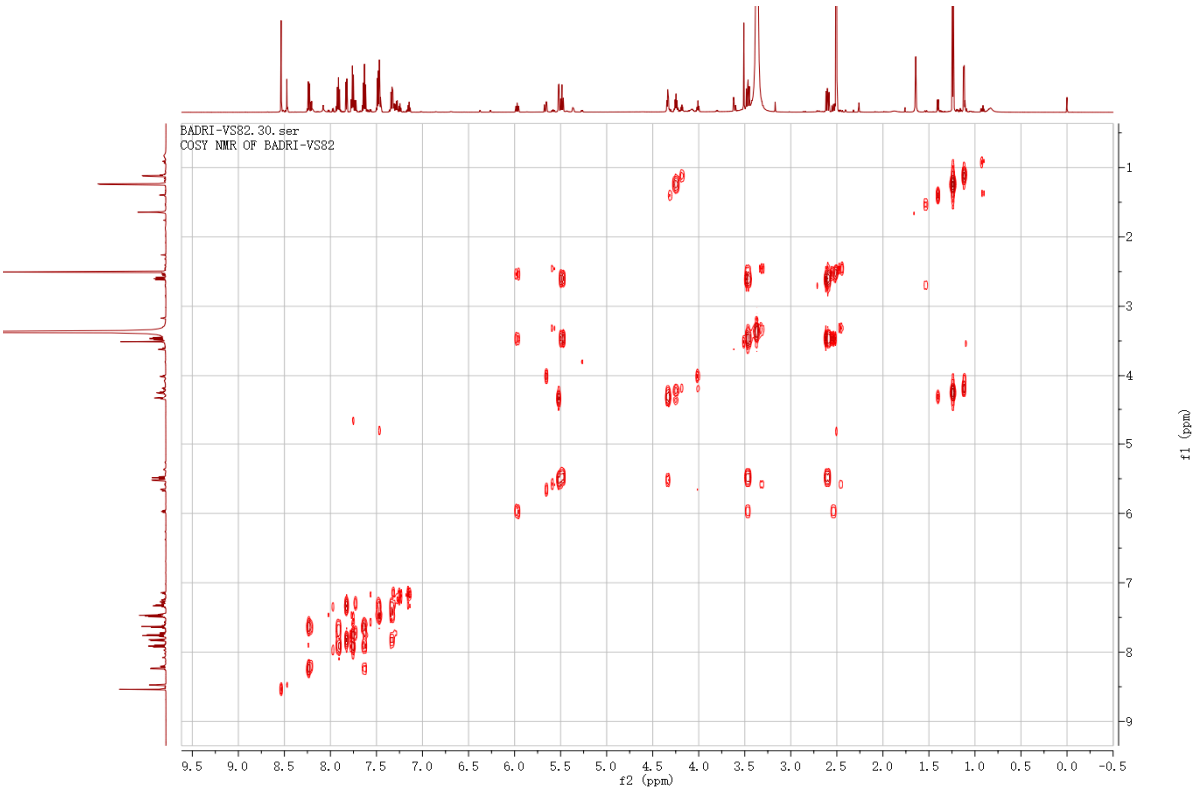

Figure S13. COSY spectra of the new compound **2**.

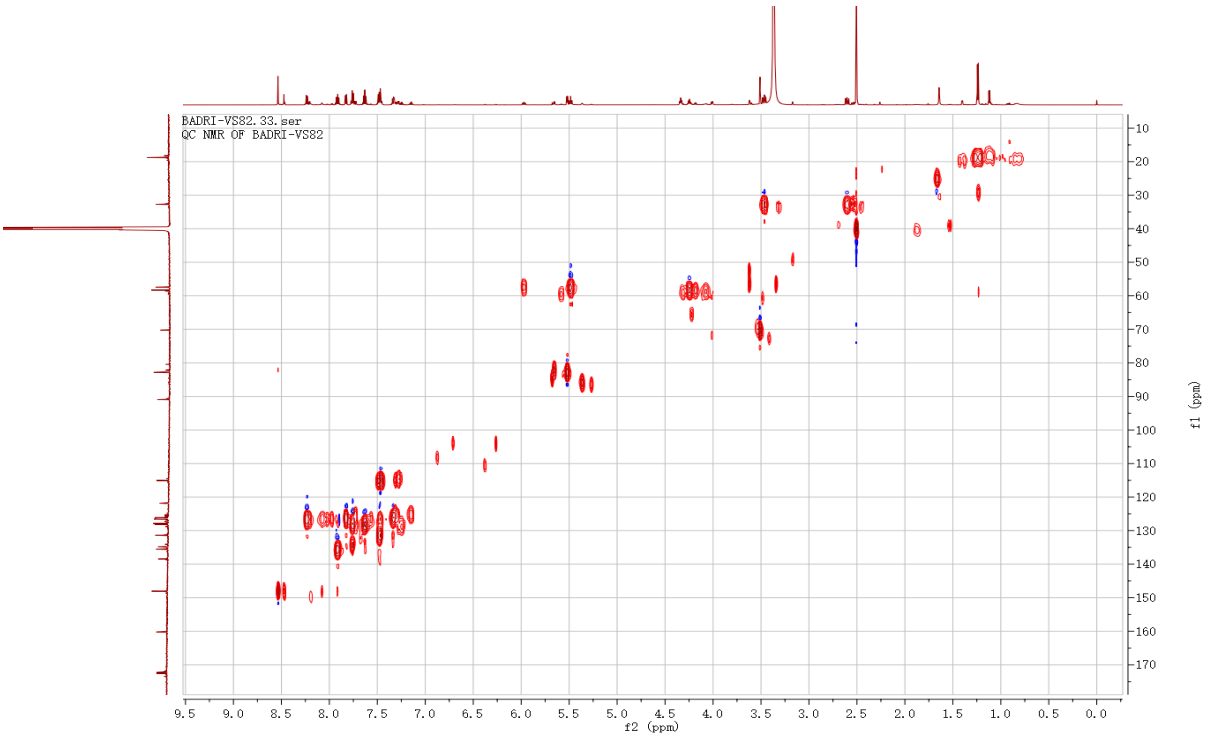

Figure S14. HMQC spectra of the new compound **2**.

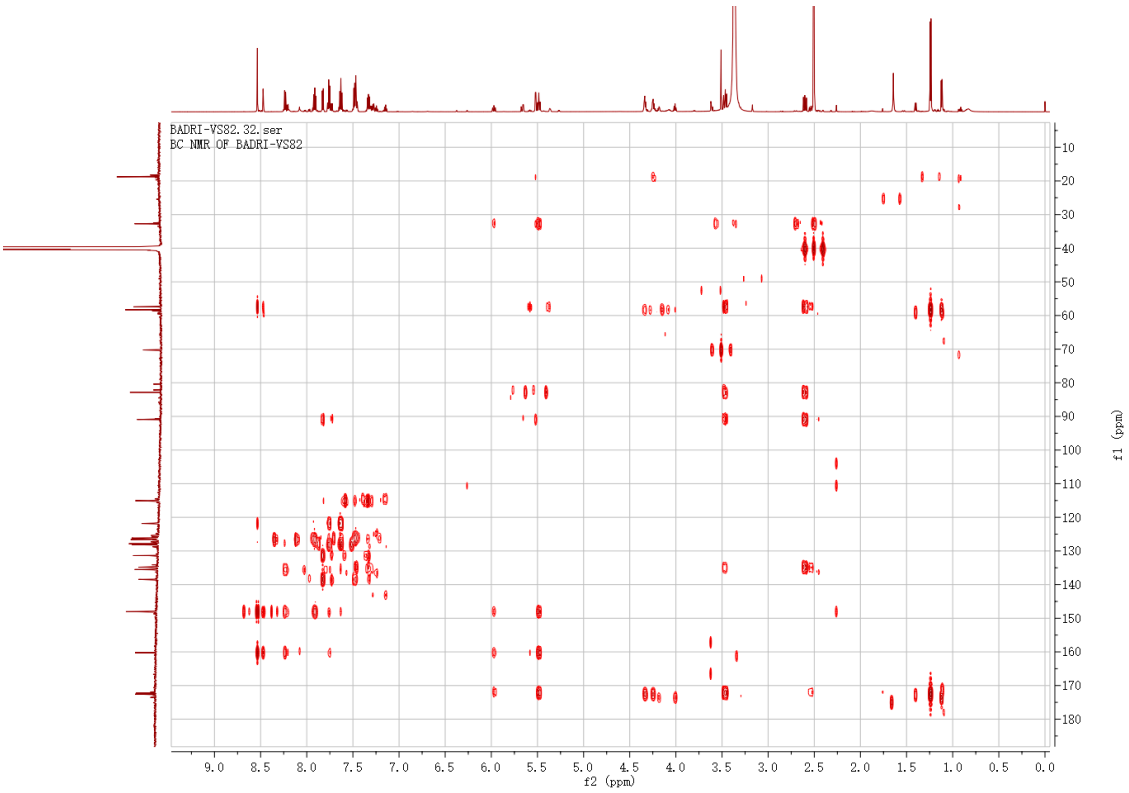

Figure S15. HMBC spectra of the new compound **2.**

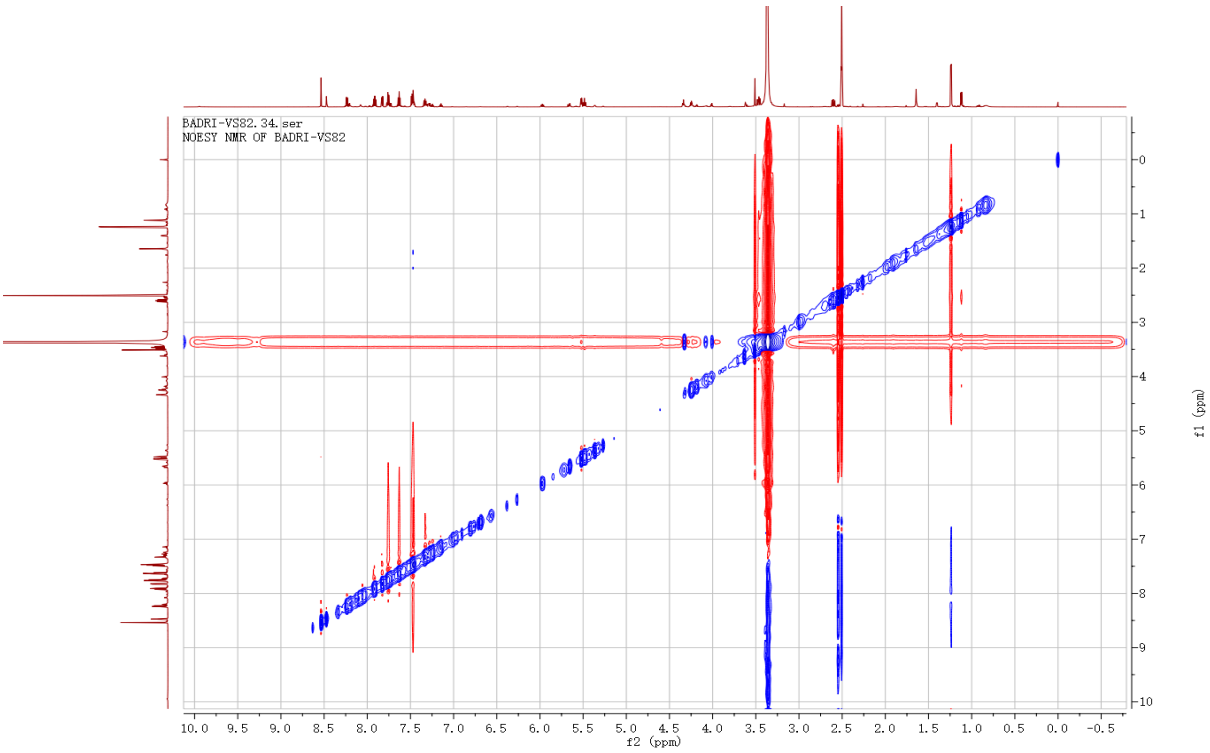

Figure S16. NOESY spectra of the new compound **2.**

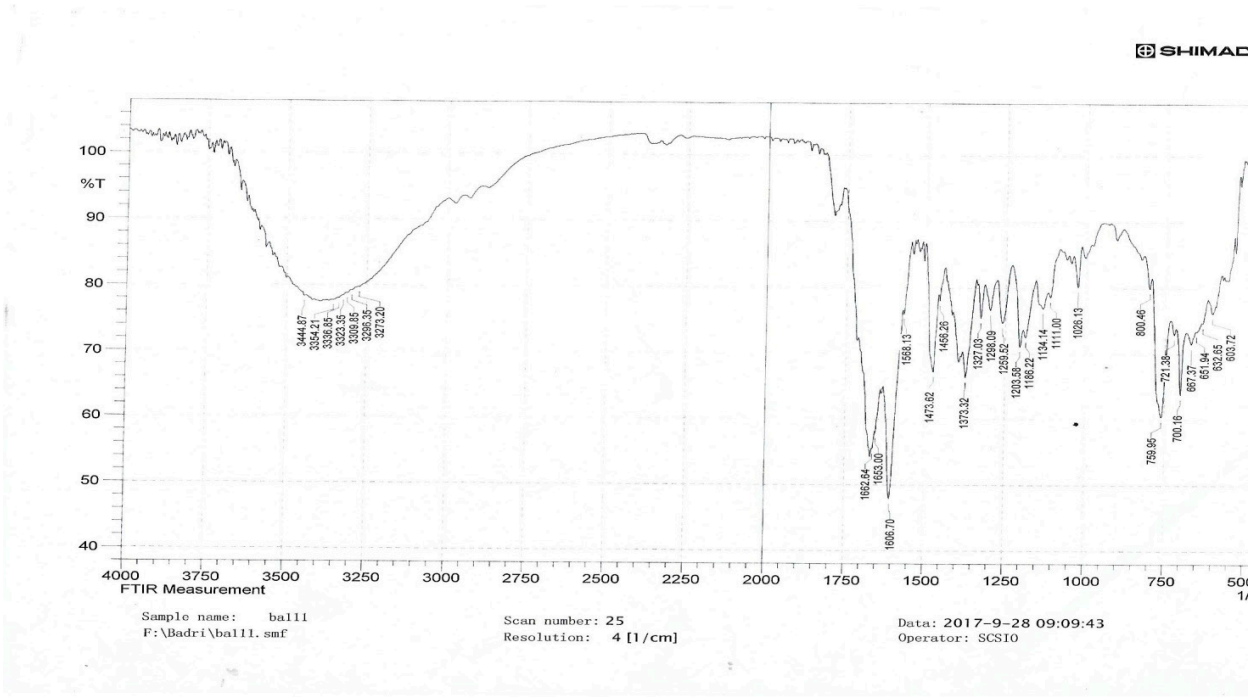

Figure S17. IR spectra of the new compound **2**.

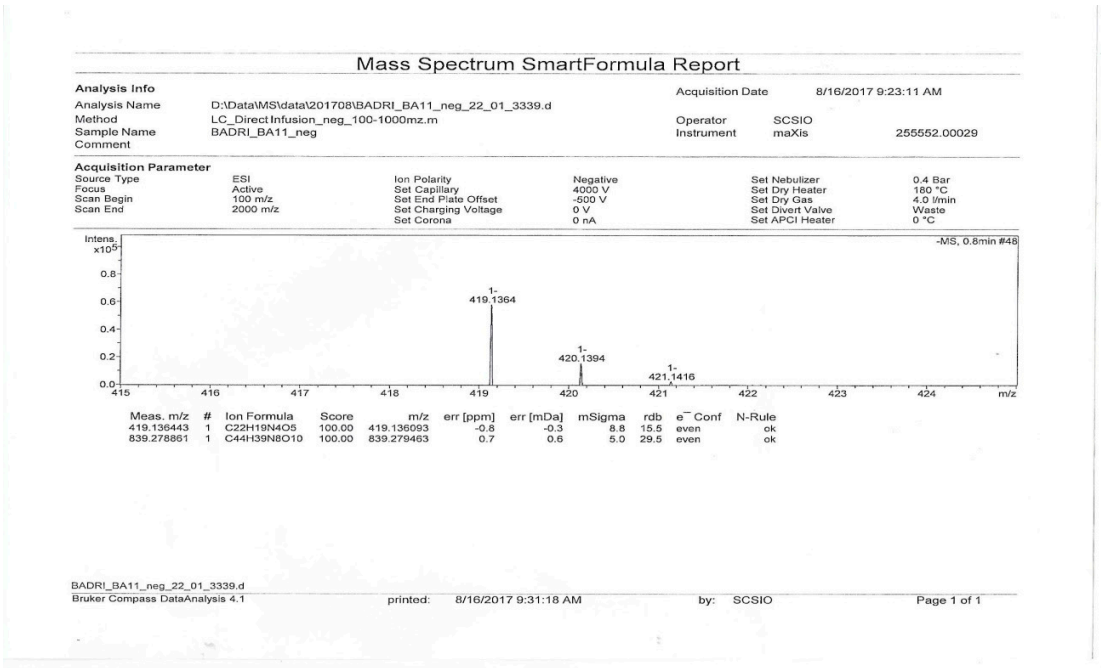

Figure S18. HRESIMS of the new compound **2**.

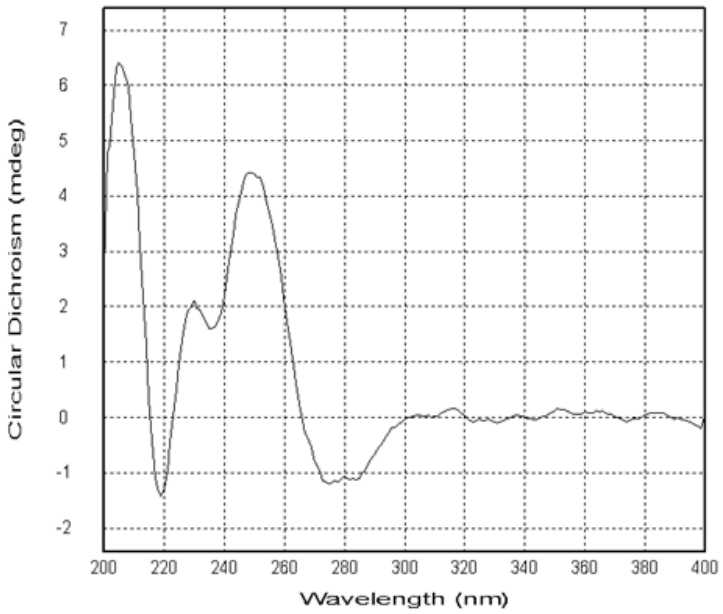

Figure S19. The experimental CD curve of the new compound **2.**

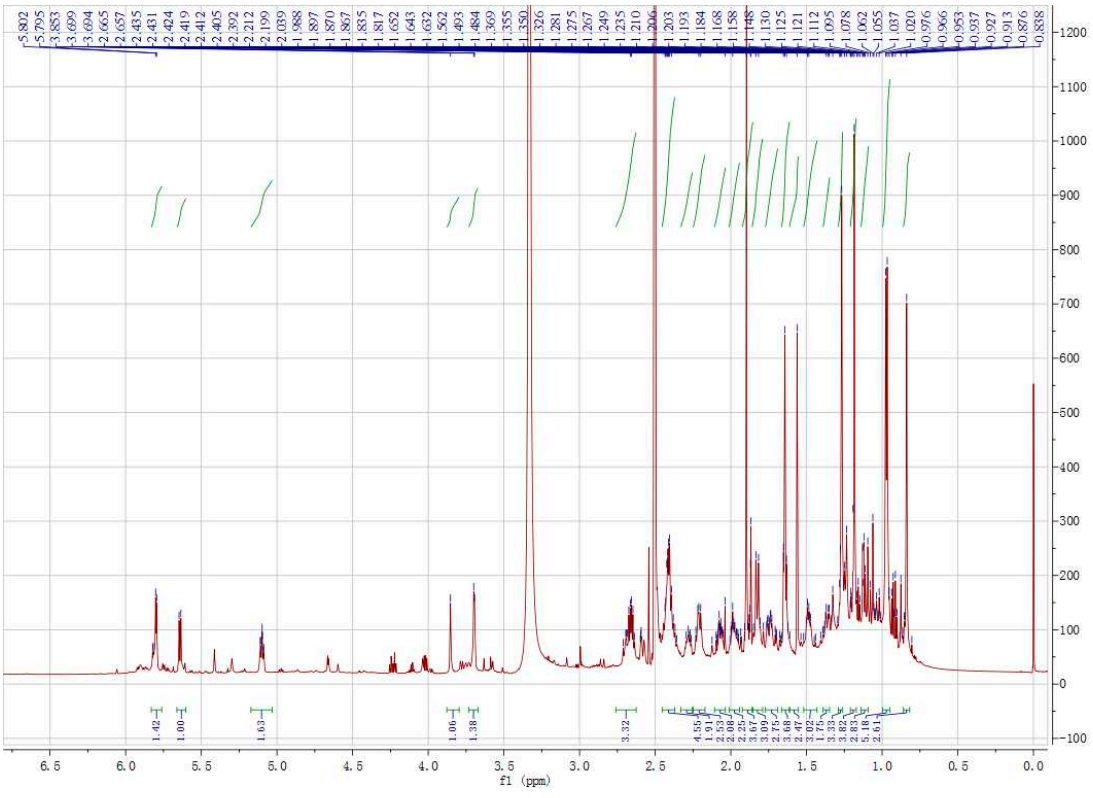

Figure S20. [1]H NMR spectra (700 MHZ, DMSO-*d6*) of the new compound **3.**

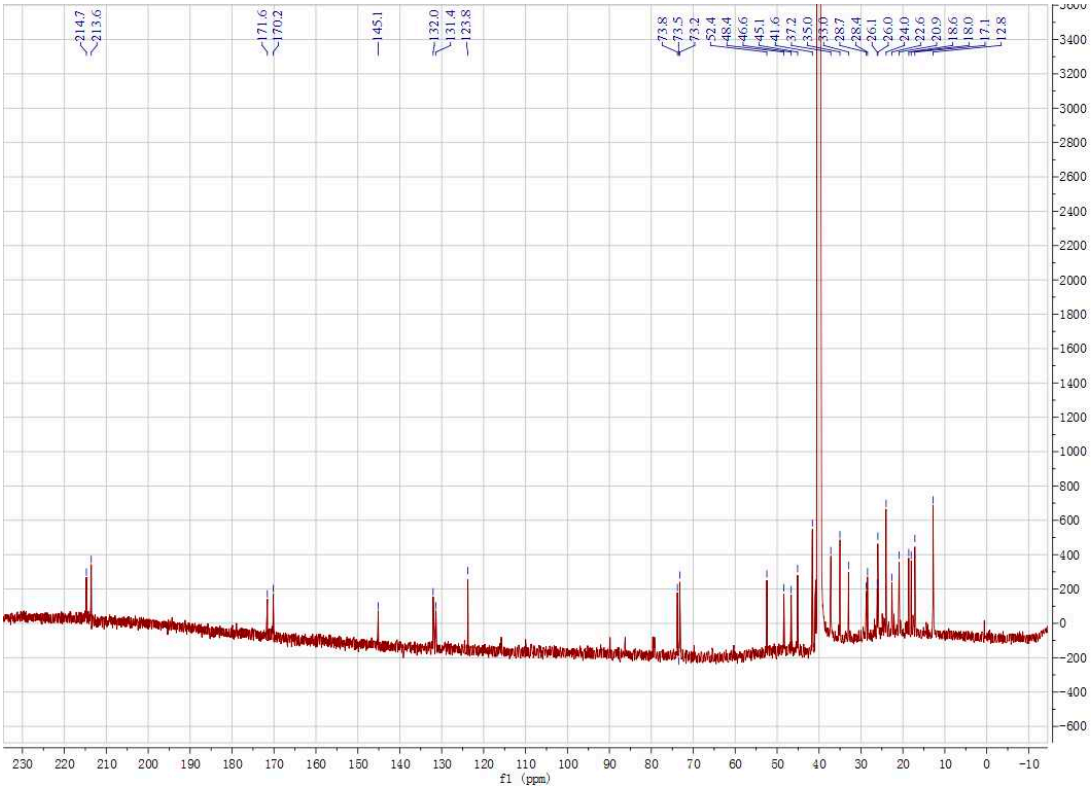

Figure S21. [13]C NMR spectra (175 MHZ, DMSO-*d6*) of the new compound **3.**

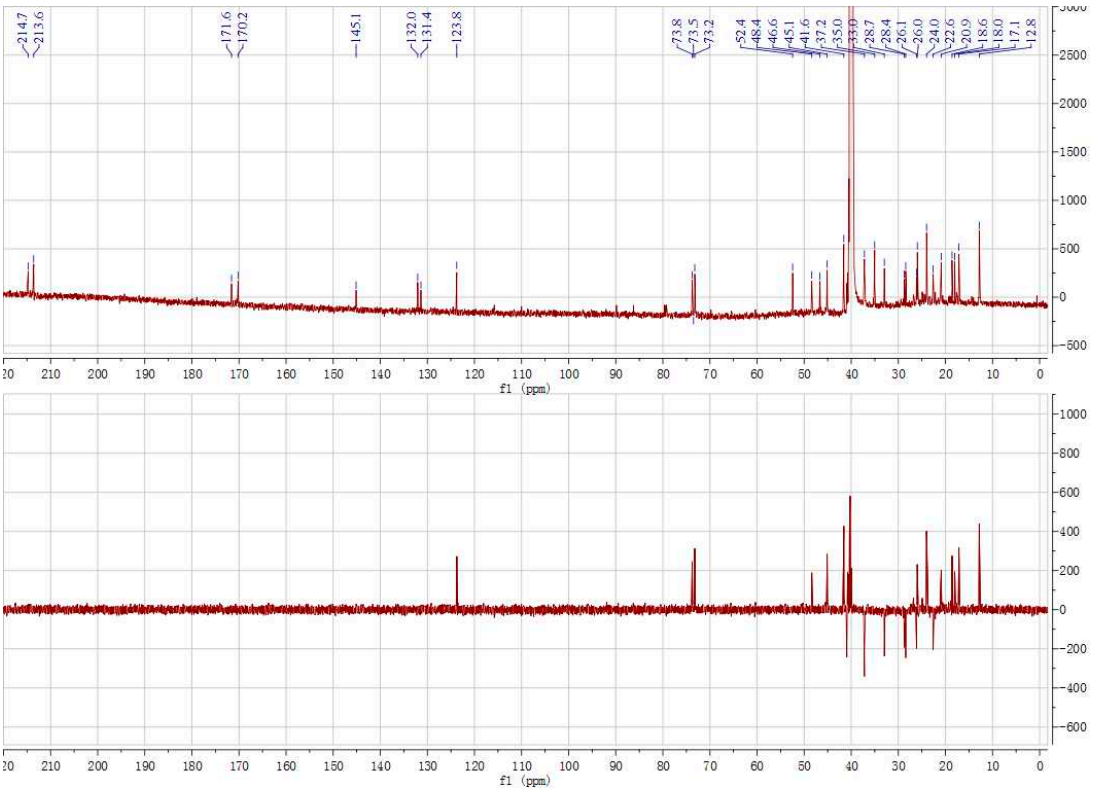

Figure S22. DEPT spectra of the new compound **3.**

Figure S23. COSY spectra of the new compound **3.**

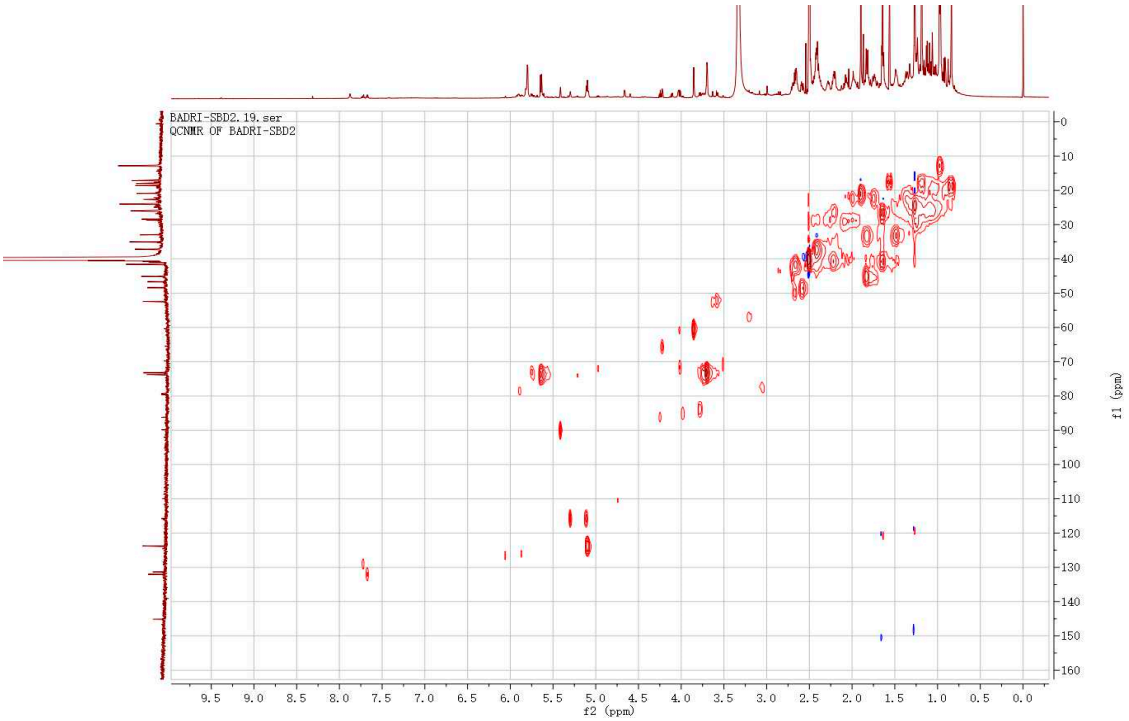

Figure S24. HMQC spectra of the new compound **3.**

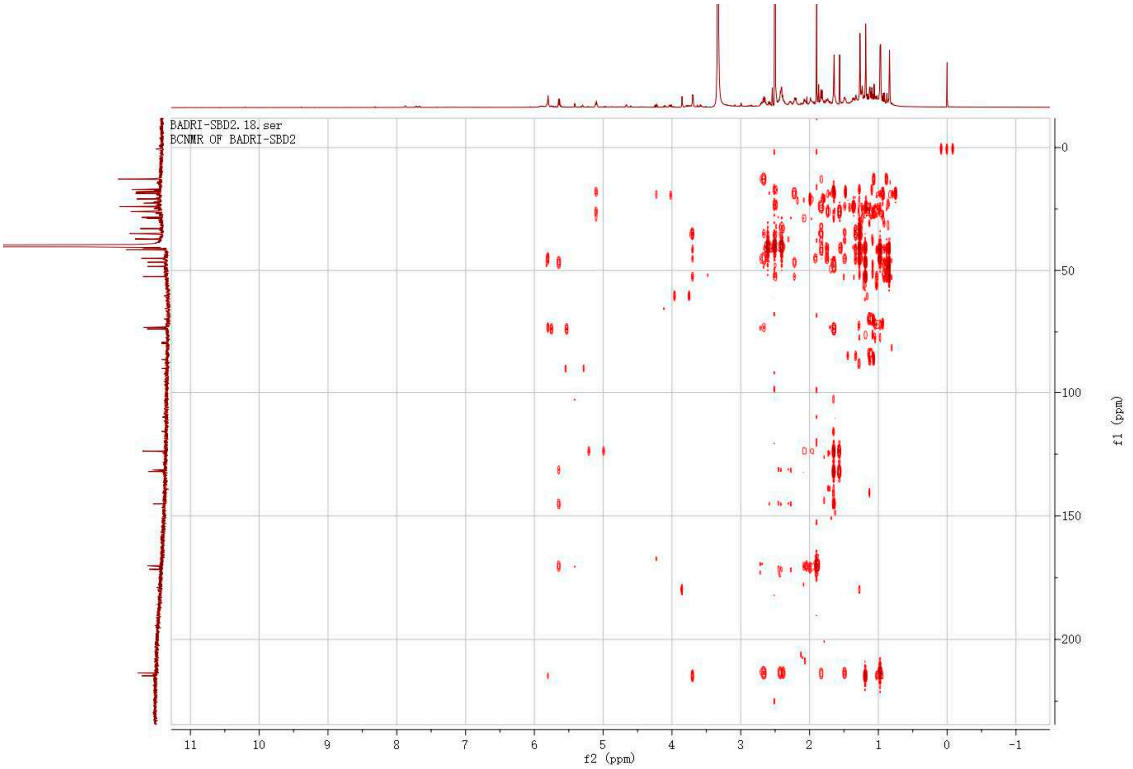

Figure S25. HMBC spectra of the new compound **3.**

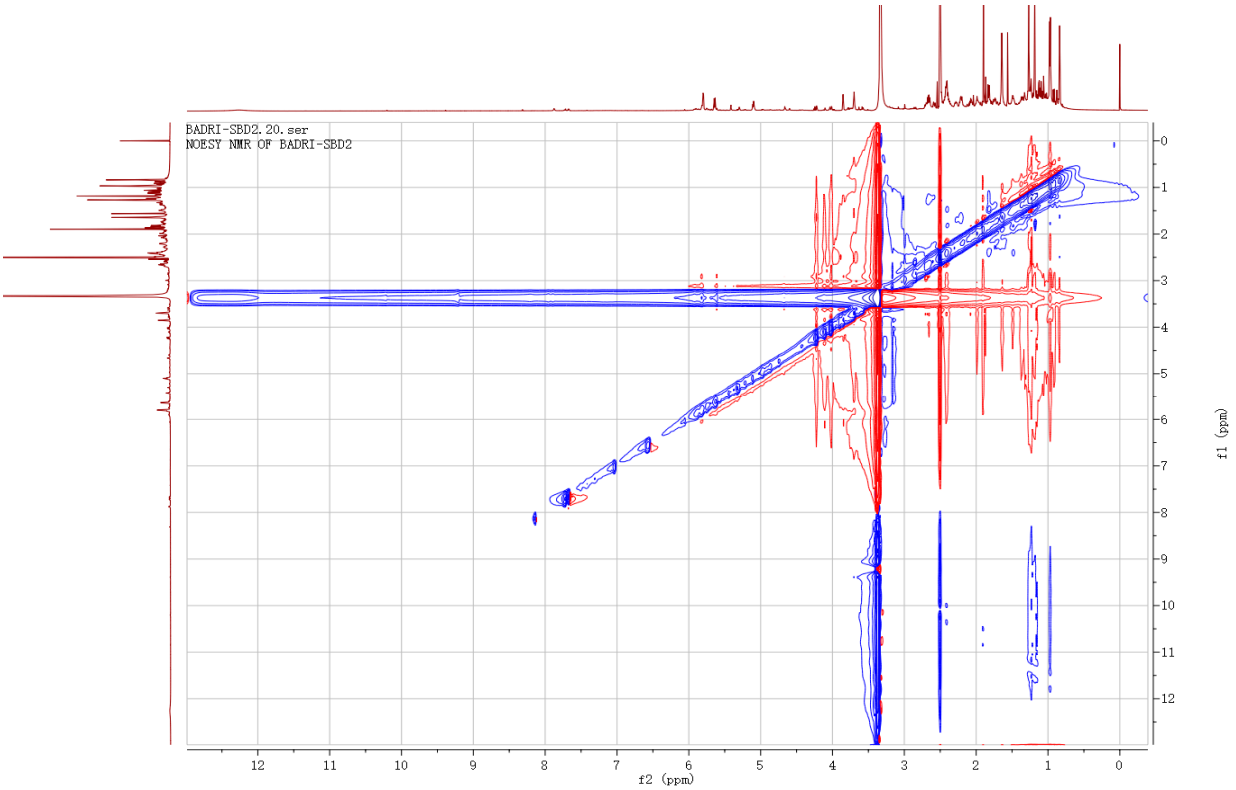

Figure S26. NOESY spectra of the new compound **3.**

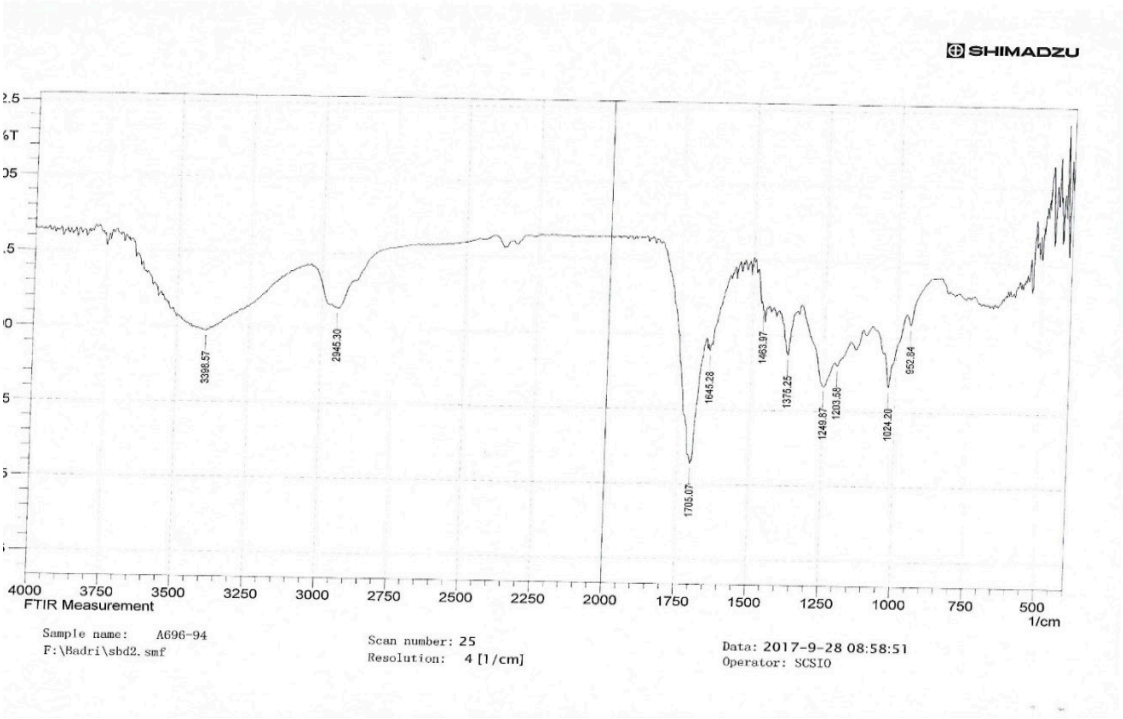

Figure S27. IR spectra of the new compound **3.**

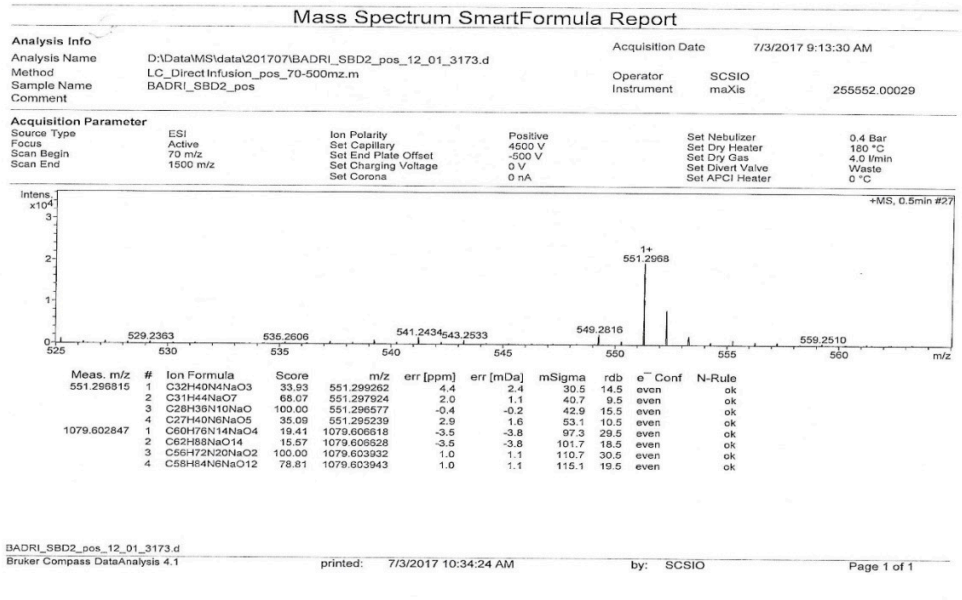

Figure S28. HR-ESIMS of the new compound **3.**

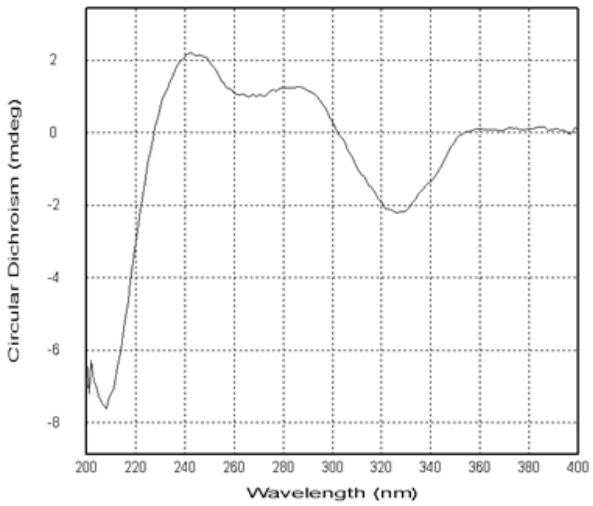

Figure S29. The experimental CD curve of the new compound **3**.

The ITS gene sequence data of *Aspergillus fumigatus* SCSIO 41012

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ggaa