

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 P₁ (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. baumannii* 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

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Figure S28: HRESIMS of the new compound **3**.

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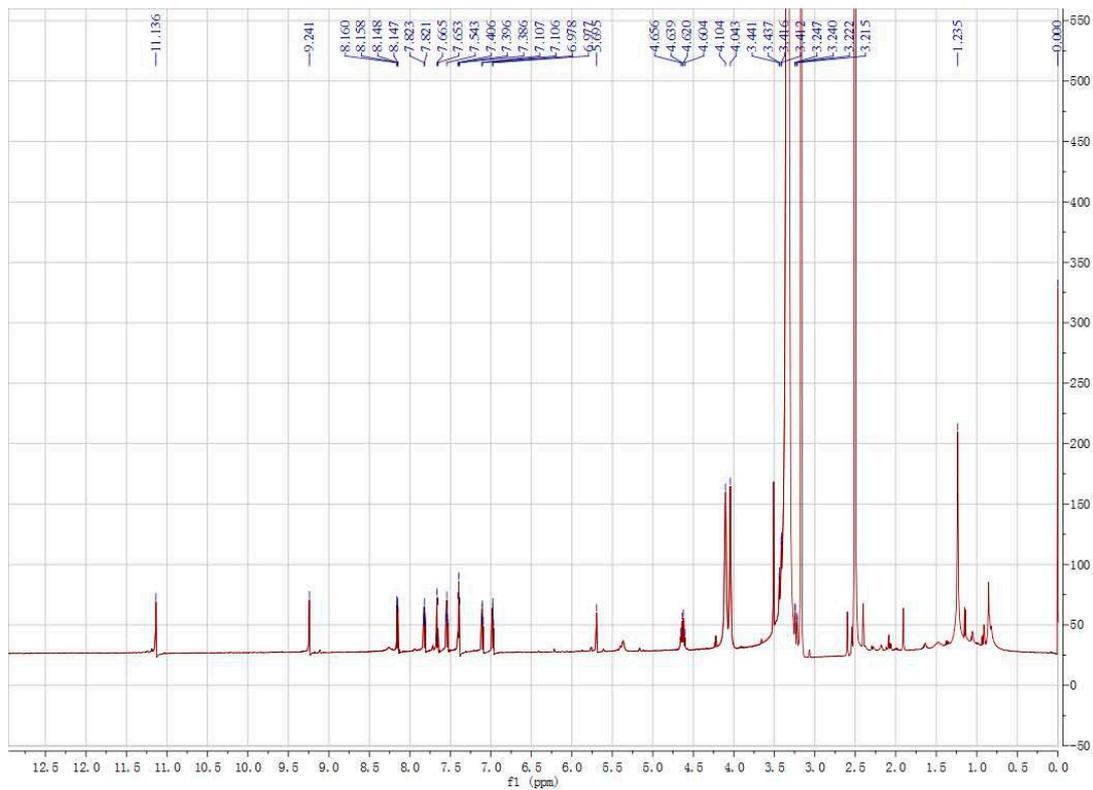


Figure S1. ¹H NMR spectra (700 MHz, DMSO-*d*₆) of the new compound **1**.

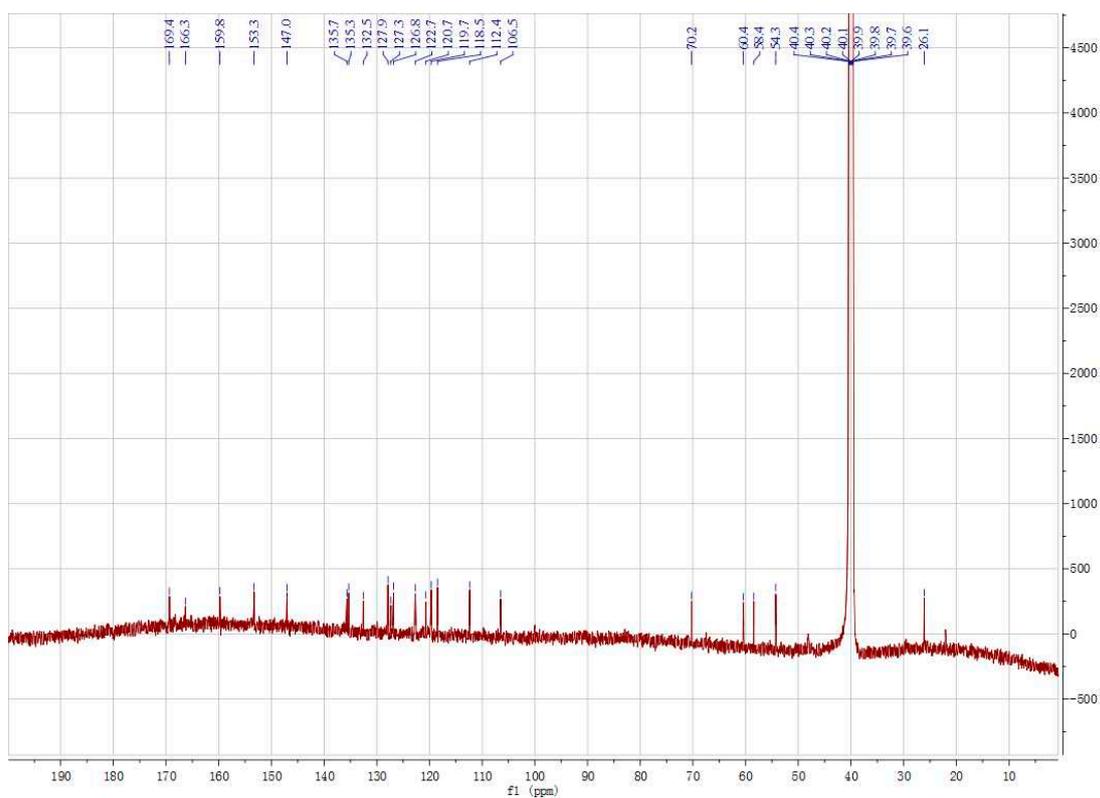


Figure S2. ^{13}C NMR spectra (175 MHz, $\text{DMSO-}d_6$) of the new compound **1**.

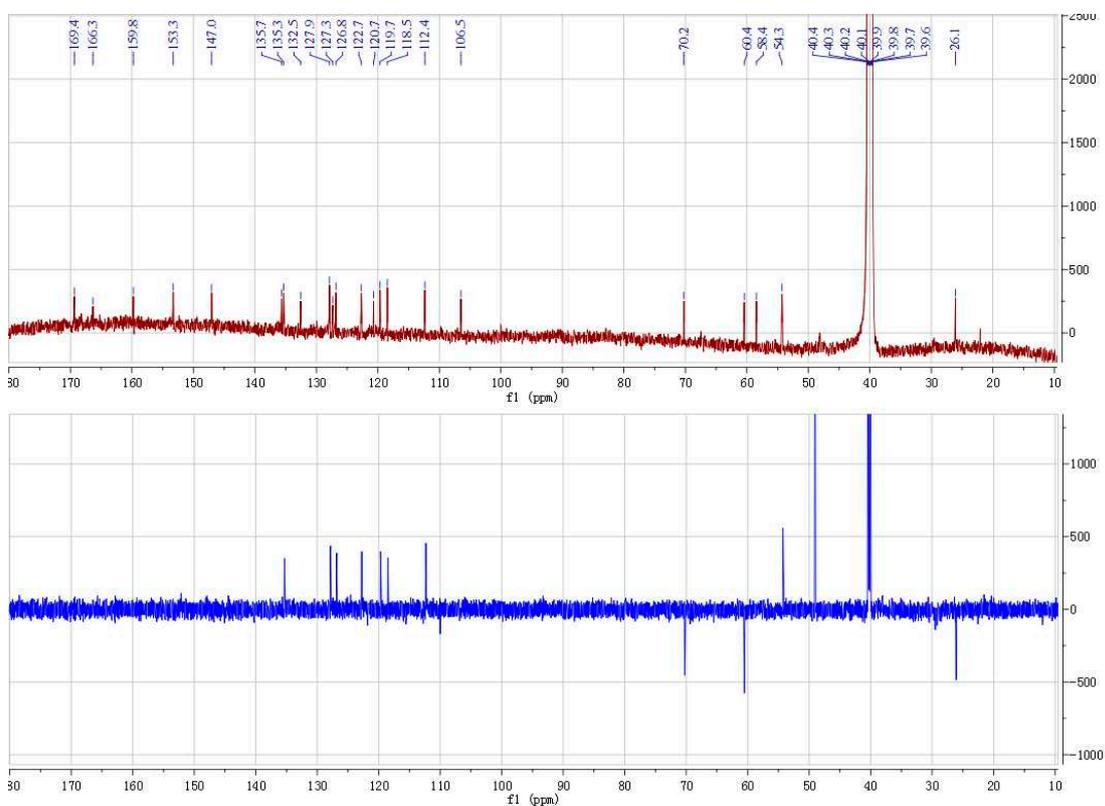


Figure S3. DEPT spectra of the new compound 1.

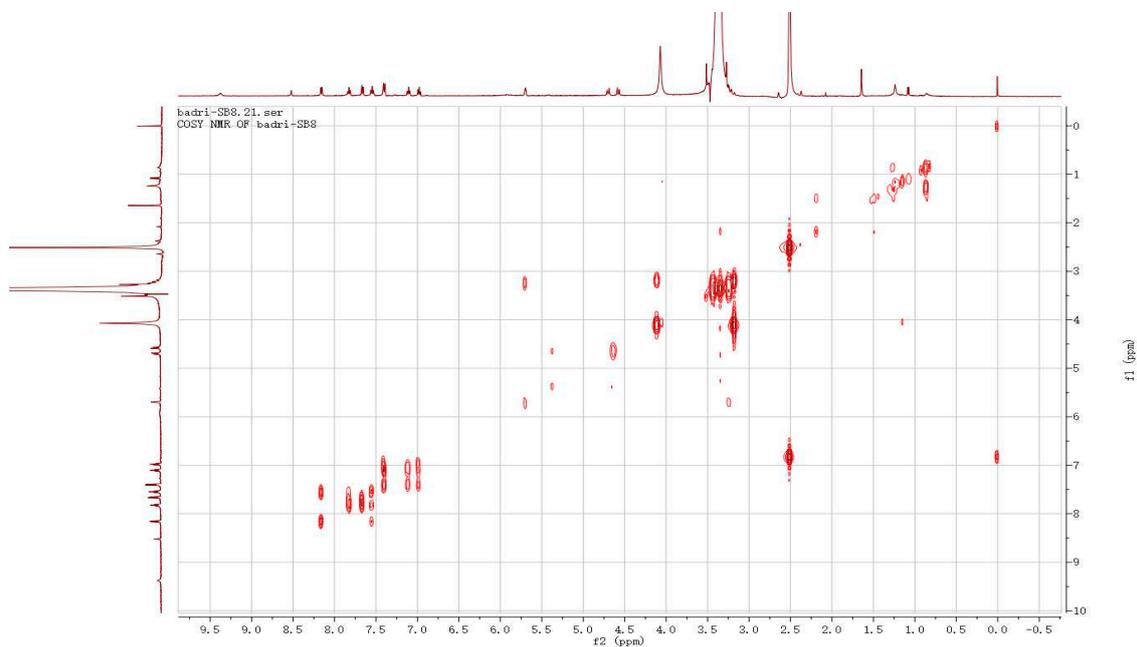


Figure S4. COSY spectra of the new compound 1.

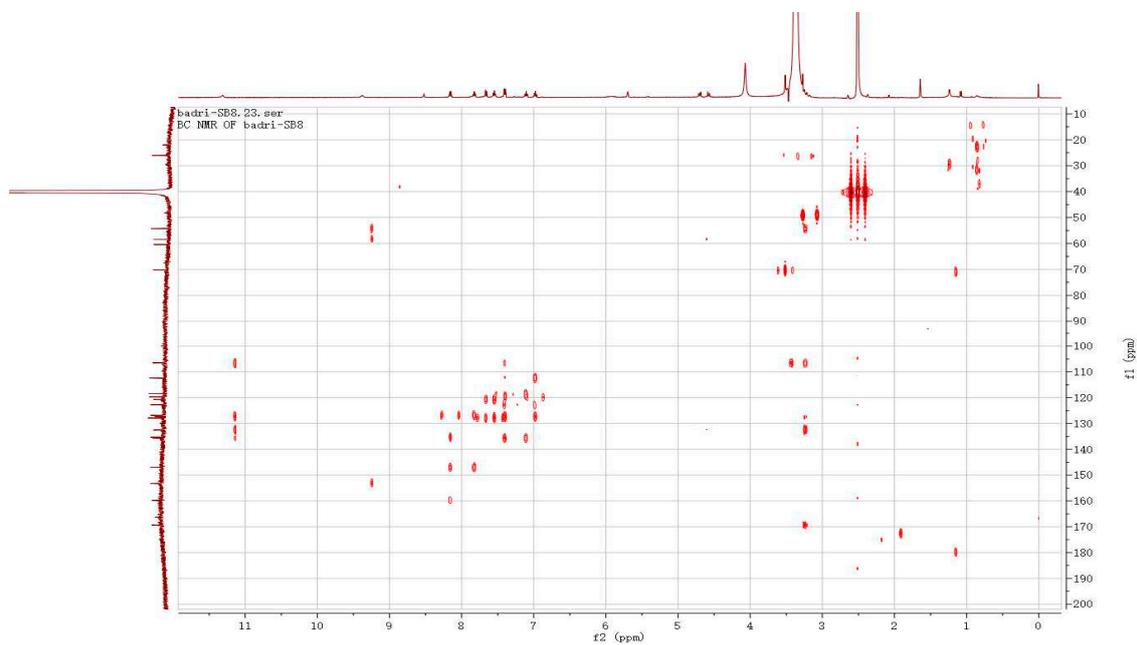


Figure S5. HMBC spectra of the new compound 1.

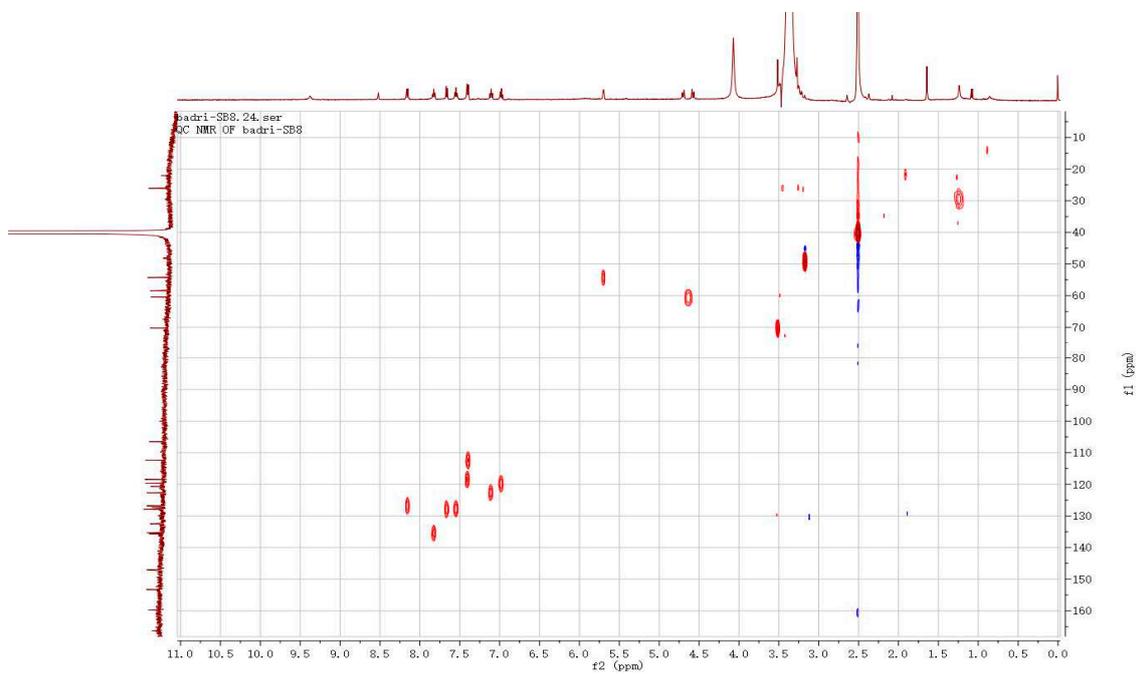


Figure S6. HMQC spectra of the new compound 1.

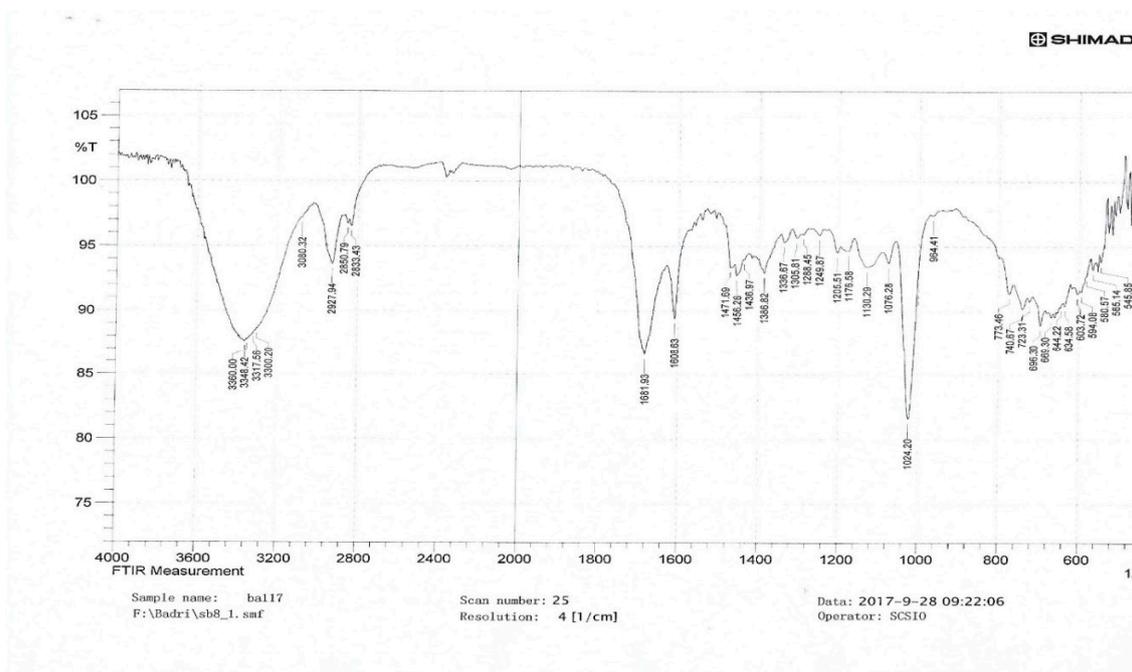
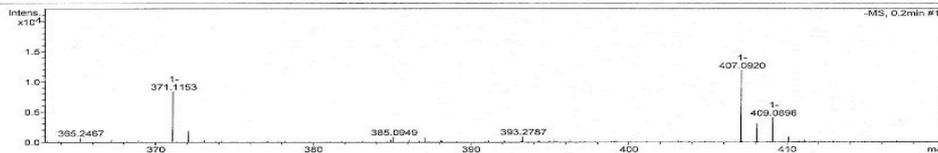


Figure S7. IR spectra of the new compound 1.

Mass Spectrum SmartFormula Report

Analysis Info
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 Method: LC_Direct Infusion_neg_100-1000mz.m
 Operator: SCSIO
 Sample Name: BADRI_SB8_neg
 Instrument: maXis
 Comment: 255552.00029

Acquisition Parameter
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 Focus: Active
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 Scan End: 2000 m/z
 Ion Polarity: Negative
 Set Capillary: 4000 V
 Set End Plate Offset: -500 V
 Set Charging Voltage: 0 V
 Set Corona: 0 nA
 Set Nebulizer: 0.4 Bar
 Set Dry Heater: 150 °C
 Set Dry Gas: 4.0 l/min
 Set Dwell Valve: Waste
 Set APCI Heater: 0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdB	e ⁻ Cnfr	N-Rule
371.115323	1	C23H19O7	52.08	371.113627	-4.6	-1.7	4.6	11.5	even	ok
	2	C21H15N4O3	100.00	371.114964	1.0	0.4	11.2	16.5	even	ok
407.091999	1	C21H16ClN4O3	100.00	407.091642	-0.9	-0.4	9.0	16.5	even	ok
	2	C23H19O7	39.62	407.093094	4.2	1.7	16.9	16.5	even	ok
779.213223	1	C40H40ClO14	42.44	779.211207	-2.5	-2.0	20.5	20.5	even	ok
	2	C42H32ClN8O8	92.37	779.213692	0.8	0.7	24.3	30.5	even	ok

Figure S8. HRESIMS of the new compound 1.

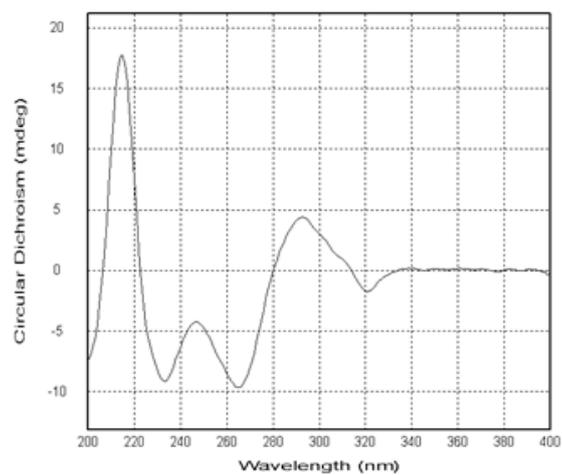


Figure S9. The experimental CD curve of the new compound **1**.

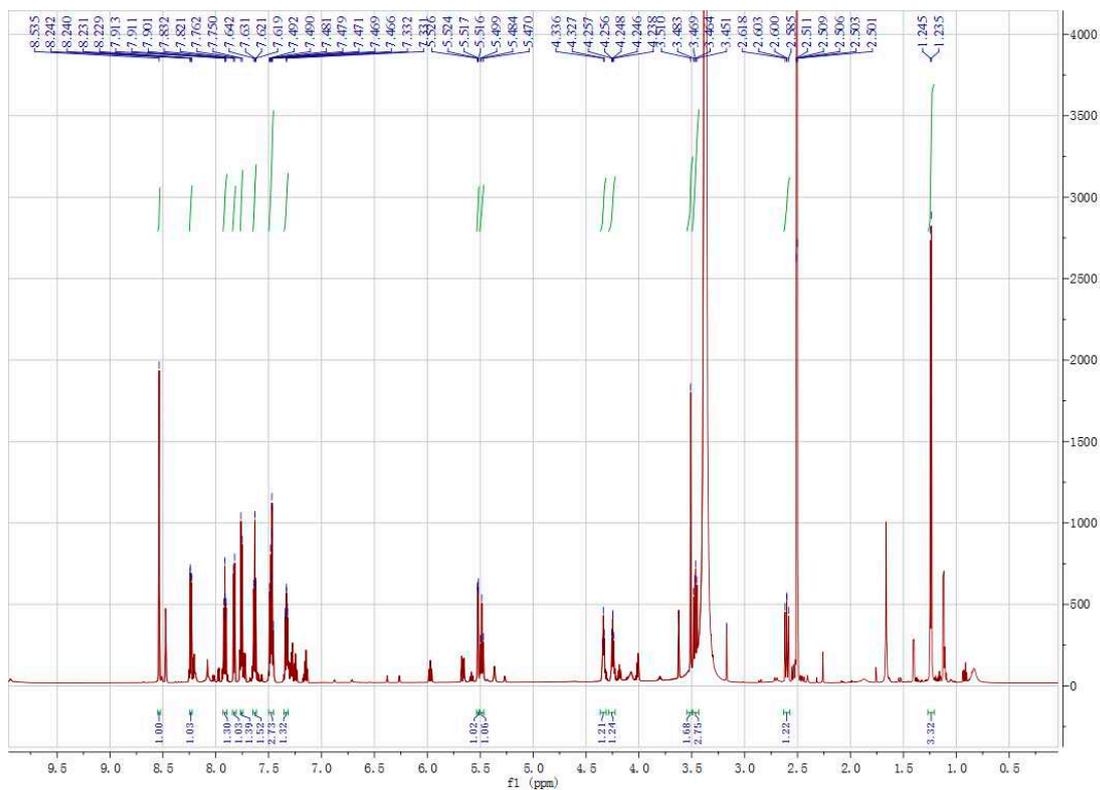


Figure S10. ^1H NMR spectra (700 MHz, $\text{DMSO-}d_6$) of the new compound **2**.

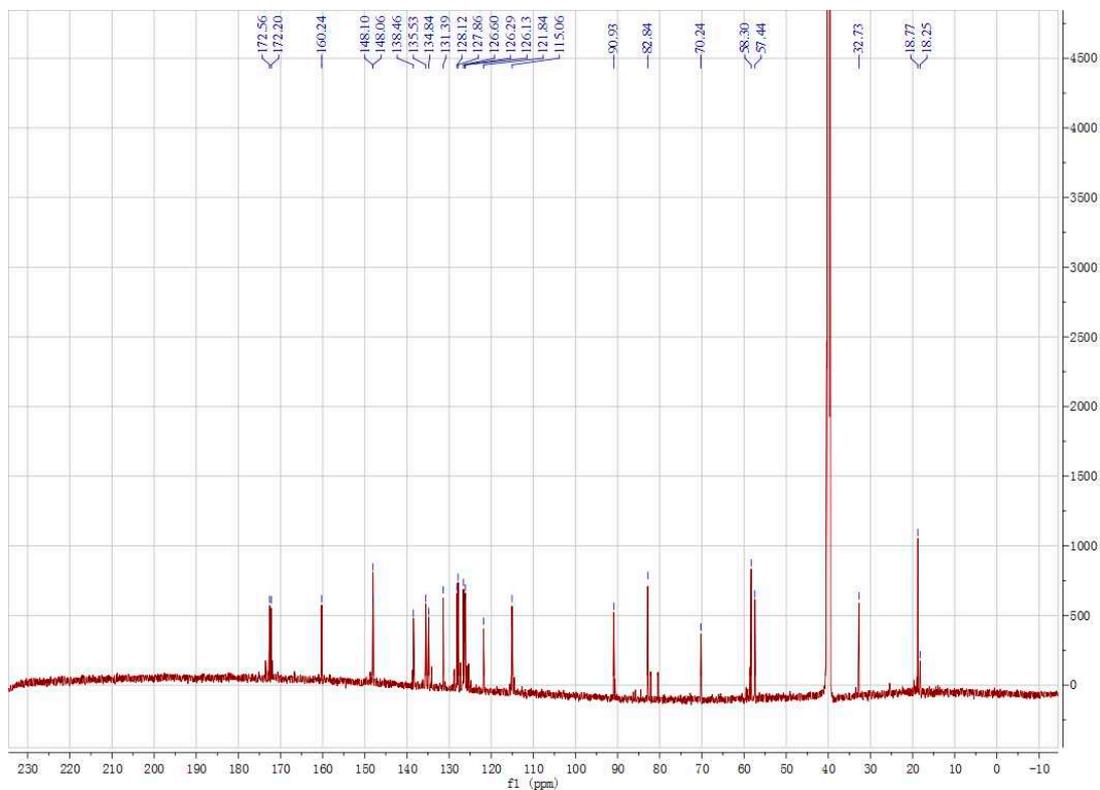


Figure S11. ^{13}C NMR spectra (175 MHz, DMSO-*d*₆) of the new compound **2**.

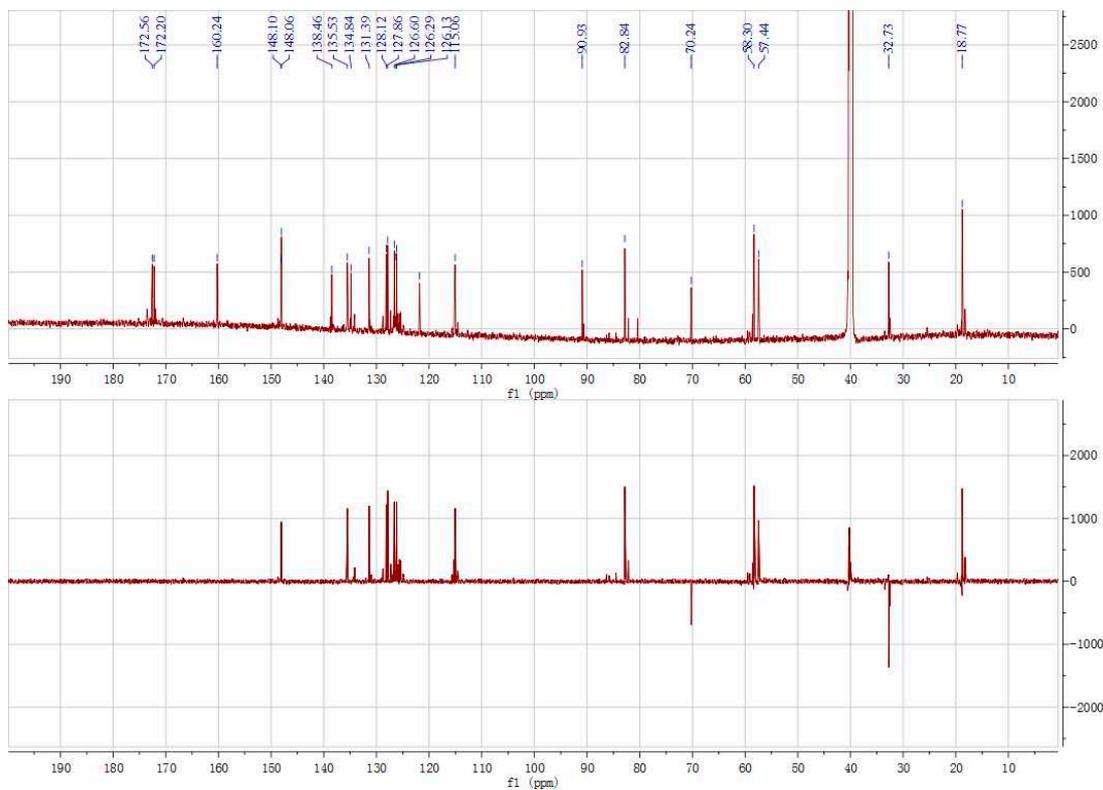


Figure S12. DEPT spectra of the new compound **2**.

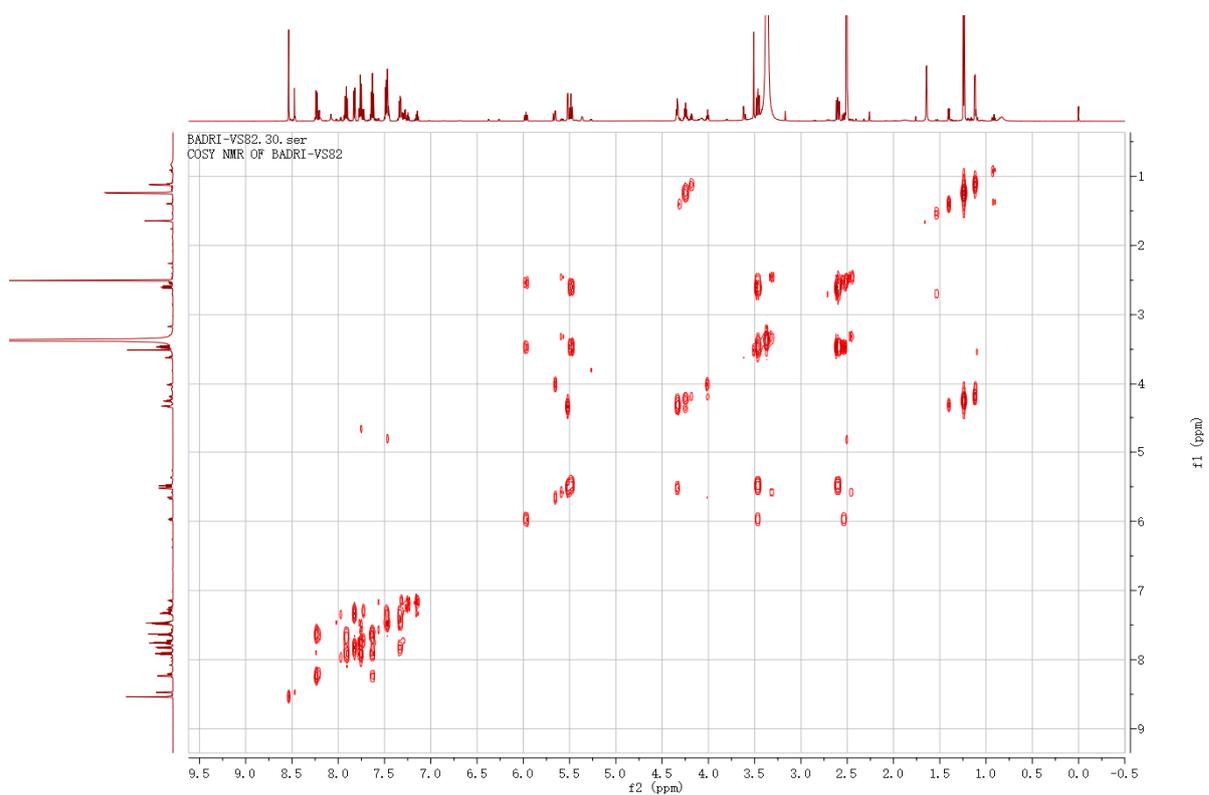


Figure S13. COSY spectra of the new compound **2**.

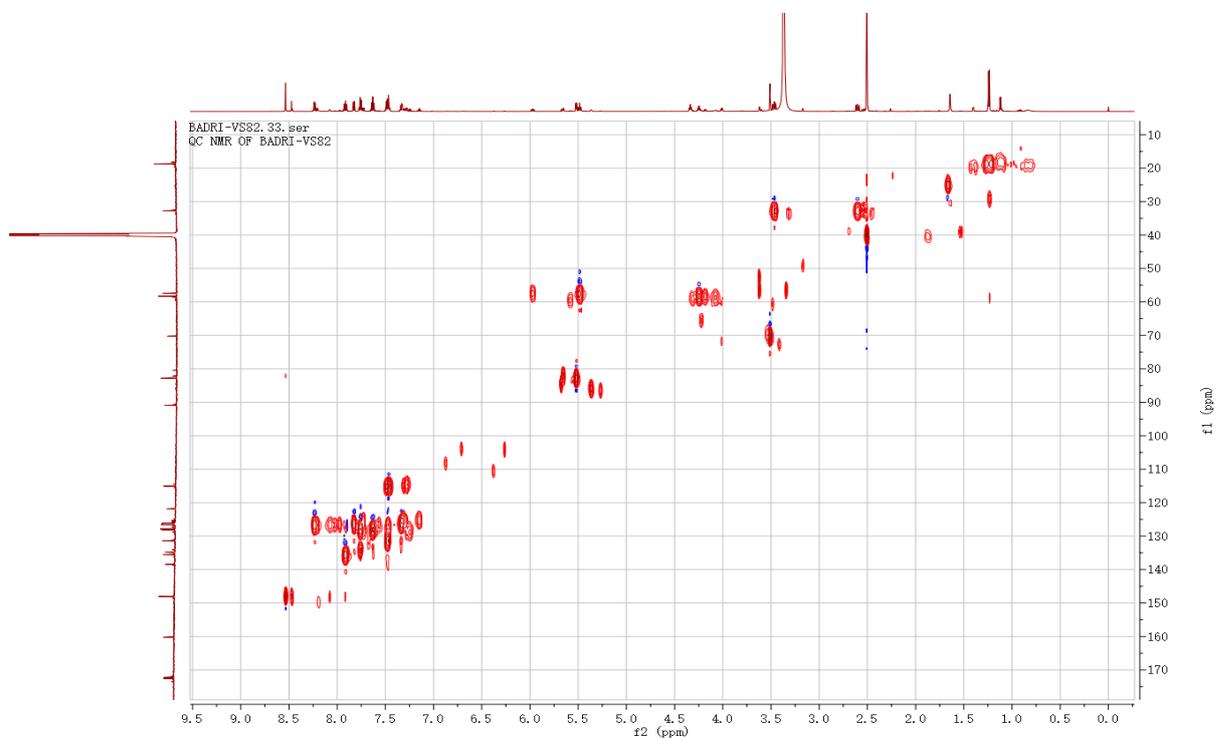


Figure S14. HMQC spectra of the new compound **2**.

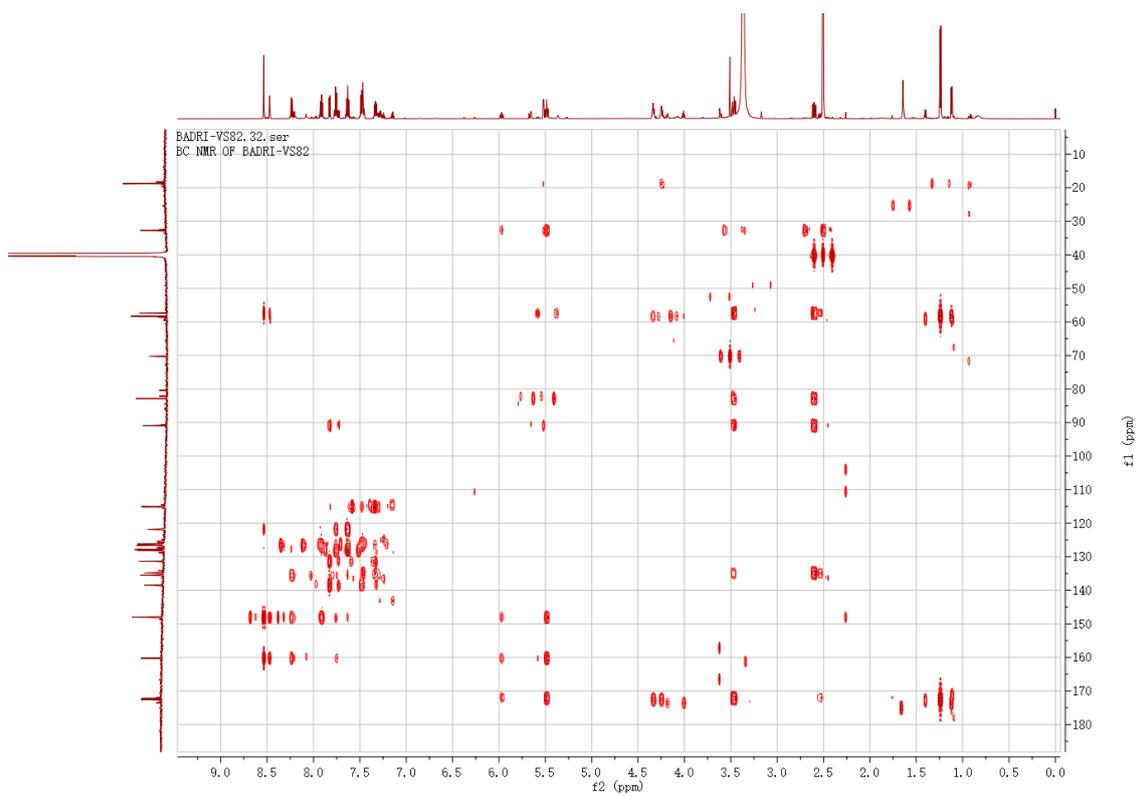


Figure S15. HMBC spectra of the new compound 2.

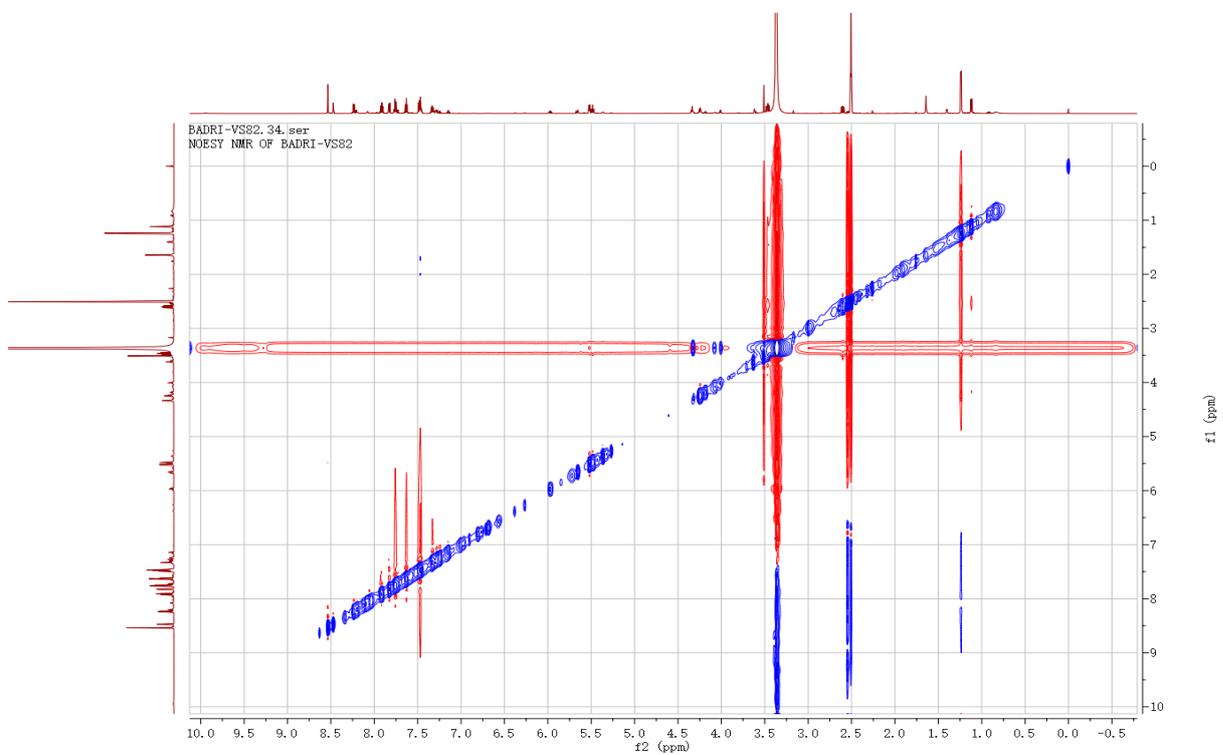


Figure S16. NOESY spectra of the new compound 2.

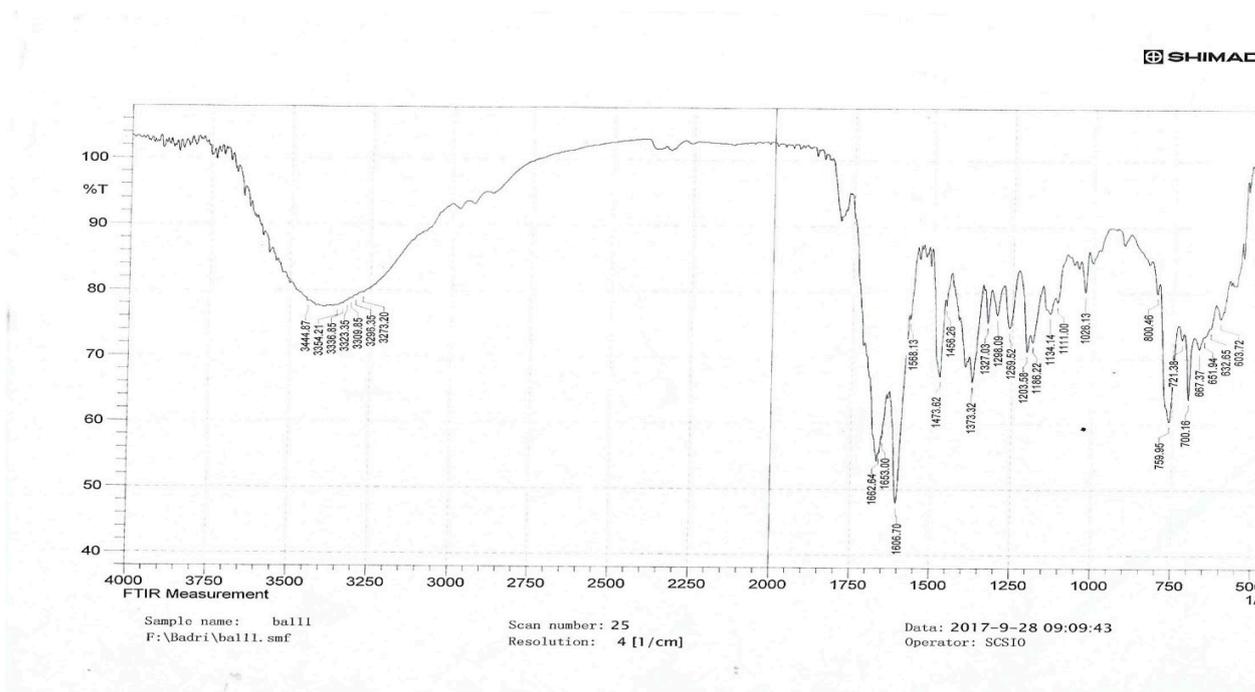


Figure S17. IR spectra of the new compound 2.

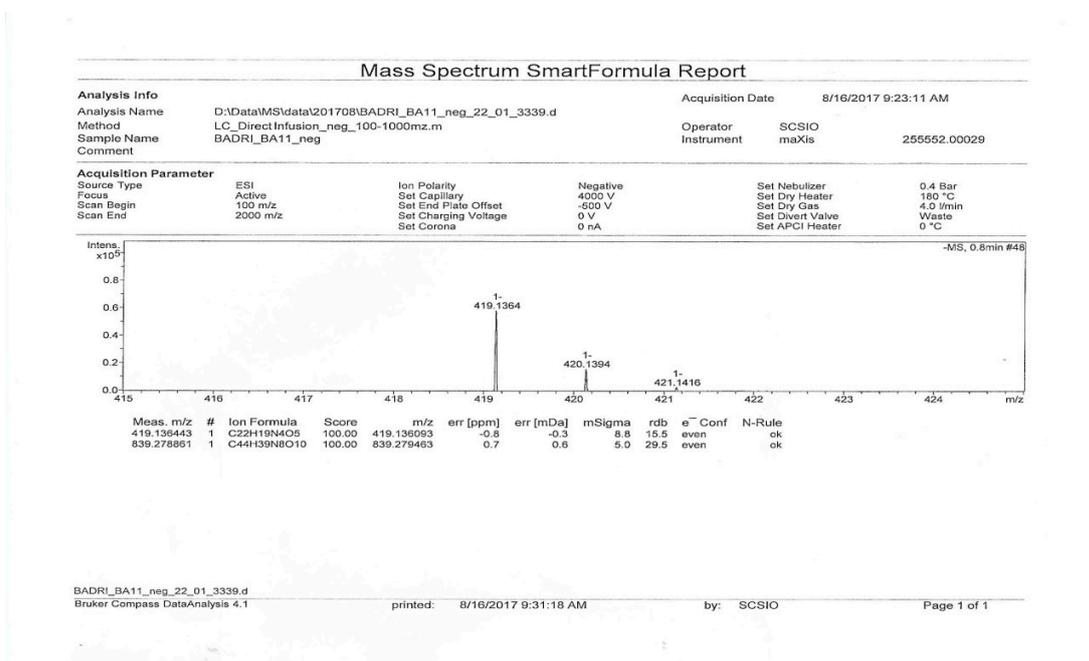


Figure S18. HRESIMS of the new compound 2.

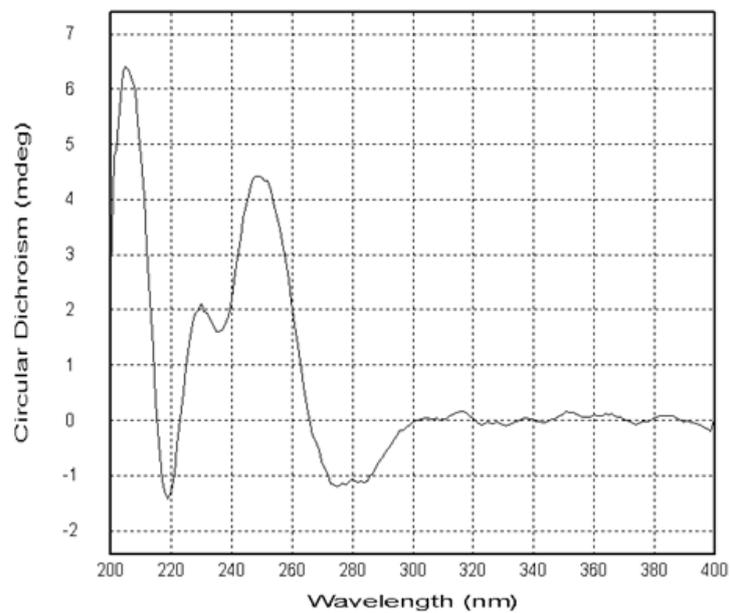


Figure S19. The experimental CD curve of the new compound **2**.

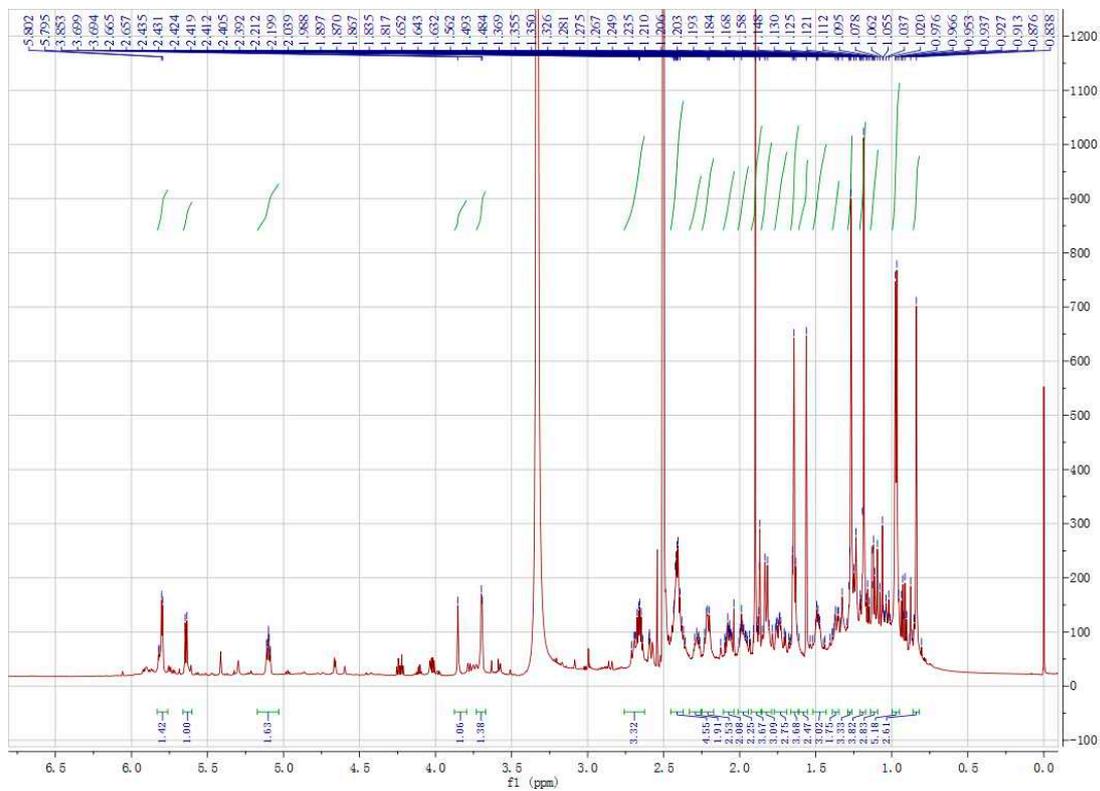


Figure S20. ^1H NMR spectra (700 MHz, $\text{DMSO-}d_6$) of the new compound **3**.

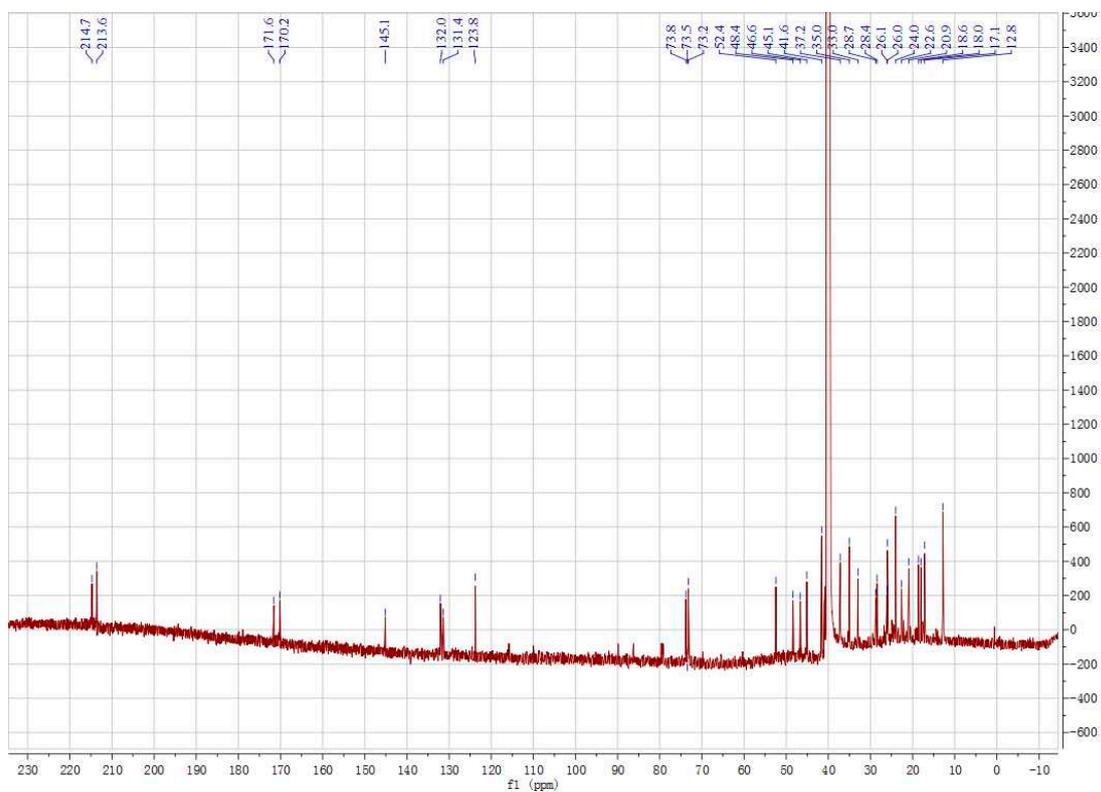


Figure S21. ^{13}C NMR spectra (175 MHz, $\text{DMSO-}d_6$) of the new compound **3**.

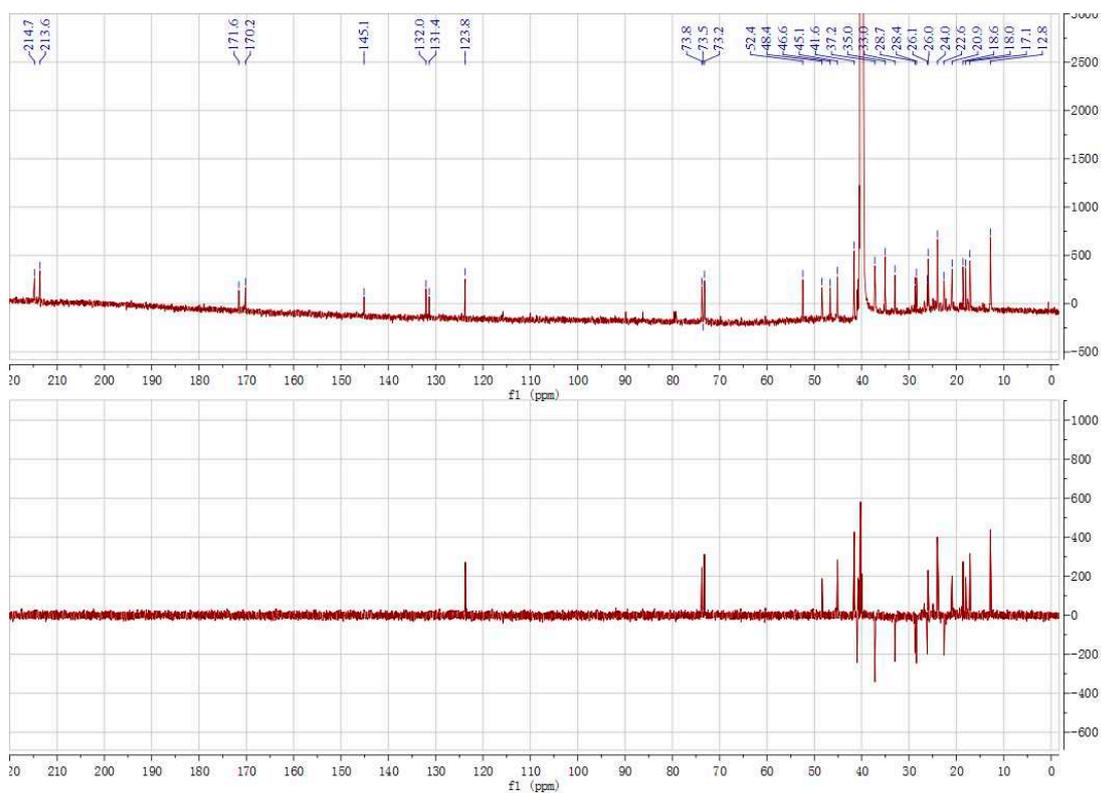


Figure S22. DEPT spectra of the new compound 3.

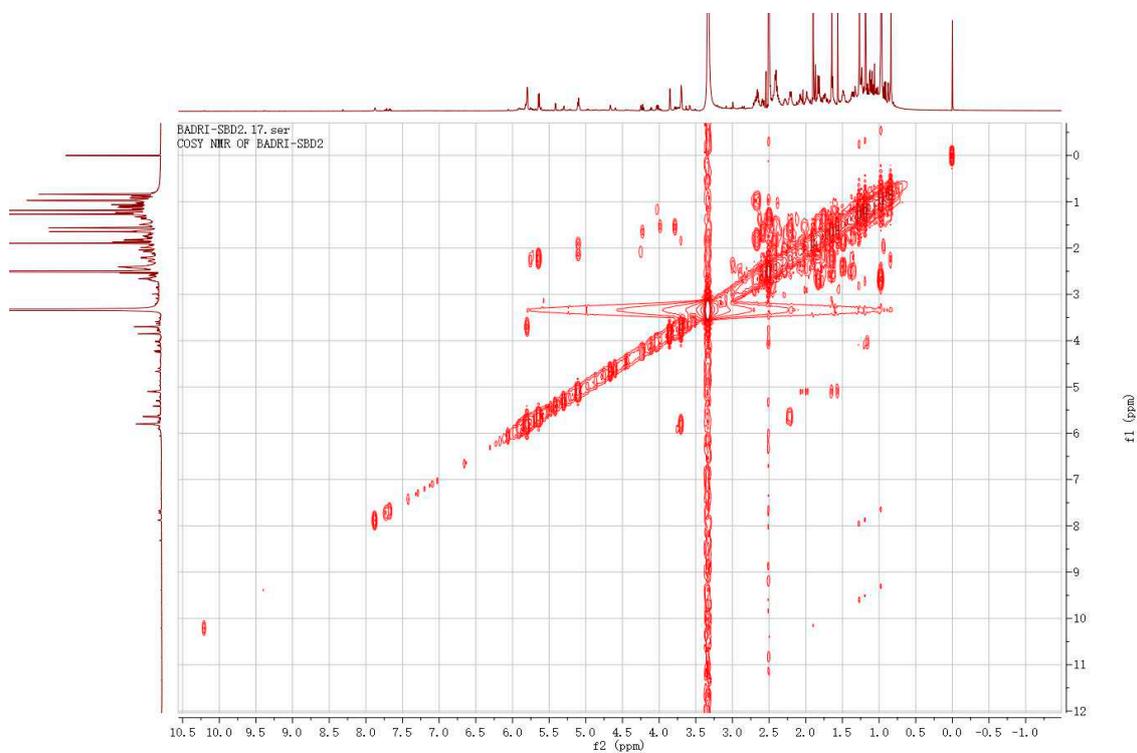


Figure S23. COSY spectra of the new compound **3**.

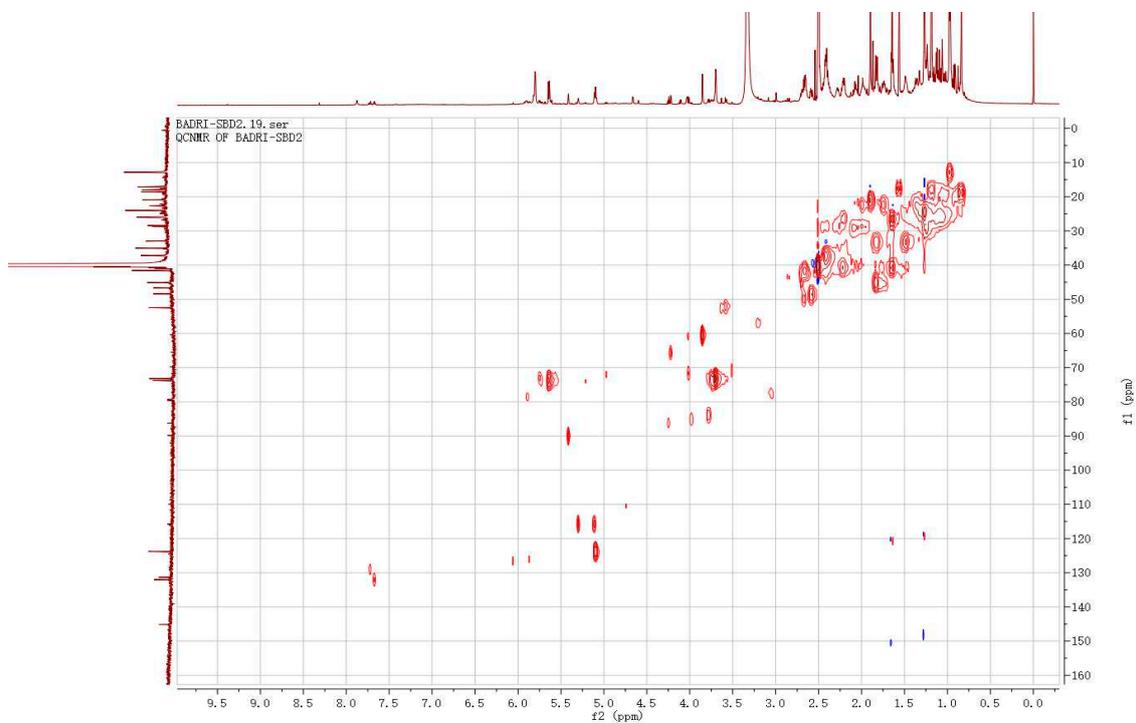


Figure S24. HMQC spectra of the new compound **3**.

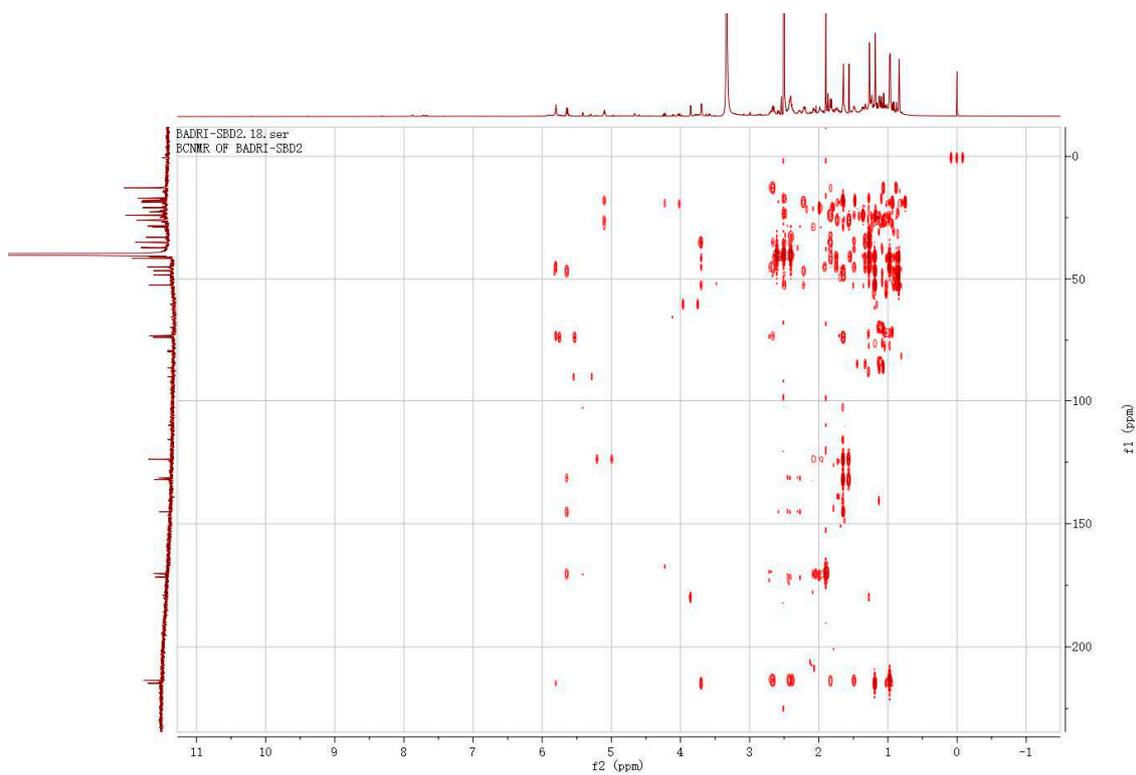


Figure S25. HMBC spectra of the new compound **3**.

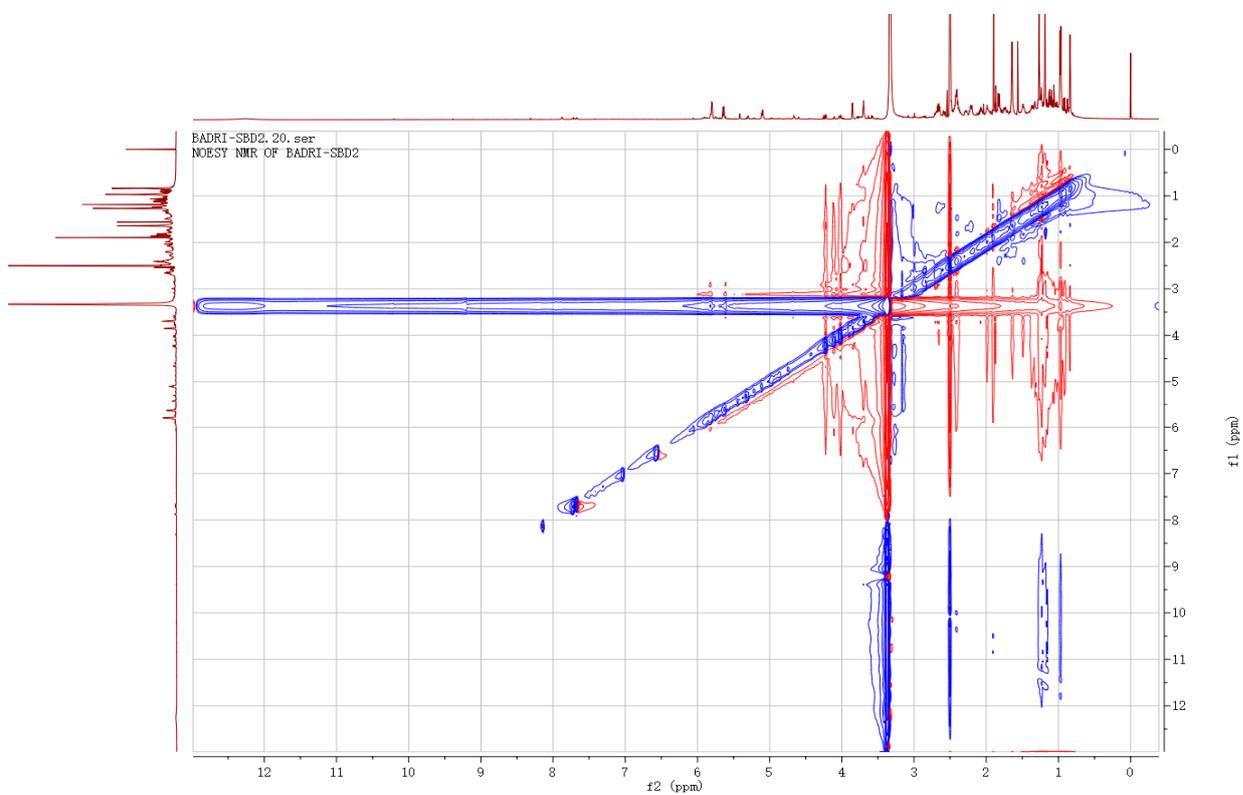


Figure S26. NOESY spectra of the new compound 3.

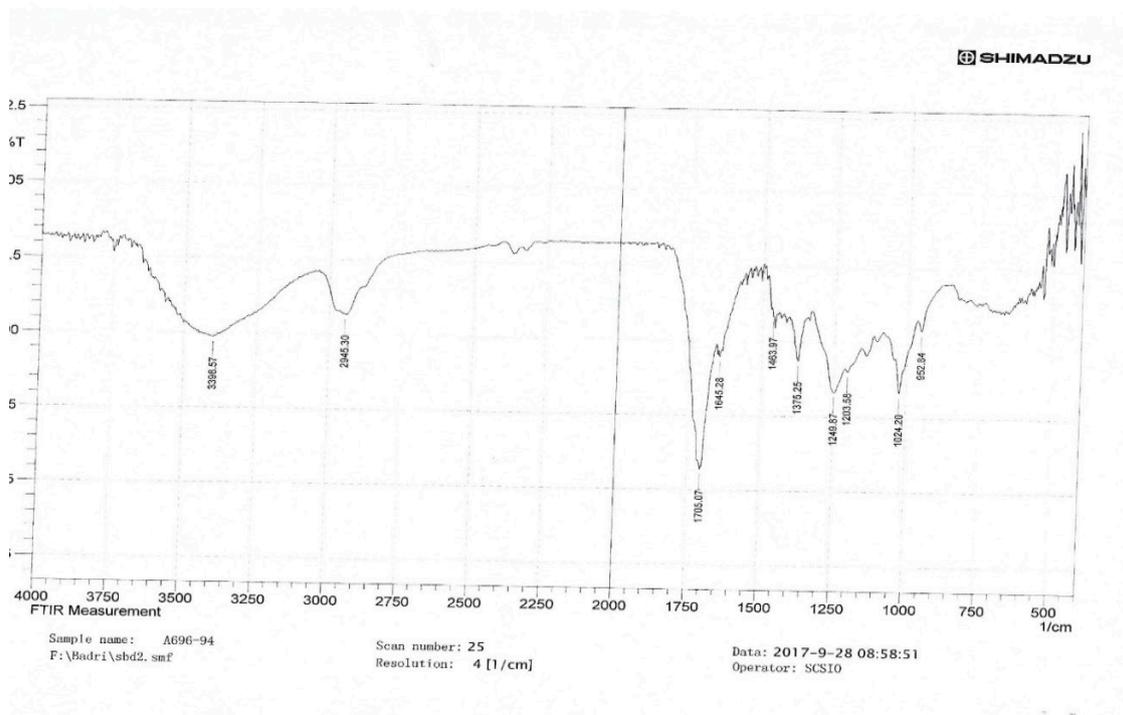


Figure S27. IR spectra of the new compound 3.

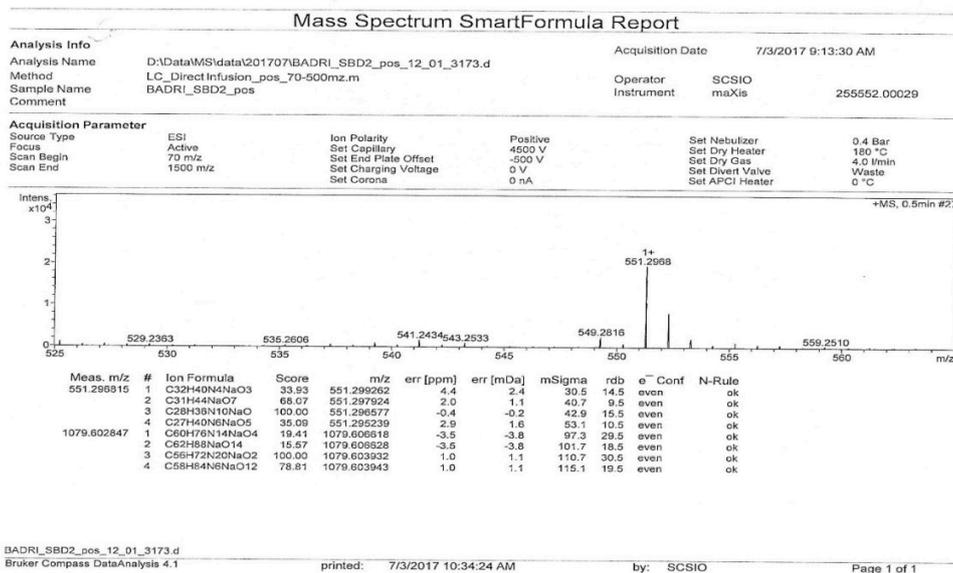


Figure S28. HR-ESIMS of the new compound 3.

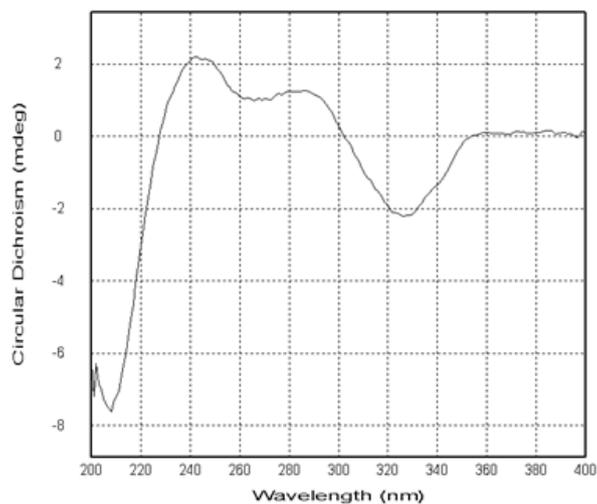


Figure S29. The experimental CD curve of the new compound **3**.

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

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ggaa