Supplementary Information

Abinukitrine A, a unique 17,18-cyclolanostane triterpenoid from *Abies nukiangensis*

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Content

Experimental procedures

General Experimental Procedures. Infrared spectra were recorded on a Bruker IFS-66/S FT-IR spectrometer. NMR spectra were recorded on a Varian UNITY INOVA 500 NMR spectrometer. Optical rotations were measured on a Hanon P850 polarimeter. HRESIMS spectra were obtained on a Q-Tof mass spectrometer. Semi-preparative HPLC was performed using a Waters 600 pump with a waters 2489 uv/visible detector and a YMC C18 5 μm column (10 mm ×250 mm). Column chromatography was performed on ODS, silica gel, and Sephadex LH-20. TLC analysis was using the precoated silica gel plates.

Plant Material. The aerial parts of *Abies nukiangensis* were collected in Lushui, Yunnan Province, China in September 2015. The plant was identified by Yuan-Chun Zhou. A voucher specimen (SMMC-AB 1501) was deposited in the herbarium of physical and chemical analysis laboratory, Shanghai Institute of Measurement and Testing Technology, Shanghai, China.

Extraction and Isolation. The twigs and leaves of *A. nukiangensis* (5.0 kg) was extracted with EtOH under reflux and filtered. The filtrate was evaporated under reduced pressure to provide an EtOH extract (320 g), which was suspended in distilled H_2O and successively partitioned with CH_2Cl_2, EtOAc, and *n*-BuOH, yielding 110 g, 75 g, and 102 g of residues, respectively. The CH_2Cl_2-soluble fraction (110 g) was subjected to CC on silica gel and eluted with $CHCl_3$-MeOH (50:1 to 20:1) to yield five fractions (C1-C5). Fraction C4 (8.0 g) was separated over a RP-C_{18} silica gel column with 80% MeOH to yield four subfractions (C4A-C4D). Subfraction C4D (1.2 g) was

separated on a silica gel column ($CHCl_3$-MeOH, 14:1), followed by CC on Sephadex LH-20 ($CHCl_3$-MeOH, 1:1) to give **1** (20.8 mg).

Crystal preparation. Compound **1** (2.0 mg) was dissolved in 0.5 mL pyridine-MeOH (1:1) solution, slow evaporation over days afforded crystals.

Anti-HCV assay on GT1b cells. Compound **1** was serially diluted in DMSO (0.016, 0.08, 0.4, 2, 10, 20 μM) and then added to 96-well plates, in duplicate. Subsequently, GT1b cells were seeded and cultured in a humidified incubator containing 5% CO_2 at 37°C for 3 days. The cell viability was determined with the CellTiter-Fluor kit in accordance with the protocol provided by the supplier. While the antiviral activity was determined by monitoring replicon reporter firefly luciferase using Bright-Glo.

Inhibition rate (%) = (ZPE-CPD)/(ZPE-HPE) × 100 %, where

CPD: Signals of tested compounds.

ZPE: Signals of DMSO control.

HPE: Signals of medium control.

50% effective concentrations (EC_{50}) value will be calculated with the GraphPad Prism software.

Table S1. X-ray crystal data for abinukitrine A (1)

Identification code	mjl18542	
Empirical formula	C35 H49 N O4	
Formula weight	547.75	
Temperature	169.96 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	C 1 2 1	
Unit cell dimensions	a = 36.5813(18) Å	α = 90°
	b = 6.2452(3) Å	β = 91.068(4)°
	c = 13.6063(7) Å	γ = 90°
Volume	3107.9(3) $Å^3$	
Z	4	
Density (calculated)	1.171 mg/m^3	
Absorption coefficient	0.378 mm^{-1}	
F(000)	1192	
Crystal size	0.12 x 0.08 x 0.03 mm^3	
Theta range for data collection	3.491 to 55.114°.	
Index ranges	$-44 \leq h \leq 44$, $-7 \leq k \leq 7$, $-16 \leq l \leq 16$	
Reflections collected	43183	
Independent reflections	5924 [R(int) = 0.0559]	
Completeness to theta = 53.594°	99.60%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.5776	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	5924 / 1 / 372	
Goodness-of-fit on F2	1.052	
Final R indices [I>2sigma(I)]	R_1 = 0.0355, wR_2 = 0.0892	
R indices (all data)	R_1 = 0.0373, wR_2 = 0.0908	
Absolute structure parameter	0.07(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.174 and -0.177 $e.Å^{-3}$	

Figure S1. ^{1}H NMR spectrum of compound 1 in $CDCl_3$.

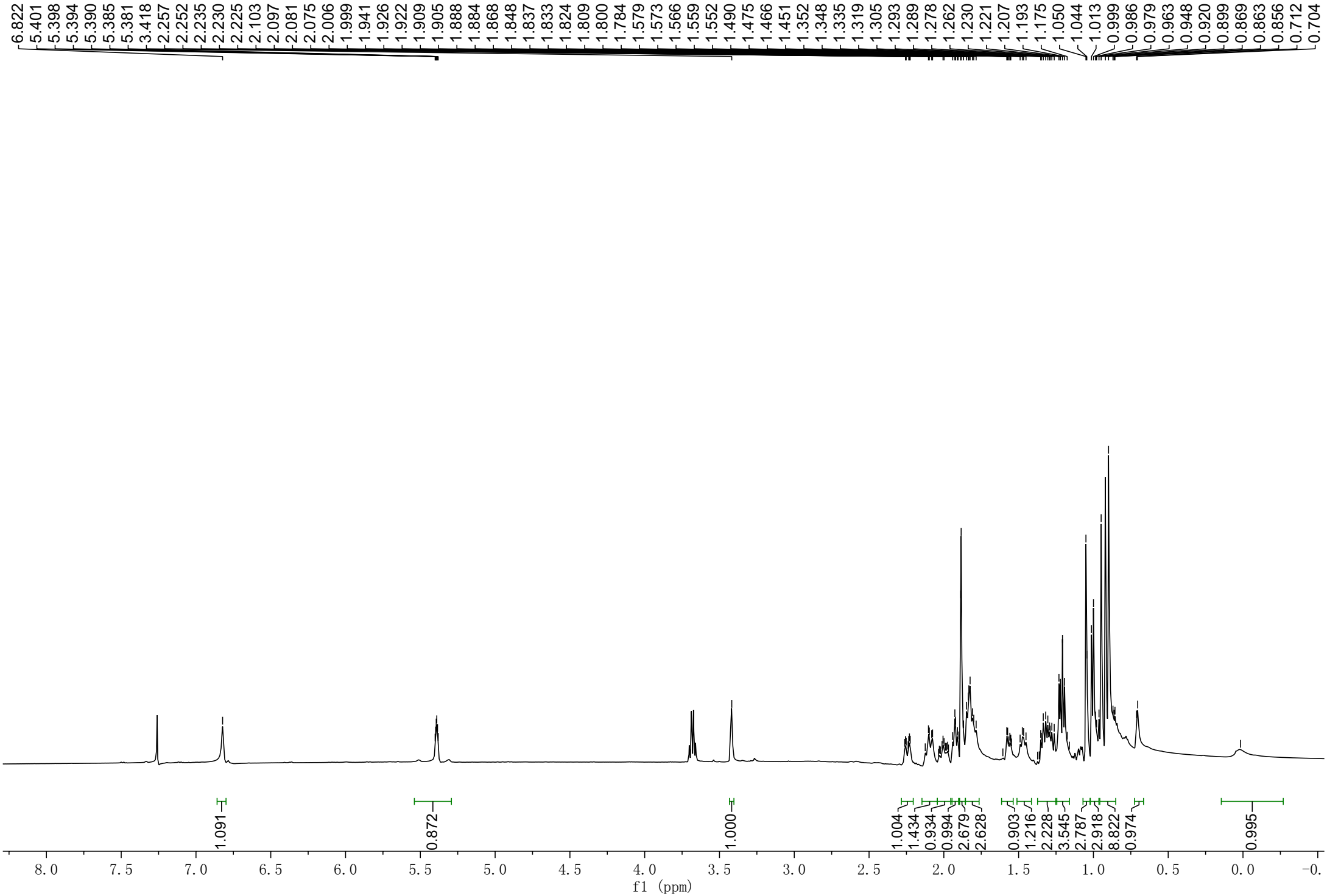

Figure S2. ^{13}C NMR spectrum of compound 1 in $CDCl_3$.

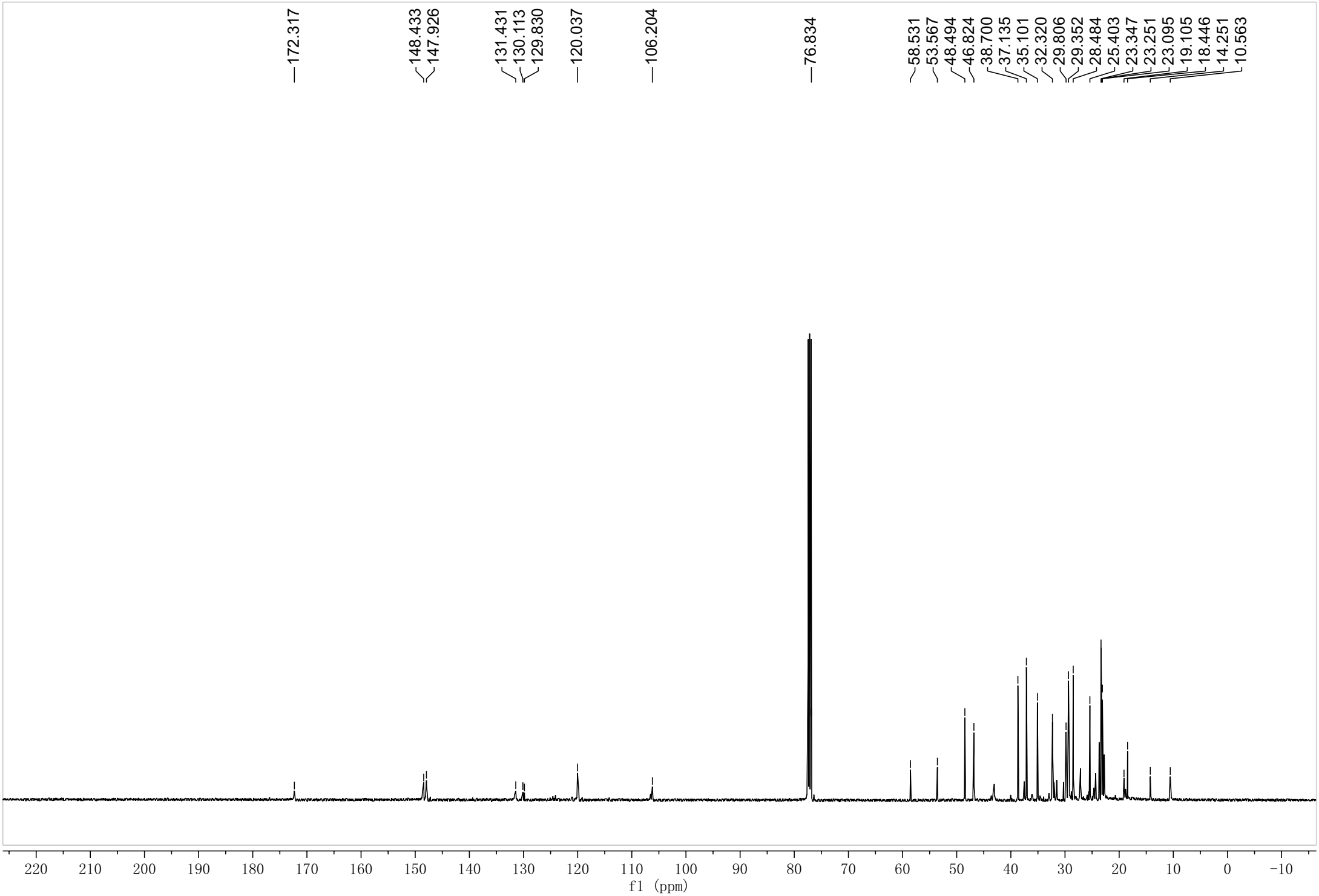

Figure S3. DEPT NMR spectrum of compound 1 in CDCl3.

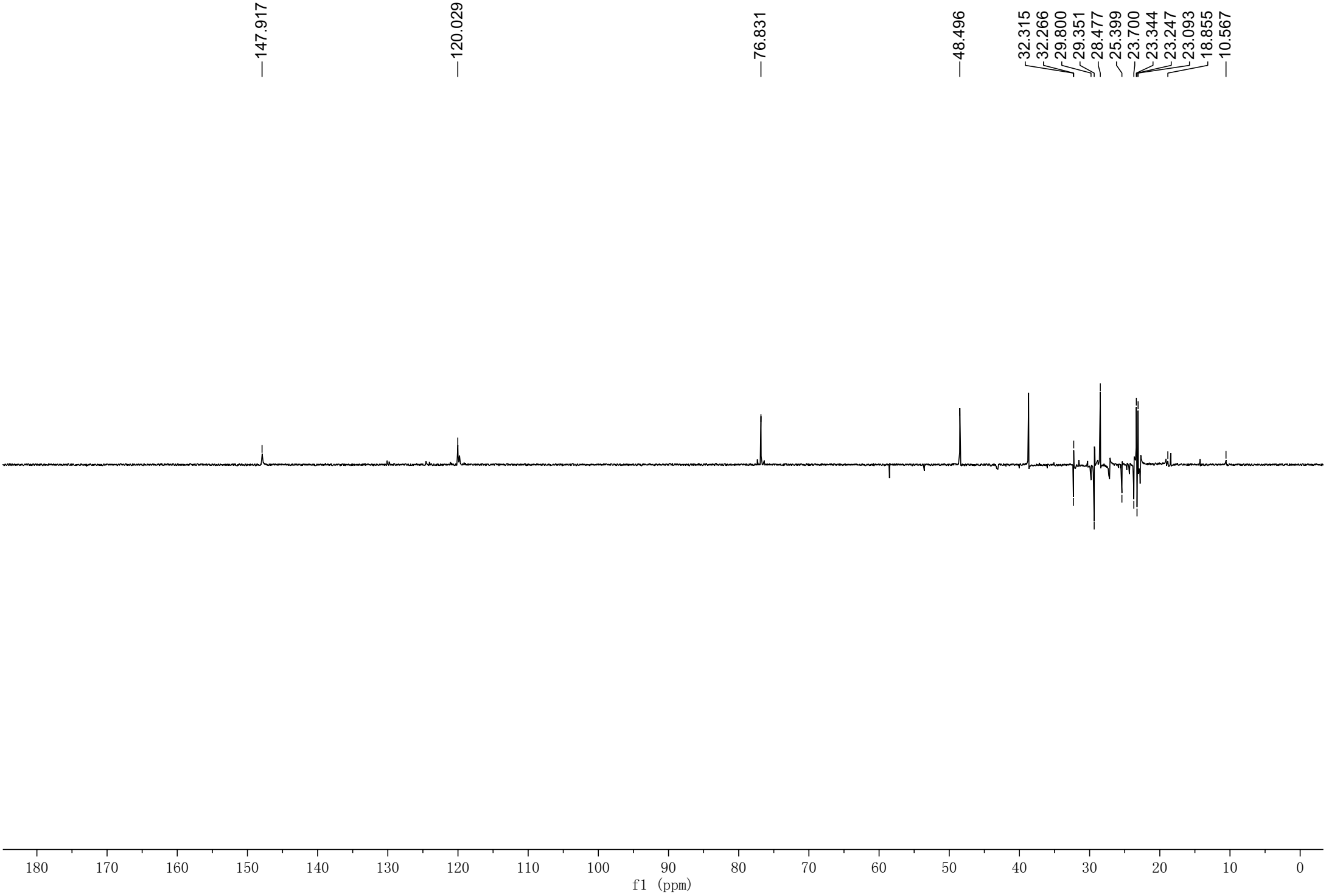

Figure S4. HSQC spectrum of compound 1 in $CDCl_3$.

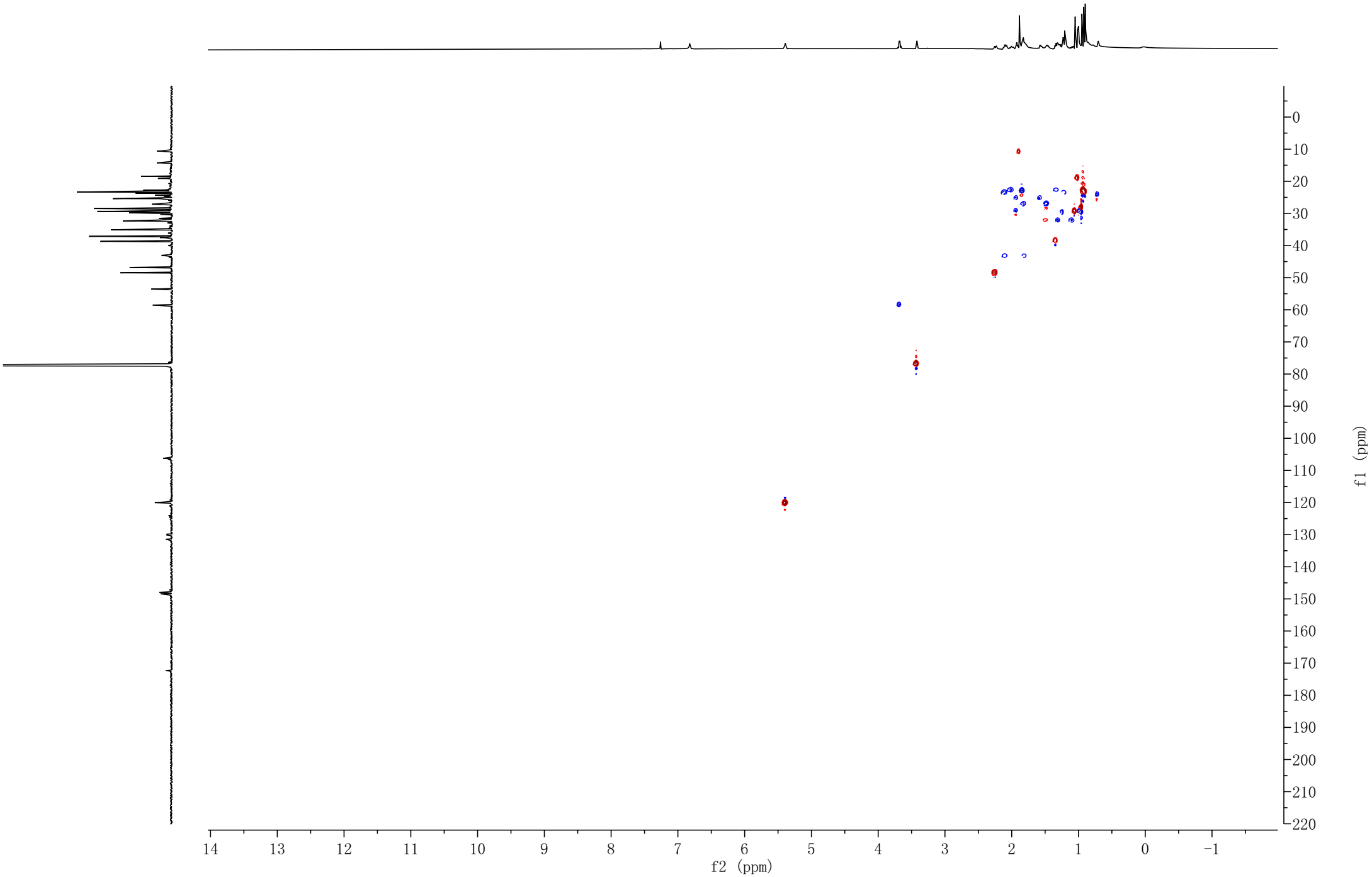

Figure S5. HSQC expansion spectrum of compound 1 in $CDCl_3$.

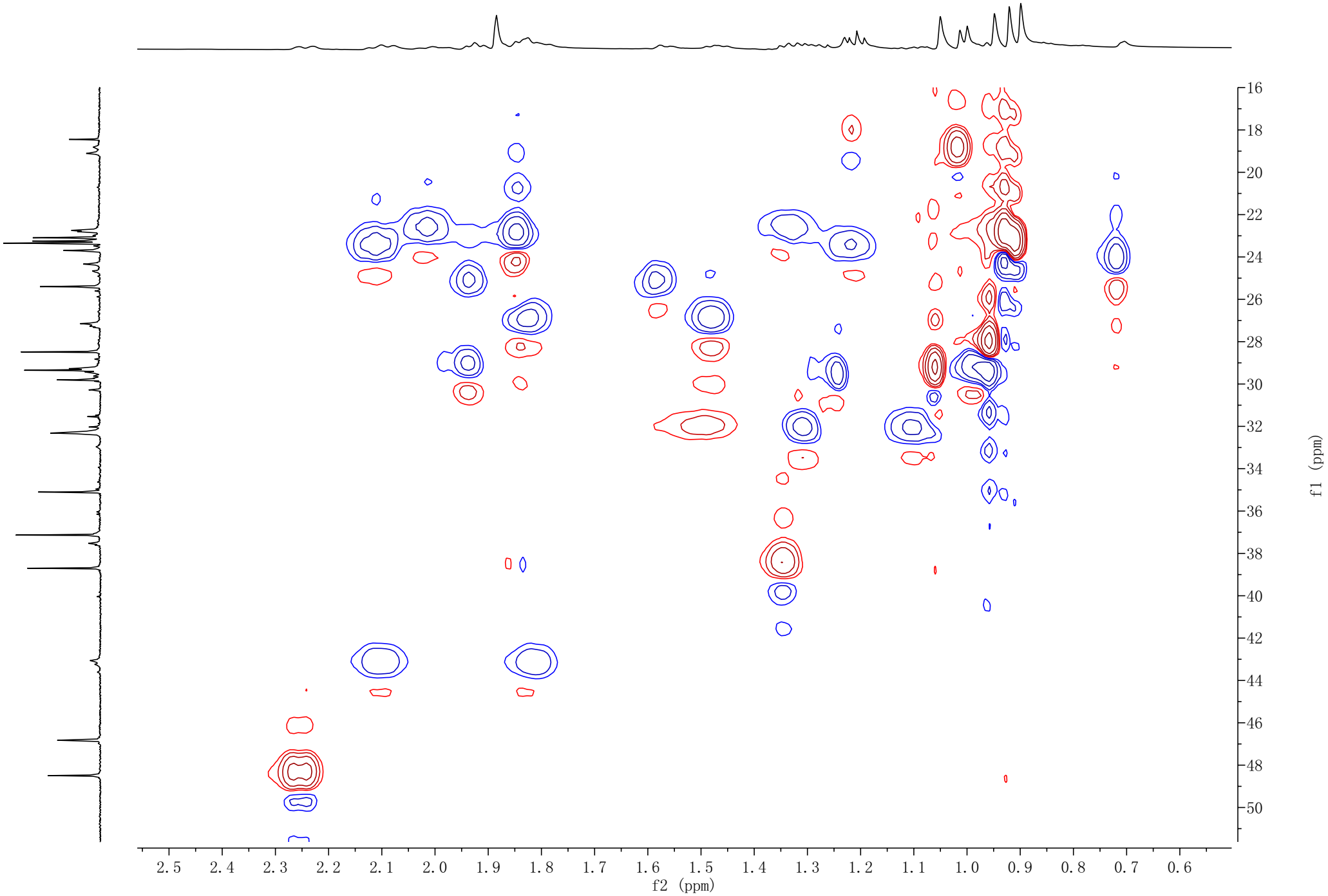

Figure S6. HMBC spectrum of compound 1 in $CDCl_3$.

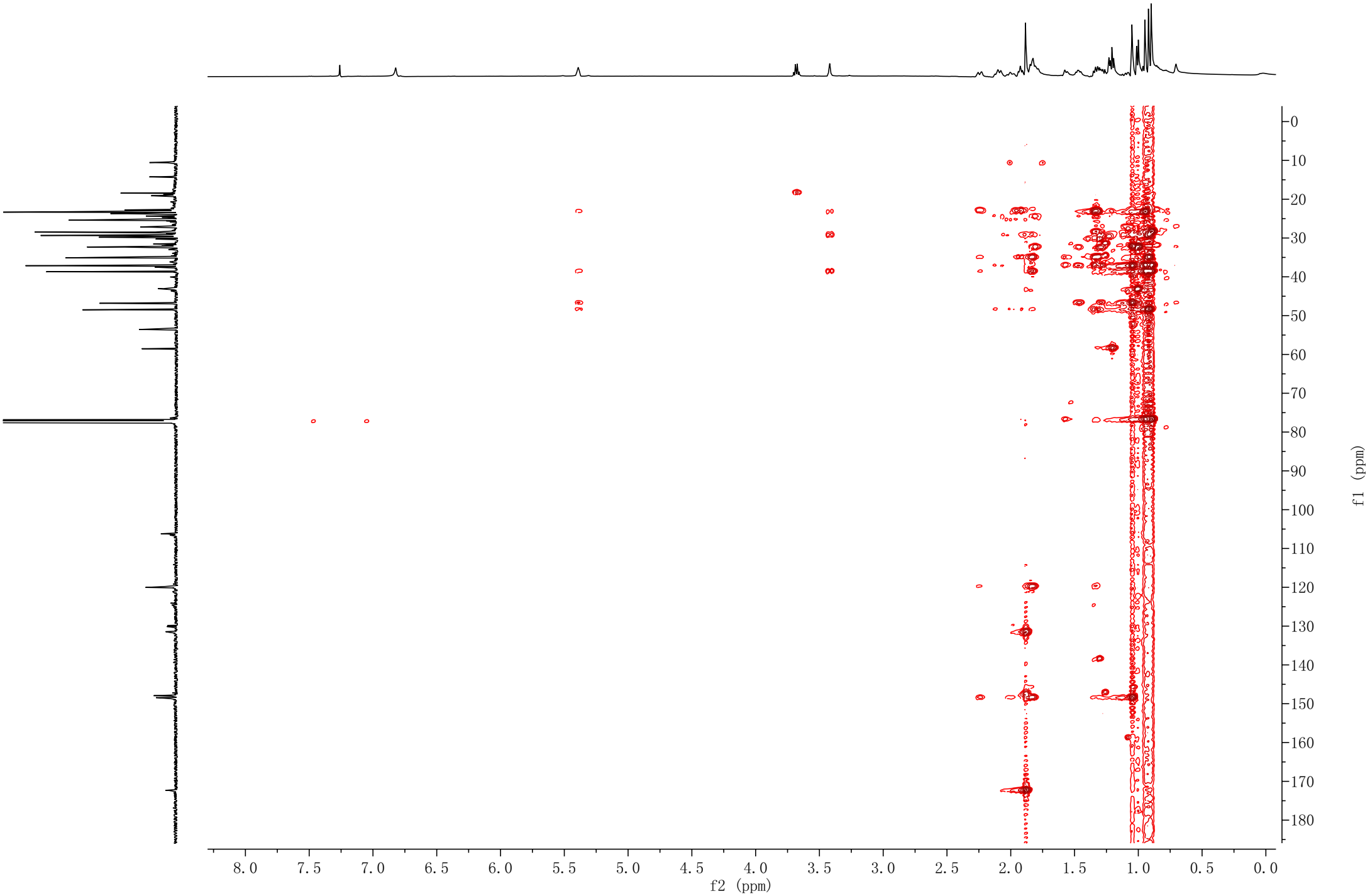

Figure S7. HMBC expansion spectrum of compound 1 in $CDCl_3$.

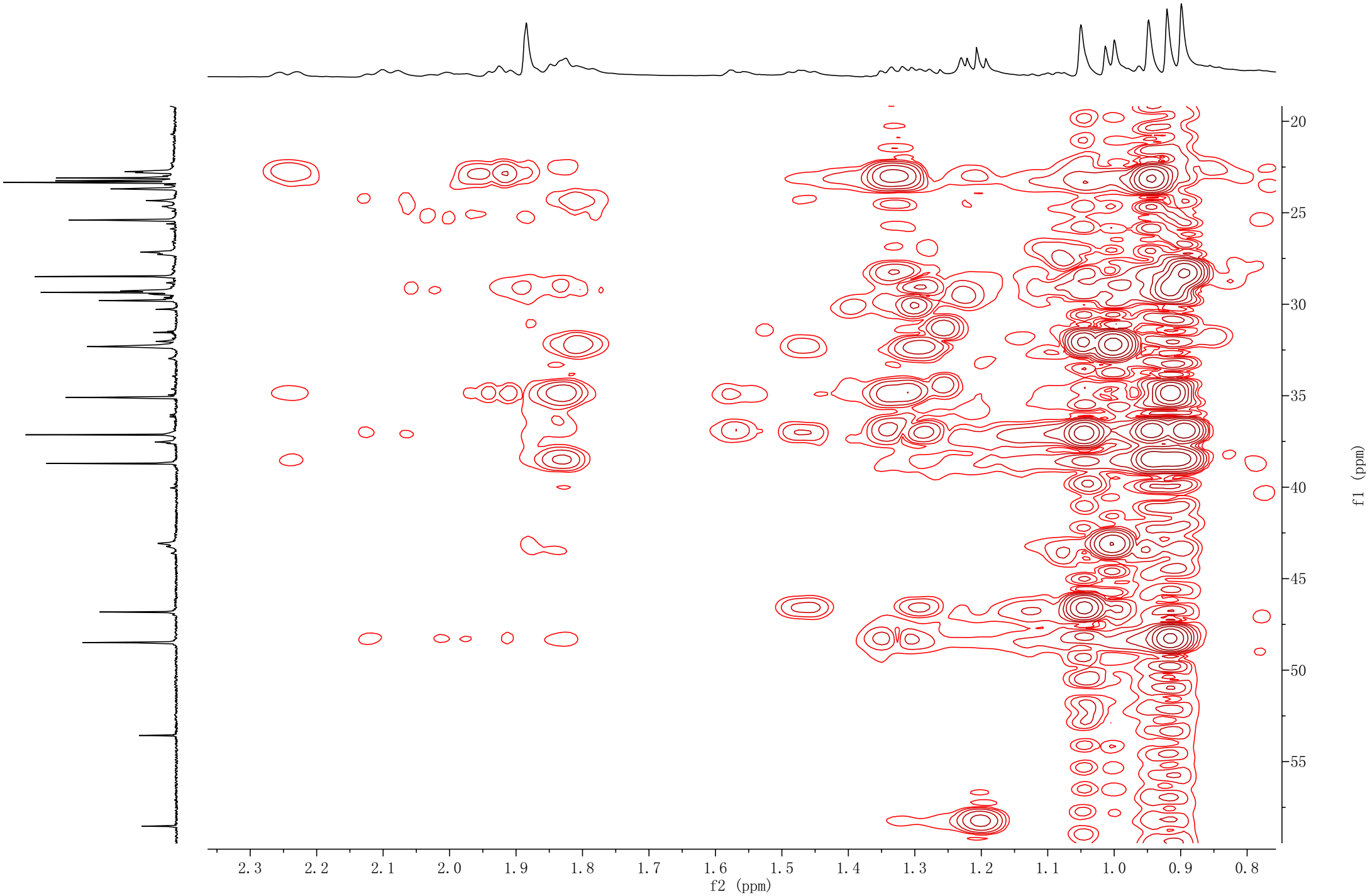

Figure S8. ^{1}H-^{1}H COSY spectrum of compound 1 in $CDCl_3$.

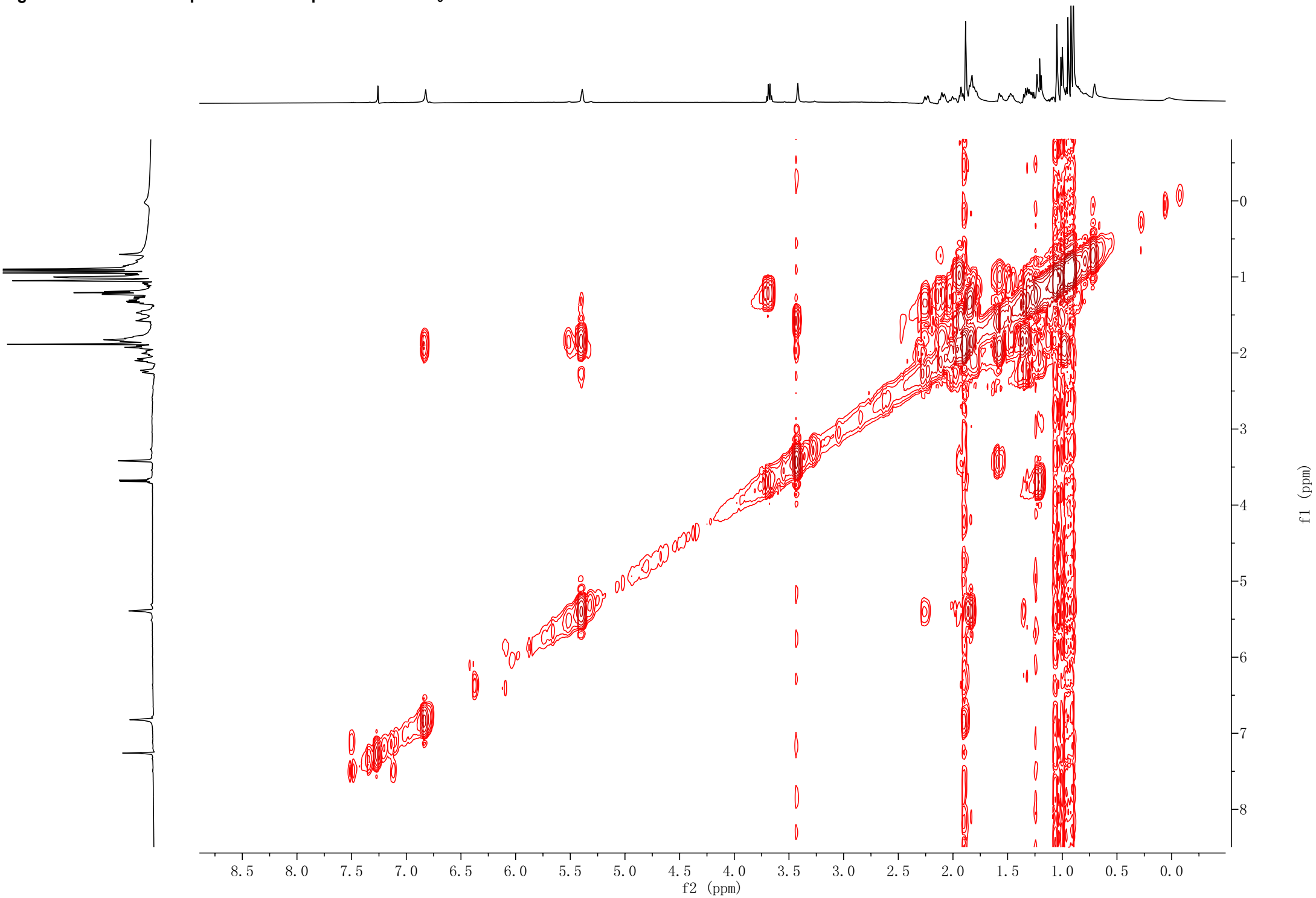

Figure S9. ^{1}H-^{1}H COSY expansion spectrum of compound 1 in $CDCl_3$.

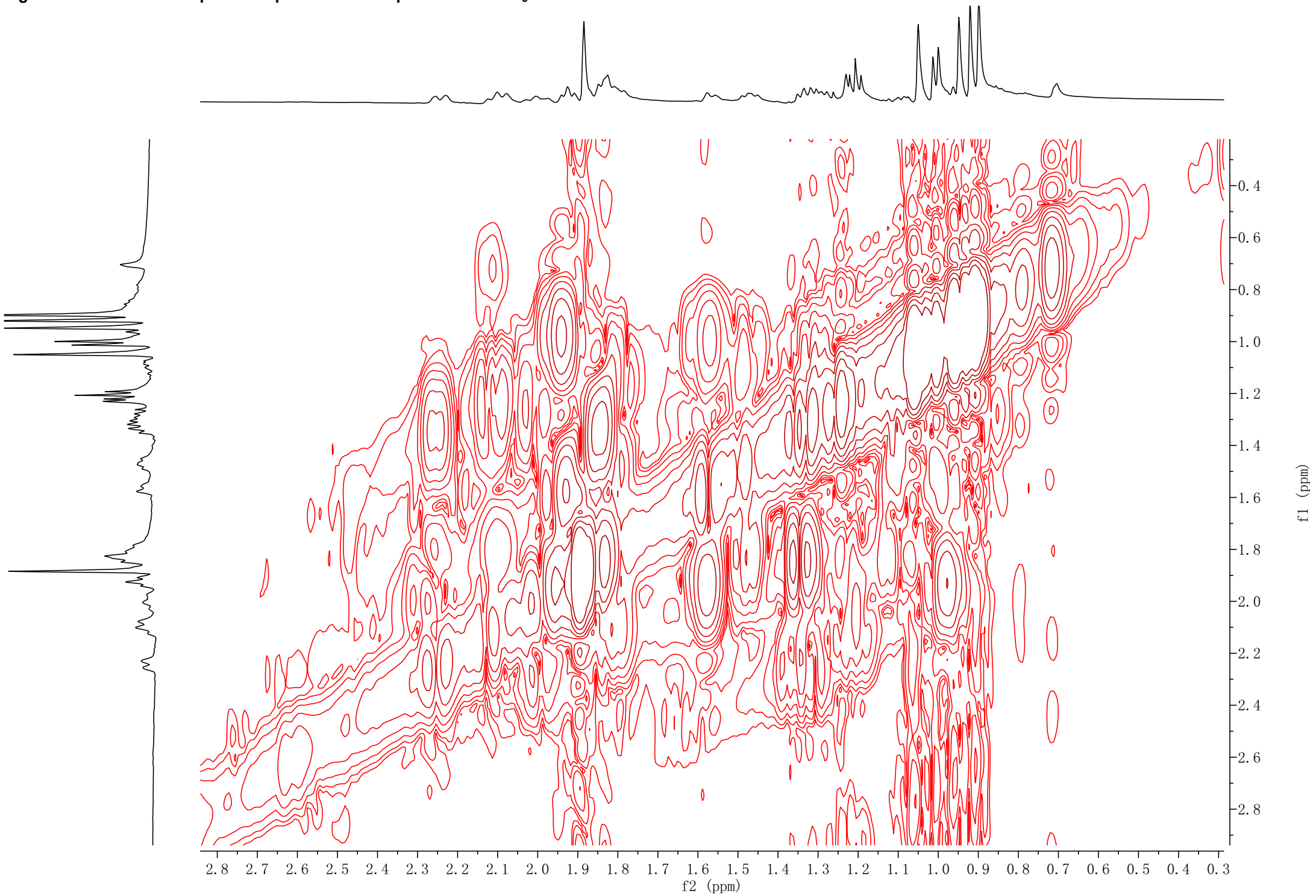

Figure S10. NOESY spectrum of compound 1 in $CDCl_3$

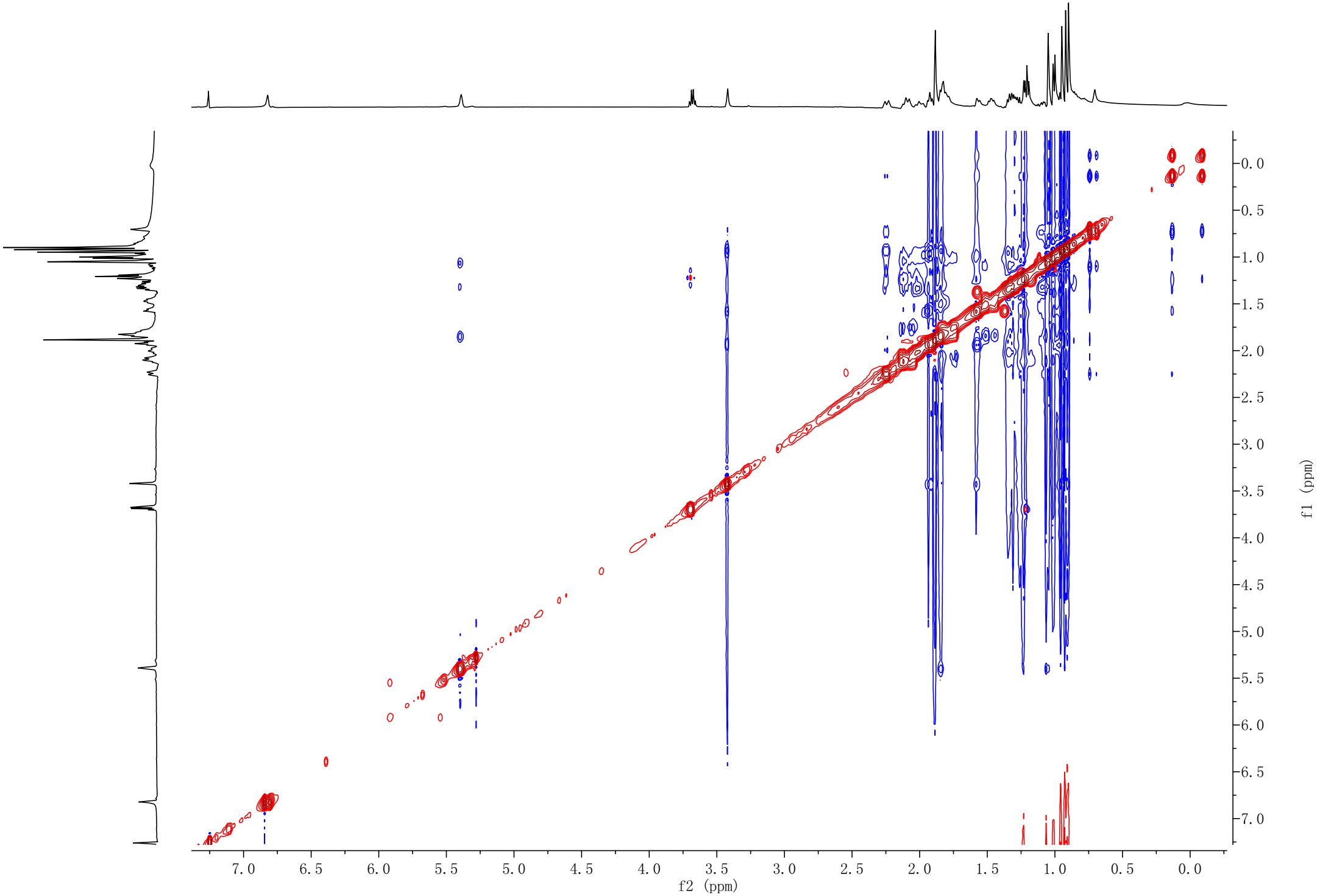

Figure S11. NOESY expansion spectrum of compound 1 in $CDCl_3$