Supporting Information

Rec. Nat. Prod. **14:4 (2020) 286-291**

Cytotoxic Lathyrane Diterpenoids from the Roots of *Euphorbia fischeriana*

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Table of Contents	Page

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1. General Experimental Procedures

Optical rotations were measured on a Perkin-Elmer 341 polarimeter. UV spectra were recorded on a Shimadzu UV-2450 spectrophotometer. IR spectra were determined on a Bruker Tensor 37 infrared spectrophotometer with KBr disks. NMR spectra were measured on a Bruker AM-400 spectrometer at 25 °C. HRESIMS data were carried out on a Finnigan LCQ Deca instrument. A Shimadzu LC-20AT equipped with an SPD-M20A PDA detector was used for HPLC, and a YMC-pack ODS-A column (250 × 10 mm, S-5 μm, 12 nm) was used for semipreparative HPLC separation. Silica gel (300−400 mesh, Qingdao Haiyang Chemical Co. Ltd.), reversed-phase C_{18} (Rp-C_{18}) silica gel (12 nm, S-50 μm, YMC Co. Ltd.), Sephadex LH-20 gel (Amersham Biosciences), and MCI gel (CHP20P, 75−150 μm, Mitsubishi Chemical Industries Ltd.) were used for column chromatography (CC). All solvents were of analytical grade (Guangzhou Chemical Reagents Company, Ltd.). V/FITC and Cell cycle were purchased from Keygen Biotech, China. MTT was purchased from Sigma, USA.

2. Plant Material

The roots of *Euphorbia fischeriana* Steud. were collected in November 2018 from Benxi city, Liaoning province, P. R. China and identified by Prof. You-Kai Xu of Xishuangbanna Tropical Botanical Garden, Chinese Academy of Sciences, and a voucher specimen (accession number: LD201812) was deposited at the Second People's Hospital of Yunnan Province

3. Extraction and Isolation

The air-dried powder of the roots of *E. fischeriana* (5 kg) was extracted by 95% EtOH (3 × 5 L) at room temperature to give 500 g of crude extract, which was suspended in H_2O (3 L) and partitioned with EtOAc (3 × 3 L). The EtOAc fraction (200 g) was subjected to silica gel CC eluted with a CH_2Cl_2/MeOH gradient (10:0 → 10:1) to obtain three fractions (I–VI). Fr. III (20 g) was subjected to MCI gel CC eluted with a MeOH/H_2O gradient (60:40 → 100:0) to give three fractions (IIIa–IIIc). Fr. IIIc was separated by silica gel CC eluted with a CH_2Cl_2/MeOH gradient (200:1 → 50:1) to give two subfractions (IIIc1 and IIIc2). Fr. IIIc1 was purified by sephadex LH-20 to obtain **5** (100 mg). Fr. IIIc2 was purified by semi-preparative HPLC (MeCN/H_2O, 70:30, 3 mL/min) to obtain **1** (10 mg, t_R = 12.5 min), **3** (16 mg, t_R = 14 min), and **2** (7 mg, t_R = 15 min). Fr. IV was subjected to silica gel CC eluted with CH_2Cl_2/MeOH (50:1) to give two fractions (IVa and IVb). Fr. IVa was purified by CH_2Cl_2/MeOH (80:1) and followed by sephadex LH-20 and to obtain **4** (23 mg).

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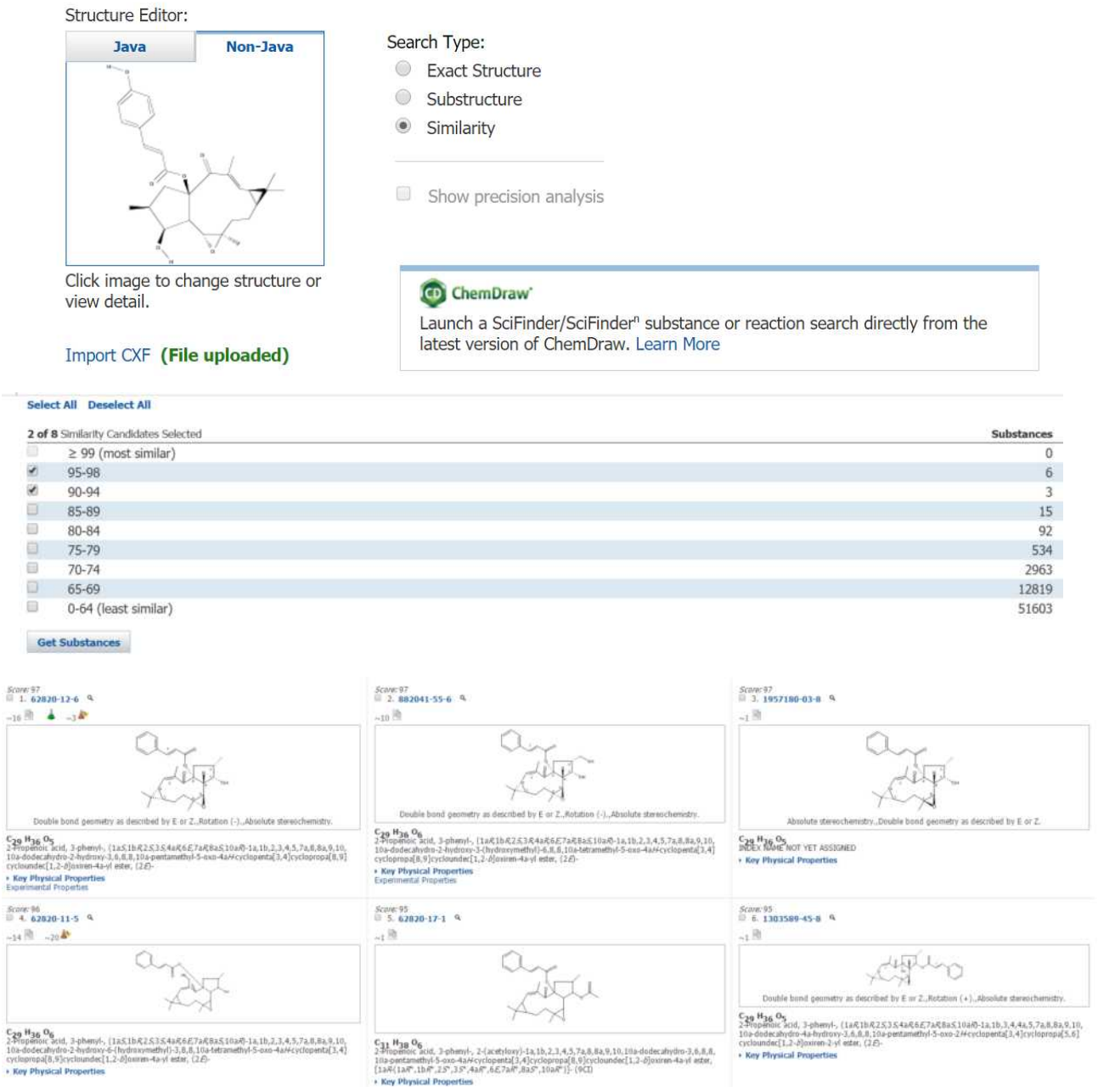

Figure S1: Scifinder search of new compound **1**

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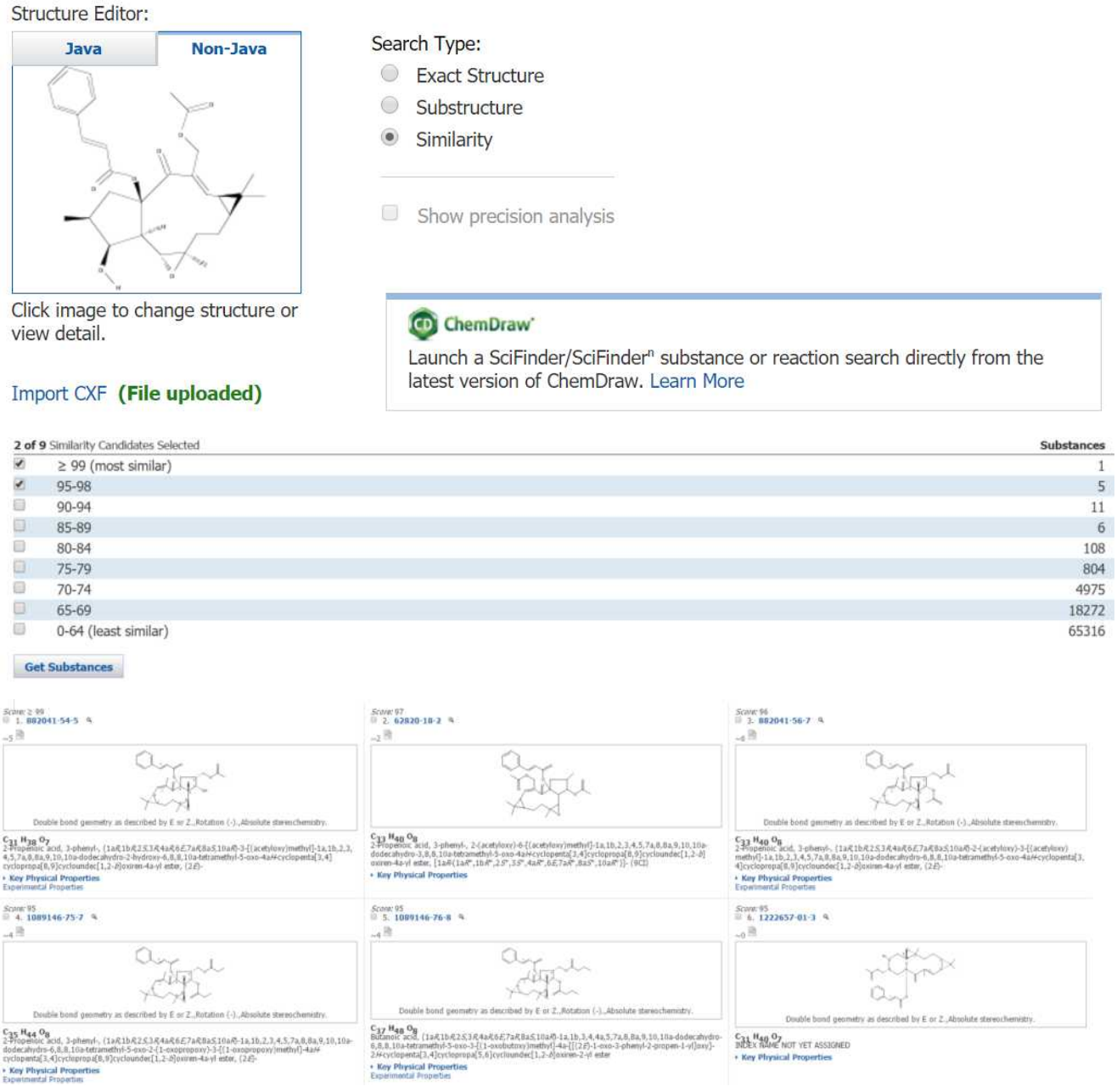

Figure S2: Scifinder search of new compound **2**

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Table S1. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for **1-5** (δ in ppm, J in Hz)

No.	**1**		**2**		**3**		**4**		**5**	
1α	3.53, dd (13.3, 7.6)	45.0	3.53, dd (13.4, 7.4)	44.3	3.53, dd (13.5, 7.4)	44.9	3.31, dd (13.6, 8.4)	46.8	3.47, dd (13.5, 7.2)	44.6
1β			1.75, dd (13.4, 13.4)		1.73, dd (13.5, 13.5)		1.56, dd (13.6, 12.1)		1.76, dd (13.5, 13.5)	
2	2.02, m	38.5	2.02, m	38.4	2.01, m	38.5	1.91, m	38.4	1.99, m	38.6
3	4.15, dd (3.7, 3.7)	78.8	4.14, dd (3.6, 3.6)	78.5	4.13, dd (3.3, 3.3)	78.6	4.15, dd (3.2, 3.2)	79.7	4.13, dd (3.5, 3.5)	78.4
4	1.57, dd (9.4, 3.7)	52.1	1.63, m	51.6	1.57, dd (9.4, 3.3)	52.2	1.43, dd (9.6, 3.2)	53.1	1.61, dd (9.4, 3.5)	52.1
5	3.67, d (9.4)	58.5	3.64, d (9.3)	58.1	3.63, d (9.4)	58.2	3.44, d (9.6)	58.6	3.63, d (9.4)	58.1
6		64.5		63.6		63.9		63.8		63.9
7a	1.62, m	38.6	1.63, m	38.5	1.62, m	38.7	1.60, m	38.9	1.58, m	38.6
7b	2.05, m		2.05, m		2.06, m		2.03, m		2.03, m	
8α	2.01, m	23.2	2.10, m	23.3	2.07, m	23.3	2.06, m	23.1	2.07, m	23.3
8β	1.51, m		1.56, m		1.52, m		1.64, m		1.60, m	
9	1.12, m	33.8	1.27, m	35.2	1.14, m	33.8	1.27, m	35.8	1.24, m	34.8
10		26.3		28.0		26.3		27.9		27.5
11	1.47, dd (11.0, 7.8)	29.7	1.67, dd (10.8, 7.8)	29.8	1.49, dd (11.0, 7.8)	29.7	1.71, dd (11.9, 7.9)	29.9	1.68, dd (11.3, 7.8)	29.5
12	6.97, d (11.0)	144.4	7.27, d (10.8)	150.7	6.99, d (11.0)	144.3	7.84, d (11.9)	152.5	7.10, d (11.3)	147.6
13		134.0		132.4		134.0		136.9		136.8
14		195.2		193.1		195.1		199.2		196.3
15		91.7		91.8		92.0		89.1		91.8
16	1.10, d (6.9)	13.2	1.10, d (6.7)	13.1	1.10, d (6.9)	13.2	1.11, d (6.9)	13.7	1.09, d (6.7)	13.2
17	1.18, s	20.0	1.24, s	20.0	1.19, s	20.0	1.22, s	20.3	1.26, s	20.2
18	1.09, s	29.0	1.12, s	29.0	1.11, s	29.0	1.21, s	29.0	1.10, s	28.9
19	0.81, s	16.1	0.87, s	16.2	0.85, s	16.2	1.12, s	16.2	0.84, s	16.1
20	1.86, s	12.4	a 4.92, d (11.5)	58.1	1.87, s	12.4	4.35, d (12.0)	58.4	4.30, d (12.3)	57.9
			b 4.98, d (11.5)				4.46, d (12.0)		4.49, d (12.3)	
1′		166.0		165.4		165.6				165.6
2′	6.21, d (15.8)	114.5	6.44, d (16.0)	117.1	6.44, d (16.0)	117.4			6.43, d (16.0)	117.2
3′	7.56, d (15.8)	146.2	7.69, d (16.0)	146.8	7.68, d (16.0)	146.5			7.67, d (16.0)	146.8
4′		126.5		133.8		133.9				133.9
5′/9′	7.30, d (8.5)	130.1	7.47, d (7.5)	128.2	7.47, m	128.1			7.46, m	128.1
6′/8′	6.82, d (8.5)	115.9	7.40, m	129.0	7.39, m	129.0			7.38, m	128.9
7′		158.5	7.40, m	130.8	7.39, m	130.7			7.38, m	130.8
20-OAc				170.9						
			1.98, s	20.9						

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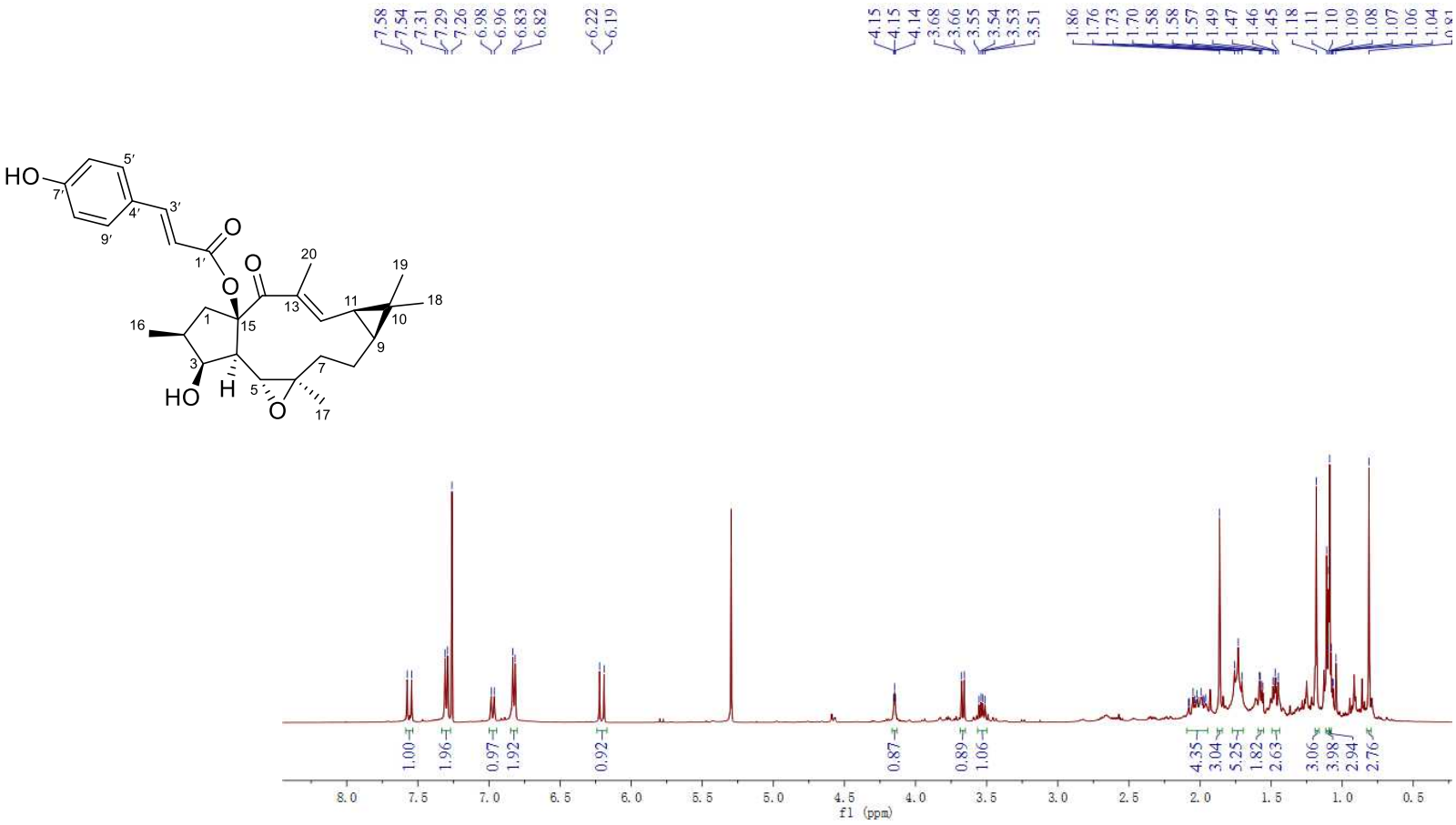

Figure S3: ^{1}H NMR spectrum of **1** in $CDCl_3$

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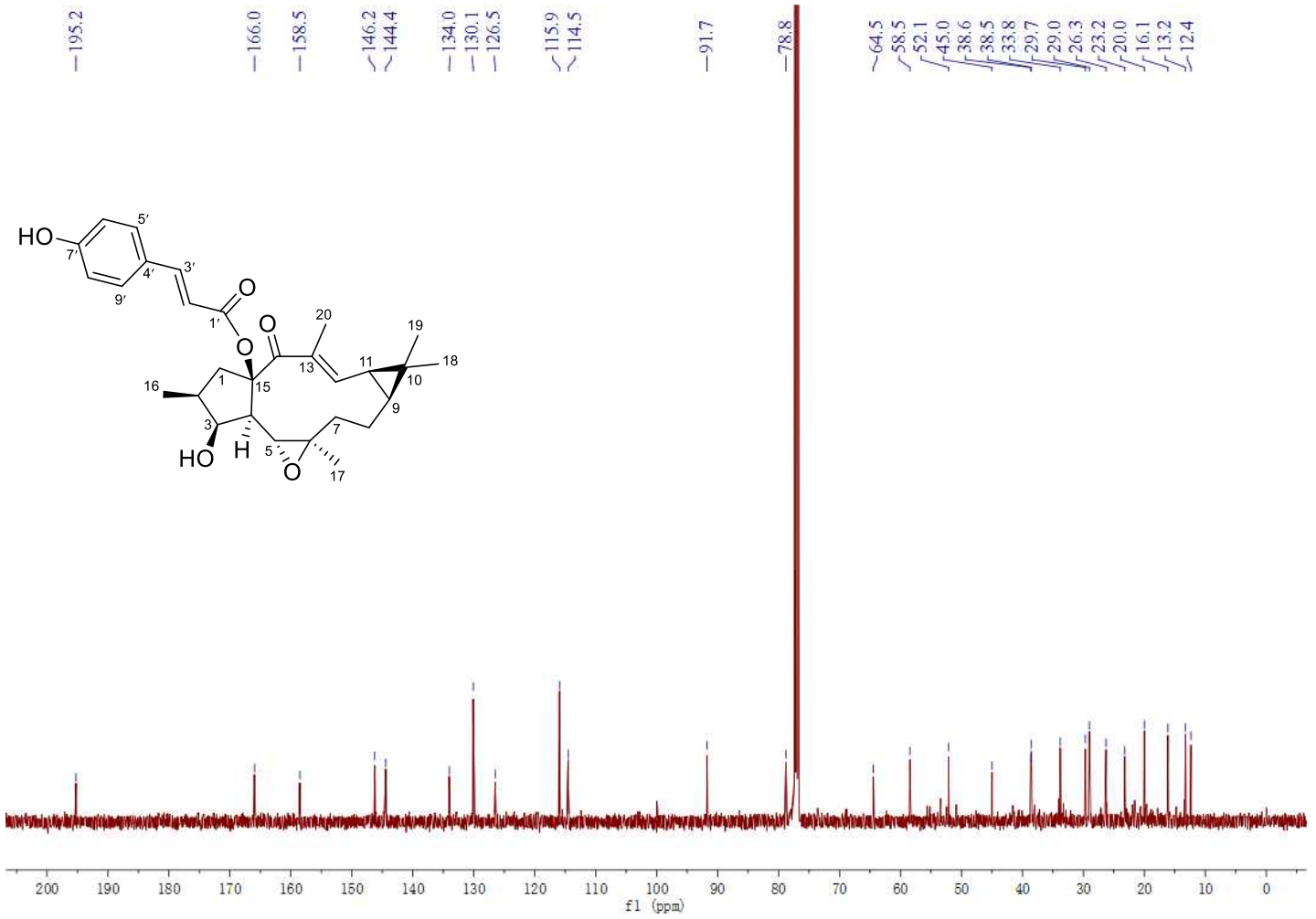

Figure S4: ^{13}C NMR spectrum of **1** in $CDCl_3$

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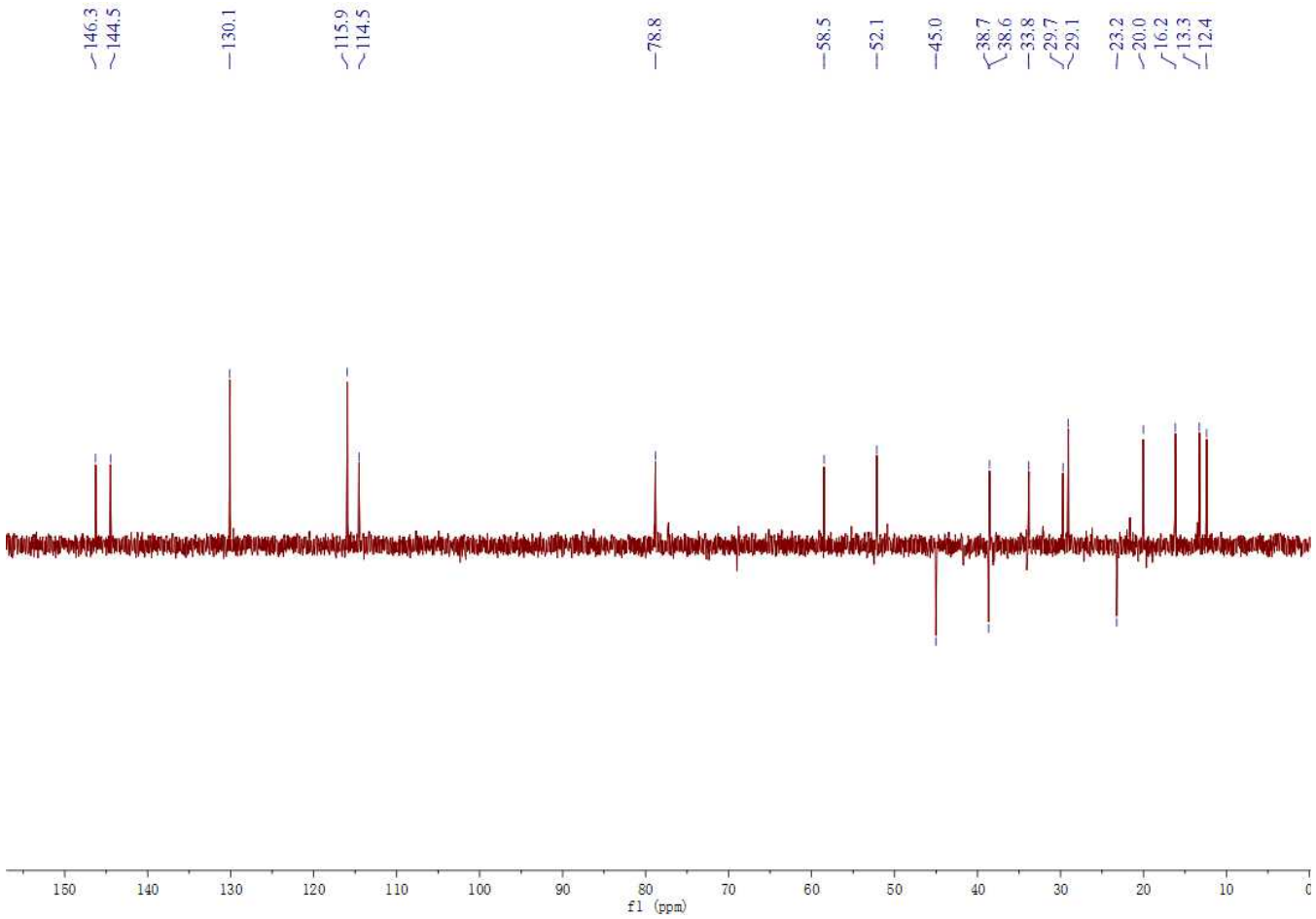

Figure S5: DEPT spectrum of **1** in $CDCl_3$

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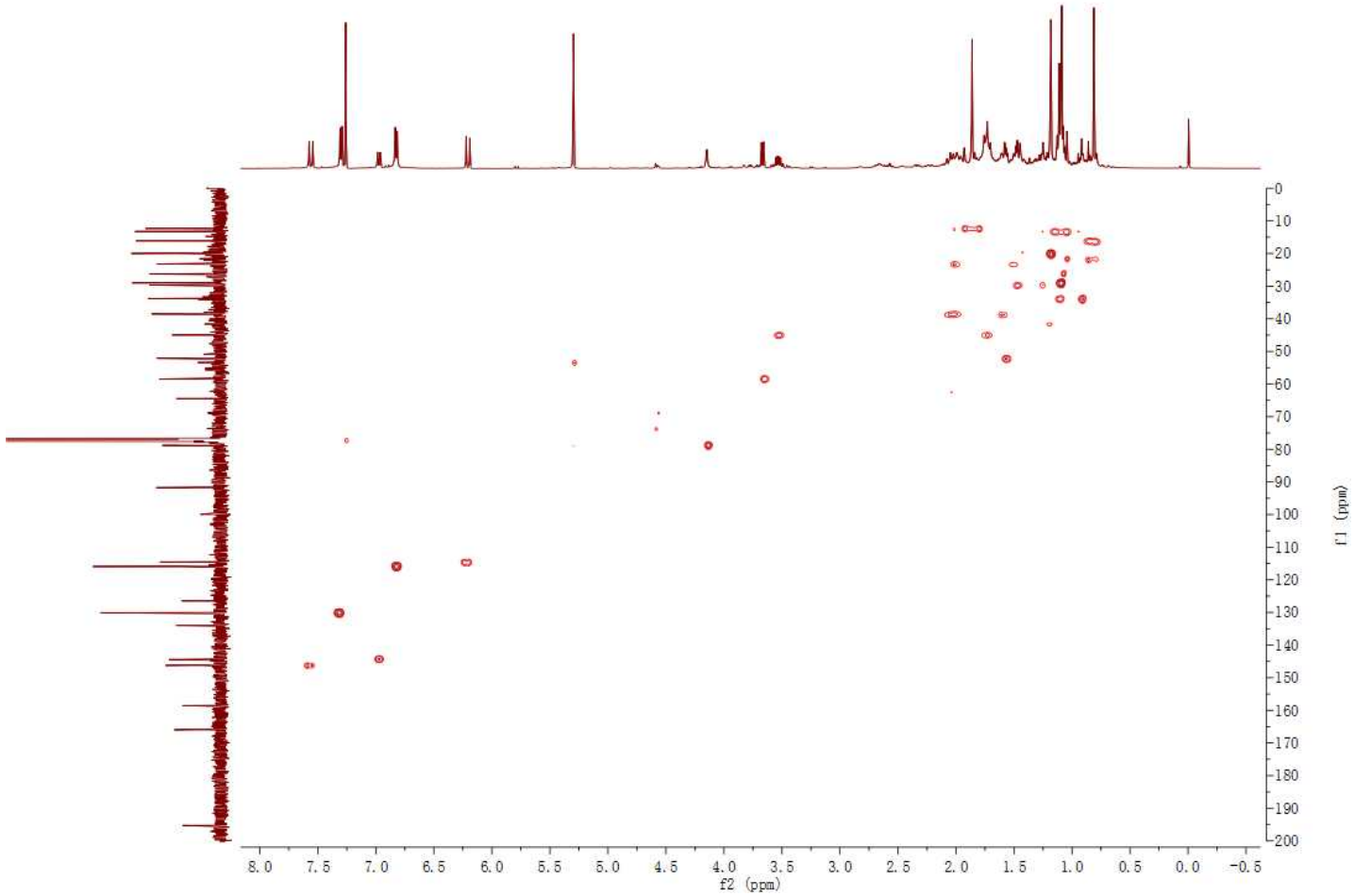

Figure S6: HSQC spectrum of **1** in $CDCl_3$

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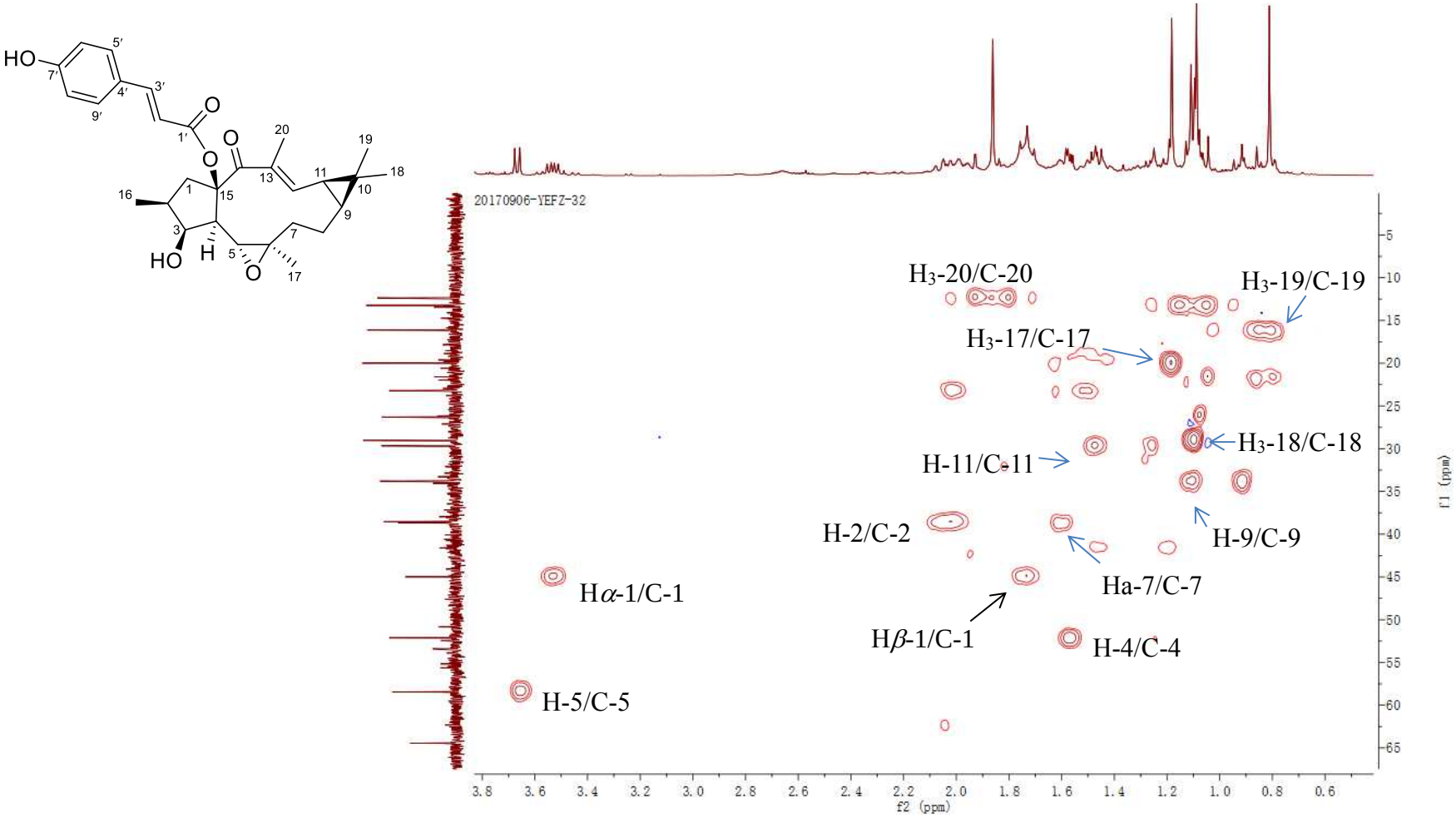

Figure S7: HSQC spectrum of **1** in $CDCl_3$ (δ_C 5–65 ppm)

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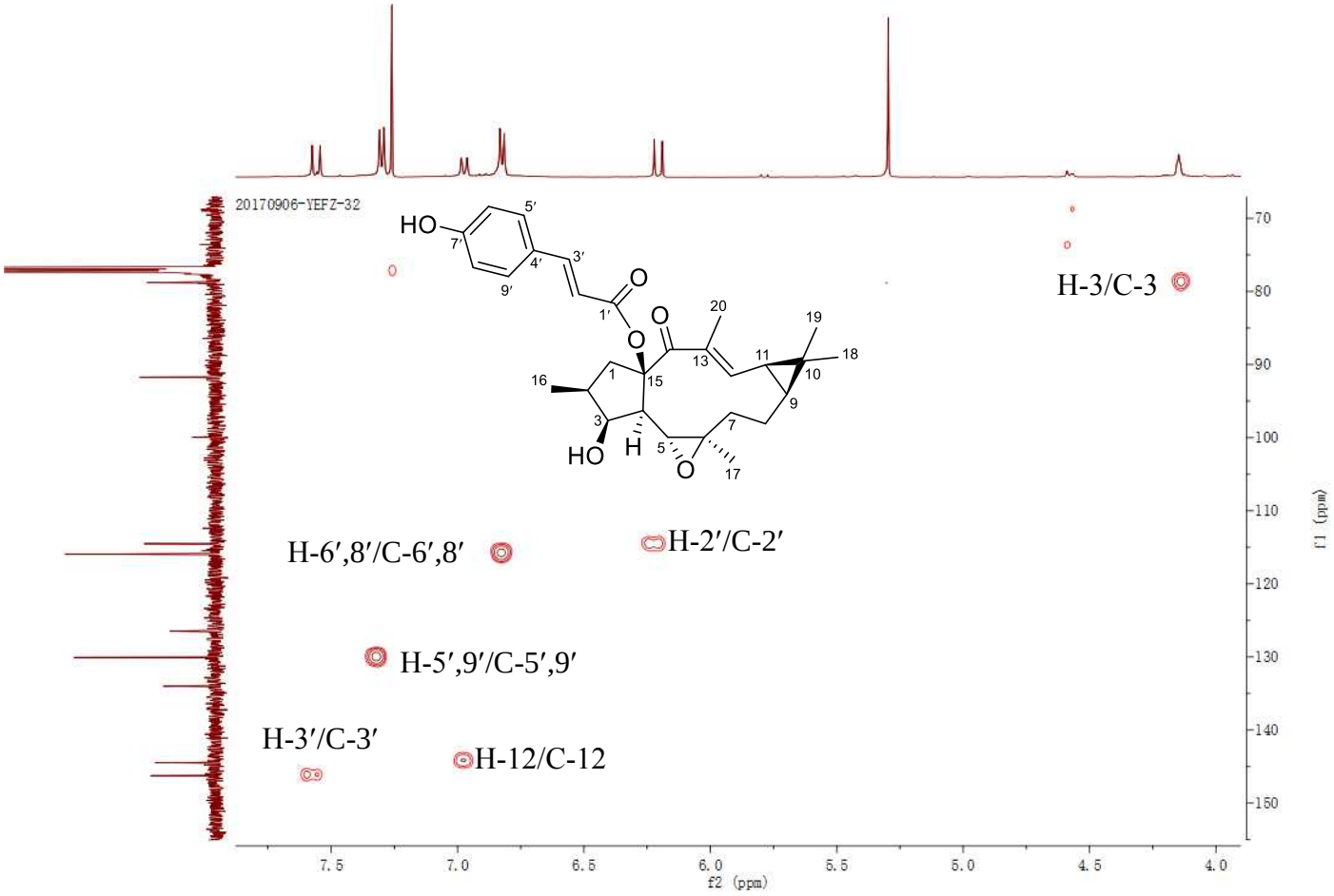

Figure S8: HSQC spectrum of **1** in $CDCl_3$ (δ_C 70–150 ppm)

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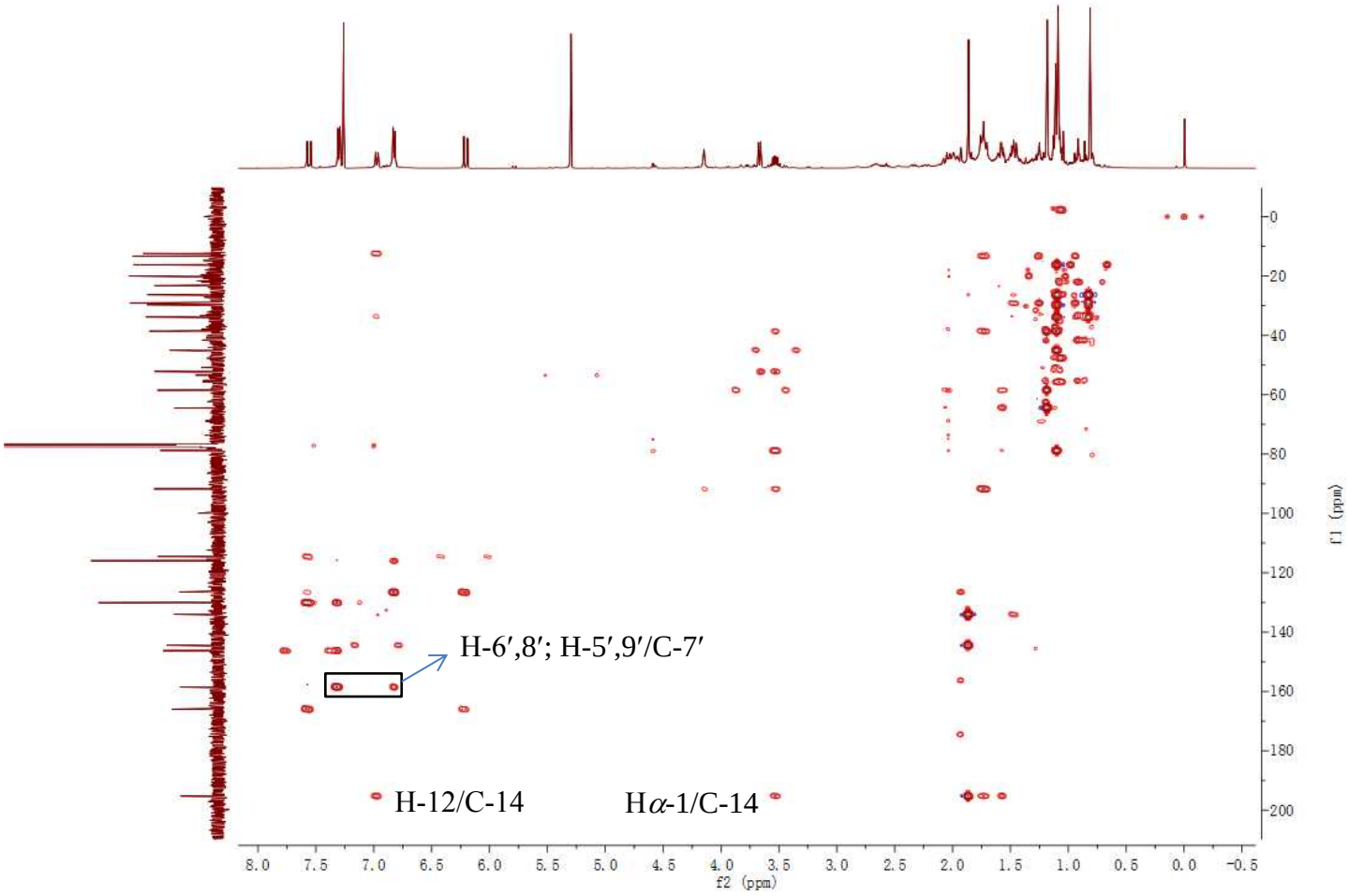

Figure S9: HMBC spectrum of **1** in $CDCl_3$

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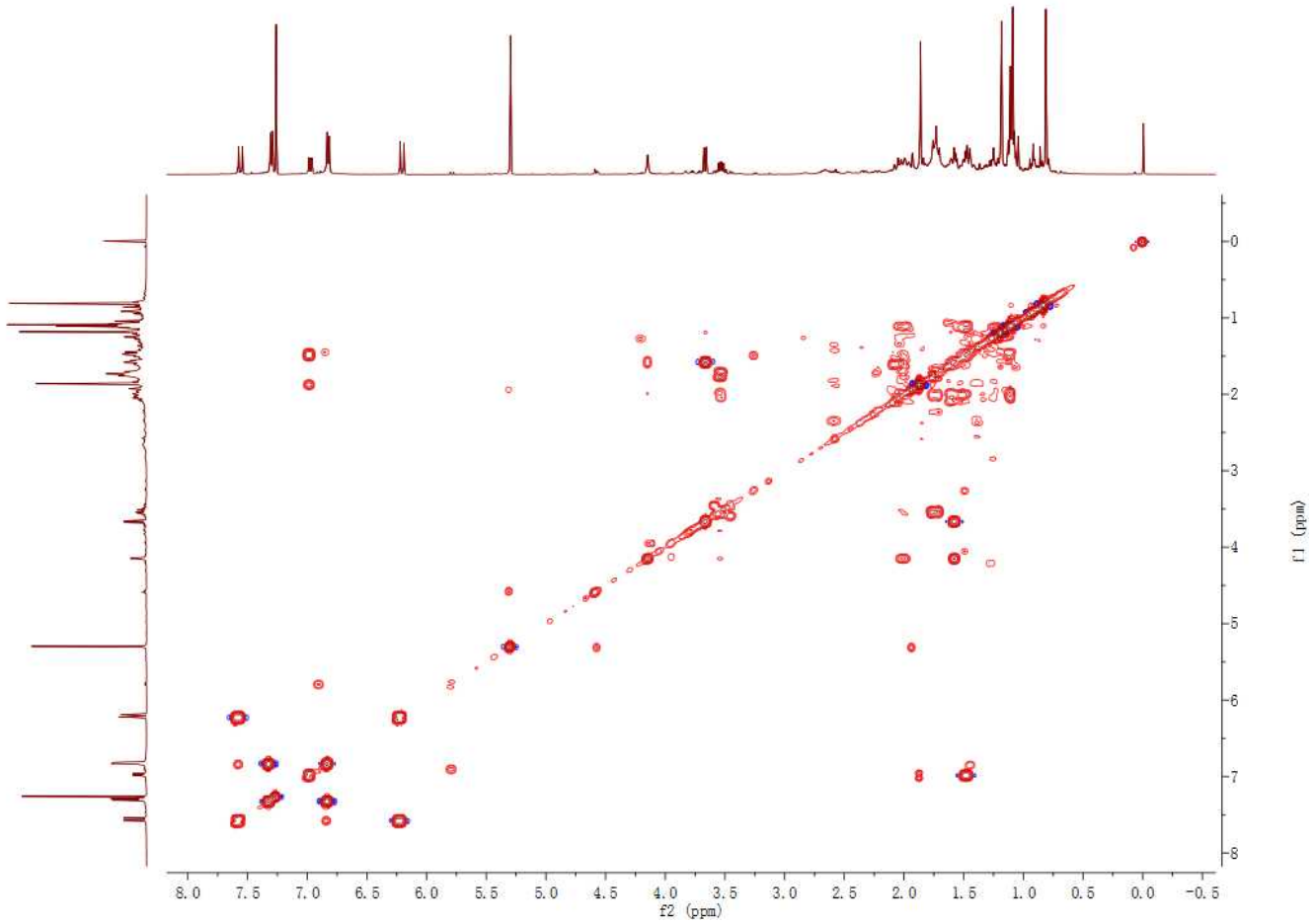

Figure S10: $^{1}H–^{1}H$ COSY spectrum of **1** in $CDCl_3$

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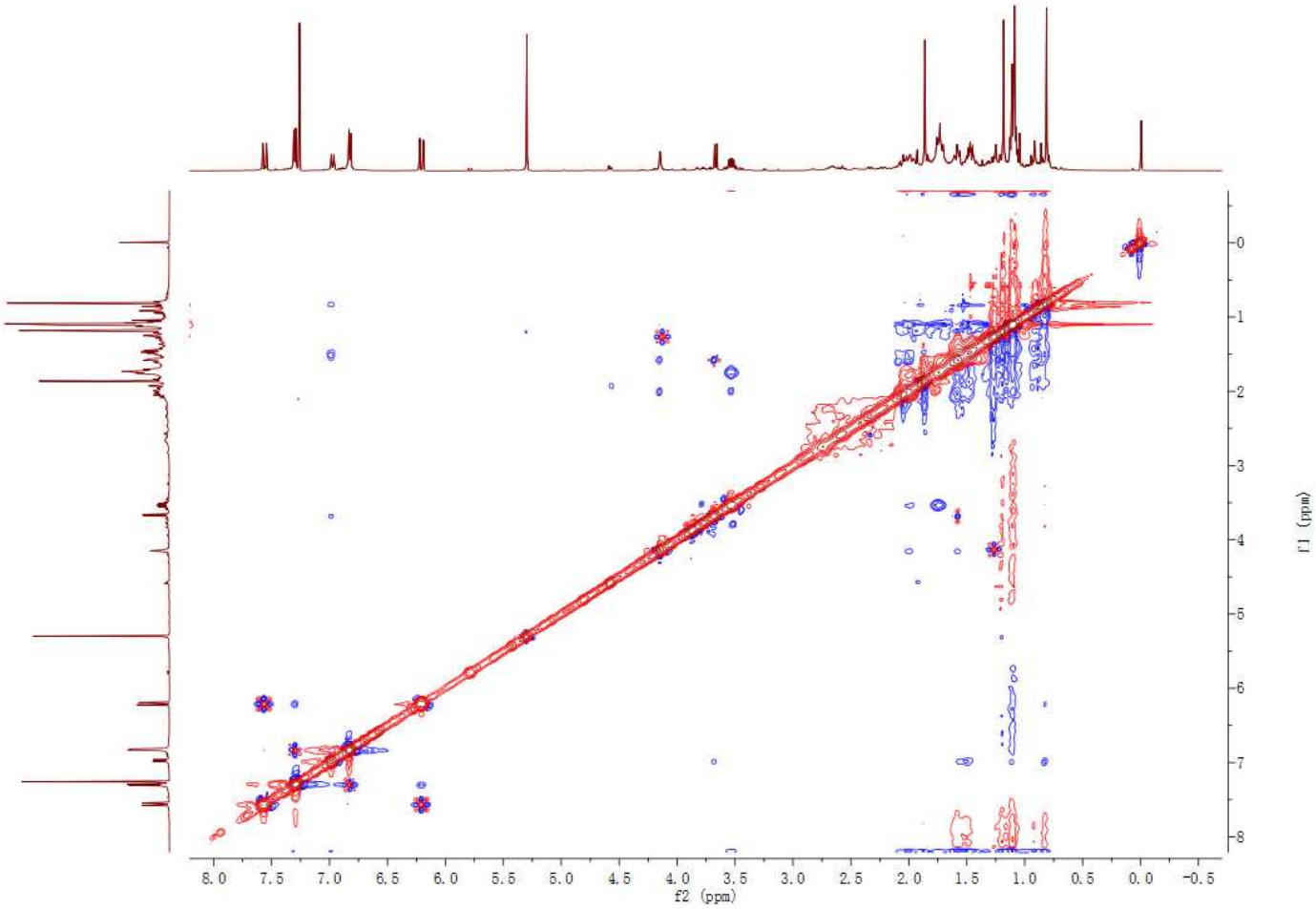

Figure S11: NOESY spectrum of **1** in $CDCl_3$

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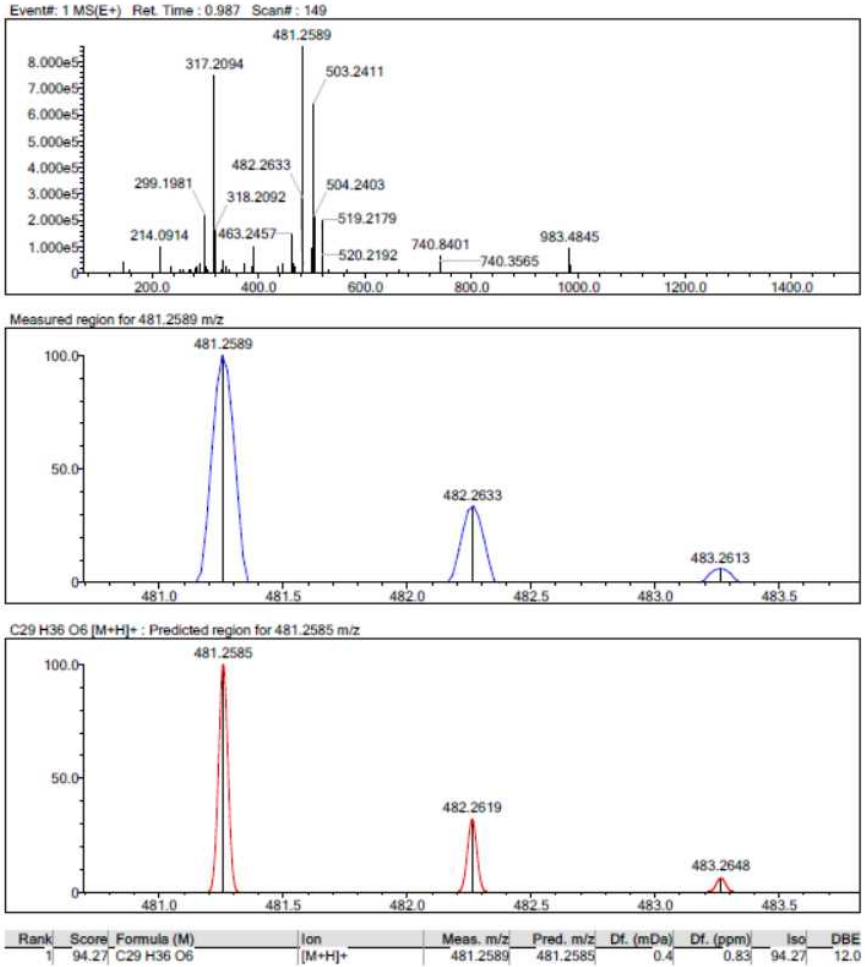

Figure S12: HRESIMS $[M + H]^+$ spectrum of **1**

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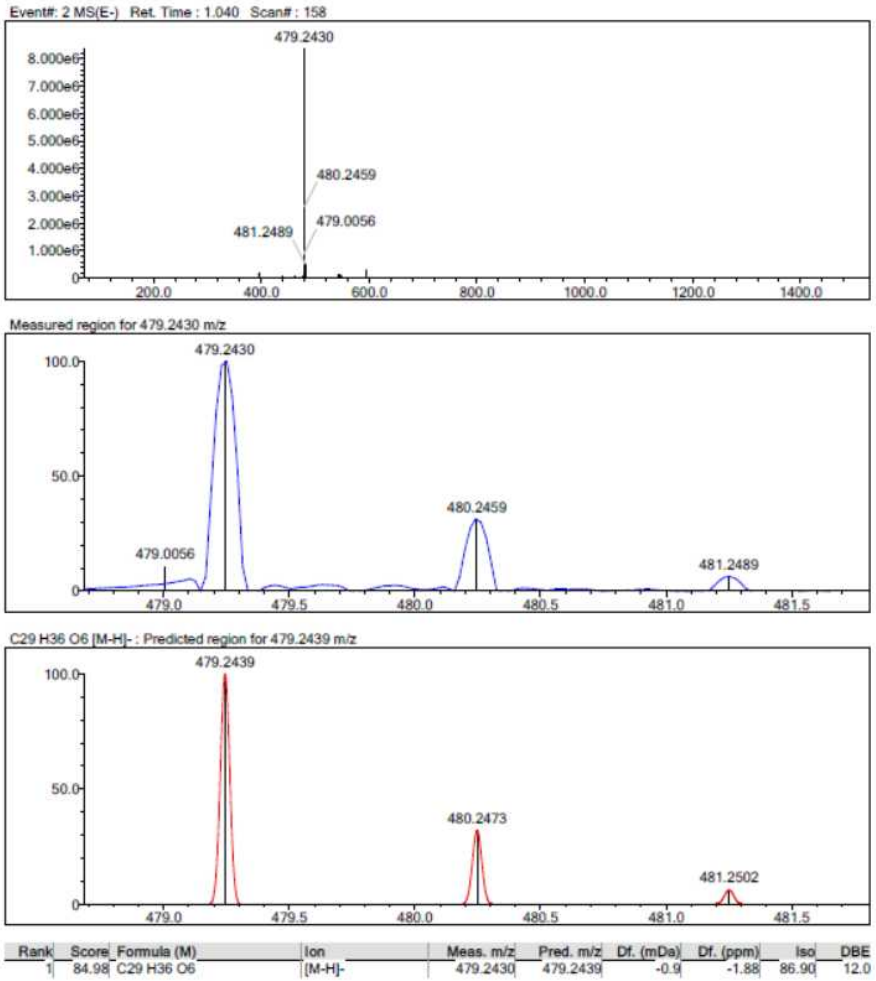

Figure S13: HRESIMS $[M - H]^-$ spectrum of **1**

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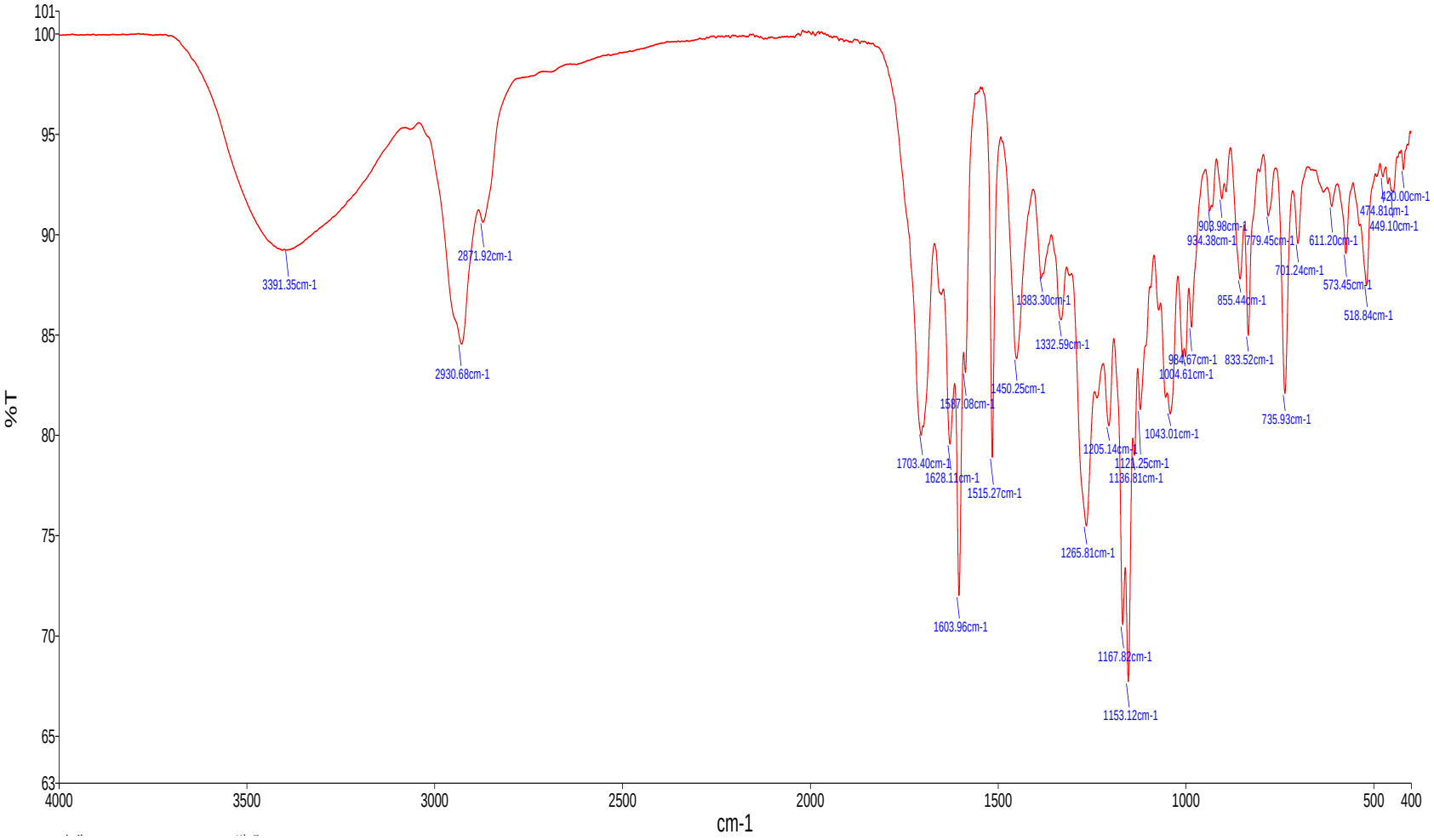

Figure S14: IR (KBr disc) spectrum of **1**

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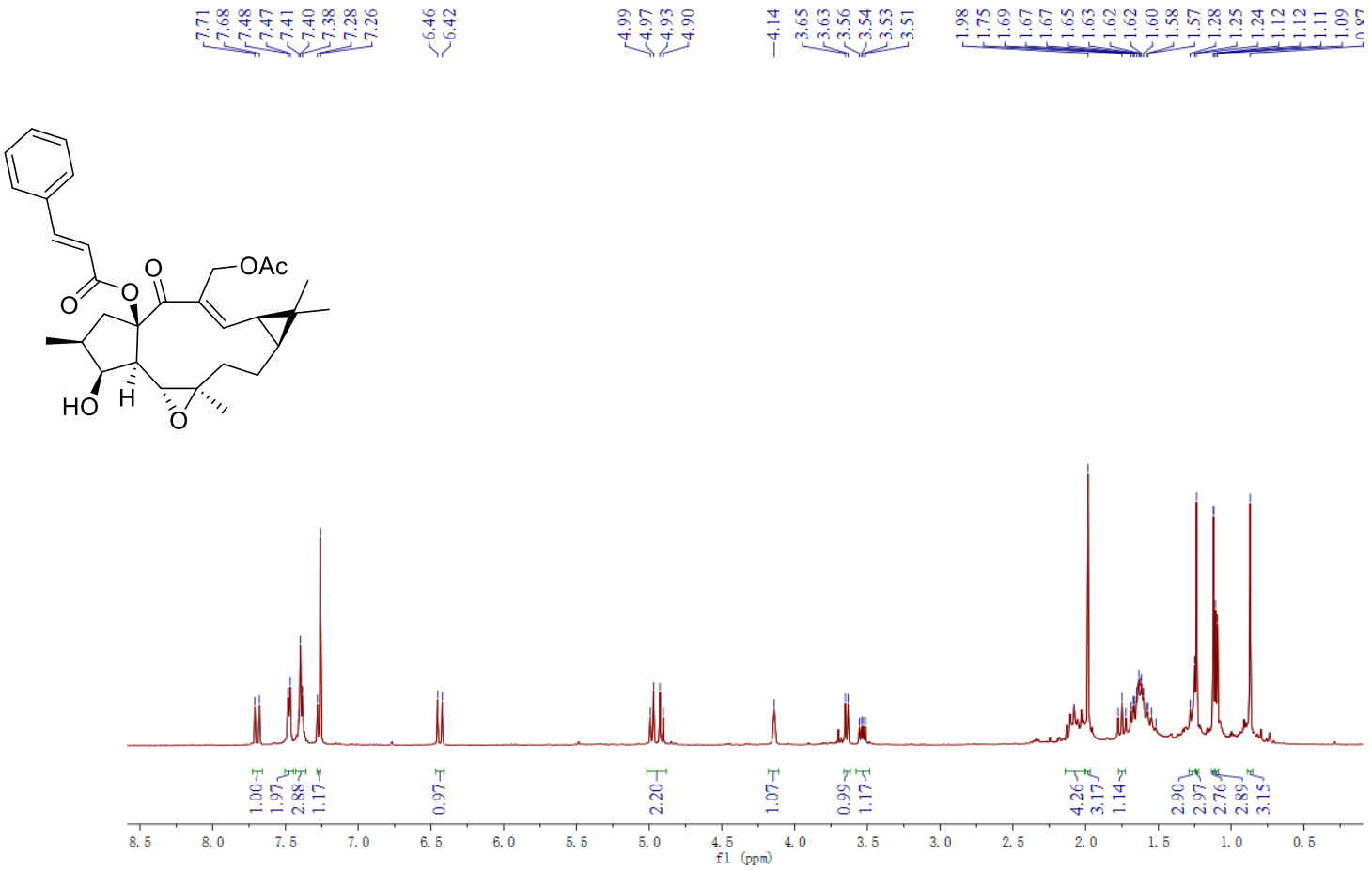

Figure S15: ^{1}H NMR spectrum of **2** in $CDCl_3$

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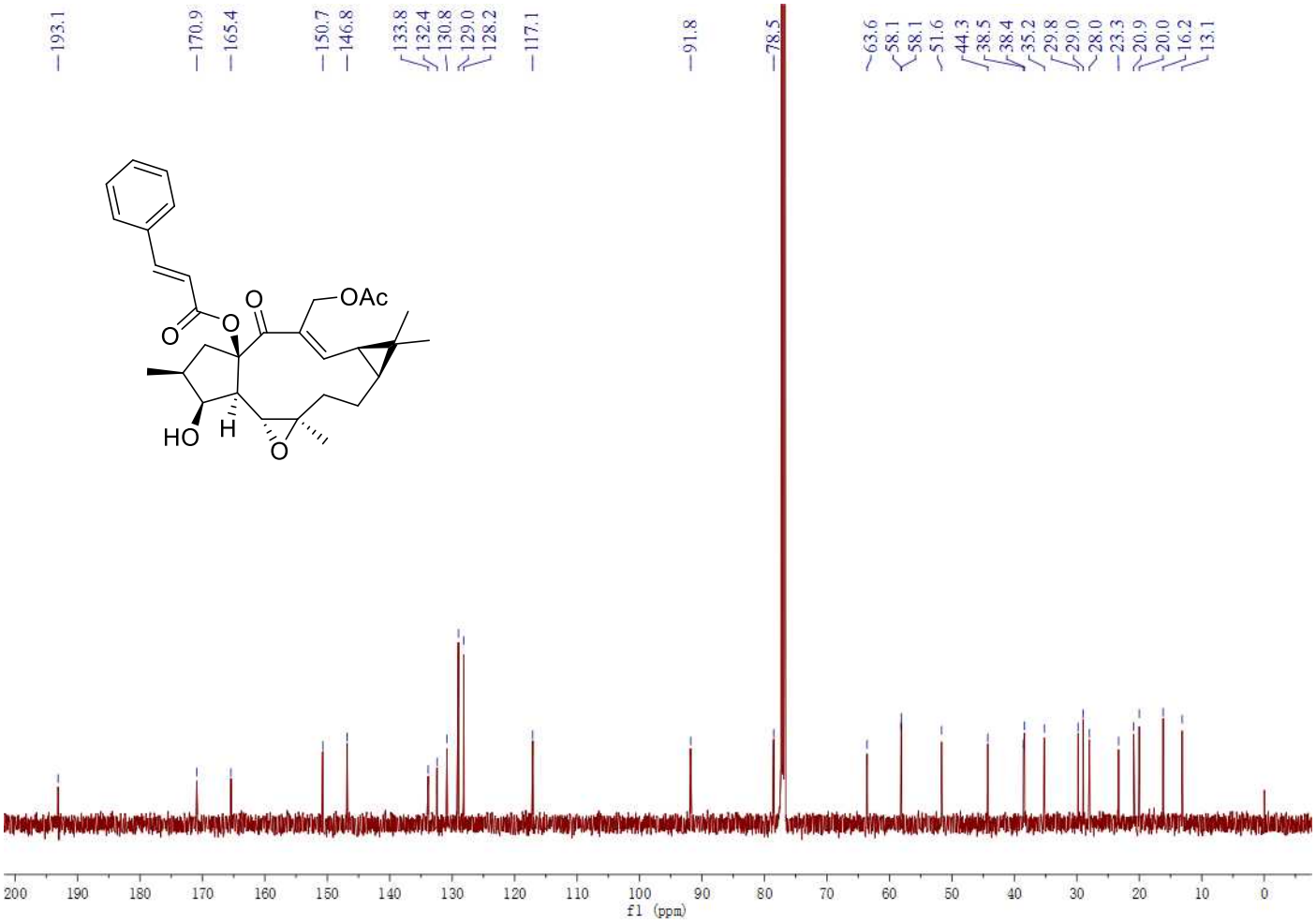

Figure S16: ^{13}C NMR spectrum of **2** in $CDCl_3$

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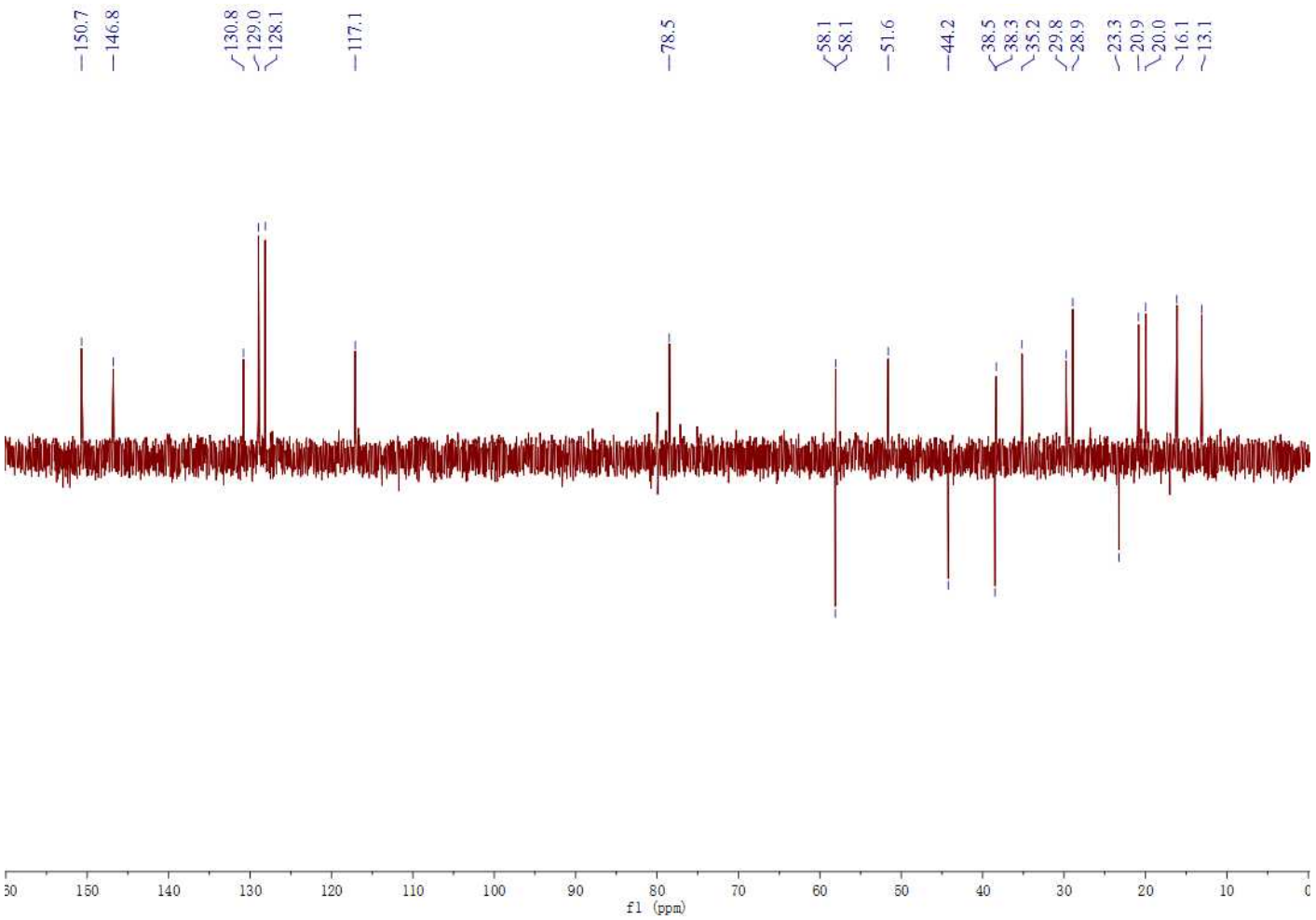

Figure S17: DEPT spectrum of **2** in $CDCl_3$

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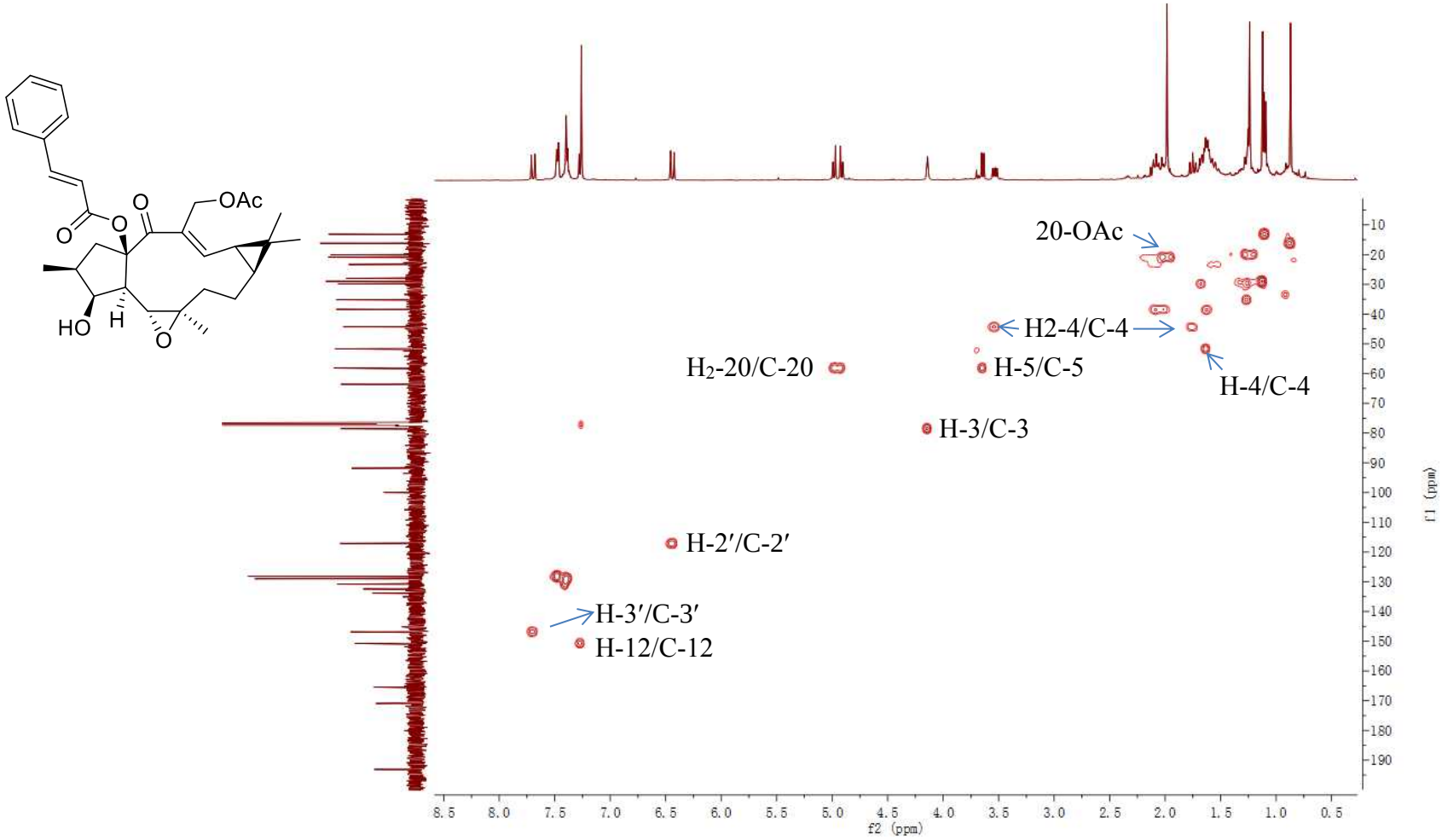

Figure S18: HSQC spectrum of **2** in $CDCl_3$

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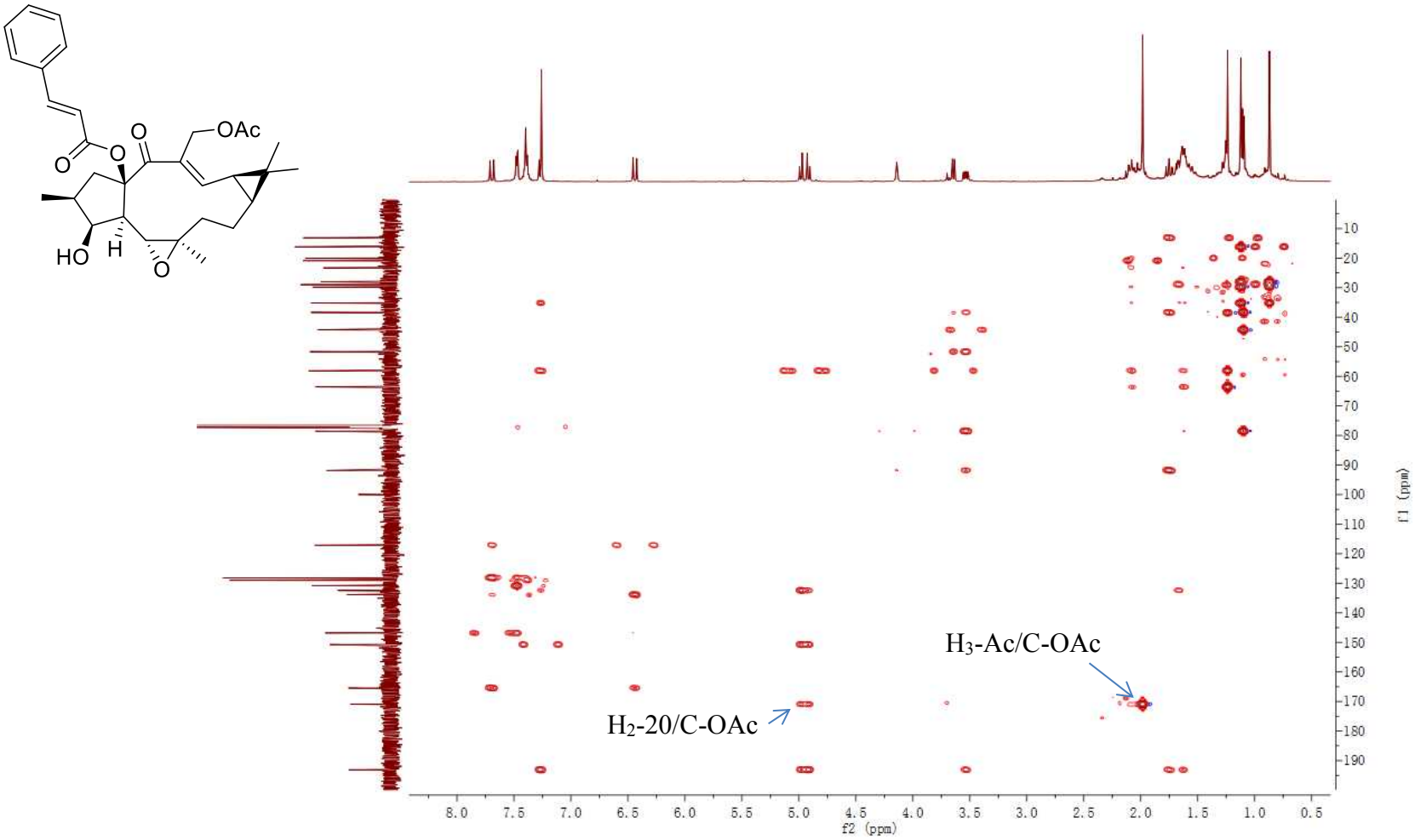

Figure S19: HMBC spectrum of **2** in $CDCl_3$

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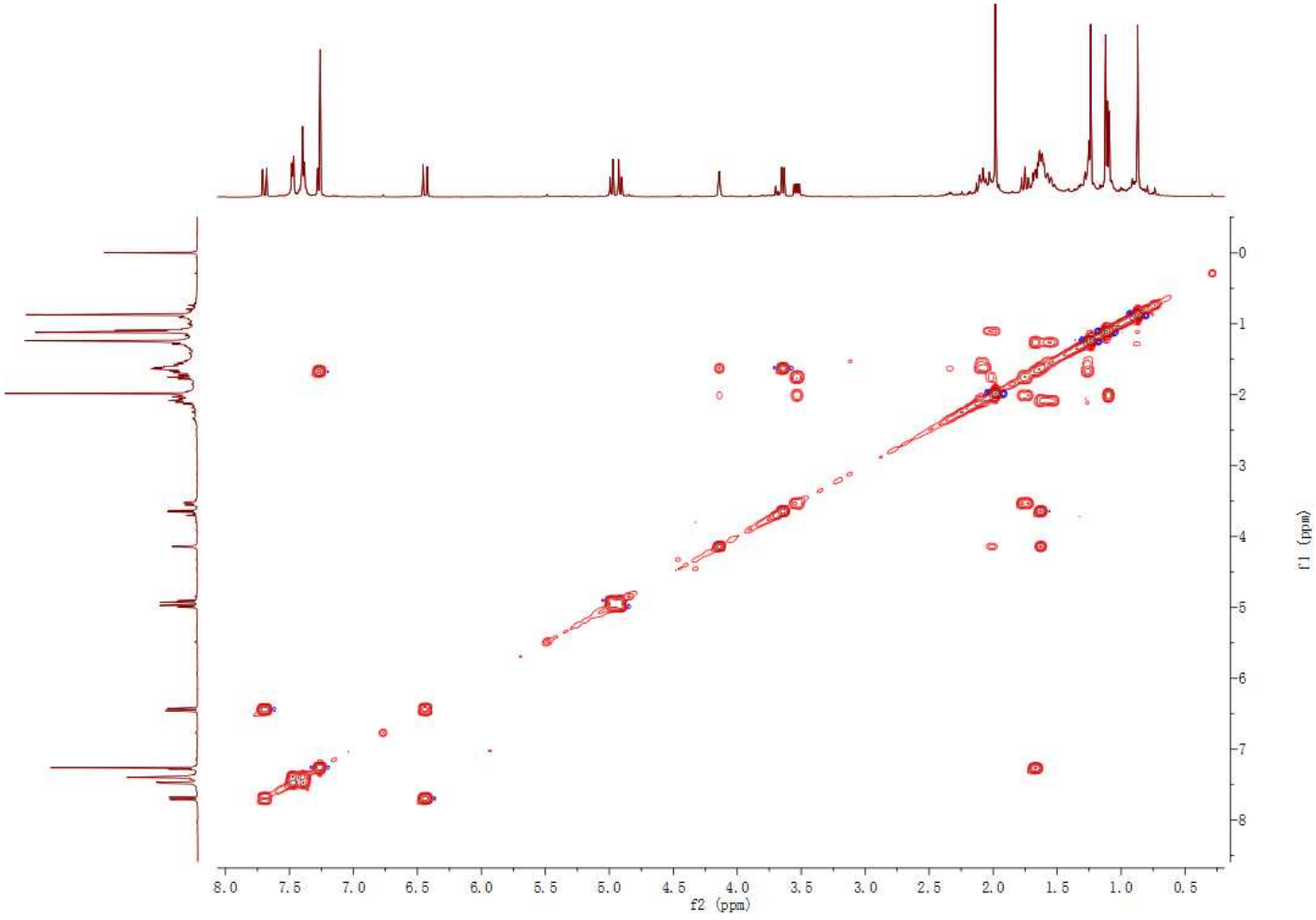

Figure S20. $^{1}H–^{1}H$ COSY spectrum of **2** in $CDCl_3$

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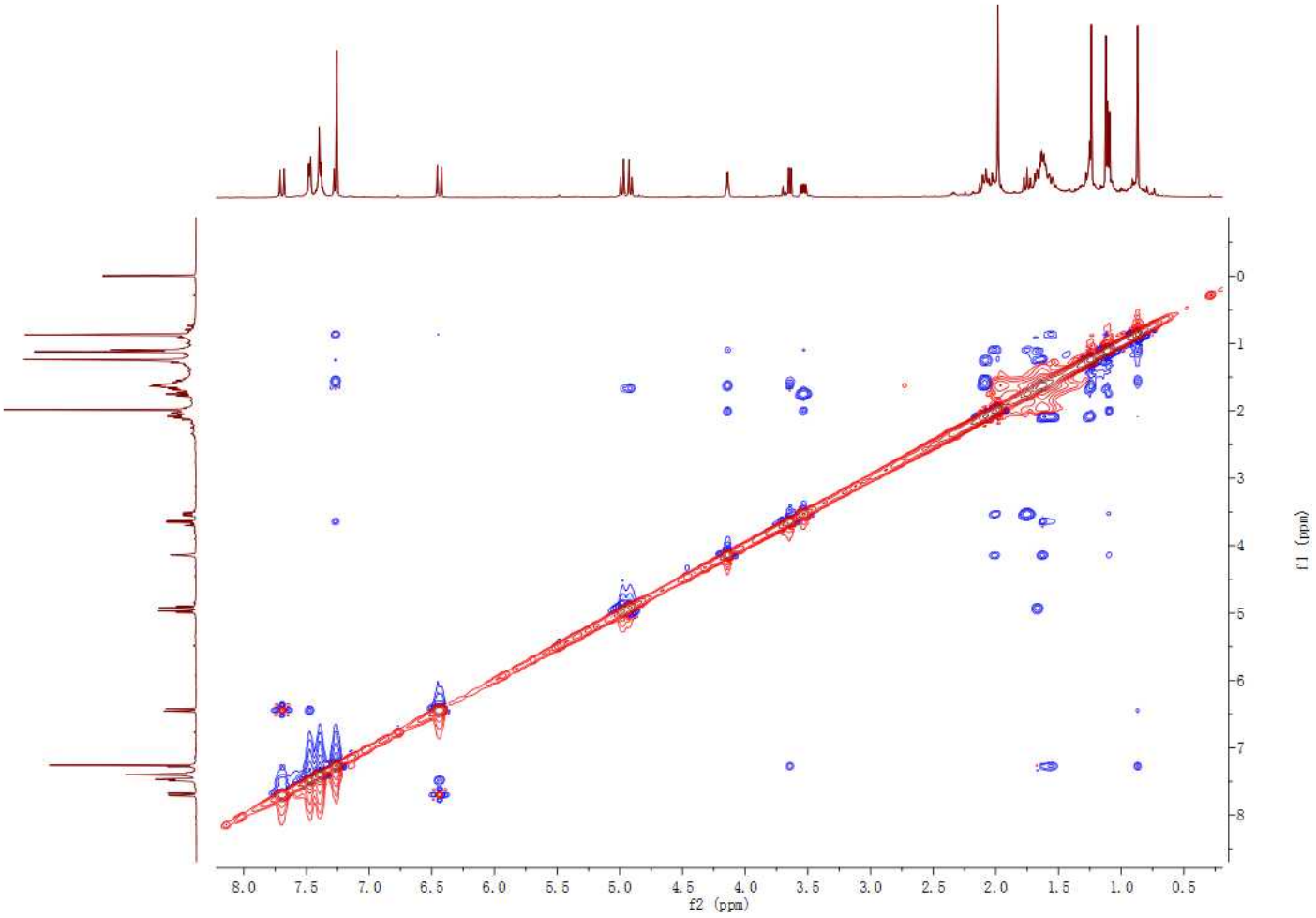

Figure S21: NOESY spectrum of **2** in $CDCl_3$

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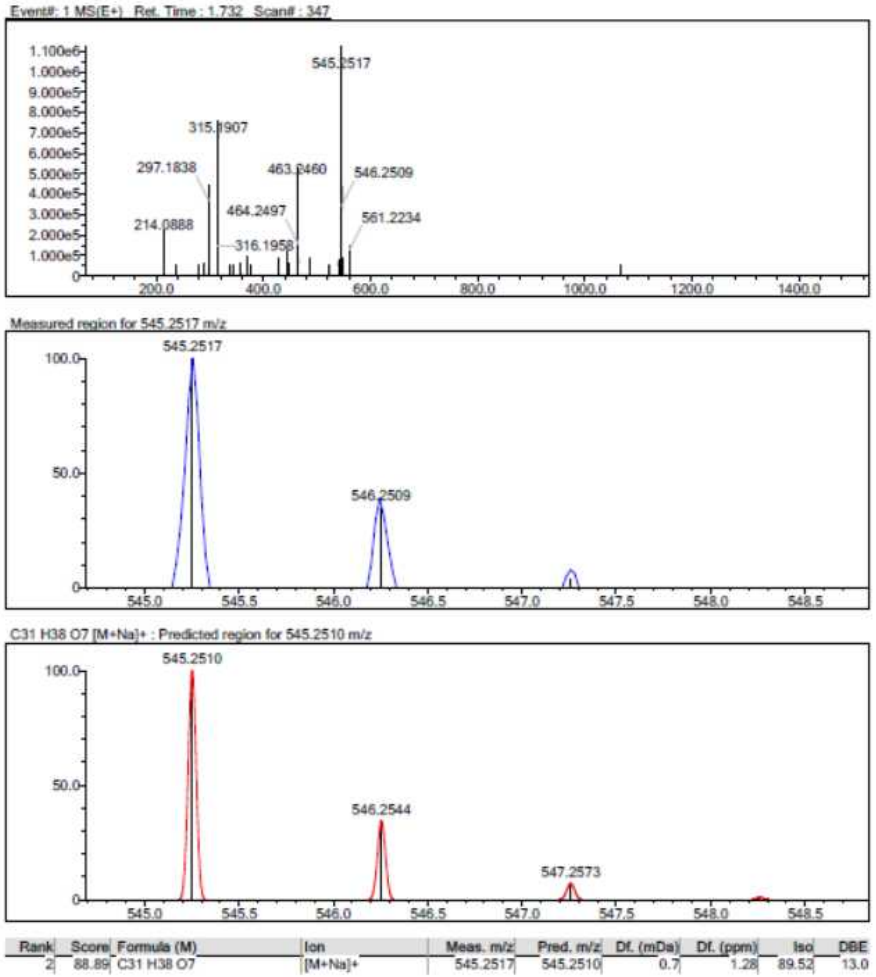

Figure S22: HRESIMS spectrum of **2**

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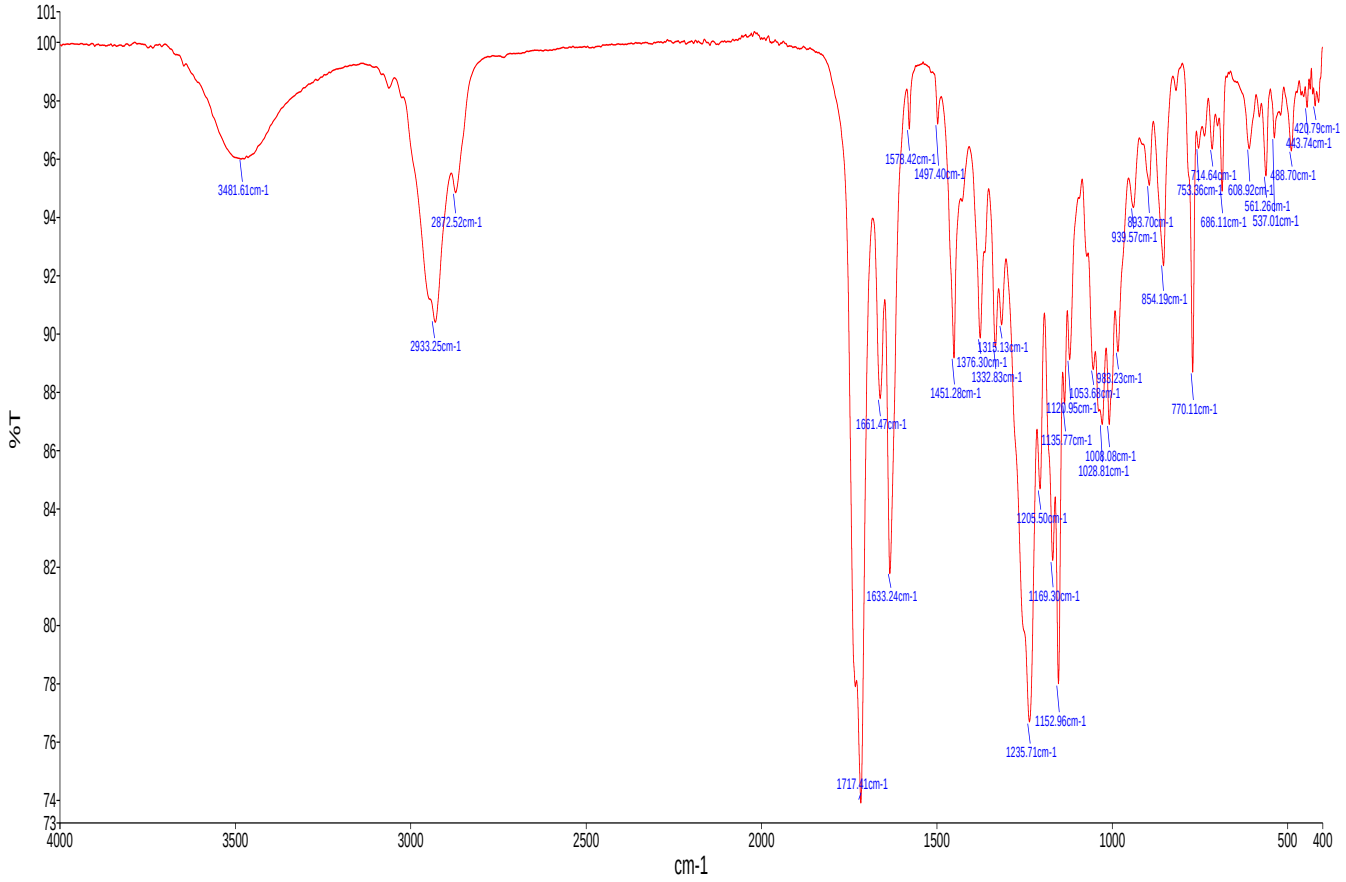

Figure S23: IR (KBr disc) spectrum of **2**

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