

## SUPPLEMENTARY MATERIAL

### Two new terpenoids from *Kalimeris indica*

Guo-Kai Wang<sup>a, b</sup>, Yang Yu<sup>a</sup>, Zheng Wang<sup>a</sup>, Bai-Xiang Cai<sup>a</sup>, Zhong-yu Zhou<sup>c</sup>, Gang Wang<sup>a, b\*</sup>, Jin-Song Liu<sup>a, b\*</sup>

<sup>a</sup>*School of Pharmacy, Anhui University of Chinese Medicine, Anhui Key Laboratory of Modern Chinese Materia Medica, Hefei 230012, China*

<sup>b</sup>*Synergetic Innovation Center of Anhui Authentic Chinese Medicine Quality Improvement, Hefei, P.R China*

<sup>c</sup>*Guang dong Provincial Key Laboratory of Applied Botany, South China Botanical Garden, Chinese Academy of Sciences, Guangzhou 510650, China*

\*To whom correspondence should be addressed. E-mail: jinsongliu108@163.com (J.-S. Liu); kunhong\_8@163.com (G. Wang)

Tel.: +86-551-68129167; Fax: +86-551-68129125

Address: School of Pharmacy, Anhui University of Chinese Medicine, Hefei, Anhui 230012, P.R.China.

**Abstract:** A new sesquiterpenoid kalimerislactone A (**1**), a new nor-triterpenoid kalimerislactone B (**2**) and with eight known compounds 7-hydroxy-4'-methoxyisoflavone (**3**), episingaresinol (**4**), epipinoresinol (**5**), rhamnetin (**6**), vanillin (**7**), *p*-hydroxybenzaldehyde (**8**), syringic acid (**9**), and 3, 4-dihydroxybenzaldehyde (**10**) were isolated from the herbs of *Kalimeris indica*. The structures of these compounds were elucidated and determined using spectroscopic techniques such as NMR and MS. All of the compounds were isolated from this genus for the first time. The cytotoxicities against four cancer cell lines (including SMMC-7721, MCF-7, K-562, and A-549) were evaluated in vitro, but were inactive.

**Keywords:** *Kalimeris indica*; Nor-triterpenoid; Sesquiterpenoids; Cytotoxicity

Table S1  $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shifts of compounds **1** ( $J$  in Hz)

Table S2  $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shifts of compounds **2** ( $J$  in Hz)

Figure S1. Selected HMBC ( $\rightarrow$ ) correlations of **1** and **2**.

Figure S2. Key NOE correlations ( $\leftarrow\cdots\rightarrow$ ) of **1** and **2**.

Figure S3. HR-EIMS spectrum of compound **1**

Figure S4. UV spectrum of compound **1**

Figure S5. IR spectrum of compound **1**

Figure S6.  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

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Figure S8. HSQC spectrum of compound **1** in  $\text{CD}_3\text{OD}$

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Figure S10. H-H COSY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

Figure S11. ROESY spectrum of compound **1** in  $\text{CD}_3\text{OD}$

Figure S12. HR-EIMS spectrum of compound **2**

Figure S13. UV spectrum of compound **2**

Figure S14. IR spectrum of compound **2**

Figure S15.  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

Figure S16.  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

Figure S17. HSQC spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

Figure S18. HMBC spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

Figure S19. H-H COSY spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

Figure S20. ROESY spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

**Table S1**  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR chemical shifts of compound **1** ( $J$  in Hz)

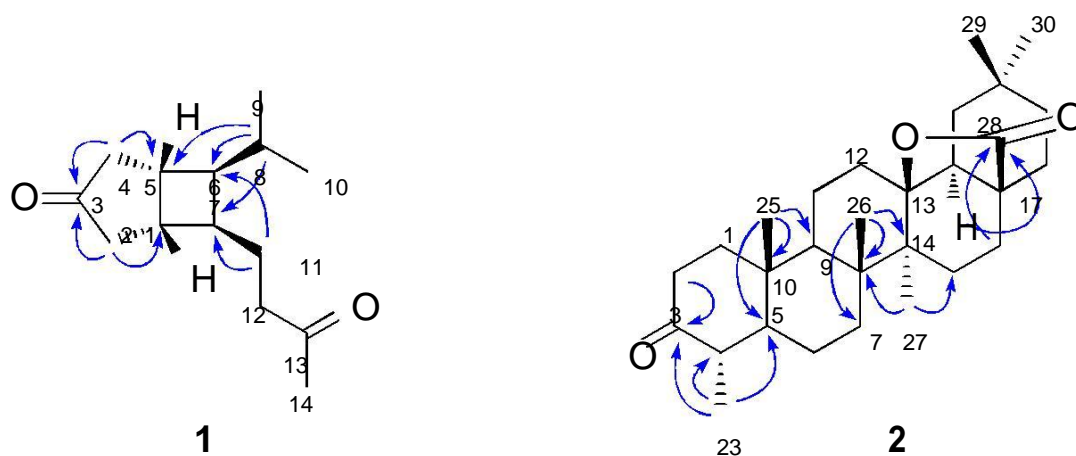
Position	$\delta$ (H) <sup>a)</sup>	$\delta$ (C) <sup>b)</sup>
1	1.19 ( <i>m</i> )	31.8 ( <i>d</i> )
2	2.14 ( <i>m</i> ), 1.98 ( <i>m</i> )	33.7 ( <i>t</i> )
3		217.8 ( <i>s</i> )
4	2.14 ( <i>m</i> ), 2.07 ( <i>m</i> )	23.9 ( <i>t</i> )
5	1.98 ( <i>m</i> )	29.7 ( <i>d</i> )
6	1.62 ( <i>m</i> )	35.6 ( <i>d</i> )
7	0.73 ( <i>m</i> )	47.6 ( <i>d</i> )
8	1.79 ( <i>m</i> )	32.4 ( <i>d</i> )
9	0.93 ( <i>d</i> , 6.8)	19.4 ( <i>q</i> )
10	0.94 ( <i>d</i> , 6.8)	20.1 ( <i>q</i> )
11	1.74 ( <i>m</i> ), 1.65 ( <i>m</i> )	25.7 ( <i>t</i> )
12	2.63 ( <i>m</i> )	42.2 ( <i>t</i> )
13		211.9 ( <i>s</i> )
14	2.17 ( <i>s</i> )	29.7 ( <i>q</i> )

a) Measured at 400 MHz. in  $\text{CD}_3\text{OD}$ , b) Measured at 100 MHz. in  $\text{CD}_3\text{OD}$

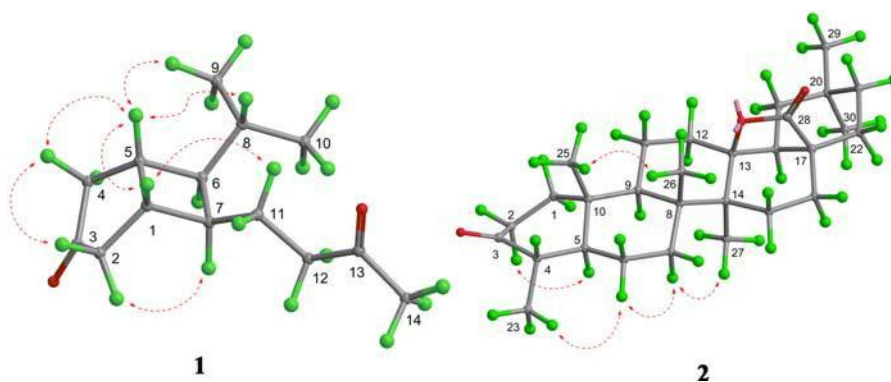
**Table S2**  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR chemical shifts of compound **2** ( $J$  in Hz)

Position	$\delta$ (H) <sup>c)</sup>	$\delta$ (C) <sup>d)</sup>	Position	$\delta$ (H) <sup>c)</sup>	$\delta$ (C) <sup>d)</sup>
1	1.31 ( <i>m</i> )	40.7 ( <i>t</i> )	16	1.39 ( <i>m</i> )	27.9 ( <i>t</i> )
2	1.25 ( <i>m</i> )	35.3 ( <i>t</i> )	17		47.5 ( <i>s</i> )
3		213.8 ( <i>s</i> )	18	2.25 ( <i>dd</i> , 12.3, 4.9)	45.0 ( <i>d</i> )
4	2.33 ( <i>m</i> )	44.7 ( <i>d</i> )	19	2.46 ( <i>m</i> )	37.6 ( <i>t</i> )
5	1.08 ( <i>m</i> )	53.3 ( <i>d</i> )	20		30.1 ( <i>s</i> )
6	1.57 ( <i>m</i> )	21.7 ( <i>t</i> )	21	1.23 ( <i>m</i> )	36.3 ( <i>t</i> )
7	1.48 ( <i>m</i> )	33.7 ( <i>t</i> )	22	1.65 ( <i>m</i> )	31.7 ( <i>t</i> )
8		41.2 ( <i>s</i> )	23	0.98 ( <i>d</i> , 6.6)	11.8 ( <i>q</i> )
9	1.32 ( <i>m</i> )	47.7 ( <i>d</i> )	24		
10		36.7 ( <i>s</i> )	25	1.08 ( <i>s</i> )	13.9 ( <i>q</i> )
11	1.55 ( <i>m</i> )	19.0 ( <i>t</i> )	26	1.22 ( <i>s</i> )	18.0 ( <i>q</i> )
12	1.86 ( <i>d</i> , 6.5)	26.7 ( <i>t</i> )	27	1.12( <i>s</i> )	19.5 ( <i>q</i> )
13		89.7 ( <i>s</i> )	28		179.5 ( <i>s</i> )
14		44.0 ( <i>s</i> )	29	0.88 ( <i>s</i> )	33.2 ( <i>q</i> )
15	1.33 ( <i>m</i> )	26.0 ( <i>t</i> )	30	0.83 ( <i>s</i> )	23.3 ( <i>q</i> )

c) Measured at 500 MHz. in  $\text{CD}_3\text{Cl}_3$ , d) Measured at 125 MHz. in  $\text{CD}_3\text{Cl}_3$



**Fig. S1.** Selected HMBC ( $\rightarrow$ ) correlations of **1** and **2**



**Fig S2.** Key NOE correlations ( $\leftarrow$ ----- $\rightarrow$ ) of **1** and **2**.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 1-3

LZ-22

12.03.47 10-Aug-2012

Voltage ESI+

100V

K1B  
M120805EA-10AFAMM 19 (1.745)  
222.1627

Autospec Premier  
P775  
1

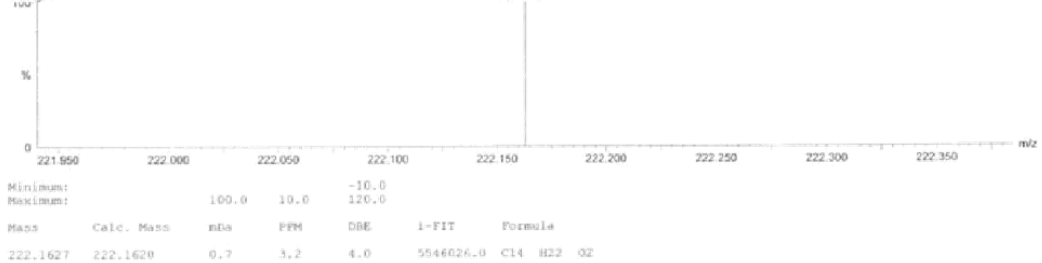


Figure S3. HR-EIMS spectrum of compound 1

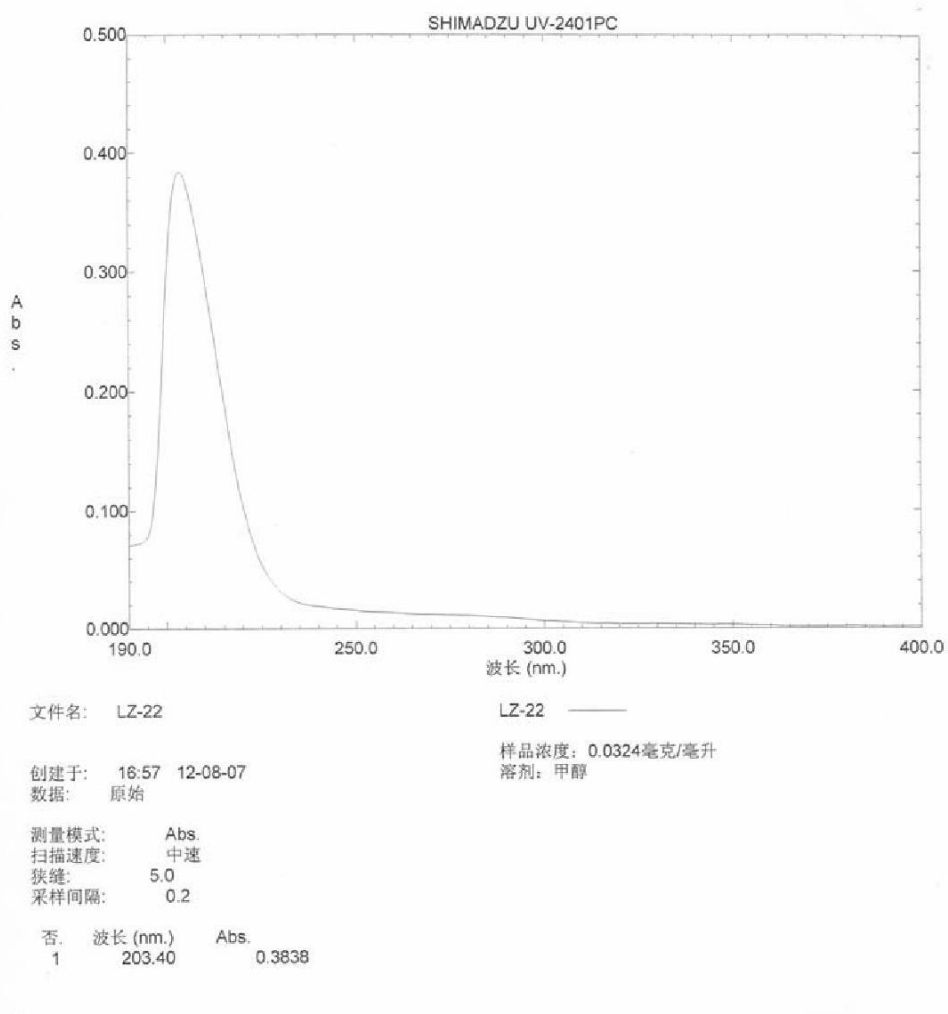
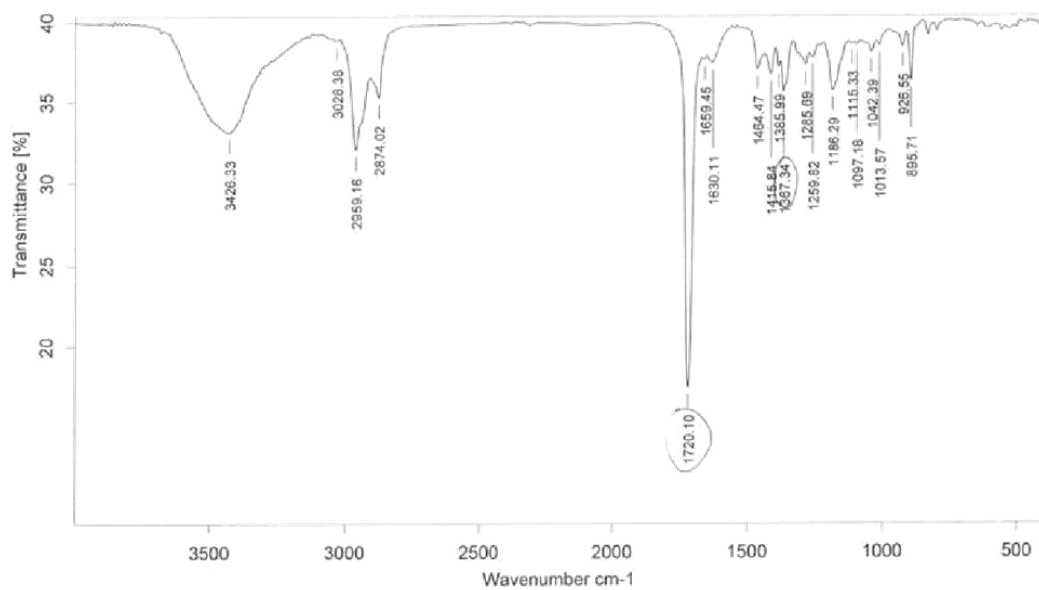


Figure S4. UV spectrum of compound 1



Sample : LZ-22	Frequency Range : 399.246 - 3996.32	Measured on : 31/12/2002
Technique : KBr压片	Resolution : 4	Instrument : Tensor27
Customer : 120810IR5	Zerofilling : 2	Sample Scans : 16
	Acquisition : Double Sided, For	

Figure S5. IR spectrum of compound 1

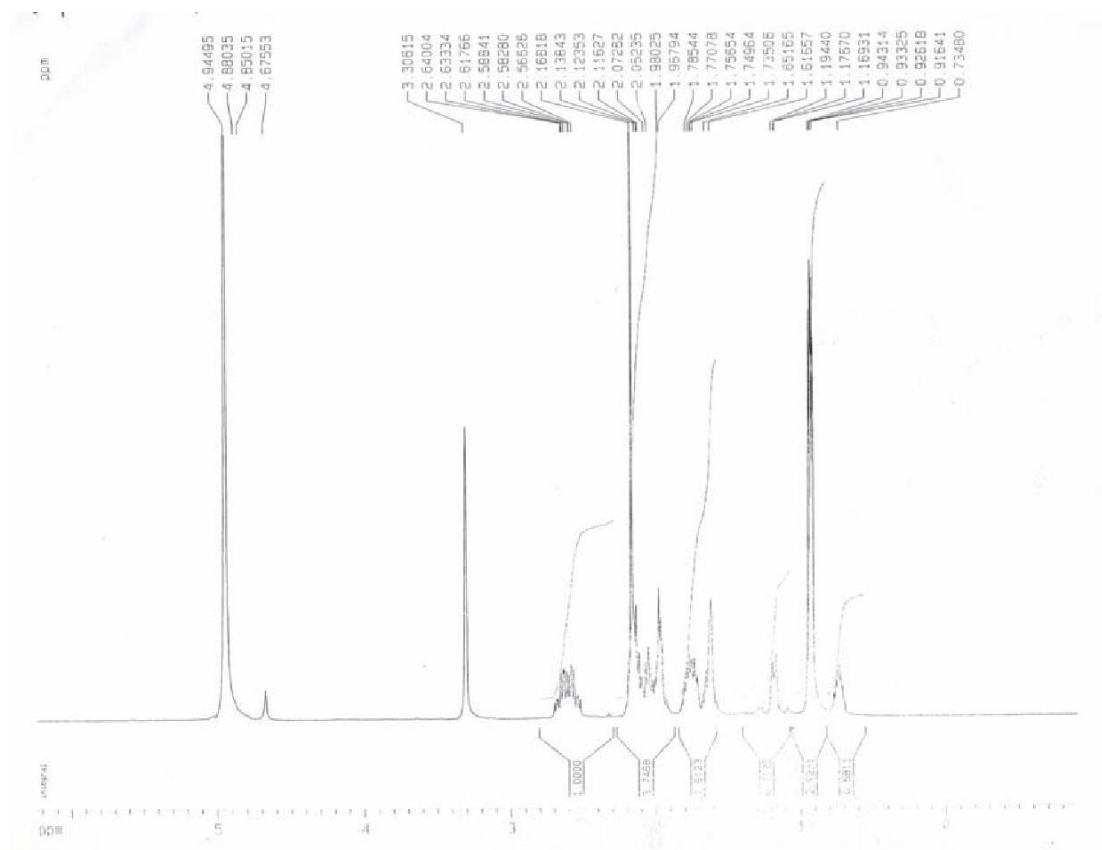


Figure S6.  $^1\text{H}$  NMR spectrum of compound 1 in  $\text{CD}_3\text{OD}$

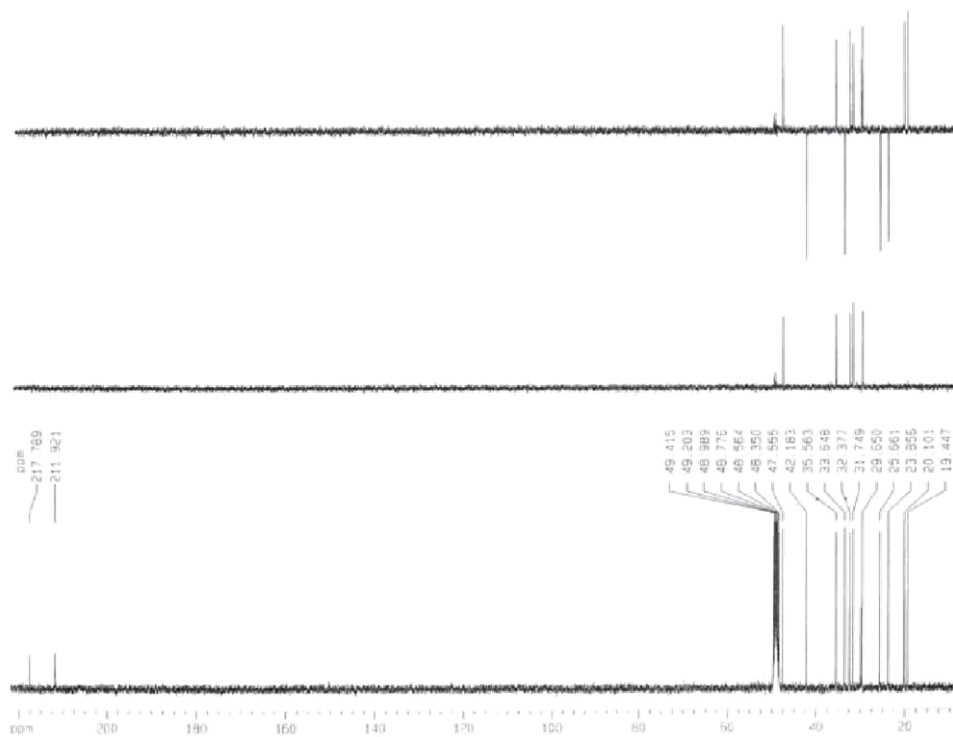


Figure S7.  $^{13}\text{C}$  NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

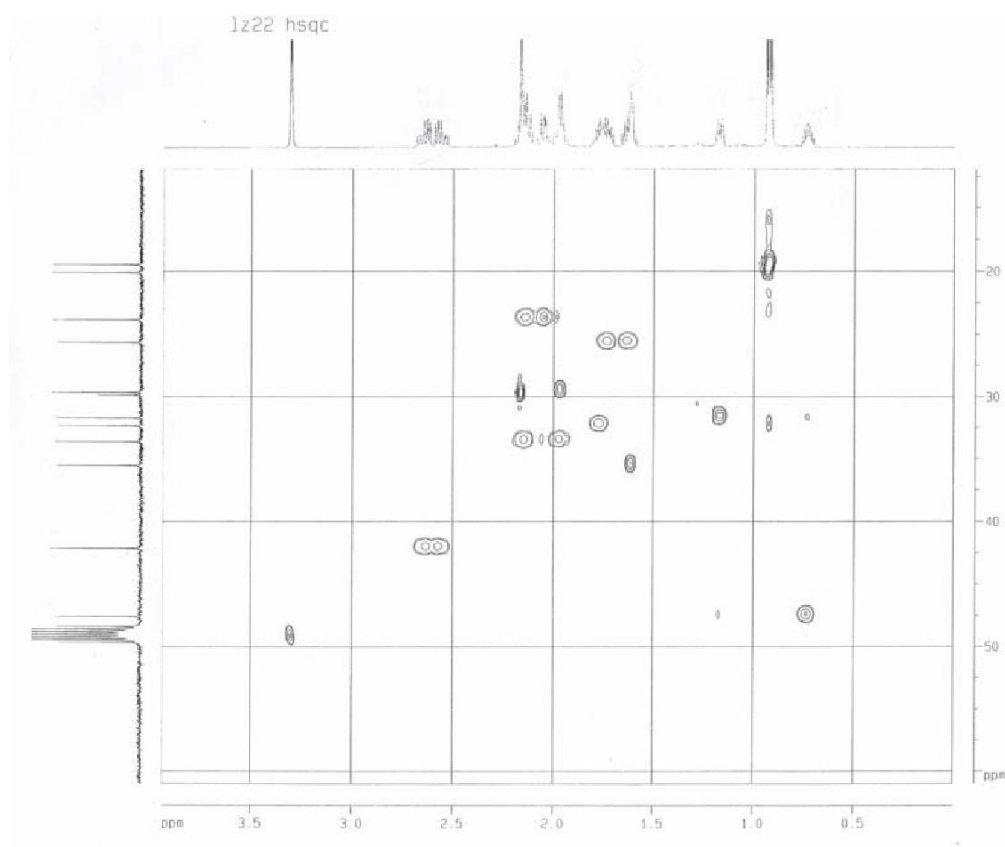


Figure S8. HSQC spectrum of compound **1** in  $\text{CD}_3\text{OD}$

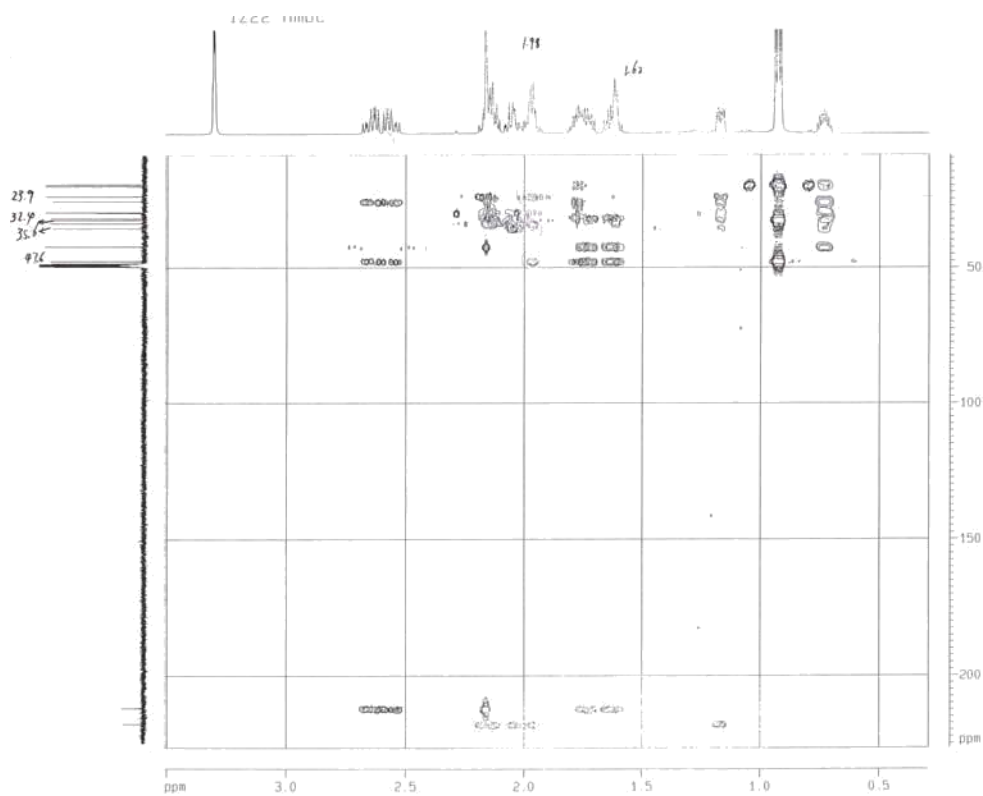


Figure S9. HMBC spectrum of compound **1** in CD<sub>3</sub>OD

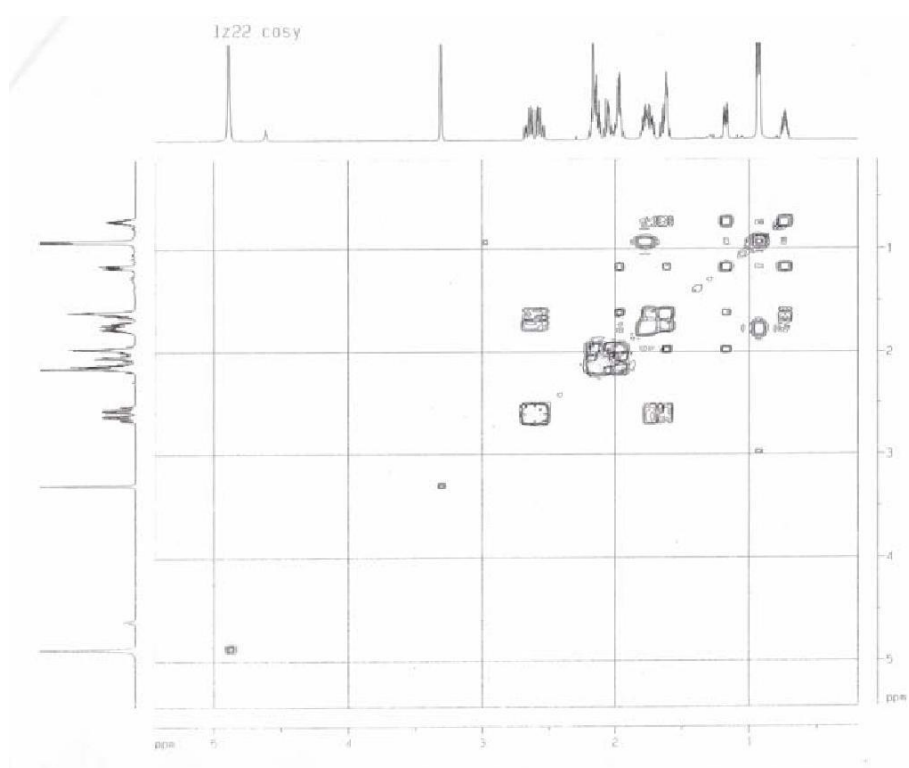


Figure S10. H-H COSY spectrum of compound **1** in CD<sub>3</sub>OD



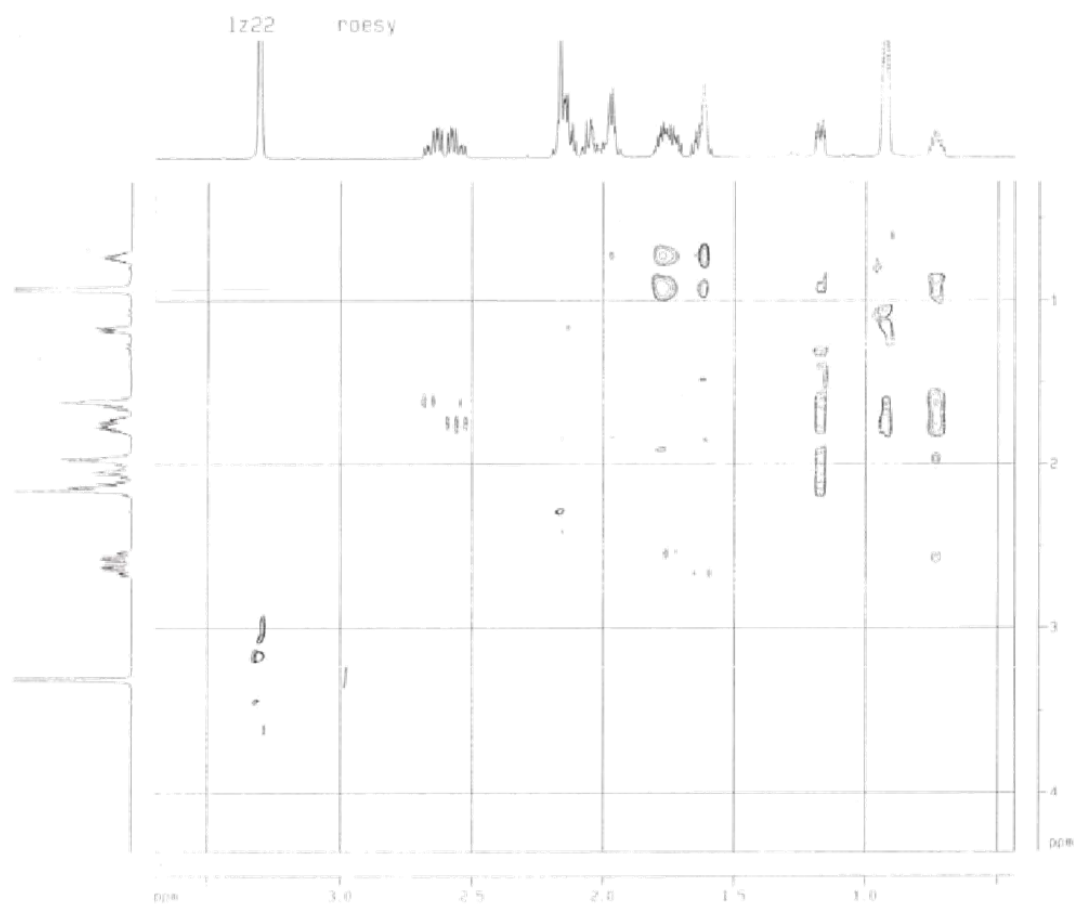


Figure S11. ROESY spectrum of compound **1** in CD<sub>3</sub>OD

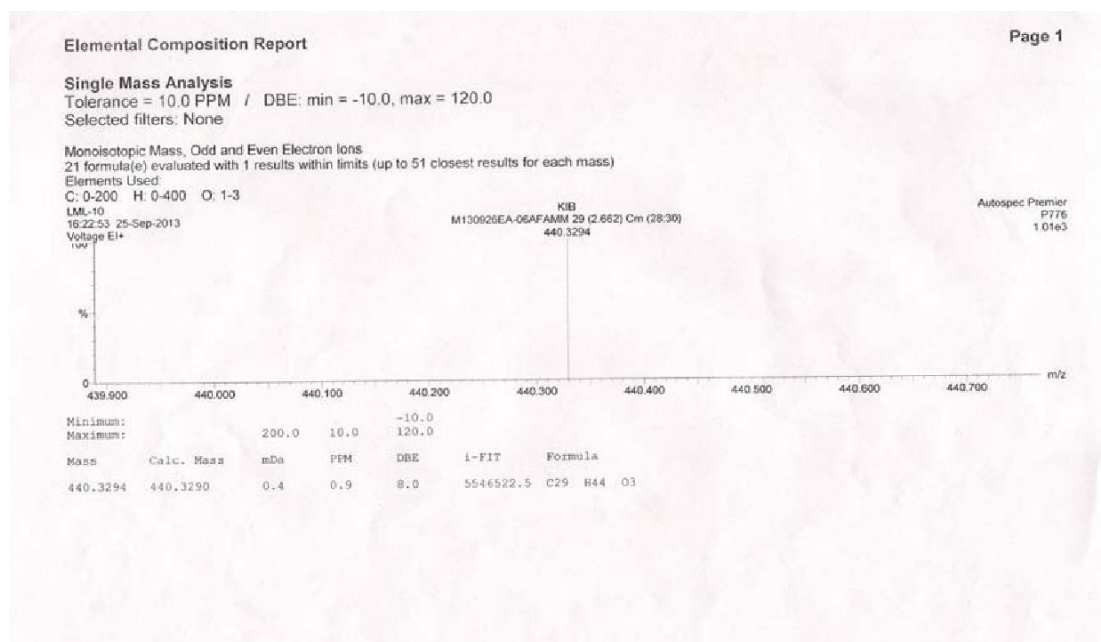


Figure S12. HR-EIMS spectrum of compound **2**

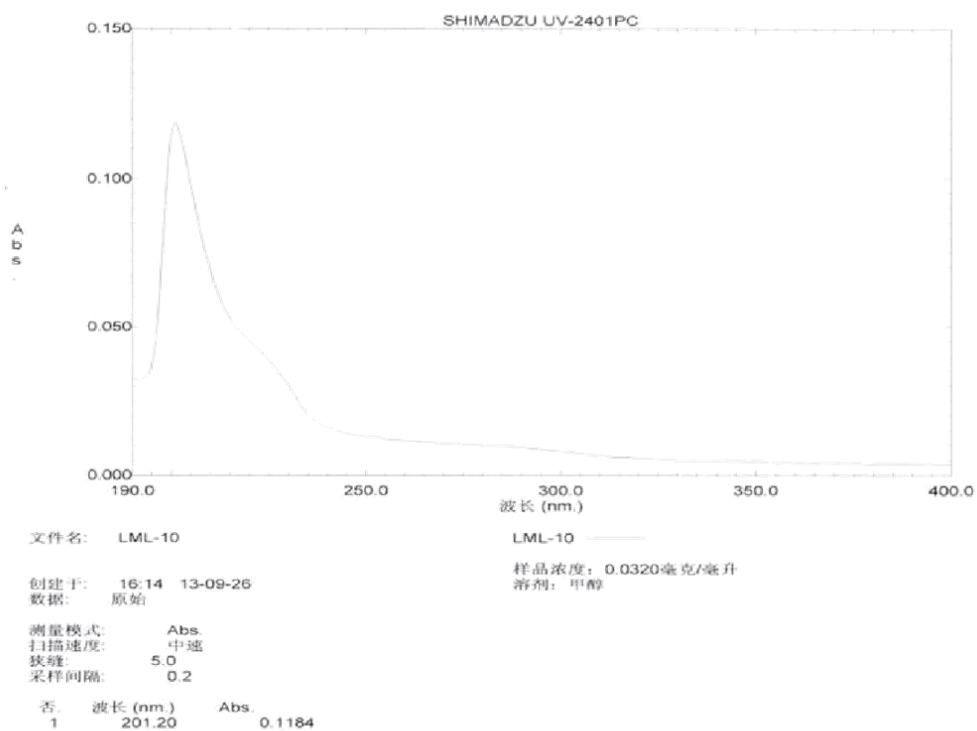


Figure S13. UV spectrum of compound 2

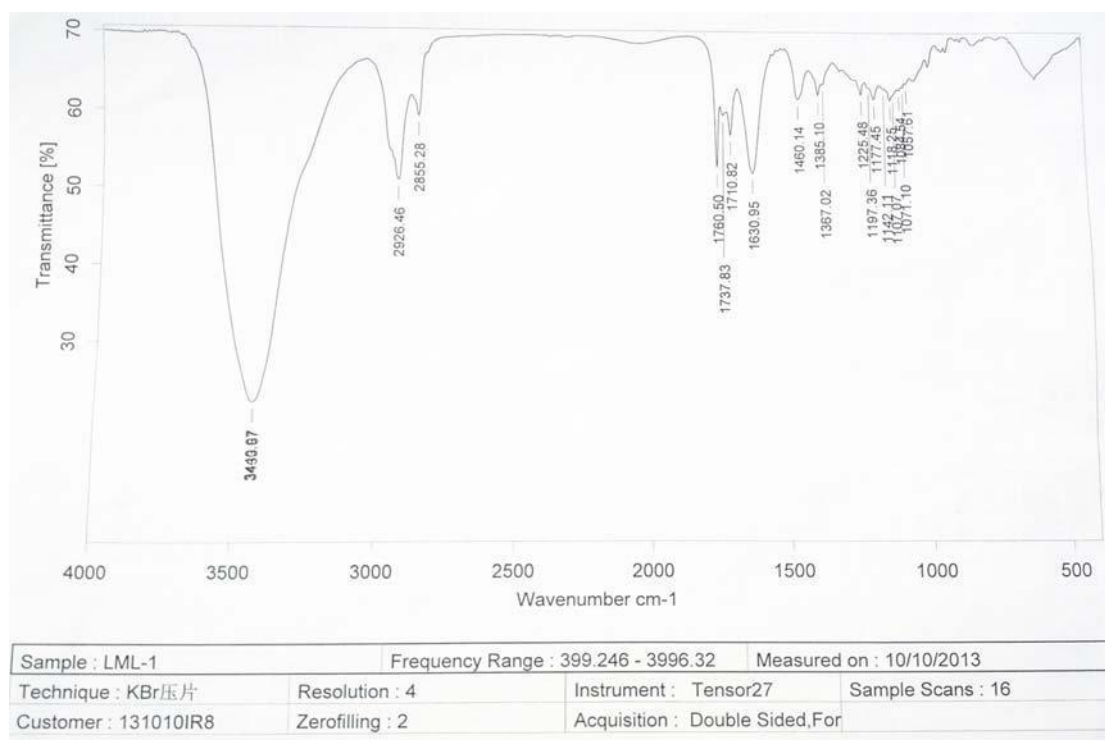


Figure S14. IR spectrum of compound 2



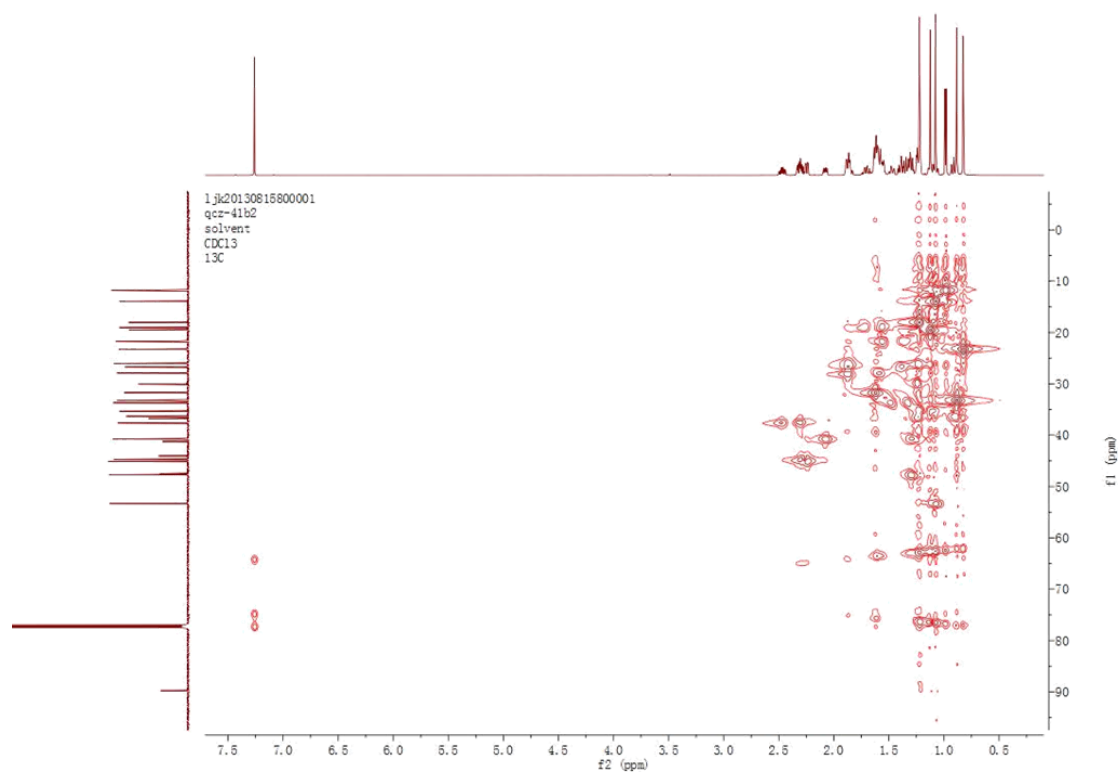


Figure S17. HSQC spectrum of compound **2** in CD<sub>3</sub>Cl<sub>3</sub>

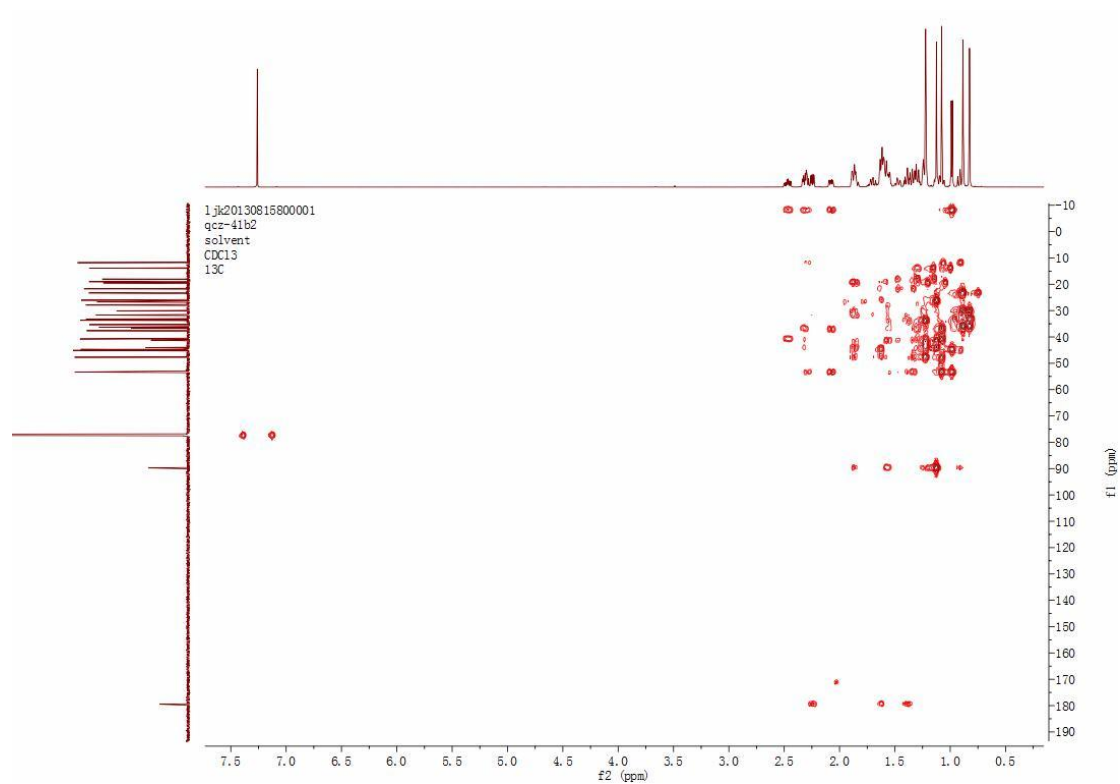


Figure S18. HMBC spectrum of compound **2** in CD<sub>3</sub>Cl<sub>3</sub>

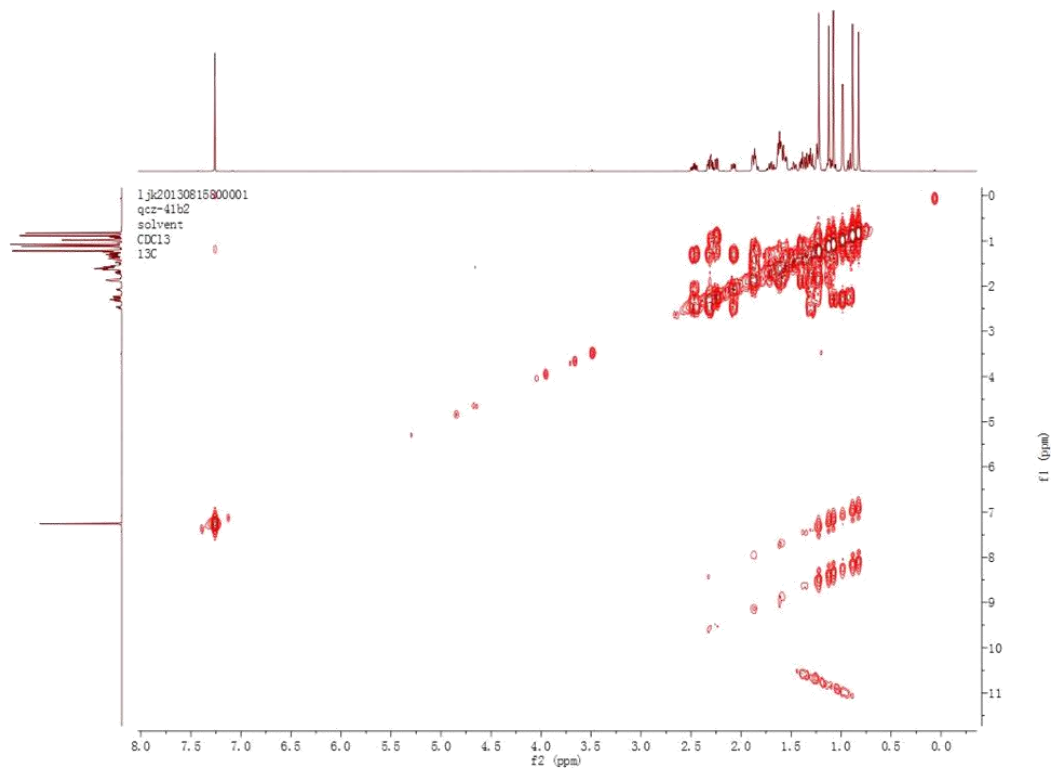


Figure S19. H-H COSY spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

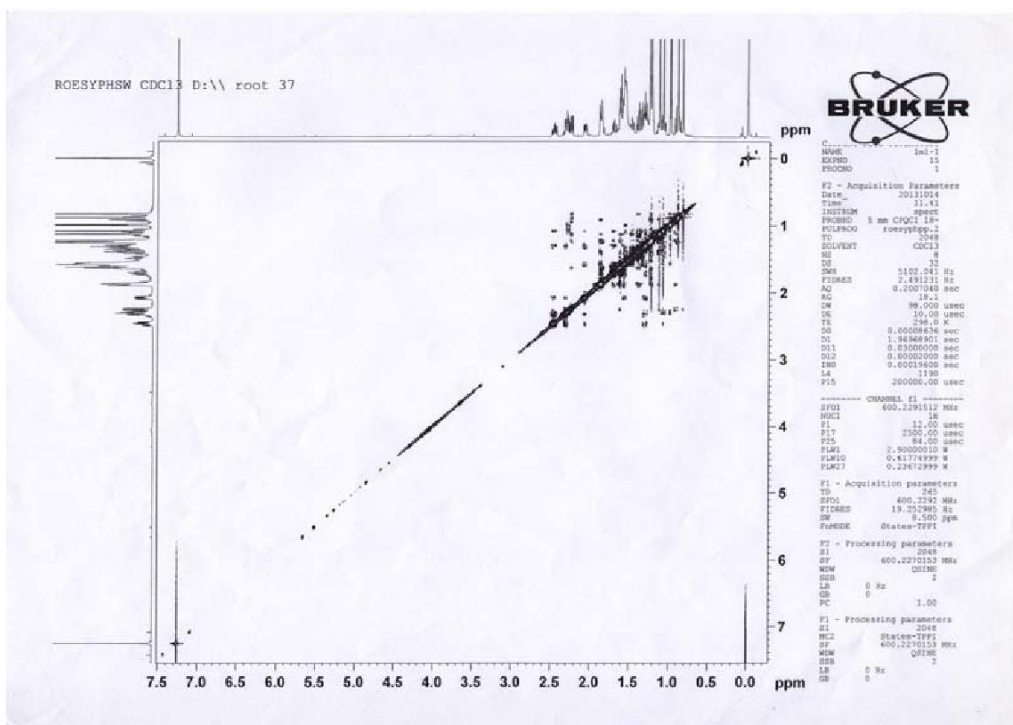


Figure S20. ROESY spectrum of compound **2** in  $\text{CD}_3\text{Cl}_3$

