SUPPLEMENTARY MATERIAL

Two New Clerodane-Type Diterpenoids from Bornean Liverwort *Gottschelia schizopleura* and Their Cytotoxic Activity

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Abstract: The Bornean liverwort *Gottschelia schizopleura* was investigated phytochemically for the first time. Two new and four previously known clerodane-type diterpenoids were isolated from the MeOH extract of *G. schizopleura* through a series of chromatographic techniques. The structures of the new metabolites were established by analyses of their spectroscopic data (1D NMR, 2D NMR, HRESIMS and IR). All the isolated compounds **1**-**6** were tested against human promyelocytic leukemia (HL-60), human colon adenocarcinoma (HT-29) and Mus musculus skin melanoma (B16-F10). Compound **1** and **2** showed active inhibition against HL-60 and B16-F10 cells.

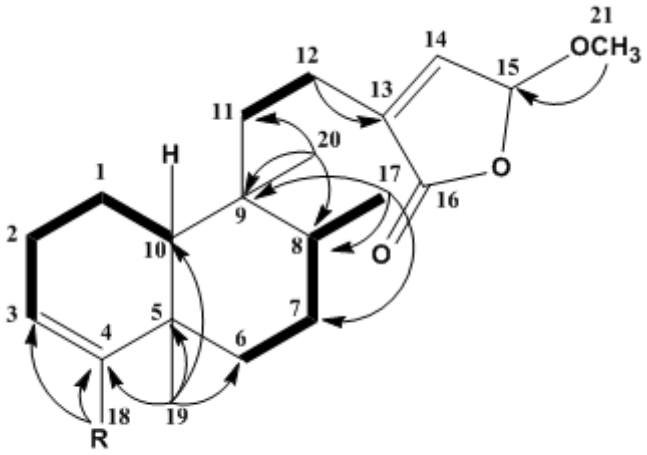
Keywords: clerodane diterpenoids, *Gottschelia schizopleura*, Jungermanniaceae, liverwort, Borneo, cytotoxic activity

Supplementary Information

Table S1. ^{13}C and ^{1}H NMR (150 and 600 MHz) data of 1 and 2 ($CDCl_3$, d in ppm).

	1		**2**	
Position	δ_C	δ_H (*J*, Hz)	δ_C	δ_H (*J*, Hz)
1	18.1	1.80 (1H, m)	17.6	1.88 (1H, m)
		2.02 (1H, m)		2.03 (1H, m)
2	24.3	2.13 (1H, m)	26.4	2.42 (1H, m)
		2.18 (1H, m)		2.53 (1H, m)
3	125.5	5.62 (1H, t, *J* = 3.4)	156.4	6.70 (1H, t, *J* = 3.4)
4	143.8		148.1	
5	36.9		37.3	
6	37.4	1.17 (1H, m)	36.0	1.11 (1H, m)
		2.07 (1H, m)		3.11 (1H, m)
7	29.5	1.25 (1H, m)	29.2	1.08 (1H, m)
		1.30 (1H, m)		1.31 (1H, m)
8	38.1	1.47 (1H, m)	38.2	1.50 (1H, m)
9	40.8		40.9	
10	45.8	1.37 (1H, brd, *J* = 6.2)	45.8	1.42 (1H, brd, *J* = 6.2)
11	35.9	1.45 (1H, m)	36.2	1.49 (1H, m)
		1.72 (1H, t, *J* = 8.9)		1.70 (1H, t, *J* = 8.9)
12	19.4	2.19 (1H, dd, *J* = 6.9, 10.3)	19.5	2.20 (1H, dd, *J* = 6.9, 10.3)
		2.19 (1H, dd, *J* = 6.9, 10.3)		2.20 (1H, dd, *J* = 6.9, 10.3)
13	140.3		140.1	
14	141.8	6.76 (1H, brs)	142.0	6.77 (1H, brs)
15	103.2	5.73 (1H, brs)	103.3	5.73 (1H, brs)
16	172.2		172.2	
17	16.5	0.77 (3H, d, *J* = 6.9)	16.6	0.76 (3H, d, *J* = 6.9)
18	65.4	4.12 (1H, d, *J* = 13.1)	194.7	9.40 (1H, s)
		4.23 (1H, d, *J* = 13.1)		
19	35.6	1.13 (3H, s)	33.8	1.14 (3H, s)
20	17.8	0.80 (3H, s)	18.5	0.74 (3H, s)
21	57.7	3.57 (3H, s)	57.8	3.58 (3H, s)

Figure S2. HMBC (solid arrows) and ^{1}H-^{1}H COSY (bold lines) correlations of **1** and **2**.



1: R = CH_2OH

2: R = CHO

Figure S3. ^{1}H NMR spectrum of **1** in $CDCl_3$ (600 MHz).

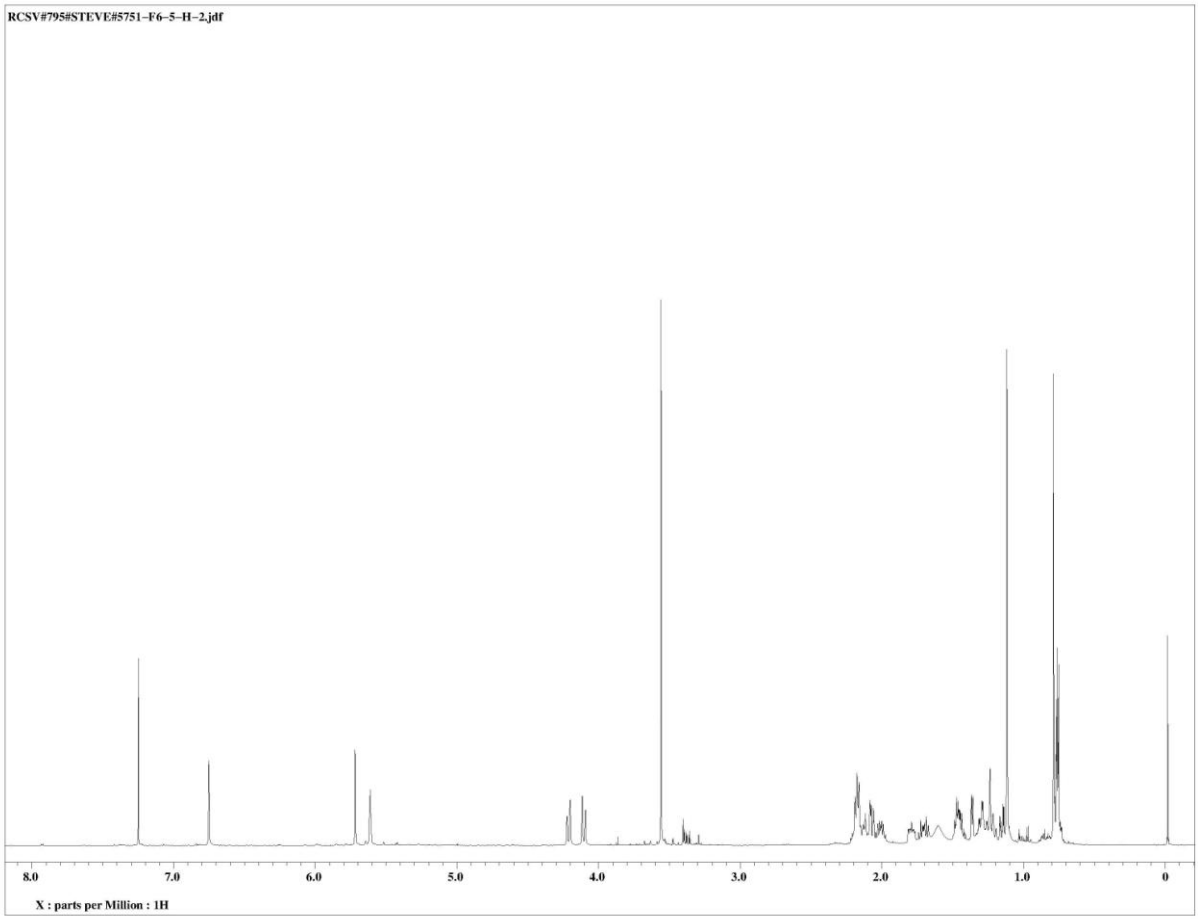


Figure S4. ^{13}C NMR spectrum of **1** in $CDCl_3$ (150 MHz).

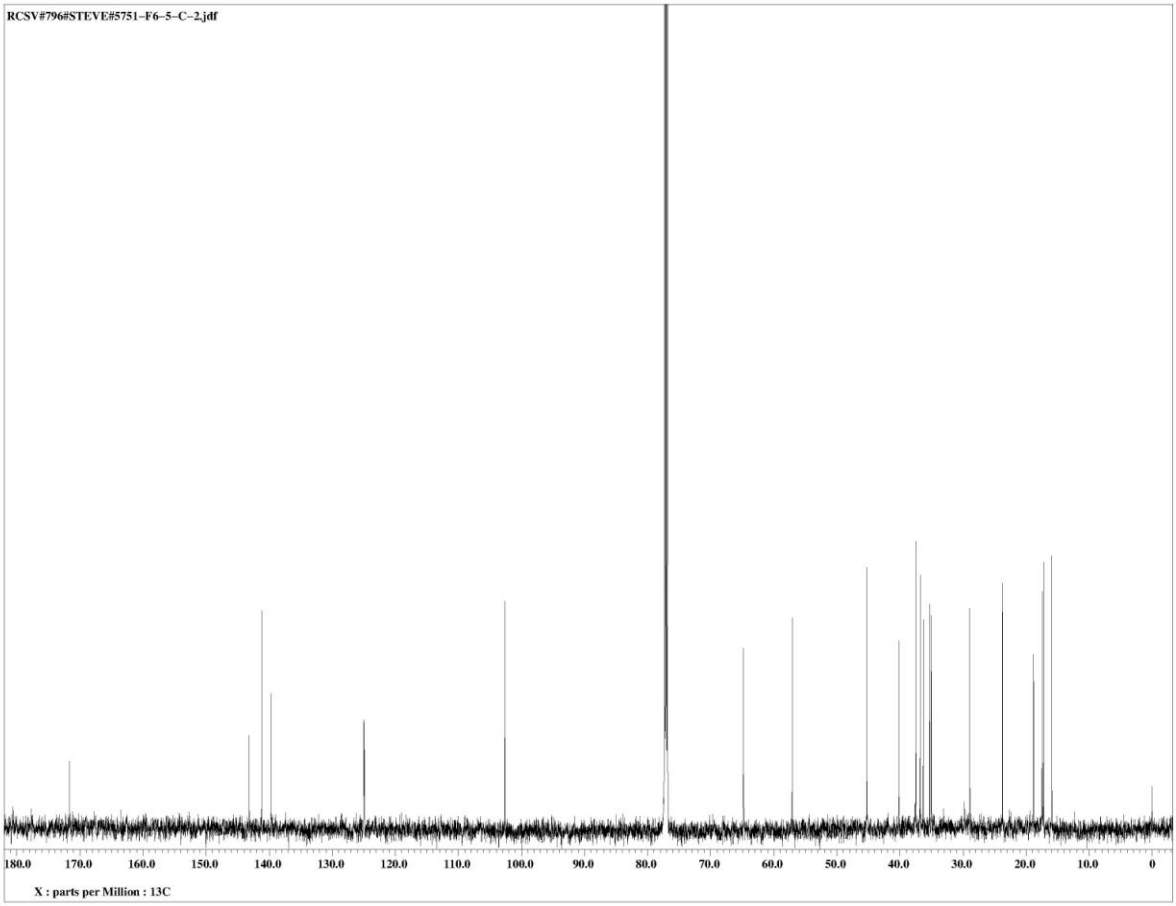


Figure S5. HSQC spectrum of **1** in $CDCl_3$.

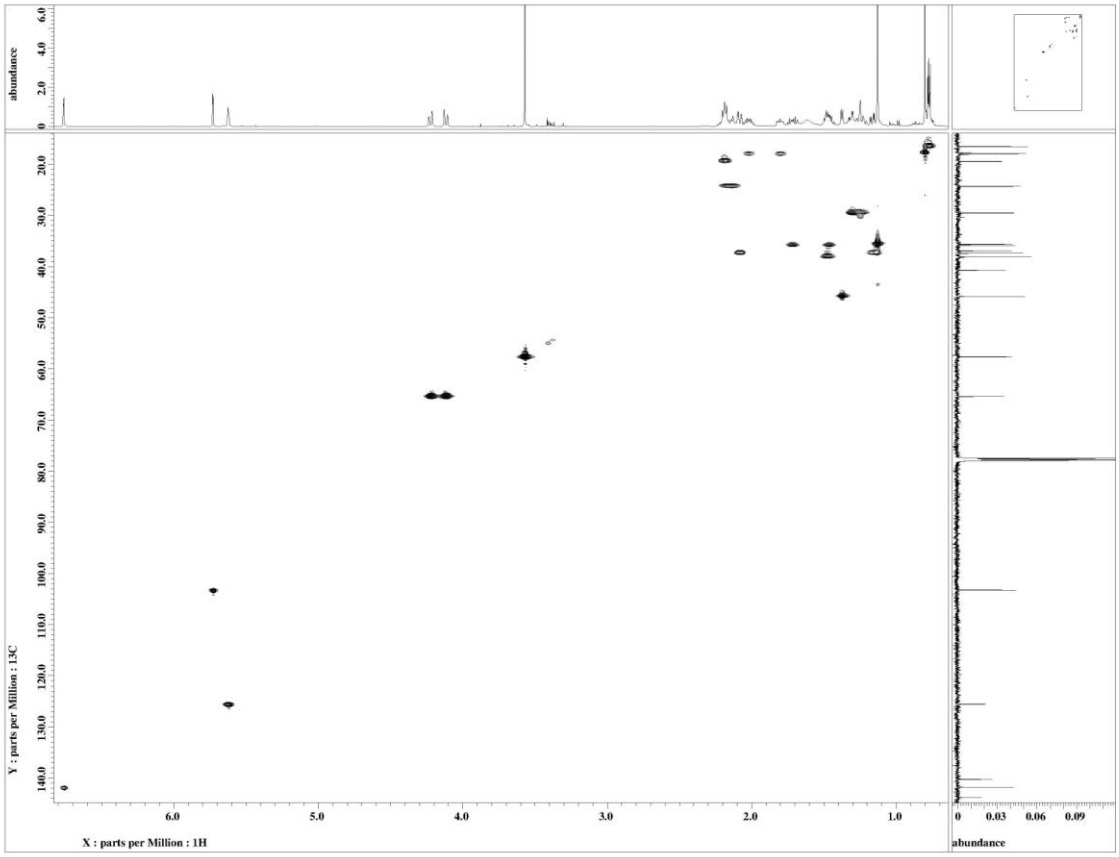


Figure S6. ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_3$.

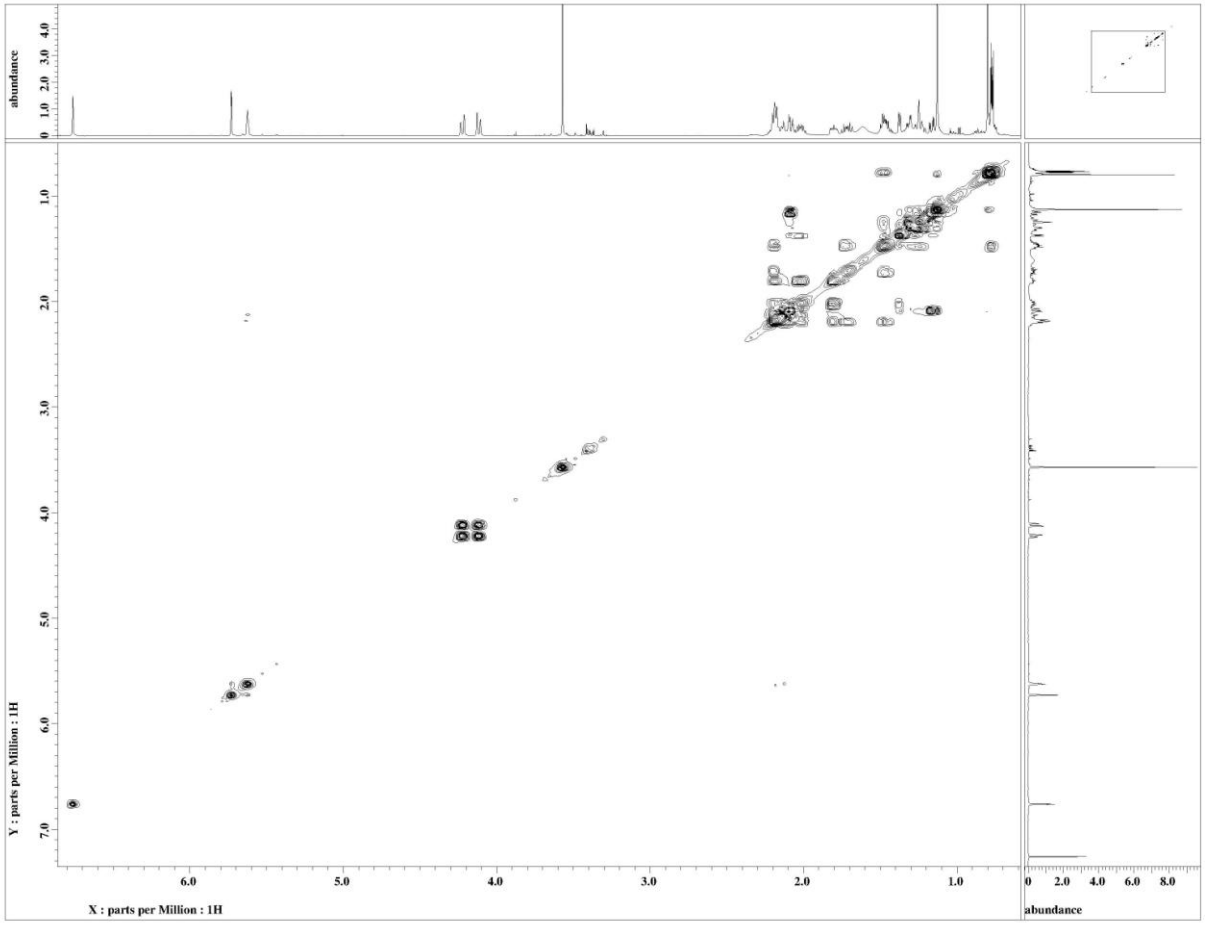


Figure S7. HMBC spectrum of **1** in $CDCl_3$.

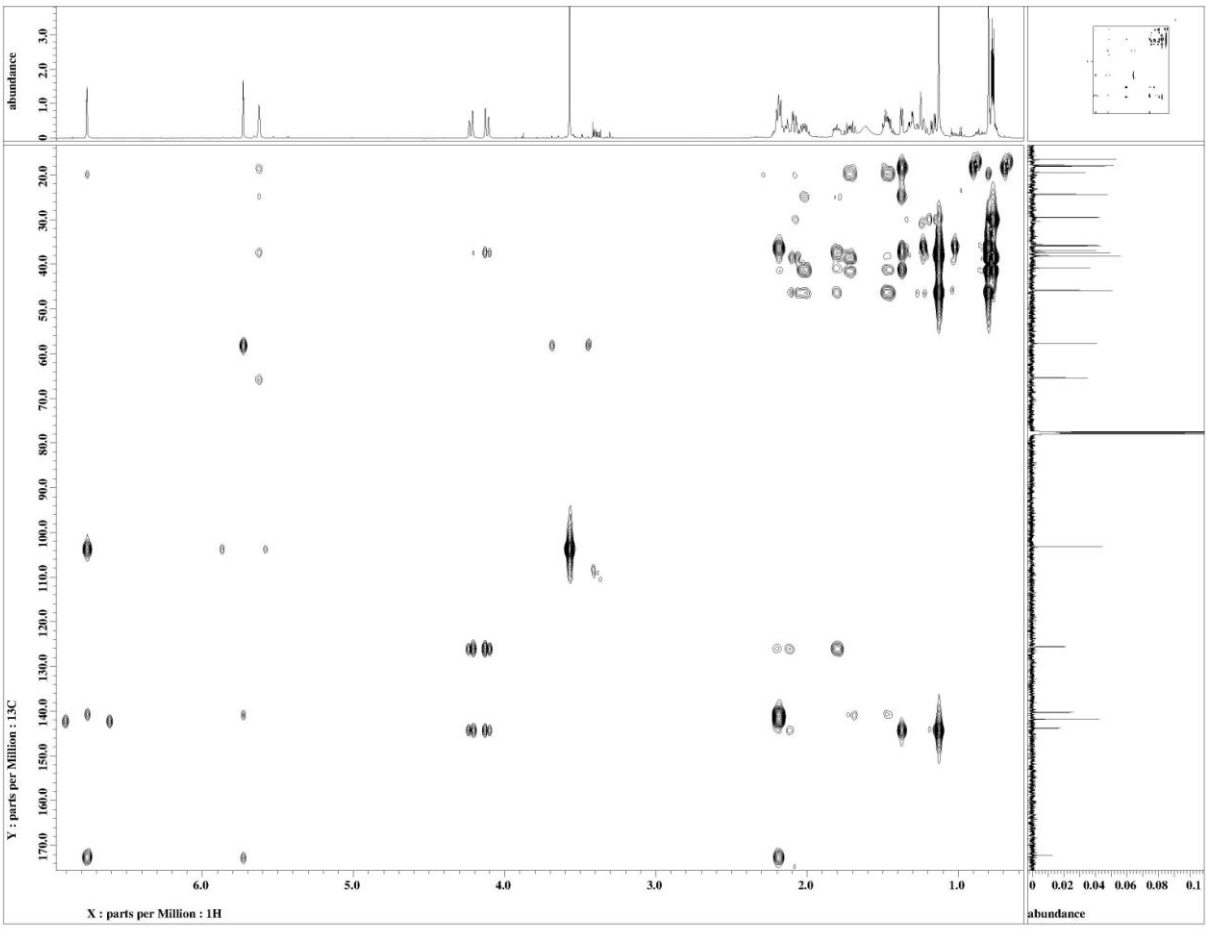


Figure S8. NOESY spectrum of **1** in $CDCl_3$.

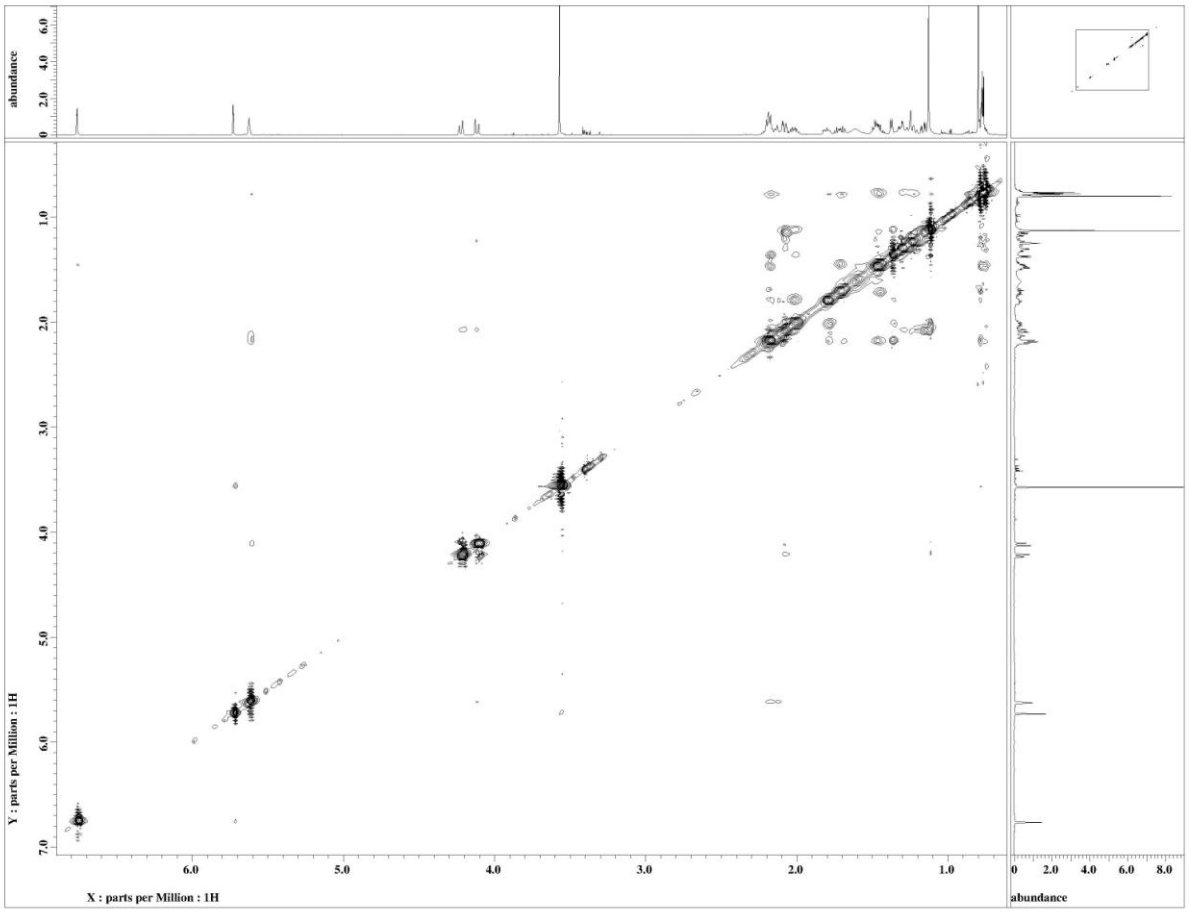


Figure S9. ^{1}H NMR spectrum of **2** in $CDCl_3$ (600 MHz).

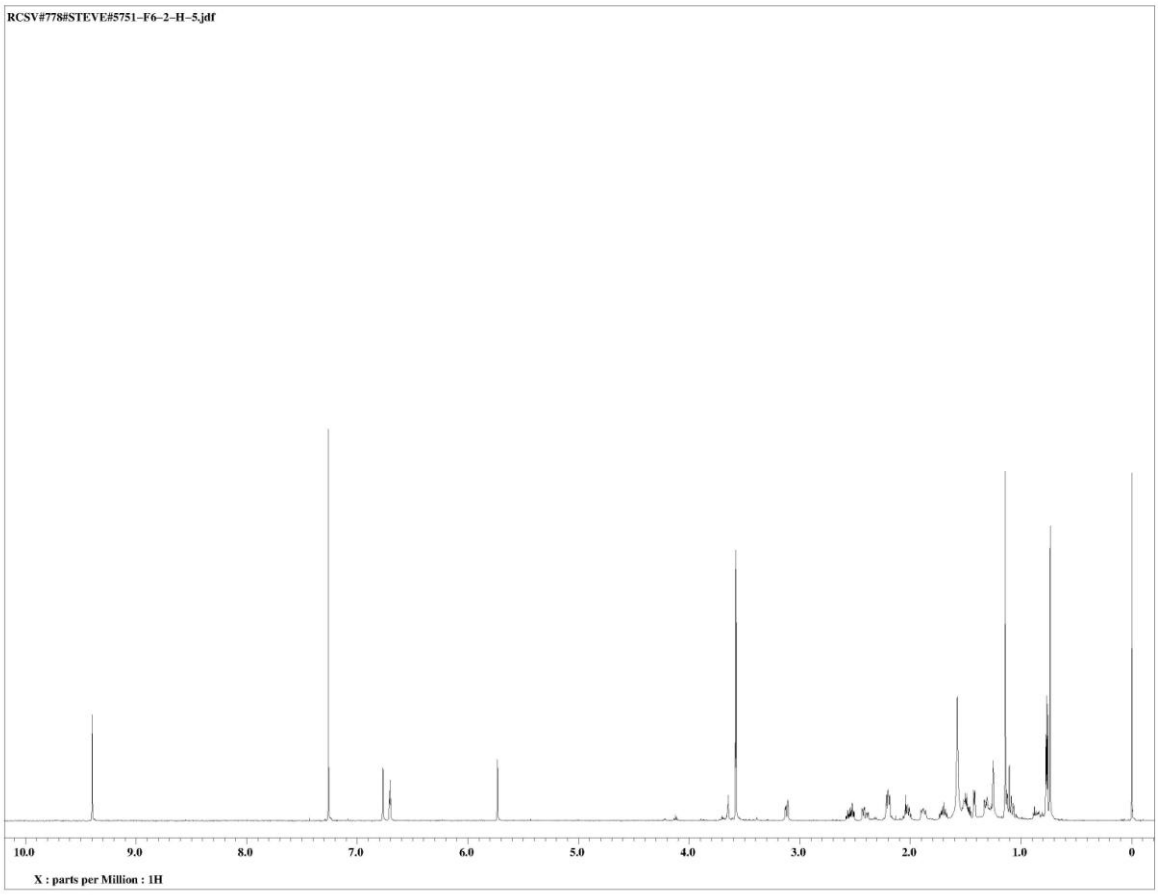


Figure S10. ^{13}C NMR spectrum of **2** in $CDCl_3$ (150 MHz).

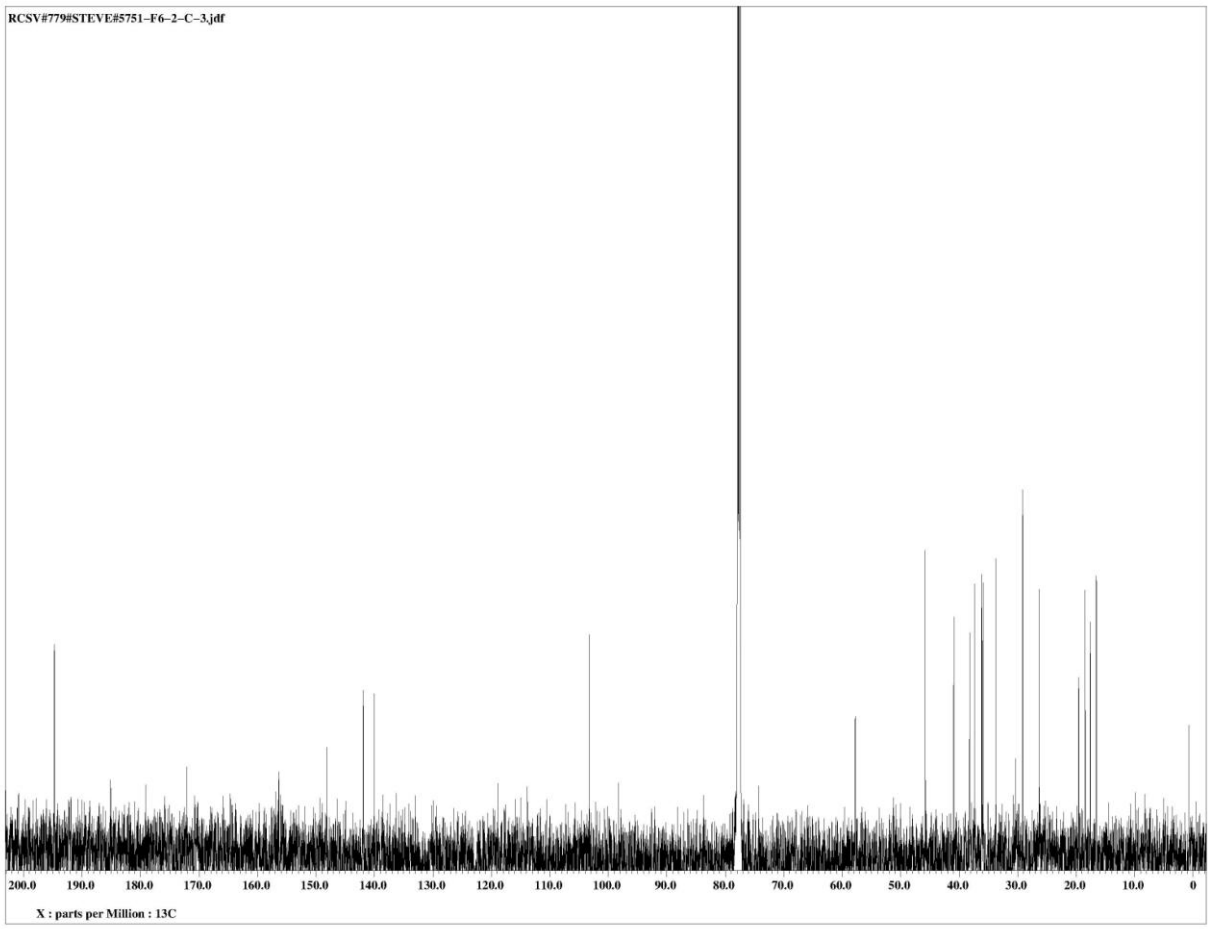


Figure S11. HSQC spectrum of **2** in $CDCl_3$.

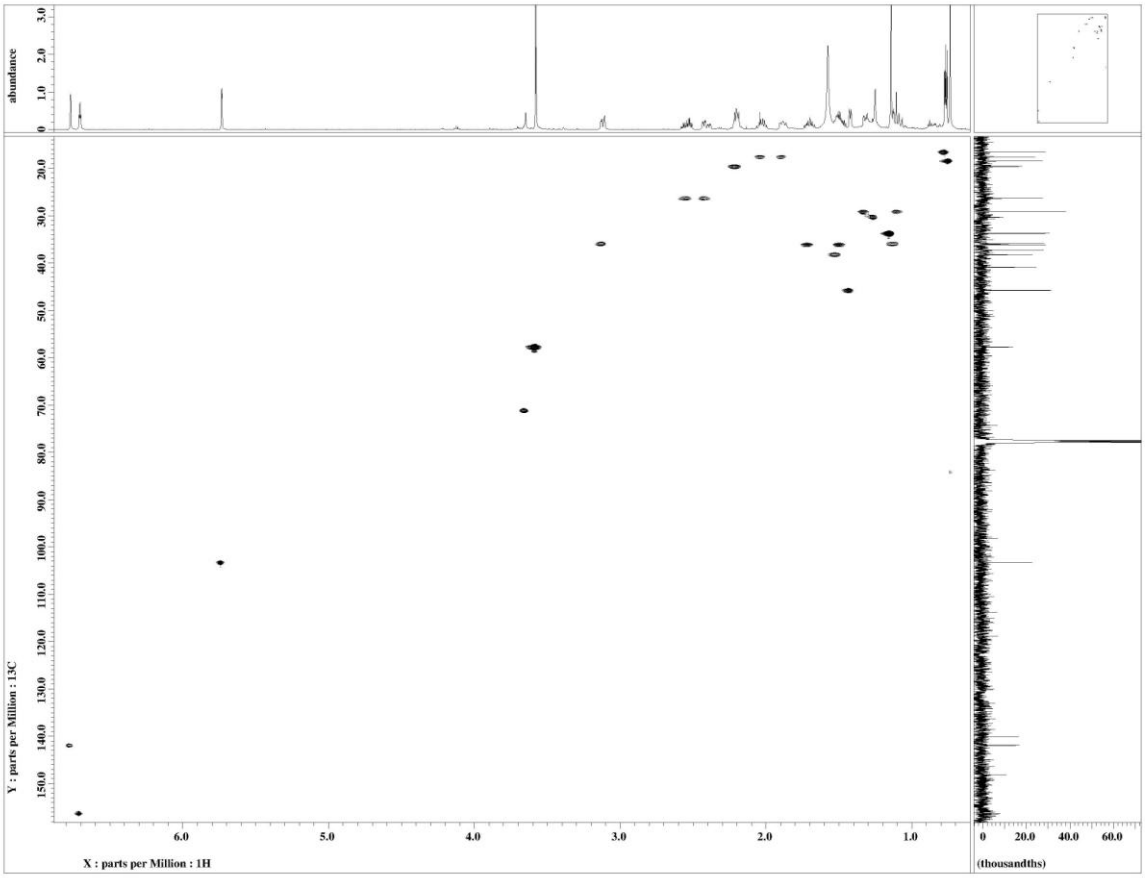


Figure S12. ^{1}H-^{1}H COSY spectrum of **2** in $CDCl_3$.

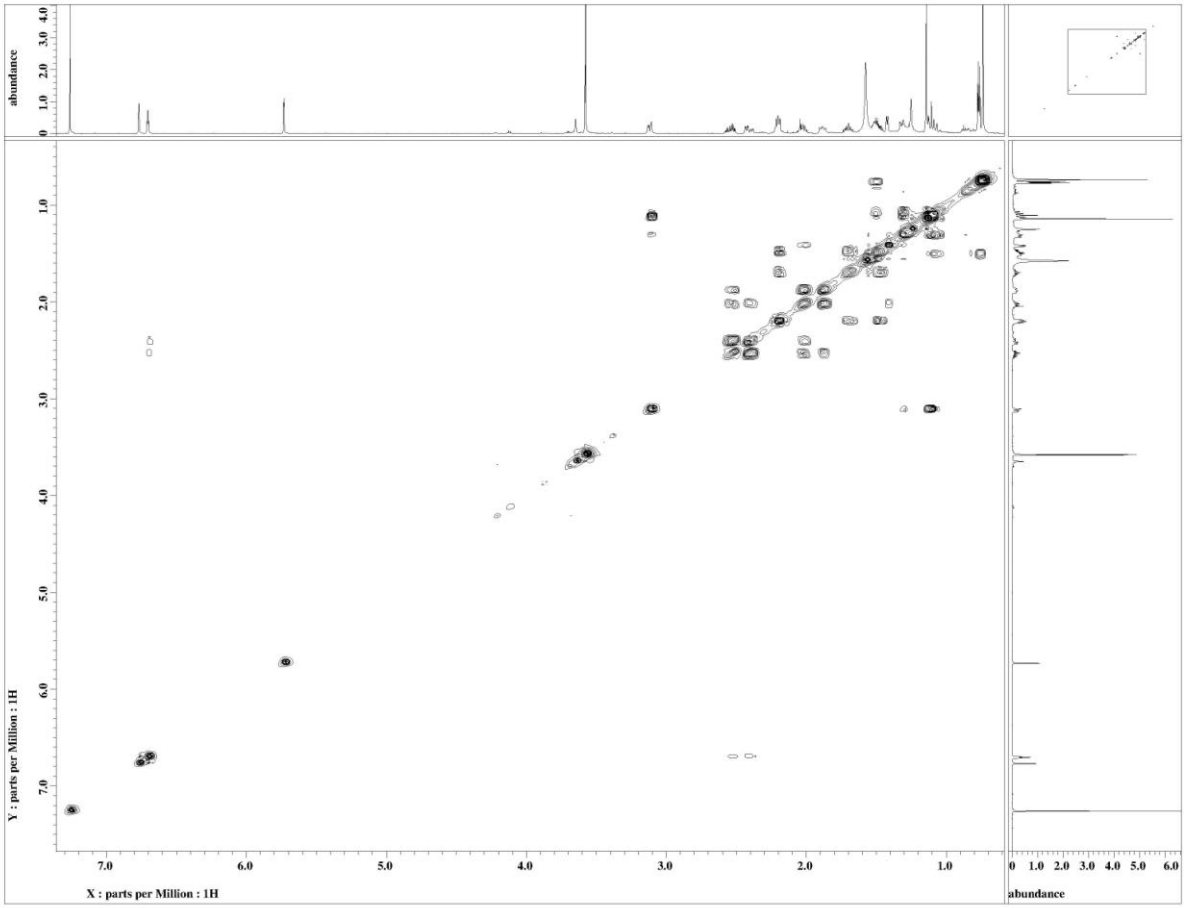


Figure S13. HMBC spectrum of **2** in $CDCl_3$.

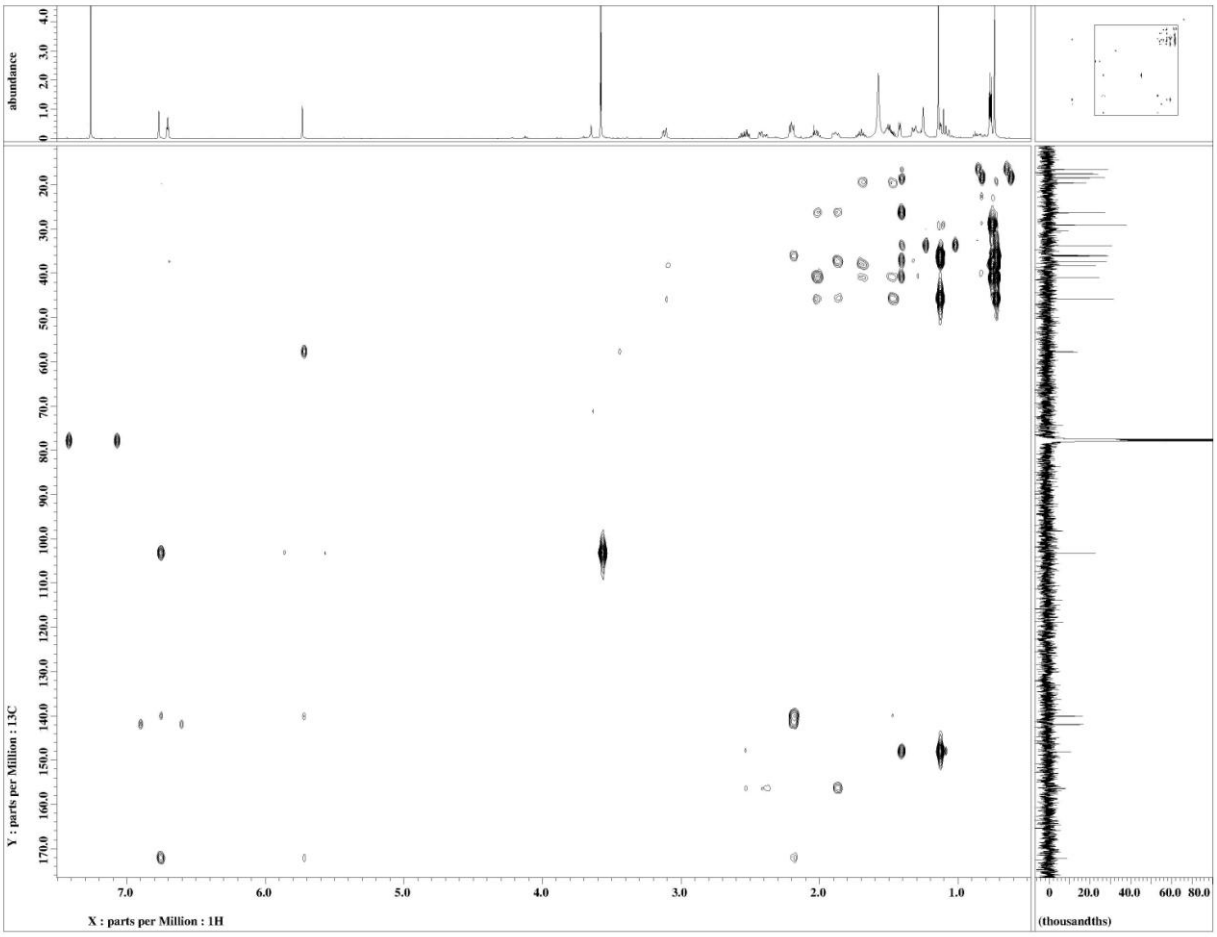


Figure S14. NOESY spectrum of **2** in $CDCl_3$.