SUPPLEMENTARY MATERIAL

Two new triterpenoids from *Gardenia jasminoides* fruits

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ABSTRACT

A new cycloartane triterpenoid, named gardenolic acid C (**1**), a new ursane triterpenoid, named 3*β*,16*β*,21*β*,23,24-pentahydroxy urs-12,18,20-trien-28-oic acid γ-lactone (**2**), together with three know triterpenoids, gardenolic acid A (**3**), gardenolic acid B (**4**), and 3*α*,16*β*,23,24-tetrahydroxy-28-nor-ursane-12,17,19,21-tetraen (**5**) were isolated from the fruits of *Gardenia jasminoides* Ellis. The structures of these compounds were elucidated by analyses of spectroscopic data. All isolates were evaluated for their neuroprotective effects *in vitro*.

KEYWORDS

Gardeniae Fructus, gardenolic acid C, ursane-type triterpenoid, neuroprotective effect

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Supplementary Materials

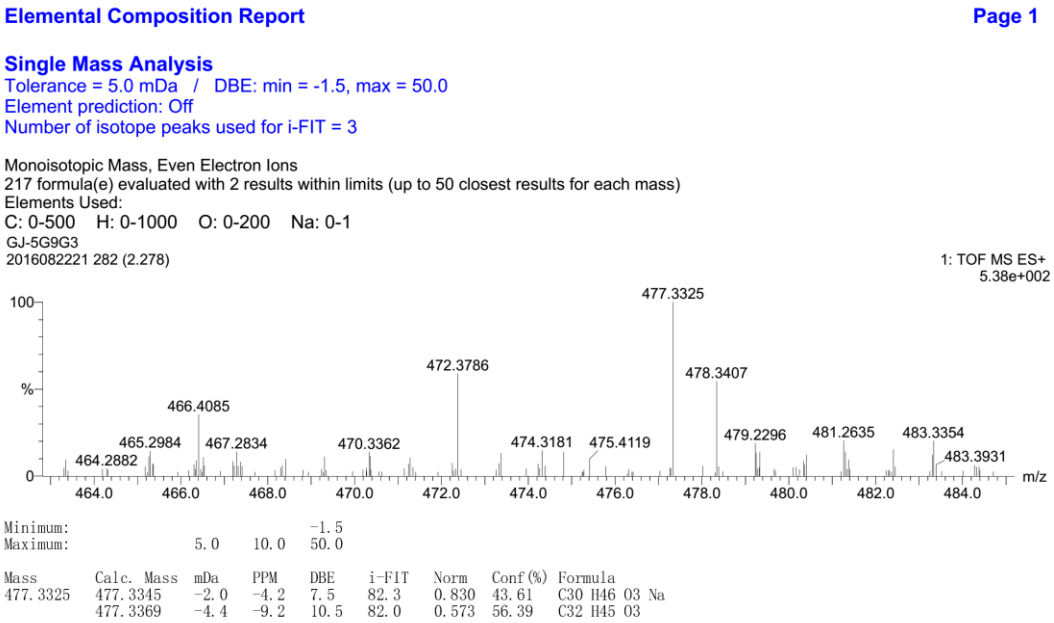


Figure S1 HRESIMS spectrum of compound 1

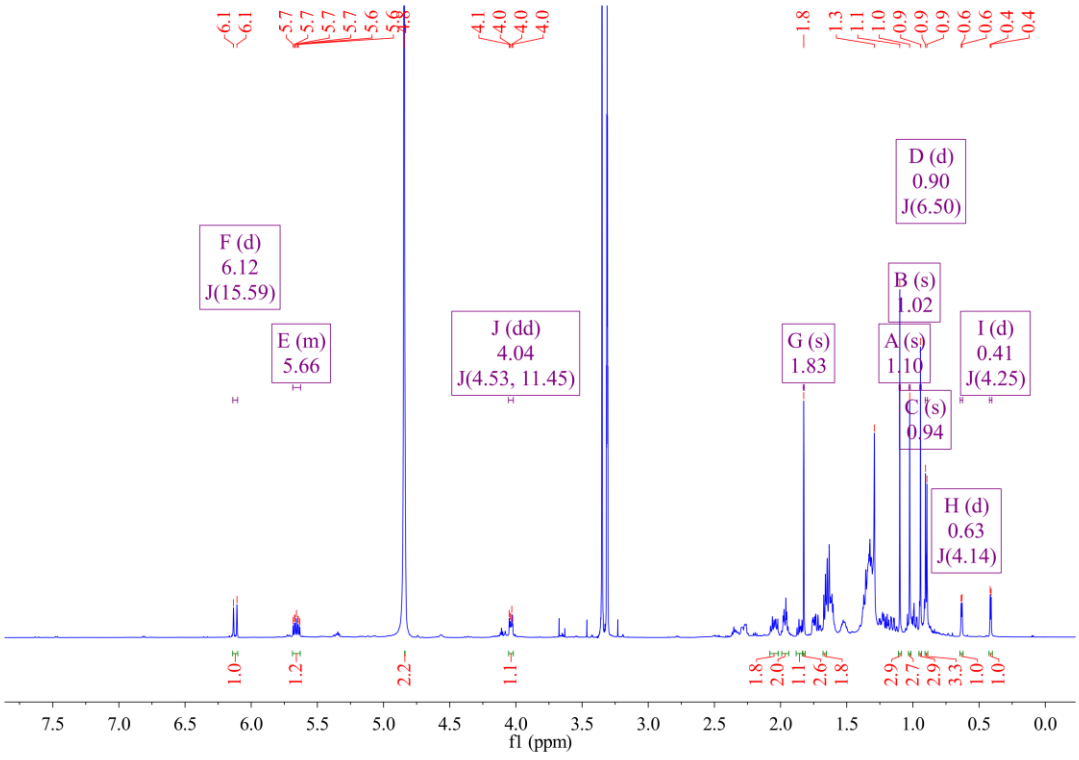


Figure S2 ^{1}H-NMR spectrum of compound 1

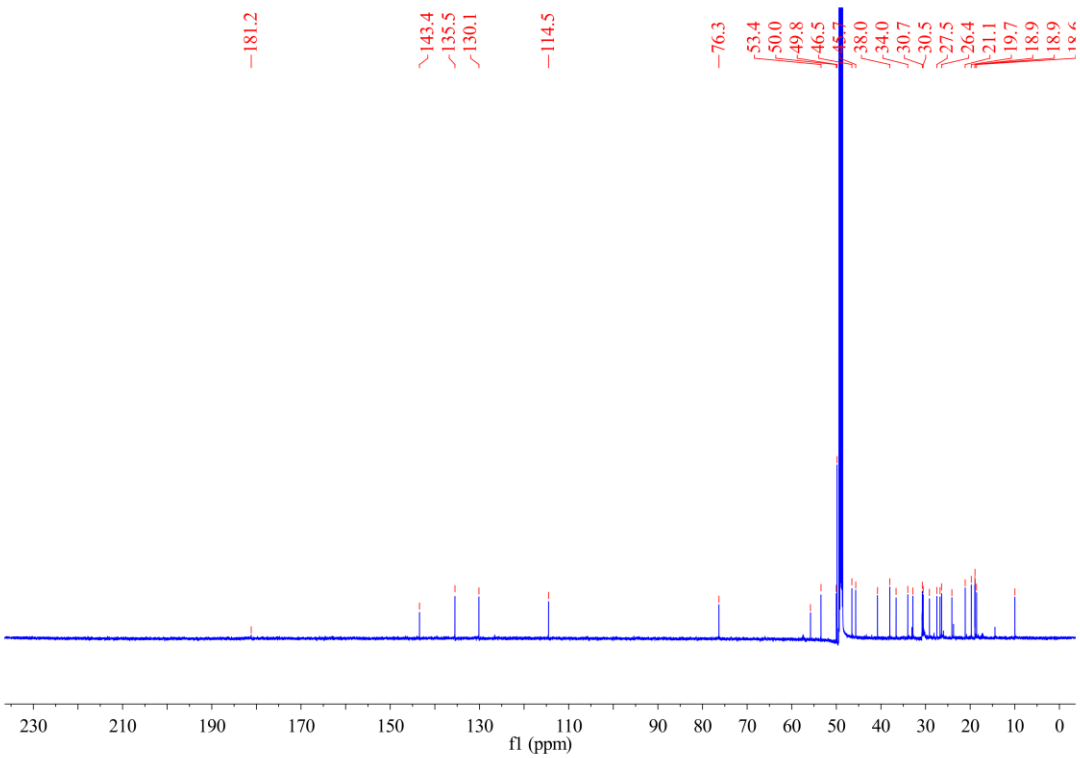


Figure S3 ^{13}C-NMR spectrum of compound 1

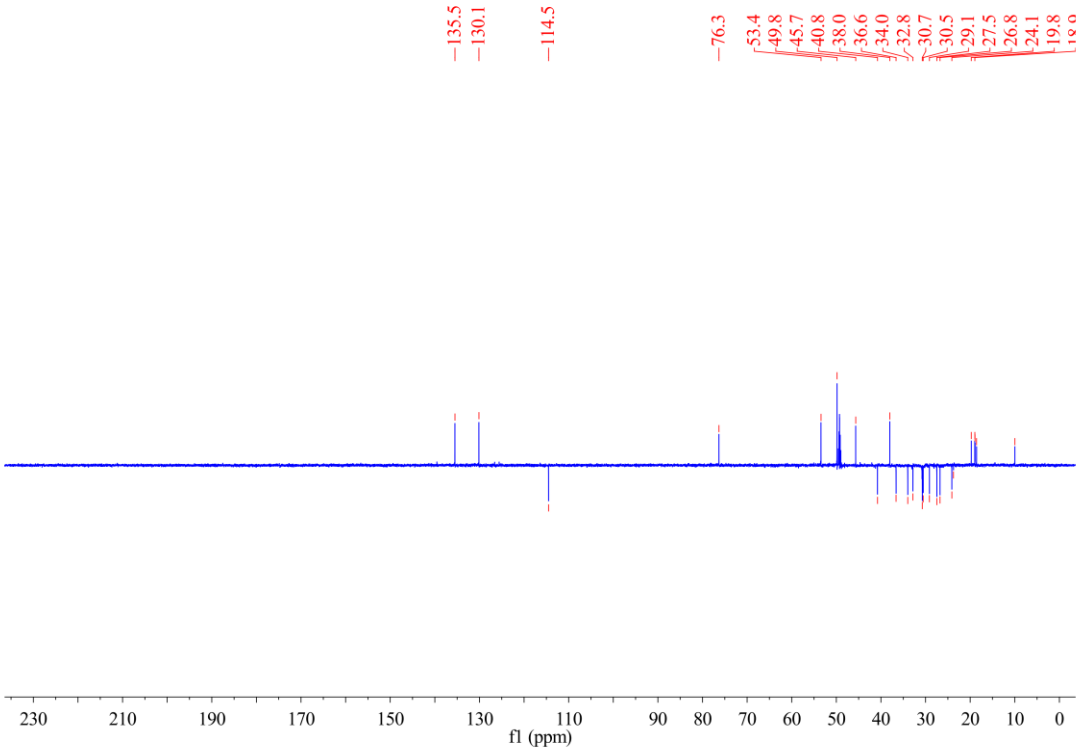


Figure S4 DEPT-135 spectrum of compound 1

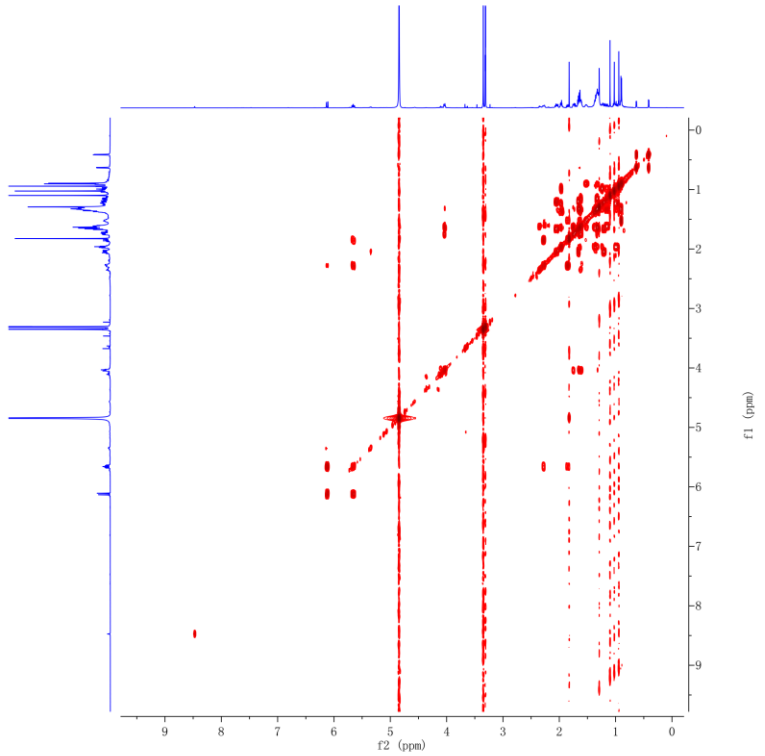


Figure S5 ^{1}H-^{1}H COSY spectrum of compound 1

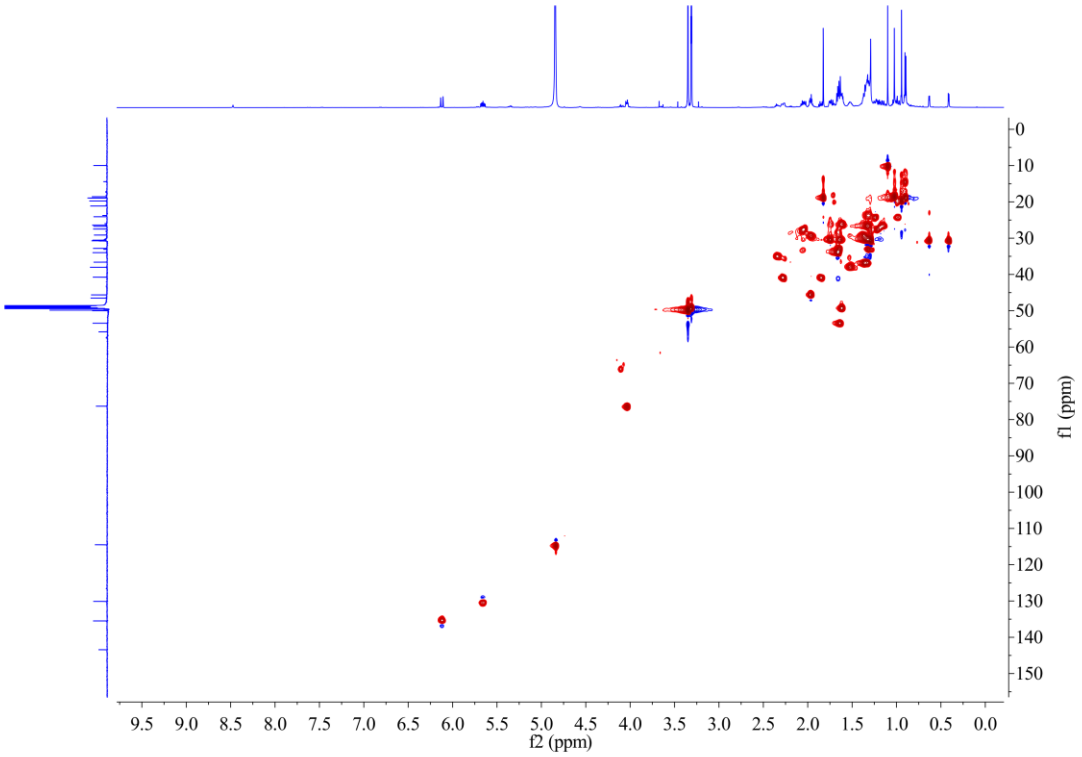


Figure S6 HSQC spectrum of compound 1

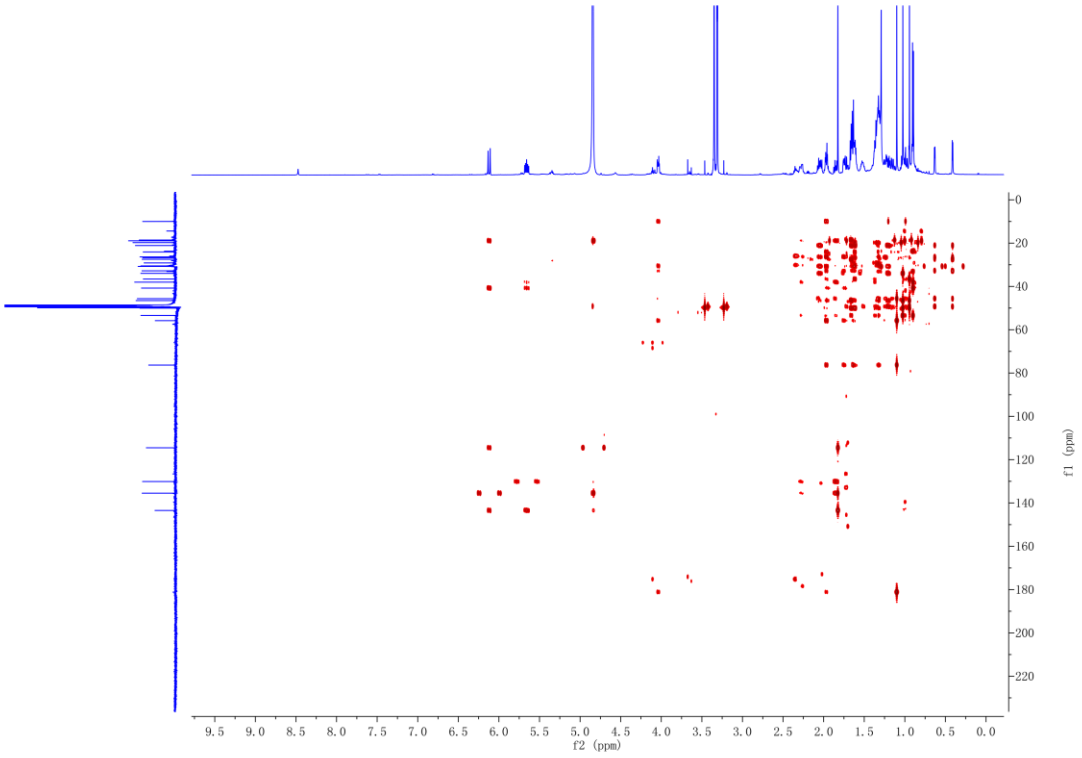


Figure S7 HMBC spectrum of compound 1

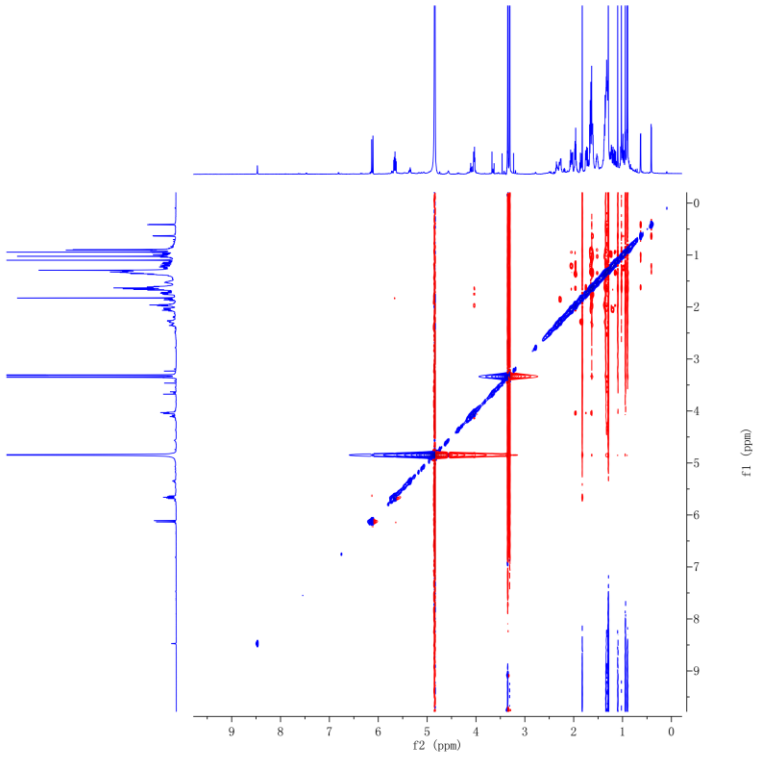
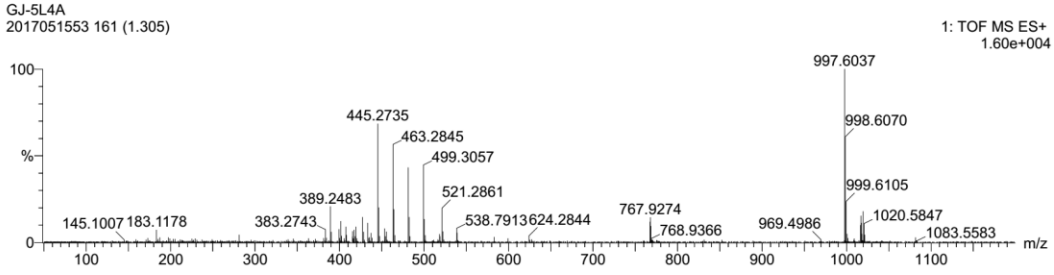


Figure S8 NOESY spectrum of compound 1

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 30-65 H: 0-100 O: 0-15 Na: 0-1
GJ-5L4A
2017051553 161 (1.305)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
499.3057	499.3060	-0.3	-0.6	9.5	122.9	n/a	n/a	C30 H43 O6

Figure S9 HRESIMS spectrum of compound 2

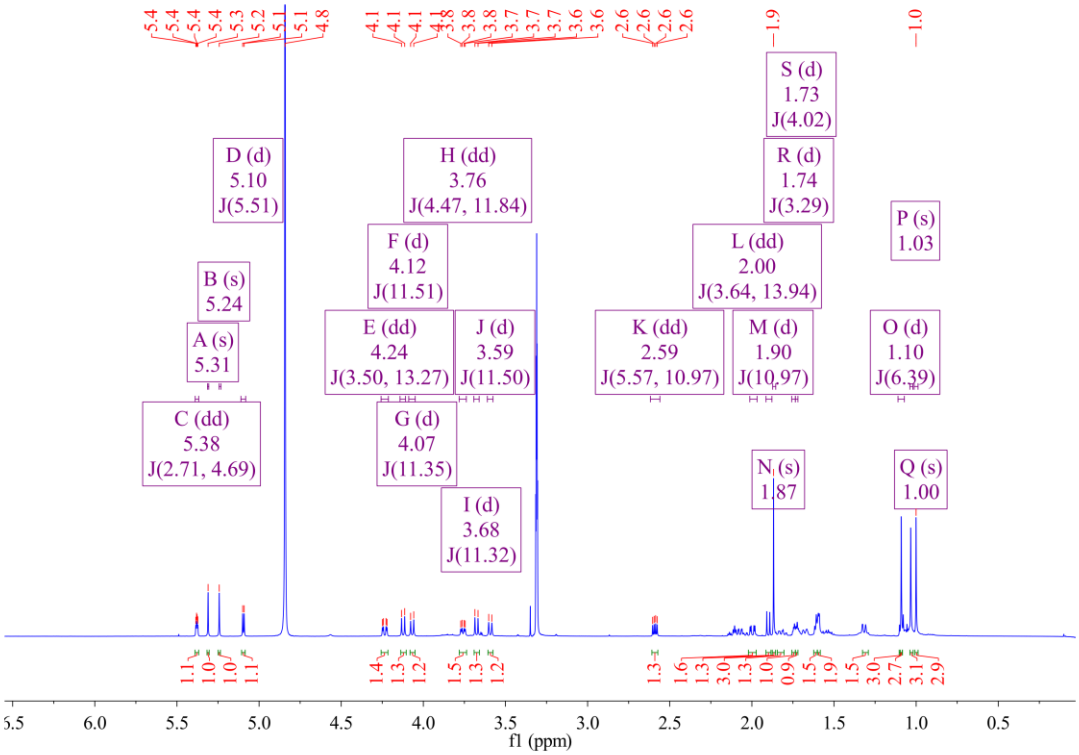


Figure. S10 ^{1}H-NMR spectrum of compound 2

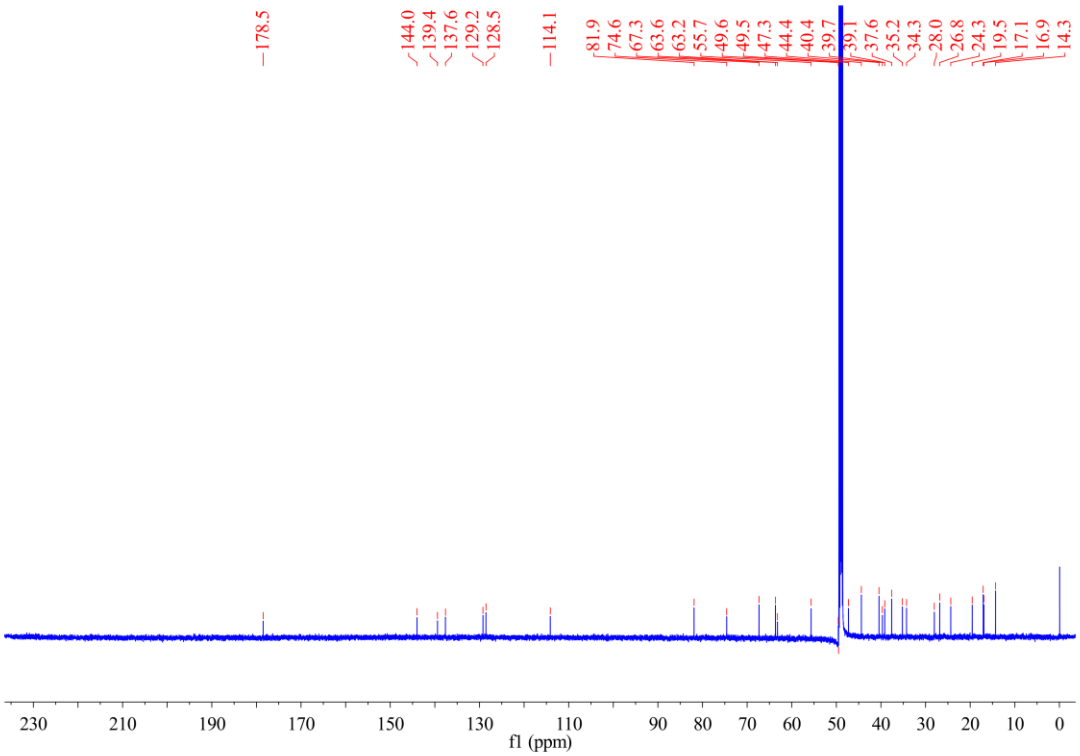


Figure S11 ^{13}C-NMR spectrum of compound 2

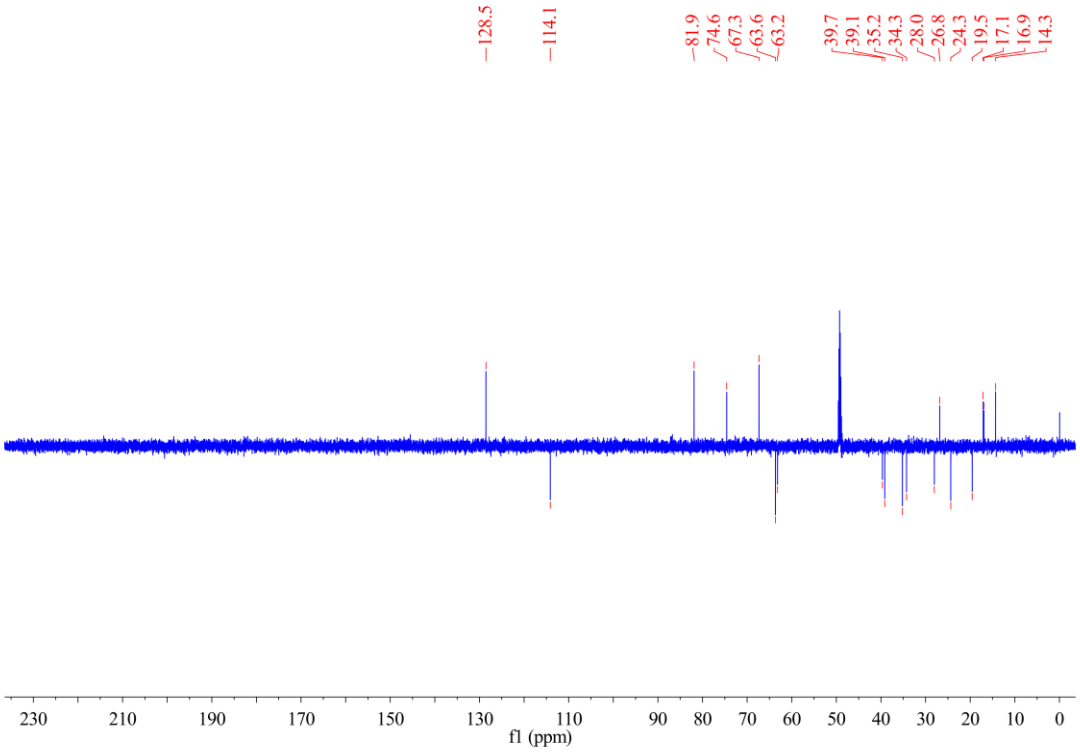


Figure S12 DEPT-135 spectrum of compound 2

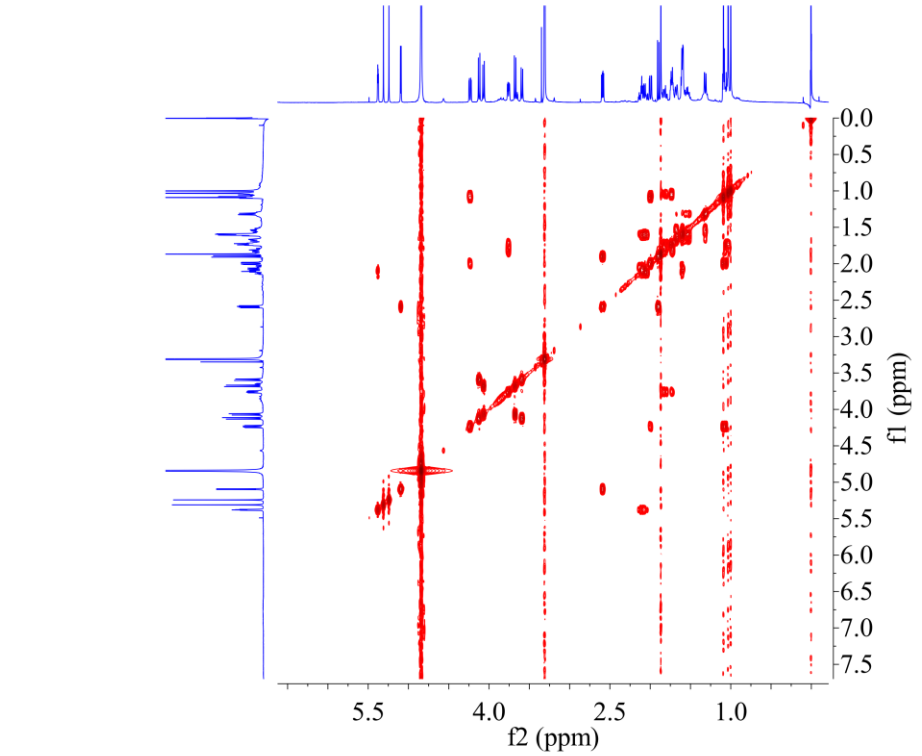


Figure S13 ^{1}H-^{1}H COSY spectrum of compound 2

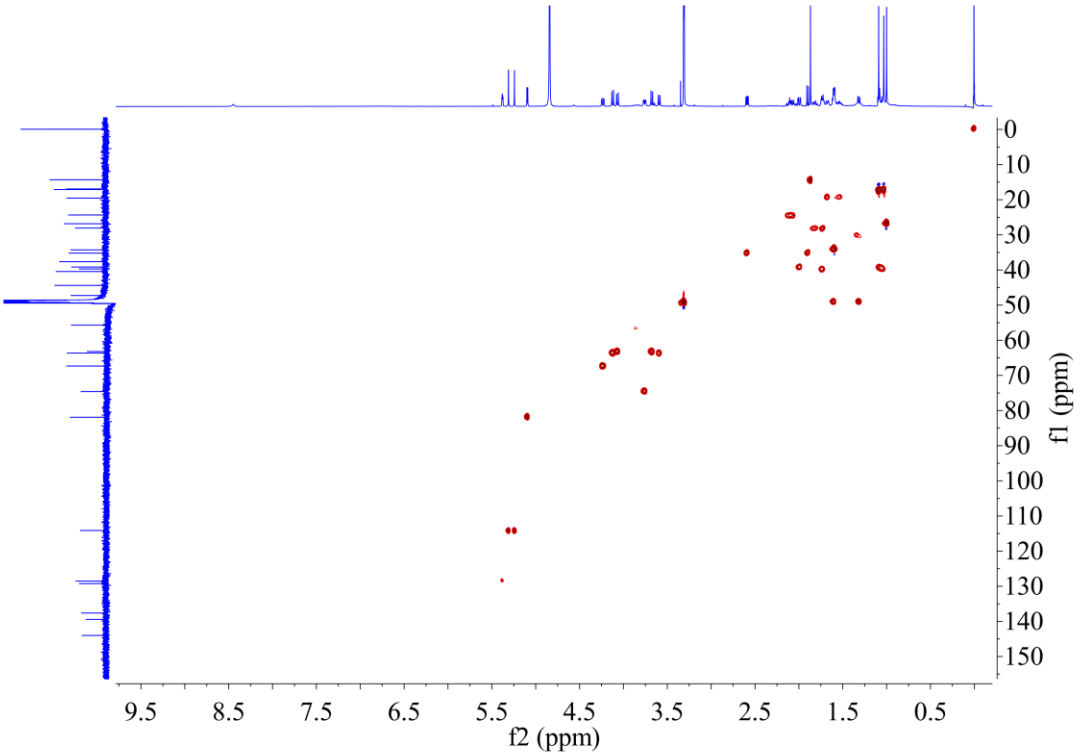


Figure S14 HSQC spectrum of compound 2

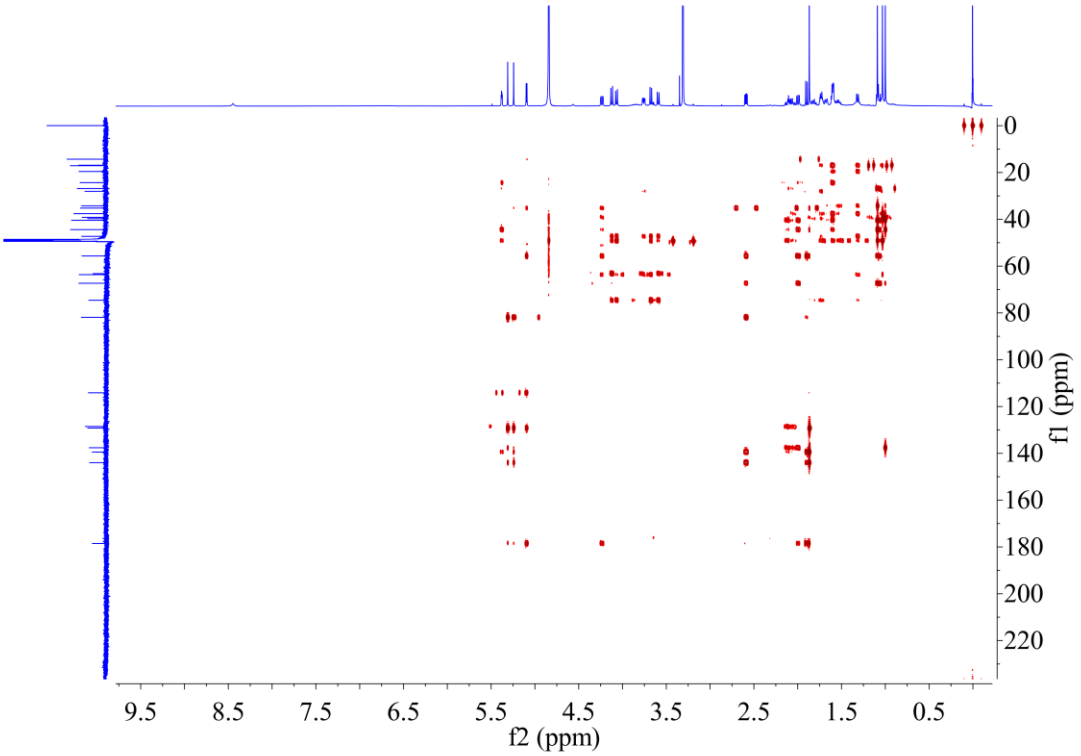


Figure S15 HMBC spectrum of compound 2

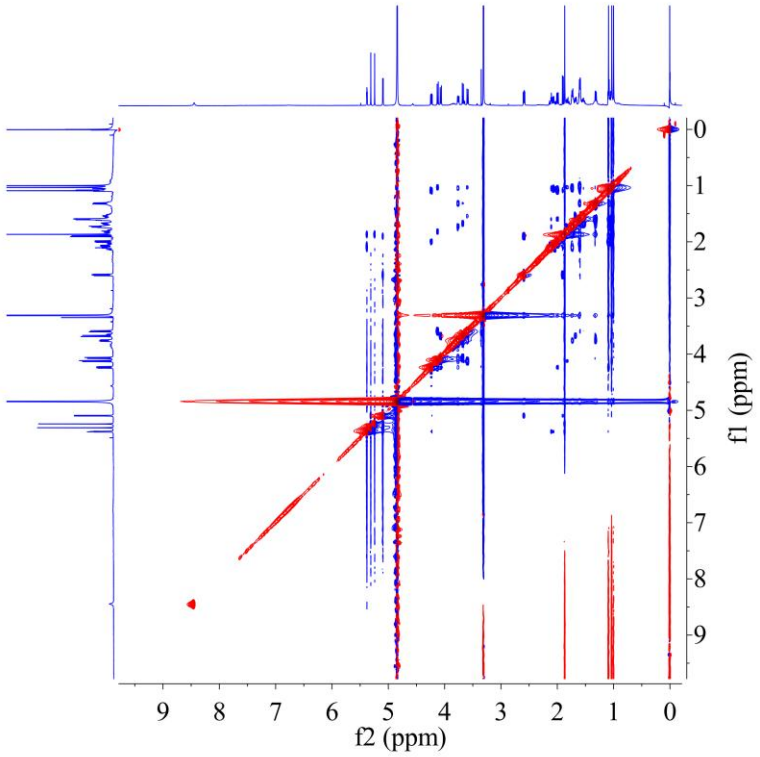


Figure S16 NOESY spectrum of compound 2

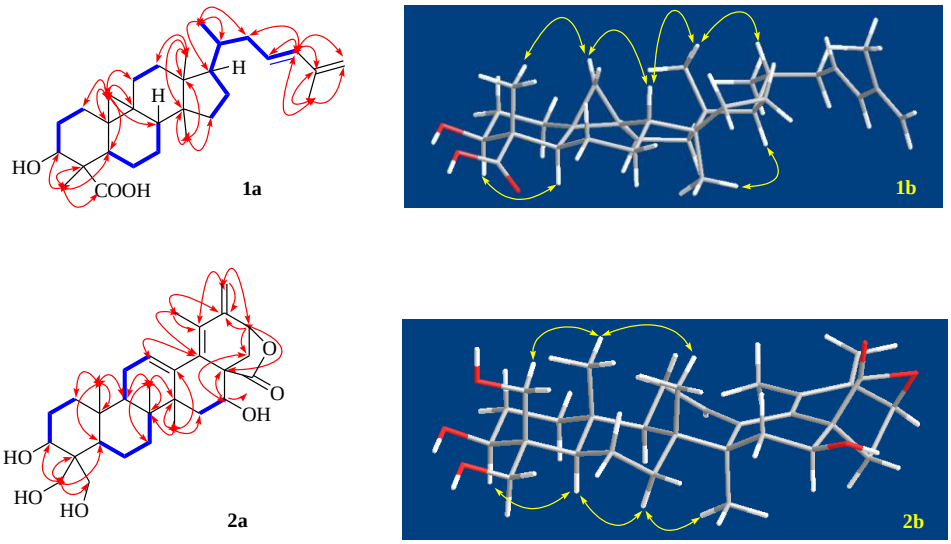


Figure S17. ^{1}H-^{1}H COSY (▬) and key HMBC correlations (1a and 2a) NOESY correlations (1b and 2b) of compounds **1** and **2**.

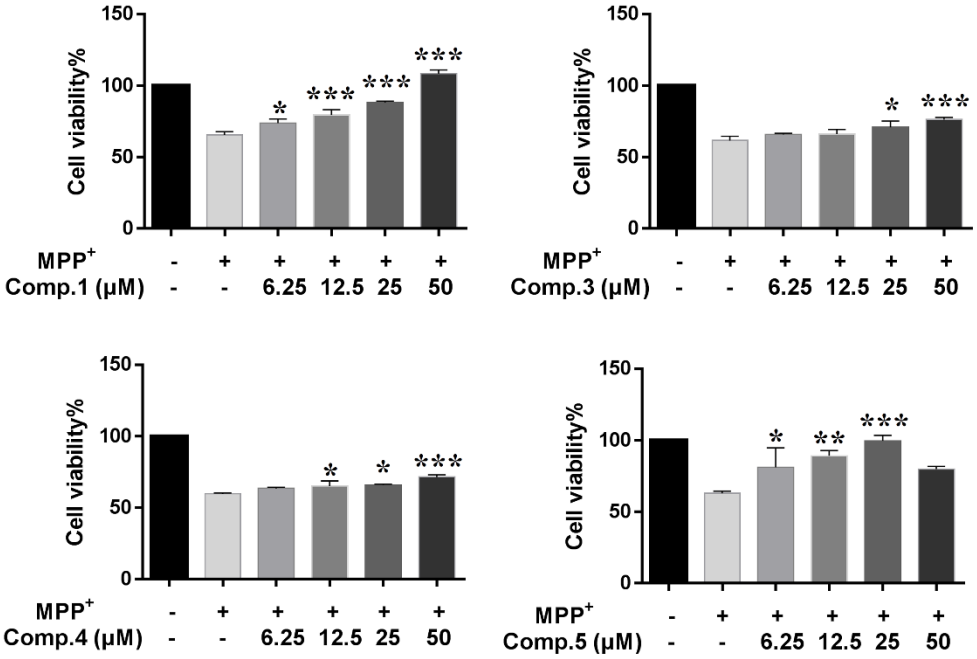


Figure S18. Cell viabilities of MPP^{+}-challenged SH-SY5Y cells, and effects of compounds **1**, **3-5** (mean ± SD %, n = 3), $^{*}P$ <0.05, $^{**}P$ <0.01, $^{***}P$ <0.001, * vs. MPP^{+}-challenged group.

Table S1. NMR spectroscopic data (in CD_3OD) of compounds 1 and 2

No.	1		2	
	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	32.8	1.32	39.7	1.73, 1.05
2	30.5	1.75, 1.64	28.0	1.82, 1.73
3	76.3	4.04 (dd, 11.4, 4.5)	74.6	3.76, dd (11.8, 4.5)
4	55.8		47.3	
5	45.7	1.96	49.1	1.32
6	24.1	1.24, 0.99	19.5	1.67, 1.53
7	26.8	1.33,1.16	34.3	1.59
8	49.3	1.62	40.4	
9	21.1		49.2	1.61
10	26.4		37.6	
11	27.5	2.05	24.3	2.09
12	34.0	1.66	128.5	5.38, dd (4.7, 2.7)
13	46.5		137.6	
14	50.0		44.4	
15	36.6	1.36	39.1	1.99, dd (13.7, 3.6) 1.08, t (13.7)
16	29.1	1.96, 1.51	67.3	4.24, dd (13.7, 3.6)
17	53.4	1.64	55.7	
18	18.6	1.03, s	139.4	
19	30.7	0.61, d (4.2), 0.43, d (4.2)	144.0	
20	38.0	1.51	129.2	
21	18.9	0.90, d (6.5)	81.9	5.10, d (5.5)
22	40.8	2.28, 1.84	35.2	2.59, dd (11.0, 5.5), 1.90, d (11.0)
23	130.1	5.66	63.2	4.07, d (11.4), 3.68, d (11.4)
24	135.5	6.12, d (15.6)	63.6	4.12, d (11.5), 3.59, d (11.5)
25	143.4		16.9	1.03, s
26	114.5	4.84	17.1	1.10, s
27	18.9	1.83, s	26.8	1.00, s
28	181.2		178.5	
29	10.0	1.10, s	14.3	1.87, s
30	19.7	0.94, s	114.1	5.31, s, 5.24, s

Multiplets or overlapped signals are reported without designating multiplicity