Supplementary Material

A new demethyl abietane diterpenoid from the roots of *Tripterygium wilfordii*

Peng Li[a,b], Shao-xin Shen[b], Ling-xue Liu[b], Jian-hua Xu[b], Xin-hua Ma[a], Dong-mei Shi[a] and Zhi-qiang Zhang[b]

[a] Department of Natural Medicine, School of Pharmacy, Fujian Medical University, Fuzhou, P.R.China; [b] Fujian Key Laboratory of Natural Medicine Pharmacology, School of Pharmacy, Fujian Medical University, Fuzhou, P.R.China

Correspondence to: Zhi-qiang Zhang, email: zzq@fjmu.edu.cn

ABSTRACT

A new demethyl abietane diterpenoid, Triptotin K (**3**) together with three known compounds, friedelin (**1**), canophyllal (**2**), and triptonoterpene (**4**) were isolated from the roots of *Tripterygium wilfordii* Hook. f. by silica gel column and preparative high performance liquid chromatography. Their structures were determined by extensive NMR data and mass spectroscopic analysis. Triptotin K showed cytotoxic activities against KB, KBv200, HepG2, and MCF-7/ADM cells lines with IC_{50} values of 29.88, 36.50, 39.55, and 41.38 μM, respectively.

Keywords: *Tripterygium wilfordii;* diterpenoids; triterpenes; cytotoxicity

List of Supporting Information

Table S1. ^{13}C NMR (125 MHz) and ^{1}H NMR (500 MHz) spectral data of compound **3** (*J* in Hz, δ in ppm, recorded in CD_3OD)

carbon	δ_C	δ_H	carbon	δ_C	δ_H
1	84.4 (d)	4.25 (dd,5.2,13.6)	11	93.7 (s)	
2	40.5 (t)	2.59 (m), 2.81 (m)	12	133.2 (d)	6.24 (s)
3	206.7 (s)		13	147.1 (s)	
4	45.2 (d)	2.39 (m)	14	184.8 (s)	
5	43.9 (d)	1.27 (m)	15	26.5 (d)	2.99 (m)
6	20.0 (t)	1.60 (m), 1.99 (m)	16	21.5 (q)*	1.11 (d, 6.8)*
7	23.7 (t)	2.26 (m), 2.77 (m)	17	21.4 (q)*	1.06 (d, 6.8)*
8	131.2 (s)		18	12.0 (q)	1.16 (d, 6.6)
9	147.5 (s)		19	13.1 (q)	1.57 (s)
10	37.5 (s)				

* Assignments may be interchanged.

Table S2. ^{13}C NMR (125 MHz) and ^{1}H NMR (500 MHz) spectral data of compound **1**-**2** and **4** (*J* in Hz, δ in ppm, recorded in CD_3OD)

	1		2		4	
No.	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C
1	1.96(m), 1.72(m)	22.3	1.67(m), 1.96(m)	22.3	1.90(m), 2.49(m)	37.6
2	2.38(m), 2.28(m)	41.5	2.29(m), 2.39(m)	41.5	2.55(m), 2.71(m)	34.7
3		213.3		213.1		217.2
4	2.25(q, 7.3)	58.2	2.23(q,6.7)	58.2		47.3
5		42.2		42.0	1.90(m)	50.1
6	1.74(m), 1.29(m)	41.3	1.27(m), 1.74(m)	41.1	1.81(m), 1.93(m)	19.5
7	1.50(m), 1.37(m)	18.2	1.37(m)	18.1	2.61(m), 2.92(m)	24.6
8	1.39(m)	53.1	1.39(m)	52.8		120.8
9		37.4		37.1		146.4
10	1.54(m)	59.5	1.52(m)	59.3		37.1
11	1.46(m), 1.27(m)	35.6	1.48(m)	35.4	6.85(d,8.2)	117.3
12	1.34(m), 1.32(m)	30.5	1.25(m)	30.6	7.04(d,8.2)	123.6
13		39.7		38.7		130.4
14		38.3		37.7		150.1
15	1.48(m), 1.28(m)	32.4	1.23(m)	32.4	3.12(m)	26.9
16	1.59(m), 1.36(m)	36.0	1.24(m)	33.4	1.23(d,6.9)	22.5
17		30.0		47.7	1.26(d,6.9)	22.7
18	1.57(m)	42.8	2.19(m)	36.5	1.32(s)	24.4
19	1.38(m), 1.22(m)	35.3	1.41(m)	35.0	1.17(s)	26.6
20		28.2		28.3	1.14(s)	21.2
21	1.51(m), 1.32(m)	32.8	1.23(m)	32.4		
22	1.50(m), 0.93(m)	39.3	1.63(m), 2.06(m)	28.0		
23	0.88(d,5.4)	6.8	0.87(d,6.7)	6.8		
24	0.72(s)	14.7	0.72(s)	14.6		
25	0.87(s)	18.0	0.84(s)	17.2		

26	1.01(s)	20.3	0.67(s)	20.0
27	1.05(s)	18.7	1.07(s)	18.8
28	1.18(s)	32.1	9.48(s)	209.1
29	1.00(s)	35.6	0.95(s)	34.5
30	0.95(s)	32.8	0.98(s)	29.4

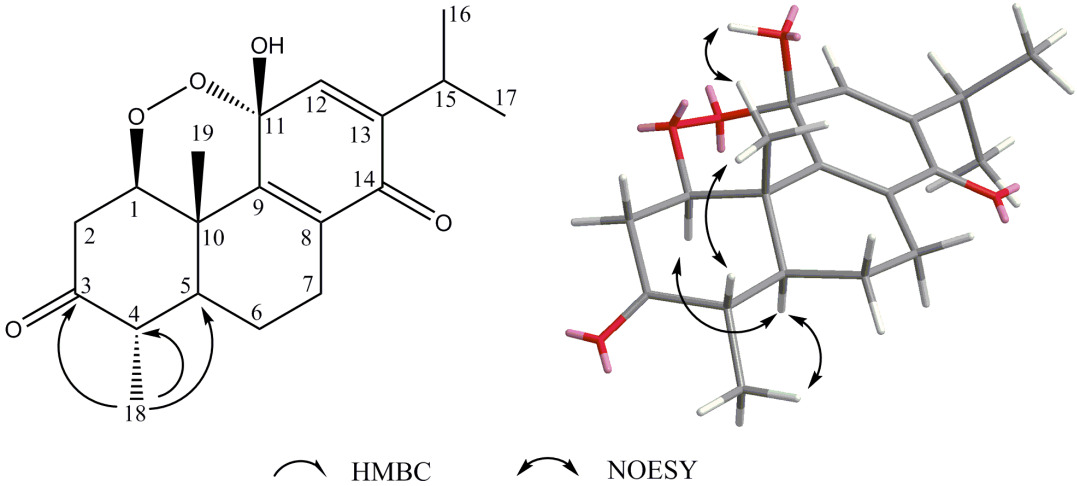

Figure S1. Key HMBC and NOESY correlations of compound **3.**

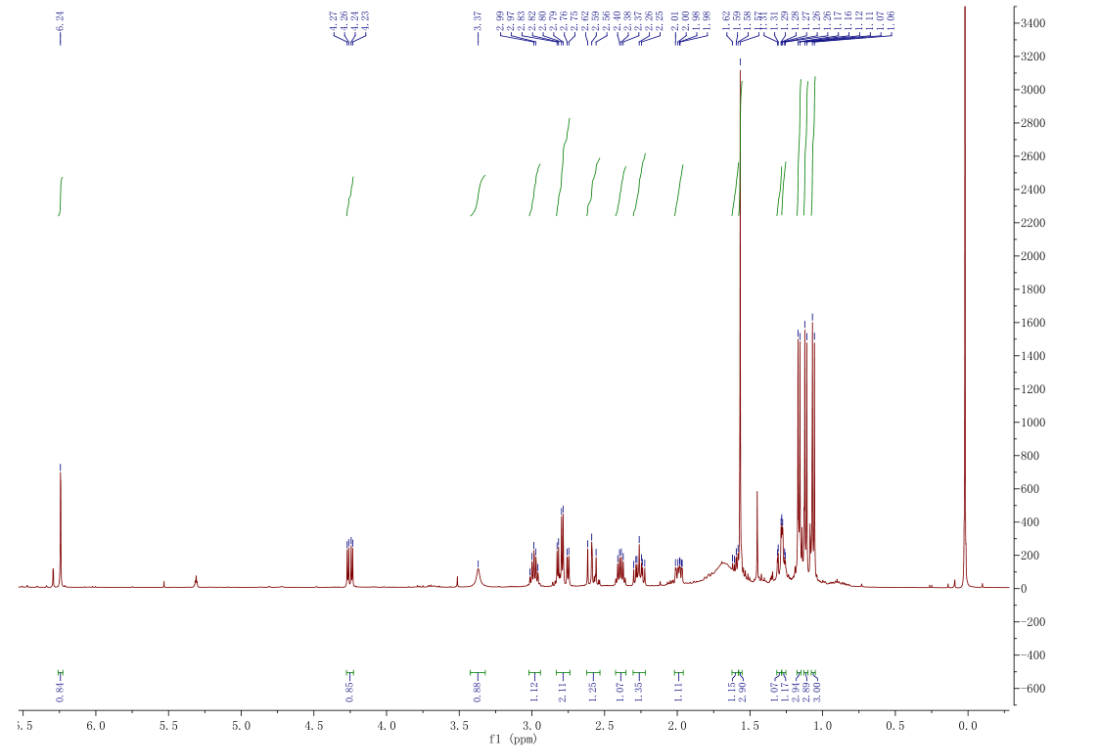

Figure S2. ^{1}H NMR Spectrum (500 MHz) of **3** in CD_3OD

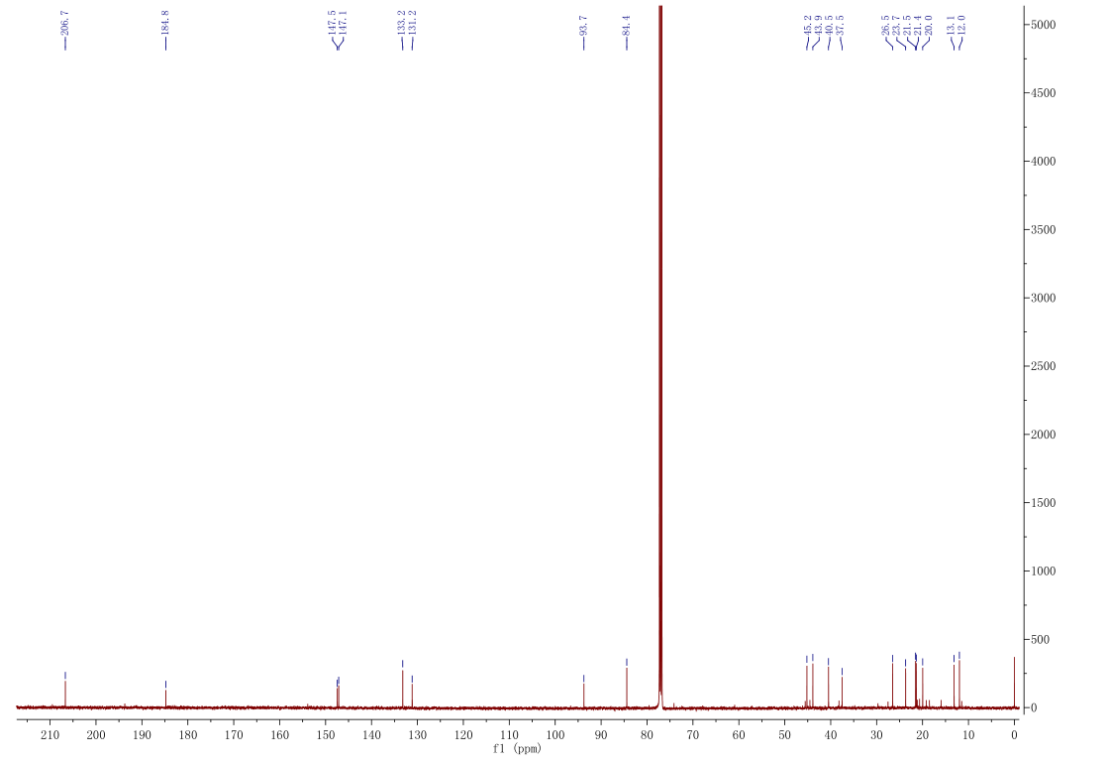

Figure S3. ^{13}C NMR Spectrum (125 MHz) of **3** in CD_3OD

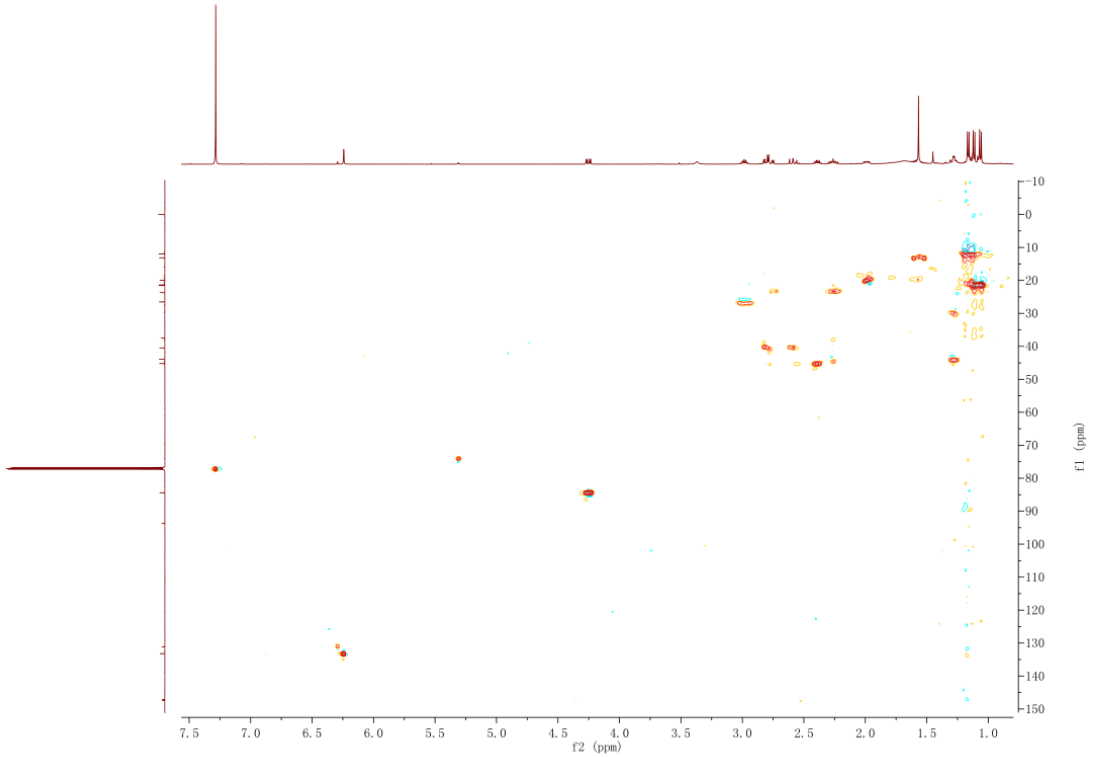

Figure S4. HSQC Spectrum of **3** in CD_3OD

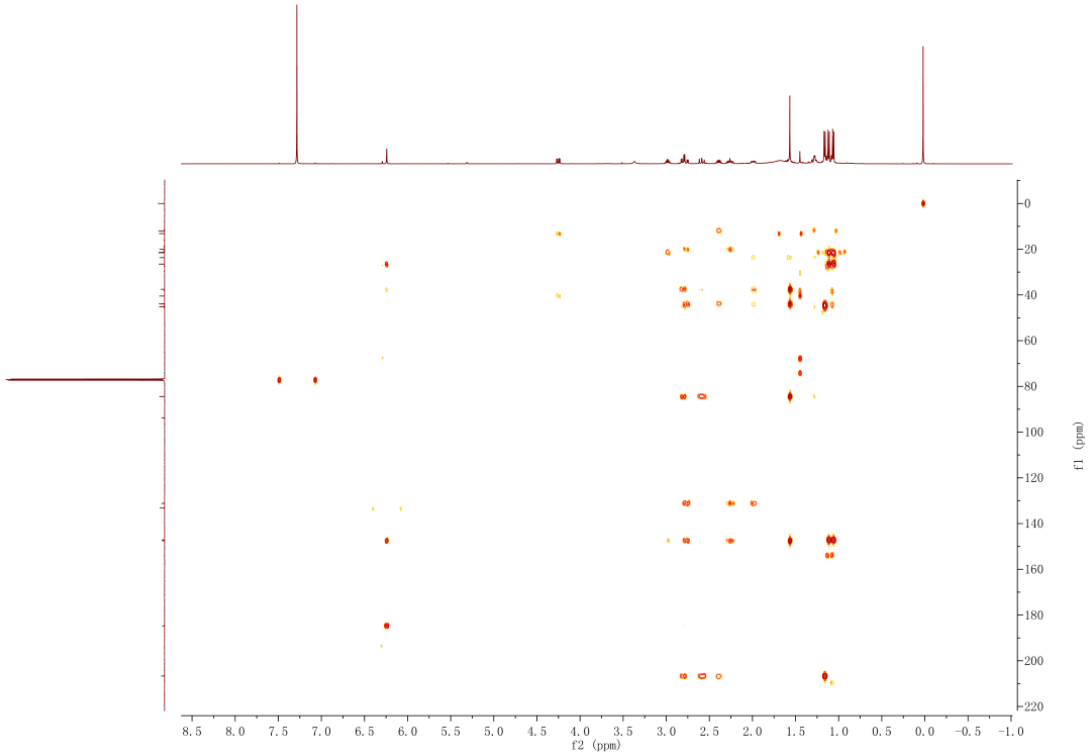

Figure S5. HMBC Spectrum of **3** in CD_3OD

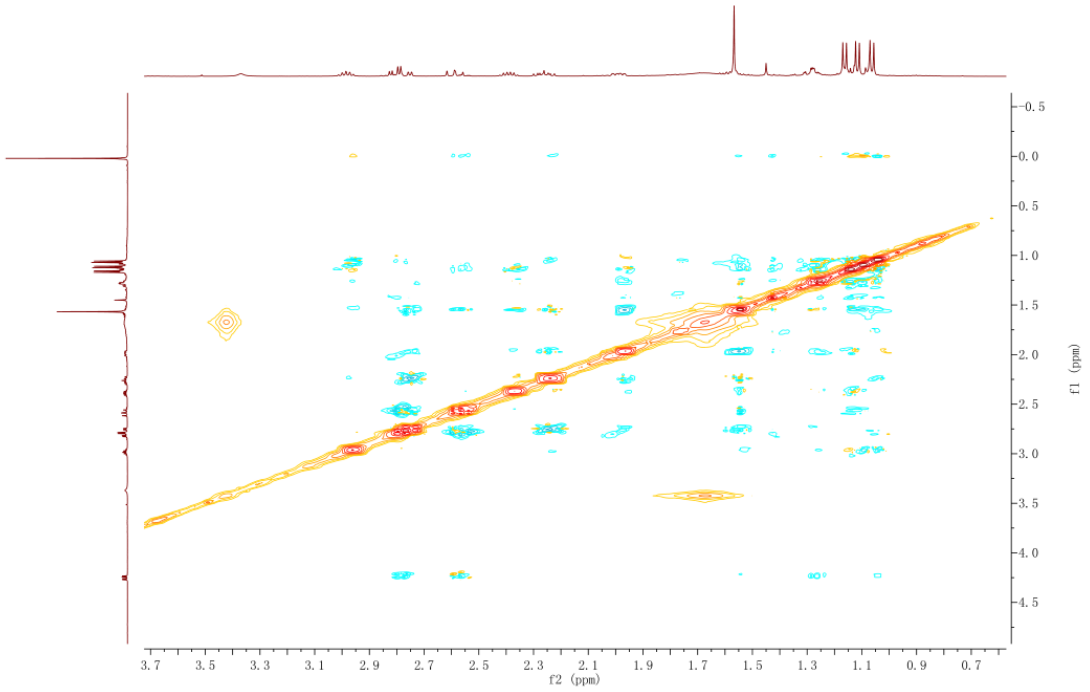

Figure S6. NOSEY Spectrum of **3** in CD_3OD

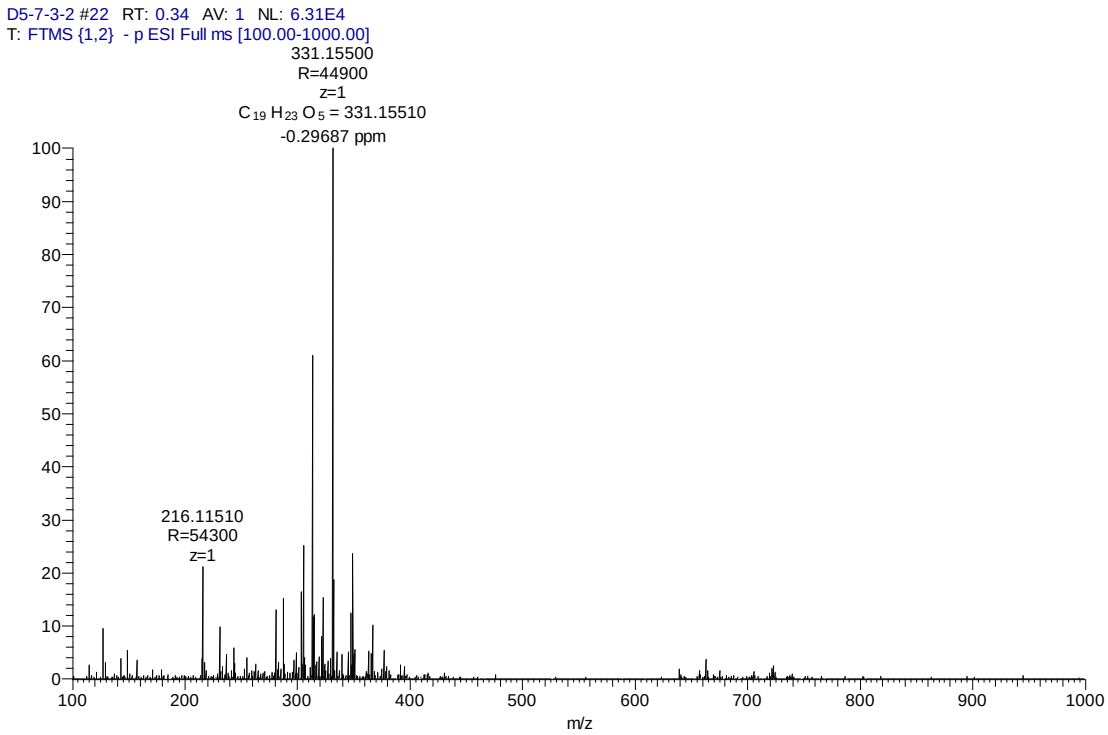

Figure S7. HR-ESI-MS Spectrum of **3**