SUPPLEMENTARY MATERIAL

Two new triterpenoids from *Gypsophila oldhamiana*

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Abstract

Two new triterpenoids (**1-2**) were isolated and elucidated from the roots of *Gypsophila oldhamiana*, together with four known triterpenoids (**3-6**). Their structures were identified to be 3 β -hydroxyolean-13(18)-ene-23, 28-dioic acid (**1**), 3 β , 12 α -dihydroxy-23-carboxyolean-28, 13 β -olide (**2**), 3 β , 16 α -dihydroxy-23-oxoolean-13(18)-en-28-oic acid (**3**), gypsogenin (**4**), quillaic acid (**5**) and gypsogenic acid (**6**) by spectral methods. All compounds were tested for their cytotoxicities against human tumor cell lines (lung cancer H460 and gastric cancer SGC-7901) and for their antiangiogenic effects using a zebrafish model. All compounds showed interesting antiangiogenic activities and the significant cytotoxicities against H460.

Keywords: *Gypsophila oldhamiana*; triterpenoid; cytotoxic activity; antiangiogenic effect

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Table S1. ^1H and ^{13}C NMR spectral data for compounds **1** and **2**. At 400/100 MHz, resp., in $\text{C}_5\text{D}_5\text{N}$; d in ppm.

Atom	1		2	
	δ_{C}	δ_{H}	δ_{C}	δ_{H}
1	38.6	1.82~1.75(m), 1.26~1.17(m)	38.6	1.83~1.76(m), 1.23~1.14(m)
2	27.2	2.02~1.95(m), 1.11~1.04(m)	26.9	2.03~1.97(m), 1.91~1.85(m)
3	74.6	4.74 (dd, $J=12$ Hz, 4 Hz)	74.6	4.70 (dd, $J=12$ Hz, 4 Hz)
4	53.7		53.7	
5	51.1	2.06~2.00(m)	50.9	2.02~1.95(m)
6	20.9	2.05~1.97(m), 1.61~1.54(m)	17.8	1.81~1.73(m), 1.59~1.52(m)
7	34.4	1.63~1.54(m), 1.38~1.32(m)	33.9	1.76~1.68(m), 1.26~1.19(m)
8	43.9		41.3	
9	50.6	1.73~1.66(m)	48.9	1.57~1.50(m)
10	36.2		35.8	
11	21.3	1.45~1.36(m)	22.7	2.37~2.28(m), 2.11~2.04(m)
12	24.7	2.88~2.80(m), 1.98~1.87(m)	68.5	4.06 (d, $J=4$ Hz)
13	128.5		90.0	
14	41.3		43.5	
15	32.7	2.24~2.17(m), 1.64~1.53(m)	34.1	2.16~2.09(m), 1.64~1.56(m)
16	35.6	2.57~2.50(m), 1.48~1.38(m)	20.3	2.08~2.04(m), 1.61~1.57(m)
17	48.0		52.4	
18	136.9		38.0	3.15 (dd, $J=11$ Hz, 4 Hz)
19	40.7	2.64~2.57(m), 2.23~2.15(m)	35.4	1.42~1.35(m), 1.10~1.00(m)
20	32.1		29.1	

21	36.5	1.69~1.59(m), 1.34~1.27(m)	34.9	1.70~1.59(m), 1.33~1.27(m)
22	26.9	2.02~1.95(m), 1.11~1.04(m)	27.1	1.73~1.67(m)
23	179.7		179.7	
24	11.3	1.64 (s)	11.1	1.66 (s)
25	16.2	0.98 (s)	16.0	0.98 (s)
26	17.2	1.16 (s)	17.1	1.30 (s)
27	20.4	1.18 (s)	20.3	1.57 (s)
28	178.1		177.4	
29	31.5	0.96 (s)	32.1	0.87 (s)
30	23.6	0.85 (s)	21.9	0.93 (s)

Table S2 In vitro cytotoxicities of **1-6** against three different human cell lines

compound	IC ₅₀ ^a (μM)	
	H460	SGC-7901
1	7.14±0.14	29.55±0.22
2	9.90±0.04	44.82±0.07
3	7.76±0.03	42.30±0.06
4	14.02±0.05	14.36±0.06
5	6.91±0.10	8.00±0.05
6	8.31±0.09	127.16±0.13
cisplatin ^b	0.03±0.01	0.93±0.10

^a Means ± S.D. From three independent experiments (n=3)^b Positive controlTable S3 Antiangiogenic Activities of Compounds **1-6**

Compound	Concentration	intersegmental vessels	inhibition ratio
	(μM)	(ISV) ^c	(%)
1	10.29	0	100
2	9.96	3.5±0.55	86.74
3	10.29	2.86±0.14	89.16
4	10.64	6.5±0.11	75.37
5	10.29	9.25±0.06	64.96
6	10.29	2.8±0.08	89.39
PTK787 ^d	2.38	0	100

^c Means $\pm$ S.D. From three independent experiments (n=5)

^d Positive control

Figure S1. IR spectrum of compound **1**

Figure S2. ¹H NMR spectrum of compound **1** in C₅D₅N (400MHz)

Figure S4. DEPT135 spectrum of compound **1** in C₅D₅N (100MHz)

[illegible]

Figure S6. HSQC spectrum of compound **1** in C₅D₅N (100MHz)

Figure S7. HMBC spectrum of compound **1** in C₅D₅N (100MHz)

Figure S8. NOESY spectrum of compound **1** in C₅D₅N (100MHz)

Figure S9. HR-ESI-MS of compound **1**

Figure S10. IR of compound **2**

Figure S11. ^1H NMR spectrum of compound **2** in $\text{C}_5\text{D}_5\text{N}$ (400MHz)

Figure S12. ^{13}C NMR spectrum of compound **2** in $\text{C}_5\text{D}_5\text{N}$ (100MHz)

Figure S13. DEPT135 spectrum of compound **2** in C₅D₅N (100MHz)

Figure S14. DEPT90 spectrum of compound **2** in C₅D₅N (100MHz)

Figure S17. NOESY spectrum of compound **2** in C₅D₅N (100MHz)

Figure S18. HR-ESI-MS of compound **2**

Figure S19. Key NOESY correlations of compounds **1** and **2**

Figure S20. Key HMBC correlations of compound **1** and **2**