SUPPLEMENTARY MATERIAL

Two new polyhydroxylated triterpenoids from *Salvia urmiensis* and their cytotoxic activity

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Abstract

Two new polyhydroxylated triterpenoids were isolated from the acetone extract of the aerial parts of *Salvia urmiensis* Bunge. Their structures were elucidated by 1D and 2D NMR and HRESIMS analyses as olean-12-ene-1 β ,3 β ,11 α ,22 α -tetraol (**1**) and urs-12-ene-1 β ,3 β ,11 β ,22 α -tetraol (**2**). The effect of these compounds on cell viability of MCF-7 cells was investigated with the MTT assay. Compounds **1** and **2** showed weak cytotoxicity with IC₅₀ values of 110 and 88 μ M, respectively.

Keywords: *Salvia urmiensis*; triterpenoid; polyhydroxylation; cytotoxic activity

Table S1: ^1H and ^{13}C NMR spectroscopic data of compounds **1** and **2** ($\text{CDCl}_3 + \text{CD}_3\text{OD}$, 500 MHz for ^1H , 125 MHz for ^{13}C).

C No.	1		2	
	$\delta_{\text{C}}(\text{ppm})$	$\delta_{\text{H}}(\text{ppm}), (J \text{ in Hz})$	$\delta_{\text{C}}(\text{ppm})$	$\delta_{\text{H}}(\text{ppm}), (J \text{ in Hz})$
1	76.7	3.39, <i>dd</i> (11.5, 5.0)	77.0	3.39, <i>dd</i> (11.5, 4.4)
2 α	34.7	1.65 ^a	34.9	1.72 ^a
2 β		1.72 ^a		1.63 ^a
3	75.6	3.10, <i>dd</i> (11.5, 4.5)	75.4	3.14, <i>dd</i> (11.6, 4.4)
4	38.7	—	38.9	—
5	52.1	0.58, <i>dd</i> (11.5, 2.0)	52.4	0.55, <i>d</i> (9.9)
6 α	18.0	1.45 ^a	18.0	1.49 ^a
6 β		1.57 ^a		1.57, <i>d</i> (8.4)
7 α	33.1	1.44 ^a	33.2	1.23 ^a
7 β		1.24 ^a		1.45 ^a
8	42.5	—	43.0	—
9	55.5	1.63, <i>d</i> (8.5)	56.0	1.59, <i>d</i> (8.4)
10	44.4	—	43.7	—
11	66.0	4.15, <i>dd</i> (8.5, 3.8)	66.1	4.15, <i>dd</i> (8.4, 3.5)
12	124.5	5.15, <i>d</i> (3.8)	127.4	5.18, <i>d</i> (3.5)
13	147.0	—	142.0	—
14	43.0	—	43.0	—
15 α	25.7	0.98 ^a	26.3	0.95 ^a
15 β		1.55 ^a		1.68 ^a
16 α	18.8	1.65 ^a	27.6	0.86 ^a
16 β		1.28 ^a		1.84, <i>dt</i> (13.2, 4.5)
17	38.1	—	37.5	—
18	46.7	1.95, <i>dd</i> (10.0, 3.5)	53.0	1.64 ^a
19 α	45.3	1.01 ^a	38.8	1.32 ^a
19 β		1.65 ^a		
20	31.0	—	31.6	1.35 ^a
21	42.2	1.30 ^a	37.7	1.53 ^a
22	75.0	3.43, <i>dd</i> (11.5, 4.5)	75.1	3.27, <i>brt</i> (2.9)
23	27.7	0.89, <i>s</i>	27.7	0.90, <i>s</i>
24	15.1	0.69, <i>s</i>	15.0	0.70, <i>s</i>
25	12.2	0.97, <i>s</i>	12.9	0.98, <i>s</i>
26	17.6	0.94, <i>s</i>	17.6	0.98, <i>s</i>
27	25.0	1.18, <i>s</i>	23.1	1.11, <i>s</i>
28	24.1	0.90, <i>s</i>	21.8	0.81, <i>s</i>
29	33.0	0.84, <i>s</i>	17.2	0.85, <i>d</i> (5.8)
30	23.9	0.86, <i>s</i>	20.9	0.86, <i>d</i> (5.9)

^a Overlapping signals.

Figure S1: Key HMBC & NOESY correlations of **1**

Figure S2: ^1H NMR (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S3: Expanded ^1H NMR (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S4: APT (125 MHz, CDCl₃+ CD₃OD) spectrum of compound **1**

Figure S5: Expanded APT (125 MHz, CDCl₃+ CD₃OD) spectrum of compound **1**

Figure S6: ^1H ^1H COSY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S7: Expanded ^1H ^1H COSY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S8: HSQC (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S9: Expanded HSQC (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S10: HMBC (500 MHz, CDCl₃+ CD₃OD) spectrum of compound **1**

Figure S11: Expanded HMBC (500 MHz, CDCl₃+ CD₃OD) spectrum of compound **1**

Figure S12: NOESY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S13: Expanded NOESY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **1**

Figure S14: ^1H NMR (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S15: Expanded ^1H NMR (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S16: APT (125 MHz, CDCl₃) spectrum of compound **2**

Figure S17: Expanded APT (125 MHz, CDCl₃) spectrum of compound **2**

Figure S18: ^1H - ^1H COSY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S19: Expanded ^1H - ^1H COSY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S20: HMQC (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S21: Expanded HMQC (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S22: HMBC (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S23: Expanded HMBC (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S24: NOESY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**

Figure S25: Expanded NOESY (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) spectrum of compound **2**