SUPPLEMENTARY MATERIAL

Isolation of a new β -carboline alkaloid from aerial parts of *Triclisia sacleuxii* and its antibacterial and cytotoxicity effect.

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Abstract.

A new β -carboline alkaloid named sacleuximine A (**1**) together with known compounds palmatine (**2**), isotetrandrine (**3**), *trans*-N-feruloyltyramine (**4**), *trans*-N-caffeoyltyramine (**5**), yangambin (**6**), syringaresinol (**7**), sesamin (**8**), (+) epi-quercitol (**9**), 4-hydroxybenzaldehyde (**10**), β -sitosterol (**11**), quercetin 3-O-rutinoside (**12**) and myricetin 3-O- β -glucose (1 $\rightarrow$ 6) α -rhamnoside (**13**) have been isolated from methanol extract of *Triclisia sacleuxii* aerial parts. Compounds **1-10** were evaluated for their cytotoxicity against human adenocarcinoma (HeLa), human hepatocarcinoma (Hep3B), and human breast carcinoma (MCF-7) cells lines and also for antibacterial activities against both Gram-positive and Gram-negative bacteria. The cytotoxicity (IC₅₀) values ranged between 0.15 and 36.7 μ M while the minimum inhibitory concentrations (MICs) were found to be in the range of 3.9 and 125 μ M, respectively. This is the first report of antibacterial compounds and the isolation of lignans together with a β -carboline alkaloid from *Triclisia sacleuxii*.

Keywords: *Triclisia sacleuxii*; Menispermaceae; secondary metabolites; cytotoxicity; antibacterial, aerial parts.

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LC-MS Display report

Analysis info

Instrument: Agilent 6320 Ion Trap
Operator: AKOPATZ

Print Date: 31.01.2013 10:57:03

Acq. Date: 31.01.2013 10:48:29

Sample Name: TS10

Acquisition Parameter:

Mass Range Mode	Ultra Scan	Trap Drive	47.4	Scan Begin	25 m/z
Ion Polarity	Positive	Octopole RF Amplitude	171.0 Vpp	Scan End	800 m/z
Ion Source Type	ESI	Capillary Exit	121.0 Volt	Averages	3 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	250000 µs
Nebulizer (Set)	40.00 psi	Oct 1 DC	12.00 Volt	(Smart) ICC Target	200000
Dry Gas (Set)	9.00 l/min	Oct 2 DC	1.70 Volt	ICC	on

Fig. S1. LC-MS chromatogram report for **1**

Mass List:

#	m/z	I	I %	S/N
1	337.2	236098	19.7	593684.3
2	444.4	135100	11.3	339716.6
3	488.4	196677	16.4	494557.4
4	576.4	189078	15.8	475447.6
5	644.4	546547	45.7	1374325.8
6	645.5	1196479	100.0	3008620.9
7	647.5	126974	10.6	319283.1
8	667.5	224950	18.8	565650.0
9				

Fig. S2. ESI-MS spectrum for **1**

Fig. S3. ¹H NMR spectrum of **1** (CDCl₃, 600 MHz)

Fig. S4. ^{13}C NMR and DEPT spectra of **1** (CDCl_3 , 150 MHz)

Fig. S5. HMQC spectrum of **1** (CDCl₃, 600 MHz)

Fig. S6. HMBC spectrum of **1** (CDCl₃, 600 MHz)

Fig. S2. NOESY spectrum of **1** (CDCl₃, 600 MHz)

Fig. S9. Significant NOESY and HMBC cross-peaks of compound **1**

Fig. S10. Proposed ESI-MS fragmentation of compound 1

Figure S11: Cytotoxicity (IC₅₀ μM) of Compounds 1–10.

Table S1: ^1H and ^{13}C NMR (CDCl_3) data of Sacleuximine A (1)

Atom	^{13}C (ppm)	^1H (ppm)	HMBC
1	51.1	5.82 (1H, dd, $J=9.6, 4.3$)	H-3 α,β , H-1'
3	41.0	4.07 (1H, dd, $J=13.7, 4.1\text{Hz}$) 3.38 (1H, dd, $J=13.0, 4.6\text{Hz}$)	
4	22.9	2.76 (2H, m)	
4a	107.7		
4b	127.1		
5	102.9	6.86 (1H, d, $J=2.4\text{Hz}$)	H-7
6	149.5		H-8
7	111.3	6.67 (1H, dd, $J=8.6, 2.4\text{Hz}$)	
8	111.6	7.00 (1H, d, $J=8.6\text{Hz}$)	
8a	131.1		H-7
9a	135.2		
-NH	-	6.90 (1H, s)	
1'	39.3	3.14 (1H, dd, $J=13.0, 4.6\text{Hz}$) 2.93 (1H, dd, $J=12.9, 9.8\text{Hz}$)	
2'	129.8		H4'/6'
3', 7'	131.0	7.15 (2H, d, $J=8.4\text{Hz}$)	H-1' α,β
4', 6'	115.7	6.82 (2H, d, $J=8.4\text{Hz}$)	
5'	154.9		
1''	177.1		H-2''
2''	34.1	2.35 (1H, t, $J=7.5\text{Hz}$)	
3''	24.9	1.67 (2H, m)	
(-CH ₂ -) ₂₀	29.9-32.1	1.25 (br m)	
-CH ₃	14.1	0.88 (3H, t, $J=6.7\text{ Hz}$)	

Table S2: Minimum Inhibitory Concentrations (µg/ml) of Compounds 1-10 Isolated from aerial parts of *Triclisia sacleuxii* against Selected Bacterial Strains.

Compound	<i>E.coli</i> ^a	<i>P. aeruginosa</i> ^a	<i>S. epidermis</i> ^b	<i>S. aureus</i> ^b
1	125	31.3	62.5	<i>S. aureus</i> ^b
2	62.5	31.3	31.3	62.5
3	31.3	15.7	7.8	15.7
4	15.7	15.7	15.7	7.8
5	31.3	62.5	31.3	15.7
6	7.8	7.8	7.8	62.5
7	7.8	7.8	3.9	3.9
8	7.8	7.8	7.8	3.9
9	125	125	62.5	7.8
10	125	125	125	125
Tetracycline	0.97	0.97	0.97	125
^a Gram negative bacteria		^b Gram positive bacteria		