SUPPLEMENTARY MATERIAL

Title : Three new monoterpene glucosides from *Sibiraea angustata*

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Abstract

Three new monoterpene glycosides, named sibiraglycoside I(**1**), J(**2**) and K(**3**), were isolated from an aqueous extract of the aerial portion of *Sibiraea angustata*. Their structures were elucidated on the basis of extensive spectroscopic data analysis (including 1 D and 2 D NMR and MS experiments) and compared to literature data.

Keywords: *Sibiraea angustata*, Rosaceae, sibiraglycoside I, sibiraglycoside J, sibiraglycoside K

Fig S1 Structures of compounds 1–4

Fig S2 Key HMBC ($\rightarrow$), COSY (—) and ROESY ($\leftrightarrow$) correlations observed for compound 1

[Comment]		Memory-5	
Sample Name	YZZ-49		
Comment	0.02		
User			
Division	UV		
Company	324		
[Measurement Information]			
Instrument Name	V-850		
Model Name	V-850		
Serial No.	A034461150		
Accessory	PSC-718	[Data Information]	
Accessory S/N	A001761114	Creation Date	2015-6-15 10:17
Position	2		
Cell Length	10 mm	Data array type	Linear data array
Temperature	19.96 C	Horizontal	Wavelength [nm]
Control Sensor	Holder	Vertical	Abs
Monitor Sensor	Holder	Start	400 nm
Start Mode	Start immediately	End	190 nm
		Data pitch	0.2 nm
		Data points	1051
Photometric Mode	Abs		
Measurement range	400 - 190 nm		
Data pitch	0.2 nm		
Band width(UV/Vis)	2.0 nm		
Response	Medium		
Scanning speed	200 nm/min		
Source Change	340 nm		
Light Source	D2/WI		
Filter Exchange	Step		
Correction	Baseline		

Fig S3 UV spectrum of compound **1**

Fig S4 IR spectrum of compound 1

Qualitative Analysis Report

Data Filename	2015052201.d	Sample Name	YZZ-49
Sample Type	Sample	Position	P1-C2
Instrument Name	Instrument 1	User Name	
Acq Method		IRM Calibration Status	Success
DA Method	TEST LCMS.m	Comment	

User Chromatograms

Fragmentor Voltage: 120 Collision Energy: 0 Ionization Mode: ESI

Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	4.053	4.254	4.496	1073010	8898538	100	63.5

Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	4.172	4.258	4.397	77	248.89	100	307

User Spectra

Fragmentor Voltage: 120 Collision Energy: 0 Ionization Mode: ESI

MS Formula Results: + Scan (4.254 min) Sub (2015052201.d)

m/z	Ion	Formula	Abundance
371.1675	(M+Na)+	C16 H28 Na O8	1478698.3

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C16 H28 O8	C16 H28 Na O8	99.96		348.1783	348.1784	371.1676	0.33	0.33	100	99.9	99.95	3
✗	C17 H24 N4 O4	C17 H24 N4 Na O4	99.6		348.1783	348.1798	371.169	4.17	4.17	99.5	99.57	99.83	8

Fig S5 HR-ESI-MS Spectrum of compound 1

Fig S6 ^1H NMR spectrum of compound **1**

Fig S7 ^{13}C NMR spectrum of compound **1**

Fig S8 ^1H - ^1H COSY spectrum of compound **1**

Fig S9 HSQC spectrum of compound **1**

Fig S10 HMBC spectrum of compound **1**

Fig S11 ROESY spectrum of compound **1**