SUPPLEMENTARY MATERIAL

A new *ent*-kaurane diterpene from *Euphorbia stracheyi* Boiss

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Abstract:

The chemical investigation of whole plants *Euphorbia stracheyi* Boiss from China led to the isolation of one new *ent*-kaurane diterpene, *ent*-Kaurane-16 β ,17,19-triol-3-one (**1**), along with three known *ent*-kaurane diterpenoids (**2–4**) as *ent*-Kaurane-3 α ,16 β ,17-triol (**2**), *ent*-16*S*,17-dihydroxy-kaurane-3-one (**3**), and *ent*-3*S*,16*S*,17-trihydroxy-kaurane-2-one (**4**). Their structures were elucidated by extensive spectroscopic analyses including 1D, 2D NMR, HR-ESI-MS, and by comparison with the literature. Compound **2** was a new natural product and firstly isolated from nature, while compounds (**3–4**) were isolated from *E. stracheyi* for the first time. All isolated compounds (**1–4**) were evaluated for their cytotoxic activities against five human cancer cell lines (including A-549, SMMC-7721, HL-60, MCF-7, and SW-480).

Contents of supplementary data

Figure S1. ^1H -NMR spectrum of compound **1** (500MHz, Pyridine- d_5)

Figure S2. ^{13}C -NMR spectrum of compound **1** (125MHz, Pyridine- d_5)

Figure S3. DEPT-90,135 NMR spectrum of compound **1** (Pyridine- d_5)

Figure S4. ^1H - ^1H COSY spectrum of compound **1** (Pyridine- d_5)

Figure S5. HMQC NMR spectrum of compound **1** (Pyridine- d_5)

Figure S6. HMBC NMR spectrum of compound **1** (Pyridine- d_5)

Figure S7. ROESY NMR spectrum of compound **1** (Pyridine- d_5)

Figure S8. ESI-MS spectrum of compound **1**

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

Figure S10. ^1H -NMR spectrum of compound **2** (500MHz, Pyridine- d_5)

Figure S11. ^{13}C -NMR spectrum of compound **2** (125MHz, Pyridine- d_5)

Figure S12. ^1H -NMR spectrum of compound **3** (500MHz, Methanol- d_4)

Figure S13. ^{13}C -NMR spectrum of compound **3** (125MHz, Methanol- d_4)

Figure S14. ^1H -NMR spectrum of compound **4** (500MHz, Pyridine- d_5)

Figure S15. ^{13}C -NMR spectrum of compound **4** (125MHz, Pyridine- d_5)

Figure S16. Key HMBC and COSY correlations of compound **1**

Table S1. ^{13}C NMR data for compounds **1-4**

Figure S1. ^1H -NMR spectrum of compound **1** (500MHz, Pyridine- d_5)

gs064a1. 22. 1. 1r
gs064a1. c13

Figure S2. ^{13}C -NMR spectrum of compound **1** (125MHz, Pyridine- d_5)

Figure S3. DEPT-90,135 NMR spectrum of compound 1 (Pyridine-d₅)

Figure S5. HMQC NMR spectrum of compound **1** (Pyridine- d_5)

Figure S6. HMBC NMR spectrum of compound **1** (Pyridine-d₅)

Figure S7. ROESY NMR spectrum of compound **1** (Pyridine-d₅)

Sample Name	GS-064A1	Position	P1-C3	Instrument Name	Instrument 1	User Name	
Inj Vol	0.1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	GS-064A1.d	ACQ Method	SIBU.m	Comment		Acquired Time	12/29/2015 10:08:50 AM

Figure S8. ESI-MS spectrum of compound 1

Qualitative Analysis Report

Data Filename	GS-064A1.d	Sample Name	GS-064A1
Sample Type	Sample	Position	P1-C3
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	12/29/2015 10:08:50 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			
Sample Group	Info.		
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra

Peak List

m/z	z	Abund	Formula	Ion
229.124	2	31378		
337.2378	1	103730.38		
359.2197	1	263610.34	C20 H32 O4	(M+Na)+
360.2228	1	52787.57	C20 H32 O4	(M+Na)+
375.1936	1	108102.98		
462.2164	1	27096.05		
695.4501	1	187137.19		
696.4533	1	75406.84		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H32 O4	336.2301	359.2193	359.2197	-0.4	-1.2	5.0000

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

Figure S10. ^1H -NMR spectrum of compound **2** (500MHz, Pyridine- d_5)

Figure S11. ^{13}C -NMR spectrum of compound **2** (125MHz, Pyridine- d_5)

Figure S12. ^1H -NMR spectrum of compound **3** (500MHz, Methanol- d_4)

Figure S13. ^{13}C -NMR spectrum of compound 3 (125MHz, Methanol- d_4)

gs064c1.21.1.1r
gs064c1 H

Figure S14. ¹H -NMR spectrum of compound 4 (500MHz, Pyridine-d₅)

Cosy $\longrightarrow$ Key HMBC

Figure S16. Key HMBC and COSY correlations of compound **1**

Table S1. ^{13}C -NMR (125 MHz) Data of Compounds **1–4**

Position	1 ^a	2 ^a	3 ^b	4 ^a
1	40.6 t	39.5 t	40.6 t	54.3 t
2	35.9 t	28.6 s	35.1 t	211.5 s
3	215.5 s	78.6 d	221.2 s	83.8. d
4	55.0 s	39.8 s	48.4 s	45.8 s
5	57.4 d	55.8 d	55.6 d	54.8 d
6	21.9 t	20.7 t	22.4 t	20.7 t
7	42.5 t	42.7 t	42.2 t	41.9 t
8	44.0 s	44.1 s	44.7 s	44.2 s
9	56.9 d	57.9 d	57.3 d	56.8 d
10	39.4 s	39.8 s	39.9 s	45.8 s
11	20.0 t	19.7 t	20.4 t	19.6 t
12	27.8 t	28.0 t	27.9 t	27.6 t
13	42.1 d	42.2 d	42.3 d	42.0 d
14	38.7 t	39.0 t	39.0 t	38.4 t
15	53.5 t	53.8 t	52.9 t	53.4 t
16	80.0 s	80.0 s	80.6 s	79.9 s
17	70.8 t	70.9 t	70.5 t	70.8 t
18	21.8 q	29.3 q	27.9 q	30.0 q
19	65.3 t	16.8 q	21.5 q	17.5 q
20	18.3 q	18.3 q	18.4 q	19.1 q

a) Measured in Pyridine- d_5 . b) Measured in Methanol- d_4 .