SUPPLEMENTARY MATERIAL

A new tigliane-type diterpene from *Euphorbia dracunculoides* Lam

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Abstract:

One new tigliane-type diterpene, 4-deoxy-4(β)H-8-hydroperoxyphorbol-12-benzoate-13-isobutyrate (**1**), together with two known diterpenoids, 3-acetyl-5,8-dibenzoyl-14 α -propanoyl-13,17-epoxy-7-myrtsinone diterpene with C9-C10 cyclized to form an additional lactone ring (**2**), Euphodendriane A (**3**) have been isolated from the whole plants of *Euphorbia dracunculoides* Lam. Their structures were elucidated by means of extensive spectroscopic analysis (NMR and HR-ESI-MS) and comparison with data reported in the literature. This is the first isolation of 8-hydroperoxy tigliane diterpene (**1**) from the genus of *Euphorbia*. All compounds were evaluated for their antifungal activities.

Key Words : *Euphorbia dracunculoides*; diterpenoids; hydroperoxy; tigliane

Contents of supplementary data

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Figure S2. ^{13}C -NMR spectrum of compound **1** (125MHz, Methanol- d_4)

Figure S3. DEPT-90 NMR spectrum of compound **1** (Methanol- d_4)

Figure S4. DEPT-135 NMR spectrum of compound **1** (Methanol- d_4)

Figure S5. ^1H - ^1H COSY spectrum of compound **1** (Methanol- d_4)

Figure S6. HMQC NMR spectrum of compound **1** (Methanol- d_4)

Figure S7. HMBC NMR spectrum of compound **1** (Methanol- d_4)

Figure S8. ROESY NMR spectrum of compound **1** (Methanol- d_4)

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Figure S10. ESI-HR-MS spectrum of compound **1**

Figure S11. ^1H -NMR spectrum of compound **2** (500MHz, CDCl_3)

Figure S12. ^{13}C -NMR spectrum of compound **2** (125MHz, CDCl_3)

Figure S13. ^1H -NMR spectrum of compound **3** (500MHz, CDCl_3)

Figure S14. ^{13}C -NMR spectrum of compound **3** (125MHz, CDCl_3)

Figure S15. Key HMBC, COSY and NOESY correlations of compound **1**.

Table S1. ^1H and ^{13}C NMR data for compound **1** in Methanol- d_4

Figure S3. DEPT-90 NMR spectrum of compound **1** (Methanol- d_4)

Figure S4. DEPT-135 NMR spectrum of compound **1** (Methanol- d_4)

Figure S5. ^1H - ^1H COSY spectrum of compound **1** ($\text{Methanol-}d_4$)

Figure S6. HMQC NMR spectrum of compound **1** (Methanol- d_4)

Figure S7. HMBC NMR spectrum of compound **1** (Methanol- d_4)

Figure S8. ROESY NMR spectrum of compound **1** (Methanol- d_4)

Sample Name	HZ-026F3	Position	P1-B7	Instrument Name	Instrument 1	User Name	
Inj Vol	0.1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	HZ-026F3.d	ACQ Method	SIBU.m	Comment		Acquired Time	5/22/2015 2:24:25 PM

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

Qualitative Analysis Report

Data Filename	HZ-026F3.d	Sample Name	HZ-026F3
Sample Type	Sample	Position	P1-B7
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	5/22/2015 2:24:25 PM
IRM Calibration Status		DA Method	Default.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
555.2588	1	30526.5		
577.2407	1	53478.79	C ₃₁ H ₃₈ O ₉	(M+Na) ⁺
578.2443	1	17621.69	C ₃₁ H ₃₈ O ₉	(M+Na) ⁺
593.215	1	31221.87		
1131.4921	1	30463.33		
1132.4949	1	20398.38		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₃₁ H ₃₈ O ₉	554.2516	577.2408	577.2407	0.0	0.1	13.0000

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Figure S10. ESI-HR-MS spectrum of compound **1**

Figure S12. ^{13}C -NMR spectrum of compound **2** (125MHz, CDCl_3)

Figure S13. ^1H -NMR spectrum of compound **3** (500MHz, CDCl_3)

Figure S15 Key HMBC and COSY correlations of compound **1**.

Figure S15 Key NOESY correlations of compound **1**

Position	δ_{C}	δ_{H}
1	164.2 (d)	7.79 (1H, s)
2	140.5 (s)	
3	211.8 (s)	
4	50.7 (d)	2.67 (1H, d, d, 4.0, 2.0 Hz)
5	71.2 (d)	4.65 (1H, s)
6	141.7 (s)	
7	133.5 (d)	5.26 (1H, t, 1.5 Hz)
8	87.7 (s)	
9	78.7 (s)	
10	48.6 (d)	3.65 (1H, m)
11	43.7 (d)	1.93 (1H, m)
12	79.8 (d)	5.69 (1H, d, 10.0 Hz)
13	68.0 (s)	
14	39.4 (d)	2.06 (1H, d, 2.0 Hz)
15	29.3 (s)	
16	24.3 (q)	1.18 (3H, s)
17	19.2 (q)	1.29 (3H, s)
18	15.2 (q)	0.72 (3H, d, 6.5 Hz)
19	10.3 (q)	1.72 (3H, m)
20	23.9 (q)	1.43 (3H, s)
1'	168.1 (s)	
2'	131.4 (s)	
3', 7'	130.8 (d)	7.96 (2H, d, d, 8.0, 1.0 Hz)
4', 6'	129.8 (d)	7.47 (2H, m)
5'	134.6 (d)	7.59 (1H, m)
1''	180.7 (s)	
2''	35.5 (d)	2.56 (1H, m)
3''	19.2 (q)	1.15 (3H, d, 3.0 Hz)
4''	19.1 (q)	1.14 (3H, d, 3.0 Hz)

Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data for compound **1** in Methanol- d_4 . (δ ppm, J in Hz).