SUPPLEMENTARY MATERIAL

Cytotoxic pimarane-type diterpenes from the marine sediment-derived fungus *Eutypella* sp. FS46

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Abstract

Two new pimarane-type diterpenes, scopararanes H-I (**1-2**), along with five known ones (**3-7**) were isolated from the culture broth of a marine sediment-derived fungus *Eutypella* sp. FS46, which was obtained from the South China Sea. Their structures were established by extensive spectroscopic analysis. All of them were evaluated for their cytotoxic activities against MCF-7, NCI-H460, and SF-268 tumor cell lines. Scopararane I (**2**) showed moderate inhibitory activities.

Keywords: pimarane diterpenes; *Eutypella* sp. FS46; scopararane H; scopararane I; cytotoxic activity

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Contents

Figure S1. ^1H NMR spectrum of **1**.

Figure S2. ^{13}C NMR spectrum of **1**.

Figure S3. DEPT spectrum of **1**.

Figure S4. ^1H - ^1H COSY spectrum of **1**.

Figure S5. HSQC spectrum of **1**.

Figure S6. HMBC spectrum of **1**.

Figure S7. NOESY spectrum of **1**.

Figure S8. HREIMS spectrum of **1**.

Figure S9. UV spectrum of **1**.

Figure S10. IR spectrum of **1**.

Figure S11. ^1H NMR spectrum of **2**.

Figure S12. ^{13}C NMR spectrum of **2**.

Figure S13. DEPT spectrum of **2**

Figure S14. ^1H - ^1H COSY spectrum of **2**.

Figure S15. HSQC spectrum of **2**.

Figure S16. HMBC spectrum of **2**

Figure S17. NOESY spectrum of **2**.

Figure S18. HREIMS spectrum of **2**.

Figure S19. UV spectrum of **2**

Figure S20. IR spectrum of **2**.

Figure S21. Key NOESY correlations of compounds **1** and **2**.

Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data of compounds **1** and **2** in CD_3OD (J in Hz, δ in ppm).

Table S2. Cytotoxic activities of compounds **1–7**.

Figure S3. DEPT spectrum of **1**

Figure S4. ¹H-¹H COSY spectrum of **1**

Figure S5. HSQC spectrum of **1**

Figure S6. HMBC spectrum of **1**

Figure S7. NOESY spectrum of **1**

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

328 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-100 H: 0-1000 N: 0-5 O: 0-200 Na: 1-1

MS+

ES19 28 (1.676) AM (Cen,6, 80.00, Ar,5000.0,556.28,0.70,LS 5); Sm (Mn, 2x3.00); Sb (1,40.00); Cm (4:33)

Page 1

Minimum:

Maximum:

20.0 5.0 -1.5

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

355.1883

355.1885

-0.2

-0.6

6.5

214.0

C20 H28 O4 Na

355.1899

-1.6

-4.5

11.5

297.2

C21 H24 N4 Na

Figure S8. HREIMS spectrum of **1**

Figure S9. UV spectrum of **1**

Figure S10. IR spectrum of **1**

Figure S11. ¹H NMR spectrum of **2**

Figure S12. ¹³C NMR spectrum of **2**

Figure S13. DEPT spectrum of **2**

Figure S14. ^1H - ^1H COSY spectrum of **2**

Figure S15. HSQC spectrum of **2**

Figure S16. HMBC spectrum of **2**

Figure S17. NOESY spectrum of **2**

Figure S18. HRESIMS spectrum of **2**

Figure S19. UV spectrum of **2**

Figure S20. IR spectrum of **2**

Figure S21. Key NOESY correlations of compounds **1** and **2**.

Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data of compounds **1** and **2** in CD_3OD (J in Hz, δ in ppm).

no.	1^a		no.	2	
	δ_{H}	δ_{C}		δ_{H}	δ_{C}
1	7.11, d, 10.4	157.3, CH	1	1.77, m	13.2, CH
2	5.93, d, 10.4	126.7, CH	2a	2.29, ddd, 3.0, 9.3, 16.0	25.8, CH ₂
3		206.9, C	2b	1.92, dd, 3.0, 6.3	
4		45.8, C	3	4.88, t, 3.0	71.7, CH
5	2.63, d, 1.5	44.2, CH	4		40.2, C
6	4.29*	71.6, CH	5	2.44, d, 12.6	43.5, CH
7	4.29*	71.4, CH	6	4.26, d, 12.6	77.4, CH
8		136.8, C	7		201.4, C
9		75.5, C	8		131.8, C
10		46.4, C	9		167.4, C
11 α	1.85, m	25.2, CH ₂	10		28.1, C
11 β	2.33, ddd, 3.0, 13.0, 13.0		11 α	2.20, ddd, 3.2, 13.0, 13.0	23.8, CH ₂
12 α	1.56, m	32.1, CH ₂	11 β	1.88, m	
12 β	1.78, m		12 α	1.95, ddd, 3.2, 13.0, 13.0	26.1, CH ₂
13		38.3, C	12 β	1.44, m	
14	5.95, dd, 1.9, 1.9	132.9, CH	13		39.8, C
15	5.92, dd, 10.7, 17.5	148.7, CH	14	4.18, s	68.0, CH
16a	5.09, dd, 1.3, 17.5	110.9, CH ₂	15	6.06, m	146.6, CH
16b	4.99, dd, 1.3, 10.7		16	5.07, d, 1.3	112.6, CH ₂
17	1.15, s	23.3, CH ₃	16	5.04, dd, 1.3, 5.1	
18	1.29, s	25.6, CH ₃	17	0.76, s	20.9, CH ₃
19	1.44, s	24.5, CH ₃	18a	4.45, d, 10.8	70.5, CH ₂
20	1.37, s	21.3, CH ₃	18b	4.07, d, 10.8	
			19	1.19, s	15.9, CH ₃
			20a	1.28, t, 5.2	18.1, CH ₂
			20b	0.69, dd, 5.2, 9.5	
			1'		171.9, C
			2'	1.99, s	21.0, CH ₃
			1''		178.1, C
			2''	2.51, dt, 7.0, 14.0	35.2, CH
			3''	1.13, d, 7.0	19.2, CH ₃
			4''	1.12, d, 7.0	19.2, CH ₃

*overlapped

Table S2. Cytotoxic activities of compounds **1–7**.

Compounds	IC ₅₀ (μg mL ⁻¹)		
	MCF-7	NCI-H460	SF-268
1	80.63	>100	>100
2	13.59	83.91	25.31
3	5.18	>100	62.34
4	5.18	34.29	13.27
5	10.03	53.91	>100
6	>100	>100	>100
7	0.84	10.74	1.37
Cisplatin	1.20	0.87	1.43