SUPPLEMENTARY MATERIAL

Non-halogenated new sesquiterpenes from Bornean *Laurencia snackeyi*

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Abstract: Two new non-halogenated sesquiterpenes, snakeol (**1**) and snakediol (**2**) were isolated together with 9 known sesquiterpenes such as (R,Z)-33-dimethyl-5-methylene-4-(3-methylpenta-24-dien-1-yl)cyclohex-1-ene (**3**), palisol (**4**), pacifigorgiol (**5**), palisadin D (**6**), palisadin A (**7**), palisadin B (**8**), 5-acetoxypalisadin B (**9**), debromolaurinterol (**10**) and α -bromocuparane (**11**) from the red algae *Laurencia snackeyi*. The structures of two new metabolites were determined from their spectroscopic data (IR, 1D and 2D NMR and MS). Compounds **1**, **2**, **10** and **11** showed strong antibacterial activity against selected human clinical bacterial pathogens.

Keywords: Red alga; Rhodomelaceae; *Laurencia snackeyi*; Sesquiterpene; Chemical race; Antibacterial activity

Supplementary Information

Table S1. ^1H and ^{13}C NMR data and HMBC data for snakeol (**1**) (recorded at 600/150 MHz in CDCl_3 , δ in ppm, J in Hz).

Table S2. ^1H and ^{13}C NMR data and HMBC data for snakediol (**2**) (recorded at 600/150 MHz in CDCl_3 , δ in ppm, J in Hz).

Table S3. ^1H and ^{13}C NMR data and HMBC data for palisadin D (**6**) (recorded at 600/150 MHz in CDCl_3 , δ in ppm, J in Hz).

Table S4. Antibacterial activities of isolated pure compounds.

Figure S2. COSY correlations (bold lines) and selected HMBC correlations ($\text{H} \rightarrow \text{C}$) of **1** and **2**.

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Figure S4. ^{13}C NMR spectrum of snakeol (**1**) in CDCl_3 (150 MHz).

Figure S5. HSQC spectrum of snakeol (**1**) in CDCl_3 .

Figure S6. ^1H - ^1H COSY spectrum of snakeol (**1**) in CDCl_3 .

Figure S7. HMBC spectrum of snakeol (**1**) in CDCl_3 .

Figure S8. NOESY spectrum of snakeol (**1**) in CDCl_3 .

Figure S9. ^1H NMR spectrum of snakediol (**2**) in CDCl_3 (600 MHz).

Figure S10. ^{13}C NMR spectrum of snakediol (**2**) in CDCl_3 (150 MHz).

Figure S11. HSQC spectrum of snakediol (**2**) in CDCl_3 .

Figure S12. ^1H - ^1H COSY spectrum of snakediol (**2**) in CDCl_3 .

Figure S13. HMBC spectrum of snakediol (**2**) in CDCl₃.

Figure S14. NOESY spectrum of snakediol (**2**) in CDCl₃.

Figure S15. ¹H NMR spectrum of palisadin D (**6**) in CDCl₃ (600 MHz).

Figure S16. ¹³C NMR spectrum of palisadin D (**6**) in CDCl₃ (150 MHz).

Figure S17. HSQC spectrum of palisadin D (**6**) in CDCl₃.

Figure S18. ¹H-¹H COSY spectrum of palisadin D (**6**) in CDCl₃.

Figure S19. HMBC spectrum of palisadin D (**6**) in CDCl₃.

Figure S20. NOESY spectrum of palisadin D (**6**) in CDCl₃.

Table S1. ^1H and ^{13}C NMR data and HMBC data for snakeol (1) (recorded at 600/150 MHz in CDCl_3 , δ in ppm, J in Hz).

C	1			
	^{13}C (δ)	^1H (δ)	multiplicity, J (Hz)	HMBC correlations
1	60.1	4.15	d $J = 7.6$	C-2, C-3
		4.15	d $J = 7.6$	C-2, C-3
2	123.7	5.40	t $J = 7.6$	C-4
3	141.1			
4	38.6	2.01	m	C-2, C-3
		1.85	m	C-2, C-3, C-5, C-12
5	25.5	1.60	m	
		1.40	m	C-6
6	53.0	1.91	dd $J = 11.7, 3.4$	C-4, C-7, C-13
7	146.4			
8	32.9	2.65	br d $J = 17.2$	C-7, C-9, C-10
		2.65	br d $J = 17.2$	C-7, C-9, C-10
9	123.7	5.49	dt $J = 9.6, 3.4$	C-7, C-8, C-10, C-11
10	137.7	5.36	d $J = 9.6$	C-6, C-8, C-9, C-11, C-14
11	37.9			
12	17.1	1.67	s	C-2, C-3, C-4
13	110.3	4.87	br s	C-6, C-8
		4.68	br s	C-6, C-8
14	26.0	0.93	s	C-6, C-9, C-10, C-15
15	31.2	1.00	s	C-6, C-9, C-10, C-14

Table S2. ^1H and ^{13}C NMR data and HMBC data for snakediol (2) (recorded at 600/150 MHz in CDCl_3 , δ in ppm, J in Hz).

2				
C	^{13}C (δ)	^1H (δ)	multiplicity, J (Hz)	HMBC correlations
1	65.7	3.63	dd $J = 11.0, 3.4$	C-2, C-3
		3.52	dd $J = 11.0, 3.4$	C-2, C-3
2	71.8	4.64	dd $J = 11.0, 3.4$	C-4
3	133.9			
4	129.6	5.28	dd $J = 17.2, 6.9$	C-2, C-3
5	25.4	2.33	m	
		1.96	m	C-6
6	53.6	1.99	dd $J = 11.0, 4.1$	C-4, C-7, C-13
7	146.2			
8	33.1	2.65	br s	C-7, C-9, C-10
		2.65	br s	C-7, C-9, C-10
9	123.8	5.50	dt $J = 10.3, 3.4$	C-7, C-8, C-10, C-11
10	137.6	5.36	d $J = 10.3$	C-6, C-8, C-9, C-11, C-14
11	37.8			
12	19.0	1.69	s	C-2, C-3, C-4
13	110.6	4.88	br s	C-6, C-8
		4.67	br s	C-6, C-8
14	31.0	1.01	s	C-6, C-9, C-10, C-15
15	25.9	0.93	s	C-6, C-9, C-10, C-14

Table S3. ^1H and ^{13}C NMR data and HMBC data for palisadin D (6) (recorded at 600/150 MHz in CDCl_3 , δ in ppm, J in Hz).

6				
C	^{13}C (δ)	^1H (δ)	multiplicity, J (Hz)	HMBC correlations
1	73.1	4.08	t $J = 8.3$	C-12
		3.49	t $J = 8.3$	C-2
2	70.5	4.99	br s	
3	142.6			
4	121.7	5.52	m	C-2
5	27.6	2.28	m	C-4, C-7, C-11
		2.12	m	
6	44.5	2.33	m	C-4, C-5, C-7, C-11, C-13
7	79.7			
8	33.2	2.17	m	
		1.34	m	
9	38.9	1.73	m	C-7
		1.63	m	C-8
10	71.7			
11	42.6	1.36	m	
12	71.9	4.40	d $J = 12.4$	
		4.32	d $J = 12.4$	
13	20.3	1.19	s	C-6, C-7, C-8
14	13.3	0.98	d $J = 6.9$	C-6, C-10, C-11
15	30.3	1.22	s	C-9, C-10, C-11

Table S4. Antibacterial activities of isolated pure compounds.

	MIC (mM)	MBC (mM)	MBC : MIC
Snakeol (1)			
<i>Escherichia coli</i>	0.45	1.36	3.02 (bactericidal)
<i>Salmonella typhi</i>	0.57	1.59	2.79 (bactericidal)
Snakediol (2)			
<i>Escherichia coli</i>	0.42	1.16	2.76 (bactericidal)
<i>Salmonella typhi</i>	0.53	1.48	2.79 (bactericidal)
Palisadin D (6)			
<i>Escherichia coli</i>	>1.98	-	-
<i>Salmonella typhi</i>	-	-	-
Palisadin A (7)			
<i>Escherichia coli</i>	>1.59	-	-
<i>Salmonella typhi</i>	-	-	-
Debromolaurinterol (10)			
<i>Escherichia coli</i>	>2.31	-	-
<i>Salmonella typhi</i>	0.58	1.62	2.79 (bactericidal)
α-Bromocuparane (11)			
<i>Escherichia coli</i>	>1.78	-	-
<i>Salmonella typhi</i>	0.36	0.98	2.72 (bactericidal)

Note: Kanamycin; MIC-0.15 mM, MBC-0.26 mM, MBC : MIC-1.73 (bactericidal).

Figure S2. COSY correlations (bold lines) and selective HMBC correlations (H → C) for 1 and 2.

Figure S3. ^1H NMR spectrum of snakeol (1) in CDCl_3 (600 MHz).

Figure S4. ^{13}C NMR spectrum of snakeol (1) in CDCl_3 (150 MHz).

Figure S5. HSQC spectrum of snakeol (1) in CDCl₃.

Figure S6. ^1H - ^1H COSY spectrum of snakeol (1) in CDCl_3 .

Figure S7. HMBC spectrum of snakeol (1) in CDCl_3 .

Figure S8. NOESY spectrum of snakeol (1) in CDCl_3 .

Figure S9. ^1H NMR spectrum of snakediol (2) in CDCl_3 (600 MHz).

Figure S10. ^{13}C NMR spectrum of snakediol (2) in CDCl_3 (150 MHz).

Figure S11. HSQC spectrum of snakediol (2) in CDCl_3 .

Figure S12. ^1H - ^1H COSY spectrum of snakediol (2) in CDCl_3 .

Figure S13. HMBC spectrum of snakediol (2) in CDCl₃.

Figure S14. NOESY spectrum of snakediol (2) in CDCl_3 .

Figure S15. ^1H NMR spectrum of palisadin D (6) in CDCl_3 (600 MHz).

Figure S16. ^{13}C NMR spectrum of palisadin D (6) in CDCl_3 (150 MHz).

Figure S17. HSQC spectrum of palisadin D (6) in CDCl₃.

Figure S18. ^1H - ^1H COSY spectrum of palisadin D (6) in CDCl_3 .

Figure S19. HMBC spectrum of palisadin D (6) in CDCl₃.

Figure S20. NOESY spectrum of palisadin D (6) in CDCl_3 .