SUPPLEMENTARY MATERIAL

A New Sesquiterpenoid from *Polyalthia petelotii*

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A New Sesquiterpenoid from *Polyalthia petelotii*

A new sesquiterpenoid (–)-ethyl dihydrophaseate (**1**), was isolated from the stems and leaves of *Polyalthia petelotii*, together with two clerodane diterpenoids, 16 α -hydroxycleroda-3,13(14)*Z*-dien-15,16-olide (**2**), 15-hydroxy-*cis-ent*-cleroda-3,13(*E*)-diene (**3**), a eudesmane sesquiterpenoid, eudesm-4(15)-ene-7 α ,11-diol (**4**), an aromatic aldehyde, vanillin (**5**), a bisisoquinolines alkaloid, spinosine (**6**), and an aporphine alkaloid, (–)-oliveroline- β -*N*-oxide (**7**). Their structures were established by extensive spectroscopic analysis, including 2D-NMR techniques. **3**, **4** and **6** were isolated from the genus *Polyalthia* for the first time and the others obtained originally from *P. petelotii*. The isolates were assessed for their cytotoxicity against five human tumor lines (HL-60, SMMC-7721, A-549, MCF-7 and SW-480), and the result showed that only **2** displayed weak inhibitory activity.

Keywords: *Polyalthia petelotii*; Annonaceae; sesquiterpenoid

Supporting information

Figure S2. Key HMBC, and COSY correlations of **1**.

Spectroscopic data of the known compounds **2-7**.

Original spectra of compound **1**.

^1H NMR Spectrum (500 MHz, CDCl_3)

^{13}C NMR Spectrum (125 MHz, CDCl_3)

COSY Spectrum

HSQC Spectrum

HMBC Spectrum

ROESY Spectrum

HRESIMS

IR

Figure S2. Key HMBC, and COSY correlations of **1**.

Spectroscopic data of the known compounds **2-7**.

16 α -hydroxycleroda-3,13(14)*Z*-dien-16,15-olide (2)

White crystal, C₂₀H₂₀O₃, MW: 318; ¹H-NMR (CDCl₃, 500 MHz): δ 6.04 (1H, d, J = 11.0 Hz, H-16), 5.84 (1H, d, J = 10.0 Hz, H-14), 5.21 (1H, brs, H-3), 2.30 (2H, m, H-12), 2.06 (2H, m, H-2), 1.76 (1H, m, Ha-6), 1.70 (1H, m, Ha-11), 1.60 (3H, s, H-18), 1.55 (2H, m, H-1), 1.50 (1H, m, Hb-11), 1.47 (1H, m, H-8), 1.46 (1H, m, H-7), 1.37 (1H, brd, J = 11.5 Hz, H-10), 1.20 (1H, m, Hb-6), 1.01 (3H, s, H-19), 0.82 (3H, d, J = 5.5 Hz, H-17), 0.79 (3H, s, H-20); ¹³C-NMR (CDCl₃, 125 MHz): δ 172.0 (s, C-13), 171.0 (s, C-15), 144.4 (s, C-4), 120.4 (d, C-3), 116.9 (s, C-14), 99.3 (d, C-16), 46.5 (d, C-10), 38.7 (s, C-5), 38.2 (s, C-9), 36.7 (t, C-6), 36.3 (d, C-8), 34.8 (t, C-11), 27.4 (t, C-1), 26.8 (t, C-7), 21.4 (t, C-12), 20.0 (q, C-19), 18.3 (t, C-2), 18.2 (q, C-20), 18.0 (q, C-18), 16.0 (q, C-17).

15-hydroxy-cis-ent-cleroda-3,13(E)-diene (3)

Colourless oil, C₂₀H₃₄O, MW: 290; ¹H-NMR (CDCl₃, 500 MHz): δ 5.86 (1H, s, H-14), 5.20 (1H, s, H-3), 4.23 (2H, m, H-15), 2.24 (1H, br, Ha-2), 2.03 (1H, d, J = 13.5 Hz, Ha-6), 1.96 (1H, m, Hb-2), 1.83 (2H, m, H-12), 1.78 (1H, d, J = 12.5 Hz, Ha-1), 1.70 (1H, d, J = 0.5 Hz, Hb-1), 1.68 (3H, s, H-18), 1.66 (3H, s, H-16), 1.60 (1H, brs, Ha-11), 1.46 (1H, m, H-8), 1.36 (1H, brs, H-10), 1.21 (1H, m, Hb-11), 1.12 (1H, m, Ha-7), 1.08 (1H, brs, Hb-7), 1.06 (1H, brs, Hb-6), 1.02 (3H, s, H-19), 0.80 (3H, s, H-17), 0.78 (3H, s, H-20); ¹³C-NMR (CDCl₃, 125 MHz): δ 144.3 (s, C-13), 139.7 (d, C-4), 123.2 (d, C-3), 123.1 (d, C-14), 44.6 (d, C-10), 40.1 (s, C-9), 37.7 (t, C-6), 37.4 (d, C-8), 36.9 (s, C-5), 36.4 (t, C-11), 34.6 (t, C-12), 33.1 (q, C-19), 28.7 (t, C-7), 24.0 (t, C-2), 19.8 (q, C-18), 17.8 (t, C-1), 17.1 (q, C-20), 16.0 (q, C-16), 15.9 (q, C-17).

eudesm-4(15)-ene-7 α ,11-diol (4)

Colourless oil, C₁₅H₂₆O₂, MW: 238; ¹H-NMR (CDCl₃, 500 MHz): δ 4.72 (1H, d, J = 1.0 Hz, Ha-15), 4.40 (1H, d, J = 1.5 Hz, Hb-15), 2.30 (1H, brd, J = 12.5 Hz, Ha-3),

2.20 (1H, brd, $J = 12.5$ Hz, H-5), 2.03 (1H, m, Hb-3), 1.76 (1H, brs, Ha-9), 1.62 (1H, brd, $J = 2.0$ Hz, Ha-1), 1.57 (1H, brs, Ha-6), 1.54 (2H, m, H-8), 1.50 (1H, brs, Hb-9), 1.48 (1H, m, Hb-6), 1.43 (1H, brs, Ha-2), 1.34 (1H, brs, Hb-1), 1.26 (6H, s, H-12, H-13), 1.25 (1H, s, Hb-2), 0.69 (3H, s, H-14); ^{13}C -NMR (CDCl_3 , 125 MHz): δ 150.9 (s, C-4), 105.2 (t, C-4), 76.3 (s, C-7), 75.5 (s, C-11), 44.2 (d, C-5), 41.4 (t, C-1), 36.9 (t, C-3), 36.3 (t, C-9), 35.5 (s, C-10), 29.4 (t, C-6), 26.5 (t, C-8), 24.7 (q, C-12), 24.6 (q, C-13), 23.5 (t, C-2), 15.3 (q, C-14).

vanillin (5)

White needles, $\text{C}_8\text{H}_8\text{O}_3$, MW: 152; ^1H -NMR (CDCl_3 , 500 MHz): δ 9.86 (1H, s, CHO), 7.46 (1H, s, H-2), 7.45 (1H, s, H-6), 7.07 (1H, d, $J = 8.5$ Hz, H-5), 3.99 (3H, s, OCH_3); ^{13}C -NMR (CDCl_3 , 125 MHz): δ 190.9 (s, CHO), 151.7 (s, C-4), 147.2 (s, C-3), 129.9 (s, C-1), 127.5 (d, C-6), 114.4 (d, C-2), 108.8 (d, C-5), 56.1 (q, OCH_3).

spinosine (6)

Colourless oil, $\text{C}_{17}\text{H}_{21}\text{NO}_4$, MW: 303; ^1H -NMR (CDCl_3 , 500 MHz): δ 6.78 (1H, s, H-1), 6.75 (1H, s, H-9), 6.69 (1H, s, H-12), 6.57 (1H, s, H-4), 3.85 (6H, s, 2^*OCH_3), 3.56 (2H, m, H-8), 3.33 (1H, m, H-14), 3.16 (1H, m, Ha-13), 3.09 (2H, m, H-6), 2.72 (1H, brs, Hb-13), 2.62 (2H, m, H-5); ^{13}C -NMR (CDCl_3 , 125 MHz): δ 146.7 (s, C-3), 146.5 (s, C-2), 144.7 (s, C-11), 144.6 (s, C-10), 129.4 (s, C-14a), 125.7 (s, C-4a), 124.9 (s, C-12a), 124.8 (s, C-8a), 112.1 (d, C-12), 111.7 (d, C-9), 111.3 (d, C-4), 111.1 (d, C-1), 59.7 (d, C-14), 57.5 (t, C-8), 55.0 (q, 2^*OCH_3), 51.3 (t, C-6), 35.3 (t, C-13), 27.8 (t, C-5).

(-)-oliveroline- β -N-oxide (7)

Yellow oil, $\text{C}_{18}\text{H}_{17}\text{NO}_4$, MW: 311; ^1H -NMR (CDCl_3 , 500 MHz): δ 8.06 (1H, d, $J = 8.0$ Hz, H-11), 7.89 (1H, d, $J = 7.5$ Hz, H-10), 7.43 (1H, m, H-8), 7.29 (1H, s, H-9), 6.63 (1H, s, H-3), 6.15 (2H, s, OCH_2O), 5.24 (1H, d, $J = 11.5$ Hz, H-11), 4.51 (1H, d, $J = 11.5$ Hz, H-6a), 3.89 (1H, brs, Ha-4), 3.72 (2H, d, $J = 6.0$ Hz, H-5), 3.89 (3H, s, N- CH_3), 1.28 (1H, brs, Hb-4); ^{13}C -NMR (CDCl_3 , 125 MHz): δ 149.0 (s, C-2), 143.9

(s, C-1), 137.0 (s, C-7a), 128.9 (d, C-10), 127.7 (d, C-9), 127.3 (s, C-11a), 126.3 (d, C-11), 124.6 (d, C-8), 122.9 (s, C-3a), 119.3 (s, C-1b), 116.1 (s, C-1a), 107.2 (d, C-3), 101.6 (t, OCH₂O), 75.2 (d, C-6a), 68.7 (d, C-7), 67.0 (t, C-5), 48.8 (q, N-CH₃), 27.2 (t, C-4).

Original spectra of compound **1**.

^1H NMR:

¹³CNMR:

H-H COSY:

HSQC:

HMBC:

ROESY:

HRESIMS:

User Spectra

Peak List

m/z	z	Abund	Formula	Ion
328.212	1	145208.75		
333.1677	1	242005.03	C17 H26 O5	(M+Na)+
349.1418	1	222159.91		
350.1451	1	41141.18		
643.346	1	171351.36		
644.3491	1	61799.57		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C17 H26 O5	310.1780	333.1672	333.1677	-0.6	-2.1	5.0000

IR:

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