SUPPLEMENTARY MATERIAL

A New (Propylphenyl)bibenzyl from *Eria bambusifolia*

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A New (Propylphenyl)bibenzyl from *Eria bambusifolia*

A new (propylphenyl)bibenzyl, bambusifolol (**1**), along with six known compounds, batatacin III (**2**), tristin (**3**), 3-hydroxy-5-methoxy bibenzyl (**4**), gigantol (**5**), 3',5-dimethoxy-9,9'-diacetyl-4,7'-epoxy-3,8'-bilign-7-ene-4'-methol (**6**), and balanophonin (**7**) were isolated from the whole plants of *Eria bambusifolia*. Their structures were elucidated by the means of extensive spectroscopic analysis. **3-7** were isolated from the genus *Eria* for the first time and **2** obtained originally from *E. bambusifolia*. All the compounds isolated were evaluated for their cytotoxicity against human tumor HL-60, SMMC-7721, A-549, MCF-7 and SW-480 cell lines, but none showed significant activity.

Keywords: *Eria bambusifolia*; Orchidaceae; bibenzyl

Supporting information

Figure 1S. Selective ^1H - ^1H COSY, HMBC and ROESY correlations of **1**.

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

Original spectra of compound **1**.

^1H NMR Spectrum (500 MHz, CDCl_3)

^1H NMR Spectrum (500 MHz, CD_3COCD_3)

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

HSQC Spectrum (125 MHz, CDCl_3)

HMBC Spectrum (125 MHz, CDCl_3)

COSY Spectrum (125 MHz, CDCl_3)

ROESY Spectrum (125 MHz, CDCl_3)

HR-EI-MS

IR

UV

Optical rotation

Figure S1. Selective ^1H - ^1H COSY, HMBC and ROESY correlations of **1**

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

batatasin III (2)

Colorless oil; MF: C₁₅H₁₆O₃, MW: 244; ¹H NMR [(CD)₃CO, 400 MHz]: δ 8.21 (s, 3'-OH), 8.19 (s, 3-OH), 7.08 (1H, dd, *J* = 7.5, 7.5, H-5'), 6.69 (1H, d, *J* = 8.0, H-6'), 6.65 (1H, d, *J* = 8.0, H-4'), 6.66 (1H, s, H-2'), 6.31 (1H, d, *J* = 1.8, H-6), 6.30 (1H, d, *J* = 2.3, H-2), 6.22 (1H, m, H-4), 3.69 (3H, s, 5-OMe), 2.78 (2H, m, H-7), 2.79 (2H, m, H-8); ¹³C NMR [(CD)₃CO, 100 MHz]: δ 161.9 (C-5), 159.3 (C-3), 158.3 (C-3'), 145.0 (C-1'), 144.3 (C-1), 130.0 (C-5'), 120.4 (C-6'), 116.2 (C-2'), 113.6 (C-4'), 108.8 (C-2), 106.2 (C-6), 99.8 (C-4), 55.3 (5-OMe), 38.5 (C-7), 38.2 (C-8).

tristin (3)

Colorless oil; MF: C₁₅H₁₆O₄, MW: 260; ¹H NMR [(CD)₃CO, 500 MHz]: δ 6.80 (1H, d, *J* = 1.9, H-2), 6.76 (1H, d, *J* = 8.0, H-5), 6.67 (1H, dd, *J* = 8.0, 1.9, H-6), 6.28 (2H, d, *J* = 2.1, H-2', 6'), 6.26 (1H, d, *J* = 2.1, H-4'), 3.79 (3H, s, 3-OMe), 2.88 (2H, m, H-7), 2.81 (2H, m, H-8); ¹³C NMR [(CD)₃CO, 125 MHz]: δ 159.6 (C-3'), 159.6 (C-5'), 148.5 (C-3), 145.7 (C-1'), 145.8 (C-4), 134.8 (C-1), 116.1 (C-5), 122.1 (C-6), 113.4 (C-2), 108.5 (C-6'), 108.5 (C-2'), 101.7 (C-3'), 56.7 (3-OMe), 39.3 (C-7), 38.3 (C-8).

3-hydroxy-5-methoxy bibenzyl (4)

Colorless oil; MF: C₁₅H₁₆O₂, MW: 228; ¹H NMR [(CD)₃CO, 400MHz] δ 7.13-7.27 (5H, m, H-2', H-3', H-4', H-5', H-6'), 6.25-6.34 (3H, m, H-2, H-4, H-6), 5.45 (1H, brs, ArOH), 3.68 (3H, s, OMe), 2.78-2.89 (4H, H-α and H-α'); ¹³C NMR [(CD)₃CO, 100MHz] δ 144.9 (C-1), 108.7 (C-2), 159.2 (C-3), 99.7 (C-4), 161.7 (C-5), 106.1 (C-6), 142.6 (C-1'), 129.0 (C-2', 6'), 129.1 (C-3', 5'), 126.5 (C-4'), 38.6 (C-7), 38.2 (C-8), 55.2 (OMe).

gigantol (5)

Colorless oil; MF: C₁₆H₁₈O₄, MW: 274; ¹H NMR [(CD₃)₂CO, 400 MHz]: δ 6.80 (1H, d, *J* = 2.0, H-2), 6.70 (1H, d, *J* = 8.0, H-5), 6.64 (1H, dd, *J* = 8.0, 2.0, H-6), 6.29 (1H, d, *J* = 2.0, H-6'), 6.28 (1H, d, *J* = 2.0, H-4'), 6.21 (1H, dd, *J* = 2.0, 2.0, H-2'), 3.78 (3H, s, 5'-OMe), 3.69 (3H, s, 3-OMe), 2.75 (4H, m, H-7, 8); ¹³C NMR [(CD₃)₂CO, 100 MHz]: δ 161.8 (C-5'), 159.3 (C-3'), 146.1 (C-3), 146.2 (C-1'), 145.2 (C-4), 134.0 (C-1), 121.5 (C-6), 115.5 (C-2), 112.8 (C-5), 108.8 (C-2'), 106.2 (C-6'), 99.6 (C-4'), 56.1 (-OCH₃), 55.2 (-OCH₃), 39.1 (C-7), 38.0 (C-8).

3',5-Dimethoxy-9,9'-diacetyl-4,7'-epoxy-3,8'-bilign-7-ene-4'-methol (6)

Colorless oil; MF: C₂₄H₂₆O₈, MW: 442; ¹H NMR [(CD₃)₂CO, 400 MHz]: δ 7.71 (1H, brs, -OH), 7.04 (1H, s, H-2), 7.03 (1H, s, H-5), 7.02 (1H, s, H-5), 6.89 (1H, dd, *J* = 8.0, 1.8, H-6'), 6.82 (1H, d, *J* = 8, H-5'), 6.64 (1H, d, *J* = 15.6, H-7), 6.27 (1H, dd, *J* = 15.6, 6.8, H-8), 5.43 (1H, d, *J* = 7.2, H-7'), 4.67 (2H, dd, *J* = 6.4, 0.8, H-9), 4.34 (1H, dd, *J* = 18, 5.2, H-9a), 4.15 (1H, dd, *J* = 18, 7.2, H-9b), 3.77 (1H, m, H-3), 3.84 (3H, s, -OCH₃), 3.79 (3H, s, -OCH₃), 2.04 (3H, s, -OAc), 1.98 (3H, s, -OAc); ¹³C NMR [(CD₃)₂CO, 100 MHz]: δ 170.1 (-OAc), 170.0 (-OAc), 149.3 (C-4), 148.4 (C-3'), 147.6 (C-4'), 145.3 (C-5), 134.7 (C-7), 133.3 (C-1'), 131.3 (C-1), 129.2 (C-3), 122.0 (C-8), 119.8 (C-6'), 116.2 (C-2), 115.7 (C-5'), 111.9 (C-6), 110.4 (C-2'), 89.0 (C-7'), 65.9 (C-9'), 65.5 (C-9), 55.6 (-OCH₃), 55.2 (-OCH₃), 51.1 (C-8'), 20.8 (-OAc), 20.7 (-OAc).

balanophonin (7)

Colorless oil; MW: 356, MF: C₂₀H₂₀O₆; ¹H NMR [(CD₃)₃CO, 500MHz]: δ 9.58 (1H, t, *J* = 7.8, H-9'), 7.61 (1H, t, *J* = 16.0, H-7'), 7.38 (2H, s, H-6, 2'), 6.99 (1H, s, H-2), 6.79 (1H, s, H-5), 6.77 (1H, dd, *J* = 16.0, 8.0, H-8'), 6.72 (1H, s, H-6'), 5.62 (1H, d, *J* = 6.6, H-7), 3.86 (3H, s, -OCH₃), 3.84 (3H, s, -OCH₃), 3.67 (2H, m, H-9), 3.54 (1H, m, H-8); ¹³C NMR [(CD₃)₃CO, 125MHz]: δ 193.8 (C-9'), 154.1 (C-7'), 150.8 (C-4'), 147.7 (C-3), 146.7 (C-4), 145.7 (C-3'), 133.8 (C-1), 131.3 (C-5'), 129.0 (C-1'), 127.2 (C-8'), 119.8 (C-6'), 119.7 (C-6), 115.8 (C-5), 113.6 (C-2'), 110.6 (C-2), 89.5 (C-7), 64.4 (C-9), 56.4 (-OCH₃), 56.3 (-OCH₃), 54.2 (C-8).

¹H NMR spectrum of compound 1 recorded in CDCl₃

^1H NMR spectrum of compound **1** recorded in $\text{CD}_3\text{CO CD}_3$

¹³C NMR and DEPT Spectrum of compound **1** recorded in CDCl₃

HSQC spectrum of compound **1** recorded in CDCl_3

HMBC spectrum of compound **1** recorded in CDCl_3

^1H - ^1H COSY spectrum of compound **1** recorded in CDCl_3

ROESY spectrum of compound **1** recorded in CDCl_3

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 mDa / DBE: min = 0.5, max = 40.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

44 formula(e) evaluated with 2 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-7

NJb-3

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Voltage EI+

Minimum: 0.5
Maximum: 10.0 10.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
452.1831	452.1835	-0.4	-0.9	13.0	2773015.0	C26 H28 O7
	452.1776	5.5	12.2	22.0	2773017.0	C33 H24 O2

HR-EI-MS spectrum of compound **1**

IR spectrum of compound **1**

UV spectrum of compound **1**

Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	9 (1/3)	Sp.Rot	-3.8520	-0.0013 0.0000	26.3 50.00 Cell	Fri May 21 14:27:10 2010 0.00068g/mlMeOH+CHCl3(1:1) JB-3	Na 589nm	2 sec 10 sec
No.2	9 (2/3)	Sp.Rot	-2.6670	-0.0009 0.0000	26.3 50.00 Cell	Fri May 21 14:27:23 2010 0.00068g/mlMeOH+CHCl3(1:1) JB-3	Na 589nm	2 sec 10 sec
No.3	9 (3/3)	Sp.Rot	-2.9630	-0.0010 0.0000	26.3 50.00 Cell	Fri May 21 14:27:37 2010 0.00068g/mlMeOH+CHCl3(1:1) JB-3	Na 589nm	2 sec 10 sec

-3.1605°

Optical rotation of compound 1