

Supplementary Data

Chemical Constituents and Chemotaxonomic studies from the Twigs of *Neobalanocarpus heimii* (King) P.S. Ashton (Dipterocarpaceae)

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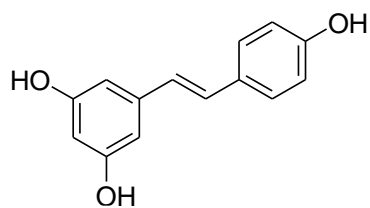
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Trans-resveratrol (1)



Molecular formula : C₁₄H₁₂O₃

UV λ_{\max} (MeOH) : 207, 285 nm

IR ν_{\max} (KBr) : 3282 (OH); 1612 cm⁻¹ (C=C Ar)

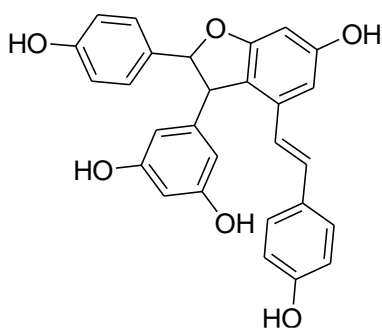
NMR data of compound 1

No	δ_{H} (<i>mult.</i> , J in Hz)	
	1*	1**
1	-	-
2,6	7.43 (d, 8.4)	7.41 (d, 8.7)
3,5	6.85 (d, 8.4)	6.83 (d, 8.7)
4	-	-
7	7.02 (d, 16.4)	7.00 (d, 16.4)
8	6.89 (d, 16.4)	6.87 (d, 16.4)
9	-	-
10	6.55 (d, 1.8)	6.53 (d, 2.0)
11	-	-
12	6.28 (t, 1.8)	6.26 (t, 2.0)
13	-	-
14	6.55 (d, 1.8)	6.53 (d, 2.0)

* measured in acetone-*d*₆

** measured in acetone-*d*₆ (Mattiviti et al. 1995)

(-)- ϵ -viniferin (2)



Molecular formula : C₂₈H₂₂O₆
UV λ_{\max} (MeOH) : 214, 282 nm
IR ν_{\max} (KBr) : 3258 (OH); 1689, 1432 cm⁻¹ (C=C Ar)

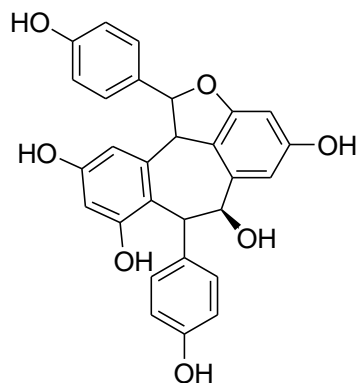
NMR data of compound 2

No	δ_{H} (<i>mult.</i> , J in Hz)	
	2*	2**
1a	-	-
2a,6a	7.21 (d, 8.8)	7.21 (d, 7.0)
3a,5a	6.84 (d, 8.8)	6.83 (d, 7.0)
4a	-	-
7a	5.43 (d, 5.4)	5.44 (d, 5.4)
8a	4.48 (d, 5.4)	4.46 (d, 5.4)
9a	-	-
10a,14a	6.25 (br s)	6.24 (br s)
11a	-	-
12a	6.25 (br s)	6.24 (br s)
13a	-	-
1b	-	-
2b,6b	7.18 (d, 8.8)	7.19 (d, 7.0)
3b,5b	6.75 (d, 8.8)	6.74 (d, 7.0)
4b	-	-
7b	6.92 (d, 16.4)	6.91 (d, 16.2)
8b	6.72 (d, 16.4)	6.71 (d, 16.2)
9b	-	-
10b	-	-
11b	-	-
12b	6.33 (d, 1.8)	6.33 (d, 2.0)
13b	-	-
14b	6.74 (d, 1.8)	6.77 (d, 2.0)

* measured in acetone-*d*₆

** measured in acetone-*d*₆ (Li et al. 1996)

Balanocarpol (3)



Molecular formula : C₂₈H₂₂O₇
UV λ_{\max} (MeOH) : 209, 283 nm
IR ν_{\max} (KBr) : 3258 (OH); 1730, 1448 cm⁻¹ (C=C Ar)

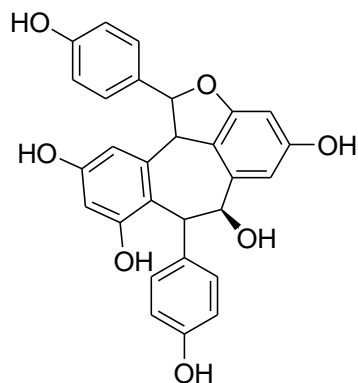
NMR data of compound 3

No	δ_{H} (<i>mult.</i> , J in Hz)	
	3*	3**
1a	-	-
2a,6a	7.50 (d, 8.4)	7.48 (d, 8.8)
3a,5a	6.95 (d, 8.4)	6.95 (d, 8.8)
4a	-	-
7a	5.70 (d, 9.6)	5.70 (d, 9.5)
8a	5.17 (d, 9.6)	5.16 (d, 9.5)
9a	-	-
10a	-	-
11a	-	-
12a	6.09 (s)	6.09 (d, 2.2)
13a	-	-
14a	5.96 (s)	5.96 (d, 2.2)
1b	-	-
2b,6b	6.75 (d, 8.4)	6.75 (d, 9.5)
3b,5b	6.42 (d, 8.4)	6.42 (d, 9.5)
4b	-	-
7b	4.89 (s)	4.89 (s)
8b	5.39 (s)	5.39 (s)
9b	-	-
10b	-	-
11b	-	-
12b	6.20 (s)	6.20 (d, 2.2)
13b	-	-
14b	6.25 (s)	6.25 (d, 2.2)

* measured in acetone-*d*₆

** measured in methanol-*d*₄ (Ito et al. 1999)

Ampelopsin A (4)



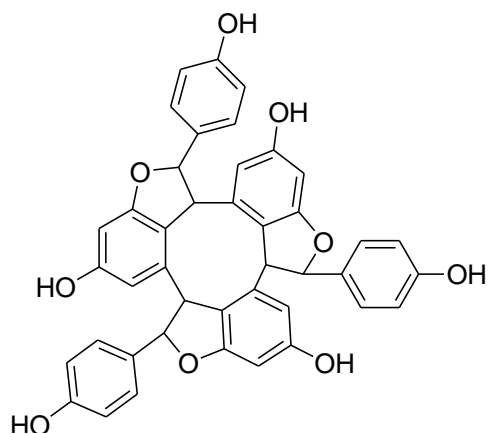
Molecular formula : C₂₈H₂₂O₇
 UV λ_{max} (MeOH) : 220, 284 nm
 IR ν_{max} (KBr) : 3339 (OH); 1600, 1450 cm⁻¹ (C=C Ar)

NMR data of compound 4

No	δ _H (mult., J in Hz)		δ _C	
	4*	4**	4*	4**
1a	-	-	131.6	132.3
2a,6a	7.10 (d, 8.6)	7.10 (d, 8.4)	129.1	129.6
3a,5a	6.75 (d, 8.6)	6.77 (d, 8.4)	115.3	115.6
4a	-	-	156.4	156.9
7a	5.76 (d, 11.4)	5.75 (d, 11.4)	48.7	49.2
8a	4.15 (d, 11.4)	4.15 (d, 11.4)	87.6	88.1
9a	-	-	142.1	142.7
10a	-	-	118.3	118.5
11a	-	-	155.4	155.7
12a	6.42 (d, 2.0)	6.42 (d, 2.2)	100.7	101.1
13a	-	-	159.2	159.8
14a	6.22 (br s)	6.22 (br s)	104.5	105.1
1b	-	-	129.9	130.6
2b,6b	6.88 (d, 8.6)	6.88 (d, 8.8)	127.9	128.3
3b,5b	6.63 (d, 8.6)	6.63 (d, 8.4)	114.6	115.0
4b	-	-	156.4	158.1
7b	5.44 (d, 4.7)	5.44 (d, 4.8)	42.9	43.5
8b	5.40 (d, 4.7)	5.40 (d, 4.8)	70.4	70.7
9b	-	-	139.3	140.1
10b	-	-	117.3	118.0
11b	-	-	158.1	159.8
12b	6.15 (d, 2.2)	6.14 (d, 2.2)	96.3	97.0
13b	-	-	157.7	158.5
14b	6.62 (d, 2.2)	6.60 (d, 2.2)	109.7	110.1

* measured in methanol-*d*₄

** measured in acetone -*d*₆ Takaya et al, (2002)

(+)- α -viniferin (5)

Formula molekul : C₄₂H₃₀O₉
 UV λ_{\max} (MeOH) : 220, 232, 284 nm
 IR ν_{\max} (KBr) : 3352 (OH); 1612, 1239 cm⁻¹ (C=C Ar)

NMR data of compound 5

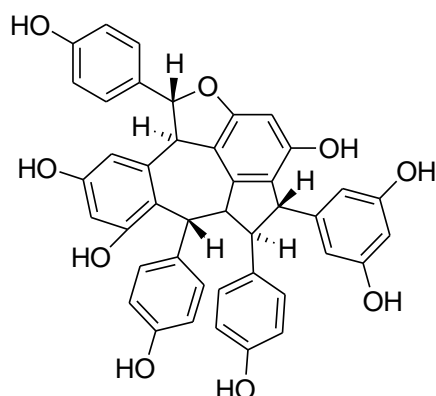
No	δ_{H} (<i>mult.</i> , J in Hz)		δ_{C}	
	6'	6''	6'	6''
1a	-	-	132.1	132.0
2a,6a	7.02 (d, 8.5)	7.03 (d, 8.5)	128.2	128.1
3a,5a	6.71 (d, 8.5)	6.72 (d, 8.5)	115.8	115.7
4a	-	-	157.9	157.9
7a	6.06 (br s)	6.07 (br s)	86.5	86.4
8a	3.96 (br s)	3.97 (br s)	46.5	46.4
9a	-	-	141.3	141.2
10a	-	-	118.9	118.8
11a	-	-	159.4	159.3
12a	5.99 (d, 1.8)	5.99 (d, 1.8)	108.6	108.5
13a	-	-	161.8	161.6
14a	6.21 (d, 1.8)	6.22 (d, 1.8)	98.1	98.0
1b	-	-	132.4	132.2
2b,6b	7.21 (d, 8.4)	7.22 (d, 8.5)	128.2	128.1
3b,5b	6.77 (d, 8.4)	6.77 (d, 8.5)	116.2	116.1
4b	-	-	158.3	158.2
7b	5.94 (d, 9.9)	5.95 (d, 9.7)	90.0	90.0
8b	4.64 (d, 9.9)	4.71 (d, 9.7)	52.9	52.9
9b	-	-	139.8	139.7
10b	-	-	121.0	120.9
11b	-	-	159.5	159.3
12b	6.71 (d, 1.8)	6.72 (d, 1.8)	106.3	106.2
13b	-	-	160.8	160.6
14b	6.24 (d, 1.8)	6.25 (d, 1.8)	96.6	96.6
1c	-	-	132.6	132.5

2c,6c	7.04 (d, 8.4)	7.08 (d, 8.5)	128.7	128.6
3c,5c	6.78 (d, 8.4)	6.79 (d, 8.5)	116.2	116.1
4c	-	-	158.4	158.3
7c	4.90 (d, 6.1)	4.9 (d, 6.4)	95.7	95.6
8c	4.68 (d, 6.1)	4.61 (d, 6.4)	55.8	55.6
9c	-	-	138.8	138.7
10c	-	-	119.8	119.7
11c	-	-	161.0	160.8
12c	6.59 (d, 1.8)	6.59 (d, 1.8)	105.8	105.8
13c	-	-	161.8	161.7
14c	6.22 (d, 1.8)	6.22 (d, 1.8)	97.0	96.9

* measured in acetone - d_6

** measured in acetone - d_6 (Kitanaka et al. 1990)

Vaticanol A (6)



Molecular formula : $C_{42}H_{32}O_9$

UV λ_{max} (MeOH) : 219, 284 nm

IR ν_{max} (KBr) : 3350 (OH); 2525, 1603, 1234 cm^{-1} (C=C Ar)

NMR data of compound 6

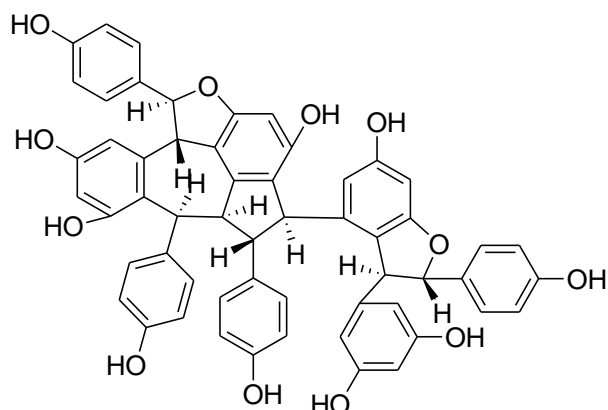
No	δ_H (mult., J in Hz)		δ_C	
	6*	6**	6*	6**
1a	-	-	134.0	134.4
2a,6a	7.27 (d, 8.5)	7.28 (d, 8.8)	127.4	128.0
3a,5a	6.82 (d, 8.5)	6.83 (d, 8.8)	115.2	116.0
4a	-	-	157.5	157.9
7a	6.16 (d, 3.5)	6.18 (br d, 3.9)	86.7	86.5
8a	4.49 (d, 3.5)	4.51 (d, 3.9)	50.0	50.3
9a	-	-	144.3	144.7
10a	-	-	118.8	119.3

11a	-	-	157.3	157.7
12a	6.07 (d, 2.2)	6.09 (d, 2.4)	1008	101.3
13a	-	-	155.9	156.3
14a	6.47 (d, 2.2)	6.48 (d, 2.4)	102.7	103.3
1b	-	-	138.3	138.7
2b,6b	7.06 (d, 8.5)	7.07 (d, 8.8)	128.8	129.2
3b,5b	6.58 (d, 8.5)	6.60 (d, 8.8)	114.7	115.4
4b	-	-	155.3	155.7
7b	5.16 (br s)	5.17 (br s)	35.7	36.0
8b	4.50 (d, 6.6)	4.52 (d, 7.3)	48.2	48.6
9b	-	-	144.5	144.9
10b	-	-	118.2	118.6
11b	-	-	159.5	159.9
12b	6.21 (br s)	6.22 (s)	94.8	95.3
13b	-	-	155.0	155.4
14b	-	-	121.9	122.2
1c	-	-	135.4	135.8
2c,6c	6.53 (d, 8.5)	6.55 (d, 8.8)	129.2	129.6
3c,5c	6.36 (d, 8.5)	6.37 (d, 8.8)	114.5	114.9
4c	-	-	156.6	156.4
7c	3.63 (d, 7.2)	3.65 (d, 7.3)	63.9	64.3
8c	4.18 (br s)	4.20 (br s)	57.1	57.5
9c	-	-	147.1	147.5
10c	6.26 (d, 2.2)	6.27 (d, 2.0)	106.2	106.7
11c	-	-	158.8	159.4
12c	6.19 (t, 2.2)	6.21 (t, 2.0)	100.7	101.2
13c	-	-	158.8	159.4
14c	6.26 (d, 2.2)	6.27 (d, 2.0)	106.2	106.7

* measured in acetone- d_6

** measured in acetone- d_6 (Tanaka et al. 2000)

Vaticanol B (7)



Molecular formula : $C_{56}H_{42}O_{12}$
 UV λ_{max} (MeOH) : 213, 284 nm
 IR ν_{max} (KBr) : 3355 (OH); 1608, 1231 cm^{-1} (C=C Ar)

NMR data of compound 7

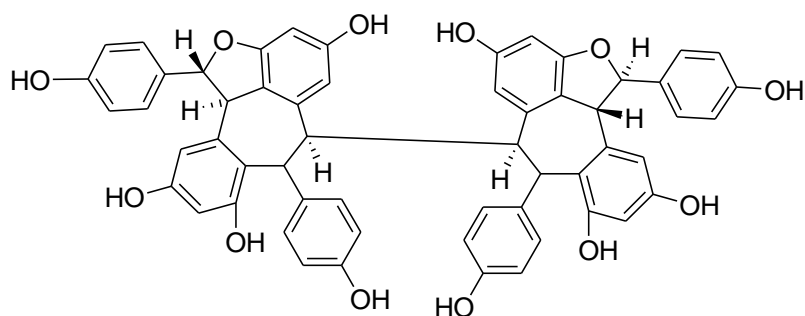
No	δ_H (mult., J in Hz)		δ_C	
	10'	10''	10'	10''
1a	-	-	130.0	130.8
2a,6a	7.22 (d, 8.5)	7.23 (d, 8.8)	130.2	130.2
3a,5a	6.78 (d, 8.5)	6.79 (d, 8.8)	115.4	116.0
4a	-	-	157.8	158.5
7a	5.76 (d, 11.8)	5.77 (d, 11.7)	89.6	90.4
8a	4.43 (d, 11.8)	4.44 (d, 11.7)	48.1	48.8
9a	-	-	140.9	141.8
10a	-	-	123.7	124.5
11a	-	-	155.1	155.7
12a	6.26 (d, 2.0)	6.29 (d, 2.0)	100.9	101.6
13a	-	-	155.9	156.7
14a	6.09 (d, 2.0)	6.12 (d, 2.0)	104.9	105.8
1b	-	-	132.7	133.5
2b,6b	7.17 (d, 8.5)	7.17 (d, 8.8)	129.8	130.7
3b,5b	6.69 (d, 8.5)	6.70 (d, 8.8)	114.7	115.5
4b	-	-	155.0	155.9
7b	5.18 (d, 3.3)	5.21 (d, 3.9)	36.3	37.1
8b	3.10 (d, 12.0)	3.13 (dd, 11.3, 3.9)	52.3	53.1
9b	-	-	142.4	143.2
10b	-	-	115.1	115.7
11b	-	-	158.0	158.8
12b	6.04 (s)	6.05 (s)	95.7	96.5
13b	-	-	154.1	154.9
14b	-	-	121.4	122.1
1c	-	-	130.6	131.4
2c,6c	6.39 (d, 8.5)	6.42 (d, 8.8)	128.4	129.2

3c,5c	6.50 (d, 8.5)	6.52 (d, 8.8)	115.1	115.8
4c	-	-	155.5	156.3
7c	4.08 (d, 11.3)	4.10 (d, 11.3)	56.9	57.6
8c	4.54 (d, 10.8)	4.55 (d, 10.7)	48.6	49.3
9c	-	-	140.9	141.6
10c	-	-	122.5	123.3
11c	-	-	160.9	161.7
12c	6.17 (t, 2.0)	6.21 (t, 2.0)	94.9	95.6
13c	-	-	158.4	159.4
14c	6.46 (d, 2.0)	6.49 (d, 2.0)	106.4	107.0
1d	-	-	133.7	134.7
2d,6d	7.16 (d, 8.5)	7.19 (d, 8.8)	127.4	128.2
3d,5d	6.76 (d, 8.5)	6.78 (d, 8.8)	115.1	115.9
4d	-	-	157.2	157.9
7d	5.36 (d, 5.2)	5.38 (d, 4.7)	93.9	94.6
8d	4.67 (d, 5.2)	4.68 (d, 4.7)	56.7	57.5
9d	-	-	147.1	147.9
10d,14d	6.10 (d, 2.2)	6.10 (d, 2.4)	106.7	107.5
11d,13d	-	-	158.0	159.8
12d	6.28 (t, 2.2)	6.20 (t, 2.4)	101.4	102.2

* measured in acetone- d_6

** measured in acetone- d_6 (Tanaka et al. 2000)

Hopeaphenol (8)



Molecular formula : C₅₆H₄₂O₁₂
 UV λ_{max} (MeOH) : 216, 292 nm
 IR ν_{max} (KBr) : 3295 (OH); 1606, 1453 cm⁻¹ (C=C Ar)

NMR data of compound 8

No	δ _H (mult., J in Hz)		δ _C	
	7*	7**	7*	7**
1a/1d	-	-	130.1	130.9
2a,6a/6a,6d	7.13 (d, 8.2)	7.15 (d, 8.6)	129.5	130.2
3a,5a/3d,5d	6.78 (d, 8.2)	6.79 (d, 8.6)	114.4	115.2
4a/4d	-	-	157.6	158.4
7a/7d	5.76 (d, 12.1)	5.78 (d, 12.1)	87.5	88.2
8a/8d	4.23 (d, 12.1)	4.25 (d, 12.1)	48.7	49.7
9a/9d	-	-	141.6	142.3
10a/10d	-	-	120.4	121.1
11a/11d	-	-	157.1	157.9
12a/12d	6.54 (d, 2.8)	6.56 (d, 1.7)	100.3	101.1
13a/13d	-	-	155.5	156.3
14a/14d	6.02 (br s)	6.31 (d, 1.7)	105.5	106.3
1b/1c	-	-	134.3	135.2
2b,6b/2c,6c	6.90 (d, 8.0)	6.92 (d, 8.4)	128.5	129.2
3b,5b/3c,5c	6.56 (d, 8.0)	6.58 (d, 8.4)	114.4	115.2
4b/4c	-	-	155.0	155.9
7b/7c	5.79 (br s)	5.81 (br s)	40.4	41.2
8b/8c	3.94 (br s)	3.96 (br s)	47.4	48.2
9b/9c	-	-	139.6	140.4
10b/10c	-	-	117.7	118.5
11b/11c	-	-	159.6	160.4
12b/12c	5.73 (d, 1.4)	5.75 (d, 2.1)	94.5	95.2
13b/13c	-	-	154.8	155.6
14b/14c	5.16 (d, 1.4)	5.18 (d, 2.1)	110.6	111.2

* measured in methanol-*d*₄

** measured in acetone-*d*₆ (Ito et al. 2001)