SUPPLEMENTARY MATERIAL

A new flavone C-glycoside and a new bibenzyl from *Bulbophyllum retusiusculum*

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Abstract

A new flavone C-glycoside, apigenin 6-C- α -arabinofuranosyl 8-C- α -arabinopyranoside (**1**) and a new bibenzyl, bulbotetusine (**2**), were isolated from the tubers of *Bulbophyllum retusiusculum*. Their structures were established on the basis of extensive spectroscopic analyses. The absolute configuration of **2** was determined by the comparison of experimental and calculated electronic circular dichroism (ECD). Compounds **1** and **2** showed no obvious cytotoxic activity against any five human tumor cell lines with IC₅₀ values > 40 μ M.

Keywords: *Bulbophyllum retusiusculum*; flavone C-glycoside; bibenzyl;

apigenin 6-C- α -arabinofuranosyl 8-C- α -arabinopyranoside; bulbotetusine

Figure S1: The key ^1H - ^1H COSY (—), HMBC (—) and ROESY (---) correlations of **1**.

Figure S2: The key ^1H - ^1H COSY (—) and HMBC (—) correlations of **2**.

Figure S3: Calculated and experimental ECD spectra of **2**.

Figure S4. ^1H NMR (600 MHz, DMSO- d_6) spectrum of compound **1**.

Figure S5. ^{13}C NMR (150 MHz, DMSO- d_6) spectrum of compound **1**.

Figure S6. ^1H - ^1H COSY spectrum of compound **1**.

Figure S7. HSQC spectrum of compound **1**.

Figure S8. HMBC spectrum of compound **1**.

Figure S9. ROESY spectrum of compound **1**.

Figure S10. HRESIMS (-) spectrum of compound **1**.

Elemental composition calculator

Target m/z: +533.1299

amu

Tolerance: +2.0000

ppm

Result type: Elemental

Max num of results: 100

Min DBE: -0.5000

Max DBE: +50.0000

Electron state: OddAndEven

Num of charges: -1

Add water: N/A

Add proton: N/A

File Name: FYS-97-----.wiff

	Elements	Min Number	Max Number
1	C	0	25
2	Cl	0	1
3	F	0	0
4	H	0	26
5	N	0	0
6	Na	0	0
7	O	0	13
8	P	0	0
9	Pd	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C25 H25 O13	533.1300	-0.1648	-0.3093	13.5

Figure S11. ^1H NMR (400 MHz, CD_3OD) spectrum of compound **2**.

Figure S12. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **2**.

Figure S13. ^1H - ^1H COSY spectrum of compound **2**.

Figure S14. HSQC spectrum of compound **2**.

Figure S15. HMBC spectrum of compound **2**.

Figure S16. ROESY spectrum of compound **2**.

Figure S17. HRESIMS (-) spectrum of compound **2**.

Elemental composition calculator

Target m/z: +273.0767

amu

Tolerance: +2.0000

ppm

Result type: Elemental

Max num of results: 100

Min DBE: -0.5000

Max DBE: +50.0000

Electron state: OddAndEven

Num of charges: -1

Add water: N/A

Add proton: N/A

File Name: FYS-80---.wiff

	Elements	Min Number	Max Number
1	C	0	20
2	Cl	0	1
3	F	0	0
4	H	0	24
5	N	0	0
6	Na	0	0
7	O	0	7
8	P	0	0
9	Pd	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C15 H13 O5	273.0768	-0.1472	-0.5394	9.5