## Article

## Cytotoxic Polyketides from a Deep-Sea Sediment Derived Fungus *Diaporthe phaseolorum* FS431

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**Abstract:** Two new chromone-derived polyketides phaseolorins, G and H (1 and 2), and one new anthraquinone derivative, phaseolorin I (3), together with three known compounds (4–6), were isolated from the deep-sea sediment-derived fungus *Diaporthe phaseolorum* FS431. The structures of the new compounds were determined by comprehensive analysis of their spectroscopic data, and the absolute configuration of 1 was established by quantum chemical calculations of electron capture detection (ECD). All the isolated compounds (1–6) were tested for their in vitro cytotoxic activities against four human tumor cell lines, of which compound 4 exhibited significant effect against MCF-7, HepG-2, and A549 tumor cell lines with IC<sub>50</sub> values of 2.60, 2.55, and 4.64 μM, respectively.

Keywords: Diaporthe phaseolorum; deep-sea derived fungus; polyketides; cytotoxicity

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Figure S1. HRESIMS spectrum of Phaseolorin G (1)



Figure S2. <sup>1</sup>H-NMR spectrum (600 MHz, acetone-d<sub>6</sub>) of Phaseolorin G (1)



Figure S3. <sup>1</sup>H-NMR spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of Phaseolorin G (1)



Figure S4. <sup>13</sup>C-NMR spectrum (150 MHz, acetone-d<sub>6</sub>) of Phaseolorin G (1)



Figure S5. <sup>1</sup>H-<sup>1</sup>H COSY spectrum (600 MHz, acetone-*d*<sub>6</sub>) of Phaseolorin G (1)



Figure S6. HSQC spectrum of Phaseolorin G (1)



Figure S7. HMBC spectrum of Phaseolorin G (1)



Figure S8. NOESY spectrum (600 MHz, acetone- $d_6$ ) of Phaseolorin G (1)



Figure S9. CD spectrum of Phaseolorin G (1)







Figure S11. IR spectrum of Phaseolorin G (1)

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Figure S12. HRESIMS spectrum of Phaseolorin G (1)



Figure S13. <sup>1</sup>H-NMR spectrum (600 MHz, CHCl<sub>3</sub>) of Phaseolorin H (2)



Figure S14. <sup>13</sup>C-NMR spectrum (150 MHz, CHCl<sub>3</sub>) of Phaseolorin H (2)



Figure S15. <sup>1</sup>H-<sup>1</sup>H COSY spectrum (600 MHz, CHCl<sub>3</sub>) of Phaseolorin H (2)



Figure S16. HSQC spectrum of Phaseolorin H (2)



Figure S17. HMBC spectrum of Phaseolorin H (2)



Figure S18. UV spectrum of Phaseolorin H (2)



Figure S19. IR spectrum of Phaseolorin H (2)



Figure S20. HRESIMS spectrum of Phaseolorin I (3)



Figure S21. <sup>1</sup>H-NMR spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of Phaseolorin I (3)



Figure S22. <sup>13</sup>C-NMR spectrum (150 MHz, DMSO-d<sub>6</sub>) of Phaseolorin I (3)



Figure S23. HMBC spectrum of Phaseolorin I (3)











Figure S26. <sup>1</sup>H-NMR spectrum (600 MHz, CHCl<sub>3</sub>) of Phomoxanthone A (4)



Figure S27. <sup>13</sup>C-NMR spectrum (150 MHz, CHCl<sub>3</sub>) of Phomoxanthone A (4)



Figure S28. <sup>1</sup>H-NMR spectrum (600 MHz, CHCl<sub>3</sub>) of Dicerandrol B (5)



Figure S29. <sup>13</sup>C-NMR spectrum (150 MHz, CHCl<sub>3</sub>) of Dicerandrol B (5)





2,2',6'-trihydroxy-4-methyl-6-methoxy-acyl-diphenylmethanone (6)



Figure S31. <sup>13</sup>C-NMR spectrum (150 MHz, CD<sub>3</sub>OD) of

2,2',6'-trihydroxy-4-methyl-6-methoxy-acyl-diphenylmethanone (6)

Compounds	CONFORMATION	E (Hartree)	E (Kcal/mol)	rel.E (Kcal/mol)	Boltzmann Dist (%)
	<b>1</b> a-1	-957.4240435	-600786.3638	0	76.40%
1.	<b>1a-</b> 2	-957.42160243	-600784.832	1.531751521	5.75%
1a	<b>1a-</b> 3	-957.42259761	-600785.4565	0.90727695	16.51%
	<b>1a-</b> 4	-957.42023030	-600783.971	2.392771468	1.34%

Table S1. Energy analysis for the Conformers of **1a** (**1**).





**1a-**2

**1a-**3

Figure S32. B3LYP/6-31G(d,p) optimized low-energy conformers of **1a** (**1**)

Compounds	Conformation	F (Hartree)	F (Kcal/mol)	rel.E	Boltzmann
compounds	comornation	E (Huitice)		(Kcal/mol)	<b>Dist (%)</b>
	<b>1b-</b> 1	-957.4240957	-600786.3966	0	76.65%
11.	<b>1b-</b> 2	-957.42169738	-600784.8916	1.50497911	6.03%
10	<b>1b-</b> 3	-957.42261675	-600785.4685	0.928069259	15.99%
	<b>1b-</b> 4	-957.42027066	-600783.9964	2.400248793	1.33%

Table S2. Energy analysis for the Conformers of **1b** (**1**).







**1b-**3



Figure S33. B3LYP/6-31G(d,p) optimized low-energy conformers of **1b** (**1**)