## **Supporting Information**

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## Two New Bibenzyls from Dendrobium hercoglossum

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Table of Contents	Page
Figure S1: Key HMBC correlations of 1 and 2	2
Figure S2: HR-ESI-MS spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)	2
Figure S3: <sup>1</sup> H-NMR (600 MHz, CDCl <sub>3</sub> ) spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)	3
Figure S4: <sup>13</sup> C-NMR (150 MHz, CDCl <sub>3</sub> ) spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)	3
Figure S5: HSQC spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)	4
Figure S6: HMBC spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)	4
Figure S7: HR-ESI-MS spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)	5
<b>Figure S8:</b> <sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> ) spectrum of <b>2</b> (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)	5
<b>Figure S9:</b> <sup>13</sup> C-NMR (100 MHz, CDCl <sub>3</sub> ) spectrum of <b>2</b> (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)	6
Figure S10: HSQC spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)	6
<b>Figure S11:</b> HMBC spectrum of <b>2</b> (4-hydroxy-3, 5, 3', $\alpha$ - tetramethoxybibenzyl)	7
<b>Figure S12:</b> ECD spectrum of <b>2</b> (4-hydroxy-3, 5, 3', $\alpha$ - tetramethoxybibenzyl)	8
Figure S13: IR spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)	8
Figure S13: The cytotoxic activities against MDA-MB-231 of compounds	9
Figure S14: The cytotoxic activities against Hela of compounds	9

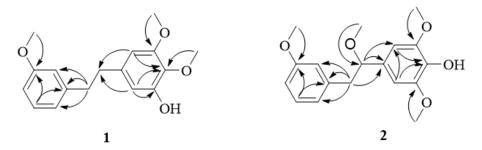


Figure S1. Key HMBC correlations of 1 and 2

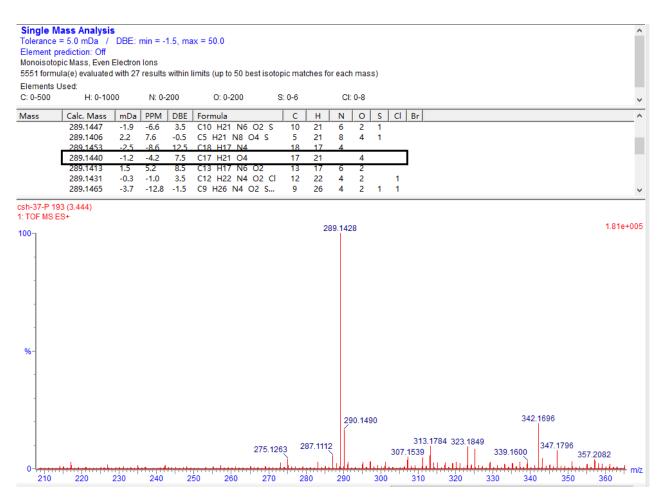


Figure S2: HR-ESI-MS spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)

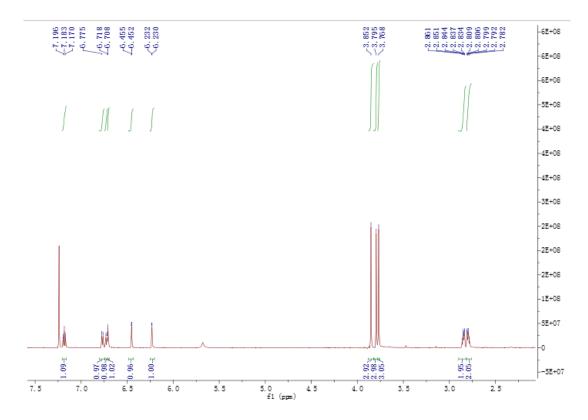


Figure S3: <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)

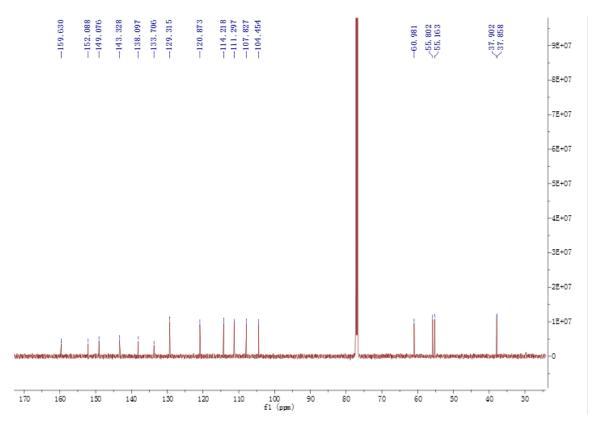


Figure S4: <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>) spectrum of **1** (3-hydroxy-4, 5, 3'-trimethoxybibenzyl) © 2021 ACG Publications. All rights reserved.

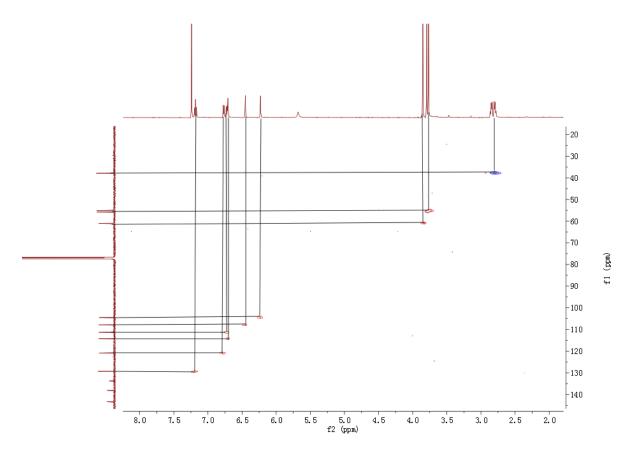


Figure S5: HSQC spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)

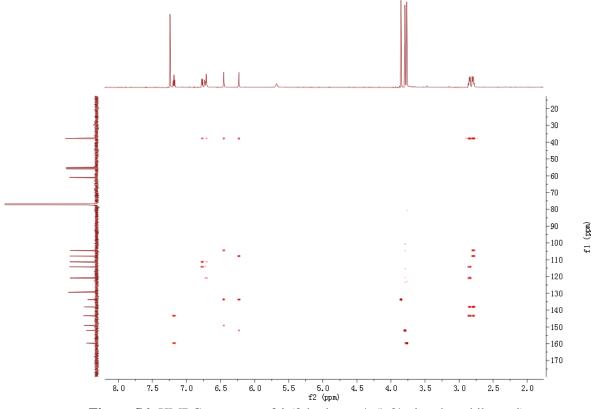


Figure S6: HMBC spectrum of 1 (3-hydroxy-4, 5, 3'-trimethoxybibenzyl)

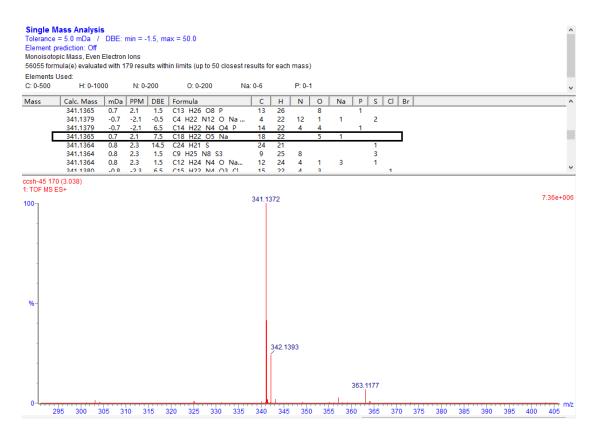


Figure S7: HR-ESI-MS spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)

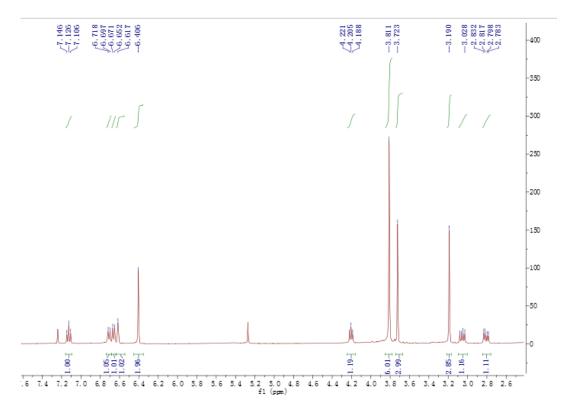


Figure S8: <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)

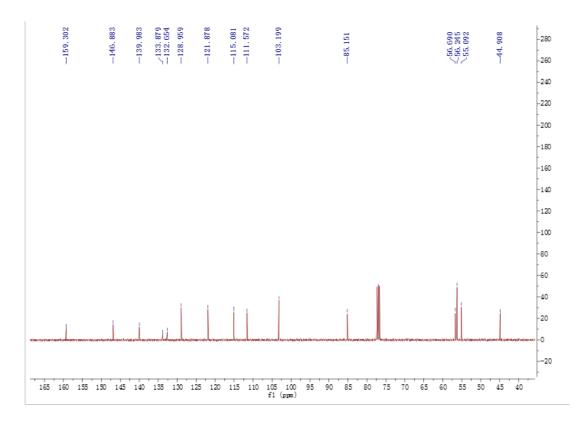


Figure S9: <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)

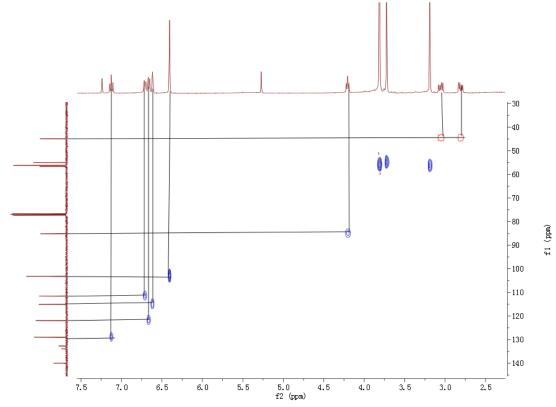
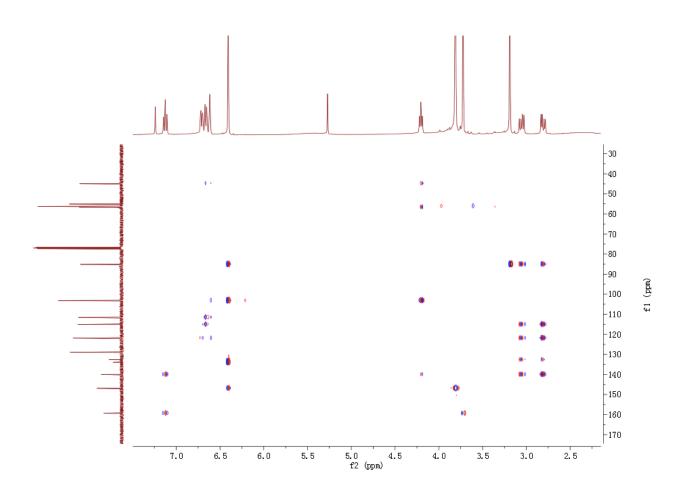
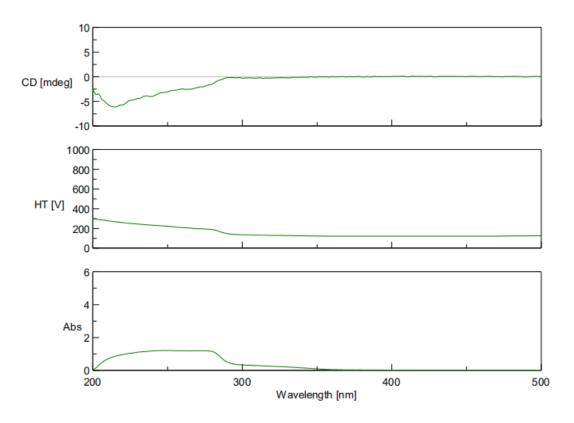


Figure S10: HSQC spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)



**Figure S11:** HMBC spectrum of **2** (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)



**Figure S12:** ECD spectrum of **2** (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)

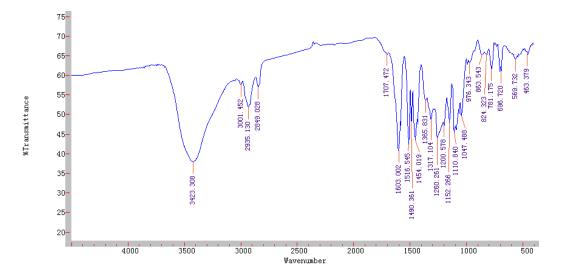


Figure S13: IR spectrum of 2 (4-hydroxy-3, 5, 3', α- tetramethoxybibenzyl)

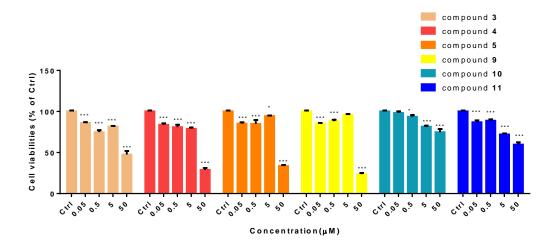


Figure S14: The cytotoxic activities against MDA-MB-231 of compounds

(Results are expressed as mean  $\pm$  SEM. Statistical significance compared to the control, \* p < 0.05, \*\* p < 0.01, \*\*\* p < 0.001.)

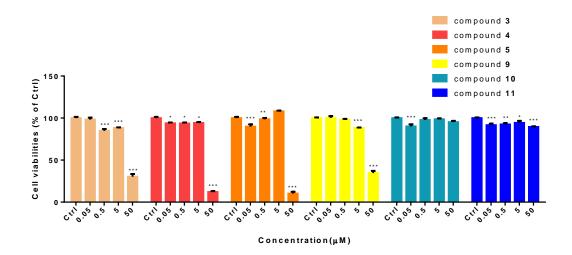


Figure S15: The cytotoxic activities against Hela of compounds

(Results are expressed as mean  $\pm$  SEM. Statistical significance compared to the control, \* p<0.05, \*\* p<0.01, \*\*\* p<0.001.)