Cytotoxic Metabolites from the Endophytic Fungus
Chaetomium globosum 7951

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Supporting Information
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<td>Figure S25. The HMBC Spectrum of Compound 6 in DMSO–d_6</td>
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EXPERIMENTAL SECTION

General experimental procedures

Optical rotations were measured using a Rudolph Research Autopol III automatic polarimeter. UV, CD, and IR spectra were recorded using a Cary 300 spectrometer, a JASCO J-815 CD spectrometer, and a Nicolet 5700 FT-IR spectrometer (FT-IR microscope transmission), respectively. $^1$H and $^{13}$C NMR spectra were obtained at 600 MHz and 150 MHz, respectively, using a Bruker-AVIIIHD-600 spectrometer with solvent peaks used as references. HR-ESIMS data were measured using an AB SCIEX QTOF MS (QSTAR Elite). ESIMS data were measured using an Agilent 1100 series LC/MSD mass spectrometer. Column chromatography was performed using silica gel (200–300 mesh, Qingdao Marine Chemical Inc., China). HPLC separation was performed using an Agilent 1200 series (quaternary pump, autosampler, diode array detector) with a Shiseido Capcell-Pak C18 MGI1, 5 μm, 250 × 10 mm column. TLC was performed using glass precoated silica gel GF254 plates (Qingdao Marine Chemical Inc., Qingdao, China).

NMR chemical shifts and ORs calculation of compound 3.

Conformational analysis of the $(3S,6S)$-3 and $(3R,6S)$-3 (Fig. S1) were carried out via Monte Carlo searching with the MMFF94s molecular mechanics force field using the spartan 14 software. $^1$ 16 of $(3S,6S)$-3 and 30 of $(3R,6S)$-3 geometries having relative energies within 4 kcal/mol were optimized using DFT at the B3LYP/6-31+G (d, p) level in vacuum with the Gaussian 09 program, respectively. $^2$ NMR chemical shifts calculation for those B3LYP/6-31+G (d, p)-optimized conformers with their Boltzmann distribution (>1%) \[(3S,6S)-3 \text{: Table S1; (3R,6S)-3 : Table S2} \] were carried out at PCM/mPW1PW91/6-311+G (d, p) level in DMSO with GIAO method. After Boltzmann weighing of the calculated chemical shift of each isomers, the DP4+ parameters were calculated using the excel file, which was provided by Ariel M. Sarotti. $^3$

In addition, those stable conformers of $(3S,6S)$-3 with their Boltzmann distribution (>1%) also were carried out at the B3LYP/DGDZVP level in the methanol for OR computation. The final OR values of $(3S,6S)$-3 was obtained according to the Boltzmann distribution theory and their relative Gibbs free energy ($\Delta G$). The theoretically calculated OR value of $(3S,6S)$-3 (+56.1, Table S8) was in good agreement with the experimental OR value of 3 (+80.0) in methanol.

Figure S1. Proposed the calculated structure of 3
Table S1. Free energies ($\Delta G$), and Boltzmann distribution abundances of conformers of (3S,6S)-3

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Table S3. Experimental $^{13}$C-NMR chemical shifts and GIAO isotropic magnetic shielding values calculated for PCM/mPW1PW91/6-31+G (d, p) geometries of (3,6S)-3

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Table S4. Experimental $^1$H-NMR chemical shifts and GIAO isotropic magnetic shielding values calculated for PCM/mPW1PW91/6-31+G (d, p) geometries of (3,6S)-3

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$^a$Averaged according to the Boltzmann-calculated contribution at B3LYP/6-31+G(d, p) level.
Table S5. Experimental $^{13}$C-NMR chemical shifts and GIAO isotropic magnetic shielding values calculated for PCM/mPW1PW91/6-311+G (d, p) geometries of (3\(R\),6\(S\))-3

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\(^a\)Averaged according to the Boltzmann-calculated contribution at B3LYP/6-31+G(d, p) level.
Table S6. Experimental $^1$H-NMR chemical shifts and GIAO isotropic magnetic shielding values calculated for PCM/mPW1PW91/6-311+G (d, p) geometries of (3R,6S)-3

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Table S7. Experimental chemical shifts, the calculated shielding tensors for (3S,6S)-3 (isomer 1) and (3R,6S)-3 (isomer 2), and the DP4+ probability of (3S,6S)-3 and (3R,6S)-3

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**Averaged** 56.1

*Averaged according to the Boltzmann-calculated contribution at B3LYP/DGDZVP level.*
Figure S2. The IR Spectrum of Compound 1
Figure S3. The (+)-HRESIMS Spectroscopic Data of Compound 1

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Figure S4. The $^1$H NMR Spectrum of Compound 1 in DMSO–$d_6$
Figure S5. The $^{13}$C NMR Spectrum of Compound 1 in DMSO–$d_6$
Figure S6. The DEPT Spectrum of Compound 1 in DMSO–d$_6$
Figure S7. The $^1$H-$^1$HCOSY Spectrum of Compound 1 in DMSO–$d_6$
Figure S8. The HSQC Spectrum of Compound 1 in DMSO–d$_6$
Figure S9. The HMBC Spectrum of Compound 1 in DMSO-\textit{d}_6
Figure S10. The ROESY Spectrum of Compound 1 in DMSO-$d_6$. 

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Figure S11. The IR Spectrum of Compound 3
Figure S12. The (+)-HRESIMS Spectroscopic of Compound 3
Figure S13. The $^1$H NMR Spectrum of Compound 3 in DMSO–$d_6$. 
Figure S14. The $^{13}$C NMR Spectrum of Compound 3 in DMSO–$d_6$
Figure S15. The DEPT Spectrum of Compound 3 in DMSO–d$_6$
Figure S16. The $^1$H-$^1$H COSY Spectrum of Compound 3 in DMSO-$d_6$. 

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Figure S17. The HSQC Spectrum of Compound 3 in DMSO–d₆
Figure S18. The HMBC Spectrum of Compound 3 in DMSO–d₆.
Figure S19. The IR Spectrum of Compound 6
Figure S20. The (+)-HRESIMS Spectroscopic Data of Compound 6
Figure S21. The $^1$H NMR Spectrum of Compound 6 in DMSO–$d_6$. 

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Figure S22. The $^{13}$C NMR Spectrum of Compound 6 in DMSO-$d_6$
Figure S23. The $^1$H-$^1$H COSY Spectrum of Compound 6 in DMSO-$d_6$
Figure S24.  The HSQC Spectrum of Compound 6 in DMSO–d$_6$
Figure S25. The HMBC Spectrum of Compound 6 in DMSO-$d_6$