## Supplementary Information

## New diketopiperazines from a marine-derived fungus strain Aspergillus versicolor MF180151

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**Figure S1.** <sup>1</sup>H NMR Spectrum of compounds ( $\pm$ )-1 in DMSO-*d*<sub>6</sub> at 600 MHz



**Figure S2.** <sup>13</sup>C NMR Spectrum of compounds ( $\pm$ )-1 in DMSO- $d_6$  at 600 MHz



Figure S3. HSQC NMR Spectrum of compounds (±)-1 in DMSO-*d*<sub>6</sub>



**Figure S4.** HMBC NMR Spectrum of compounds (±)-1 in DMSO-*d*<sub>6</sub>



**Figure S5.** <sup>1</sup>H-<sup>1</sup>H COSY NMR Spectrum of compounds ( $\pm$ )-1 in DMSO- $d_6$ 



**Figure S6.** ROESY NMR Spectrum of compounds  $(\pm)$ -1 in DMSO- $d_6$ 



Figure S7. HRESIMS and UV spectrum of compounds (±)-1 in CH<sub>3</sub>OH



**Figure S8.** Circular Dichroism spectrum of compounds (±)-1 in CH<sub>3</sub>OH



**Figure S9.** <sup>1</sup>H NMR Spectrum of compounds ( $\pm$ )-**2** in DMSO-*d*<sub>6</sub> at 600 MHz



**Figure S10.** <sup>13</sup>C NMR Spectrum of compounds ( $\pm$ )-2 in DMSO- $d_6$  at 600 MHz



**Figure S11.** HSQC NMR Spectrum of compounds  $(\pm)$ -2 in DMSO- $d_6$  at 600 MHz



**Figure S12.** HMBC NMR Spectrum of compounds  $(\pm)$ -2 in DMSO- $d_6$  at 600 MHz



**Figure S13.** <sup>1</sup>H-<sup>1</sup>H COSY NMR Spectrum of compounds ( $\pm$ )-**2** in DMSO- $d_6$ 





Figure S15. HRESIMS and UV spectrum of compounds (±)-2 in CH<sub>3</sub>OH



Figure S16. Circular Dichroism spectrum of compounds (±)-2 in CH<sub>3</sub>OH



**Figure S17.** <sup>1</sup>H NMR Spectrum of compounds ( $\pm$ )-**3** in DMSO- $d_6$  at 600 MHz



**Figure S18.** <sup>13</sup>C NMR Spectrum of compounds  $(\pm)$ -**3** in DMSO- $d_6$  at 600 MHz



**Figure S19.** HSQC NMR Spectrum of compounds  $(\pm)$ -3 in DMSO- $d_6$ 



**Figure S20.** HMBC NMR Spectrum of compounds  $(\pm)$ -3 in DMSO- $d_6$ 



fl (ppm)

**Figure S21.** <sup>1</sup>H-<sup>1</sup>H COSY NMR Spectrum of compounds (±)-**3** in DMSO-*d*<sub>6</sub>



Figure S22. ROESY NMR Spectrum of compounds (±)-3 in DMSO-*d*<sub>6</sub>



Figure S23. HRESIMS and UV spectrum of compounds (±)-3 in CH<sub>3</sub>OH



Figure S24. Circular Dichroism spectrum of compounds (±)-3 in CH<sub>3</sub>OH