Supporting Information

Harzianumnones A and B: two hydroxyanthraquinones from the coral-derived fungus Trichoderma harzianum

Ting Shi, a,b Xue-Mei Hou, a,b Zhi-Yong Li, c Fei Cao, d Ya-Hui Zhang, a,b Jia-Yin Yu, a,b Dong-Lin Zhao, a,b Chang-Lun Shao, *a,b and Chang-Yun Wang, *a,b,e

Affiliation

a Key Laboratory of Marine Drugs, The Ministry of Education of China, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, People’s Republic of China

b Laboratory for Marine Drugs and Bioproducts, Qingdao National Laboratory for Marine Science and Technology, Qingdao 266071, People’s Republic of China

c Marine Biotechnology Laboratory, State Key Laboratory of Microbial Metabolism, School of Life Sciences & Biotechnology, Shanghai Jiao Tong University, Shanghai 200240, People’s Republic of China

d Key Laboratory of Pharmaceutical Quality Control of Hebei Province, College of Pharmaceutical Sciences, Hebei University, Baoding 071002, People’s Republic of China.

e Institute of Evolution & Marine Biodiversity, Ocean University of China, Qingdao 266003, People’s Republic of China

Correspondence

* To whom correspondence should be addressed.

Tel/Fax: +86-531-82031536 (C.-Y. Wang); +86-532-82031381 (C.-L. Shao)

E-mail: changyun@ouc.edu.cn (C.-Y. Wang); shaochanglun@ouc.edu.cn (C.-L. Shao)
List of Supporting Information

Figure S1. $^1$H NMR spectrum of compound 1 (DMSO-$d_6$).
Figure S2. $^1$H NMR spectrum of compound 1 at the condition of spin (DMSO-$d_6$).
Figure S3. Partial $^1$H NMR spectrum of compound 1 at the condition of spin (DMSO-$d_6$).
Figure S4. $^{13}$C NMR spectrum of compound 1 (DMSO-$d_6$).
Figure S5. COSY spectrum of compound 1 (DMSO-$d_6$).
Figure S6. HSQC spectrum of compound 1 (DMSO-$d_6$).
Figure S7. HMBC spectrum of compound 1 (DMSO-$d_6$).
Figure S8. NOESY spectrum of compound 1 (DMSO-$d_6$).
Figure S9. ESIMS spectrum of compound 1.
Figure S10. HRESIMS spectrum of compound 1.
Figure S11. $^1$H NMR spectrum of compound 2 (DMSO-$d_6$).
Figure S12. $^{13}$C NMR spectrum of compound 2 (DMSO-$d_6$).
Figure S13. COSY spectrum of compound 2 (DMSO-$d_6$).
Figure S14. HSQC spectrum of compound 2 (DMSO-$d_6$).
Figure S15. HMBC spectrum of compound 2 (DMSO-$d_6$).
Figure S16. NOESY spectrum of compound 2 (DMSO-$d_6$).
Figure S17. ESIMS spectrum of compound 2.
Figure S18. HRESIMS spectrum of compound 2.
Figure S19. DNA Topo I inhibitory activity of compounds 5–9.
Table S1. Cytotoxic activity for compounds 5, 7 and 8.
Figure S1. $^1$H NMR spectrum of compound 1 (DMSO-$d_6$).

Figure S2. $^1$H NMR spectrum of compound 1 at the condition of spin (DMSO-$d_6$).
Figure S3. Partial $^1$H NMR spectrum of compound 1 at the condition of spin (DMSO-$d_6$).

Figure S4. $^{13}$C NMR spectrum of compound 1 (DMSO-$d_6$).
Figure S5. COSY spectrum of compound 1 (DMSO-$d_6$).

Figure S6. HSQC spectrum of compound 1 (DMSO-$d_6$).
Figure S7. HMBC spectrum of compound 1 (DMSO-$d_6$).

Figure S8. NOESY spectrum of compound 1 (DMSO-$d_6$)
Figure S9. ESIMS spectrum of compound 1.

Figure S10. HRESIMS spectrum of compound 1.
Figure S11. $^1$H NMR spectrum of compound 2 (DMSO-$d_6$).

Figure S12. $^{13}$C NMR spectrum of compound 2 (DMSO-$d_6$).
Figure S13. COSY spectrum of compound 2 (DMSO-$d_6$).

Figure S14. HSQC spectrum of compound 2 (DMSO-$d_6$).
Figure S15. HMBC spectrum of compound 2 (DMSO-$d_6$).

Figure S16. NOESY spectrum of compound 2 (DMSO-$d_6$)
Figure S17. ESIMS spectrum of compound 2.

Figure S18. HRESIMS spectrum of compound 2.
Figure S19. DNA Topo I inhibitory activity of compounds 5–9. RLX: relaxed form; SC: supercoiled form; CPT: Camptothecin.

Table S1 Cytotoxic activity for compounds 5, 7 and 8

<table>
<thead>
<tr>
<th>Compound</th>
<th>IC$_{50}$ (μM)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HCT-116</td>
</tr>
<tr>
<td>5</td>
<td>35.3</td>
</tr>
<tr>
<td>7</td>
<td>&gt;50</td>
</tr>
<tr>
<td>8</td>
<td>29.8</td>
</tr>
<tr>
<td>Adriamycin$^a$</td>
<td>0.206</td>
</tr>
</tbody>
</table>

$^a$ Adriamycin was used as a positive control.