Supplementary material

Trichosordarin A, a norditerpene glycoside from the marine-derived fungus

*Trichoderma harzianum* R5

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Abstract

A new sordarin derivative, trichosordarin A (1), with a unique norditerpene aglycone was isolated from the culture of a marine-sediment-derived fungal strain, *Trichoderma harzianum* R5. Its structure and relative configuration were unequivocally identified by a combination of 1D/2D NMR, IR, and mass spectrometric methods. Compound 1 was assayed to be toxic to the marine zooplankton *Artemia salina*.

Keywords: *Trichoderma harzianum*; norditerpene; trichosordarin A
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| No. | I (in DMSO-\textit{d}_6) | I (in acetone-\textit{d}_6) |
|-----|------------------------|-----------------------------|
|     | \(\delta_H\)            | \(\delta_C\)               | \(\delta_H\)            | \(\delta_C\)               |
| 1   | 62.4 (C)                |                             | 63.9 (C)                |                             |
| 2   | 2.11 (d, 7.4)           | 2.27 (d, 7.6)               | 43.5 (CH)               |                             |
| 3   | 1.32 (ddd, 11.5, 11.5, 6.0) | 1.46 (overlapped)        | 42.2 (CH)               |                             |
| 4a  | 1.39 (dd, 17.8, 8.2)    | 1.46 (overlapped)          | 27.5 (CH\_2)           |                             |
| 4b  | 0.95 (overlapped)       | 1.02 (overlapped)          |                             |                             |
| 5a  | 1.91 (ddd, 10.4)        | 1.96 (m)                   |                             | 32.6 (CH\_2)               |
| 5b  | 1.03 (m)                |                             | 1.09 (dddd, 12.9, 8.3, 8.3, 2.3) | 32.8 (CH)               |
| 6   | 1.98 (br q, 6.4)        | 2.03 (overlapped)          |                             |                             |
| 7   | 1.46 (overlapped)       | 1.57 (ddd, 12.4, 12.4, 5.9, 5.5) | 40.3 (CH)               |                             |
| 8a  | 2.05 (m)                | 2.13 (dd, 12.9, 5.0)       |                             | 31.8 (CH\_2)               |
| 8b  | 1.45 (overlapped)       | 1.64 (dd, 12.8, 12.8)      |                             |                             |
| 9   | 54.3 (C)                |                             | 55.7 (C)                |                             |
| 10  | 2.22 (d, 6.0)           | 2.38 (d, 6.2)              | 49.4 (CH)               |                             |
| 11  | 3.25 (overlapped)       | 3.45 (s)                   | 77.6 (CH)               | 37.9 (C)                   |
| 12  | 36.6 (C)                |                             |                             |                             |
| 13  | 173.2 (C)               |                             | 173.5 (C)               |                             |
| 14a | 1.63 (dd, 13.3, 6.2)    | 1.75 (dd, 13.6, 6.3)       | 26.4 (CH\_2)           |                             |
| 14b | 0.74 (dd, 13.4, 7.8)    | 0.86 (dd, 13.5, 7.8)       |                             |                             |
| 16  | 0.68 (d, 7.0)           | 0.73 (d, 7.0)              | 18.0 (CH\_3)           |                             |
| 17a | 4.28 (d, 8.8)           | 4.44 (d, 9.1)              | 75.0 (CH\_2)           |                             |
| 17b | 3.86 (d, 8.8)           | 4.09 (d, 9.1)              |                             |                             |
| 18  | 1.07 (m)                | 1.23 (m)                   | 12.9 (CH)               |                             |
| 19  | 0.96 (d, 6.2)           | 1.04 (d, 6.2)              | 15.7 (CH\_3)           |                             |
| 20a | 0.49 (dd, 5.5, 5.5)     | 0.64 (dd, 5.7, 5.7)        | 15.2 (CH\_2)           |                             |
| 20b | 0.34 (dd, 8.7, 4.8)     | 0.51 (dd, 8.8, 5.1)        |                             |                             |
| 1'  | 4.59 (br s)             | 98.8 (CH)                  | 4.75 (d, 1.6)           | 99.9 (CH)                 |
| 2'  | 3.58 (br d, 3.6)        | 70.0 (CH)                  | 3.77 (dd, 4.6, 1.6)     | 71.1 (CH)                 |
| 3'  | 3.94 (br s)             | 66.0 (CH)                  | 4.11 (dd, 4.7, 3.0)     | 67.4 (CH)                 |
| 4'  | 3.02 (dd, 8.8, 2.8)     | 79.9 (CH)                  | 3.15 (dd, 8.3, 3.0)     | 81.5 (CH)                 |
| 5'  | 3.66 (dq, 8.7, 6.4)     | 67.7 (CH)                  | 3.78 (overlapped)       | 69.2 (CH)                 |
| 6'  | 1.15 (d, 6.3)           | 18.4 (CH\_3)              | 1.22 (d, 6.4)           | 19.0 (CH\_3)             |
| OH-11 | 4.87 (br d, 3.4) |                             |                             |                             |
| OH-2' | 4.68 (br s)            |                             |                             |                             |
| OH-3' | 4.29 (overlapped)      |                             |                             |                             |
| OCH\_3-4' | 3.25 (s) | 55.9 (CH\_3) | 3.34 (s) | 57.0 (CH\_3) |
Figure S1. Key HMBC (arrow) and COSY (bold line) correlations of 1.
Figure S2. Key NOE correlations (double-headed arrow) of 1.
Figure S3. $^1$H NMR spectrum of compound 1 in DMSO-$d_6$. 
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Figure S6. HMBC spectrum of compound 1 in DMSO-<i>d</i><sub>6</sub>.
Figure S7. COSY spectrum of compound 1 in DMSO-d$_6$. 
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Figure S10. $^{13}$C NMR and DEPT spectra of compound 1 in acetone-$d_6$. 
Figure S11. HSQC spectrum of compound 1 in acetone-$d_6$. 

![HSQC spectrum of compound 1 in acetone-$d_6$.](image)
Figure S12. HMBC spectrum of compound 1 in acetone-$d_6$. 
Figure S13. COSY spectrum of compound 1 in acetone-$d_6$. 
Figure S14. NOESY spectrum of compound 1 in acetone-$d_6$. 
Figure S15. EIMS spectrum of compound 1.
Figure S16. ESI\textsuperscript{+}MS spectrum of compound 1;
Figure S17. ESI-MS spectrum of compound 1;
Figure S18. HREIMS spectrum of compound 1.
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