Supporting Information

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Trichothecene Sesquiterpenes with Anti-osteosarcoma Cytotoxicity from the Fungus *Fusarium* sp. XPW68

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[#] These authors contributed equally to the study.



Figure S2: Enlarged ¹H-NMR (500 MHz, CDCl₃) spectrum of 1



Figure S3: ¹³C-NMR (125 MHz, CDCl₃) spectrum of 1



Figure S4: HSQC spectrum of 1

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Figure S6: Enlarged HSQC spectrum of 1



Figure S7: HMBC spectrum of 1



Figure S8: Enlarged HMBC spectrum of 1



Figure S9: Enlarged HMBC spectrum of 1



Figure S10: ¹H-¹H COSY spectrum of 1







Figure S12: Enlarged ¹H-¹H COSY spectrum of 1





Figure S13: NOESY spectrum of 1



Figure S14: Enlarged NOESY spectrum of 1



Figure S15: Enlarged NOESY spectrum of 1



Figure S16: HRESIMS spectrum of 1

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Figure S17: Scifinder search result of 1

| Position | | 0H 2 112 113 4 0H | $3,6\alpha-dimethyl-2\beta-(1\beta-methyl-2)-enone [11]$ | $\frac{16}{9} + \frac{10}{7} + \frac{10}{5} + \frac{2}{13} + \frac{10}{15} + \frac{2}{14} + \frac{10}{7} + \frac{2}{15} + \frac{10}{14} + \frac{10}{15} + \frac{2}{14} + \frac{2}{15} + \frac{2}{15} + \frac{2}{14} + \frac{2}{15} + \frac{2}{1$ |
|----------------|---|----------------------------------|--|--|
| | $\delta_{ m H}$ | $\delta_{ m C}$ | $\delta_{\rm C}$ | $\frac{\delta_{\rm H}}{\delta_{\rm H}}$ |
| 2 | 4.32, d (4.3) | 74.7, CH | 38.4, CH ₂ | 4.33, dd (8.3, 4.5) |
| 3a | 2.16, dd (13.5, | 40.7, CH ₂ | 23.4, CH ₂ | 1.78, dd (13.8, 6.9) |
| 3b 4a 4b | 1.70, ddd (13.5, 10.9, 5.1) 4.67, dd (10.6, 6.8) | 76.6, CH | 39.0, CH ₂ | 1.71, dddd (13.8, 13.1, 6.9, 4.5) 2.60, ddd (13.1, 13.1, 6.9) 1.48, dd (13.1, 6.9) |
| 5 | | 52.2, C | 48.5, C | |
| 6 | | 49.4, C | 49.4, C | |
| 7a | 2.20, m | 31.6, CH ₂ | 30.3, CH ₂ | 2.31, ddd (13.1, 11.7, |
| 7b 8a | 1.87, ddd (13.6, 5.2, 1.7) 2.43, m | 28.9, CH ₂ | 28.4, CH ₂ | 1.97, ddd (13.1, 5.2, 2.1) 2.43, m |
| 8b | 2.24, m | | | 2.23, ddd (18.6, 5.1, 2.1) |
| 9 | | 161.6, C | 160.7, C | |
| 10 | 5.76, s | 126.9, CH | 127.2, CH | 5.73, s |
| 11 | | 207.1, C | 204.2, C | |
| 12 | | 161.0, C | 159.0, C | |
| 13a | 5.24, s | 113.5, | 106.2, CH ₂ | 5.22, s |
| 13b | 5.11, s | | | 5.12, s |
| 14 | 1.21, s | 20.8, CH ₃ | 26.1, CH ₃ | 1.10, d (0.7) |
| 15 | 1.29, s | 18.2, CH ₃ | 17.4, CH ₃ | 1.22, s |
| 16 | 1.93, s | 23.9, CH ₃ | 23.8, CH ₃ | 1.92, s |

| Table S1: | NMR data of compounds 1, $3,6\alpha$ -dimethyl- 2β -(1β -methyl- 2 -methylenecyclopentyl)cyclohex- |
|-----------|---|
| | 2-enone, and 2α-hydroxytrichodiene-11-one |

[15] T. Tokai, H. Koshino, T. Kawasaki, T. Igawa, Y. Suzuki, M. Sato, M. Fujimura, T. Eizuka, H. Watanabe, T. Kitahara, K. Ohta, T. Shibata, T. Kudo, H. Inoue, I. Yamaguchi and M. Kimura (2005). Screening of putative oxygenase genes in the *Fusarium graminearum* genome sequence database for their role in trichothecene biosynthesis, *FEMS Microbiol. Lett.* 251, 193-201.