Supporting Information

Penicamide A, a Unique $N,N'$-Ketal Quinazolinone Alkaloids from Ascidian-derived Fungus Penicillium sp. 4829

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Table S1. Energy Analysis for the Conformers of (R)-1.

Figure S17 B3LYP/6-31G(d) optimized low-energy conformers of (R)-1.

NMR data of known compounds
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Figure S3. The $^{13}$C NMR (100MHz) spectrum of compound 1 in DMSO-$d_6$.

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Figure S16. IR spectrum of compound 2.
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Figure S24. The $^{13}$C NMR (100MHz) spectrum of compound 6 in MeOH-$d_4$. 
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Figure S26. The $^{13}$C NMR (100MHz) spectrum of compound 7 in DMSO-$d_6$. 
Figure S27. The $^1$H NMR (400MHz) spectrum of compound 8 in acetone-$d_6$.

Figure S28. The $^{13}$C NMR (100MHz) spectrum of compound 8 in acetone-$d_6$. 
Experimental Section

Calculation of ECD Spectra

Molecular Merck force field (MMFF) and DFT/TD-DFT calculations were carried out with Spartan’ 14 software (Wavefunction Inc., Irvine, CA, USA) and Gaussian 09 program, respectively\(^1\). Conformers within 10 kcal/mol energy window were generated and optimized using DFT calculations at B3LYP/6-31G(d) level. Conformers with Boltzmann distribution over 1% were chosen for ECD calculations in methanol at B3LYP/6-311+g(2d,p) level. The IEF-PCM solvent model for MeOH was used. ECD spectra were generated using the program SpecDis 3.0 (University of Würzburg, Würzburg, Germany) and OriginPro 8.5 (OriginLab, Ltd., Northampton, MA, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.30 ev. All calculations were performed by Tianhe-2 in National Super Computer Center in Guangzhou.

Table S1. Energy Analysis for the Conformers of (R)-1.

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<th>Conformation</th>
<th>G (Hartree)</th>
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<th>ΔG (Kcal/mol)</th>
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Figure S17. B3LYP/6-31G(d) optimized low-energy conformers of (R)-1.
NMR data of known compounds 3-8.

**Compound 3:** $^1$H NMR (acetone-$d_6$) $\delta_{H}$ 8.73 (1H, d, $J$ = 8.4 Hz), 7.89 (1H, d, $J$ = 7.9 Hz), 7.56 (1H, m), 7.20 (1H, d, $J$ = 7.6 Hz), 2.47 (3H, q, $J$ = 6.9 Hz); $^{13}$C NMR (acetone-$d_6$) $\delta_{C}$ 197.2, 171.4, 159.9, 139.7, 133.3, 129.3, 124.3, 121.6, 121.3, 24.2.

**Compound 4:** $^1$H NMR (MeOH-$d_4$) $\delta_{H}$ 8.53 (1H, d, $J$ = 8.5 Hz), 7.73 (1H, d, $J$ = 7.8 Hz), 7.50 (1H, m), 7.16 (1H, d, $J$ = 7.6 Hz), 4.23 (1H, q, $J$ = 6.9 Hz), 1.43 (3H, q, $J$ = 6.9 Hz); $^{13}$C NMR (MeOH-$d_4$) $\delta_{C}$ 175.2, 138.2, 131.9, 128.1, 123.1, 121.4, 120.7, 68.4, 19.7.

**Compound 5:** $^1$H NMR (CDCl$_3$) 8.51 (1H, s), 8.30 (2H, d, $J$ = 8.4 Hz), 7.63 (2H, d, $J$ = 10.6 Hz), 7.47 (2H, d, $J$ = 7.8 Hz), 5.56 (1H, dt, $J$ = 7.3, 10.5 Hz), 5.56 (1H, dt, $J$ = 7.3, 10.5 Hz), 5.26 (1H, m), 4.74 (1H, dd, $J$ = 4.3, 8.7 Hz), 4.68 (1H, d, $J$ = 9.7 Hz), 4.58 (1H, d, $J$ = 4.5 Hz), 3.44 (3H, s), 2.10 (3H, m), 1.66 (3H, s), 0.97 (3H, t, $J$ = 7.5 Hz); $^{13}$C NMR (CDCl$_3$) 196.6, 195.5, 186.2, 166.9, 136.8, 134.9, 132.5, 130.9, 128.6, 126.6, 113.4, 92.9, 90.7, 73.2, 71.0, 70.8, 51.9, 21.5, 14.2, 6.2.

**Compound 6:** $^1$H NMR (MeOH-$d_4$) 9.03 (1H, s, H-3), 8.69 (1H, d, $J$ = 4.3 Hz, H-3), 8.29 (1H, d, $J$ = 8.0 Hz, H-6), 7.55 (1H, d, $J$ = 7.9, 5.0 Hz, H-3); $^{13}$C NMR (MeOH-$d_4$) 169.8, 152.8, 149.4, 137.3, 131.4, 125.1.

**Compound 7:** $^1$H NMR (DMSO-$d_6$) $\delta_{H}$ 5.55 (1H, s), 4.49 (1H, d, $J$ = 3.2 Hz), 4.51 (1H, s), 3.56 (3H, s), 2.32 (2H, m), 2.00 (3H, s), 1.77 (4H, m), 1.58 (3H, s), 1.22 (3H, s), 1.16 (3H, s), 0.90 (3H, s), 0.80 (3H, s); $^{13}$C NMR (DMSO-$d_6$) $\delta_{C}$ 178.5, 170.2, 169.6, 121.8, 114.8, 76.9, 75.2, 54.3, 51.8, 51.1, 43.0, 33.9, 30.7, 25.8, 21.7, 21.5, 20.7, 20.6, 17.1, 6.5.

**Compound 8:** $^1$H NMR (acetone-$d_6$) $\delta_{C}$ 5.63 (1H, s), 4.98 (1H, dd, $J$ = 3.6, 1.6 Hz), 4.61 (1H, dd, $J$ = 3.7, 1.5 Hz), 3.67 (3H, s), 2.78 (1H, br d, $J$ =14.4 Hz), 2.40 (1H, dd, $J$ =14.4, 3.8 Hz), 2.15 (1H, s), 1.98 (2H, m), 1.99 (3H, s), 1.78 (2H, m), 1.65 (3H, s), 1.36 (3H, s), 1.32 (3H, s), 1.21 (3H, s), 1.01 (3H, s), 0.95 (3H, s); $^{13}$C NMR (acetone-$d_6$) $\delta_{C}$ 204.6 (C-15), 201.4 (C-17), 178.1 (C-23), 170.2 (C$_3$-OAc), 168.5 (C-19), 147.2 (C-9), 124.7 (C-11), 77.6 (C-6), 76.9 (C-12), 76.2 (C-3), 76.0 (C-16), 72.6 (C-14), 54.1 (C-13), 52.5 (C$_{19}$-OMe), 50.9 (C-5), 48.5 (C-10), 39.0 (C-8), 38.7 (C-7), 35.6 (C-4), 31.9 (C-22), 26.7 (C-24), 23.8 (C-21), 23.0 (C-25), 22.7 (C-2), 20.8 (C$_3$-OAc), 20.2 (C-1), 11.2 (C-20), 7.8 (C-18).
References.
