Diverse Secondary Metabolites from the Coral-Derived Fungus *Aspergillus hiratsukae* SCSIO 5Bn1003

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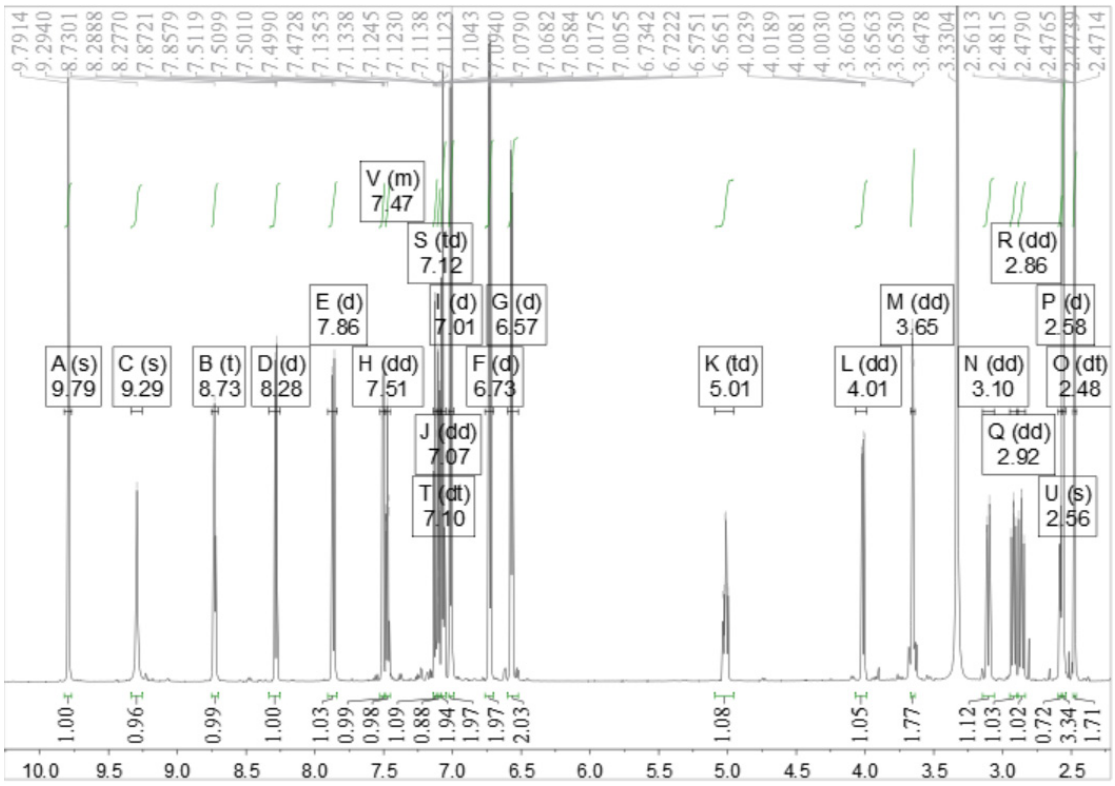


Figure S1. [1]H NMR spectrum of asperhiratide **(1)**.

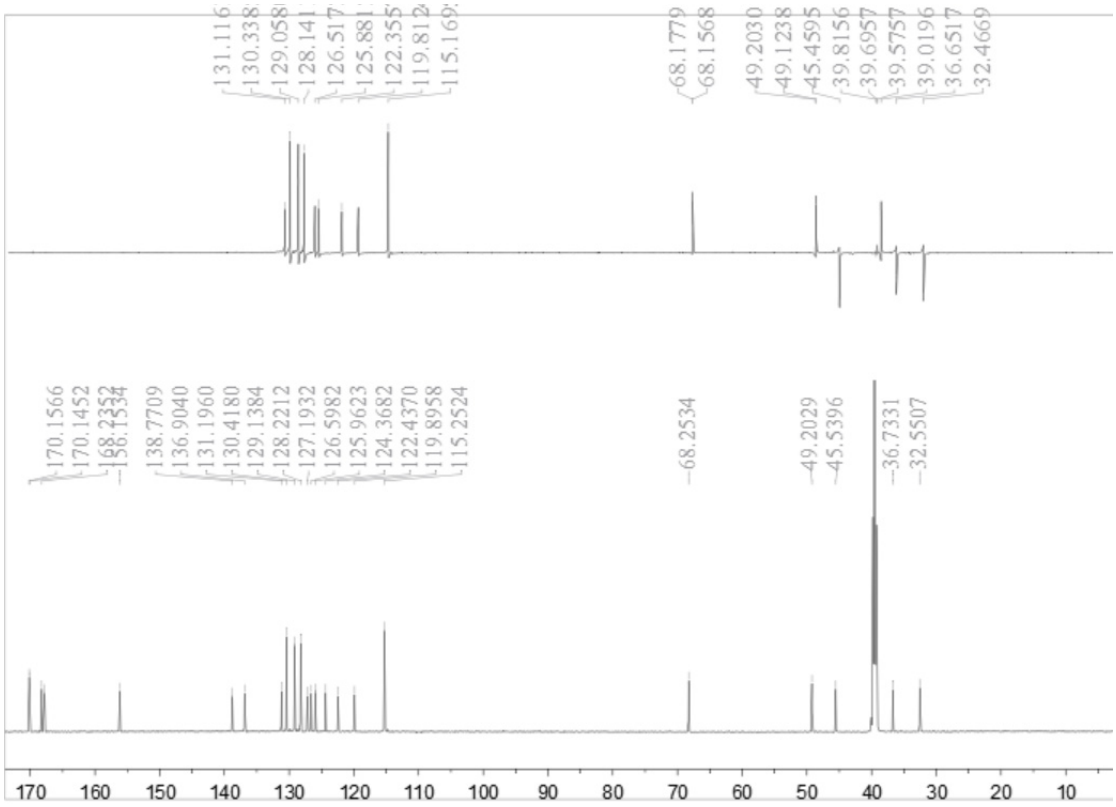


Figure S2.[13]C NMR and DEPT spectrum of asperhiratide **(1)**.

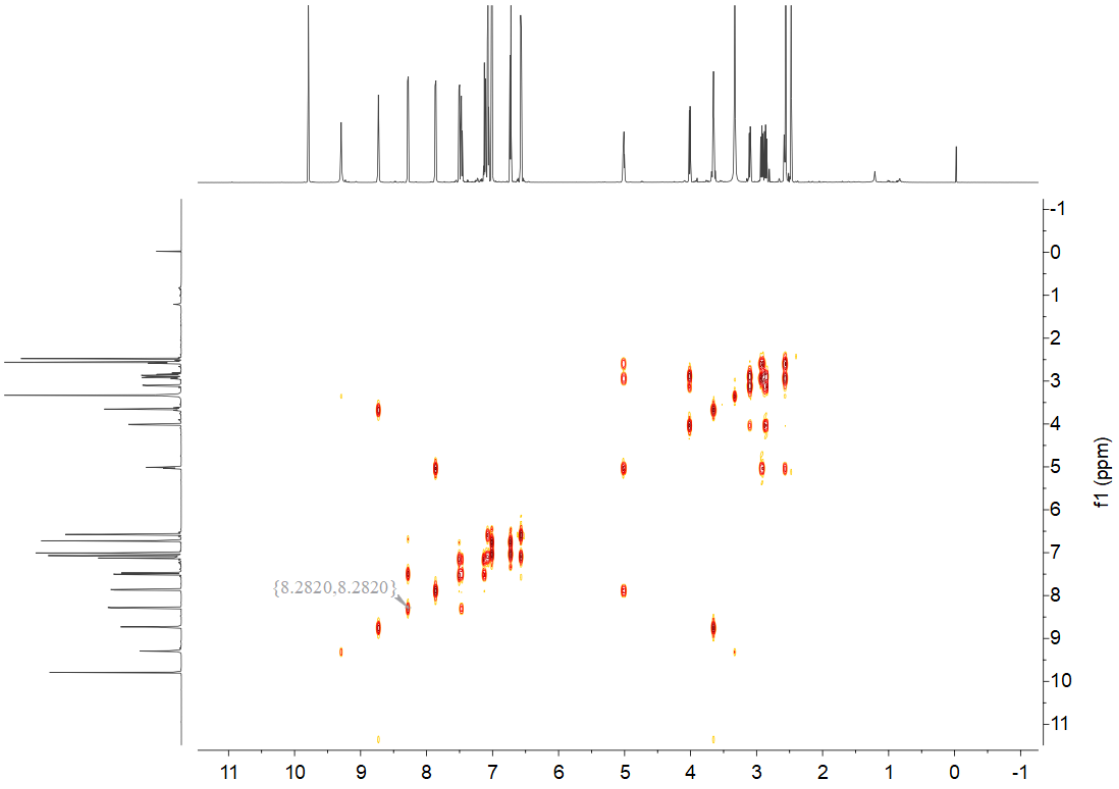


Figure S3. COSY spectrum of asperhiratide **(1)**.

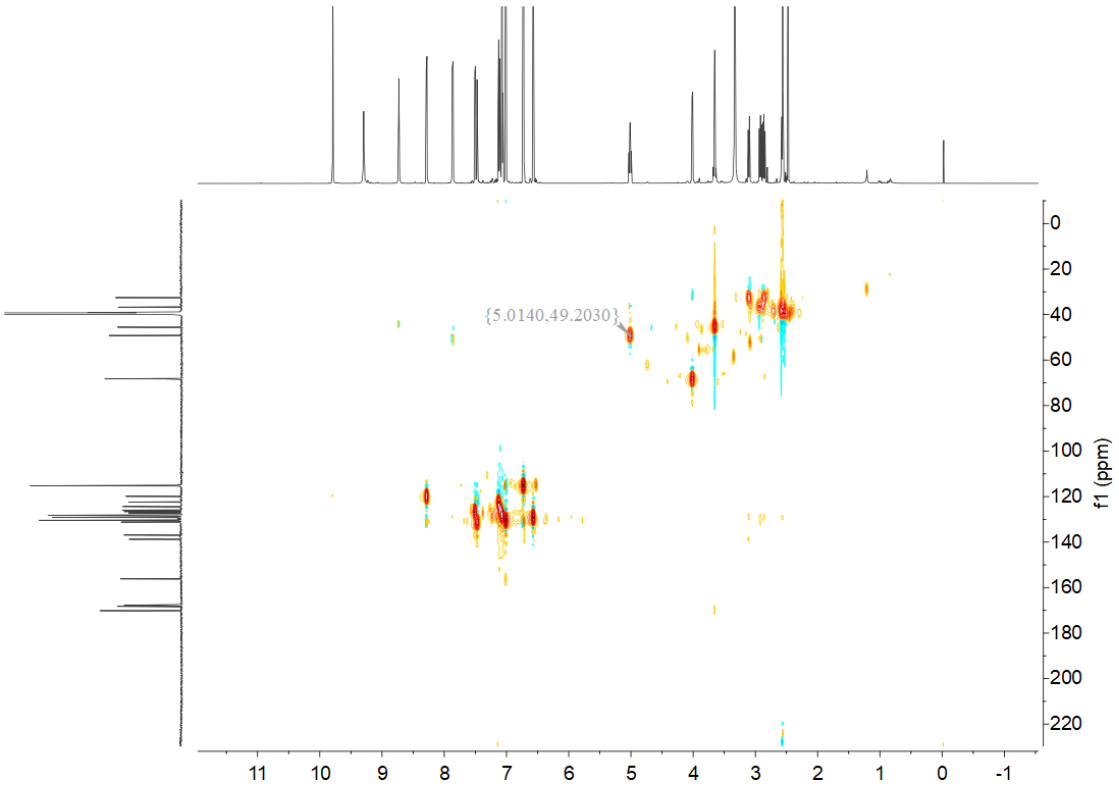


Figure S4. HSQC spectrum of asperhiratide **(1)**.

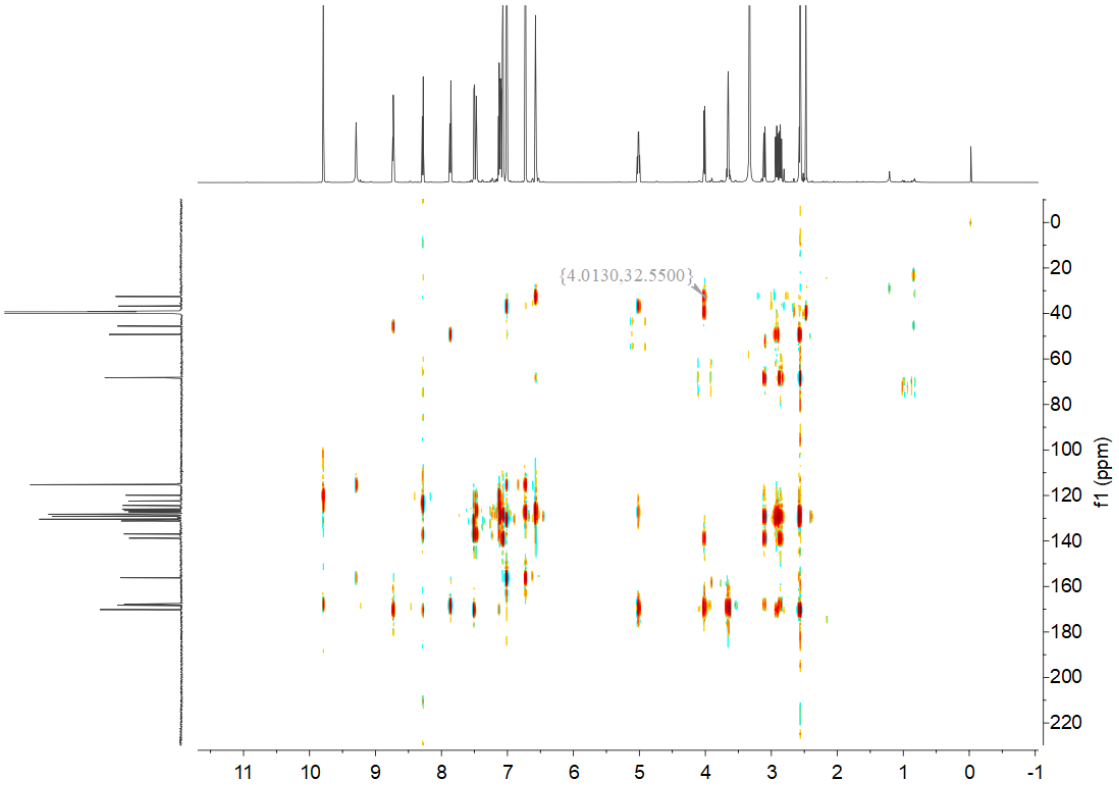
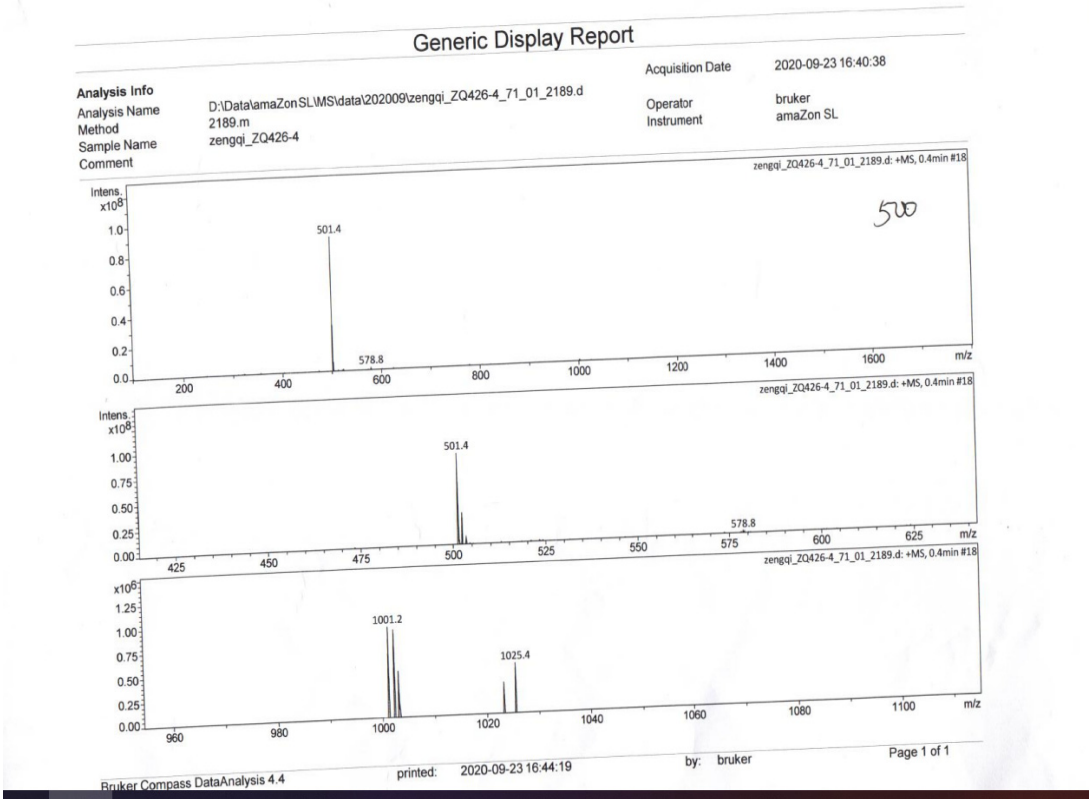


Figure S5. HMBC spectrum of asperhiratide **(1)**.



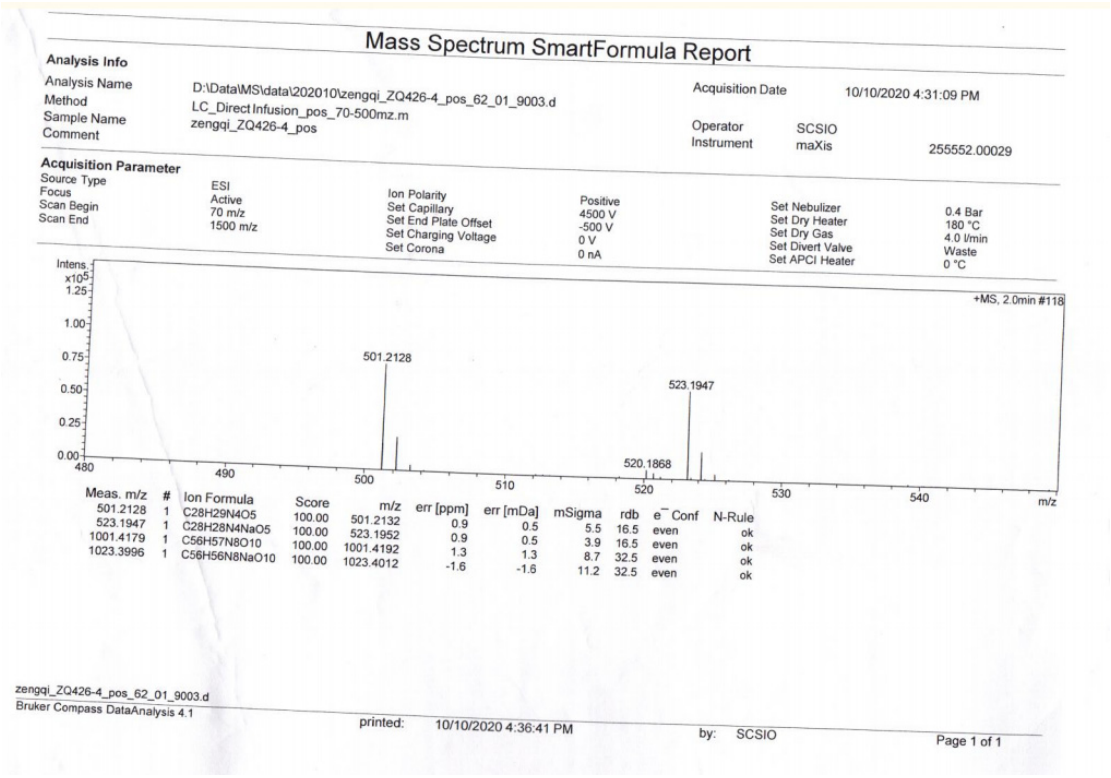


Figure S6. HRESIMS spectrum of asperhiratide **(1)**.

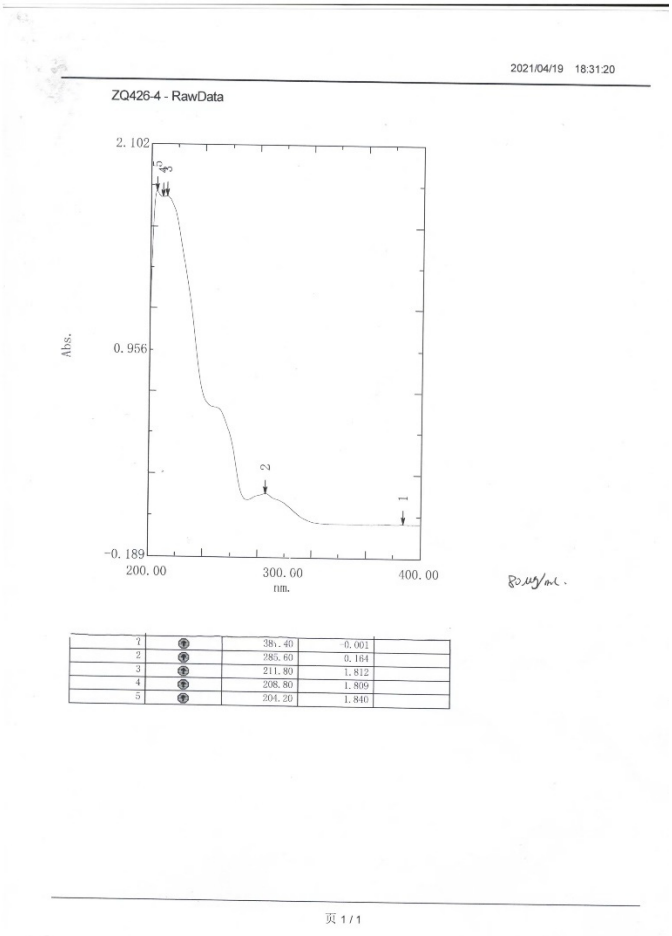


Figure S7. UV spectrum of asperhiratide **(1)** (MeOH).

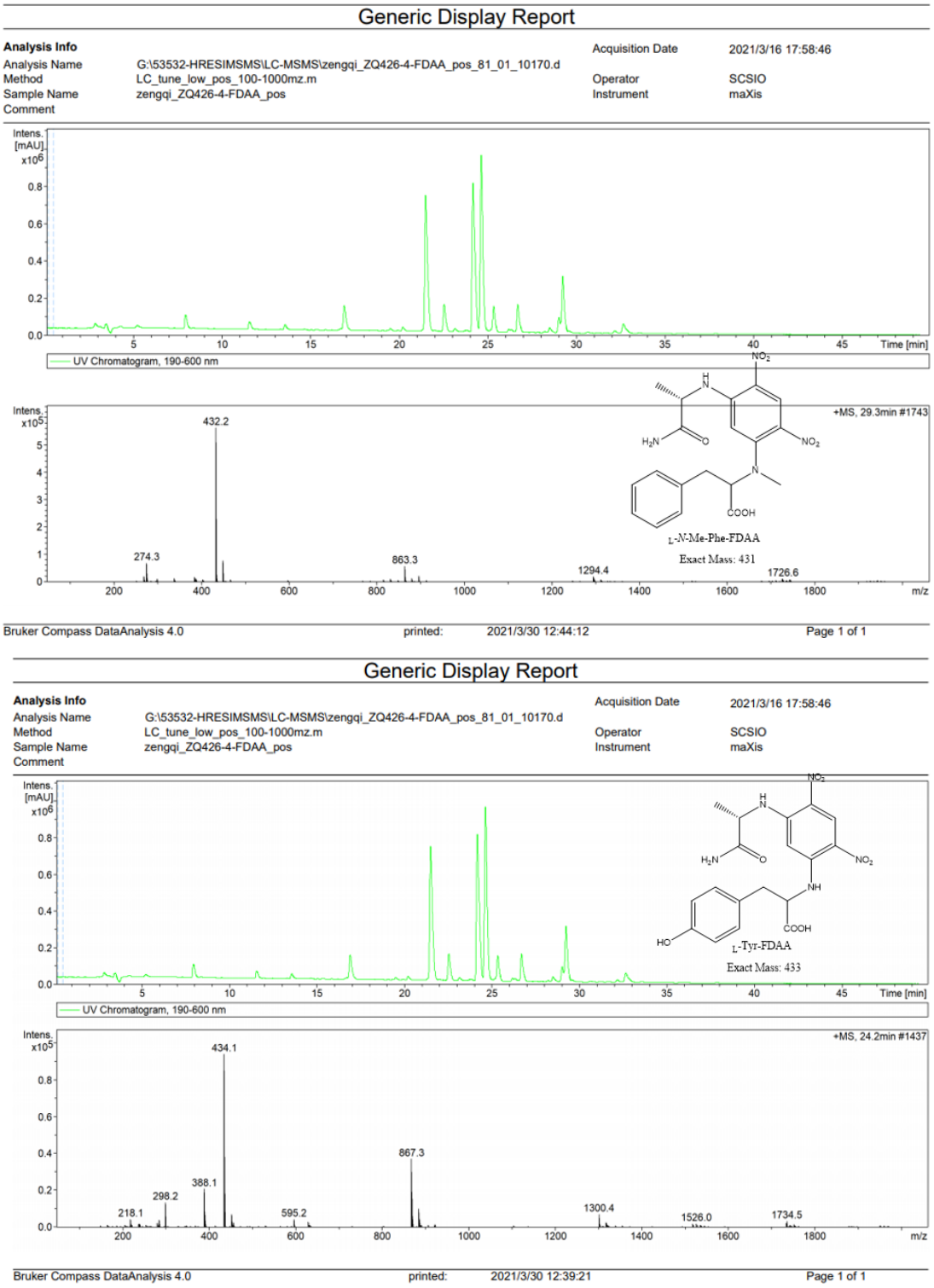


Figure S8. UPLC-MS analysis of the acid hydrolysate of asperhiratide **(1)**.

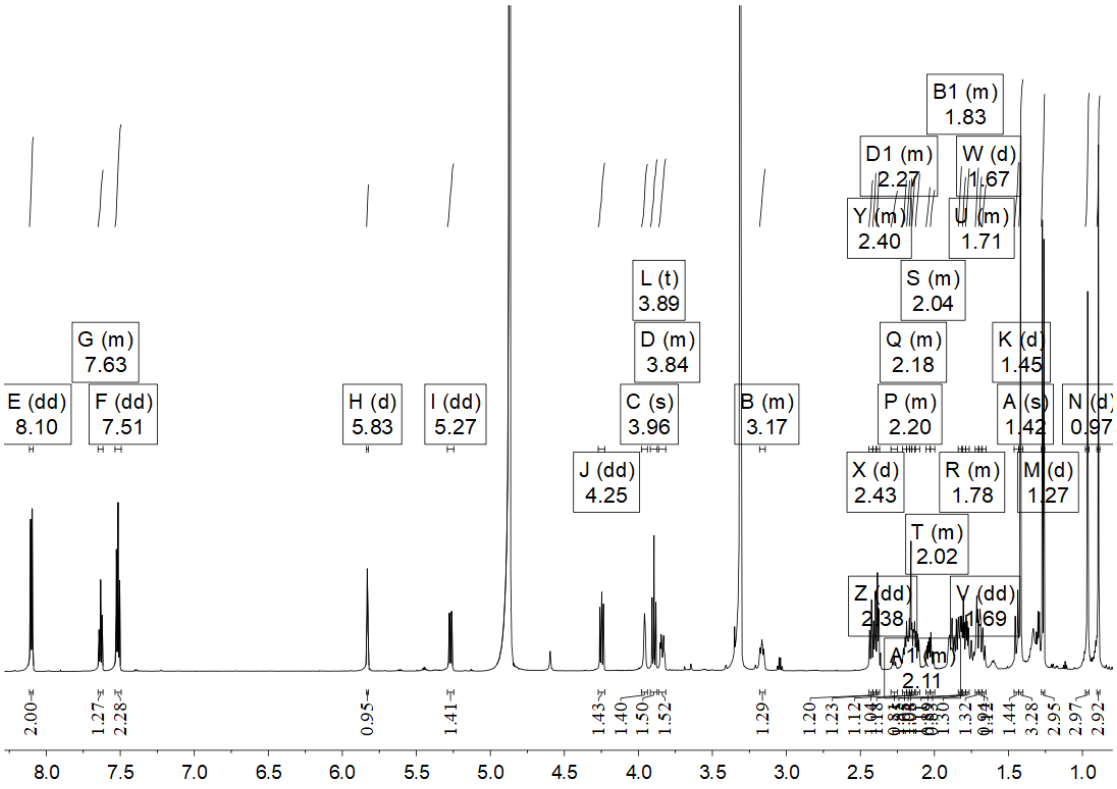


Figure S9. [1]H NMR spectrum of asperhiratine **(2)**.

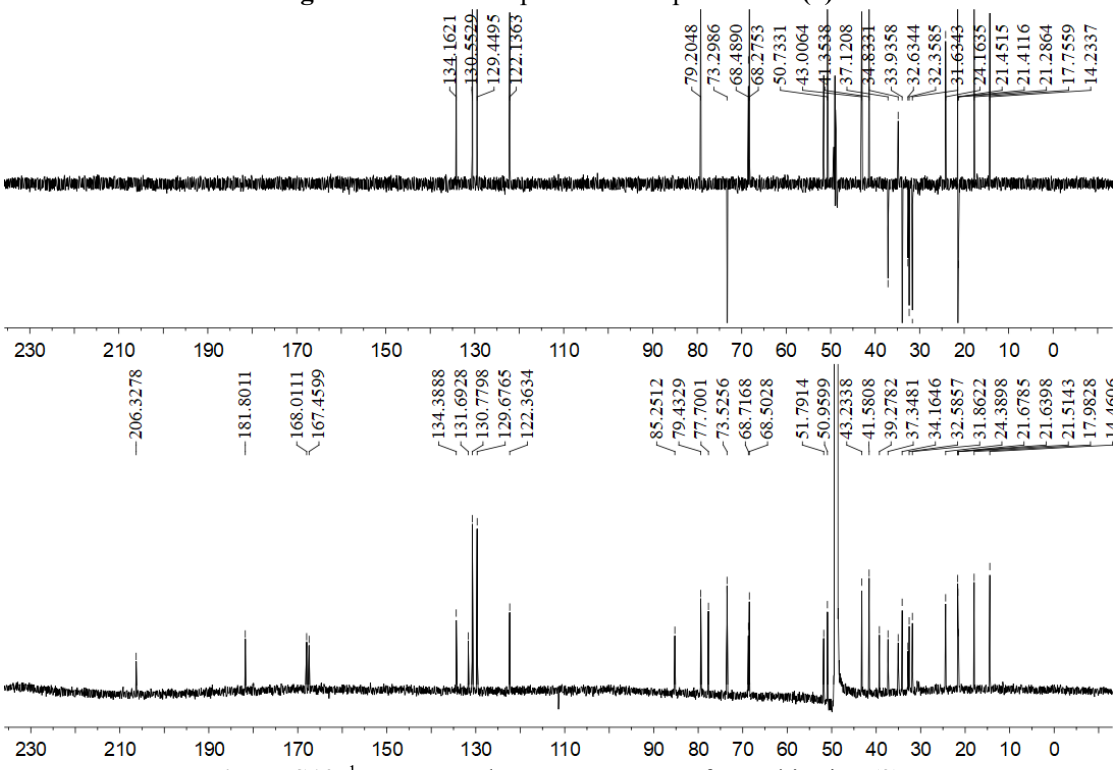


Figure S10. [1]C NMR and DEPT spectrum of asperhiratine **(2)**.

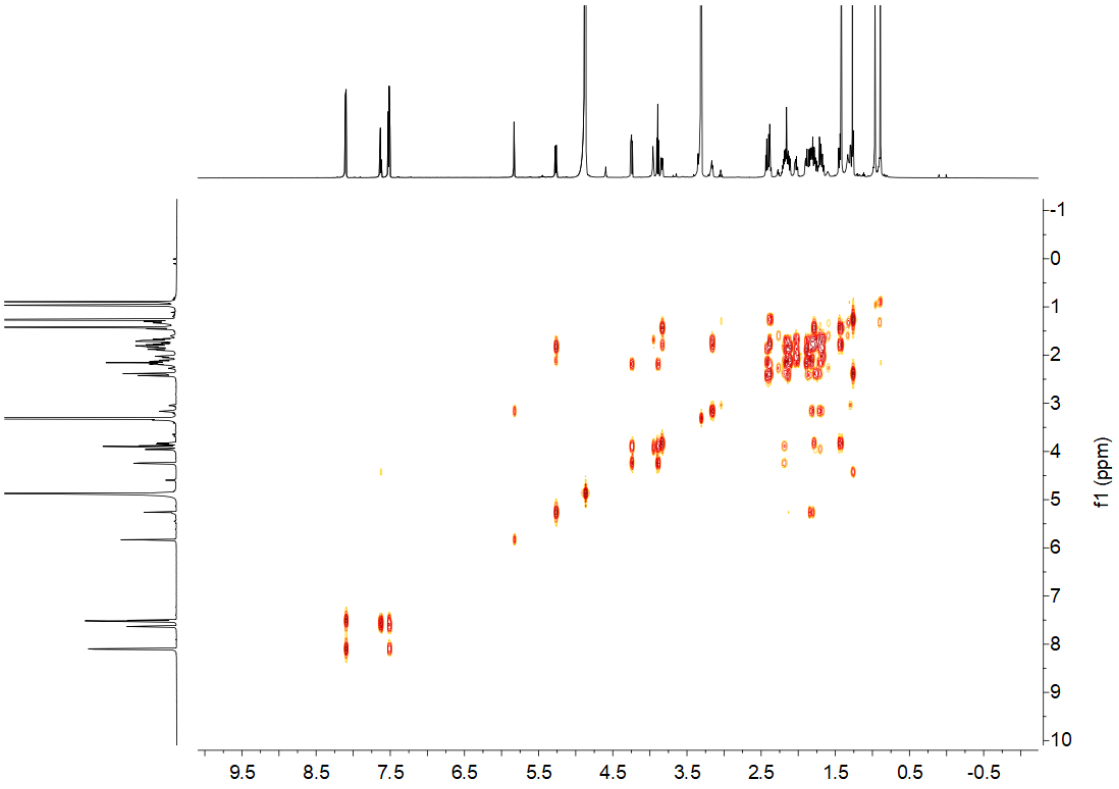


Figure S11. COSY spectrum of asperhiratine **(2)**.

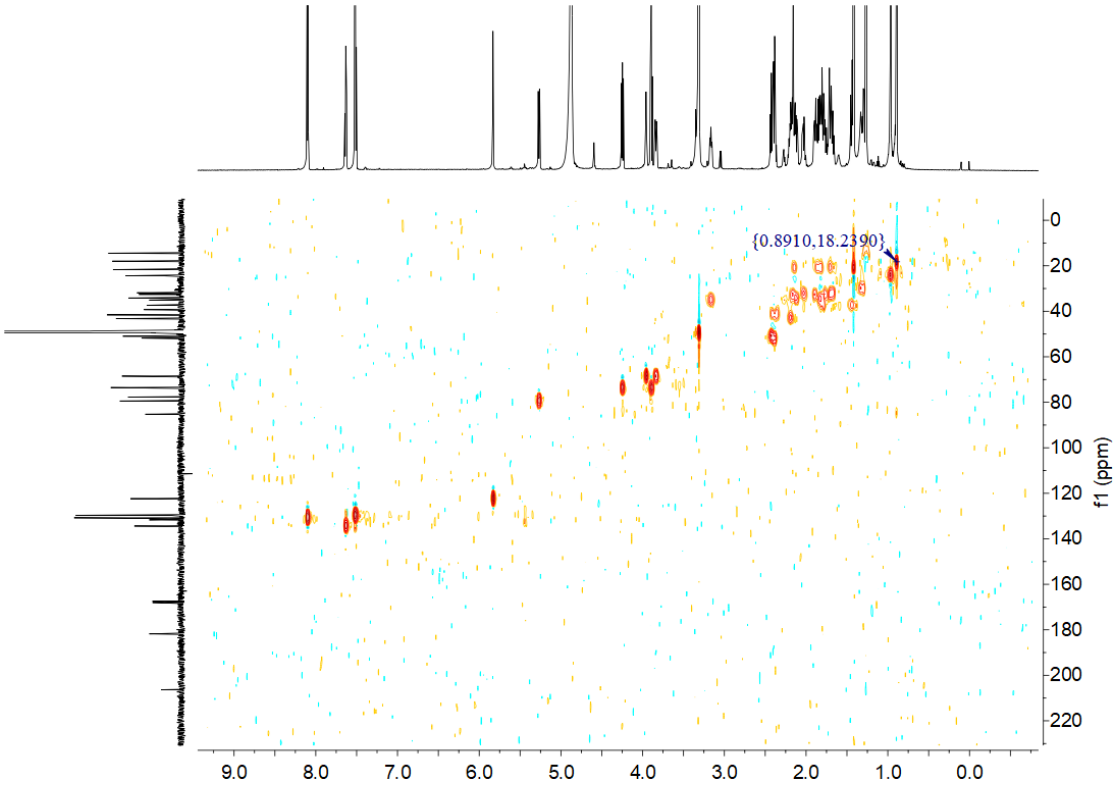


Figure S12. HSQC spectrum of asperhiratine **(2)**.

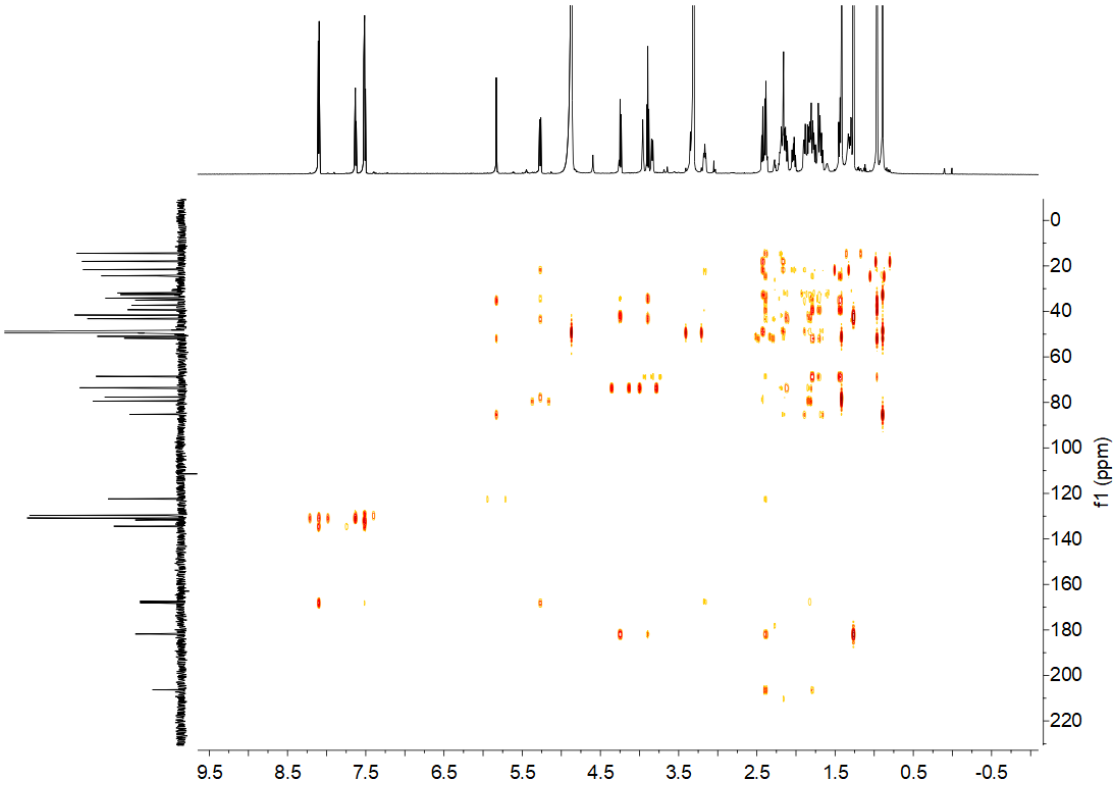


Figure S13. HMBC spectrum of asperhiratine **(2)**.

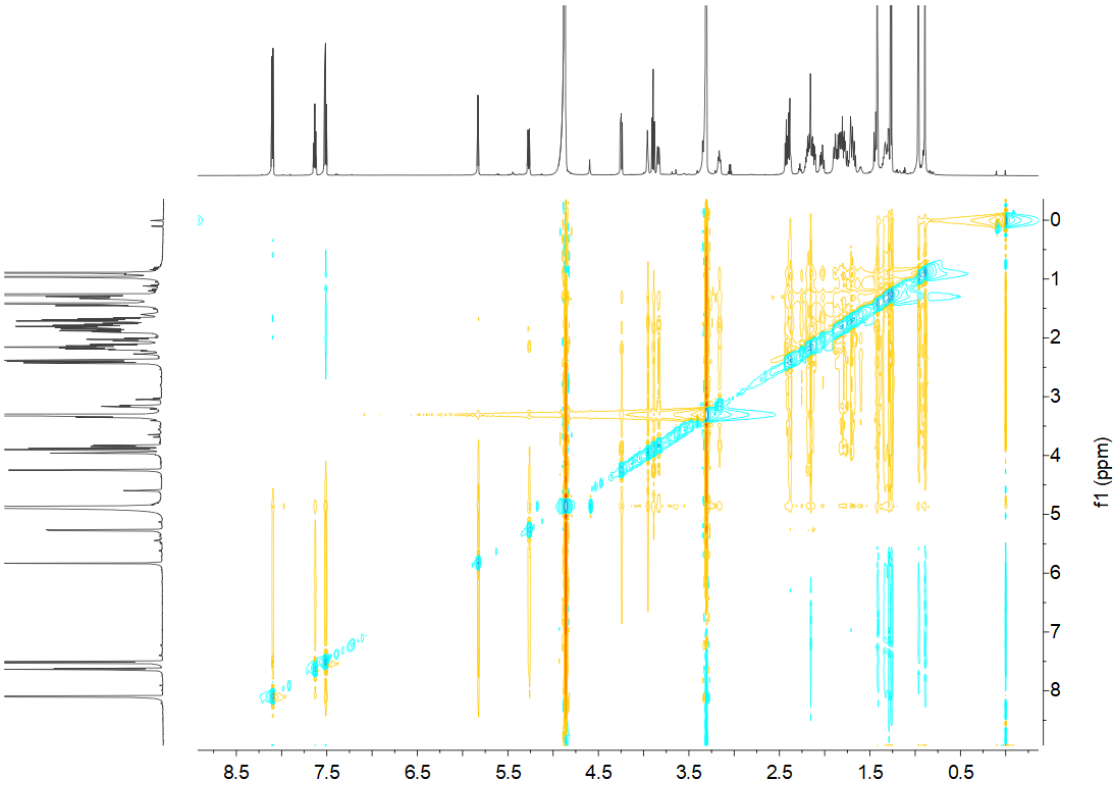
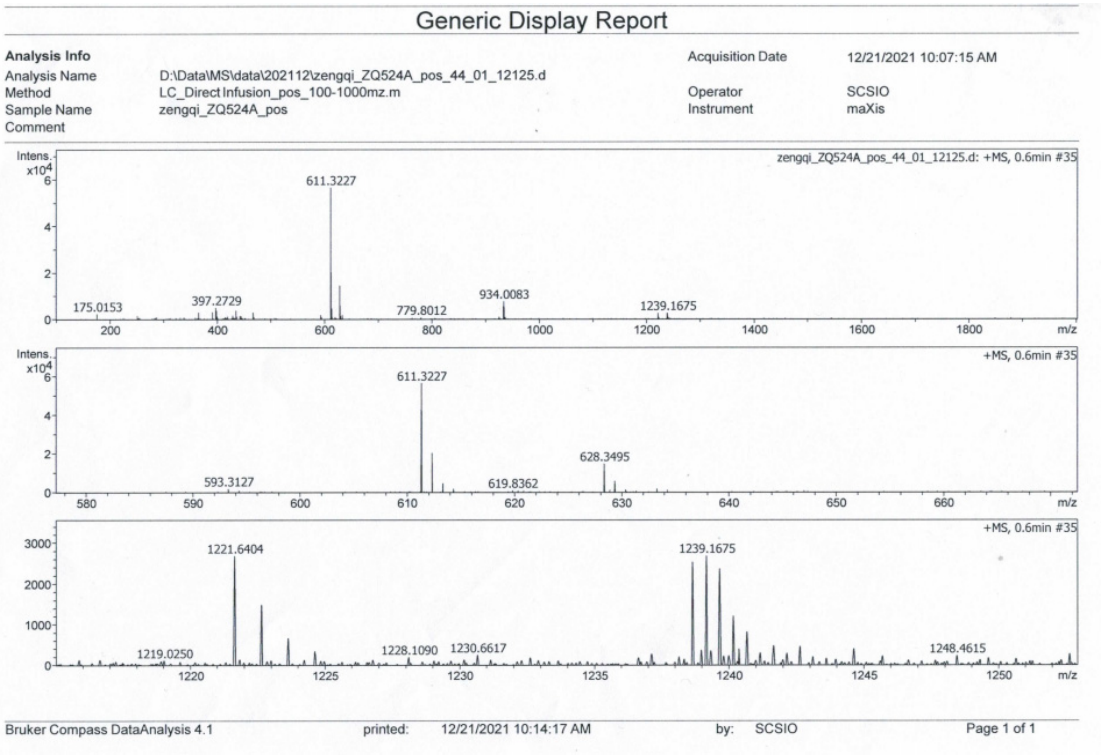


Figure S14. NOESY spectrum of asperhiratine **(2)**.



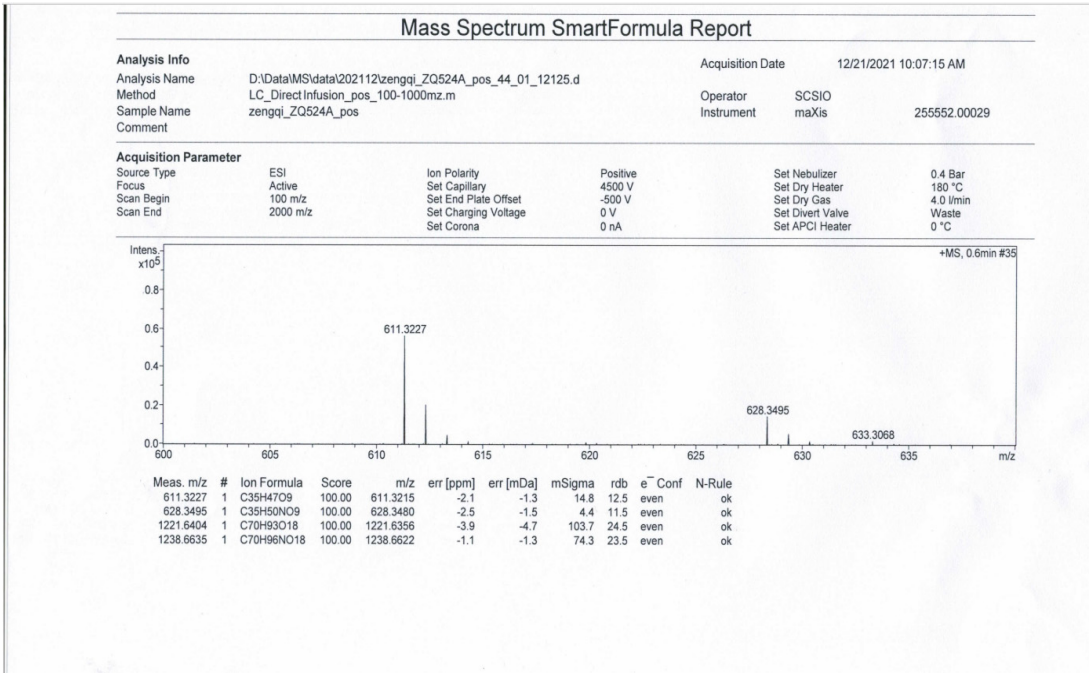


Figure S15. HRESIMS spectrum of asperhiratine **(2)**.

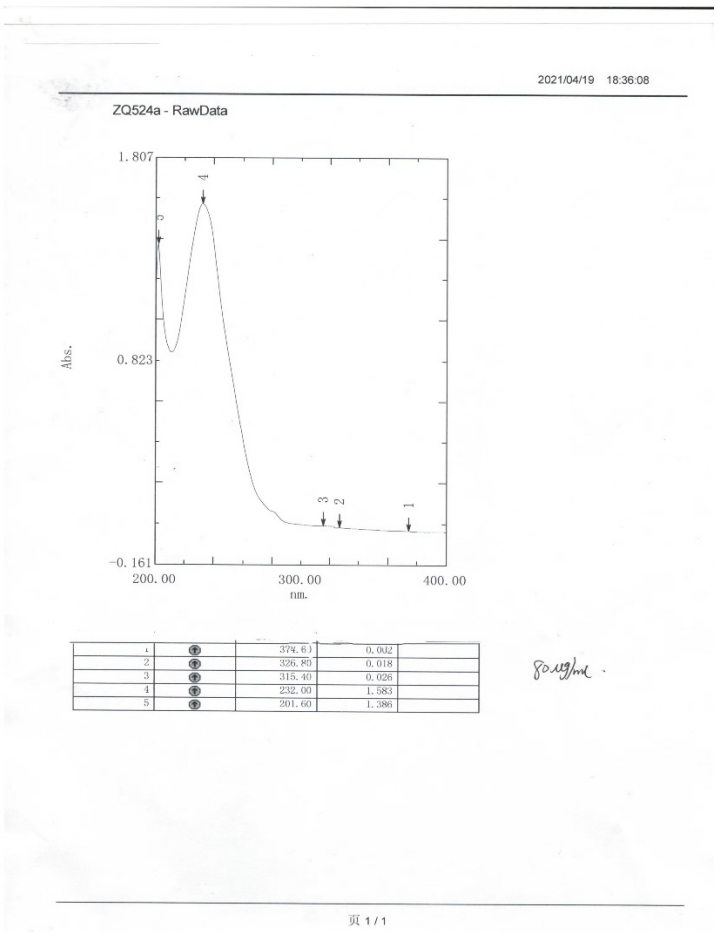


Figure S16. UV spectrum of asperhiratine **(2)**.

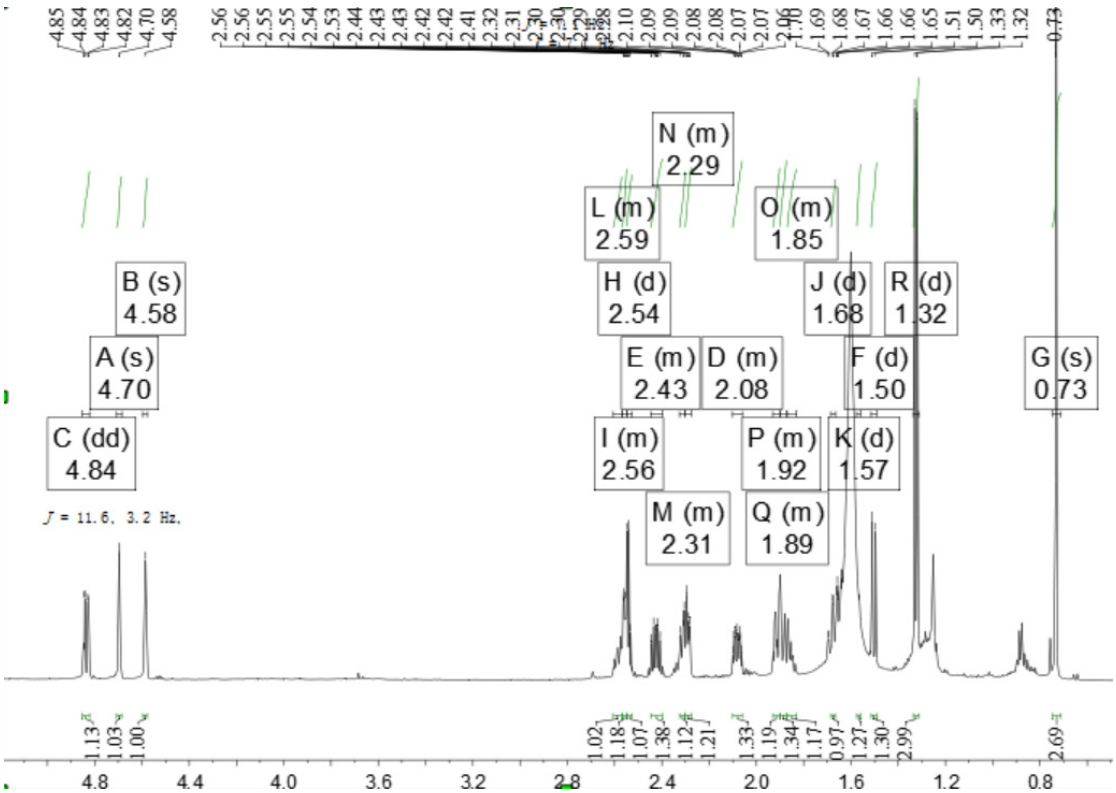


Figure S17. ^{1}H NMR spectrum of asperhiratone **(3)**.

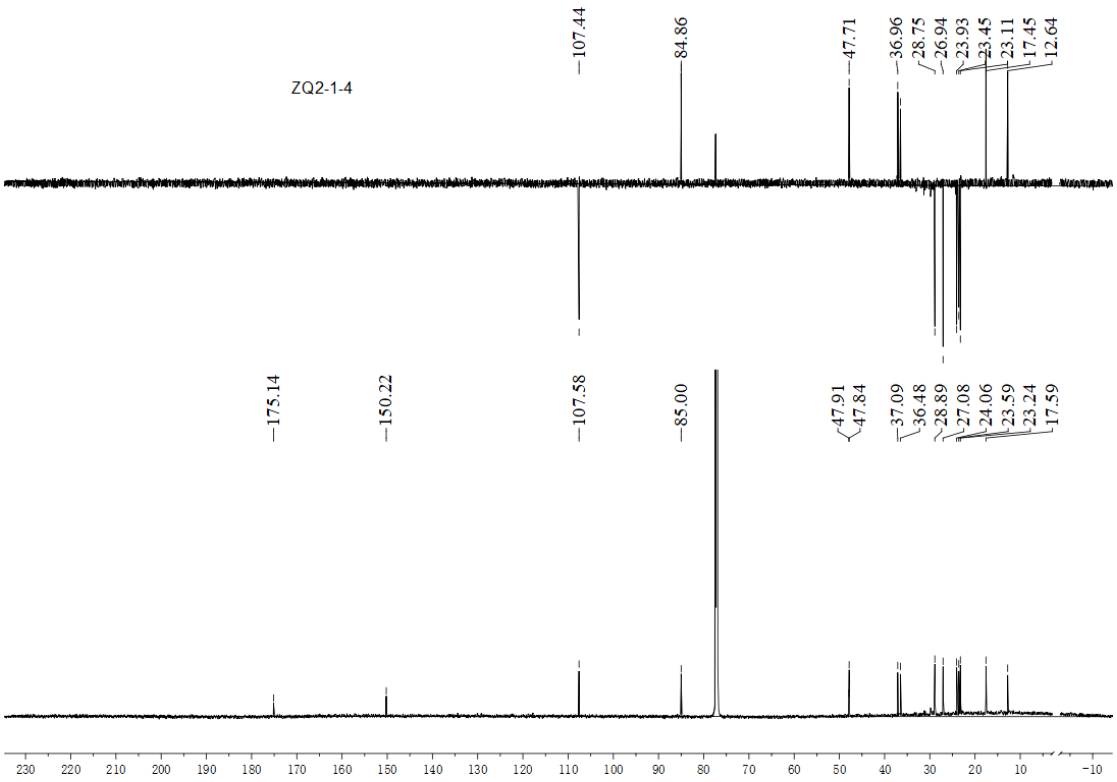


Figure S18. ^{13}C NMR and DEPT spectrum of asperhiratone **(3)**.

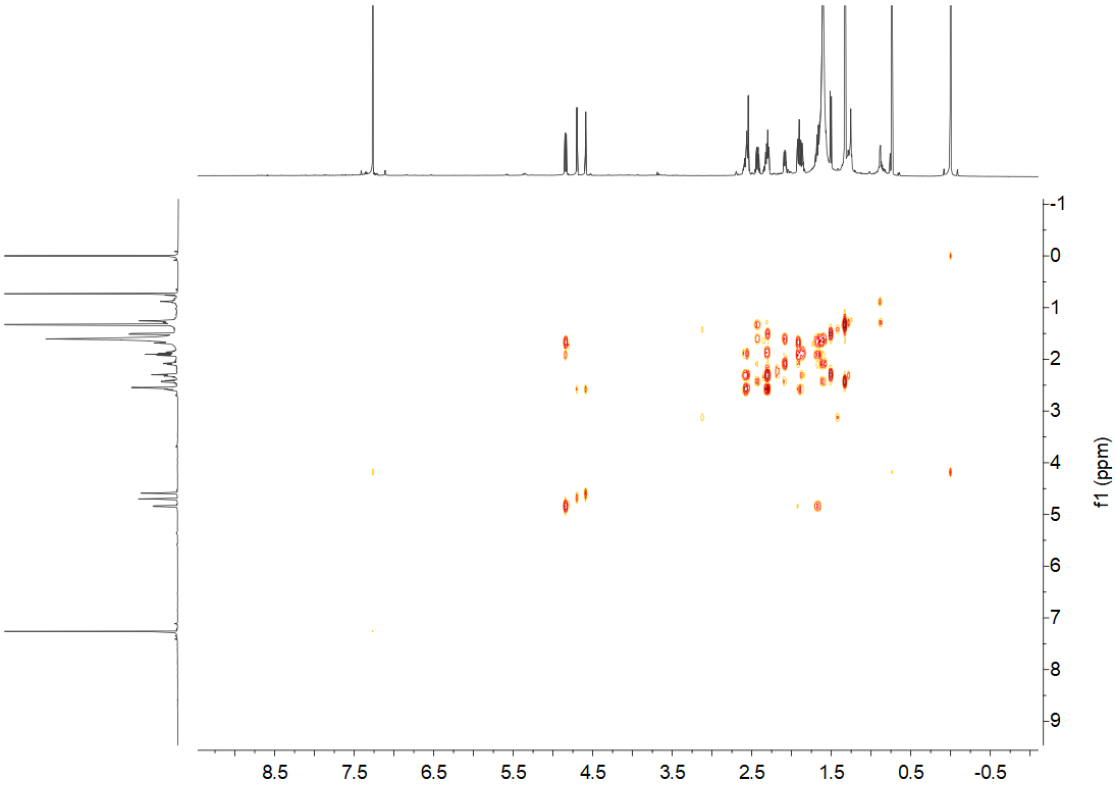


Figure S19. ^{1}H -^{1}H COSY spectrum of asperhiratone **(3)**.

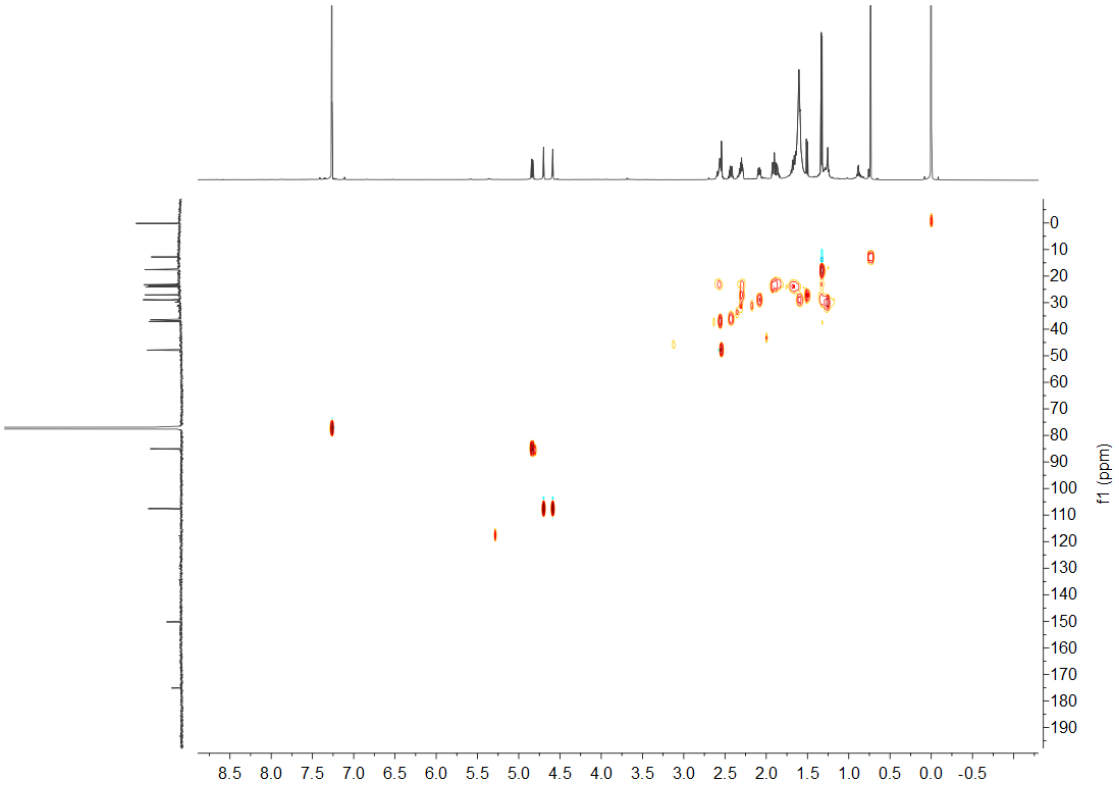


Figure S20. HSQC spectrum of asperhiratone **(3)**.

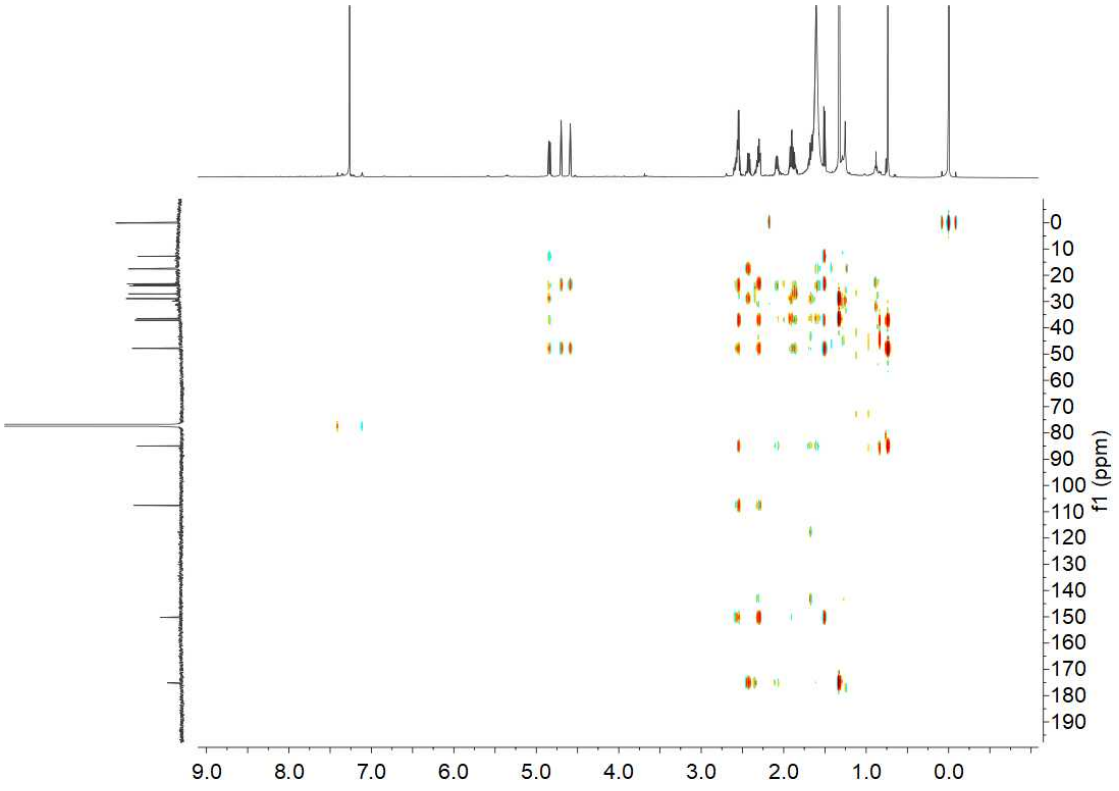
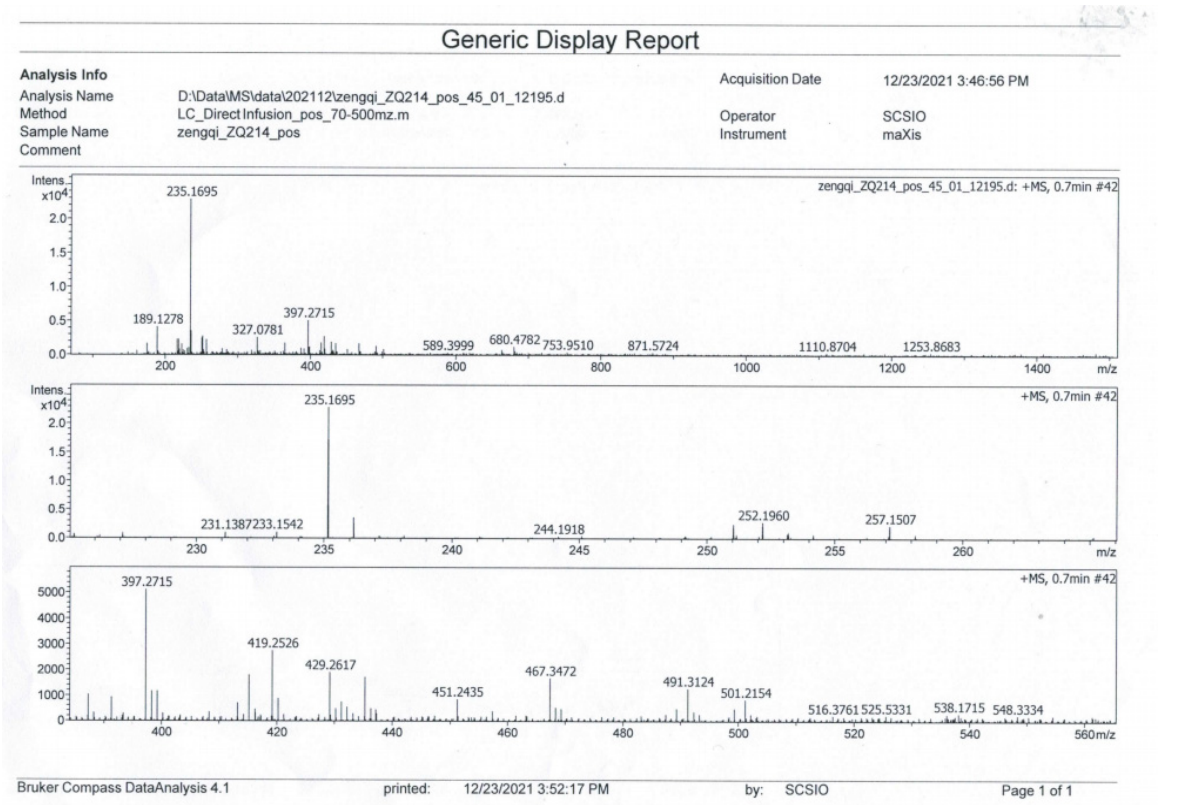


Figure S21. HMBC spectrum of asperhiratone **(3)**.



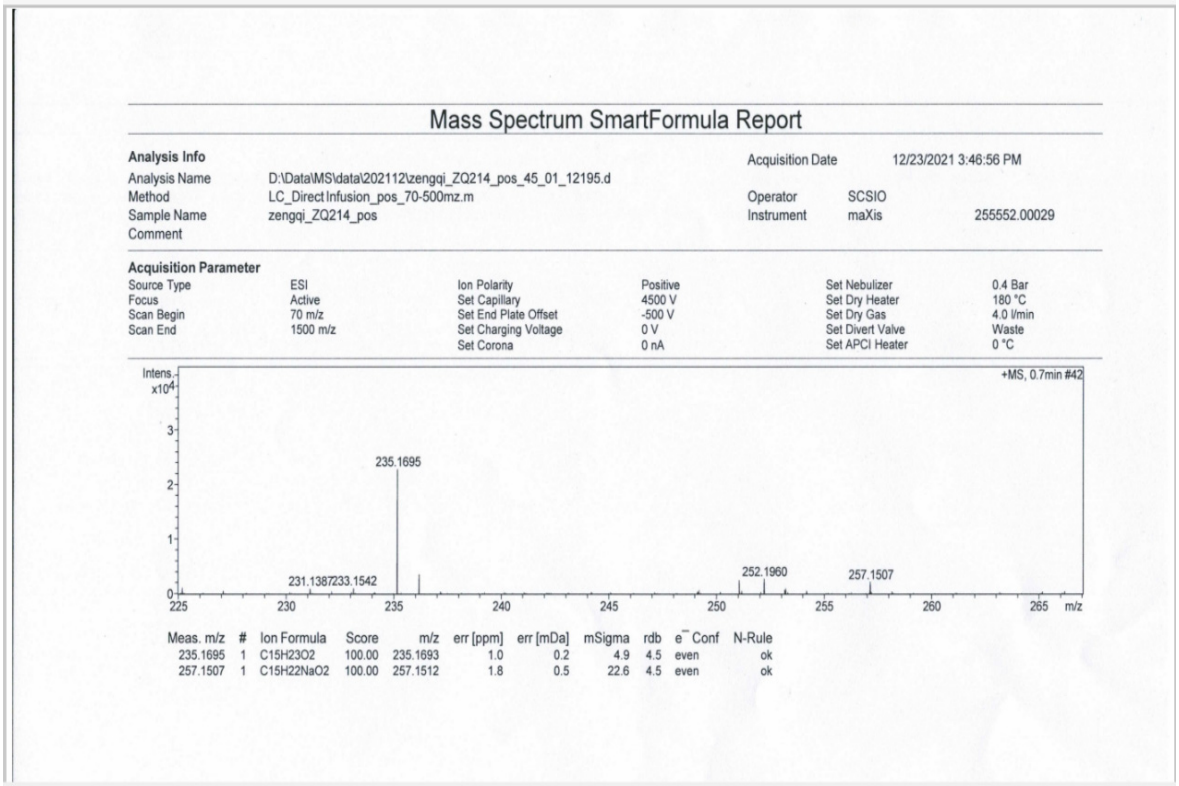


Figure S22. HRESIMS spectrum of asperhiratone **(3)**.

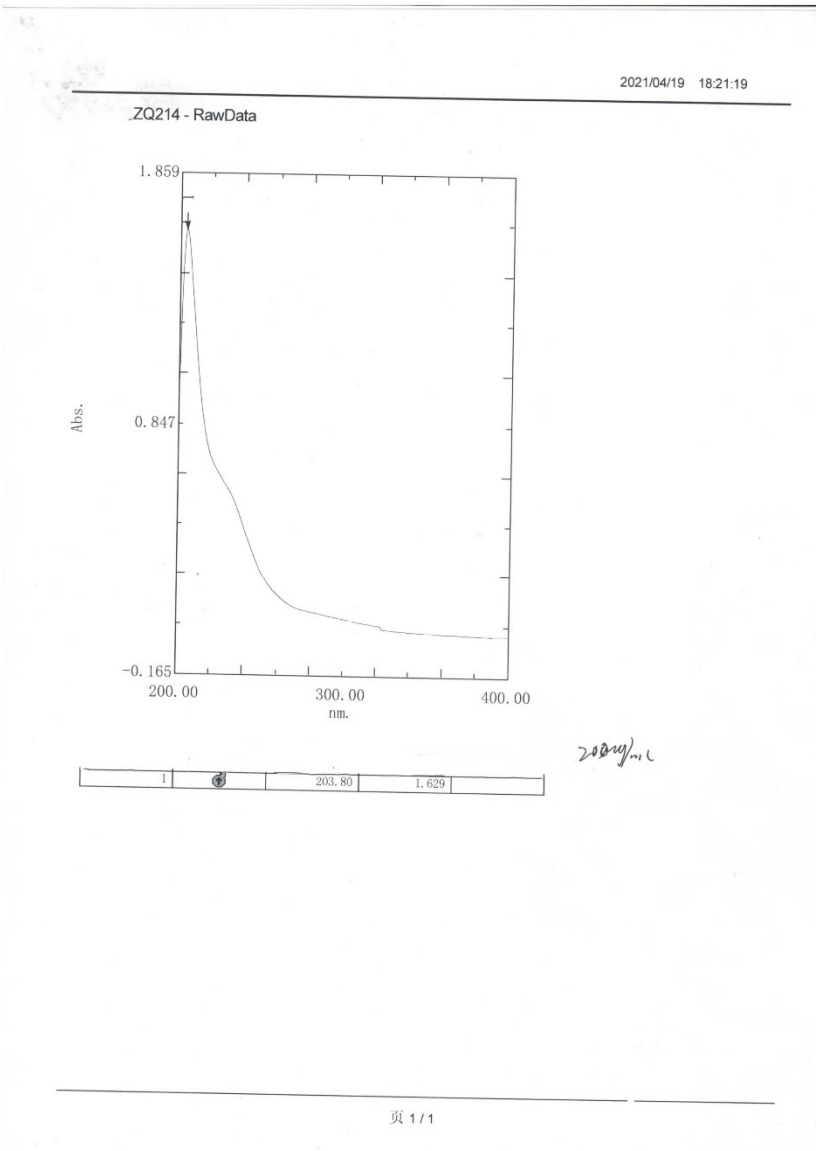


Figure S23. UV spectrum of asperhiratone **(3)**.

The ECD computational detail of compound 3

Conformational searches were done using Molecular Merck force field (MMFF) embedded in Spartan'14 software (Wavefunction Inc., Irvine, CA, USA). Density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations were performed with Gaussian09 RevD.01. [26]. Double-hybrid (DH) DFT calculations were conducted with ORCA 4.2.1 program package using RIJK approximation, tight SCF criteria, and grid 6 integrity [27]. For simulations of ECD spectrum of compound 3, low-energy conformers of (1R,2S,6S,10R,13S)- and (1R,2S,6S,10S,13R)-3 within a 10 kcal/mol energy window from MMFF conformational search were subjected to geometry optimizations followed by frequency calculations using DFT method at the B3LYP [28,29] /Def2-SVP [30] level of theory with the solvent model PCM for MeOH. The

high level of single point calculations of the optimized low-energy conformers was carried out using the DH-DFT method at the PWPB95 [31] -D3BJ [32,33] / def2-QZVPP[29]. level with the SMD [34] solvent model for MeOH. The TDDFT calculations were carried out using PBE1PBE (PBE0) [35] , M06 [36] and M06-2X [37] functionals in combination with the TZVP [38]. basis set and the PCM solvent (MeOH) model. The number of excited states was 20 for all conformers. The results were visualized and exported using the SpecDis program [39]. The calculated ECD spectra of the two stereoisomers were generated as a sum of Gaussian curve with the σ value of 0.27 eV using rotatory strengths computed in the dipole-velocity gauge from ECD data of the individual low-energy conformers. Boltzmann distributions of the conformers in equilibrium population were estimated from the relative Gibbs free energies (ΔG) at 298.15K.

The physicochemical data of the known compounds

schizaeasterone A (4): white powder; LRESIMS $[M+H]^+$ *m/z* 463.1. $[\alpha]^{25}D$ +64.3 (c 0.1 MeOH). ^1H NMR (700 MHz, DMSO): δ_H 1.56 (1H, m, H-1a), 1.31 (1H, d, *J*=11.3Hz, H-1b), 1.72 (1H, d, *J*=4.6Hz, H-2a), 1.45 (1H, d, *J*=4.9Hz, H-2b), 3.40 (1H, dd, *J*=10.8, 4.4Hz, H-3), 1.70 (1H, m, H-4a), 1.51(1H, m, H-4b), 1.89 (1H, d, *J*=3.3Hz, H-5), 5.62 (1H, d, *J*=2.4Hz, H-7), 1.87 (1H, d, *J*=4.1Hz, H-9), 1.45 (1H, d, *J*=4.5 Hz , H-11a), 1.56 (1H, m, H-11b) , 1.69 (1H, m, H-12a), 2.20 (1H, m, H-12b), 1.77 (1H, m, H-15a),1.53 (1H, d, *J*=8.7 Hz, H-15b), 1.69 (1H, m, H-16a), 2.20 (1H, m, H-16b), 2.24 (1H, t, *J*=8.7 Hz, H-17), 0.76 (3H, s, H-18), 0.80 (3H, s, H-19), 1.04 (3H, s, H-21), 3.25 (1H, dd, *J*=8.9, 5.4 Hz, H-22), 0.97 (1H, dd, *J*=8.2, 4.1Hz, H-23a), 1.37 (1H, m, H-23b), 1.59 (1H, m, H-24), 1.23 (1H, m, H-25), 0.73 (3H, d, *J*=6.9 Hz, H-26), 0.86(3H, d, *J*=6.9 Hz, H-27), 0.77 (3H, d, *J*=7.0 Hz, H-28), 4.73 (1H, s, OH-3), 4.70 (1H, s, OH-14), 3.60 (1H, s, OH-20), 4.29 (1H, s, OH-22), ^1C NMR (700 MHz, DMSO): δ_C 33.2 (CH_2, C-1), δ_C 30.5 (CH_2, C-2), δ_C 67.9 (CH, C-3), δ_C 34.3 (CH_2, C-4), δ_C 55.9 (CH, C-5), δ_C 201.3 (qC, C-6), δ_C 120.2 (CH, C-7), δ_C 165.6 (qC, C-8), δ_C 32.7 (CH, C-9), δ_C 36.0 (qC, C-10), δ_C 19.8 (CH_2, C-11), δ_C 30.9 (CH_2, C-12), δ_C 46.9 (qC, C-13), δ_C 82.9 (qC, C-14), δ_C 30.3 (CH_2, C-15), δ_C 20.3 (CH_2, C-16), δ_C 48.6 (CH, C-17), δ_C 17.1 (CH_3, C-18), δ_C 23.2 (CH_3, C-19), δ_C 75.7 (qC, C-20), δ_C 20.7 (CH_3, C-21), δ_C 73.4 (CH, C-22), δ_C 36.2 (CH_2, C-23), δ_C 34.9 (CH, C-24), δ_C 28.7 (CH, C-25), δ_C 15.8 (CH_3, C-26), δ_C 21.0 (CH_3, C-27), δ_C 15.4 (CH_3, C-28)

terretonin (5): Orange powder; LRESIMS $[M+H]^+$ *m/z* 489.2. $[\alpha]^{25}D$ -64.3 (c 0.1 MeOH). ^1NMR (700 MHz, DMSO): δ_H 1.80 (1H, dd, *J*=11.6, 6.5 Hz, H-1a), 2.07 (1H, dd, *J*=20.5, 10.3 Hz, H-1b), 2.67 (1H, d, *J*=19.0, 8.7Hz, H-2a), 2.39 (1H, m, H-2b), 2.91 (1H, d, *J*=14.4 Hz , H-11a), 2.29 (1H, d, *J*=14.6 Hz , H-11b) , 3.68 (1H, s, H-14), 1.58 (3H, s, H-20), 1.33 (3H, s, H-21), 1.35 (3H, s, H-24), 1.78 (3H, s, H-26), 4.94 (1H, s, H-27a), 5.17 (1H, s, H-27b), 1.06 (3H, s, H-28), 1.33 (3H, s, H-30), 3.70 (3H, s, H-34). ^1C NMR (700 MHz, DMSO): δ_C 32.4 (CH_2, C-1), δ_C 34.0 (CH_2, C-2), δ_C 214.5 (qC, C-3), δ_C 52.0 (qC, C-4), δ_C 130.7 (qC, C-5), δ_C 140.4 (qC, C-6), δ_C 197.1 (qC, C-7), δ_C 43.5 (qC, C-8), δ_C 77.5 (qC, C-9), δ_C 47.2 (qC, C-10), δ_C 27.9 (CH_2, C-11), δ_C 139.1 (qC, C-12), δ_C 48.9 (qC, C-13), δ_C 42.8 (CH, C-14), δ_C 168.0 (qC, C-15), δ_C 84.7 (qC, C-17), δ_C 202.5 (qC, C-18), δ_C 21.2 (CH_3, C-20), δ_C 23.8 (CH_3, C-21), δ_C 21.3 (CH_3, C-24), δ_C 18.6 (CH_3, C-26), δ_C 113.9 (CH_2, C-27), δ_C 18.2 (CH_3, C-28), δ_C 23.1 (CH_3, C-30), δ_C 167.8 (qC, C-31), δ_C 53.5 (CH_3, C-34)

demethylincisterol A2 (6): Orange powder; LRESIMS $[M+H]^+$ *m/z* 333.6. $[\alpha]^{25}D$ +10.3 (c 0.2 MeOH). ^1H NMR (700 MHz, $CDCl_3$): δ_H 5.64 (1H, d, *J*=1.7 Hz, H-2), δ_H 2.28 (1H, ddd, *J*=14.2,3.9,2.5 Hz, H-5a), δ_H1.86 (1H, m, H-5b), δ_H1.98 (1H, m, H-6a), δ_H1.64 (1H, m, H-6b), δ_H 2.64 (1H, m, H-8), δ_H1.73 (1H, m, H-9a), δ_H1.62 (1H, m, H-9b), δ_H1.92 (1H, m, H-10a), δ_H1.49 (1H, m, H-10b), δ_H 1.50 (1H, m, H-11),δ_H 0.61 (3H, s, H-12), δ_H 2.06 (1H, dd, *J*=15.6, 8.7 Hz, H-13), δ_H 1.04 (3H, d, *J*=6.6 Hz, H-14), δ_H 5.17 (1H, d, *J*=15.3, 8.5 Hz, H-15), δ_H 5.25 (1H, d, *J*=15.2, 7.9 Hz, H-16), δ_H 1.98 (1H, m, H-17), δ_H 1.63 (1H, d, *J*=4.1 Hz, H-18), δ_H 0.84 (3H, d, *J*=6.8 Hz, H-19), δ_H 0.82 (3H, d, *J*=6.7 Hz, H-20), δ_H 0.92 (3H, d, *J*=6.8 Hz, H-21). ^1C NMR (500 MHz, $CDCl_3$): δ_C 171.0 (qC, C-1), δ_C 112.5(CH, C-2), δ_C 170.6 (qC, C-3), δ_C 104.9 (qC, C-4),δ_C 35.4 (CH_2, C-5), δ_C 29.0 (CH_2, C-6), δ_C 49.0 (qC, C-7), δ_C 50.5 (CH, C-8), δ_C 21.5 (CH_2, C-9), δ_C 35.1 (CH_2, C-10), δ_C 55.5 (CH, C-11), δ_C 11.9 (CH_3, C-12), δ_C 40.3 (CH, C-13), δ_C 19.8 (CH_3, C-14), δ_C 133.0 (CH, C-15), δ_C 134.8 (CH, C-16), δ_C 42.9 (CH, C-17), δ_C 33.2 (CH, C-18), δ_C 20.1 (CH_3, C-19), δ_C 21.2 (CH_3, C-20), δ_C 17.7 (CH_3, C-21).

asperophiobolin E(7): Orange powder; LRESIMS $[M+H]^+$ *m/z* 383.8. $[\alpha]^{25}D$ +86.9 (c 0.2 MeOH);^1H NMR (700 MHz, $CDCl_3$): δ_H 1.13 (1H, dd, *J*=22.9, 9.8 Hz, H-1a), δ_H 2.04 (1H, d, *J*=4.2 Hz,H-1b), δ_H 2.84 (1H, d, *J*=12.8 Hz,H-2), δ_H 5.93 (1H, s, H-4), δ_H 3.42 (1H, d, *J*=3.7 Hz, H-6), δ_H 7.03 (1H, d, *J*=4.6 Hz,H-8), δ_H 2.09 (1H, m, H-9a), δ_H 2.75 (1H, d, *J*=19.9 Hz, H-9b), δ_H 2.54 (1H, dd, *J*=10.3, 3.4 Hz, H-10), 1.42 (1H, td, *J*=12.4, 5.1Hz, H-12a), δ_H 1.51 (1H, dt, *J*=14.3, 7.2 Hz, H-12b), δ_H 1.23 (1H,m, H-13a), δ_H 1.65 (1H,m, H-13b), δ_H 1.86 (1H, m, H-14), δ_H 2.56 (1H, dd, *J*=9.9, 3.0 Hz, H-15), δ_H 5.09 (1H, t, *J*=10.1 Hz, H-16), δ_H 6.08 (1H, t, *J*=11.2 Hz, H-17), δ_H 5.99 (1H, t, *J*=11.6Hz, H-18), δ_H 2.07 (3H, s, H-20), δ_H 0.92 (3H, s, H-22), δ_H 0.95 (3H, s, H-23), δ_H 1.75 (3H, s, H-24), δ_H 1.81 (3H, s, H-25). ^1C NMR (700 MHz, $CDCl_3$): δ_C 46.2 (CH_2, C-1), δ_C 49.5 (CH, C-2), δ_C 178.6 (qC, C-3), δ_C 129.8 (CH, C-4), δ_C 208.2 (qC, C-5), δ_C 51.4 (CH, C-6), δ_C 127.9 (qC, C-7), δ_C 148.1 (CH, C-8), δ_C 30.1 (CH_2, C-9), δ_C 44.1 (CH, C-10), δ_C 45.5 (qC, C-11), δ_C 44.5 (CH_2, C-12), δ_C 27.9 (CH_2, C-13), δ_C 52.3 (CH, C-14), δ_C 32.6 (CH, C-15), δ_C 135.9 (CH, C-16), δ_C 124.1 (CH, C-17), δ_C 120.1 (CH, C-18), δ_C 136.5 (qC, C-19), δ_C 17.5 (CH_3, C-20), δ_C 17.5 (CH_3, C-20), δ_C 171.6 (qC, C-21), δ_C 23.0 (CH_3, C-22), δ_C 21.4 (CH_3, C-23), δ_C 18.3 (CH_3, C-24), δ_C 26.7 (CH_3, C-25).

butyrolactone I (8): Pale yellow oil; LRESIMS [M-H]− m/z 423.1; [2M-H]− m/z 847.1. [α] D^{25} =+30.5（c 0.8 MeOH）.^1H NMR (700 MHz, MeOH): δ_H 3.43 (2H, dd, *J*= 31.1, 14.7Hz, H-5), δ_H 3.79 (3H, s, H-7), δ_H 7.59 (2H, m, H-2′/6'), δ_H 6.85 (2H, m, H-3′/5'), δ_H 6.49 (H, d, *J*= 8.1Hz, H-2"), δ_H 6.41 (H, d, *J*= 2.1Hz, H-5"), δ_H 6.54 (H, dd, *J*= 8.2, 2.2Hz, H-6"), δ_H 3.08 (2H, m, H-7”), δ_H 5.07 (1H, m, H-8”), δ_H 1.67 (3H, s, H-10”), δ_H 1.58 (3H, s, H-11”). ^1C NMR (700 MHz, MeOH): δ_C 168.9 (qC, C-1), δ_C 138.3 (qC, C-2), δ_C 127.8 (qC, C-3), δ_C 85.4 (qC, C-4), δ_C 38.2 (CH2, C-5), δ_C 170.2 (qC, C-6), δ_C 52.4 (OCH_3, C-7), δ_C 121.8 (qC, C-1'), δ_C 128.9 (CH, C-2′/6'), δ_C 115.2 (CH, C-3′/5'), δ_C 157.9 (qC, C-4'), δ_C 123.7 (qC, C-1"), δ_C 131.0 (CH, C-2"), δ_C 127.0 (qC, C-3"), δ_C 153.7 (qC, C-4"), δ_C 113.6 (CH, C-5"), δ_C 128.4 (CH, C-6"), δ_C 27.3 (CH_2, C-7”), δ_C 122.2 (CH, C-8”'), δ_C 131.6 (qC, C-9”'), δ_C 24.6 (CH_3, C-10”), δ_C 16.4 (CH_3, C-11”).

butyrolactones VI (9): Colorless solid; LRESIMS $[M+H]^+$ *m/z* 459.8. $[\alpha]^{25}D$ +66.8 (c 0.5 MeOH). ^1H NMR (700 MHz, MeOH): δ_H 3.45 (2H, d, J=5.7 Hz, H-5), δ_H 3.79 (3H, s, H-7), δ_H 7.58 (2H, m, H-2′/6'), δ_H 6.78 (2H, m, H-3′/5'), δ_H 6.52 (H, d, *J*= 8.1Hz, H-2"), δ_H 6.50 (H, d, J= 2.1Hz, H-5"), δ_H 6.62 (H, dd, J= 8.2, 2.2Hz, H-6"), δ_H 2.69 (1H, dd, *J*= 14.1, 2.1 Hz, H-7”a), δ_H 2.55 (1H, dd, *J*= 14.1, 10.0 Hz, H-7”b), δ_H 3.44(1H, t, *J*= 3.7 Hz, H-8”), δ_H 1.18 (3H, s, H-10”), δ_H 1.18 (3H, s, H-11”). ^1C NMR (700 MHz, MeOH): δ_C 168.9 (qC, C-1), δ_C 138.3 (qC, C-2), δ_C 127.8 (qC, C-3), δ_C 85.4 (qC,

C-4), δ_C 38.2 (CH2, C-5), δ_C 170.2 (qC, C-6), δ_C 52.4 (OCH3, C-7), δ_C 121.7 (qC, C-1'), δ_C 129.1 (CH, C-2'/6'), δ_C 115.3 (CH, C-3'/5'), δ_C 157.9 (qC, C-4'), δ_C 124.1 (qC, C-1"), δ_C 132.9 (CH, C-2"), δ_C 127.9 (qC, C-3"), δ_C 154.5 (qC, C-4"), δ_C 114.5 (CH, C-5"), δ_C 129.0 (CH, C-6"), δ_C 32.6 (CH2, C-7"), δ_C 79.2 (CH, C-8'"), δ_C 72.4 (qC, C-9'"), δ_C 24.1 (CH3, C-10"), δ_C 23.7 (CH3, C-11").

***epi*-aszonalenins B (10)**: White powder; LRESIMS $[M+H]^+$ *m/z* 402.3 $[\alpha]^{25}D$ -3.8 (c 0.1 MeOH) ^1H NMR (700 MHz, $CDCl_3$): δ_H 8.03 (1H, s, H-9), δ_H 7.59 (1H, d, *J*=8.0 Hz, H-10), δ_H 7.57 (1H, dd, *J*=8.5, 5.8 Hz, H-11), δ_H 6.89 (1H, d, *J*=5.8 Hz, H-12), δ_H 3.45 (3H, s, H-13), δ_H 1.92 (3H, s, H-14), δ_H 1.92 (3H, s, H-15), δ_H 4.25 (2H, s, H-17), δ_H 2.37 (3H, s, H-19). ^1C NMR (500 MHz, $CDCl_3$): δ_C 164.8 (qC, C-2), δ_C 125.6 (qC, C-3), δ_C 126.4 (qC, C-3a), δ_C 125.6 (qC, C-4), δ_C 165.0 (qC, C-5), δ_C 66.0 (qC, C-7), δ_C 152.7 (qC, C-8), δ_C 123.2 (CH, C-9), δ_C 132.3 (qC, C-9a), δ_C 120.2 (CH, C-10), δ_C 131.5 (CH, C-11), δ_C 105.0 (CH, C-12), δ_C 141.6 (qC, C-12a), δ_C 26.5 (CH_3, C-13), δ_C 26.8 (CH_3, C-14), δ_C 26.8 (CH_3, C-15), δ_C 167.8 (qC, C-16), δ_C 54.1 (CH_2, C-17), δ_C 201.7 (qC, C-18), δ_C 30.4 (CH_3, C-20), δ_C 30.4 (CH_3, C-22), δ_C 30.4 (CH_3, C-23), δ_C 30.4 (CH_3, C-24), δ_C 30.4 (CH_3, C-25), δ_C 30.4 (CH_3, C-26).

Flavoglaucin (11): Yellow liquid; LRESIMS $[M+H]^+$ *m/z* 305.2. $[\alpha]^{25}D$ -2.04 (c 0.2 MeOH). ^1H NMR (700 MHz, $CDCl_3$): δ_H 10.3 (1H, s, CHO-1), δ_H 6.89 (1H, s, H-4), δ_H 2.88 (1H, m, H-1'), δ_H 1.57 (2H, ddd, *J*=15.6, 8.9, 6.8Hz, H-2'), δ_H 1.39 (2H, qt, *J*=15.2, 7.1Hz, H-3'), δ_H 1.32 (2H, m, H-4'), δ_H 1.27 (2H, m, H-5'), δ_H 1.28 (2H, m, H-6'), δ_H 0.88 (3H, t, *J*=7.1Hz, H-7'), δ_H 3.29 (2H, d, *J*=7.4 Hz, H-1"), δ_H 5.28 (1H, m, H-2"), δ_H 1.76 (3H, s, H-4"), δ_H 1.70 (3H,s, H-5"), δ_H 11.9 (1H, s, OH-2), δ_H 4.47 (1H, s,OH-5). ^1C NMR (500 MHz, $CDCl_3$): δ_C 195.6 (CH, CHO-1), δ_C 117.3 (qC, C-1), δ_C 155.8 (qC, C-2), δ_C 128.6 (qC, C-3), δ_C 125.7 (CH, C-4), δ_C 145.0 (qC, C-5), δ_C 128.6 (qC, C-6), δ_C 24.0 (CH_2, C-1'), δ_C 32.0 (CH_2, C-2'), δ_C 29.6 (CH_2, C-3'), δ_C 29.2 (CH_2, C-4'), δ_C 31.8 (CH_2, C-5'), δ_C 22.7 (CH_2, C-6'), δ_C 14.1 (CH_2, C-7'), δ_C 27.0 (CH_2, C-1"), δ_C 121.2 (CH, C-2"), δ_C 133.9 (qC, C-3"), δ_C25.8 (CH_3, C-4"), δ_C 17.8 (CH_3, C-5").

6,8-Dimethoxy-3-methylisocoumar (12): Orange powder; LRESIMS $[M+H]^+$ *m/z* 223.5. $[\alpha]^{25}D$ -89.3 (c 0.1 MeOH). ^1H NMR (700 MHz, MeOH): δ_H 4.45 (1H, ddd, *J*=11.4, 6.3, 2.9 Hz, H-3), δ_H 2.85 (1H, dd, *J*=16.2, 11.4 Hz, H-4), δ_H 2.94 (1H, dd, *J*=16.3, 2.8 Hz, H-4), δ_H 6.55 (1H, d, *J*=2.2Hz, H-5), δ_H 6.48 (1H, d, *J*=2.2 Hz, H-7), δ_H 1.44 (3H, d, *J*=6.3 Hz, H-9), δ_H 3.88 (3H, s, H-10), δ_H 3.88 (3H, s, H-11). ^1C NMR (500 MHz, $CDCl_3$): δ_C 164.8 (qC, C-2), δ_C 125.6 (qC, C-3), δ_C 126.4 (qC, C-3a), δ_C 125.6 (qC, C-4), δ_C 165.0 (qC, C-5), δ_C 66.0 (qC, C-7), δ_C 152.7 (qC, C-8), δ_C 123.2 (CH, C-9), δ_C 132.3 (qC, C-9a), δ_C 120.2 (CH, C-10), δ_C 131.5 (CH, C-11), δ_C 105.0 (CH, C-12), δ_C 141.6 (qC, C-12a), δ_C 26.5 (CH_3, C-13), δ_C 26.8 (CH_3, C-14), δ_C 26.8 (CH_3, C-15), δ_C 167.8 (qC, C-16), δ_C 54.1 (CH_2, C-17), δ_C 201.7 (qC, C-18), δ_C 30.4 (CH_3, C-19).

methyl shikimate (13): Yellow liquid; HRESIMS $[M+H]^+$ *m/z* 189.1560. $[\alpha]^{25}D$ -1.38 (c 0.2 MeOH) ^1H NMR (700 MHz, DMSO): δ_H 6.48 (1H, m, H-2), δ_H 4.17 (1H, d, *J*=1.6 Hz, H-3), δ_H 3.74 (1H, s, H-4), δ_H3.61 (1H, m, H-5), δ_H 2.15 (1H, m, H-6a),δ_H2.29 (1H, dd, *J*=16.8, 5.8 Hz, H-6b), δ_H 3.65 (3H, s, H-8), δ_H 4.87 (1H, d, *J*=7.4 Hz, OH-3), δ_H 4.58 (1H, d, *J*=3.5 Hz, OH-4), δ_H 4.76 (1H, d, *J*=5.4 Hz, OH-5),^1C NMR (700 MHz, DMSO): δ_C 127.8 (qC, C-1), δ_C 140.8 (CH, C-2), δ_C 68.3 (CH, C-3), δ_C 70.9 (CH, C-4), δ_C 67.6 (CH, C-5), δ_C 29.0 (CH_2, C-6), δ_C 166.7 (qC, C-7),δ_C 51.8 (CH_3, C-8).

The strain's (*Aspergillus hiratsukae* SCSIO 5Bn$_1$003) ITS sequence of the rDNA

TCAACCTCCCACCCGTGTCTATTGTACCTTGTTGCTTCGGCGGGCCCGCCG
TTTTCGAACGGCCGCCGGGGAGGCCTCGCGCCCCCGGGCCCGCGCCCGCC

GAAGACCCCAACATGAACGCTGTTCTGAAAGTATGCAGTCTGAGTTTGAT
TATCATAATCAGTTAAAACTTTCAACAACGGATCTCTTGGTTCCGGCATCG
ATGAAGAACGCAGCGAAATGCGATAAGTAATGTGAATTGCAGAATTCAGT
GAATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGTATTCCGGGGGG
CATGCCTGTCCGAGCGTCATTGCTGCCCTCAAGCACGGCTTGTGTGTTGGG
CCCCCGTCCCCGGTTCTCCCCGGGGACGGGCCCGAAAGGCAGCGGCGGCA
CCGCGTCCGATCCTCGAGCGTATGGGGCTTTGTCACCCGCTCTGTAGGCCC
GGCCGGCGCCAGCCGACACCCCAACTTTATTTTCTAAGGTTGACCTCGGA
TCAGGTAGGGATACCCGCTGAACTTAAGCATATCAATAA

Table S1. the primary screening of cytotoxic activity of all compounds.

compounds	Inhibition rate (50 μM) %			
	SF-268	MCF-7	HepG-2	A549
1	0.82	1.03	0.38	4.40
2	1.43	1.01	1.45	1.21
3	2.31	3.24	0.13	0.83
4	8.79	19.08	1.57	8.60
5	4.58	5.62	3.52	2.97
6	93.24	92.20	81.44	0.41
7	9.64	38.75	40.71	0.58
8	41.92	50.70	69.11	21.53
9	8.47	17.74	5.43	0.29
10	32.90	42.17	6.70	0.73
11	0.81	0.49	0.39	1.53
12	4.43	6.09	2.34	2.91
13	0.59	0.66	0.66	0.36

Table S2. the primary screening of antibacterial activities of all compounds.

compounds	Inhibition rate (50 μM) %	
	Staphylococcus aureus	*Bacillus subtilis*
1	5.22	3.87
2	4.34	0.67
3	7.98	9.17
4	19.38	5.23
5	11.80	8.18
6	29.44	79.64
7	82.36	94.33
8	84.36	91.28
9	19.65	3.76
10	12.62	0.30
11	12.97	17.50
12	9.43	2.16
13	11.78	7.69

Table S3. the primary screening of antioxidative and *α*-glucosidase inhibitory activities of all compounds.

compounds	Inhibition rate (100 μM) %	
	antioxidative activity	*α*-Glucosidase Inhibitory
1	4.30	40.90
2	1.60	31.00
3	2.00	22.00
4	2.80	14.40
5	1.90	14.40
6	1.00	77.90
7	3.60	5.00
8	2.50	73.30
9	0.60	37.90
10	0.40	39.30
11	18.20	18.00
12	5.50	28.30
13	32.90	9.00