

Supporting Information

**New Chlorinated Metabolites and Antiproliferative
Polyketone from the Mangrove Sediments-Derived Fungus
Mollisia sp. SCSIO41409**

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The physicochemical data of the known compounds 2 and 4–9

5-hydroxy-2,3-dimethyl-7-methoxychromone (**2**): white needles; ^1H NMR (500 MHz, DMSO- d_6) δ 13.00 (s, 1H, 5-OH), 6.53 (d, $J = 2.3$ Hz, 1H, H-6), 6.33 (d, $J = 2.3$ Hz, 1H, H-8), 3.83 (s, 3H, H-11), 2.39 (s, 3H, H-9), 1.91 (s, 3H, H-10); ^{13}C NMR (125 MHz, DMSO) δ 181.7 (C-4), 165.4 (C-5), 164.2 (C-2), 161.6 (C-5), 157.6 (C-8a), 114.9 (C-3), 104.2 (C-4a), 98.1 (C-6), 92.3 (C-8), 56.5 (C-11), 18.8 (C-9), 9.3 (C-10).

Stemphone C (**4**): yellow needles; HRESIMS m/z 515.3003 $[\text{M}+\text{H}]^+$ (calcd $\text{C}_{30}\text{H}_{43}\text{O}_7$, 515.3003); $[\alpha]_{\text{D}}^{25} +160.9$ (c 0.01, CH_3OH); ^1H NMR (500 MHz, DMSO- d_6) δ 6.59 (s, 1H, H-11), 5.52 (q, $J = 6.5$ Hz, 1H, H-2), 5.16 (d, $J = 9.2$ Hz, 1H, H-4), 4.14 (s, 1H, 22-OH), 3.21 (dd, $J = 9.1, 6.9$ Hz, 1H, H-21), 3.17 (m, 1H, overlapped, H-21), 3.08 (dd, $J = 11.4, 3.5$ Hz, 1H, H-17), 2.36 (dd, $J = 18.4, 4.6$ Hz, 1H, H-12a), 2.09 (m, 1H, H-12b), 2.0 (m, 3H, H-15, 19a), 1.86 (s, 3H, H-30), 1.73 (m, 2H, H-16), 1.57 (s, 3H, H-28), 1.56 (d, $J = 4.0$ Hz, 3H, H-1), 1.45 (m, 3H, overlapped, H-13, 20), 1.24 (m, 1H, H-19b), 1.19 (s, 3H, H-26), 1.08 (s, 3H, H-24), 1.04 (s, 3H, H-23), 0.95 (d, $J = 7.1$ Hz, 3H, H-27), 0.81 (s, 3H, H-25); ^{13}C NMR (125 MHz, DMSO) δ 186.5 (C-10), 180.9 (C-7), 169.3 (C-29), 151.7 (C-8), 147.3 (C-6), 132.3 (C-11), 132.1 (C-3), 124.5 (C-2), 117.6 (C-9), 84.8 (C-21), 83.2 (C-17), 81.0 (C-4), 80.2 (C-14), 70.3 (C-22), 45.7 (C-13), 36.8 (C-15), 36.0 (C-19), 35.0 (C-18), 33.1 (C-5), 26.9 (C-24), 25.0 (C-16), 24.6 (C-23), 20.7 (C-30), 20.5 (C-20), 20.5 (C-26), 16.5 (C-27), 16.0 (C-12), 12.9 (C-1), 11.9 (C-25), 11.2 (C-28).

Cis-cyclo (Tyr-Ile) (**5**): white powder; ^1H NMR (500 MHz, DMSO- d_6) δ 9.15 (s, 1H, 11-OH), 8.03 (s, 1H, NH-1), 7.86 (s, 1H, NH-4), 6.95 (d, $J = 8.4$ Hz, 2H, H-9, 13), 6.61 (d, $J = 8.4$ Hz, 2H, H-10, 12), 4.11 (t, $J = 4.1$ Hz, 1H, H-3), 3.55 (s, 1H, H-6), 3.04 (dd, $J = 13.7, 4.0$ Hz, 1H, H-7a), 2.73 (dd, $J = 13.7, 4.8$ Hz, 1H, H-7b), 1.41 (m, 1H, H-14), 0.60 (d, $J = 6.8$ Hz, 1H, H-17), 0.59 (t, $J = 7.0$ Hz, 3H, H-16). ^{13}C NMR (125 MHz, DMSO) δ 166.5 (C-2), 166.4 (C-5), 156.3 (C-11), 131.3 (C-9), 131.3 (C-13), 126.2 (C-8), 114.7 (C-10), 114.7 (C-12), 58.9 (C-3), 55.3 (C-6), 37.9 (C-7), 36.9 (C-14), 23.1 (C-15), 14.6 (C-17), 11.7 (C-16).

4,8-dihydroxy-1-tetra-lone (**6**): white solid; ^1H NMR (500 MHz, DMSO- d_6) δ 12.41 (s, 1H, 8-OH), 7.55 (t, $J = 8.0$ Hz, 1H, H-6), 7.08 (d, $J = 7.5$ Hz, 1H, H-5), 6.85 (dd, $J = 8.5, 1.1$ Hz, 1H, H-7), 4.75 (dt, $J = 9.4, 4.8$ Hz, 1H, H-4), 2.74 (m, 2H, H-2), 2.19 (m, 1H, H-3); ^{13}C NMR (125 MHz, DMSO) δ 205.3 (C-1), 161.5 (C-8), 148.7 (C-4a), 136.8 (C-6), 117.4 (C-7), 115.9 (C-1a), 115.1 (C-8a), 66.0 (C-

4), 35.3 (C-2), 31.5 (C-3).

Cyclo (Phe-Tyr) (**7**): white powder; ^1H NMR (500 MHz, DMSO- d_6) δ 9.22 (1H, s, 11-OH); 7.85 (s, NH-1, 4), 7.27 (m, $J = 7.5$ Hz, 2H, H-17, 19), 7.20 (t, $J = 7.3$ Hz, 1H, H-18), 7.03 (d, $J = 7.0$ Hz, 2H, H-16, 20), 6.83 (d, $J = 8.4$ Hz, 2H, H-9, 13), 6.67 (d, $J = 8.4$ Hz, 2H, H-10, 12), 3.95 (m, 1H, H-3), 3.89 (d, $J = 6.3$ Hz, 1H, H-6), 2.18 (m, 2H, H-7); ^{13}C NMR (125 MHz, DMSO) δ 166.3 (C-2), 166.2 (C-5), 156.1 (C-11), 136.7 (C-15), 130.9 (C-9, 13), 129.8 (C-17, 19), 128.2 (C-16, 20), 126.5 (C-8), 126.4 (C-18), 115.0 (C-10, 12), 55.7 (C-3), 55.4 (C-6), 39.2 (C-14), 38.5 (C-7).

Tenuissimasatin (**8**): white solid; $[\alpha]_{\text{D}}^{25} -15.7$ (c 0.01, CH_3OH); ^1H NMR (500 MHz, DMSO- d_6) δ 7.52 (t, $J = 7.8$ Hz, 1H, H-6), 7.01 (d, $J = 7.4$ Hz, 1H, H-7), 6.90 (d, $J = 8.1$ Hz, 1H, H-5), 5.72 (dd, $J = 8.5$, 4.0 Hz, 1H, H-3), 3.64 (s, 3H, H-12), 3.19 (dd, $J = 16.6$, 3.9 Hz, 1H, H-4a), 2.76 (dd, $J = 16.6$, 8.5 Hz, 1H, H-4b); ^{13}C NMR (125 MHz, DMSO) δ 169.9 (C-1), 167.6 (C-11), 156.9 (C-8), 151.1 (C-10), 136.1 (C-6), 115.9 (C-7), 112.4 (C-5), 111.2 (C-9), 75.7 (C-3), 51.7 (C-12), 38.7 (C-4).

4-methyl-5,6-dihydro-2H-pyran-2-one (**9**): colorless oil; ^1H NMR (500 MHz, DMSO- d_6) δ 5.74 (d, $J = 1.5$ Hz, 1H, H-3), 4.29 (t, $J = 6.2$ Hz, 2H, H-6), 2.37 (t, $J = 6.4$ Hz, 2H, H-5), 1.96 (d, $J = 1.3$ Hz, 3H, H-7); ^{13}C NMR (125 MHz, DMSO) δ 164.0 (C-2), 159.7 (C-4), 115.5 (C-3), 65.7 (C-6), 28.6 (C-5), 22.5 (C-7).

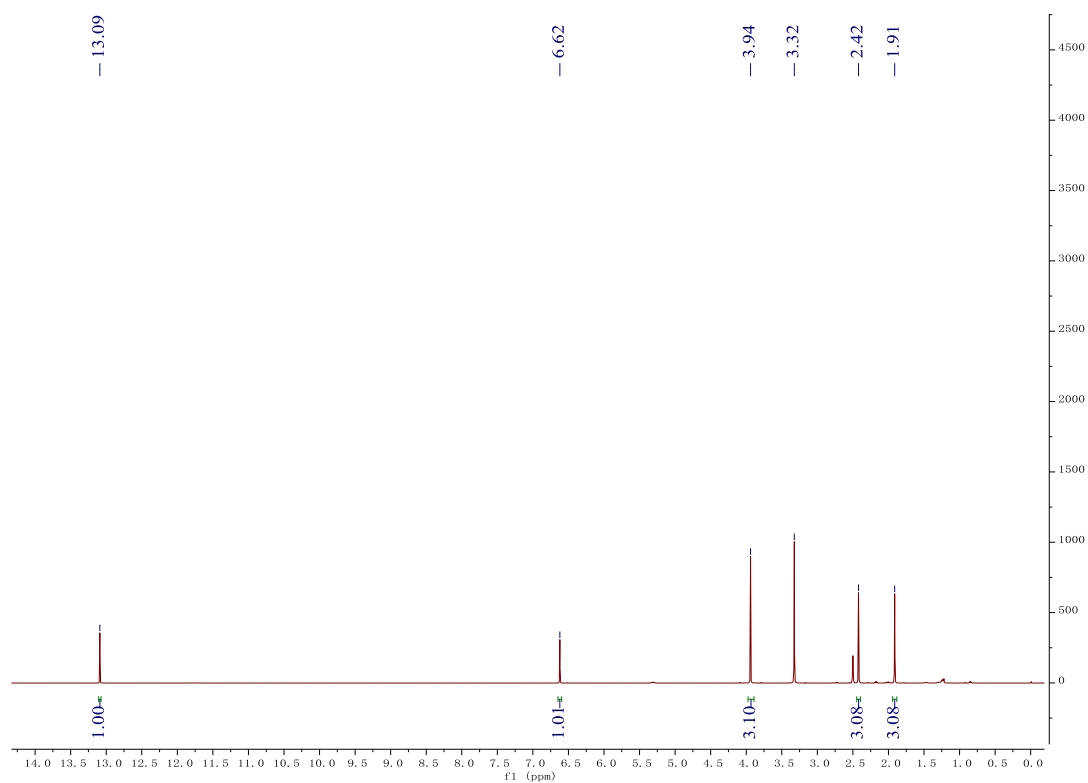


Figure S1: ¹H NMR spectrum of **1** in DMSO-*d*₆.

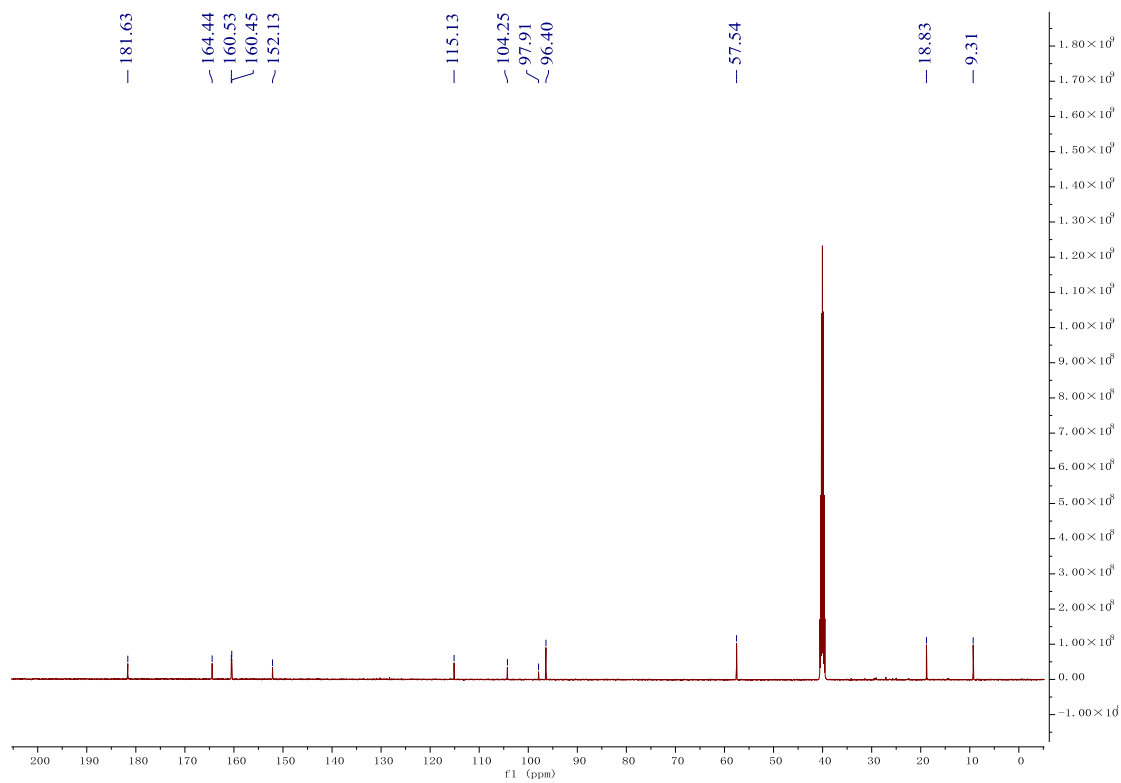


Figure S2: ¹³C NMR spectrum of **1** in DMSO-*d*₆.

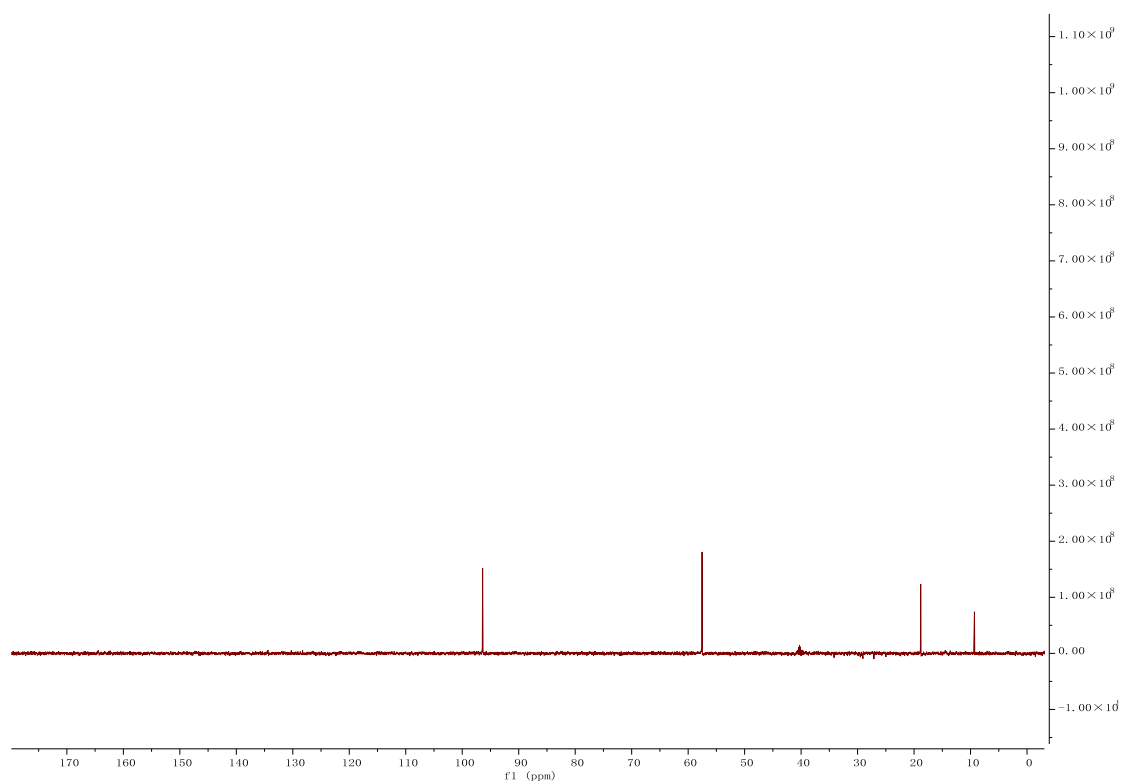


Figure S3: DEPT135 spectrum of **1** in DMSO-*d*₆.

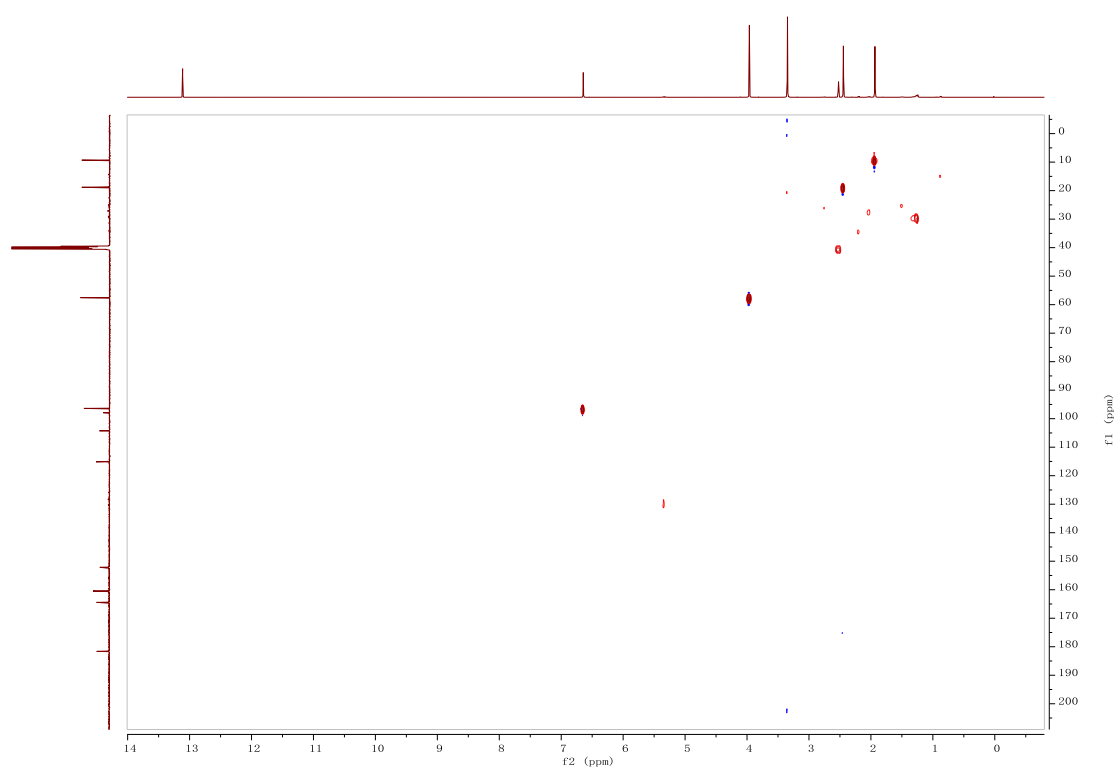


Figure S4: HSQC spectrum of **1** in DMSO-*d*₆.

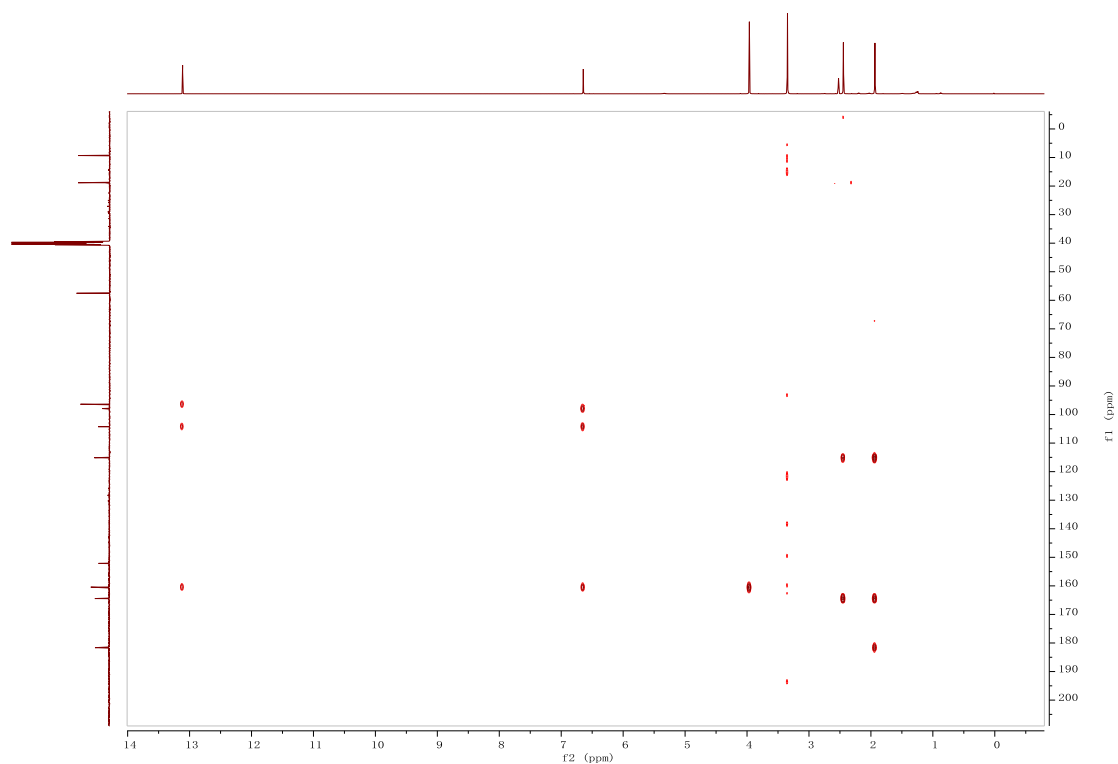


Figure S5: HMBC spectrum of **1** in DMSO- d_6 .

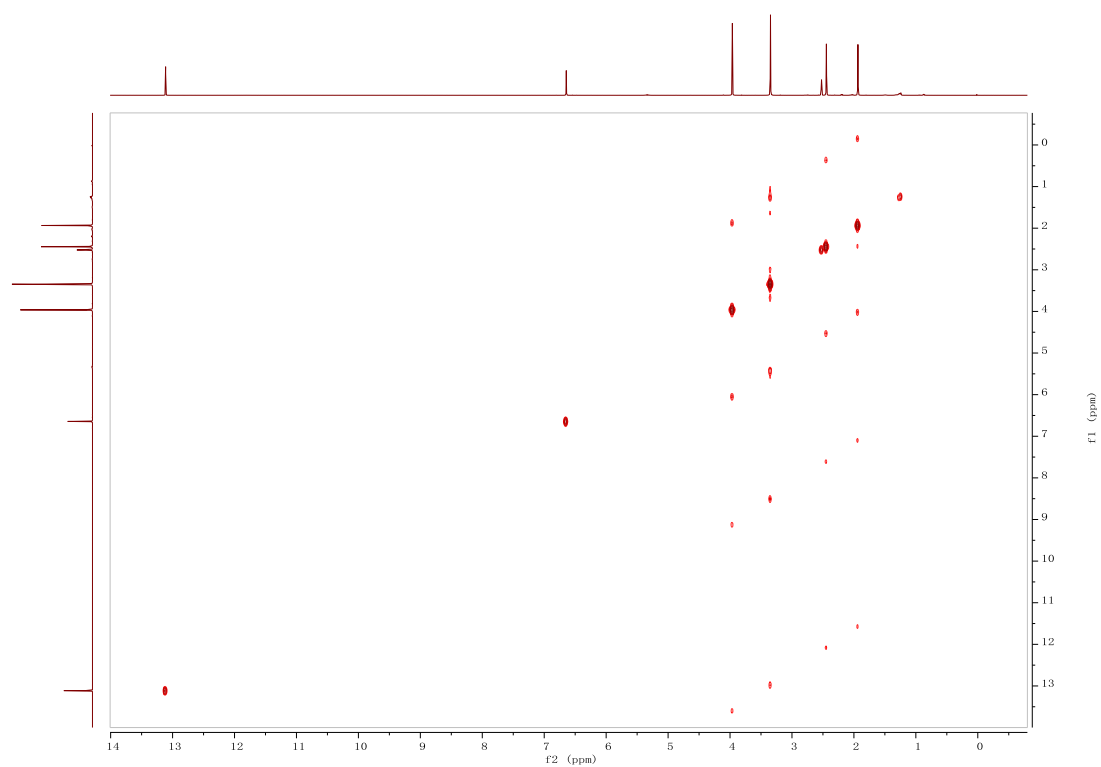


Figure S6: ^1H - ^1H COSY spectrum of **1** in DMSO- d_6 .

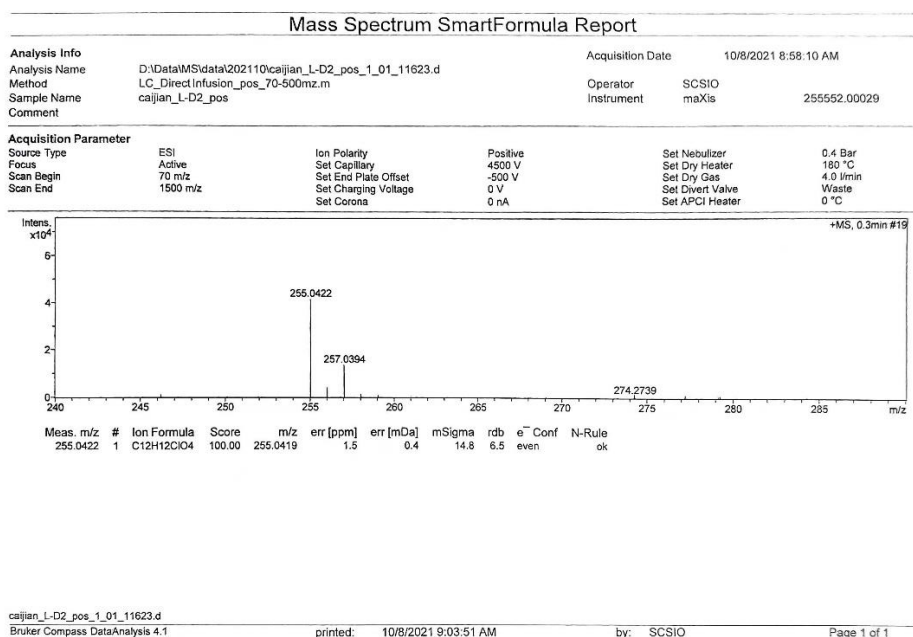


Figure S7: HRESIMS spectrum of **1**.

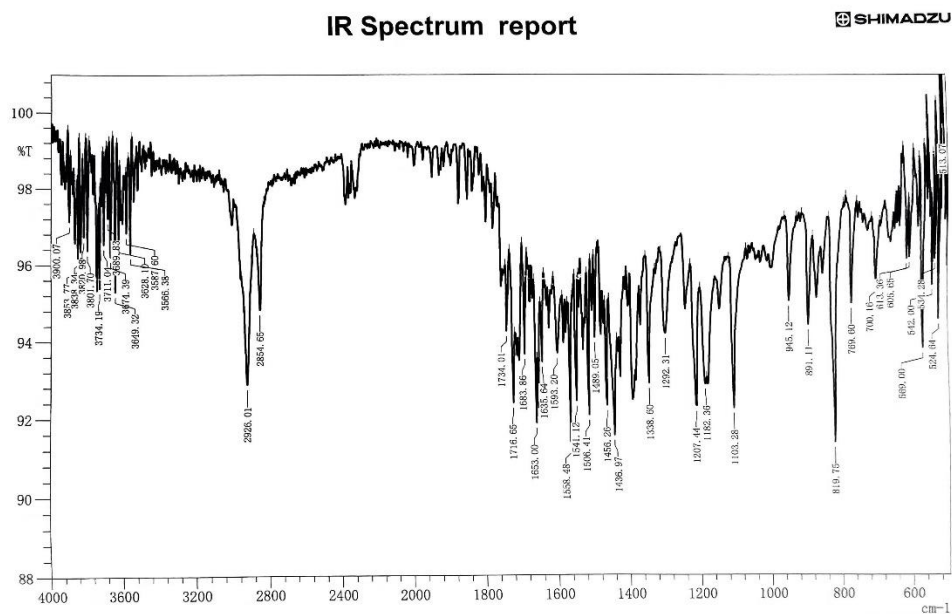


Figure S8: IR spectrum of **1**.

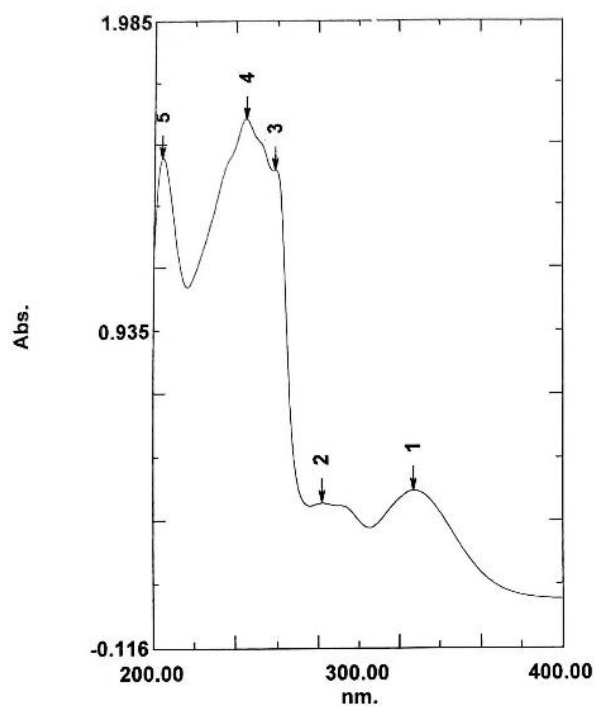


Figure S9: UV spectrum of **1** in MeOH.

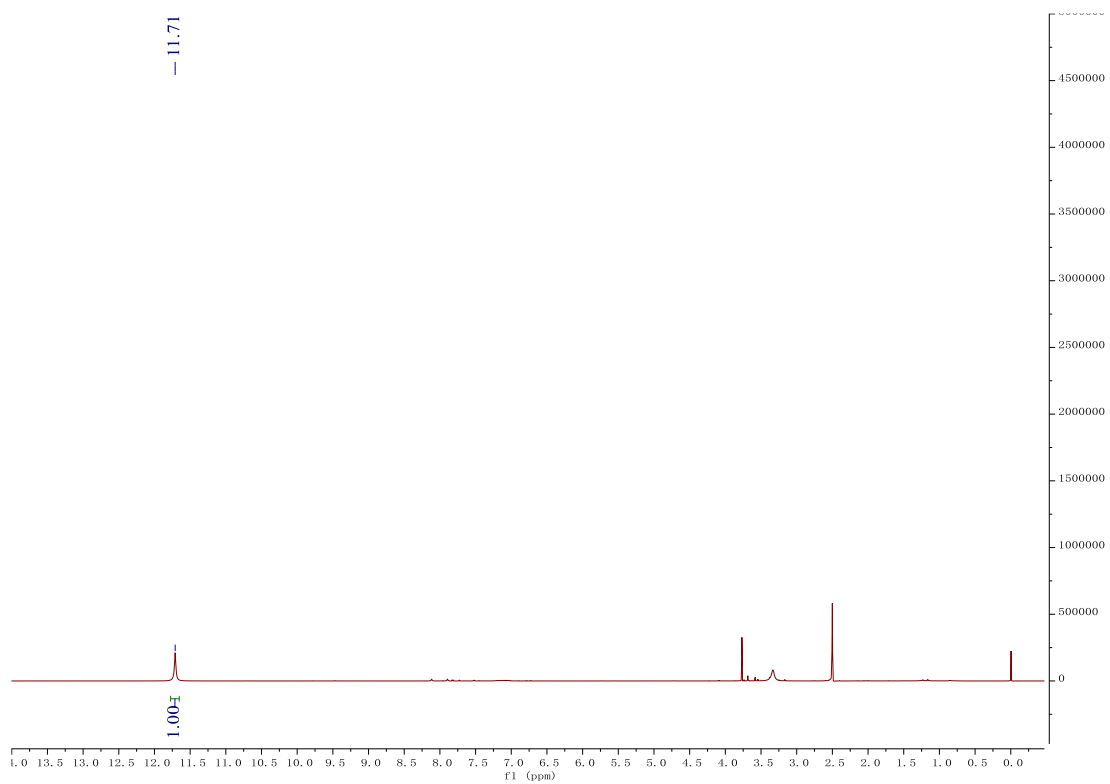


Figure S10: ^1H NMR spectrum of **3** in $\text{DMSO}-d_6$.

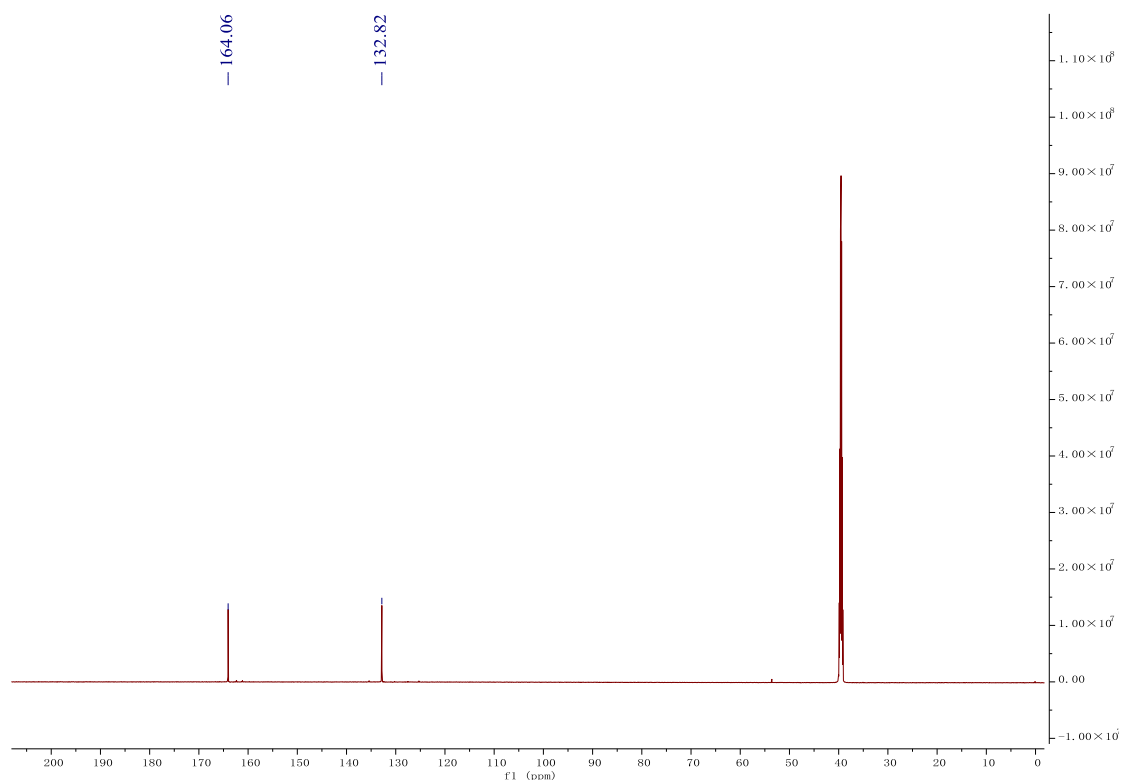


Figure S11: ^{13}C NMR spectrum of **3** in $\text{DMSO-}d_6$.

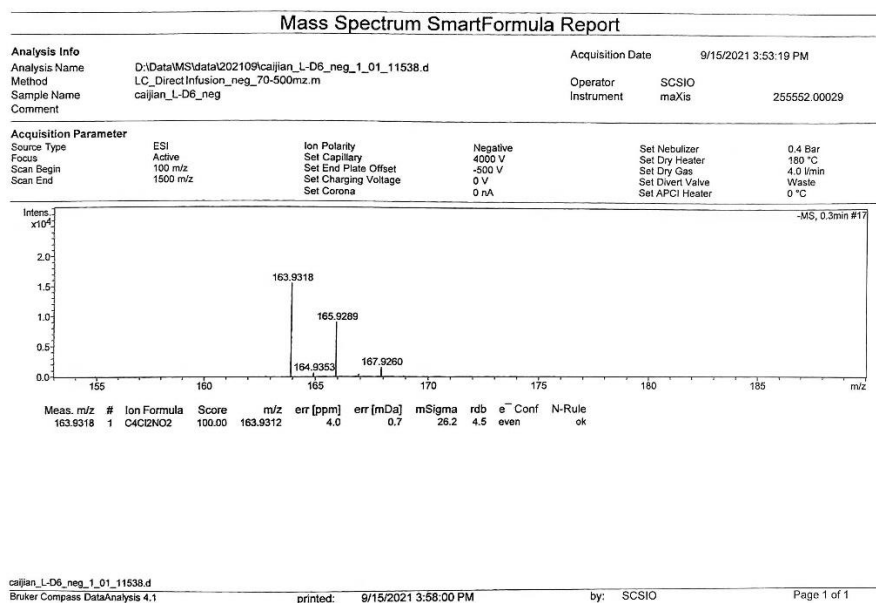


Figure S12: HRESIMS spectrum of **3**.

IR Spectrum report

SHIMADZU

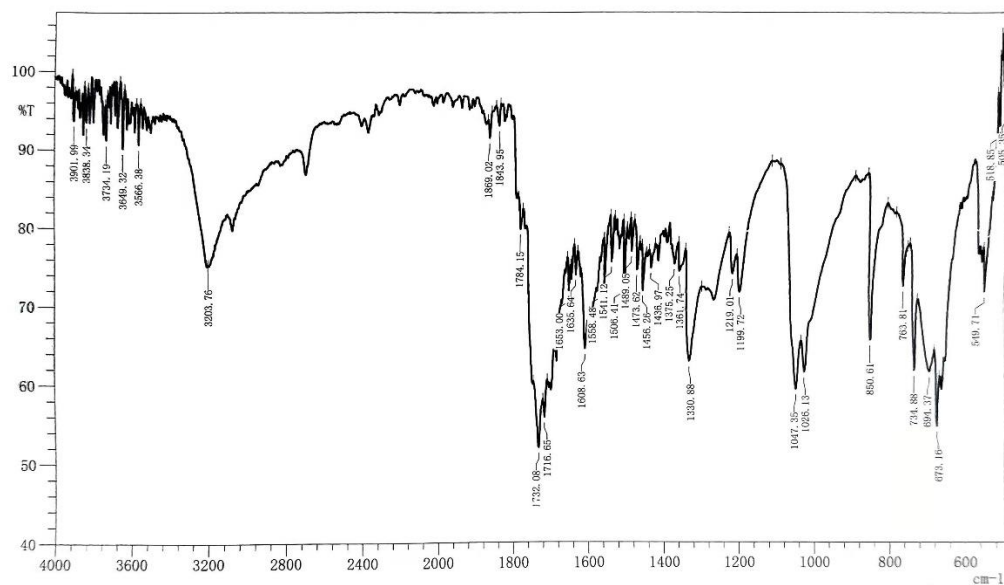


Figure S13: IR spectrum of 3.

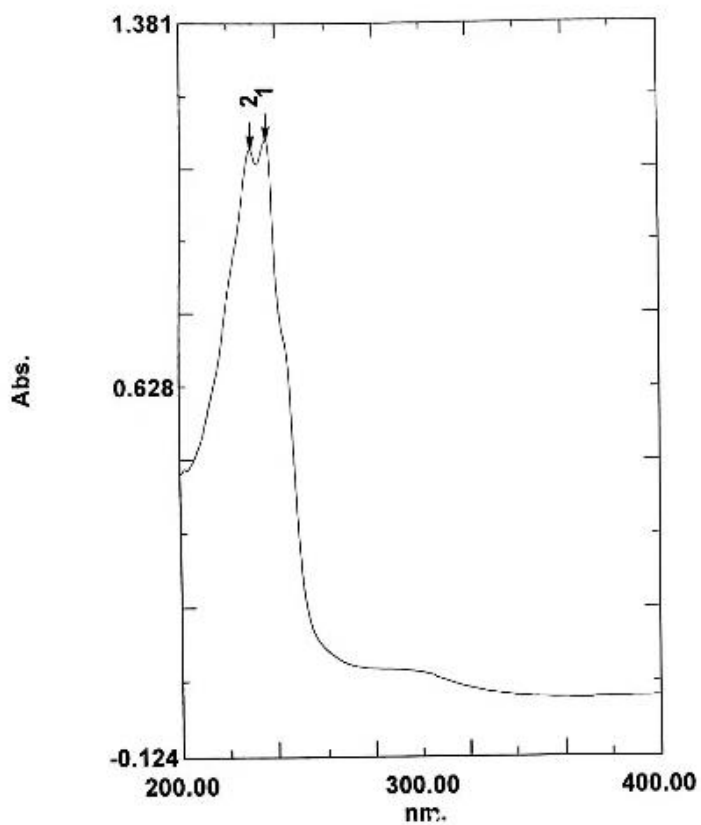


Figure S14: UV spectrum of 3 in MeOH.

ITS sequence of the strain *Mollisia* sp. SCSIO41409

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