


Assessment of Novel C-4 Methylated Tetraketide by HPLC-SPE-TT in *Saccharicola* sp., an Endophytic Fungus in *Eugenia jambolana* Lam.

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Fusaric acid (2)

Amorphous white powder; UV (CH₃OH) λ_{\max} / nm 225, 271; ¹H NMR (600 MHz, CD₃OD) δ 0.96 (t, 3H, *J* 7.4 Hz, CH₃), 1.39 (m, 2H, CH₂), 1.66 (m, 2H, CH₂), 2.77 (t, 1H, *J* 7.30 Hz, CH₂), 7.93(d, 1H, *J* 7.5 Hz, CH), 8.11 (d, 1H, *J* 7.5Hz, CH), 8.51 (s, 1H, CH); ¹³C NMR (150 MHz, CD₃OD) δ 13.7, 22.9, 33.4, 34.1, 125.8, 139.8, 144.3, 148.8; HRMS (ESI-Qq-TOF-HRMS) C₁₀H₁₃NO₂ [M + H]⁺ calcd.: 180.0980; found: 180.1018.

***trans*-4-Hydroxymellein (3)**

Amorphous white powder; UV (CH₃OH) λ_{\max} / nm 209, 245, 312; ¹H NMR (600 MHz, CD₃OD) δ 1.47 (d, 3H, *J* 6.5 Hz, CH₃), 4.55 (m, 1H, CH), 4.60 (m, 1H, CH), 4.62 (s, 1H, OH), 6.94 (dd, 1H, *J* 8.4, 1.0 Hz, CH), 7.08 (dt, 1H, *J* 8.0, 1.0 Hz, CH), 7.58 (tap, 1H, *J* 8.4, 7.5 Hz, CH); ¹³C NMR (150 MHz, CD₃OD) δ 17.1, 68.0, 81.0, 116.4, 116.5, 136.5, 176.2; HRMS (ESI-Qq-TOF-HRMS) C₁₀H₁₀O₄ [M + H]⁺ calcd.: 195.0613; found: 195.0650.

Thymidine (4)

Amorphous white powder; UV (CH₃OH) λ_{\max} / nm 203, 263, 323; ¹H NMR (600 MHz, DMSO-*d*₆) δ 1.77 (d, 3H, *J* 1.0 Hz, CH₃), 2.06 (m, 2H, CH₂), 3.56 (m, 2H, *J* 3.0, 12.0 Hz, CH₂), 3.75 (q, 1H, CH), 4.23 (m, 1H, CH), 5.04 (t, 1H, OH), 5.25 (d, 1H, OH), 6.16 (d, 1H, *J* 7.6, 6.2 Hz, CH), 7.69 (d, 1H, *J* 1.0 Hz, CH), 11.27 (sl, 1H, NH); ¹³C NMR (150 MHz, DMSO-*d*₆) δ 12.5, 40.0, 61.8, 70.5, 83.8, 87.5, 136.6; HRMS (ESI-Qq-TOF-HRMS) C₁₀H₁₄N₂O₅ [M + H]⁺ calcd.: 243.0936; found: 243.0974.

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Adenosine (5)

Amorphous white powder; UV (CH₃OH) λ_{max} / nm 258; ¹H NMR (600 MHz, D₂O) δ 3.80 (dd, 1H, *J* 12.0 Hz, CH), 3.88 (dd, 2H, *J* 12.0 Hz, CH), 4.26 (m, 1H, *J* 3.6, 6.6 Hz, CH), 4.39 (m, 1H, *J* 3.6, 5.5 Hz, CH), 6.03 (d, 1H, *J* 6.2 Hz, CH), 8.19 (s, 1H, CH), 8.29 (s, 1H, CH); ¹³C NMR (150 MHz, D₂O) δ 61.4, 70.5, 73.5, 85.8, 88.1, 118.9, 140.3, 148.5, 152.4, 155.6.

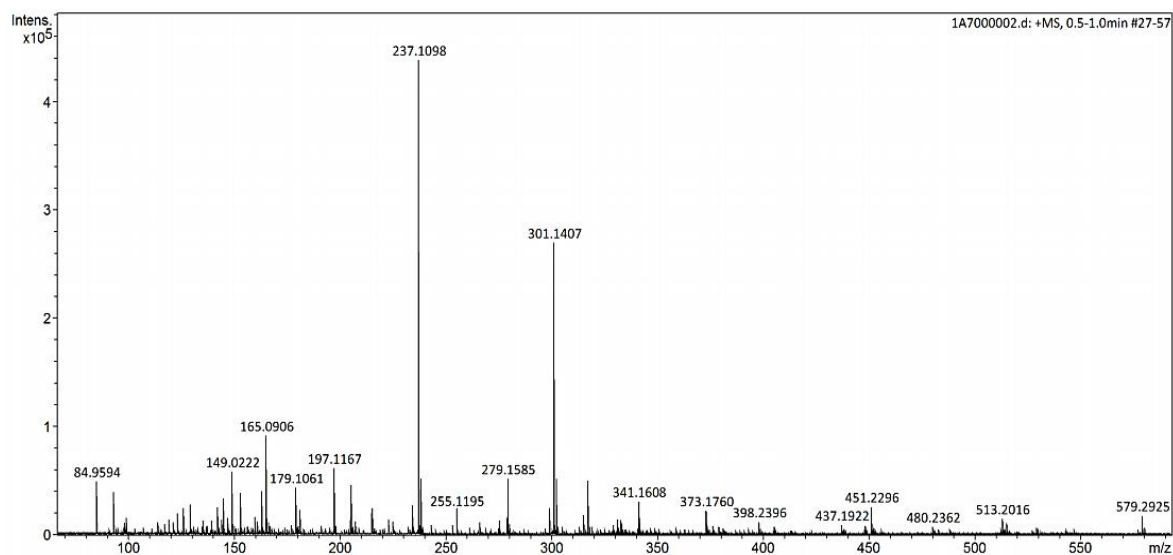


Figure S1. ESI-Qq-TOF-HRMS spectrum of compound **1** (*m/z* 301.1407 refers to the dopant phthalate).

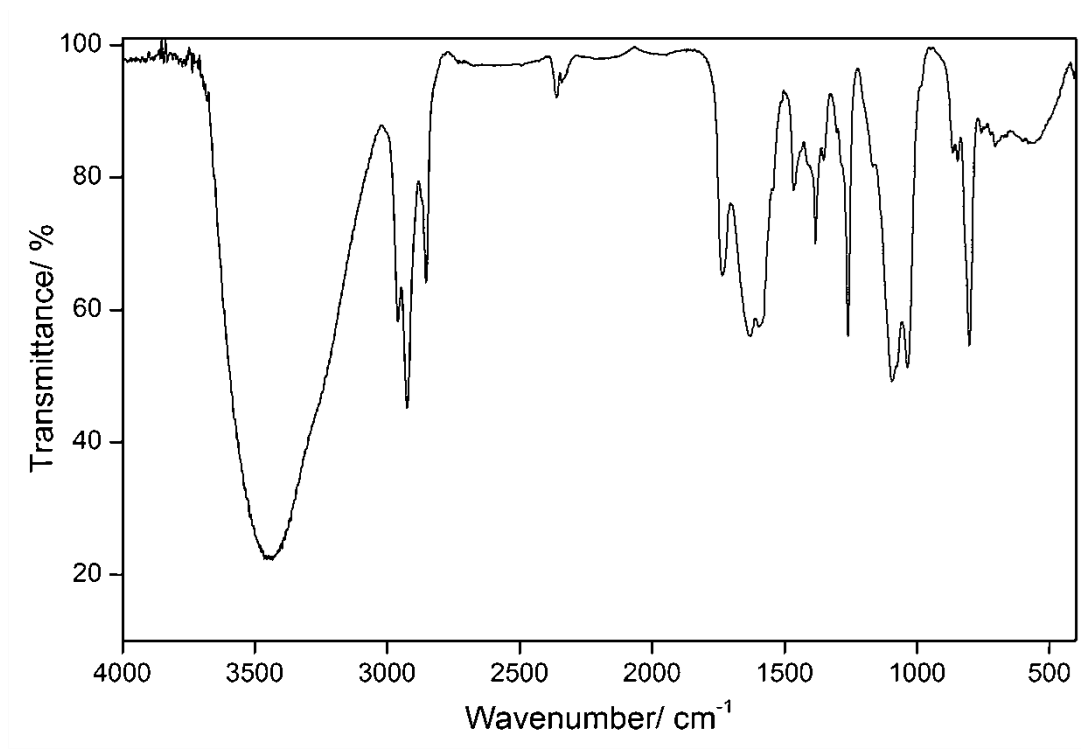


Figure S2. FTIR (KBr) spectrum of compound **1**.

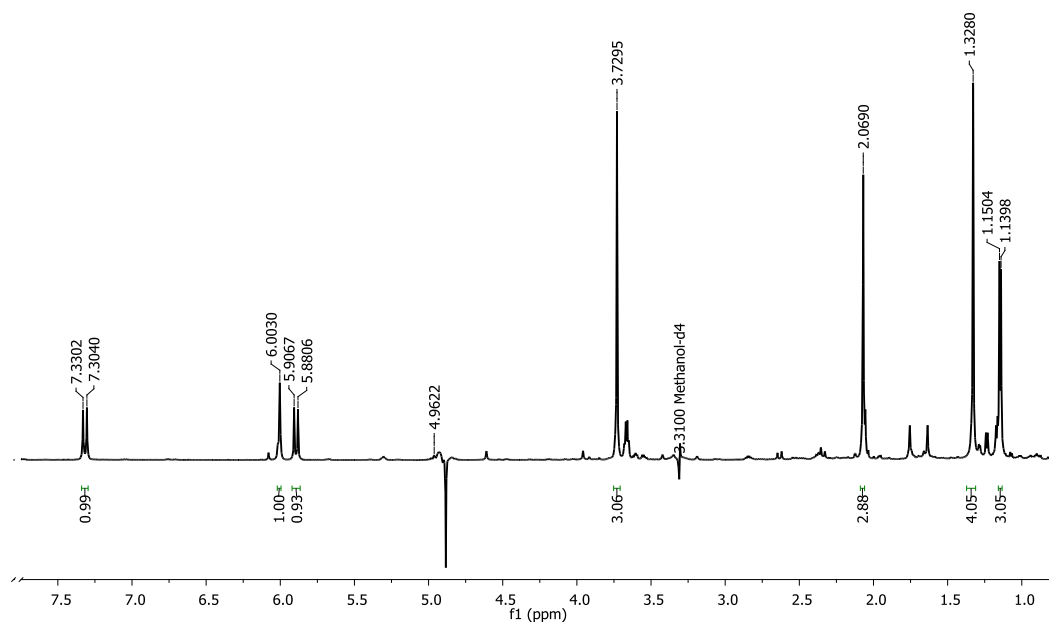


Figure S3. ^1H NMR spectrum (600 MHz, CD_3OD) of compound **1**.

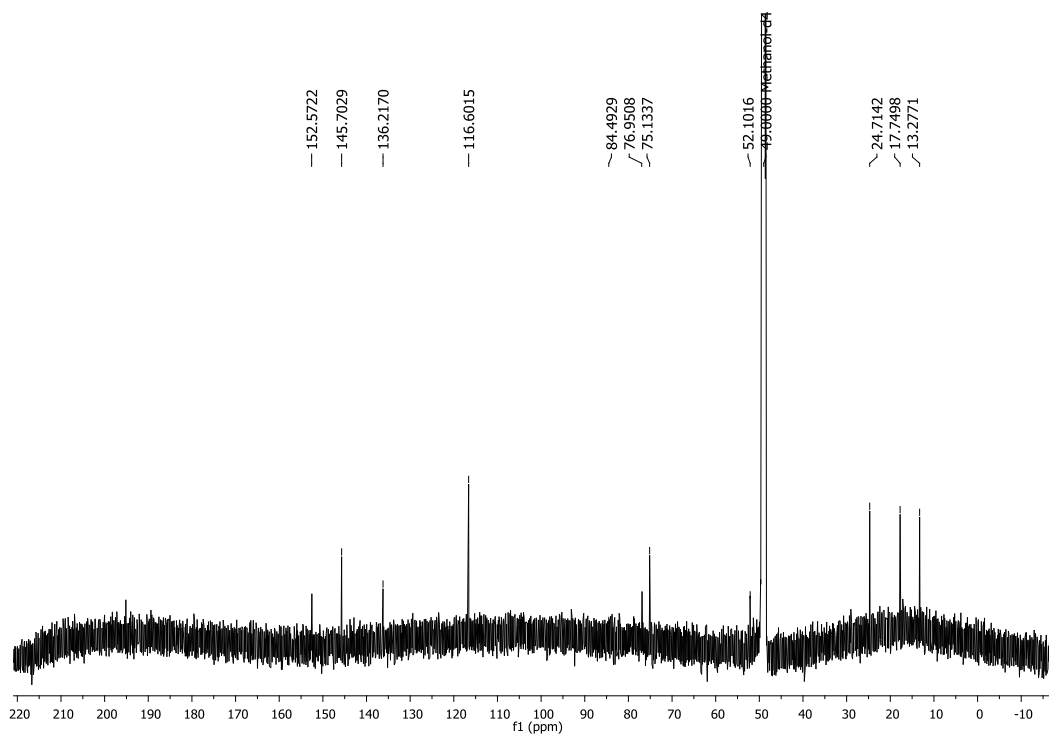


Figure S4. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound **1**.

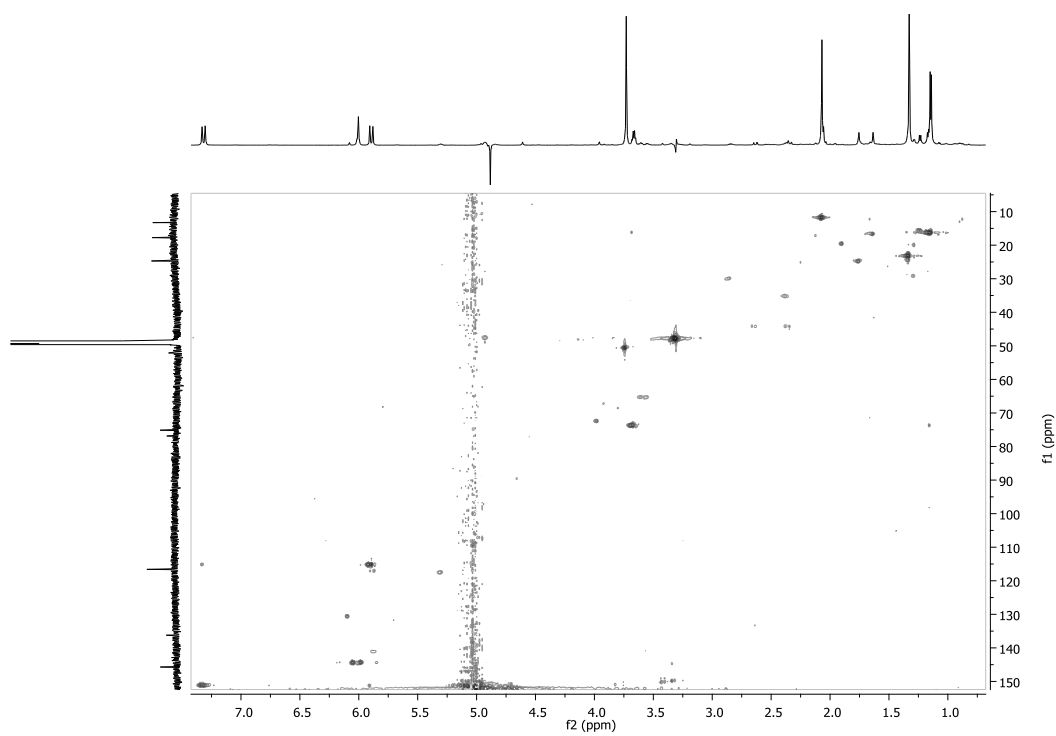


Figure S5. HSQC contour map (^1H : 600 MHz, ^{13}C : 150 MHz, CD_3OD) of compound **1**.

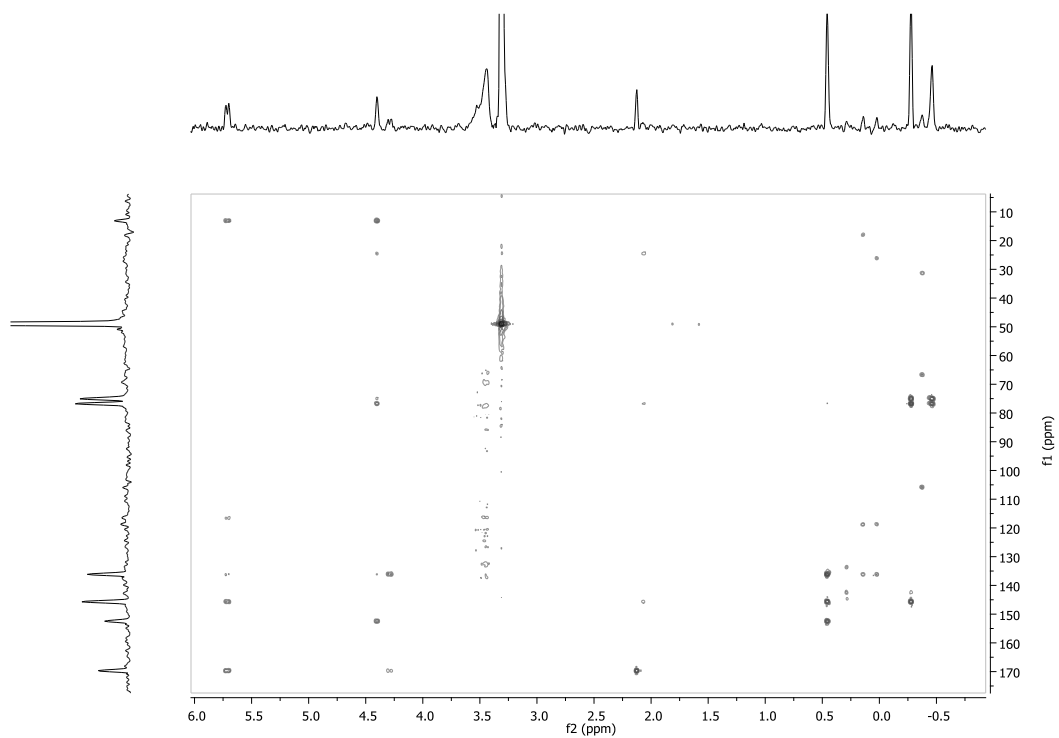


Figure S6. HMBC contour map (^1H : 600 MHz, ^{13}C : 150 MHz, CD_3OD) of compound **1**.

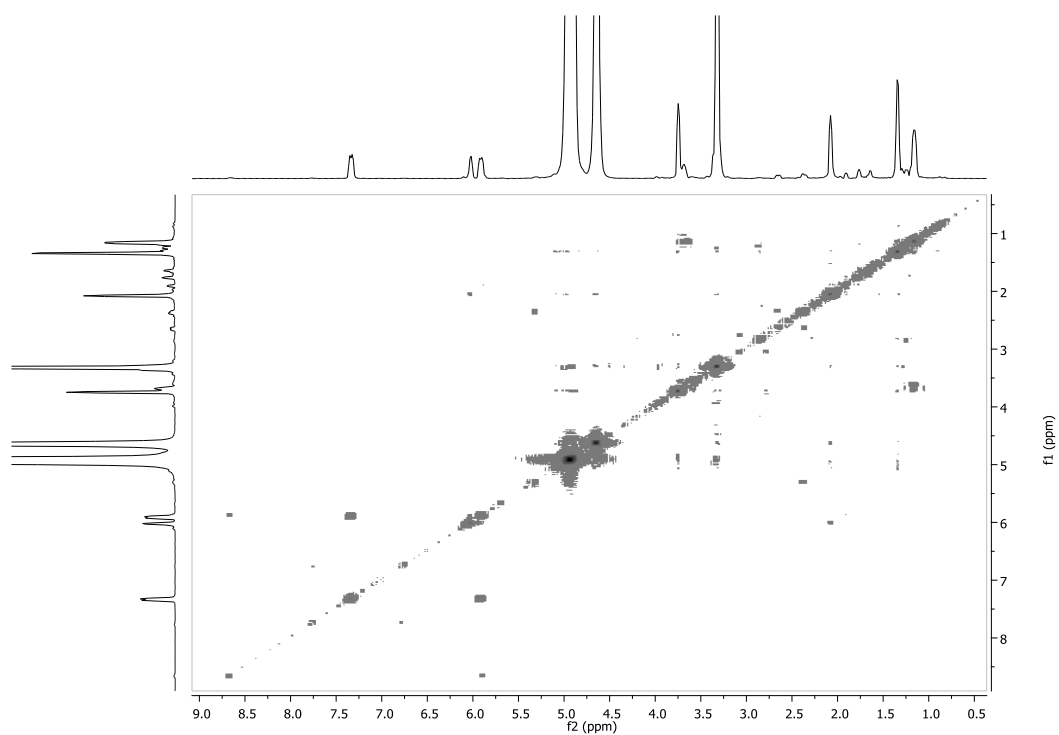


Figure S7. COSY (600 MHz, CD_3OD) of compound **1**.

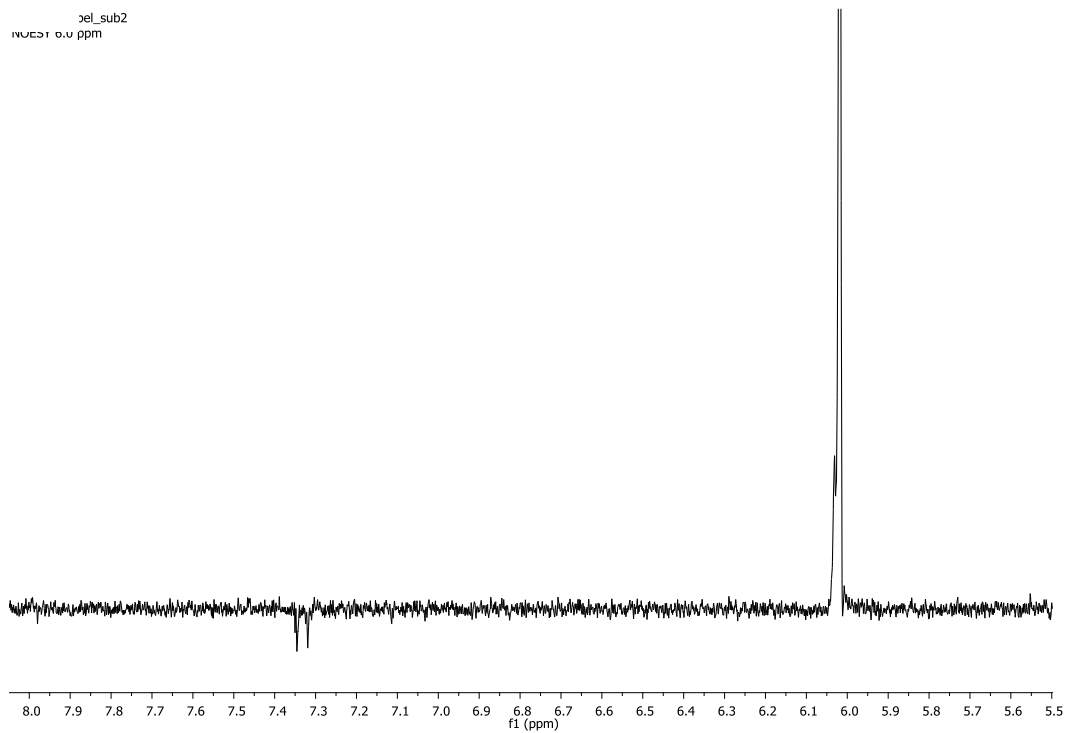


Figure S8. 1D NOESY irradiation (600 MHz, CD₃OD) at d 6.00 (H-5) of compound **1**.