

Supplementary Information

Compounds of *Anthostomella brabeji*, an Endophytic Fungus Isolated from *Paepalanthus planifolius* (Eriocaulaceae)

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(+)-(6*R**,7*S**,8*R**)-6,7,8-Trihydroxy-2,2-dimethyl-5,6,7,8-tetrahydro-chroman-4-one (1)

Amorphous white powder; $[\alpha]_D^{20} = +50$, $c = 0.08$ (CH₃OH); UV (CH₃OH) λ_{\max} / nm 280; ¹H NMR (600 MHz, CD₃OD) δ 1.42 (s, 3H, CH₃), 1.44 (s, 3H, CH₃), 2.02 (ddd, 1H, J 16.0, 9.5, 1.8 Hz, CH₂), 2.52 (d, 1H, J 16.6 Hz, CH₂), 2.56 (d, 1H, J 16.0 Hz, CH₂), 2.72 (dd, 1H, J 16.0, 5.5 Hz, CH₂), 3.51 (dd, 1H, J 9.3, 7.3 Hz, CH), 3.60 (ddd, 1H, J 9.5, 9.3, 5.5 Hz, CH), 4.05 (dd, 1H, J 7.3, 1.8 Hz, CH); ¹³C NMR (150 MHz, CD₃OD) δ 25.9, 26.6, 28.1, 47.8, 69.6, 73.7, 77.8, 82.0, 107.9, 167.6, 194.8; HRMS (ESI-Qq-TOF-HRMS) C₁₁H₁₆O₅ [M + H]⁺ calcd.: 229.1070; found: 229.1070; HR-ESI-MS/MS: 229.1070 (14), 173.0444 (33), 155.0338, (65), 137.0232 (34), 109.0232 (46), 83.0493 (100).

6-Hydroxy-2,2-dimethyl-5,6,7,8-tetrahydro-7,8-epoxychroman-4-one (2)

Amorphous white powder; UV (CH₃OH) λ_{\max} / nm 287; ¹H NMR (600 MHz, CD₃OD) δ 1.43 (s, 3H, CH₃), 1.48 (s, 3H, CH₃), 1.96 (dd, 1H, J 16.5, 4.5 Hz, CH₂), 2.50 (d, 1H, J 16.6 Hz, CH₂), 2.62 (d, 1H, J 16.6 Hz, CH₂), 2.69 (ddd, 1H, J 16.5, 2.0, 1.9 Hz, CH₂), 3.40 (d, 1H, J 3.9 Hz, CH), 3.60 (m, 1H, CH), 4.43 (m, 1H, CH); ¹³C NMR (150 MHz, CD₃OD) δ 25.3, 24.6, 27.1, 47.8, 50.3, 57.7, 63.9, 82.7,

106.4, 165.9, 193.8; MS (ESI-QTRAP-MS) C₁₁H₁₄O₄ [M + H]⁺ calcd.: 211.1; found: 211.2.

Siccayne (3)

Amorphous yellow powder, UV (CH₃OH) λ_{\max} / nm 269, 322; ¹H NMR (600 MHz, CD₃OD) δ 1.97 (dd, 3H, J 1.6, 1.1 Hz, CH₃), 5.28 (dq, 1H, J 2.1, 1.6 Hz, CH₂), 5.35 (dq, 1H, J 2.1, 1.1 Hz, CH₂), 6.63 (dd, 1H, J 2.8, 8.7 Hz, Ar-H), 6.67 (d, 1H, J 8.7 Hz, Ar-H), 6.70 (d, 1H, J 2.8 Hz, Ar-H); ¹³C NMR (150 MHz, CD₃OD) δ 23.7, 85.8, 94.9, 112.1, 117.2, 118.1, 119.4, 121.7, 128.6, 151.0, 152.2; MS (ESI-QTRAP-MS) C₁₁H₁₀O₂ [M - H]⁻ calcd.: 173.1; found: 173.2.

Eutypinol (4)

Amorphous yellow powder, UV (CH₃OH) λ_{\max} / nm 269, 306; ¹H NMR (600 MHz, CD₃OD) δ 1.98 (dd, 3H, J 1.6, 1.1 Hz, CH₃), 4.47 (s, 2H, CH₂), 5.28 (dq, 1H, J 2.1, 1.6 Hz, CH₂), 5.36 (dq, 1H, J 2.1, 1.1 Hz, CH₂), 6.81 (d, 1H, J 8.4 Hz, Ar-H), 7.16 (dd, 1H, J 2.1, 8.4 Hz, Ar-H), 7.27 (d, 1H, J 2.1 Hz, Ar-H); ¹³C NMR (150 MHz, CD₃OD) δ 23.7, 64.6, 85.8, 95.1, 111.6, 116.2, 121.7, 128.7, 130.0, 133.0, 133.8, 158.5; MS (ESI-QTRAP-MS) C₁₂H₁₂O₂ [M - H]⁻ calcd.: 187.1; found: 186.9.

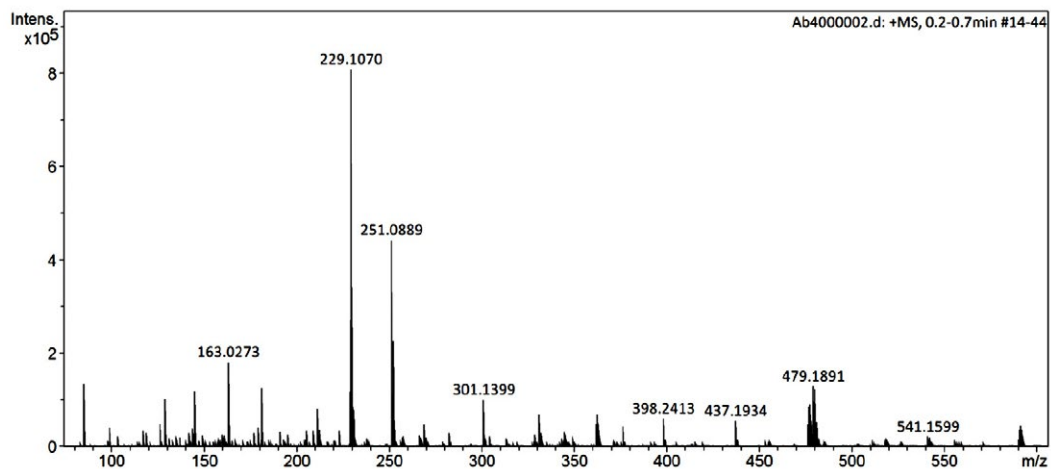


Figure S1. ESI-Qq-TOF-HRMS spectrum of compound **1**.

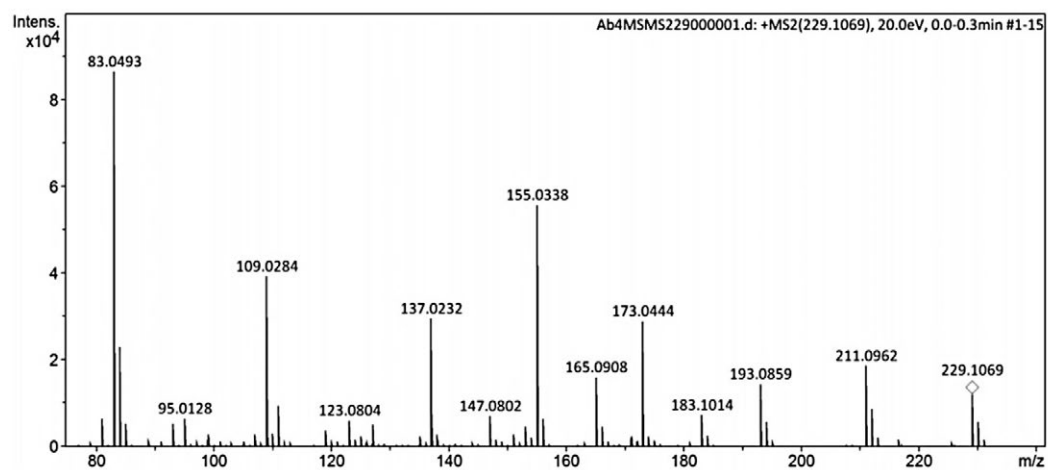


Figure S2. ESI-MS/MS spectrum of *m/z* 229.1069 of compound **1**.

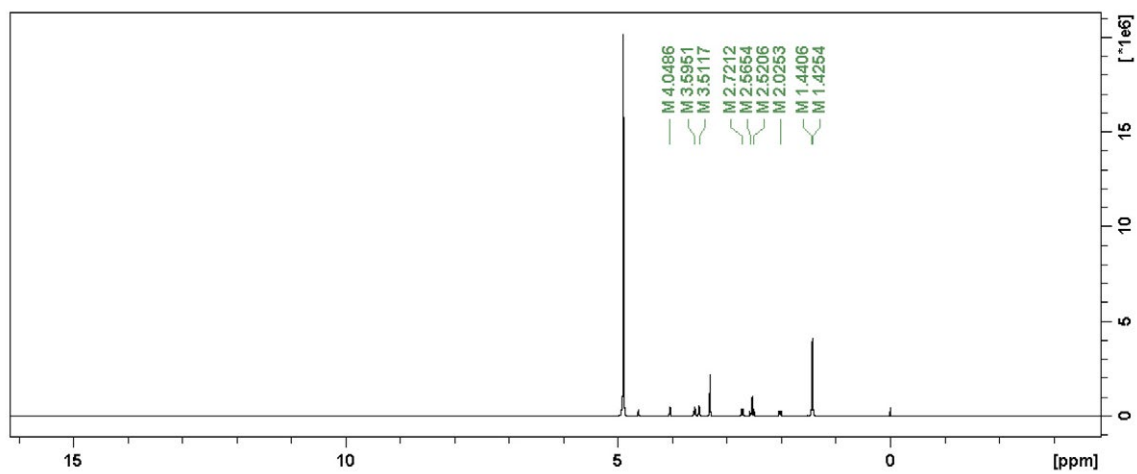


Figure S3. ¹H NMR spectrum (600 MHz, CD₃OD) of compound **1**.

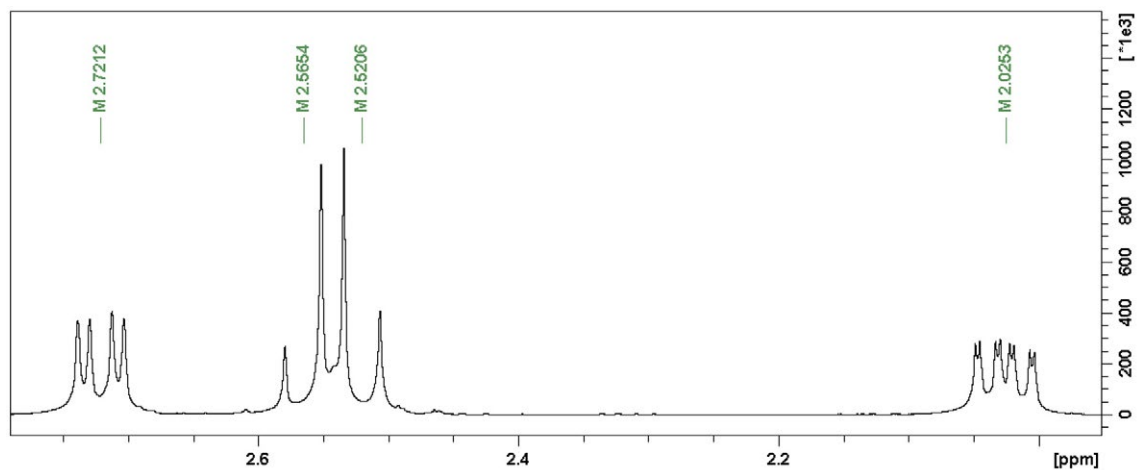


Figure S4. ^1H NMR spectrum (600 MHz, CD_3OD) expansion of compound 1.

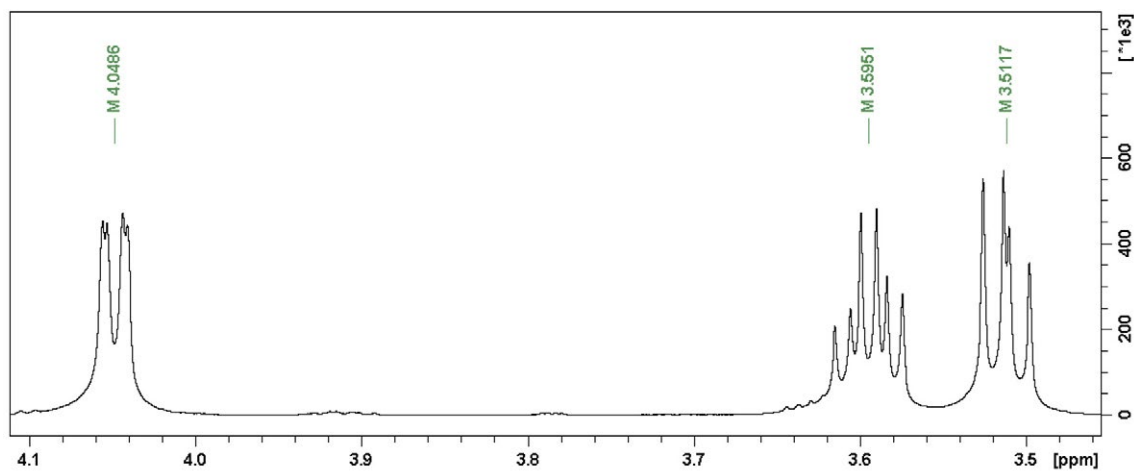


Figure S5. ^1H NMR spectrum (600 MHz, CD_3OD) expansion of compound 1.

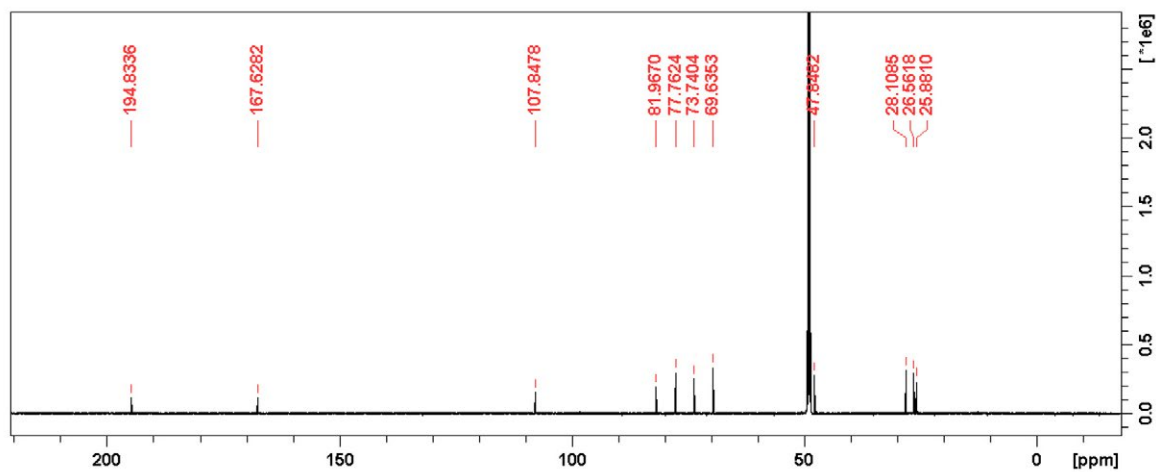


Figure S6. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 1.

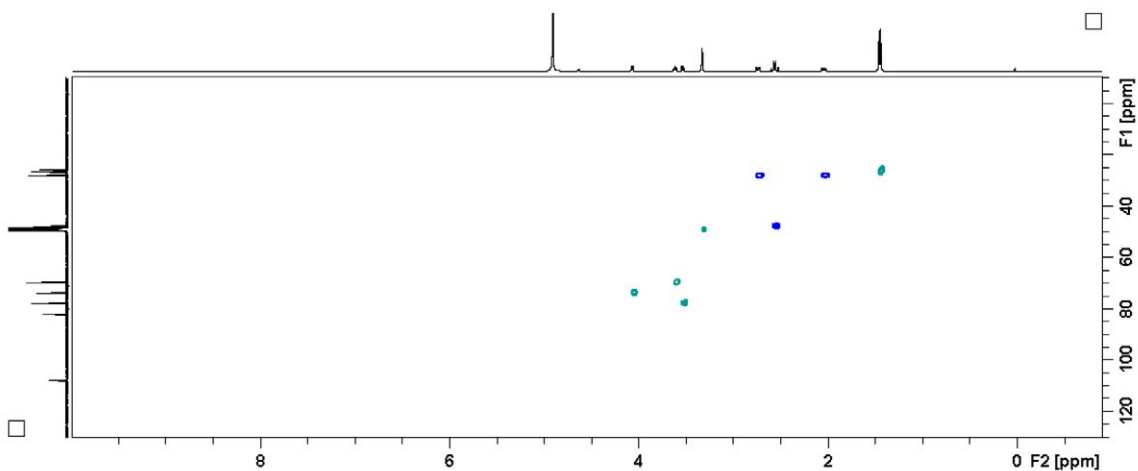


Figure S7. HSQC contour map (^1H : 600 MHz, ^{13}C : 150 MHz, CD_3OD) of compound 1.

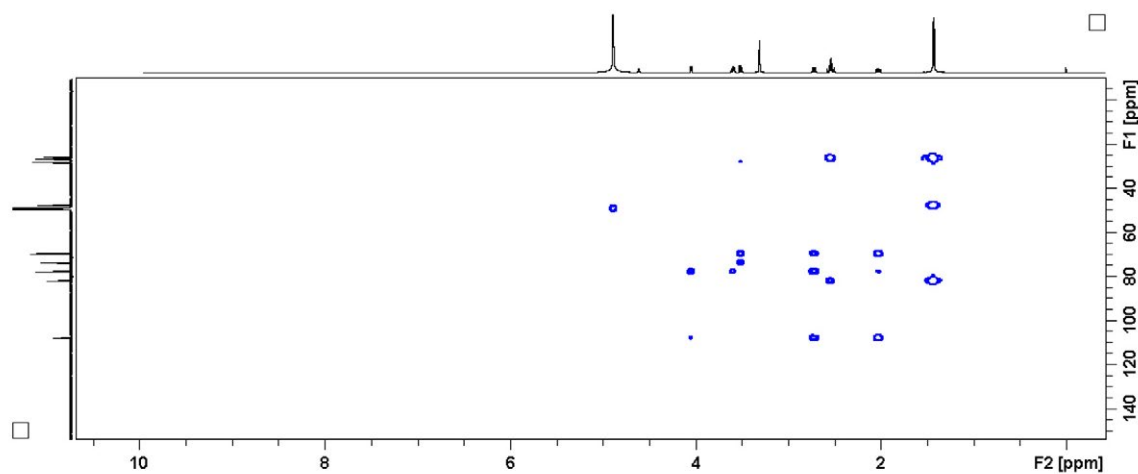


Figure S8. HMBC contour map (^1H : 600 MHz, ^{13}C : 150 MHz, CD_3OD) of compound 1.

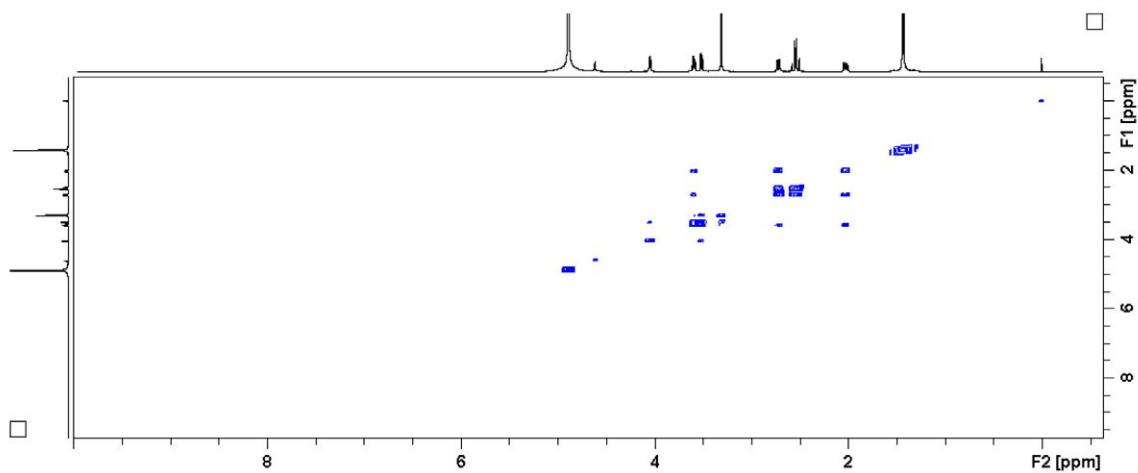


Figure S9. COSY (600 MHz, CD_3OD) of compound 1.

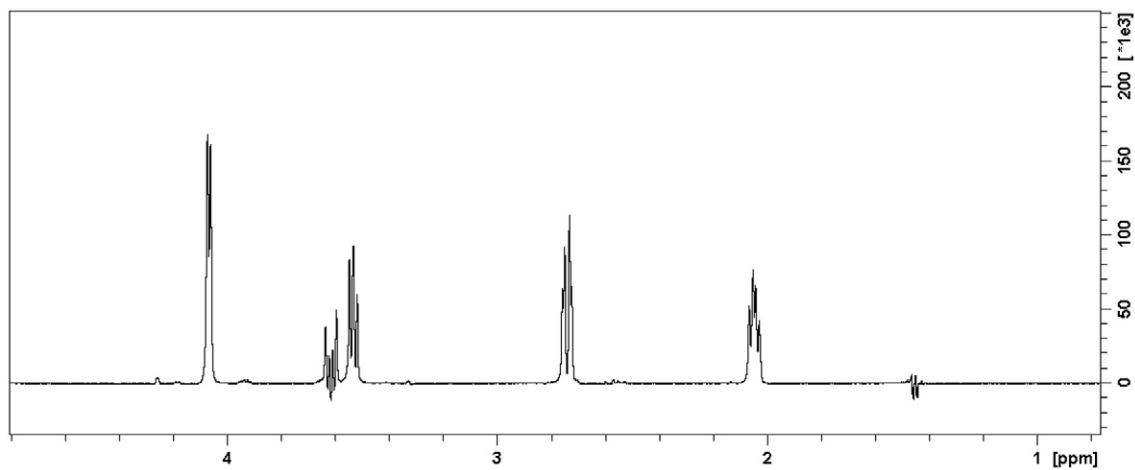


Figure S10. 1D TOCSY (600 MHz, CD_3OD) of compound **1**.

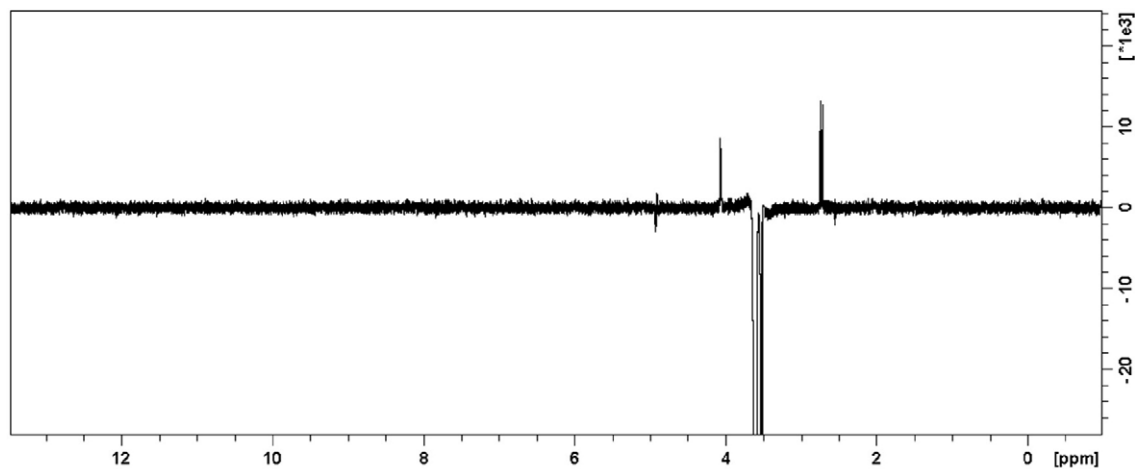


Figure S11. 1D NOESY irradiation (600 MHz, CD_3OD) at δ 3.60 (H-6) of compound **1**.

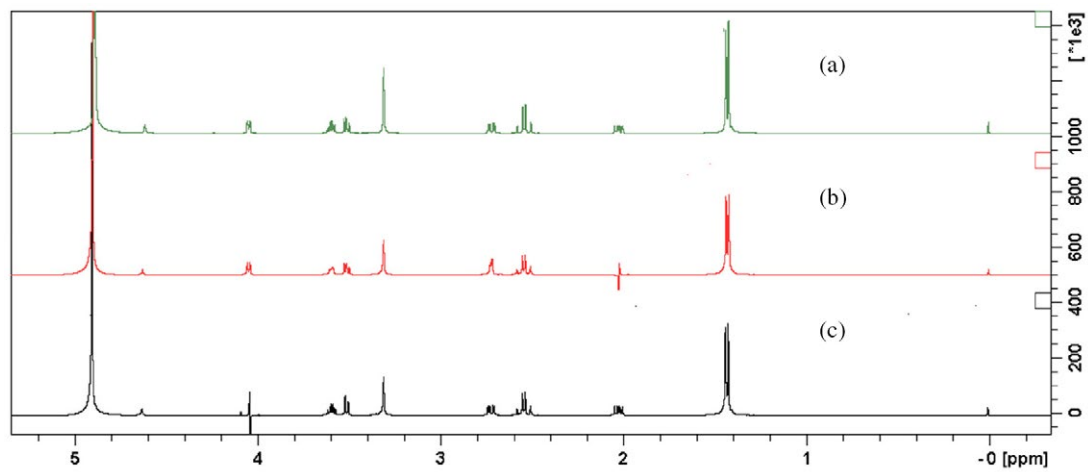


Figure S12. ^1H NMR spectrum (600 MHz, CD_3OD) (a), HOMODEC at δ 4.05 (b) and at δ 2.02 (c) of compound **1**.

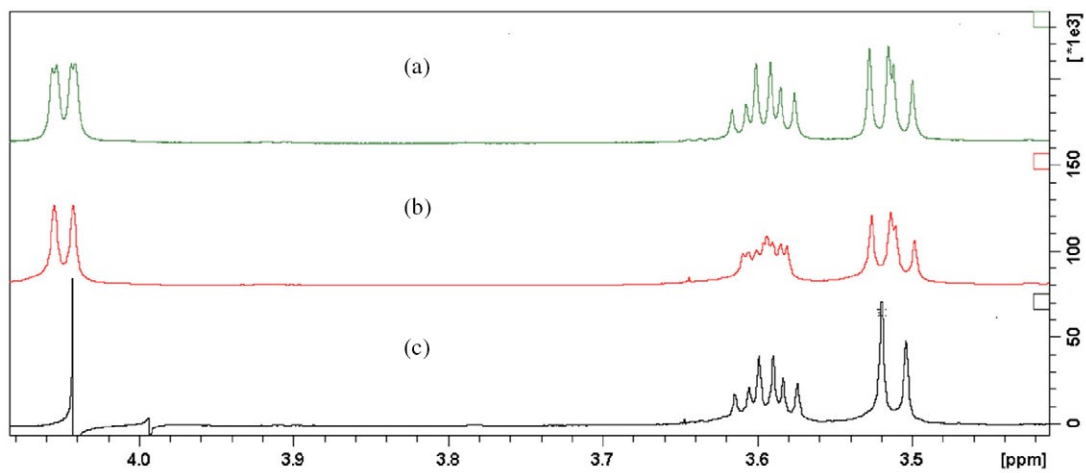


Figure S13. ¹H NMR spectrum (600 MHz, CD₃OD) expansion (a), HOMODEC at δ 4.05 (b) and at δ 2.02 (c) of compound 1.

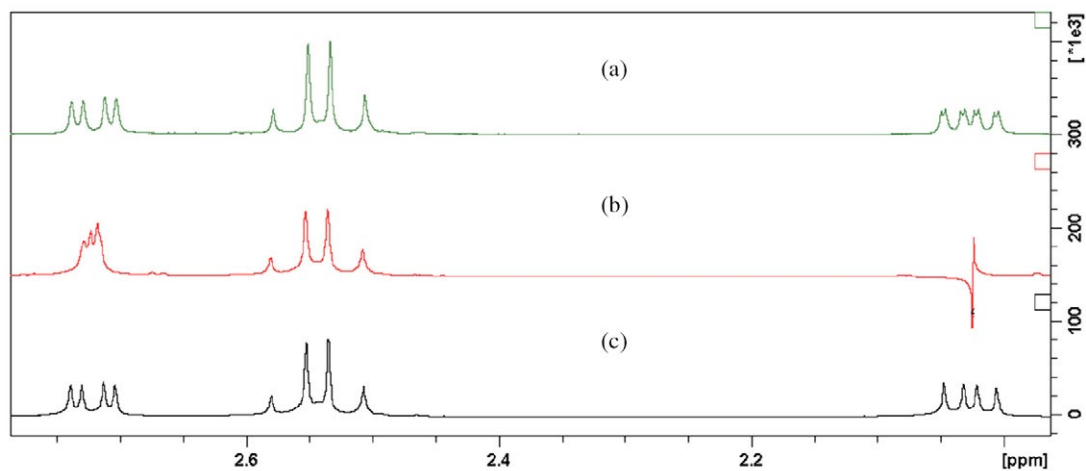


Figure S14. ¹H NMR spectrum (600 MHz, CD₃OD) expansion (a), HOMODEC at δ 4.05 (b) and at δ 2.02 (c) of compound 1.

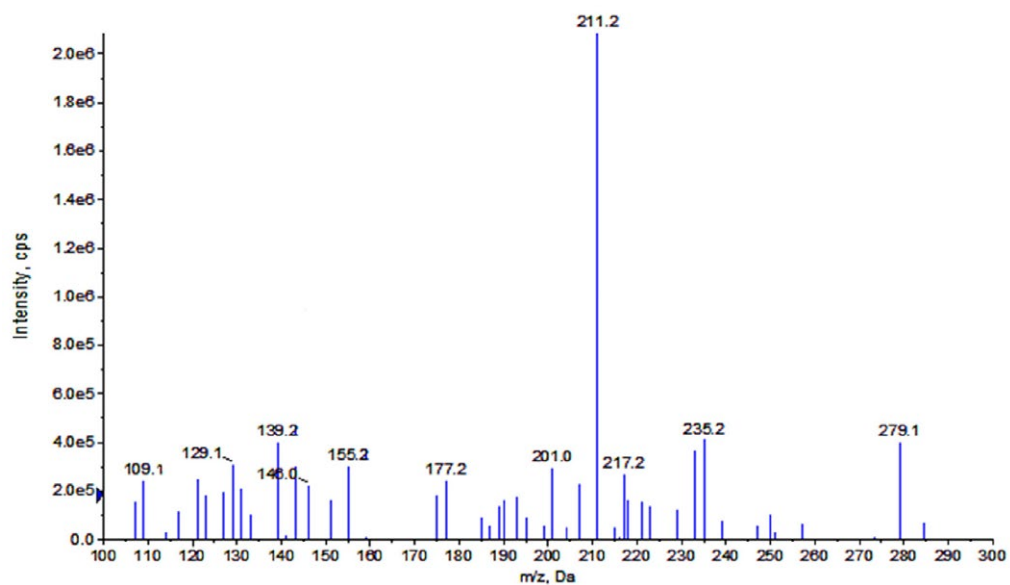


Figure S15. ESI-MS spectrum of compound 2.

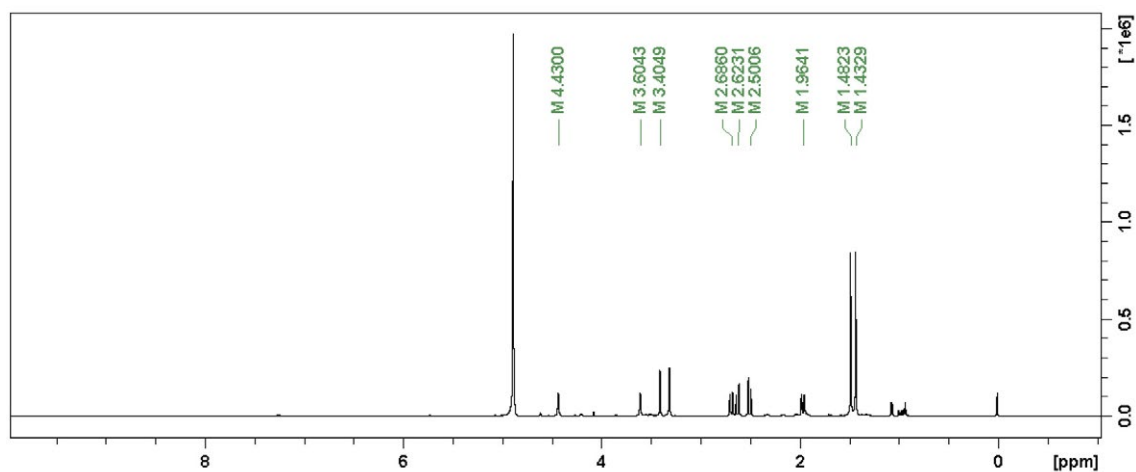


Figure S16. ^1H NMR spectrum (600 MHz, CD_3OD) of compound 2.

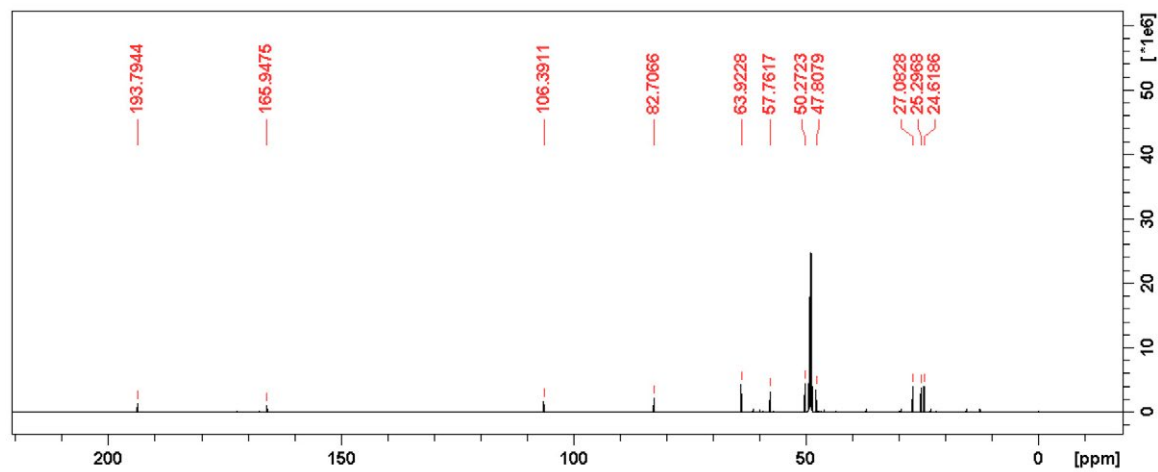


Figure S17. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 2.

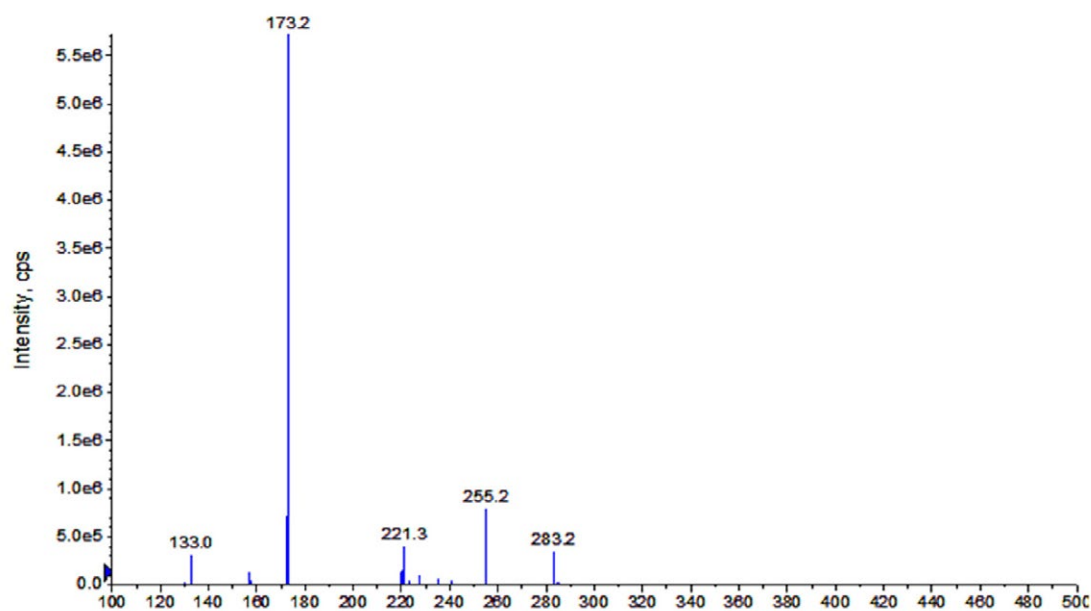


Figure S18. ESI-MS spectrum of compound 3.

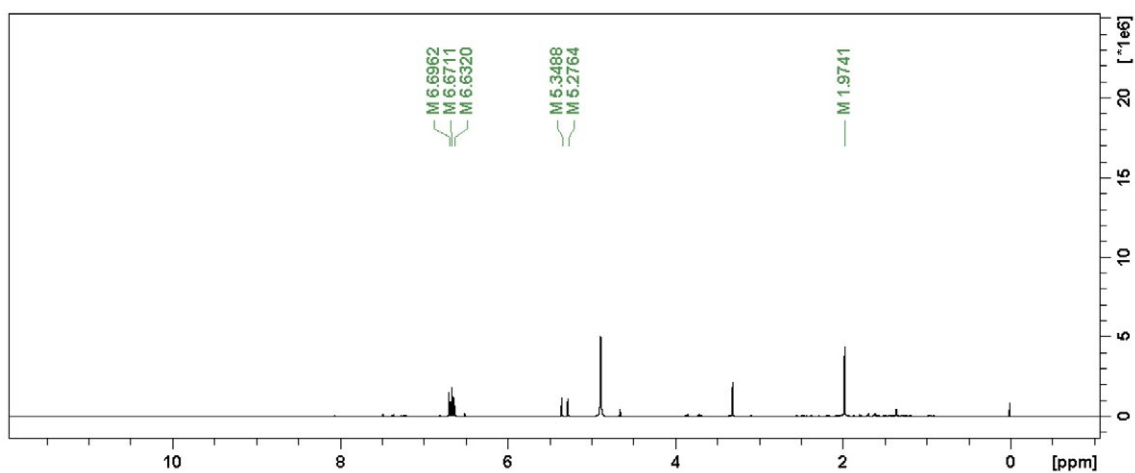


Figure S19. ^1H NMR spectrum (600 MHz, CD_3OD) of compound 3.

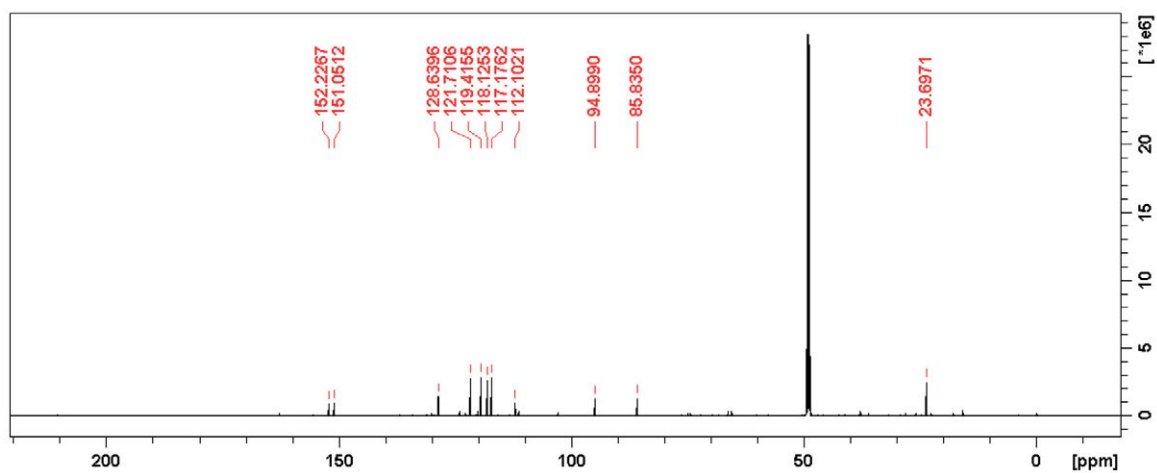


Figure S20. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 3.

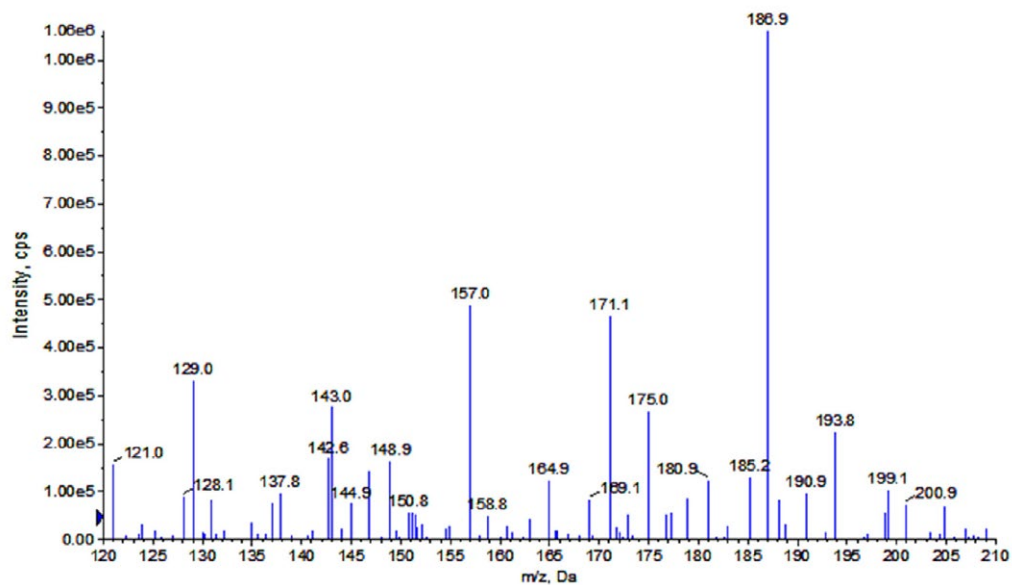


Figure S21. ESI-MS spectrum of compound 4.

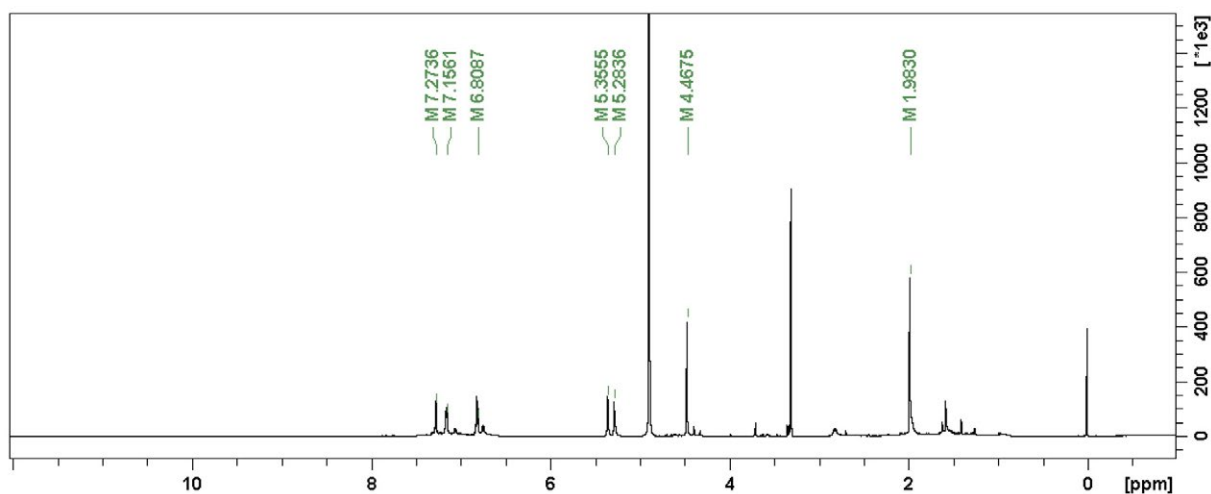


Figure S22. ^1H NMR spectrum (600 MHz, CD_3OD) of compound 4.

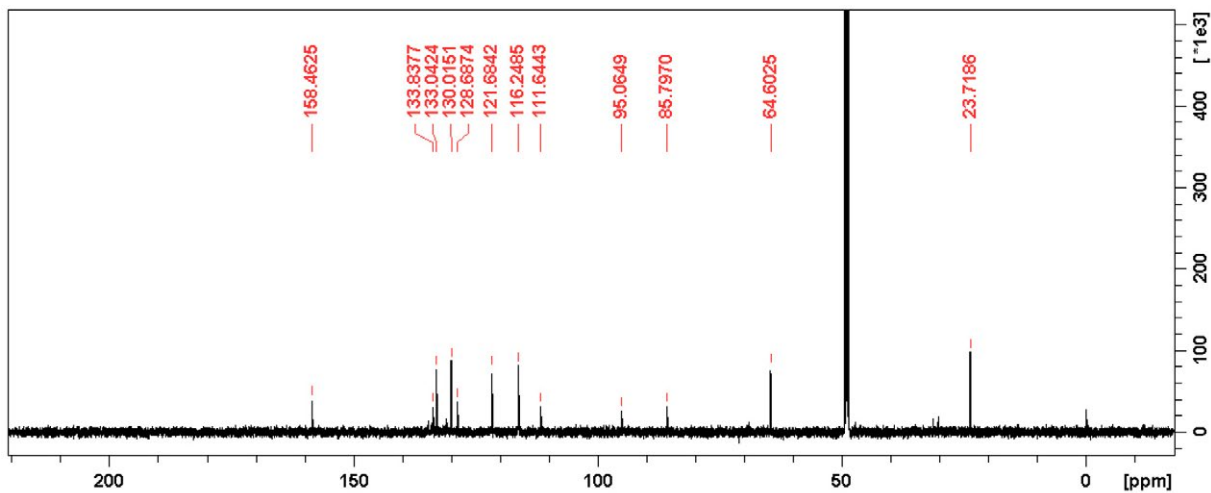


Figure S23. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 4.