Supplementary Information

Antimicrobial Activity of *Paepalanthus planifolius* and its Major Components against Selected Human Pathogens

Marcelo R. de Amorim,[a] Felipe Hilário,[b] Paulo T. Sano,[c] Tais M. Bauab[b] and Lourdes C. dos Santos*[a]

[a]Departamento de Química Orgânica, Instituto de Química and
[b]Departamento de Ciências Biológicas, Escola de Ciências Farmacêuticas, Universidade Estadual Paulista (UNESP), 14800-900 Araraquara-SP, Brazil

[c]Departamento de Botânica, Instituto de Biociências, Universidade de São Paulo (USP), 05508-090 São Paulo-SP, Brazil

Planifoliusin A (**9**)

Yellow amorphous solid; ($[\alpha]_D^{25}$ = +6.5, *c* = 0.1, $CHCl_3$); UV (CH_3OH) λ_{max} / nm 280, 380; ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.56 (d, 3H, *J* 6.0 Hz, CH_3), 2.32 (s, 3H, CH_3), 3.03 (m, 2H, CH_2), 3.86 (s, 3H, CH_3), 3.91 (s, 3H, CH_3), 3.93 (s, 3H, CH_3), 4.78 (m, 1H, CH), 6.57 (s, 1H, CH), 6.72 (s, 1H, CH), 6.97 (s, 1H, CH), 7.06 (s, 1H, CH), 9.74 (s, 1H, OH), 9.75 (s, 1H, OH), 13.44 (s, 1H, OH), 13.81 (s, 1H, OH); ^{13}C NMR (150 MHz, $CDCl_3$) δ 19.8, 20.9, 34.9, 56.1, 56.2, 62.0, 76.7, 92.3, 96.9, 98.3, 99.5, 99.5, 108.1, 108.5, 108.6, 108.9, 116.3, 122.3, 133.1, 135.6, 140.2, 140.6, 152.4, 155.5, 155.9, 158.9, 161.6, 162.1, 163.0, 168.4, 171.7; HRMS (LC-ESI-TOF-HRMS) *m/z*, observed: 575.1547; $C_{31}H_{26}O_{11}$ $[M + H]^+$ required: 575.1548; CD (CH_3CN) λ / nm (mdeg) 225 (+3.1), 263 (+6.4), 293 (–14.7), 402 (–3.4).

Vioxanthin (**7**)

Yellow amorphous solid; ($[\alpha]_D^{25}$ = +5.1, *c* = 0.1, $CHCl_3$); UV (CH_3OH) λ_{max} / nm 270, 372; ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.56 (d, 3H, *J* 6.0 Hz, CH_3), 3.00 (m, 2H, CH_2), 3.86 (s, 3H, CH_3), 4.77 (m, 1H, CH), 6.71 (s, 1H, CH), 6.96 (s, 1H, CH), 9.78 (s, 1H, OH), 13.78 (s, 1H, OH); ^{13}C NMR (150 MHz, $CDCl_3$) δ 20.9, 34.9, 56.1, 76.7, 98.2, 99.4, 108.2, 108.6, 116.2, 133.0, 140.2, 155.5, 161.6, 163.0, 171.8; HRMS (LC-ESI-TOF-HRMS) *m/z*, observed: 547.1597; $C_{30}H_{26}O_{10}$ $[M + H]^+$ required: 547.1599; CD (CH_3CN) λ / nm (mdeg) 221 (+2.3), 250 (–10.0), 273 (+9.2), 381 (+1.6).

*e-mail: loursant@gmail.com

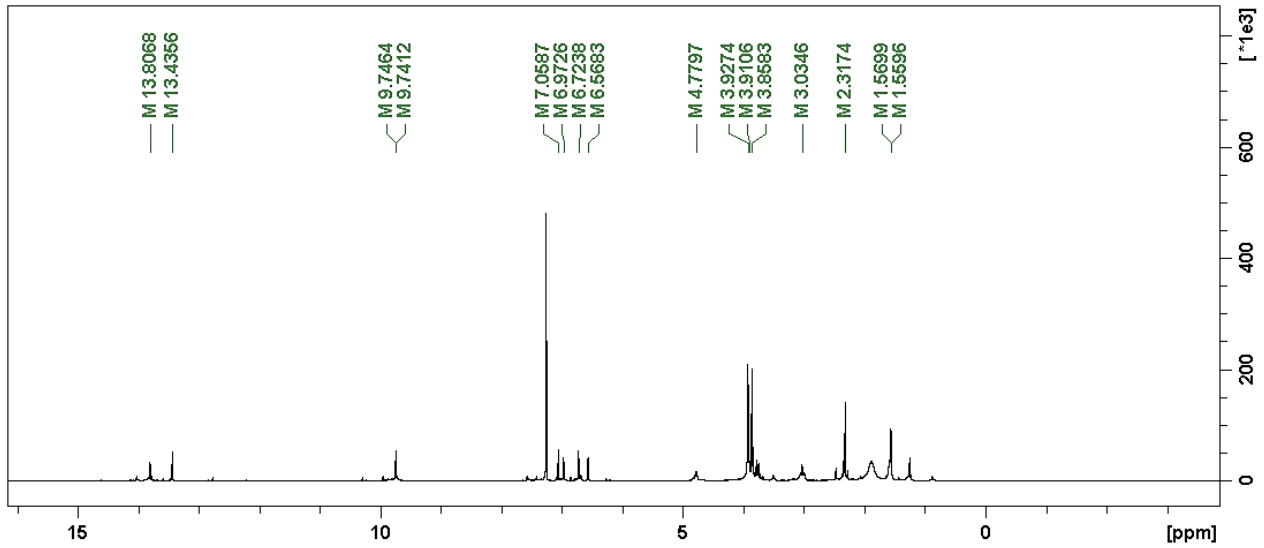

Figure S1. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **9**.

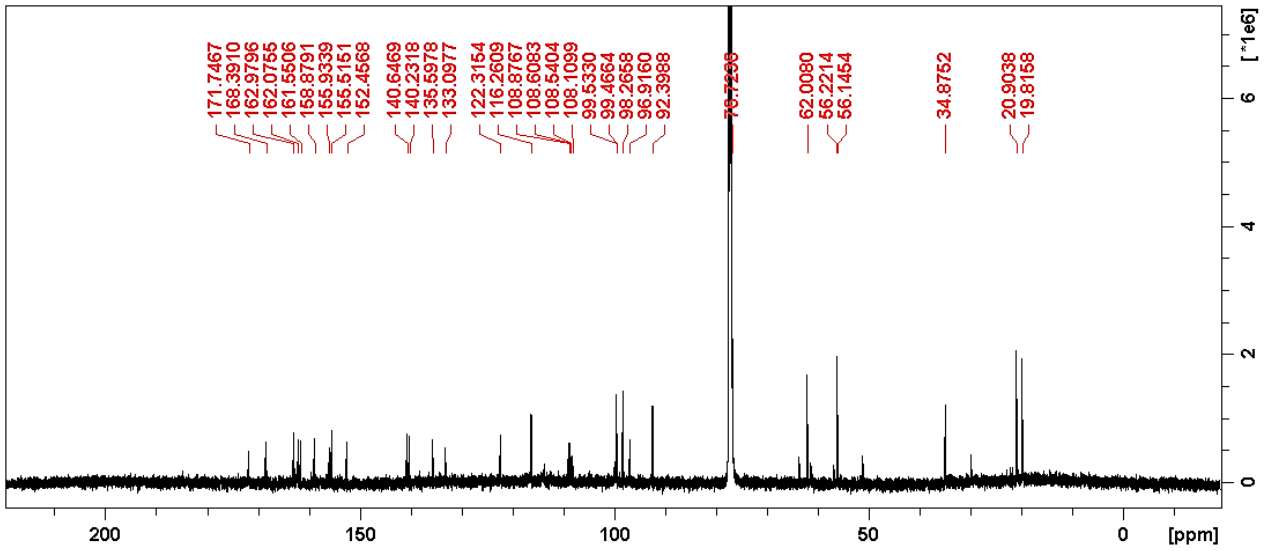

Figure S2. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **9**.

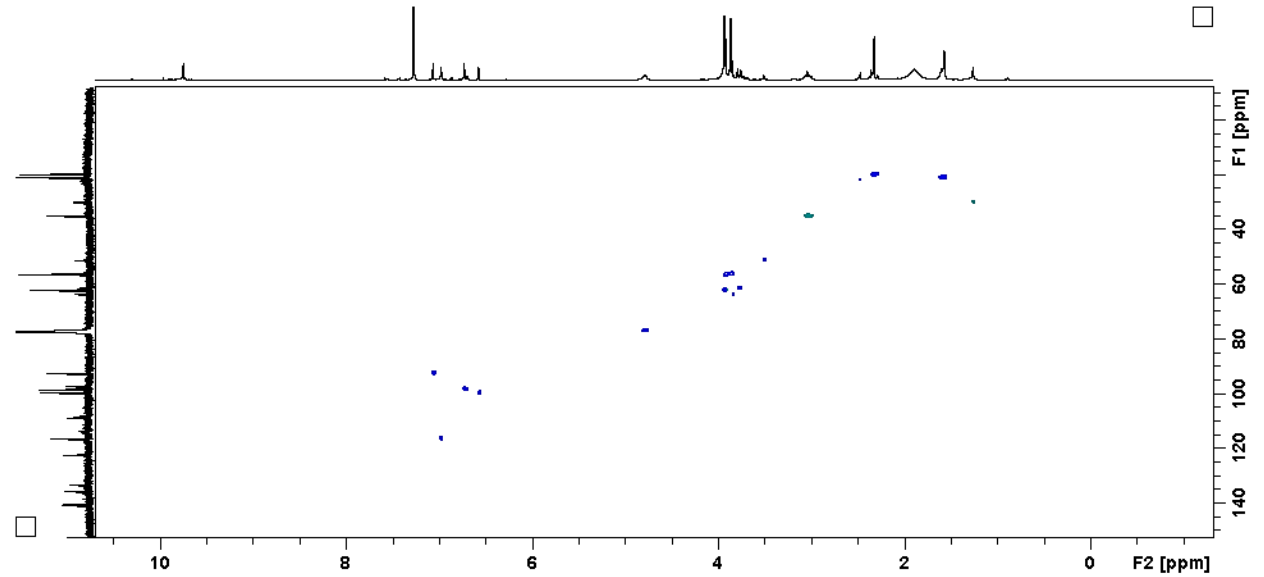

Figure S3. Contour map HSQC (^{1}H: 600 MHz, ^{13}C: 150 MHz, $CDCl_3$) of compound **9**.

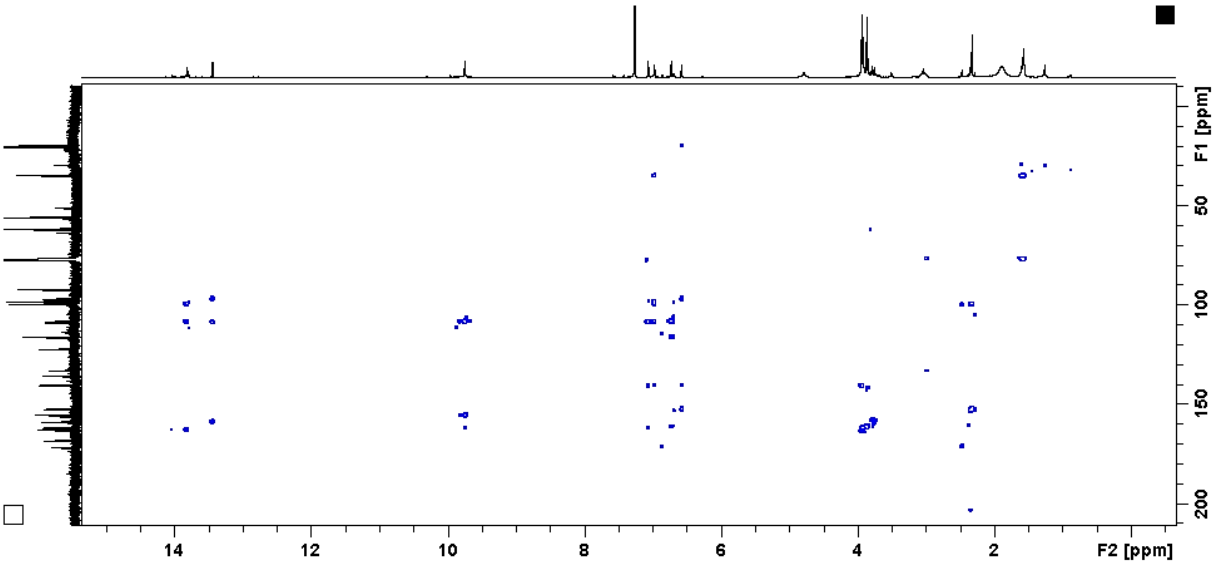

Figure S4. Contour map HMBC (^{1}H: 600 MHz, ^{13}C: 150 MHz, $CDCl_3$) of compound **9**.

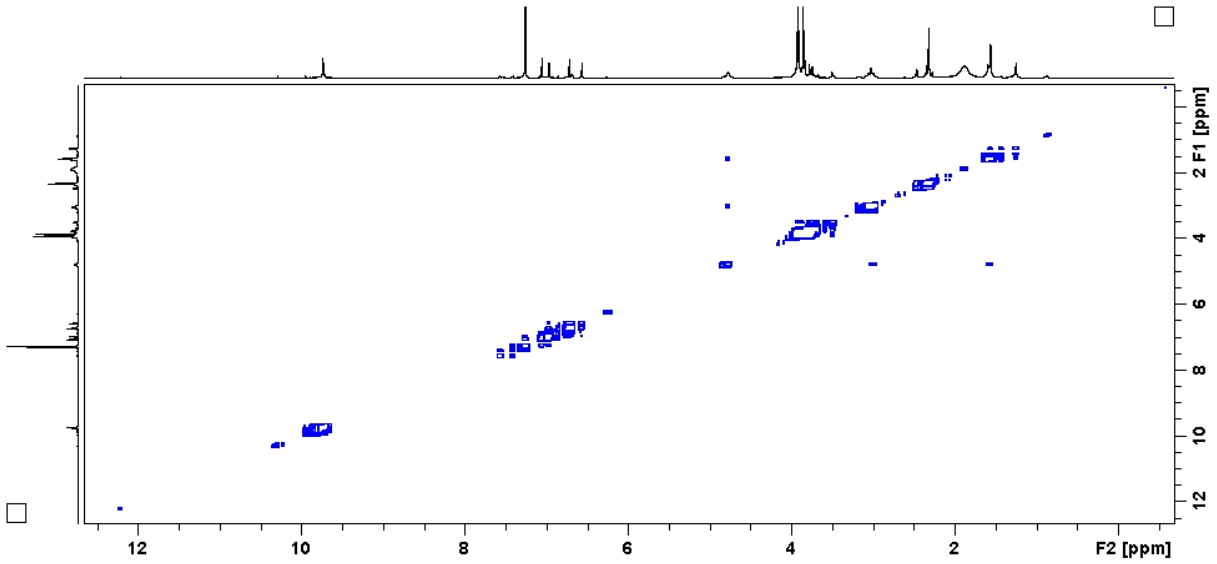

Figure S5. COSY (600 MHz, $CDCl_3$) of compound **9**.

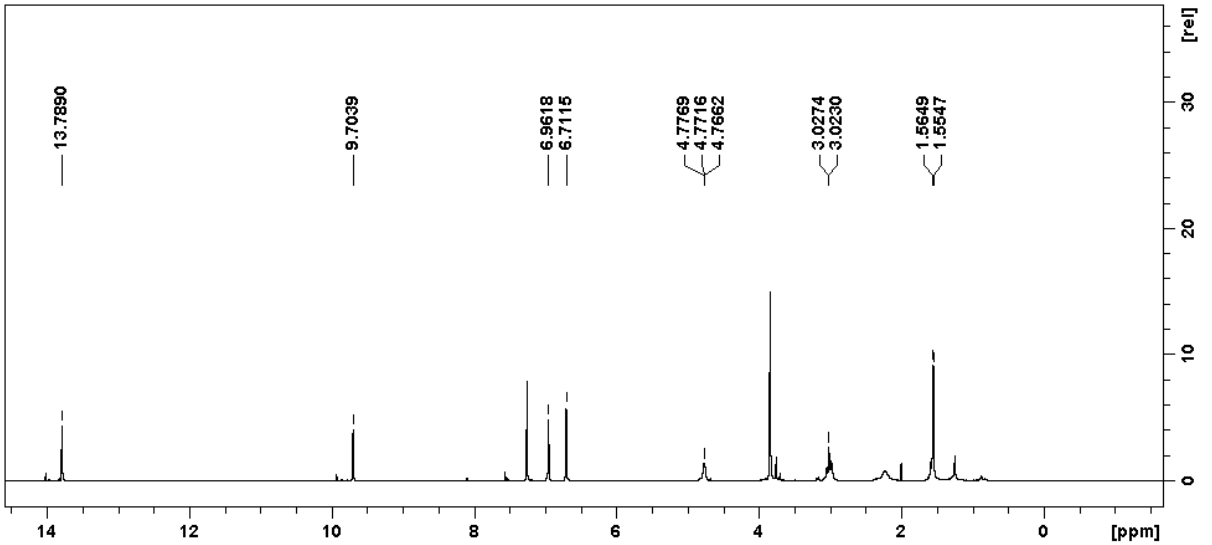

Figure S6. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **7**.

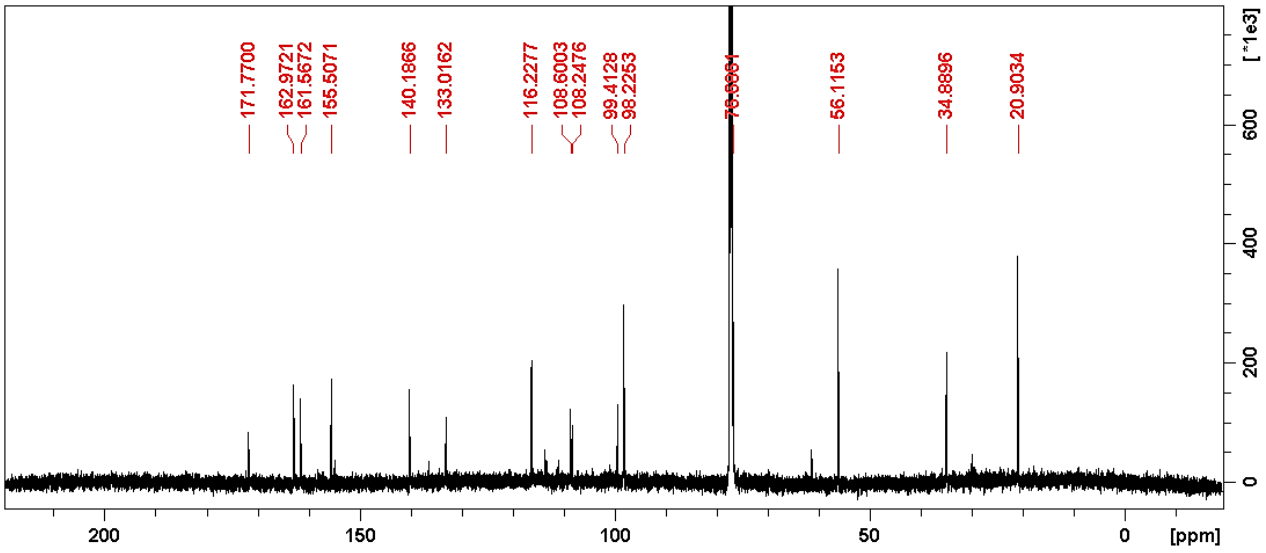

Figure S7. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **7**.

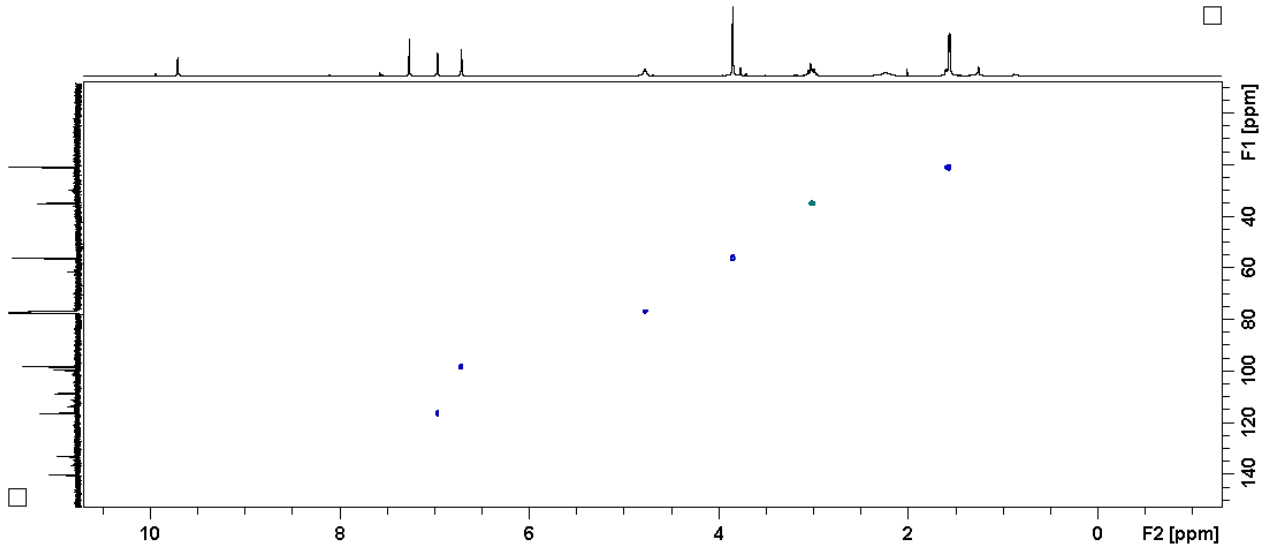

Figure S8. Contour map HSQC (^1H: 600 MHz, ^{13}C: 150 MHz, $CDCl_3$) of compound **7**.

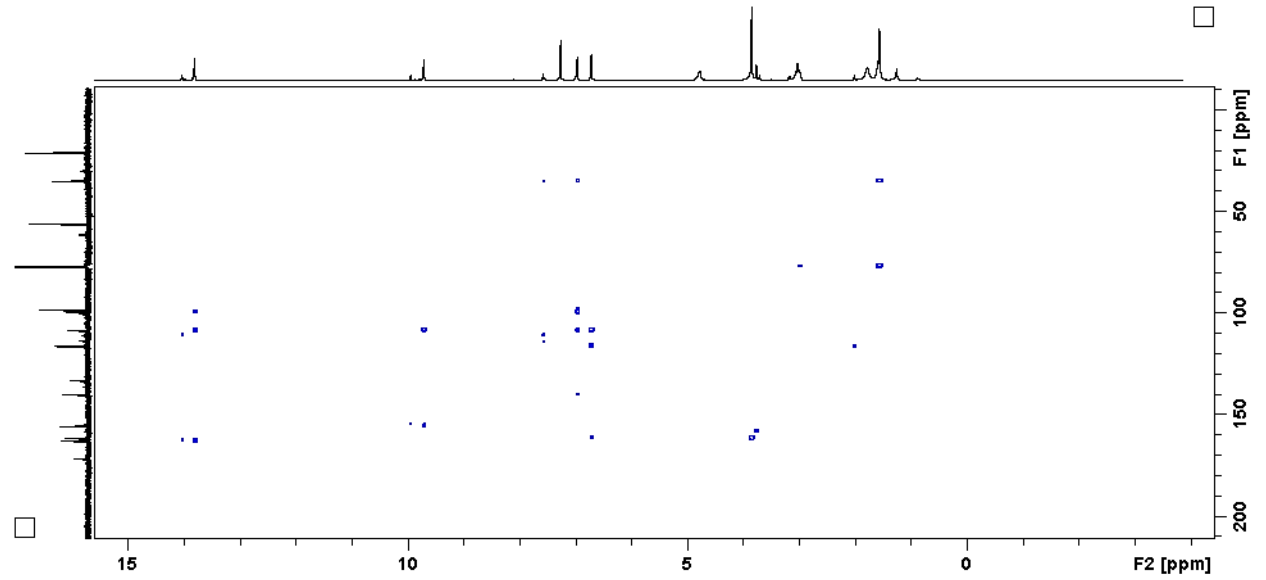

Figure S9. Contour map HMBC (^1H: 600 MHz, ^{13}C: 150 MHz, $CDCl_3$) of compound **7**.

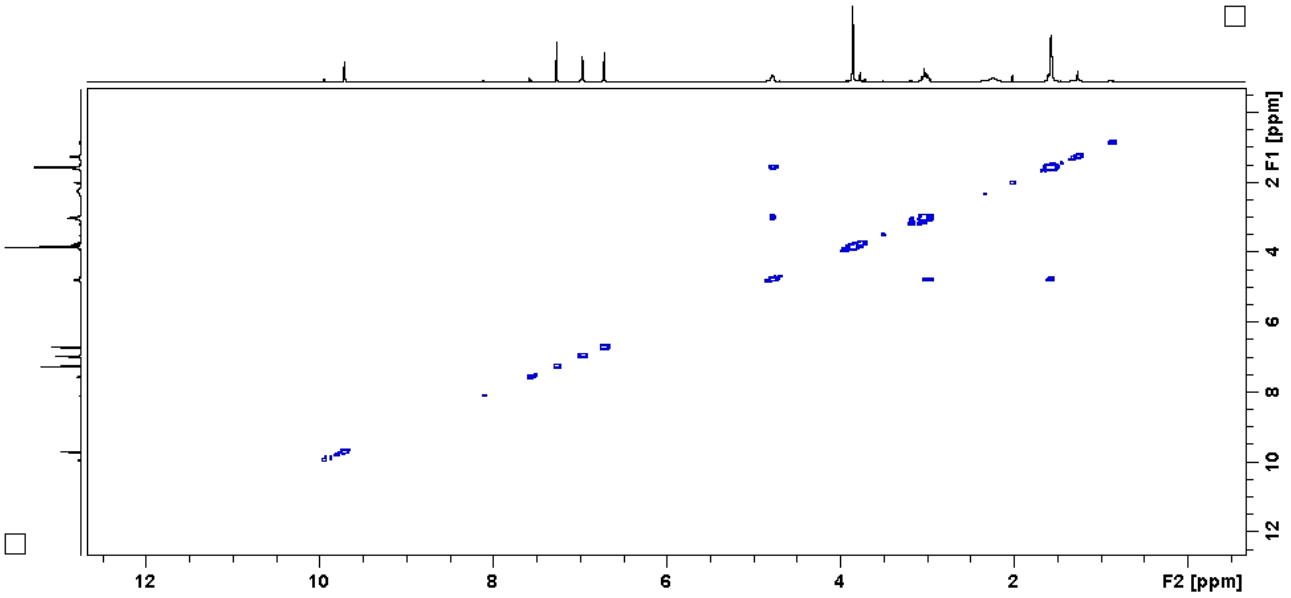

Figure S10. COSY (600 MHz, $CDCl_3$) of compound **7**.

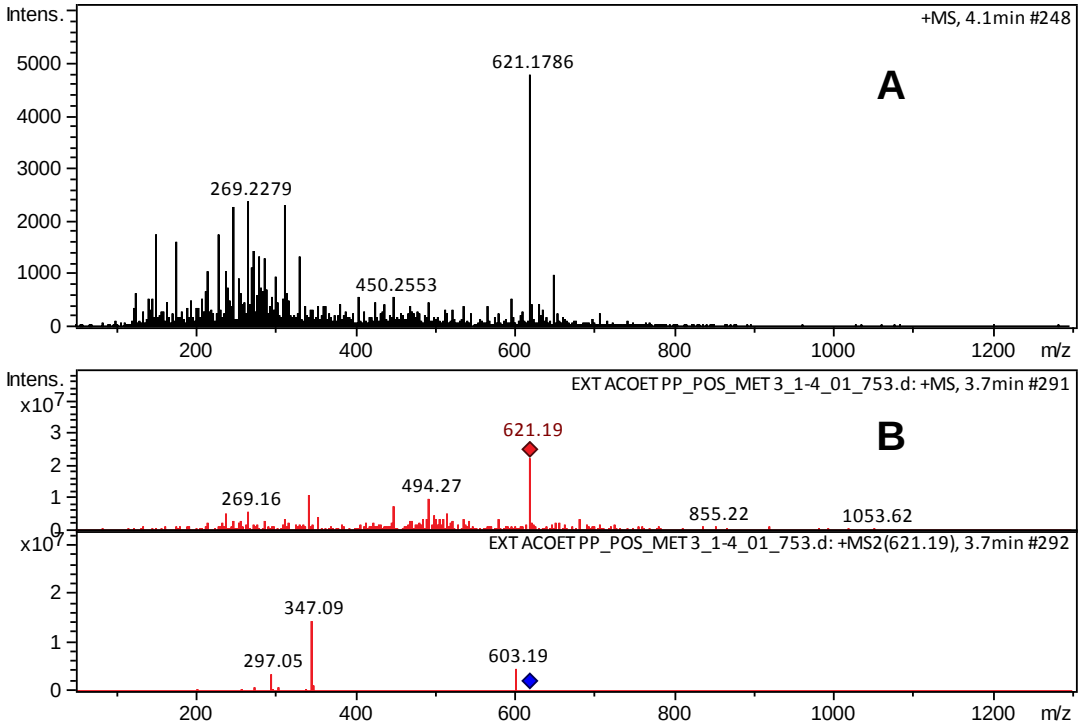

Figure S11. (A) LC-ESI-TOF-HRMS spectrum of compound **1**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 621 of compound **1**.

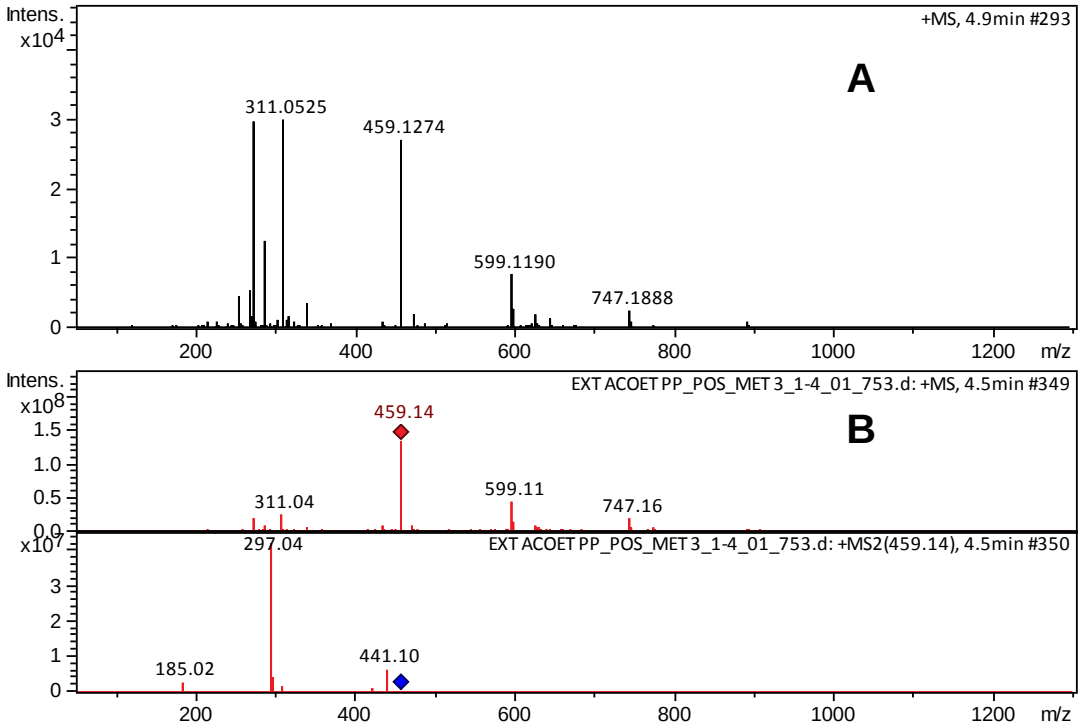

Figure S12. (A) LC-ESI-TOF-HRMS spectrum of compound **2**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 459 of compound **2**.

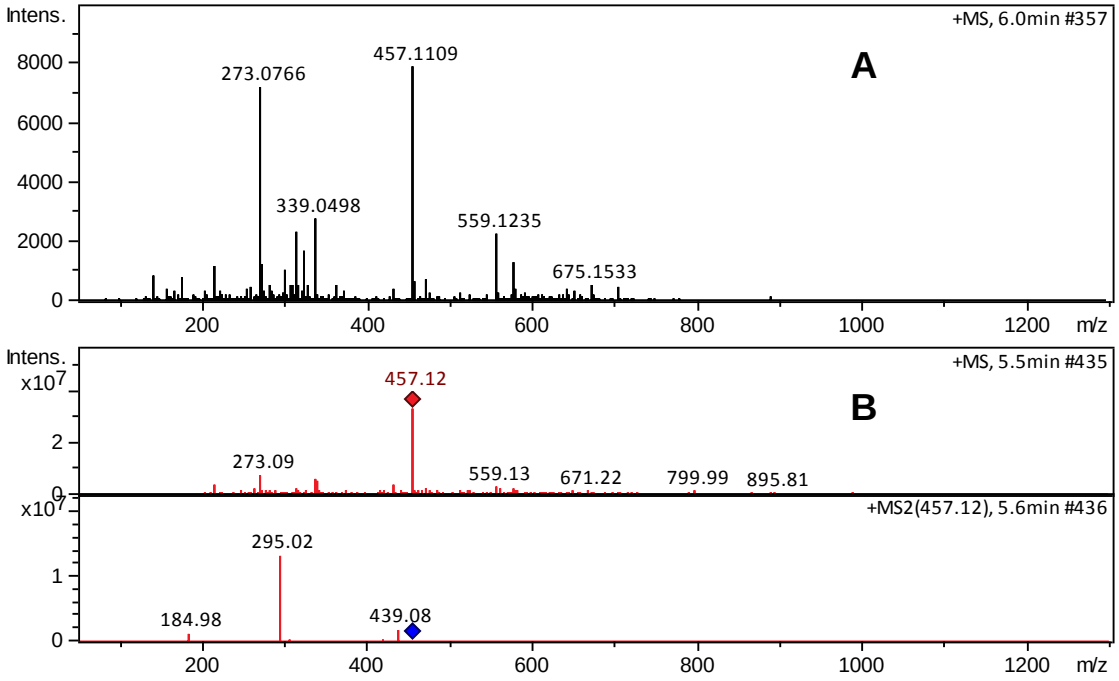

Figure S13. (A) LC-ESI-TOF-HRMS spectrum of compound **3**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 457 of compound **3**.

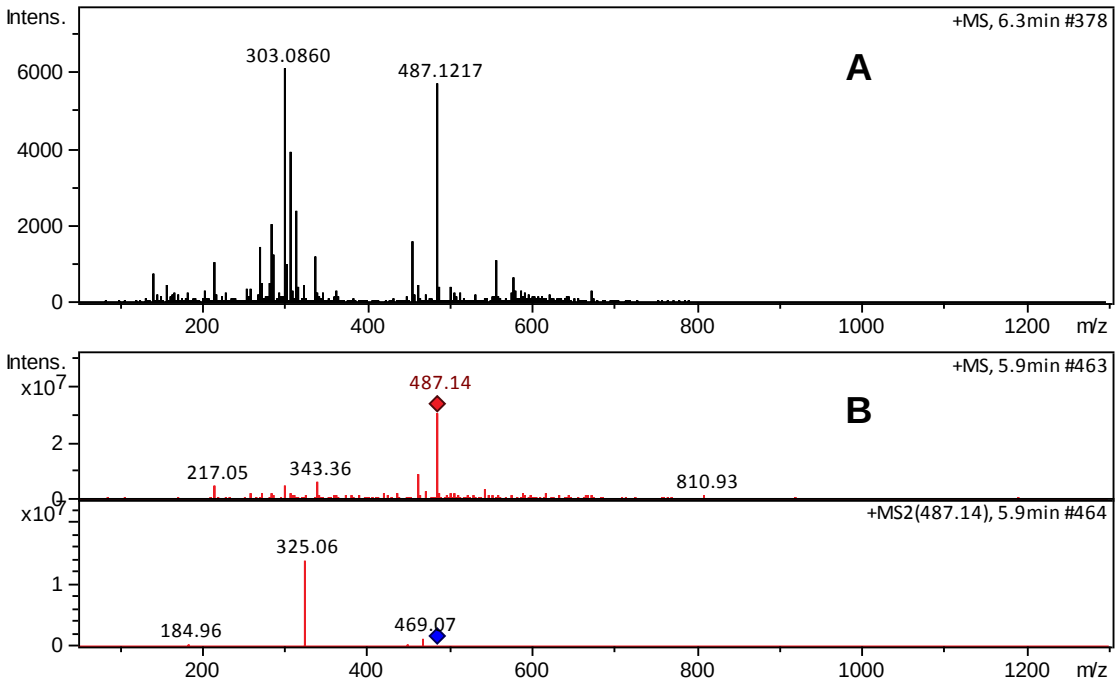

Figure S14. (A) LC-ESI-TOF-HRMS spectrum of compound **4**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 487 of compound **4**.

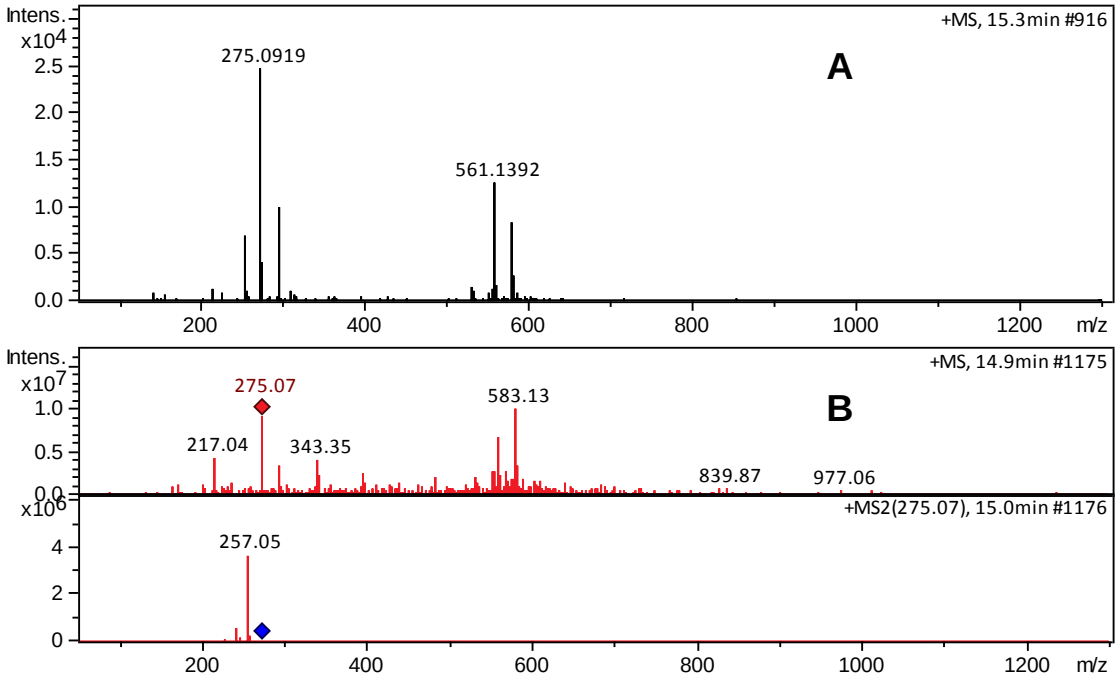

Figure S15. (A) LC-ESI-TOF-HRMS spectrum of compound **5**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 275 of compound **5**.

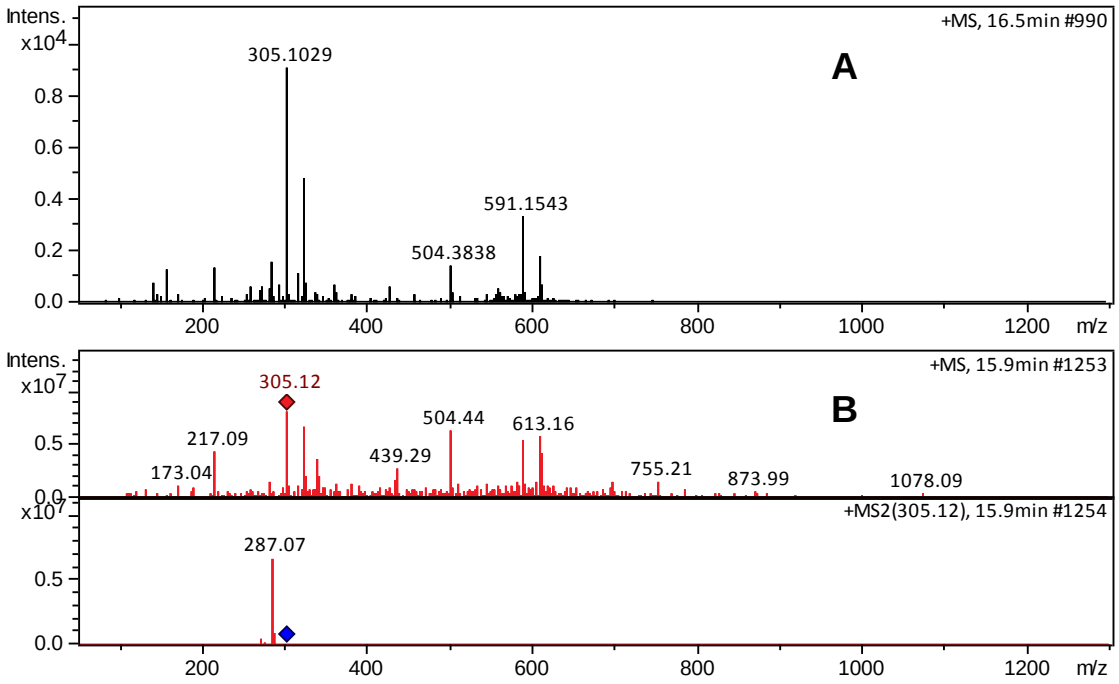

Figure S16. (A) LC-ESI-TOF-HRMS spectrum of compound **6**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 305 of compound **6**.

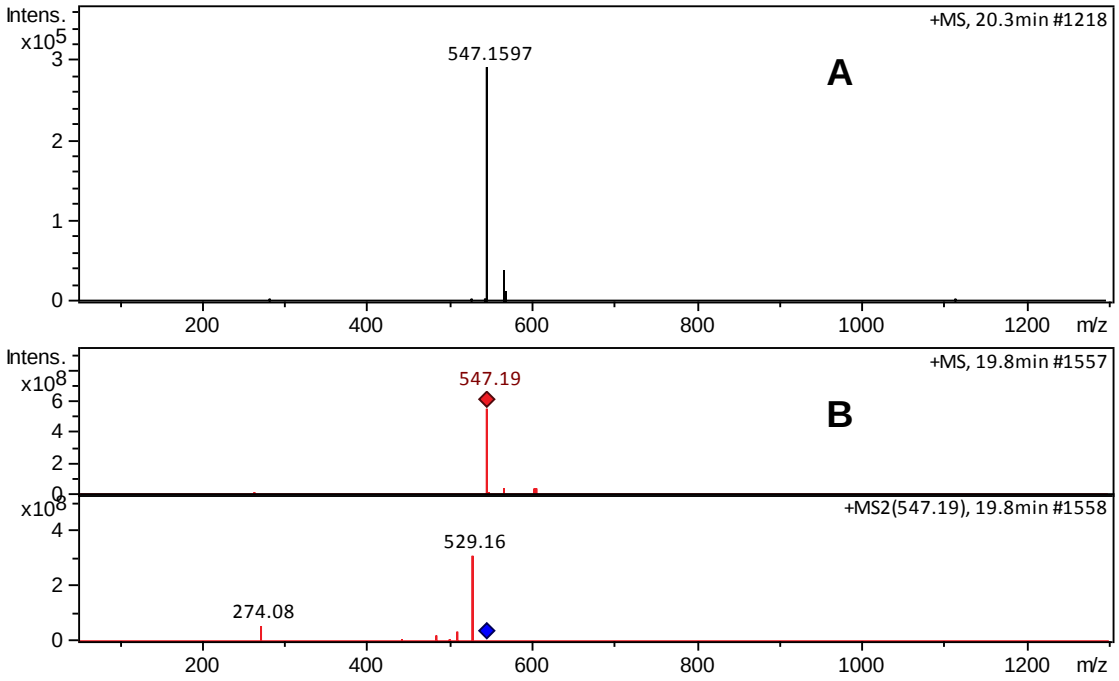

Figure S17. (A) LC-ESI-TOF-HRMS spectrum of compound **7**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 305 of compound **7**.

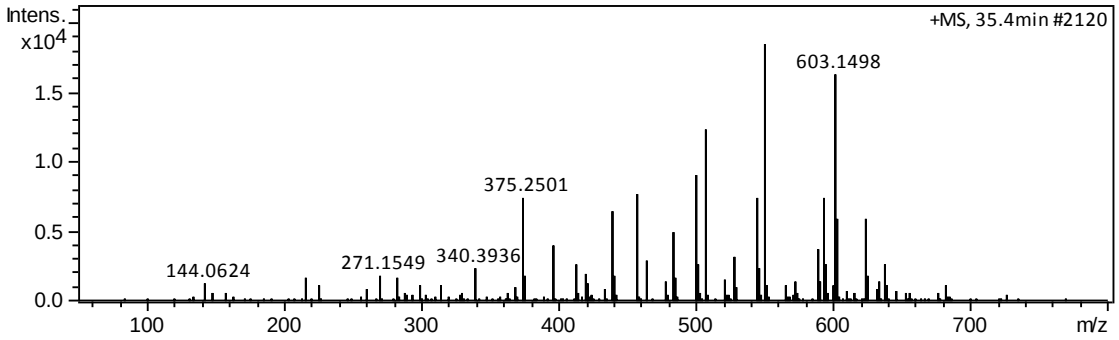

Figure S18. LC-ESI-TOF-HRMS spectrum of compound **8**.

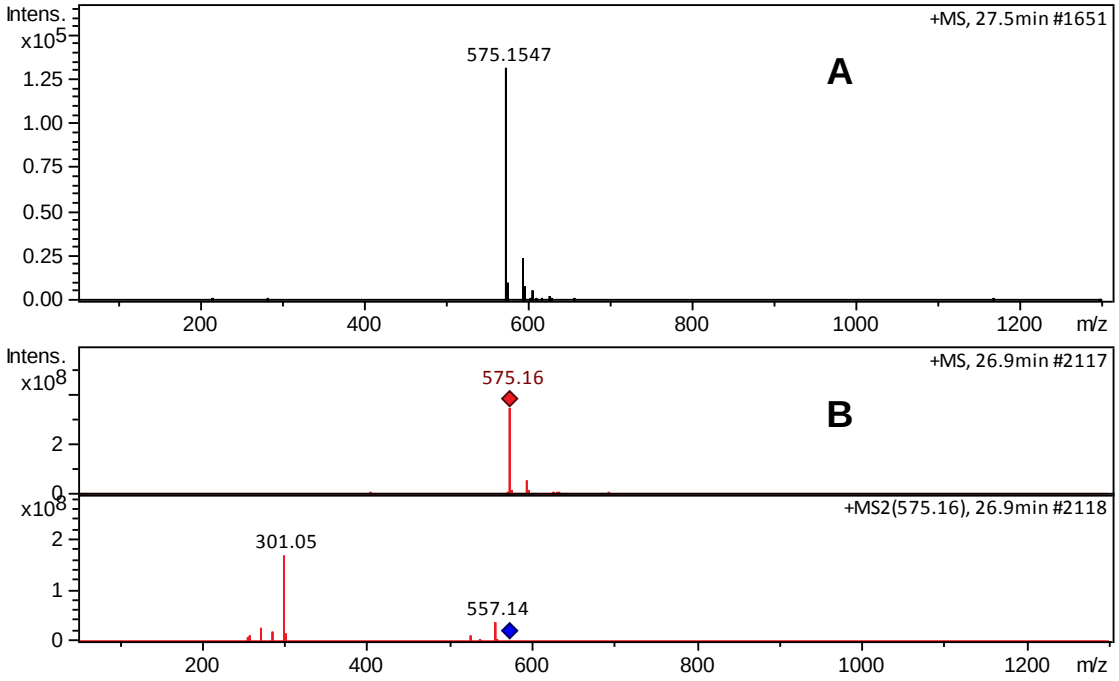

Figure S19. (A) LC-ESI-TOF-HRMS spectrum of compound **9**; (B) LC-ESI-IT-MS/MS spectrum of *m*/*z* 575 of compound **9.**

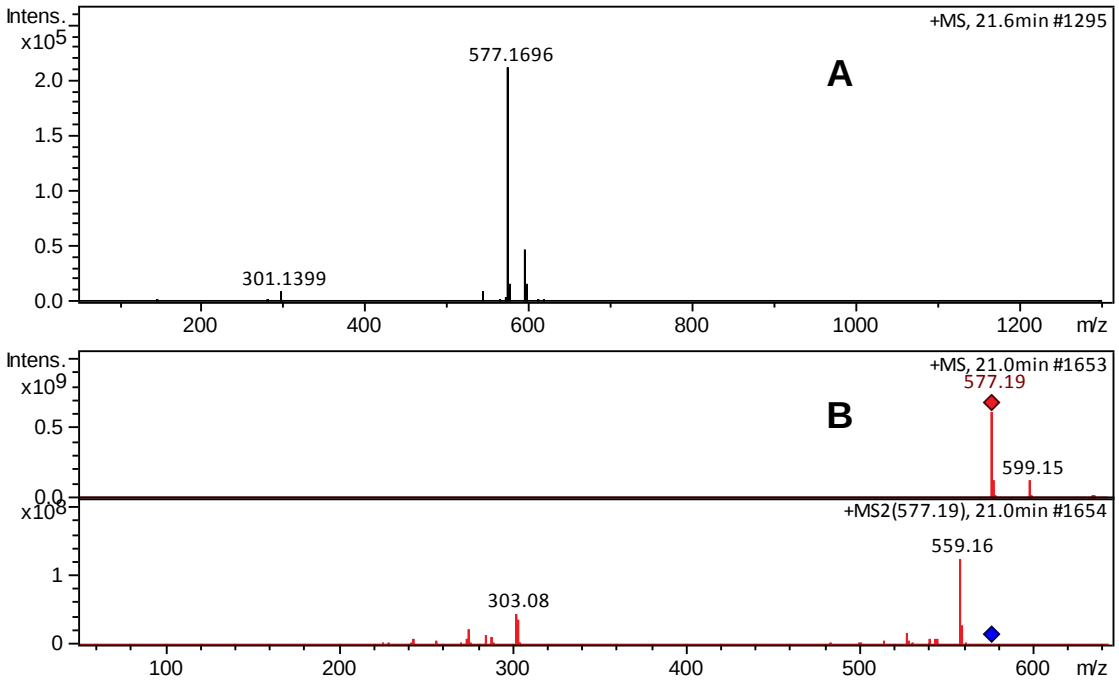

Figure S20. (A) LC-ESI-TOF-HRMS spectrum of compound **10**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 577 of compound **10**.

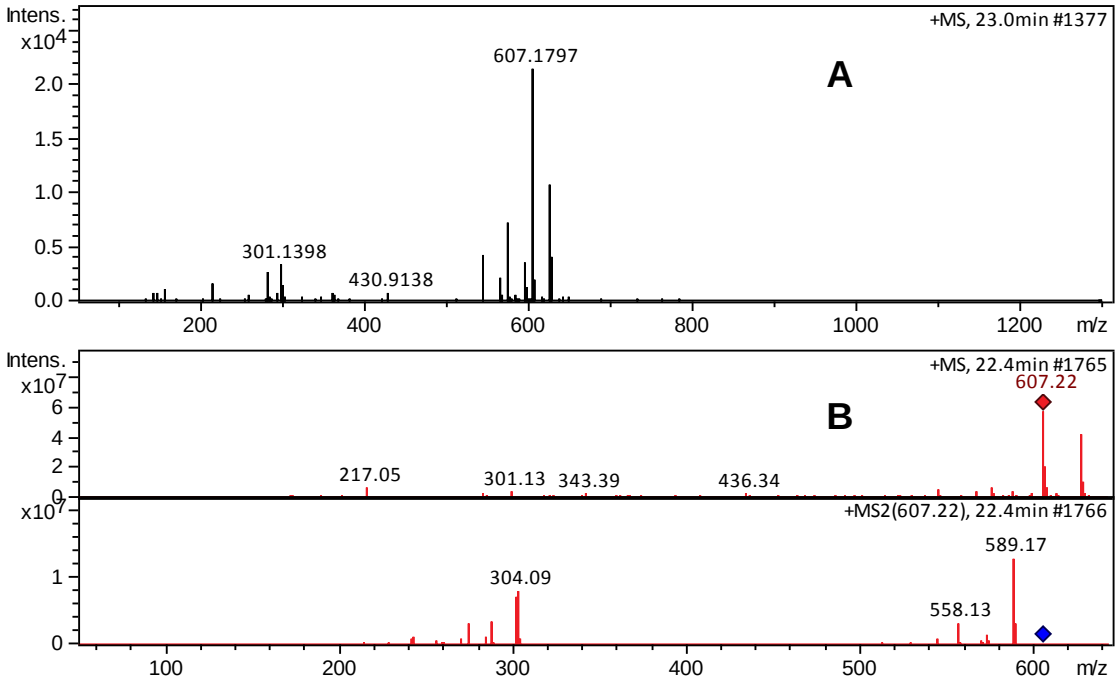

Figure S21. (A) LC-ESI-TOF-HRMS spectrum of compound **11**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 607 of compound **11**.

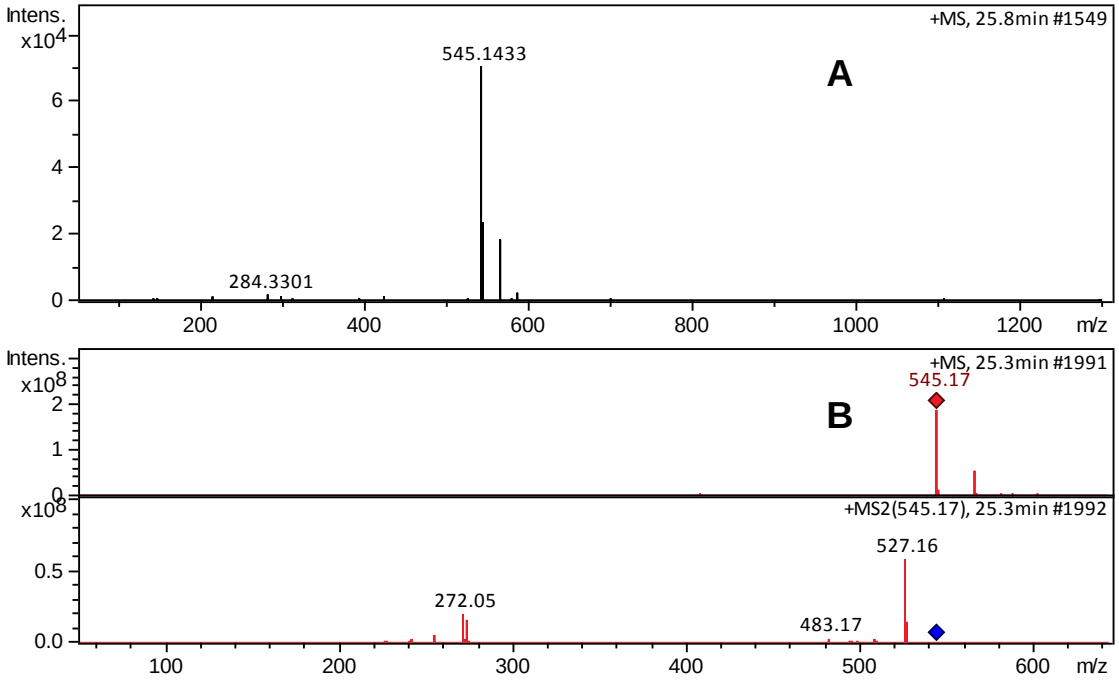

Figure S22. (A) LC-ESI-TOF-HRMS spectrum of compound **12**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 545 of compound **12**.

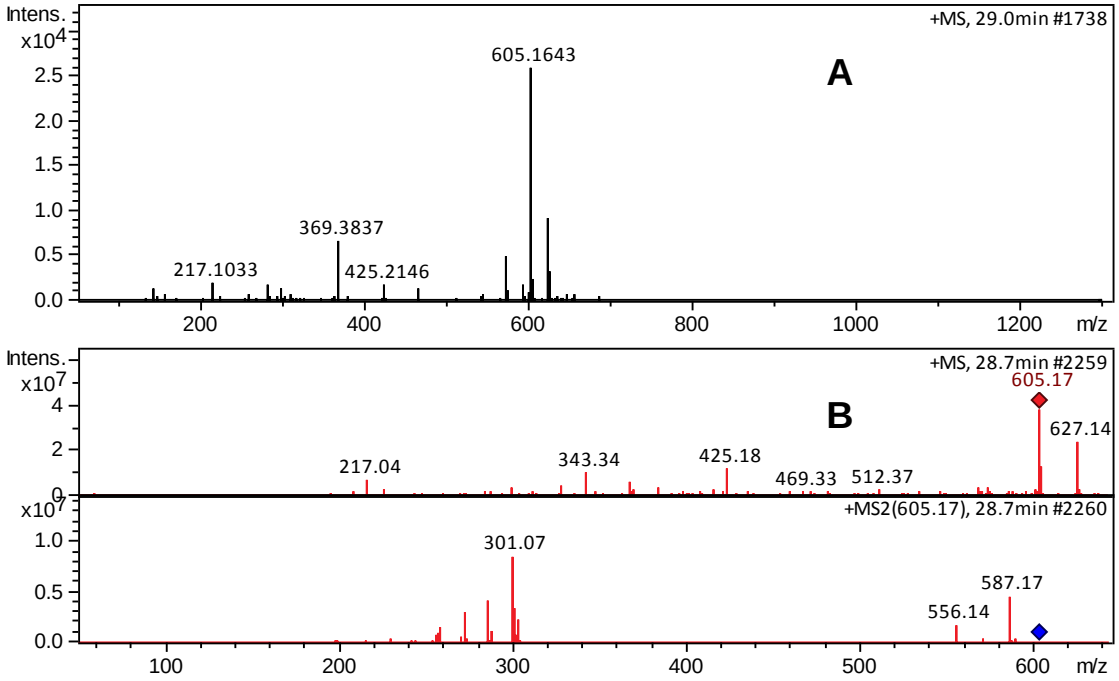

Figure S23. (A) LC-ESI-TOF-HRMS spectrum of compound **13**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 605 of compound **13**.

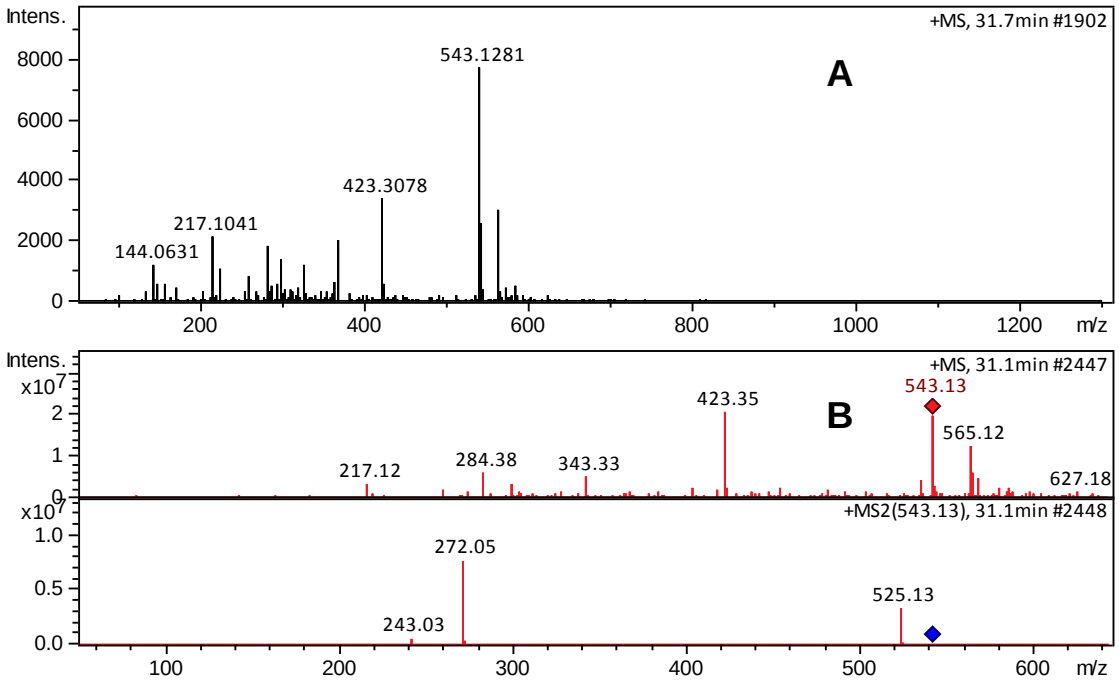

Figure S24. (A) LC-ESI-TOF-HRMS spectrum of compound **14**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 543 of compound **14**.

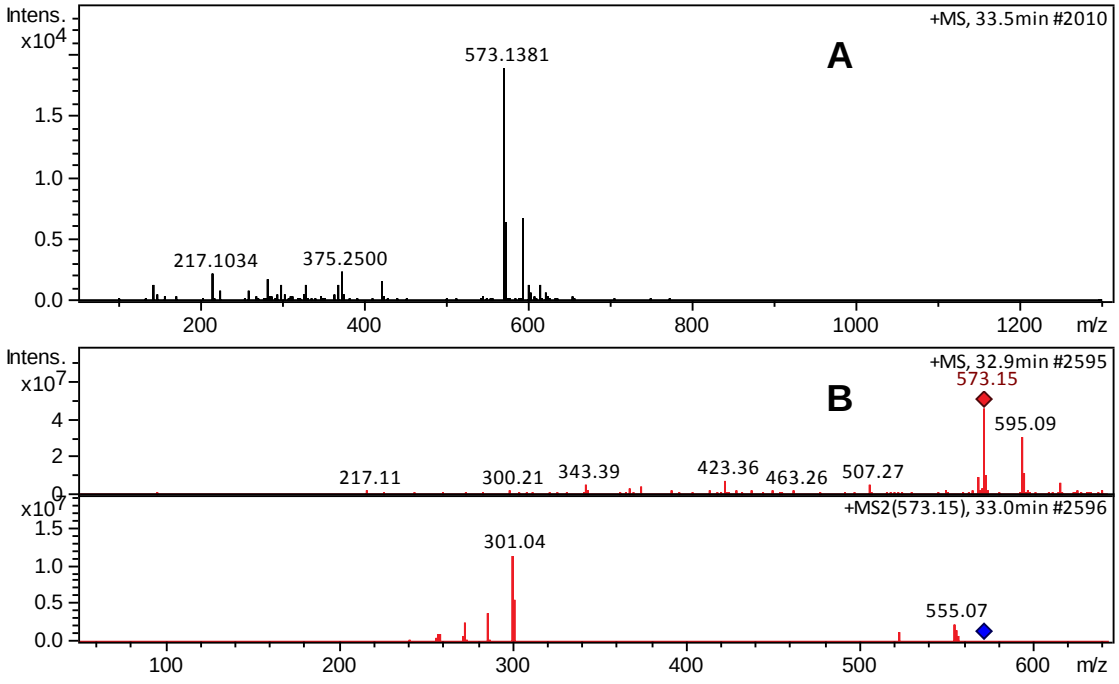

Figure S25. (A) LC-ESI-TOF-HRMS spectrum of compound **15**; (B) LC-ESI-IT-MS/MS spectrum of *m/z* 573 of compound **15**.

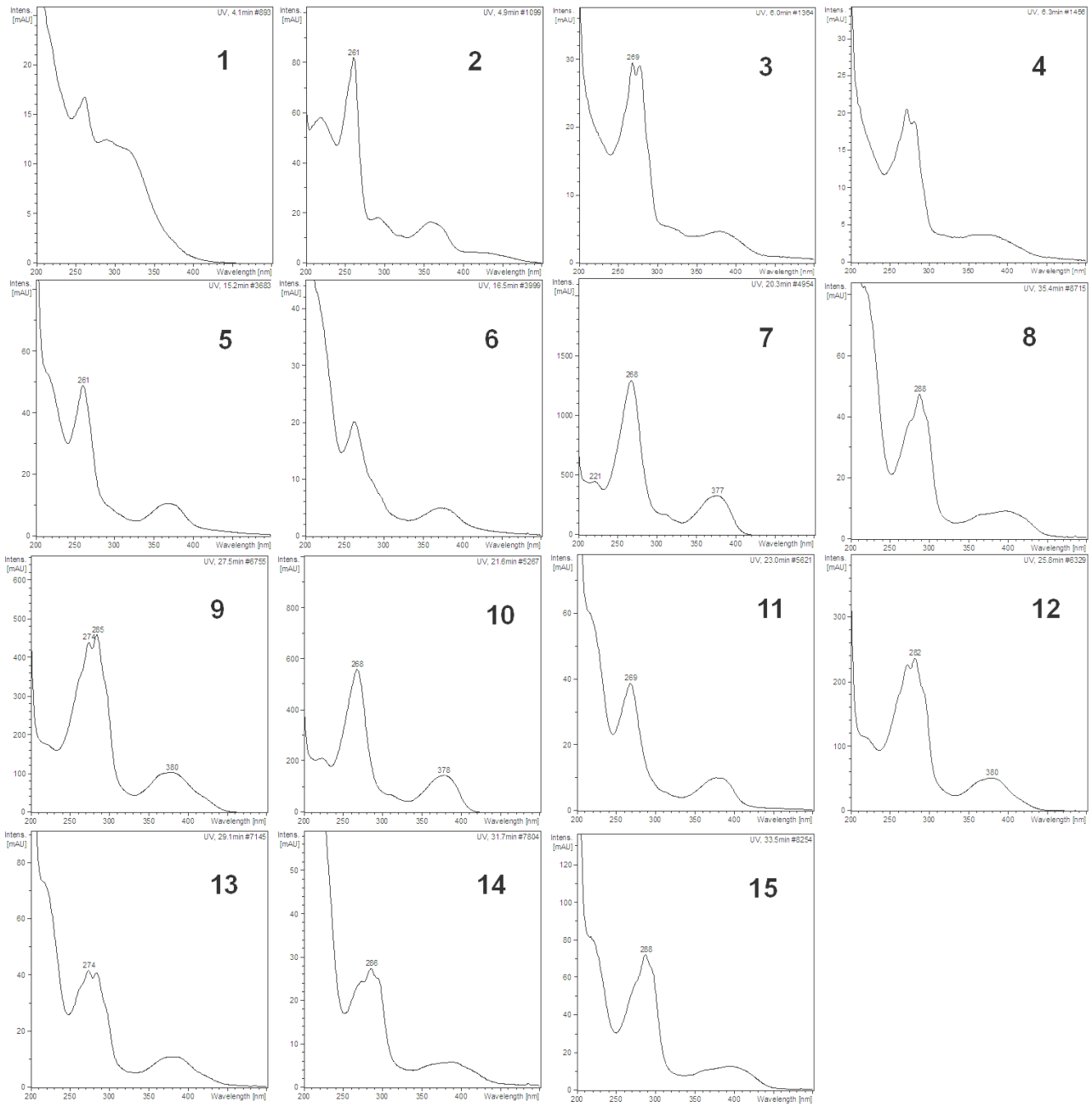

Figure S26. UV spectra of compounds **1-15** present in the EtOAc extract of the capitula from *P. planifolius*.

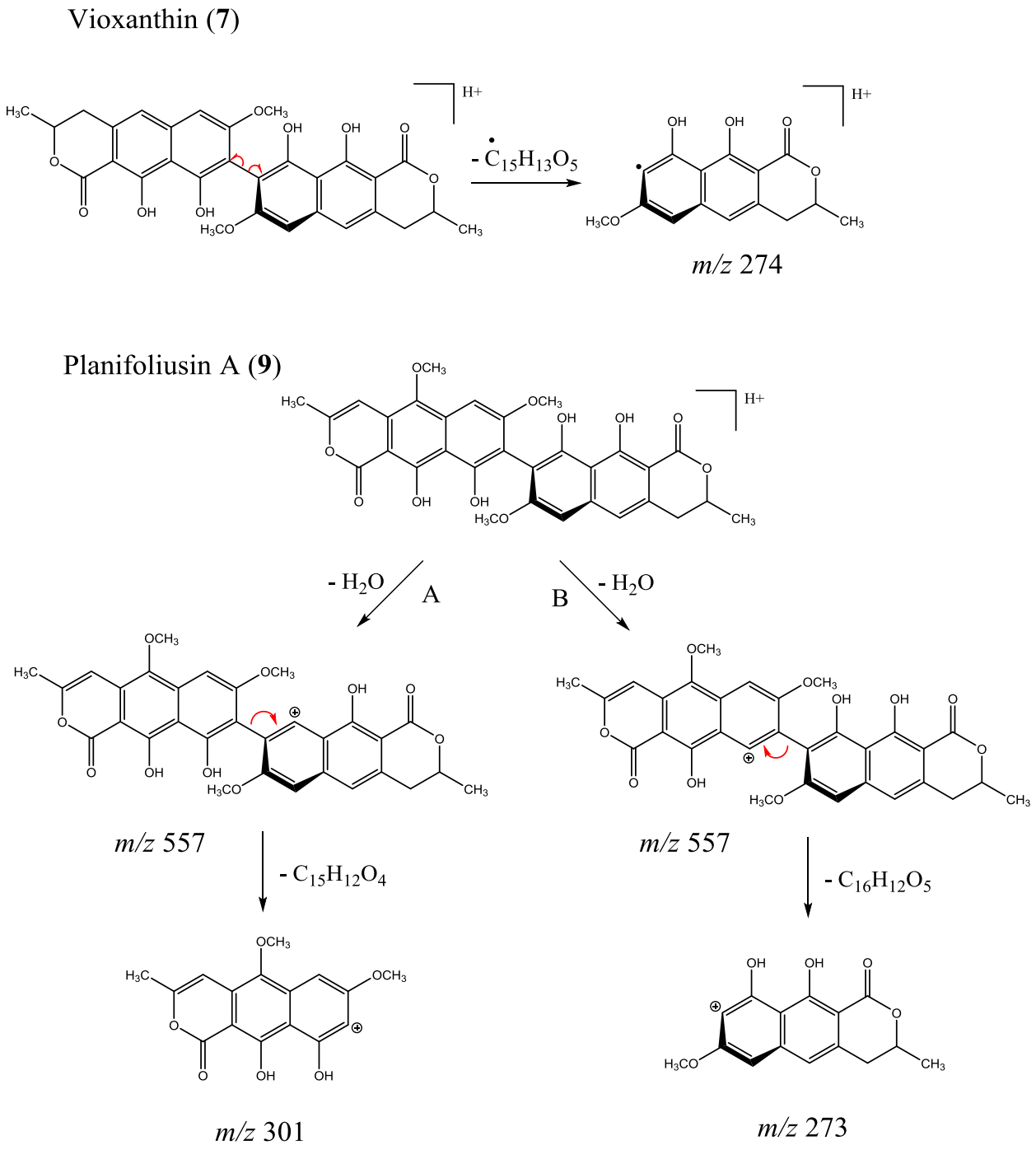

Figure S27. Proposed fragmentation pathways of compounds **7** and **9**.

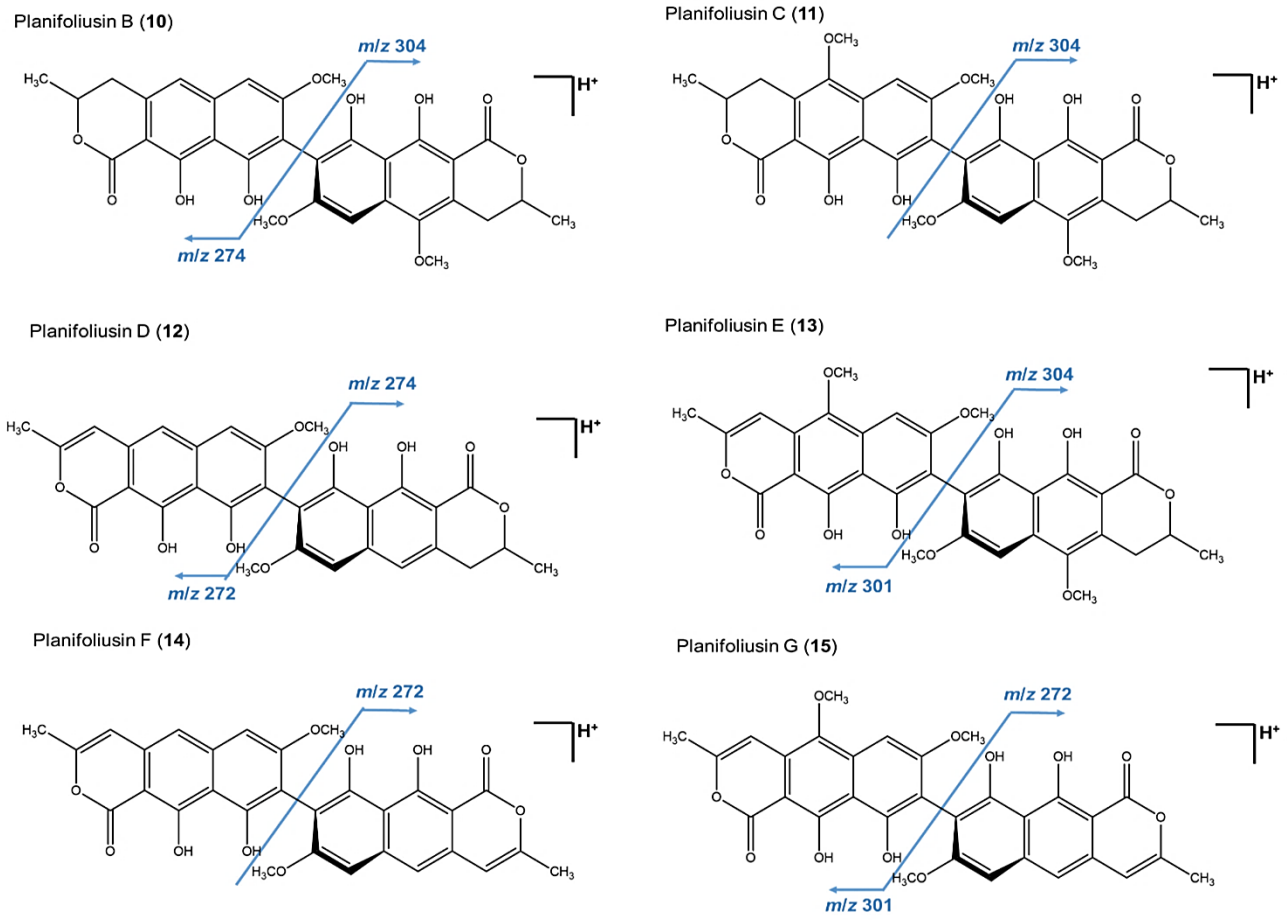

Figure S28. Proposed fragmentation pathways of naphthopyranones **10**-**15**.

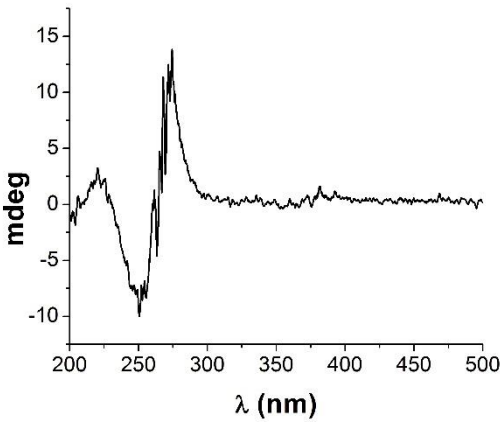

Figure S29. CD spectrum (solvent: acetonitrile) of vioxanthin (**7**).