

An integrated LC-ESI-MSⁿ and High Resolution LC-ESI-QTOF approach for the identification of phloroglucinols from Nepalese *Hypericum japonicum*

Gregorio Peron ^{a*}, Deepak Raj Pant ^b, Shyam Sharan Shrestha ^b, Sangeeta Rajbhandary ^b, Stefano Dall'Acqua ^{a*}

Affiliations

^a Department of Pharmaceutical and Pharmacological Sciences, University of Padova, Via Marzolo 5, 35131 Padova, Italy. **Gregorio Peron:** e-mail: gregorio.peron@unive.it; ORCID number: 0000-0002-6007-6184. **Stefano Dall'Acqua:** e-mail: stefano.dallacqua@unipd.it; ORCID number: 0000-0001-8264-6953.

^b Central Department of Botany, Tribhuvan University, 44600 Kirtipur, Kathmandu, Nepal. **Sangeeta Rajbhandary:** e-mail: s.rajbhandary@cdbtu.edu.np; **Deepak Raj Pant:** drpant_agbot@yahoo.com; **Shyam Sharan Shrestha:** e-mail: shyamsharan999@gmail.com.

*Correspondence: Stefano Dall'Acqua: stefano.dallacqua@unipd.it; Gregorio Peron: gregorio.peron@unive.it.

SUPPLEMENTARY MATERIAL

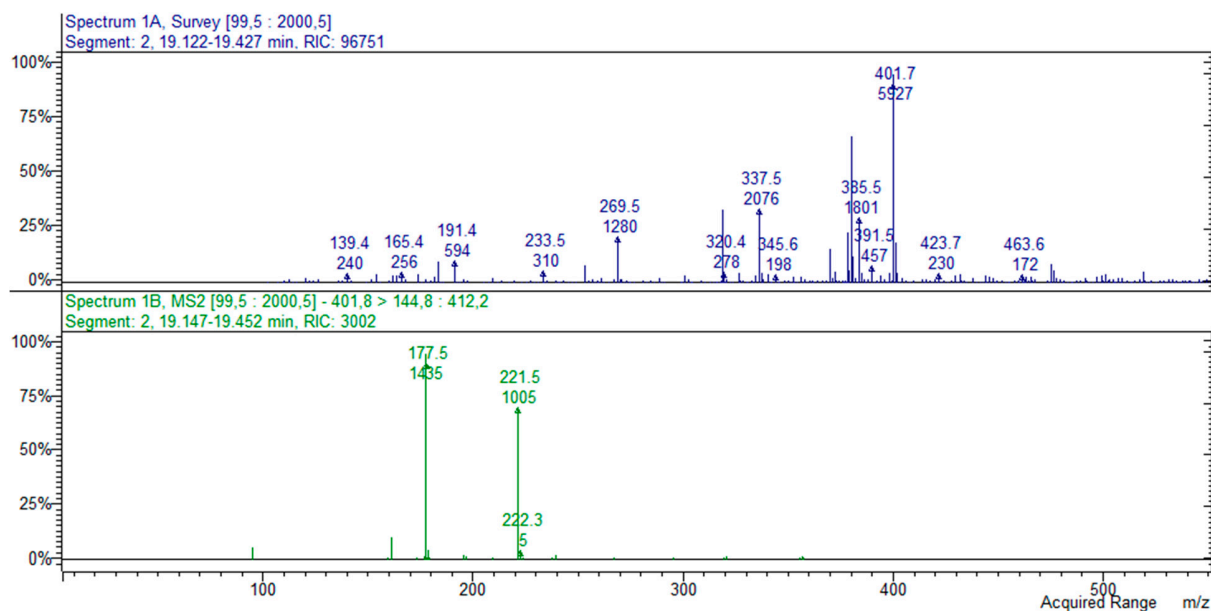
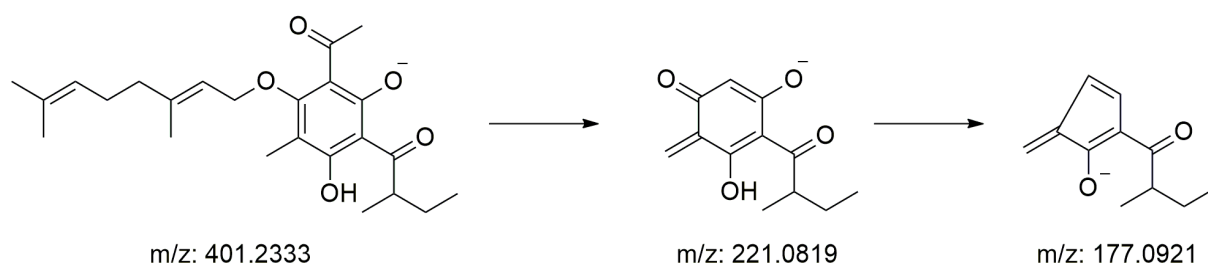


Figure S1. MS/MS spectrum of 2-acetyl-3,5-dihydroxy-1-geranoxy-6-methyl-4-(2-methyl)butyryl-benzene, $[M-H]^- = 401$.



Fragmentation Scheme 1. 2-acetyl-3,5-dihydroxy-1-geranoxy-6-methyl-4-(2-methyl)butyryl-benzene, $[M-H]^- = 401$.

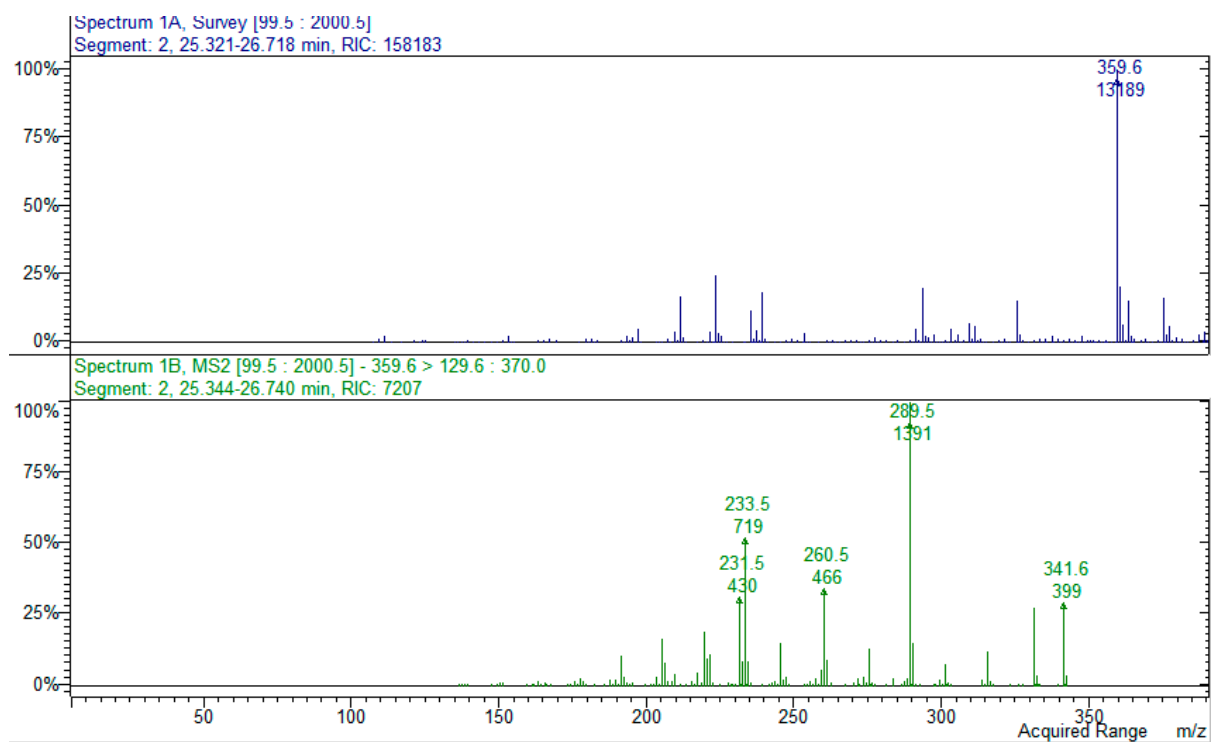
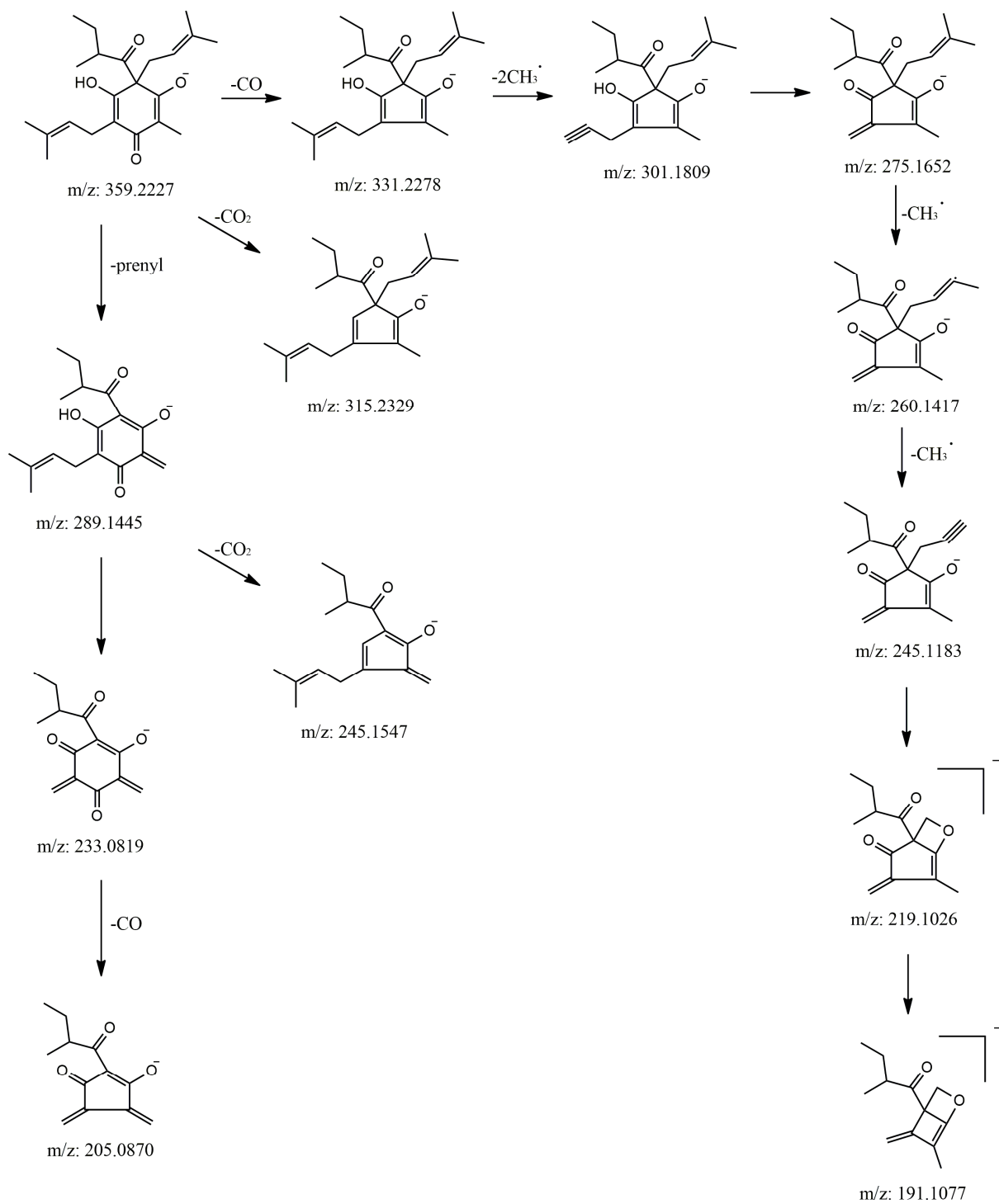


Figure S2. MS/MS spectrum of 1'3'pren45'me4'oxoPIB, $[M-H]^- = 359$.



Fragmentation Scheme 2. 1'3'pren45'me4'oxoPIB, $[M-H]^- = 359$.

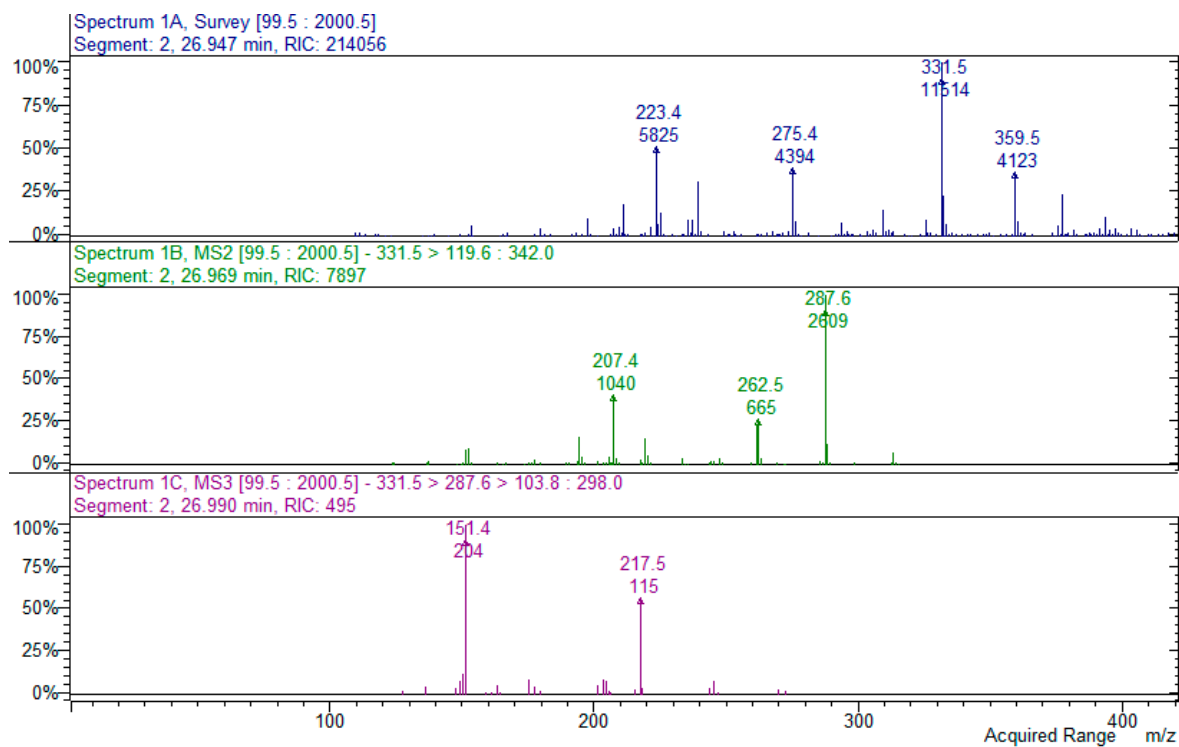
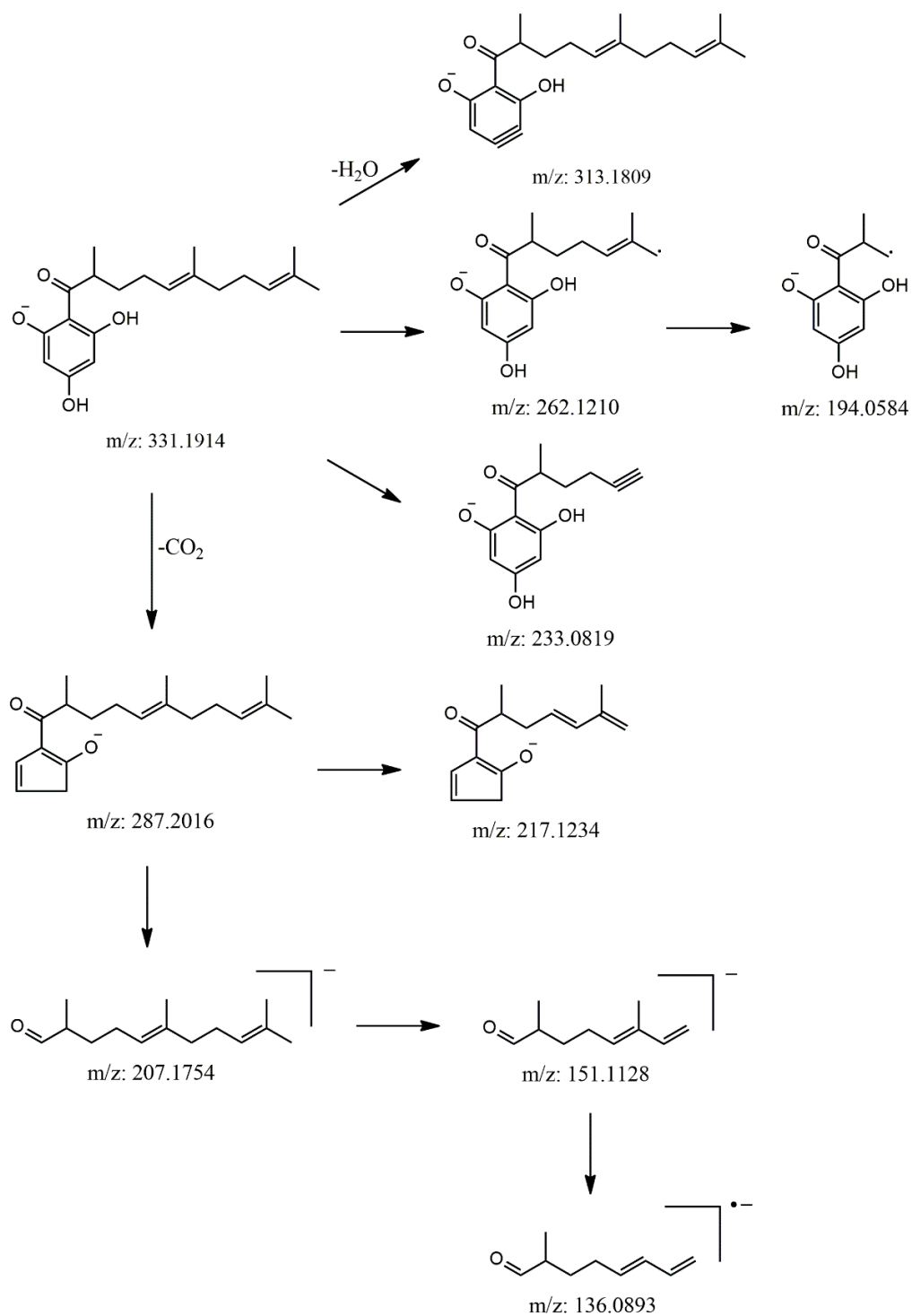


Figure S3. MSⁿ spectra (n=3) of geranyl phlorisobutyrophenone, [M-H]⁻ = 331.



Fragmentation Scheme 3. Geranyl phlorisobutyrophenone, $[M-H]^- = 331$.

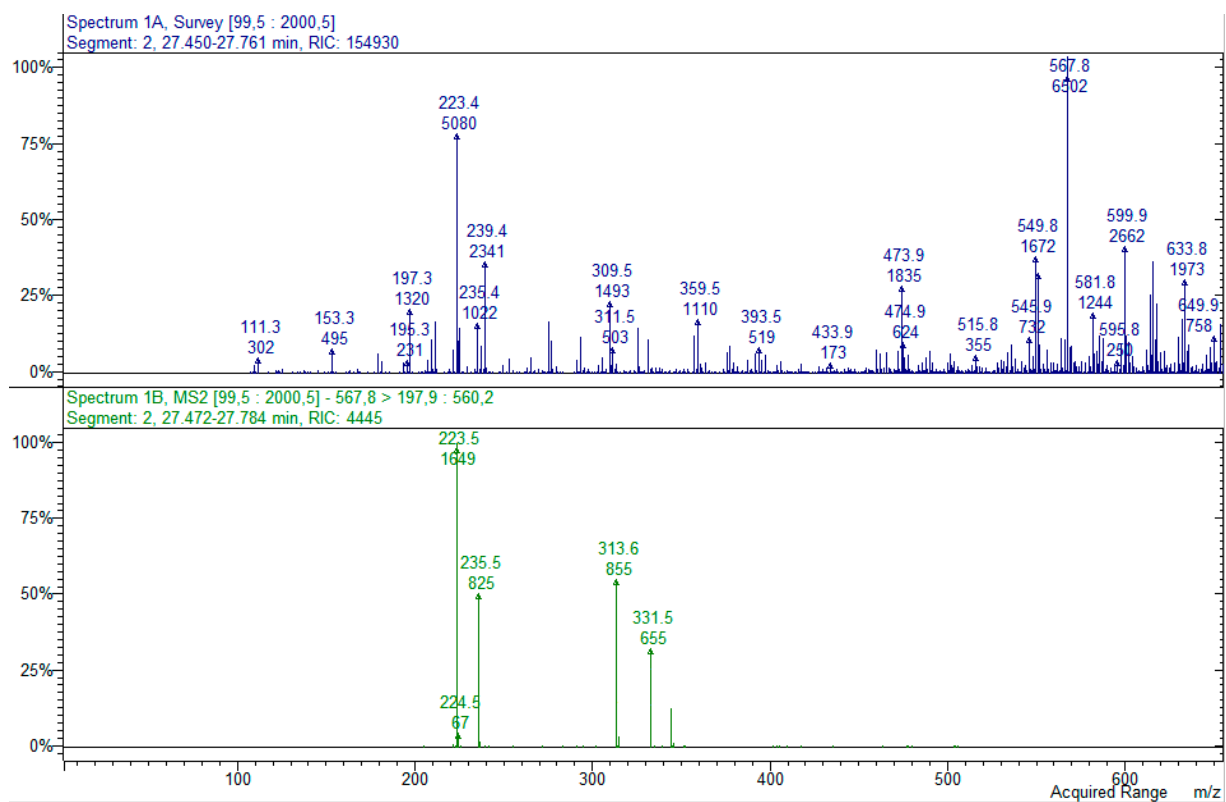
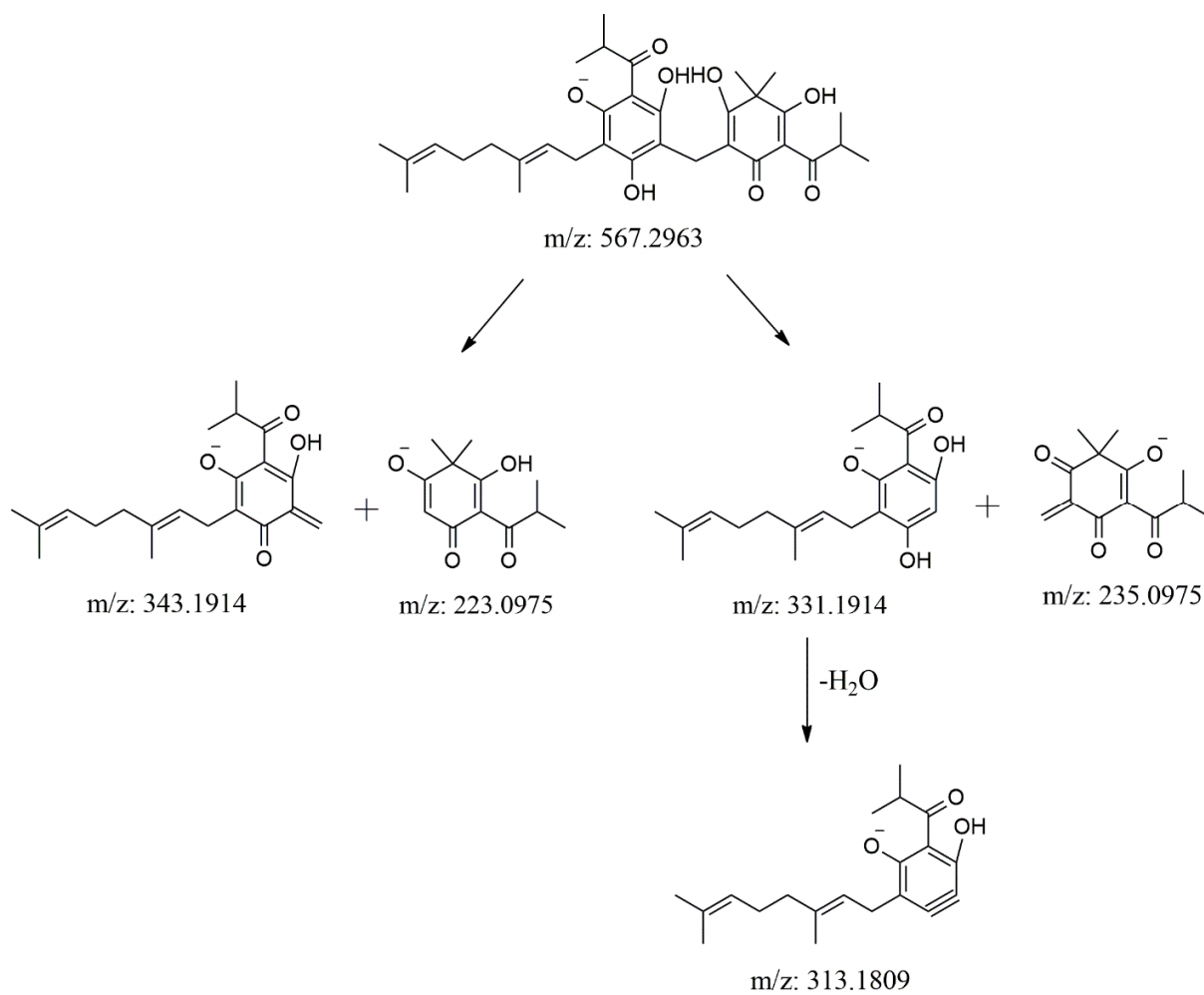


Figure S4. MS/MS spectrum of sarothralen A, $[M-H]^- = 567$.



Fragmentation Scheme 4. Sarothralen A, $[M-H]^- = 567$.

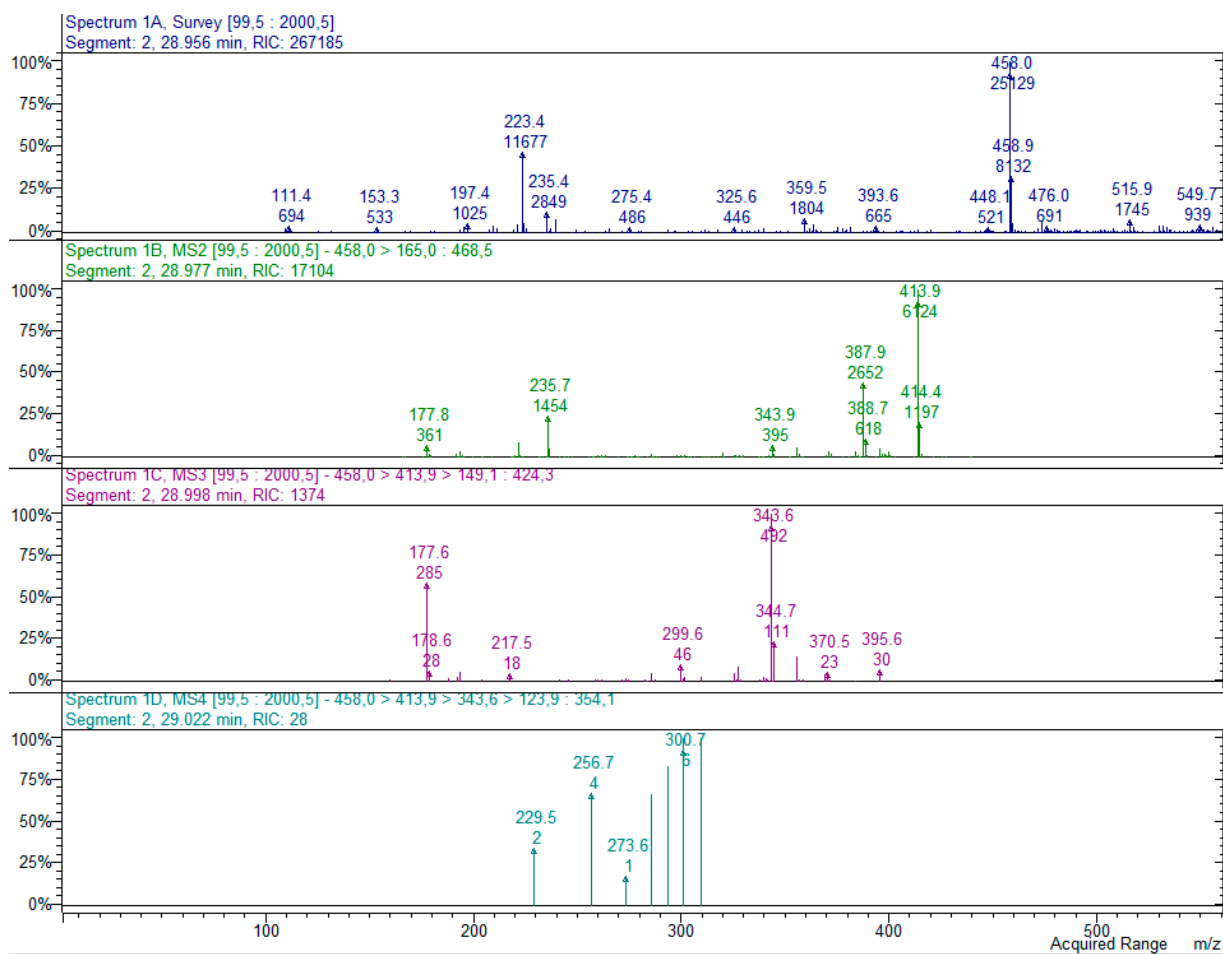
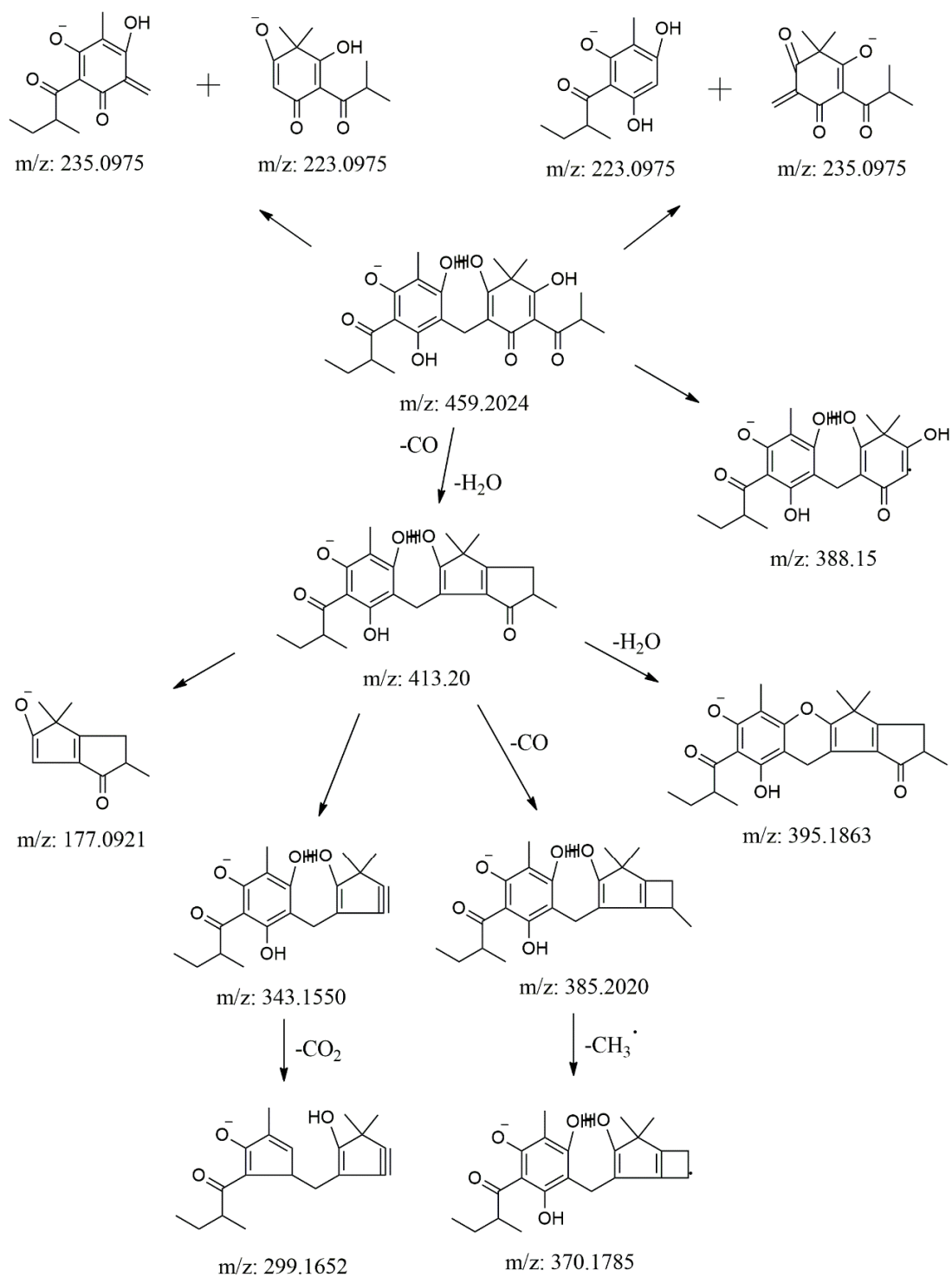


Figure S5. MSⁿ spectra (n = 4) of sarospidin B, [M-H]⁻ = 459.



Fragmentation Scheme 5. Saroaspidin B, $[M-H]^- = 459$.

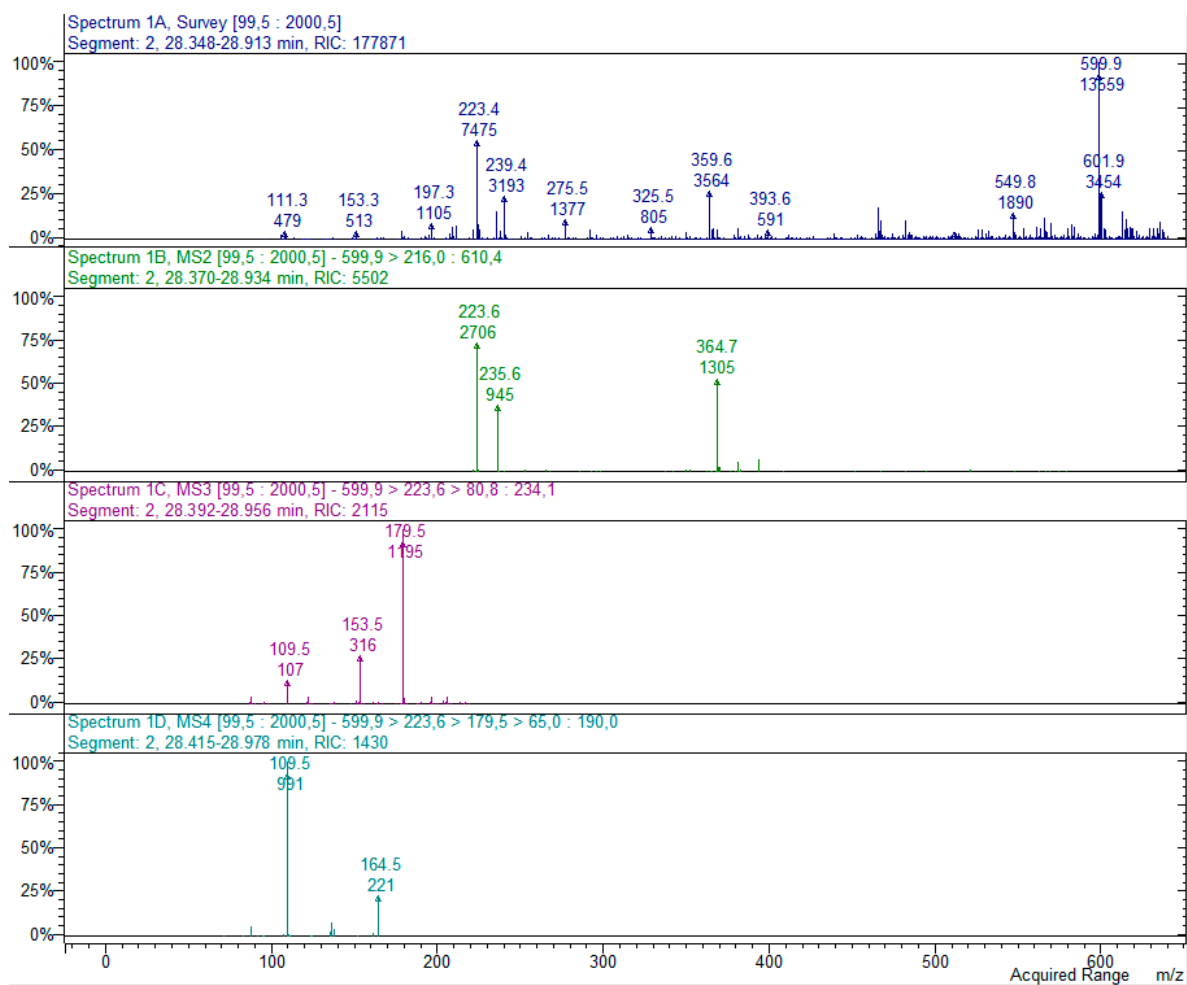
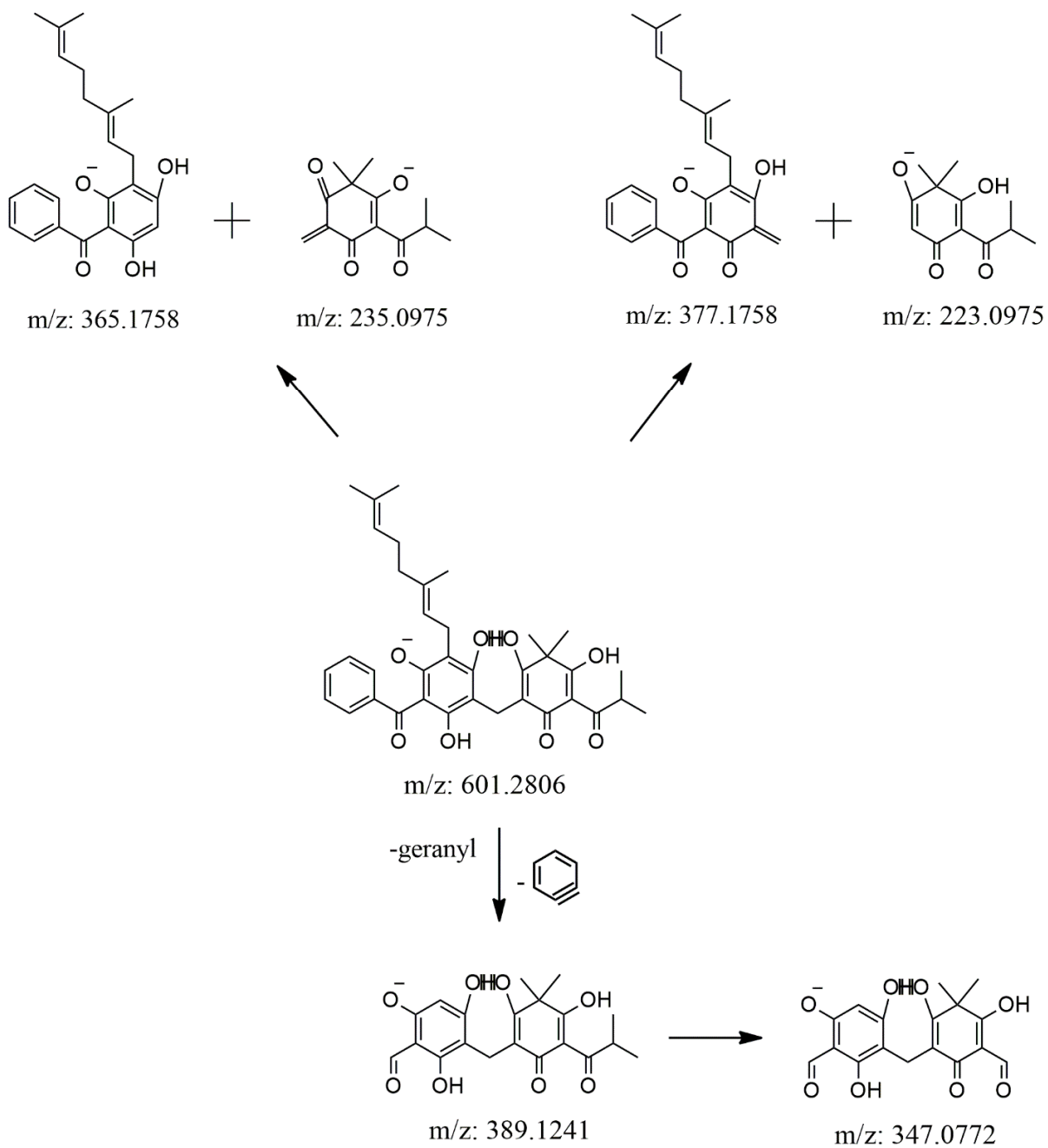


Figure S6. MSⁿ spectra (n = 4) of sarothralen G, [M-H]⁻ = 601.



Fragmentation Scheme 6. Sarothralen G, $[M-H]^- = 601$.

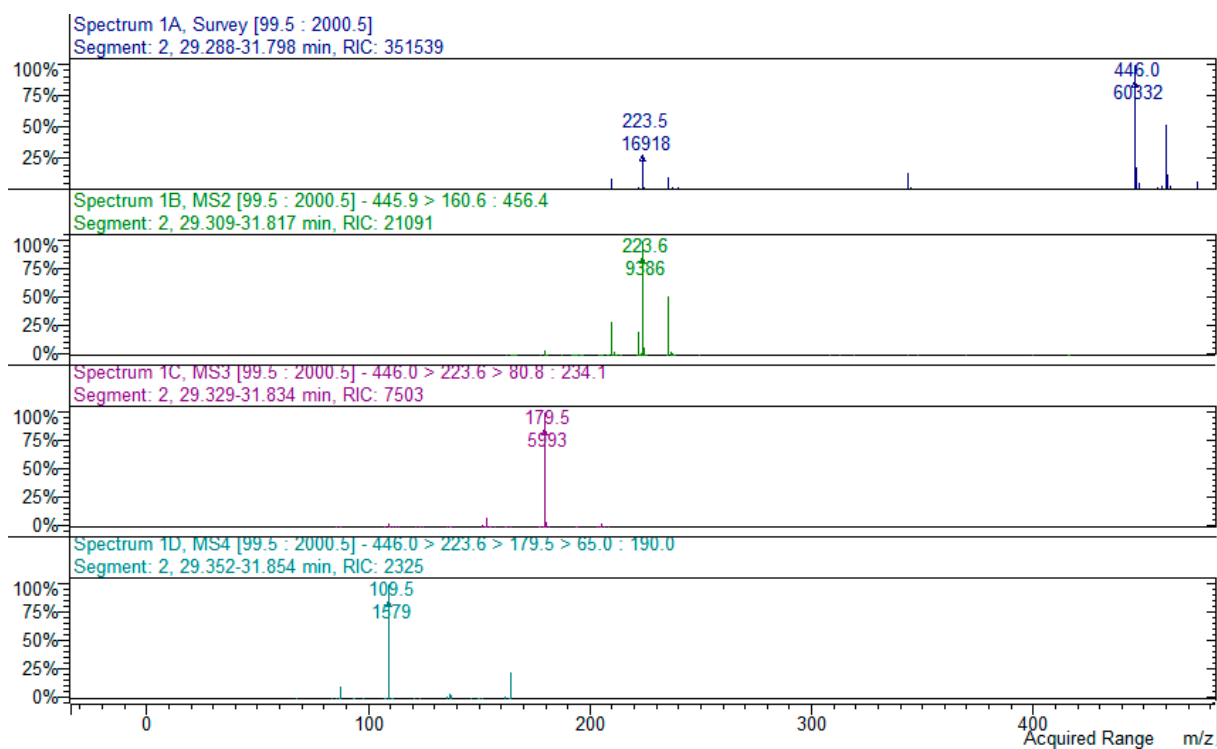
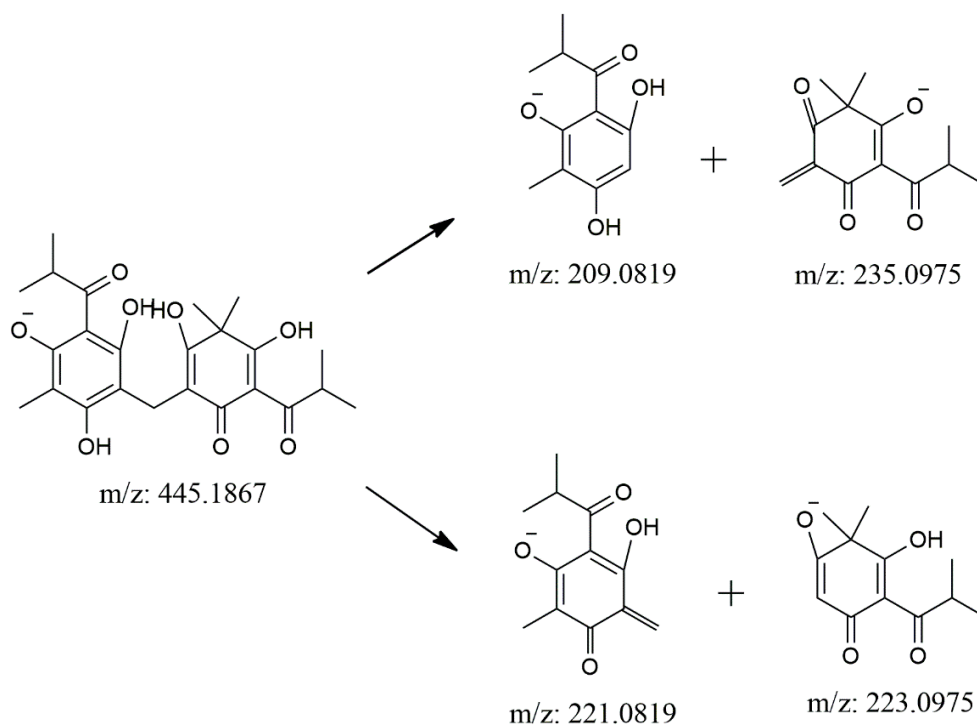
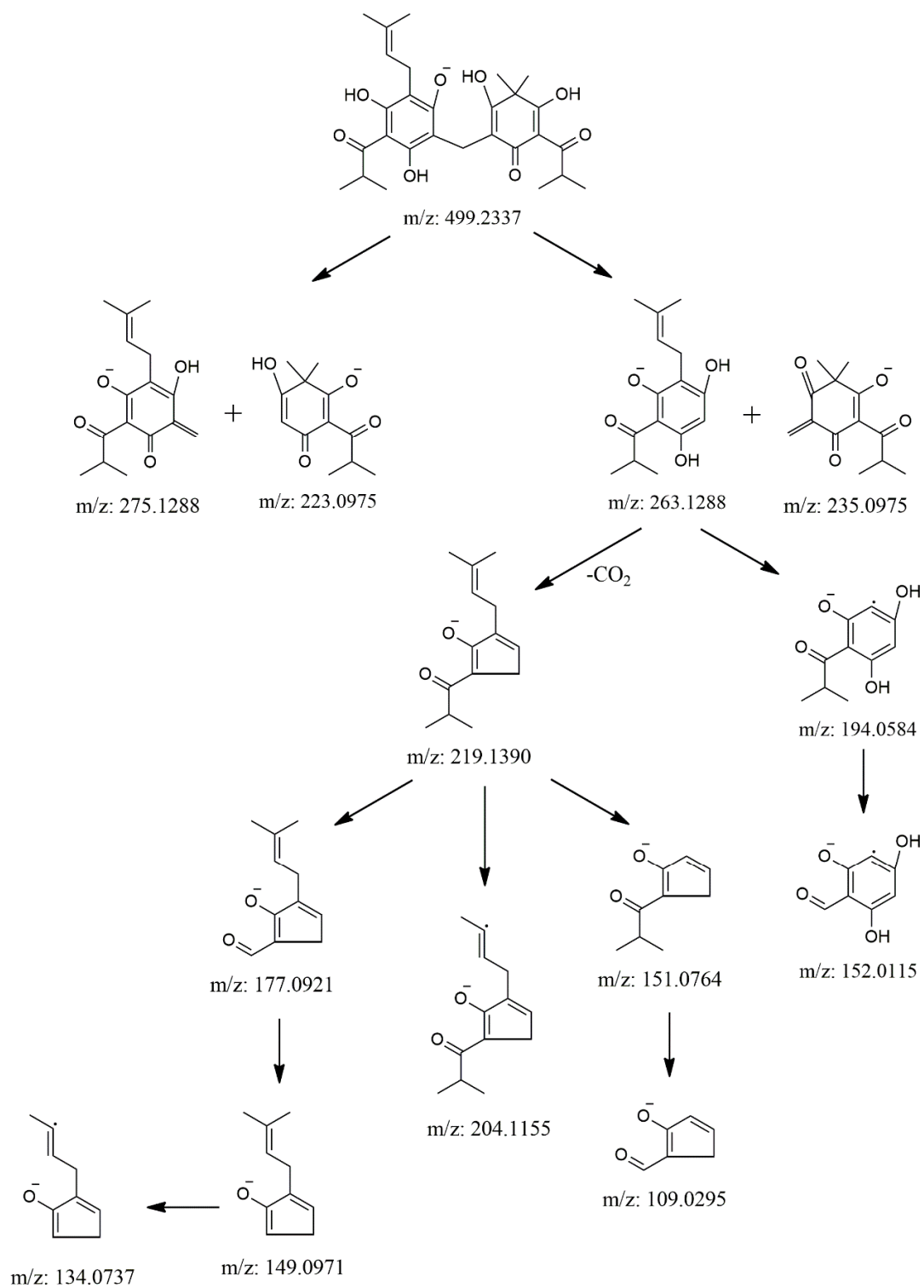


Figure S7. MS/MS spectrum of sarospidin A, $[M-H]^- = 445$.



Fragmentation Scheme 7. Saroaspidin A, $[M-H]^- = 445$.



Fragmentation Scheme 8. Uliginosin A, $[M-H]^- = 499$.

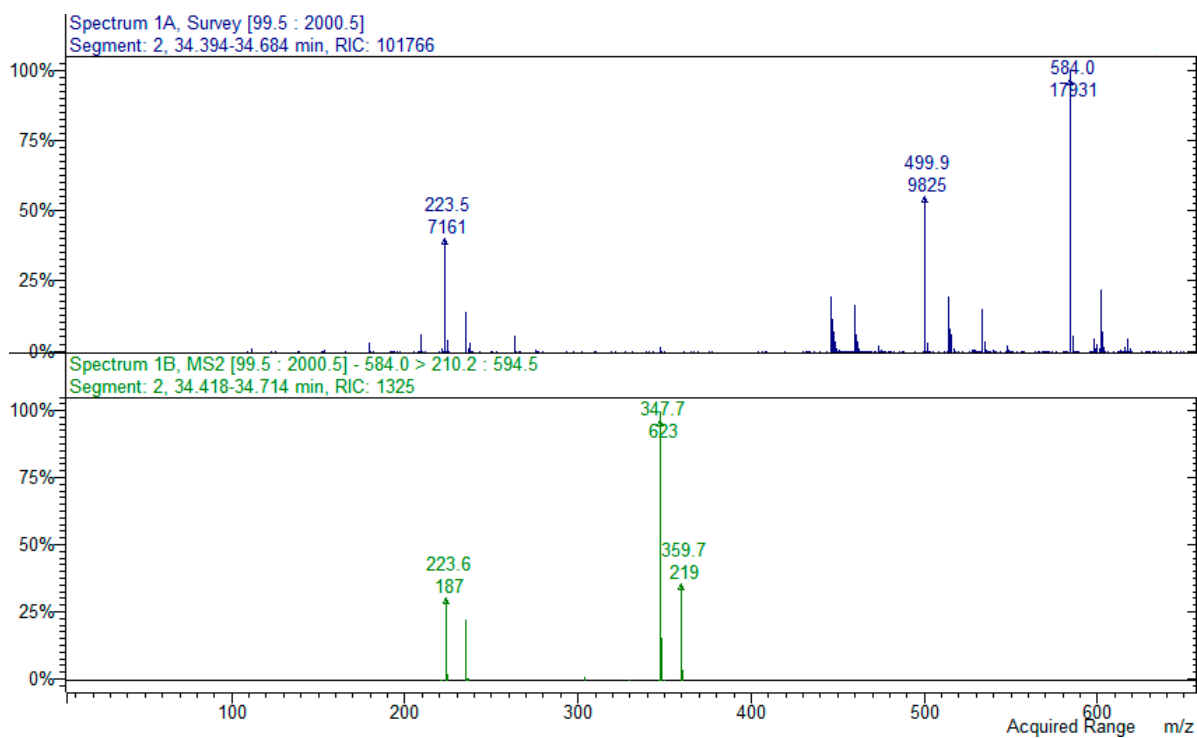
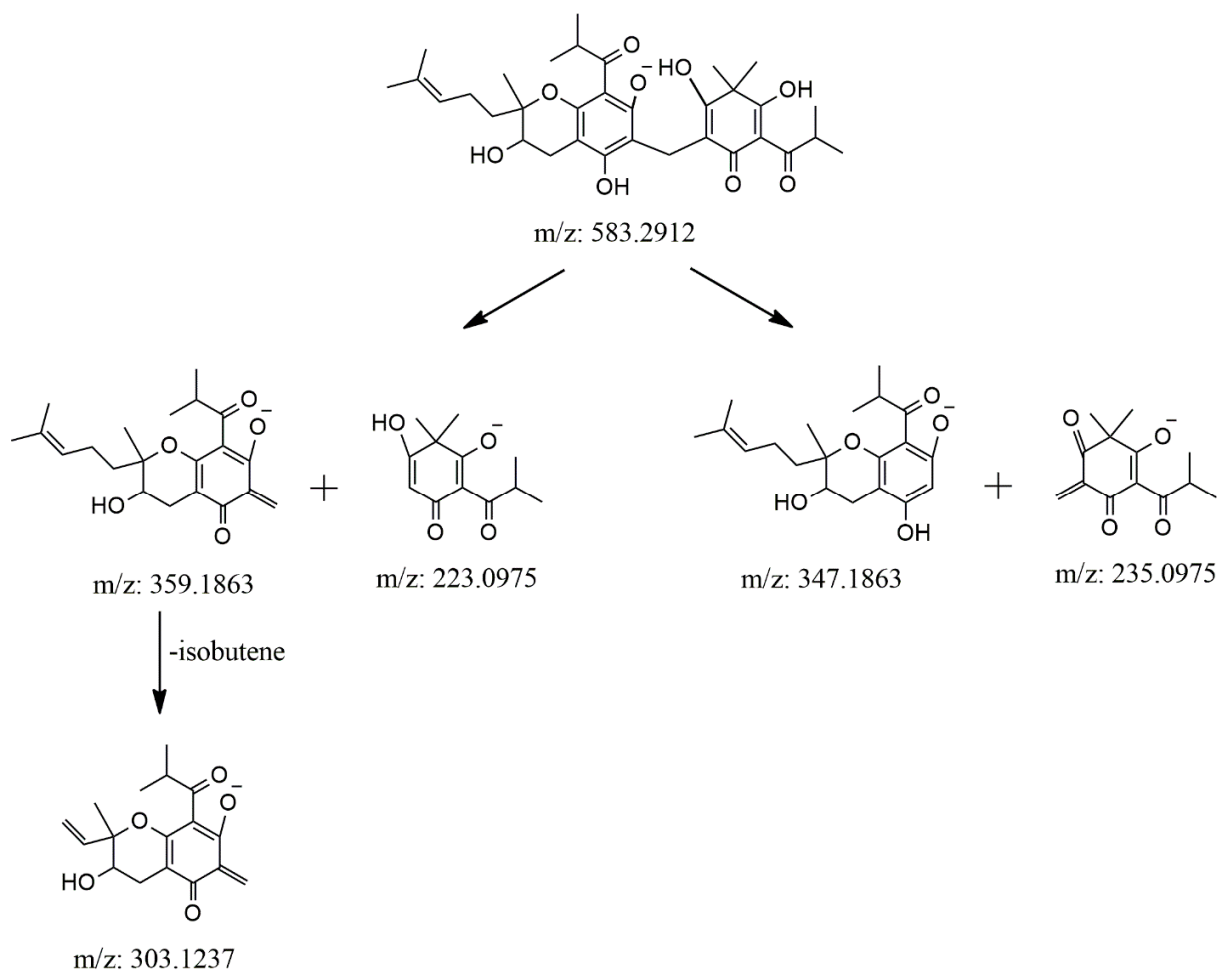


Figure S8. MS/MS spectrum of sarothralens C and D, $[M-H]^- = 583$.



Fragmentation Scheme 9. Sarothralens C and D, $[M-H]^- = 583$.