

Cytotoxic Potential of *Alternaria tenuissima* AUMC14342 Mycoendophyte Extract: A Study Combined with LC-MS/MS Metabolic Profiling and Molecular Docking Simulation

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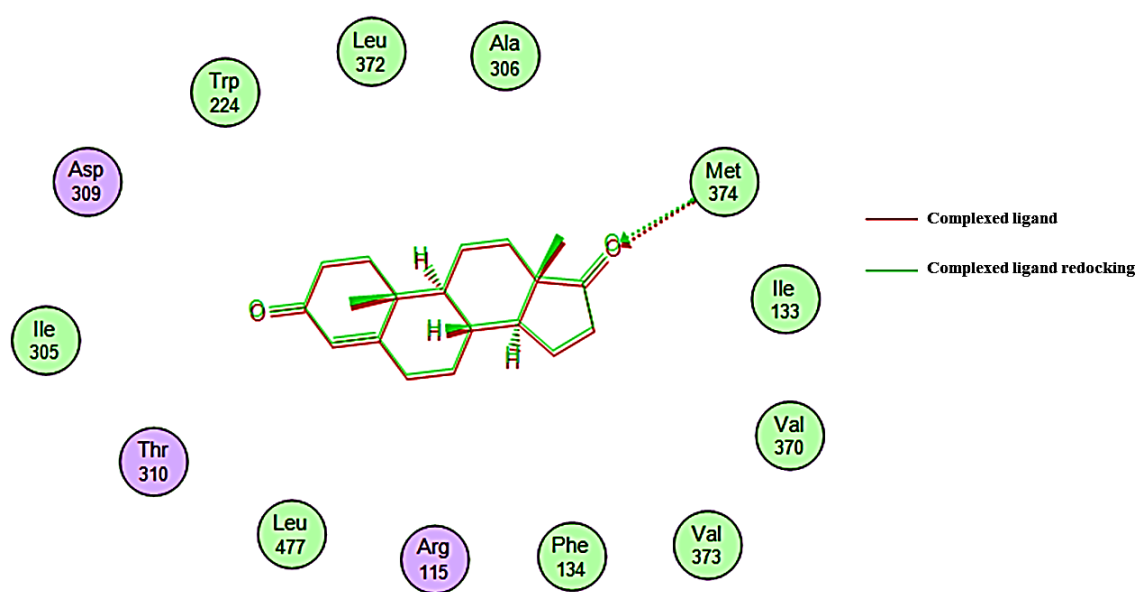


Figure S1. Validation of docking protocol by complexed ligand redocking.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 4.485 min
Precursor: 167.2 Da, Charge: 1

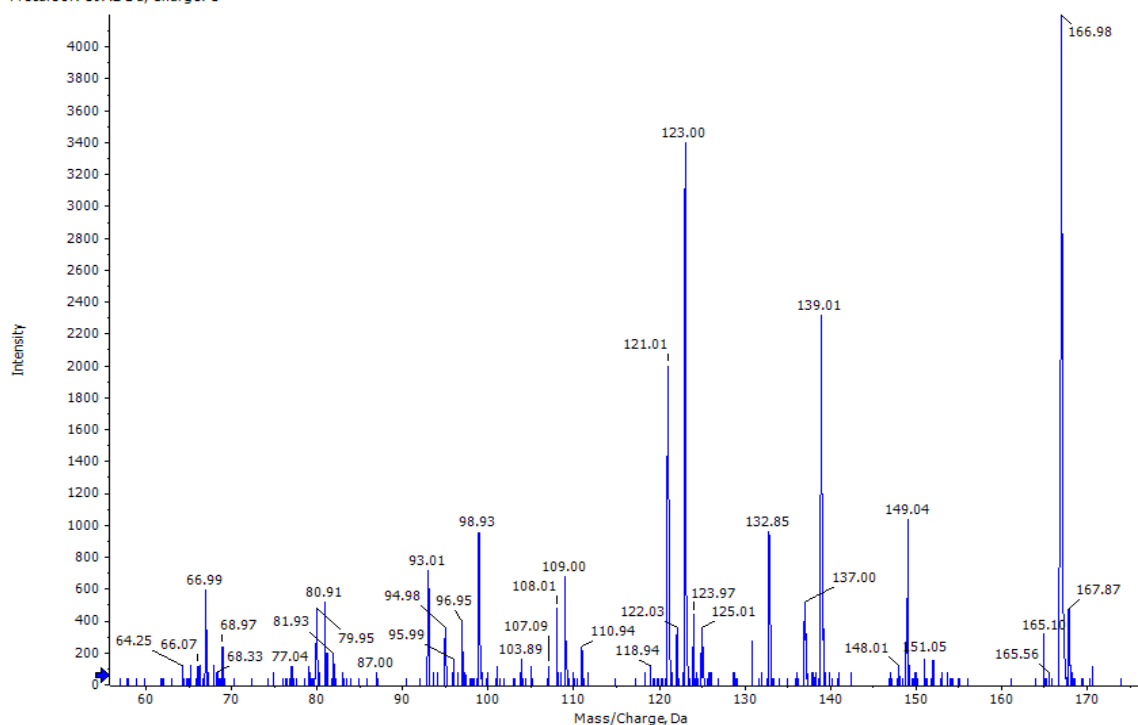


Figure S2. MS² mass chromatogram of Cyclo-Ala-Pro-Diketopiperazine.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 12.432 min
Precursor: 233.4 Da, Charge: 2

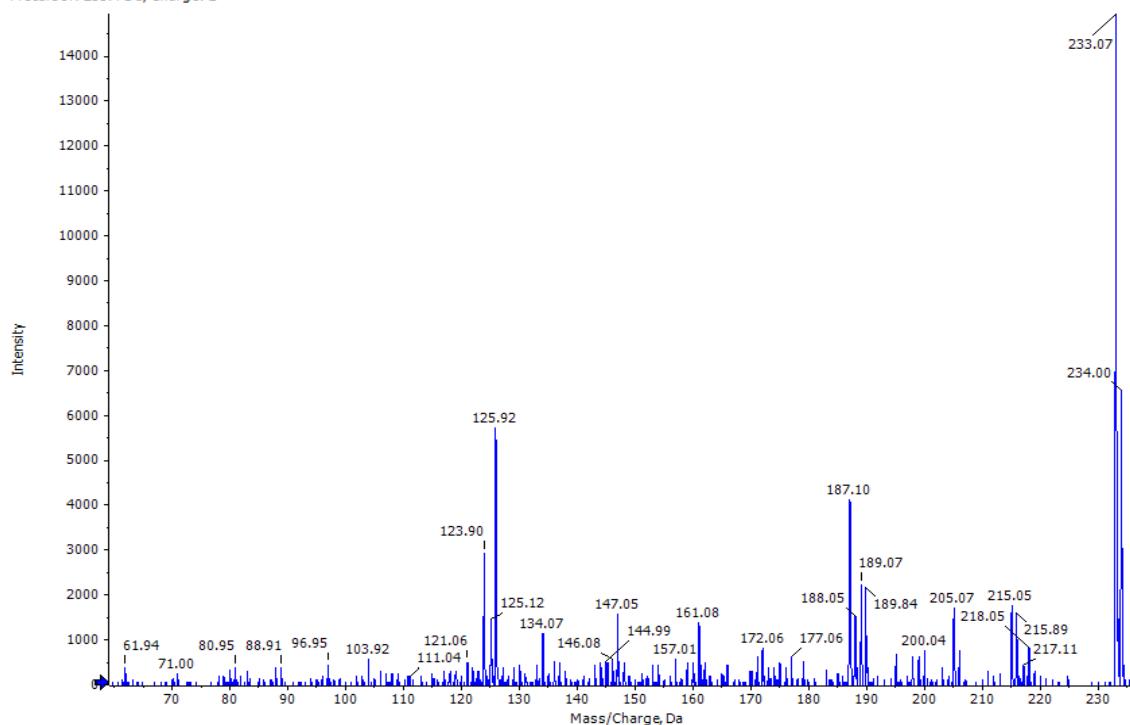


Figure S3. MS² mass chromatogram of (S)-alternariphent A.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 12.837 min
Precursor: 161.4 Da

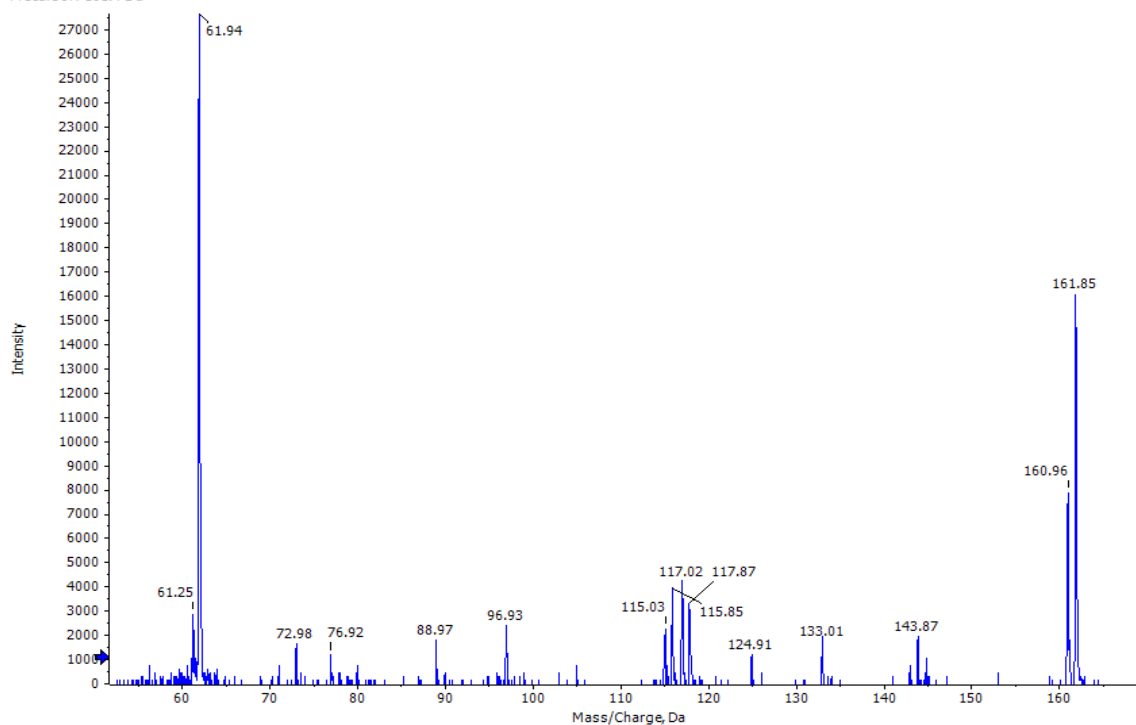


Figure S4. MS² mass chromatogram of Alternapyran.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 14.321 min
Precursor: 291.4 Da, Charge: 1

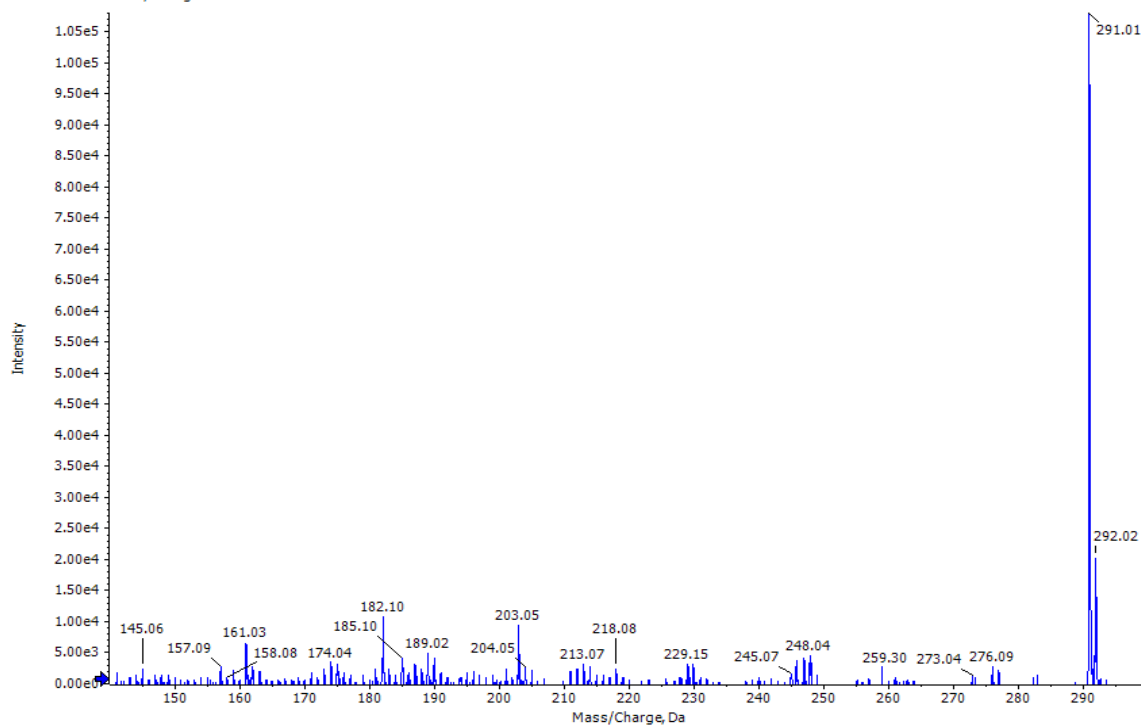


Figure S5. MS² mass chromatogram of Altenuene (4'-Epialtenuene).

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 14.713 min
Precursor: 286.4 Da, Charge: 1

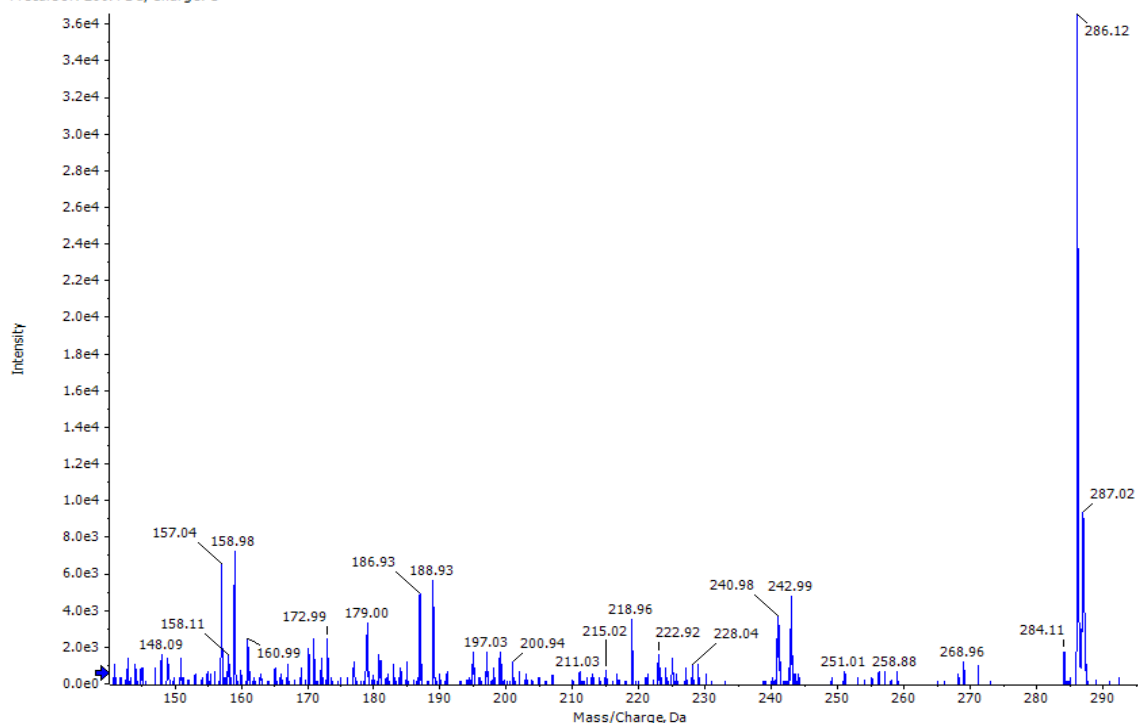


Figure S6. MS² mass chromatogram of Solanapyrone G.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 15.037 min
Precursor: 209.7 Da

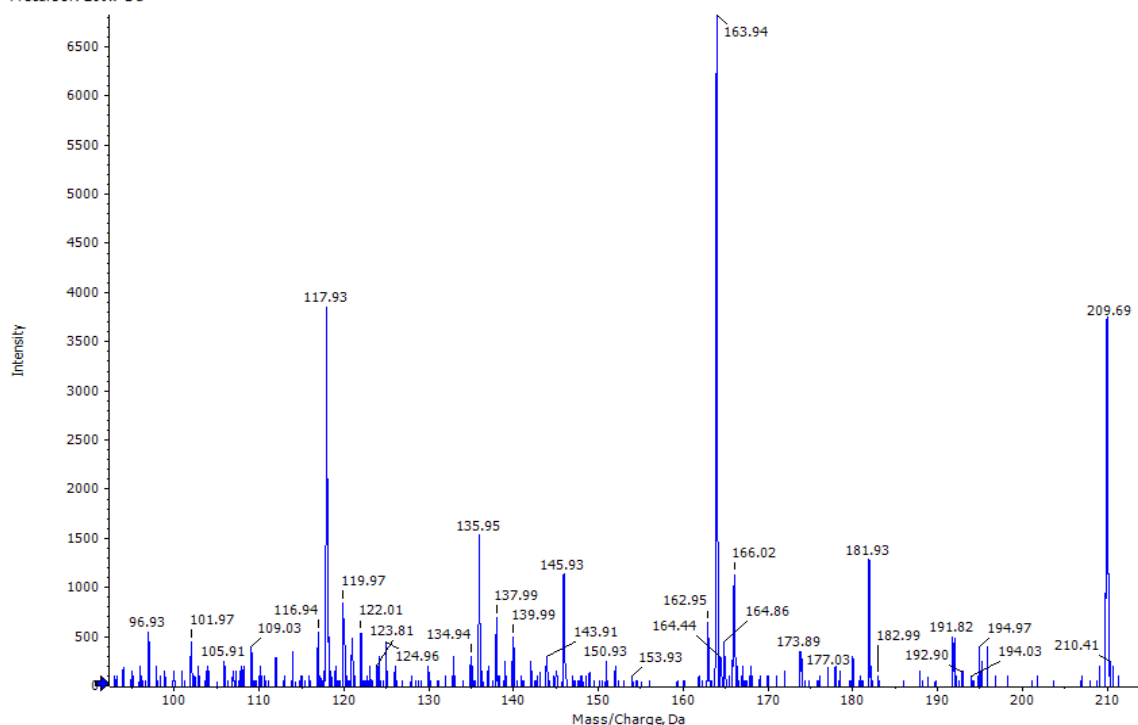


Figure S7. MS² mass chromatogram of 4-methoxy-6-methyl-5-(3-oxobutyl)-2H-pyran-2-one.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 15.825 min
Precursor: 180.4 Da, CE: 35.0

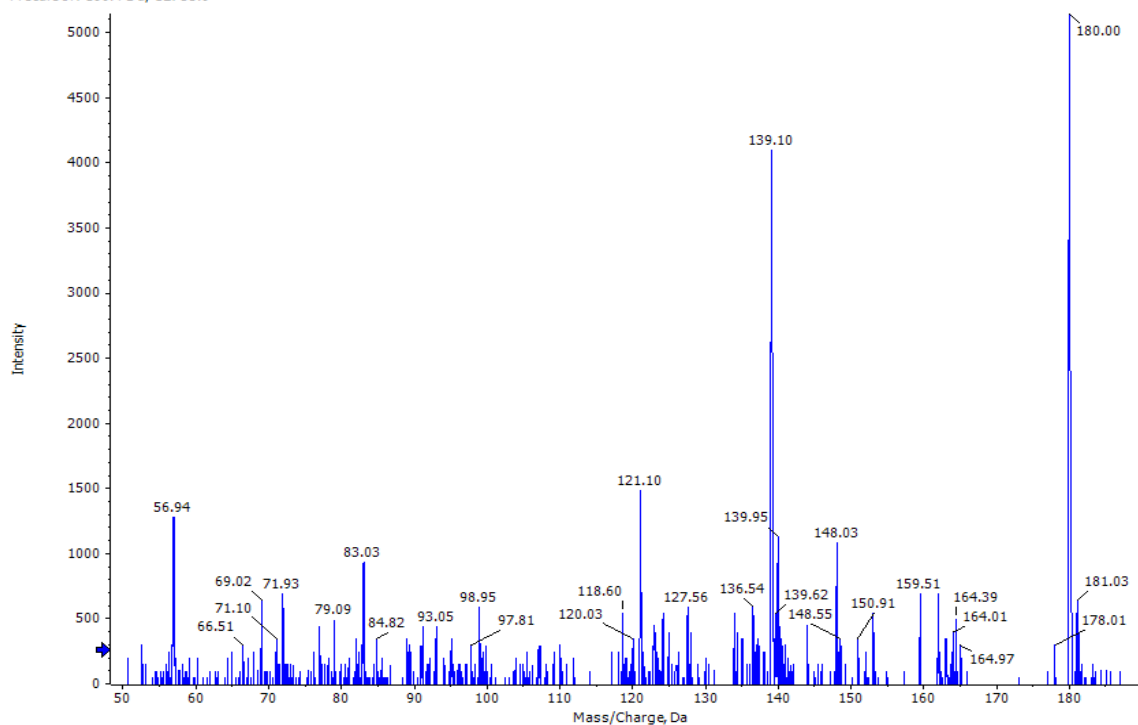


Figure S8. MS² mass chromatogram of Nacetyltyramine.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 16.036 min
Precursor: 196.0 Da

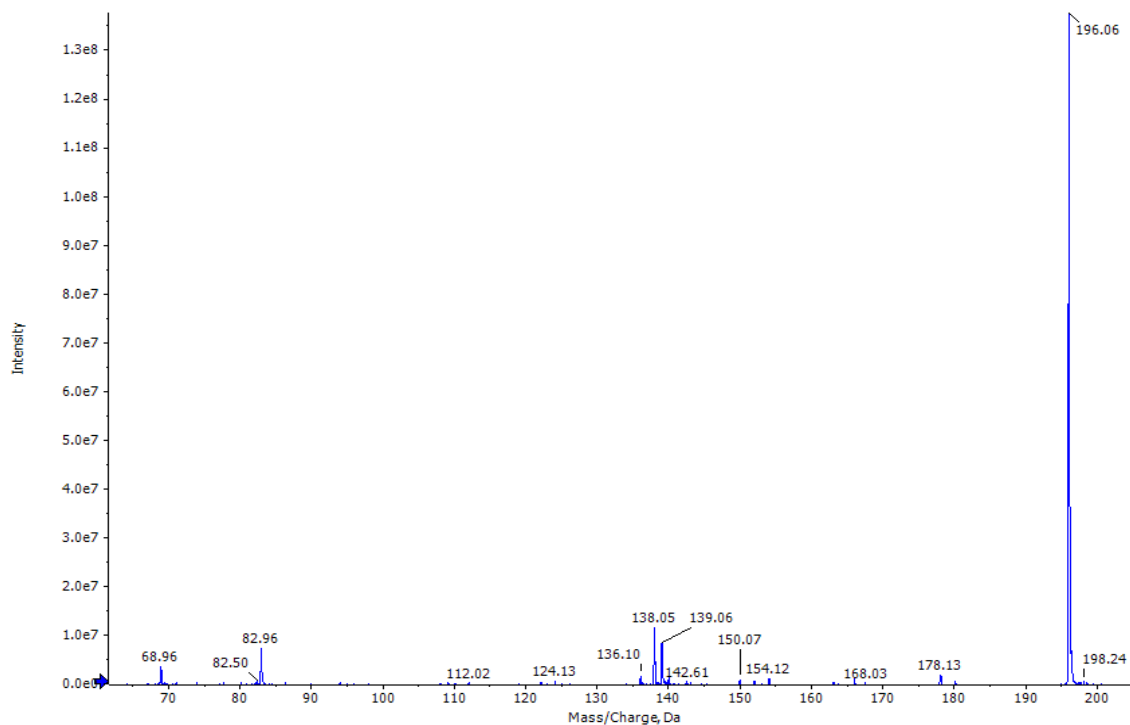


Figure S9. MS² mass chromatogram of Versimide.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 16.207 min
Precursor: 279.4 Da, Charge: 1, CE: 35.0

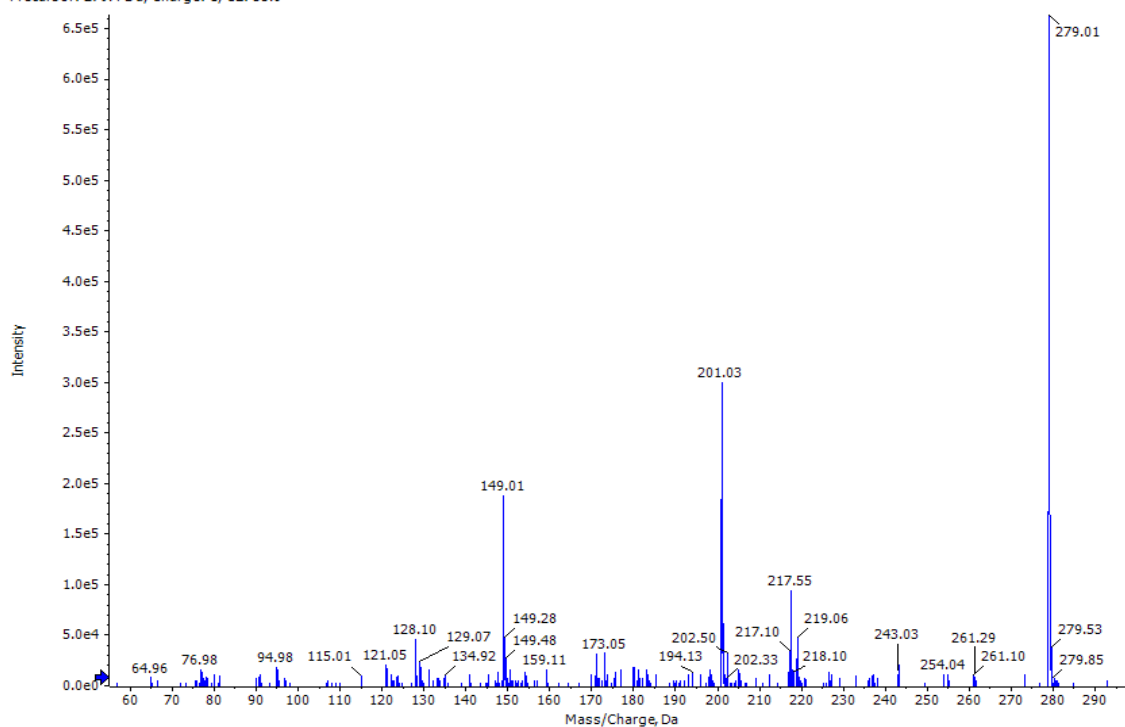


Figure S10. MS² mass chromatogram of 7-dehydrobrefeldin A.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 16.843 min
Precursor: 257.5 Da, Charge: 1

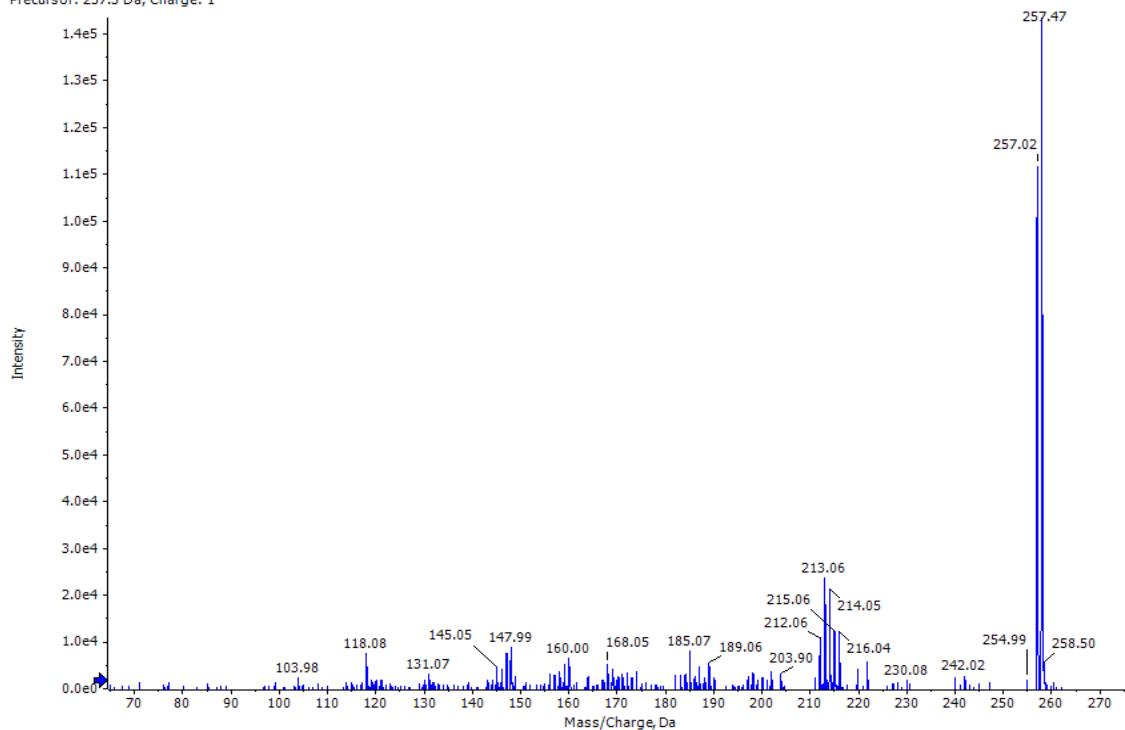


Figure S11. MS² mass chromatogram of Alternariol.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 17.214 min
Precursor: 197.8 Da, CE: 35.0

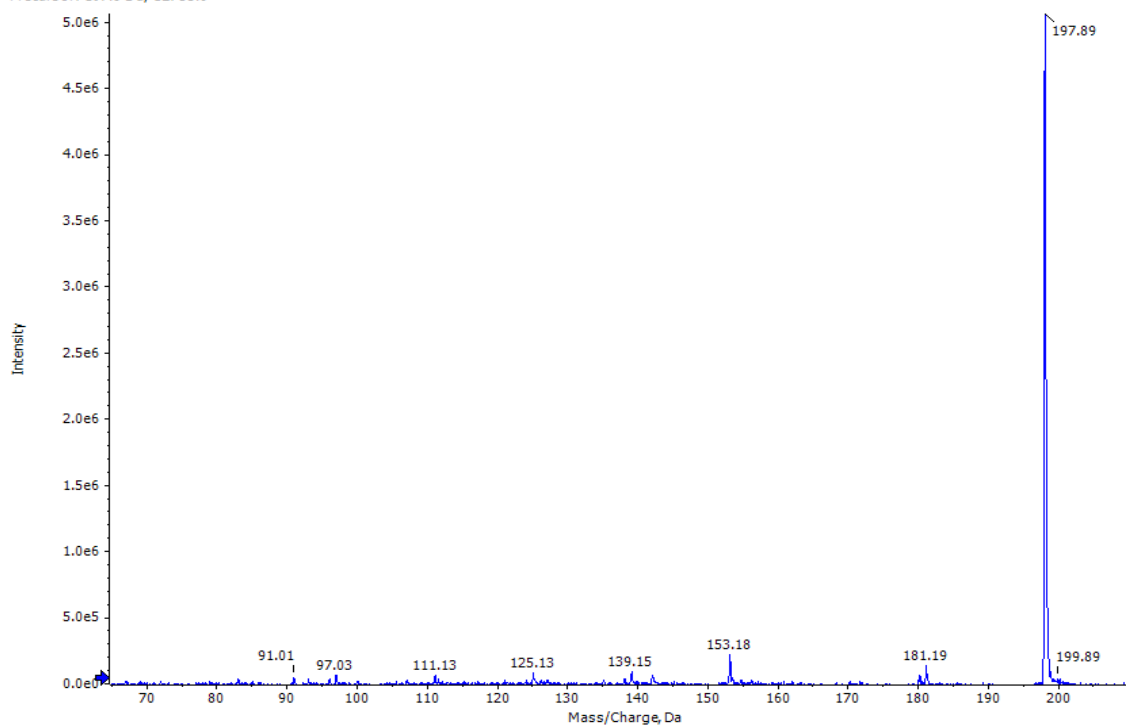


Figure S12. MS² mass chromatogram of 5-butyl-4-methoxy-6-methyl-2H-pyran-2-one.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 18.035 min
Precursor: 275.3 Da, Charge: 1, CE: 35.0

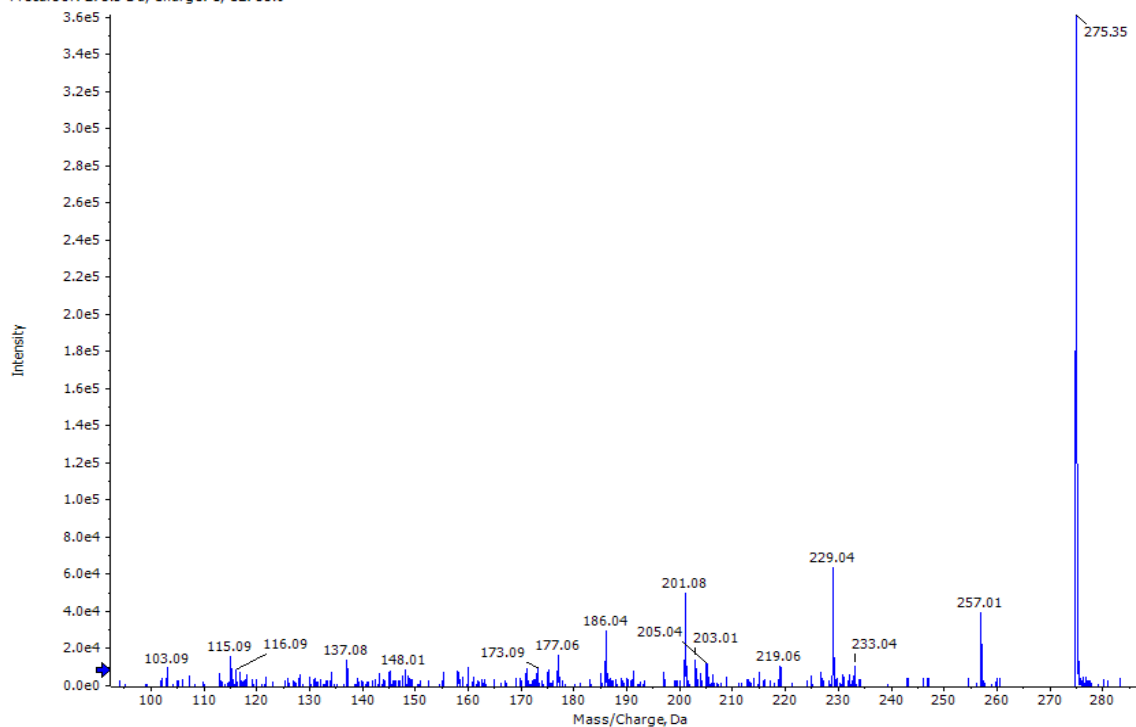


Figure S13. MS² mass chromatogram of Alvertenuol.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 18.084 min
Precursor: 259.2 Da, Charge: 1

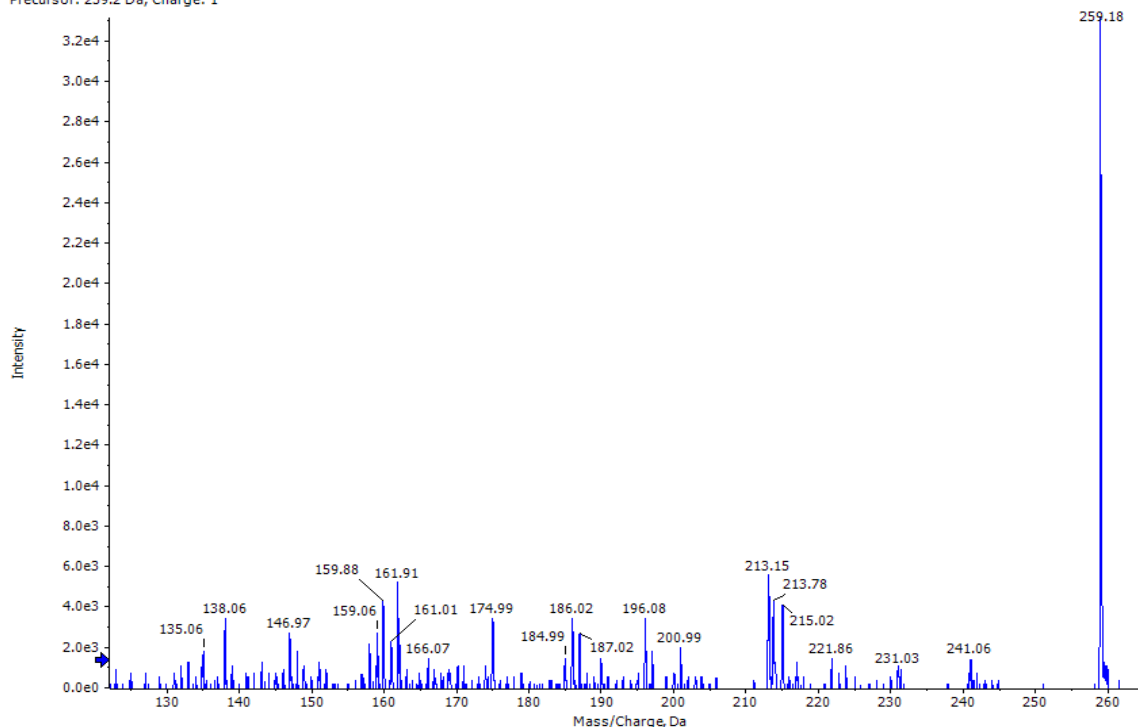


Figure S14. MS² mass chromatogram of 3-O-demethylaltenuisol.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 18.845 min
Precursor: 258.8 Da

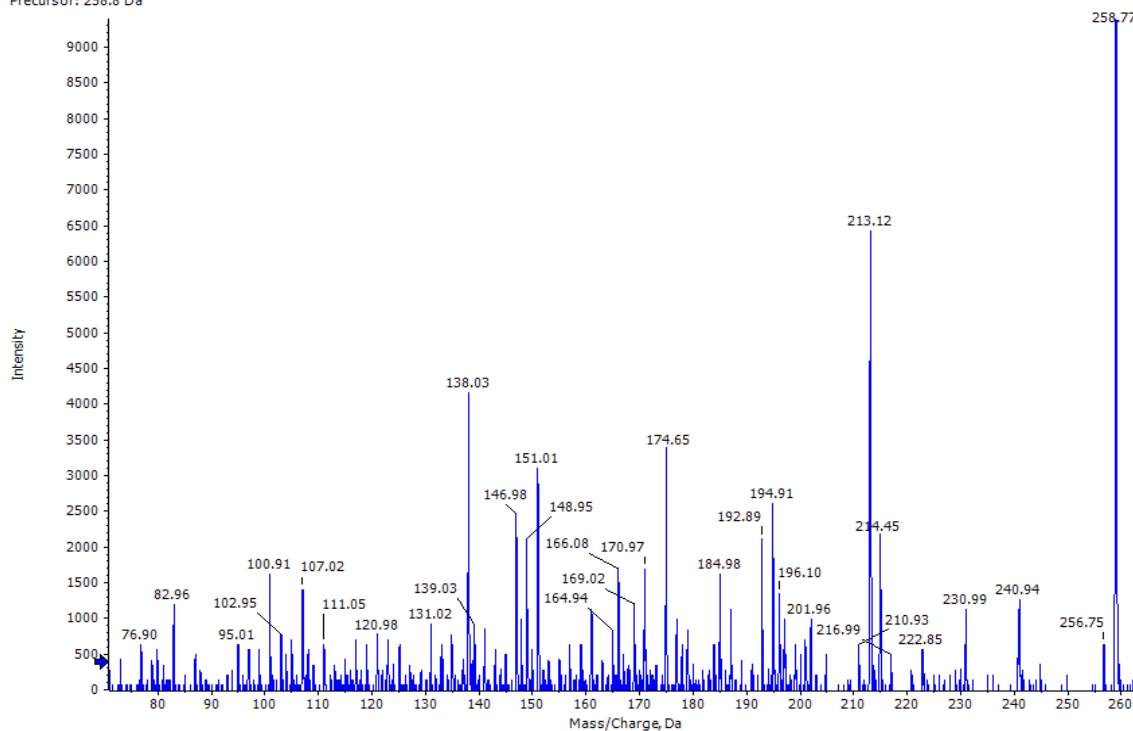


Figure S15. MS² mass chromatogram of (-)-alternarlactam.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 19.770 min
Precursor: 184.1 Da, Charge: 1, CE: 35.0

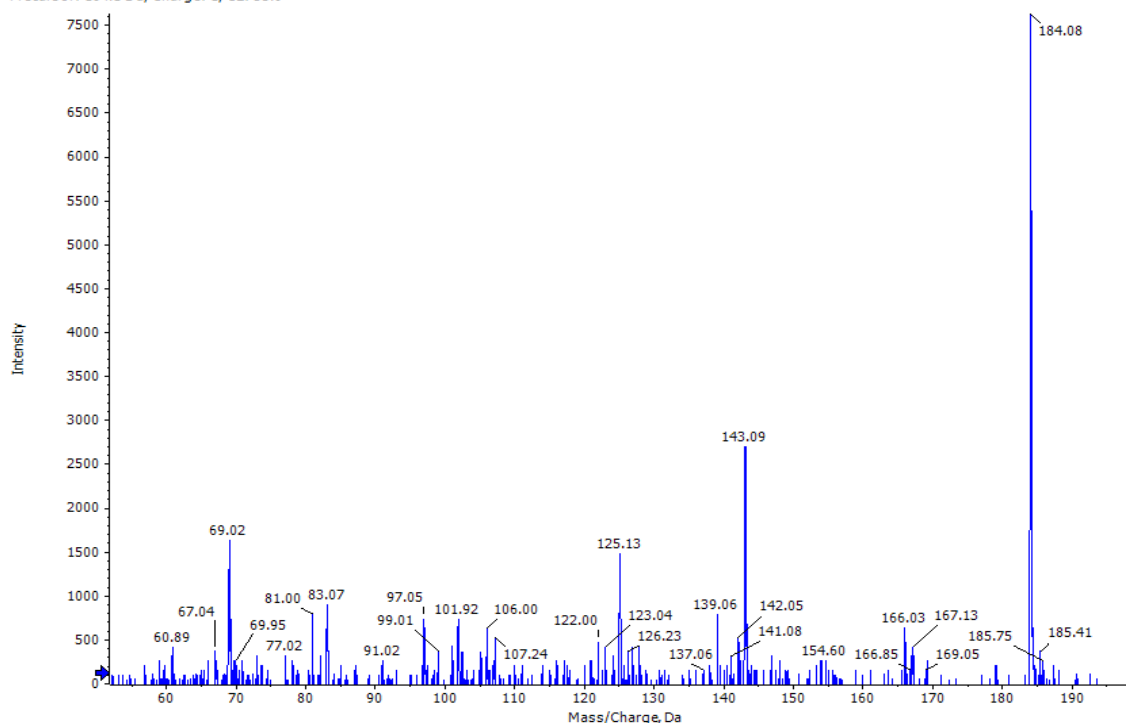


Figure S16. MS² mass chromatogram of 2-(N-vinylacetamide)-4-hydroxymethyl-3-enebutyrolactone.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 25.337 min
Precursor: 271.6 Da

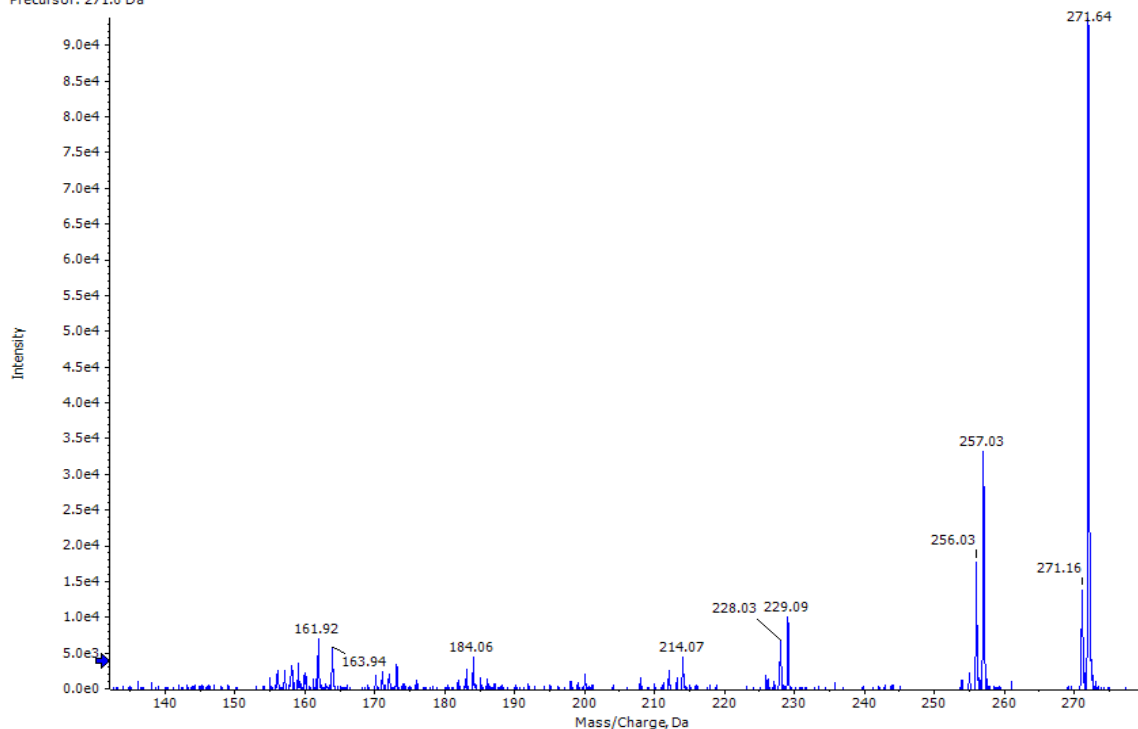


Figure S17. MS² mass chromatogram of Alternariol-9-methyl ether.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 30.177 min
Precursor: 255.7 Da
With 1 other merged spectrum

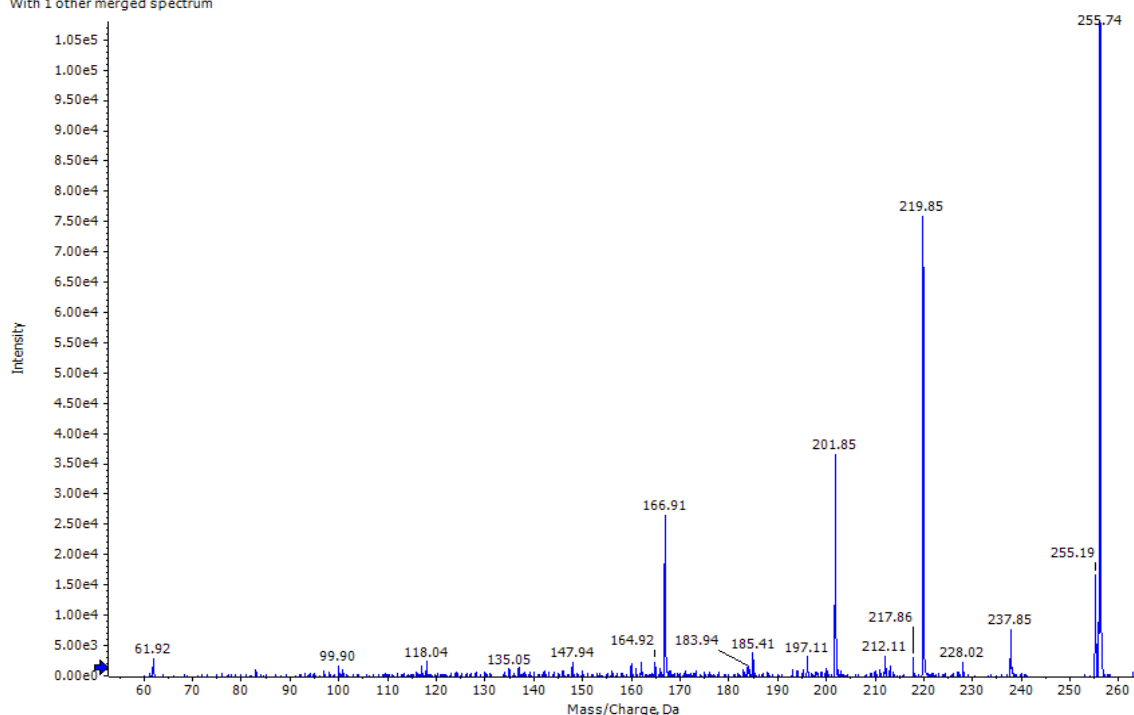


Figure S18. MS² mass chromatogram of Resveratroldehyde C.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 30.235 min
Precursor: 263.4 Da, Charge: 1, CE: 35.0

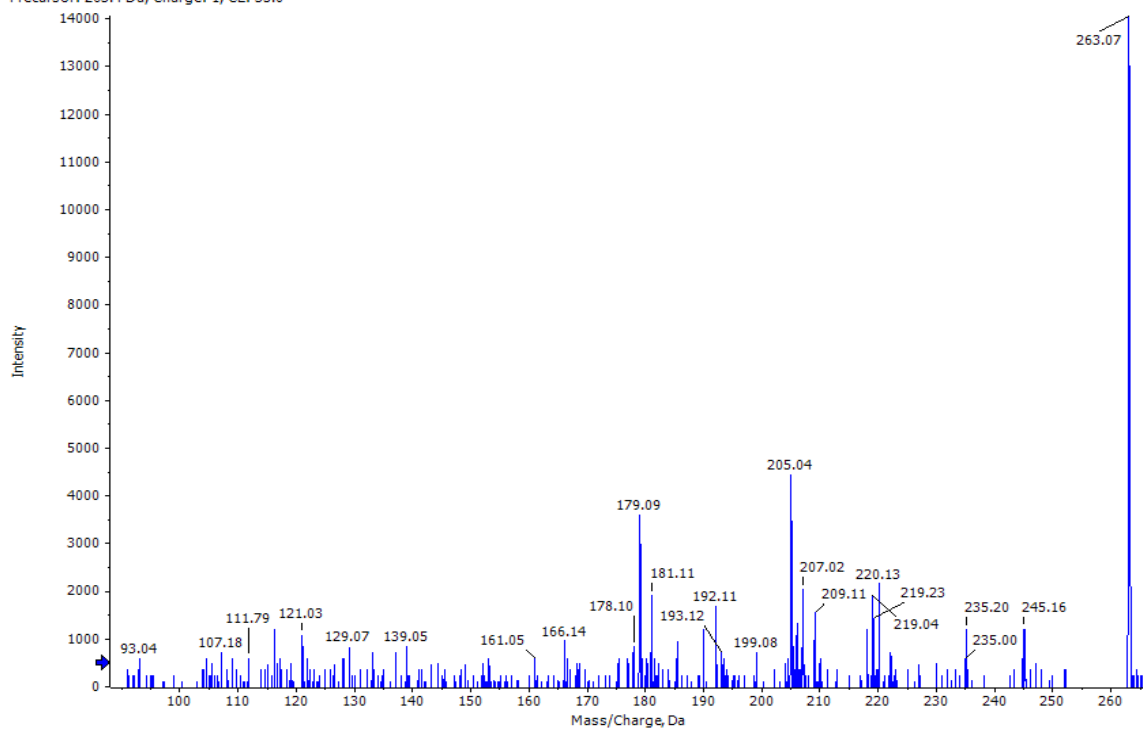


Figure S19. MS² mass chromatogram of Solanapyrone P.

Spectrum from AT -ve 1-6-2022 .wiff (sample 1) - AT -ve, Experiment 2, -EPI (50 - 800) from 31.128 min
Precursor: 265.8 Da, Charge: 1

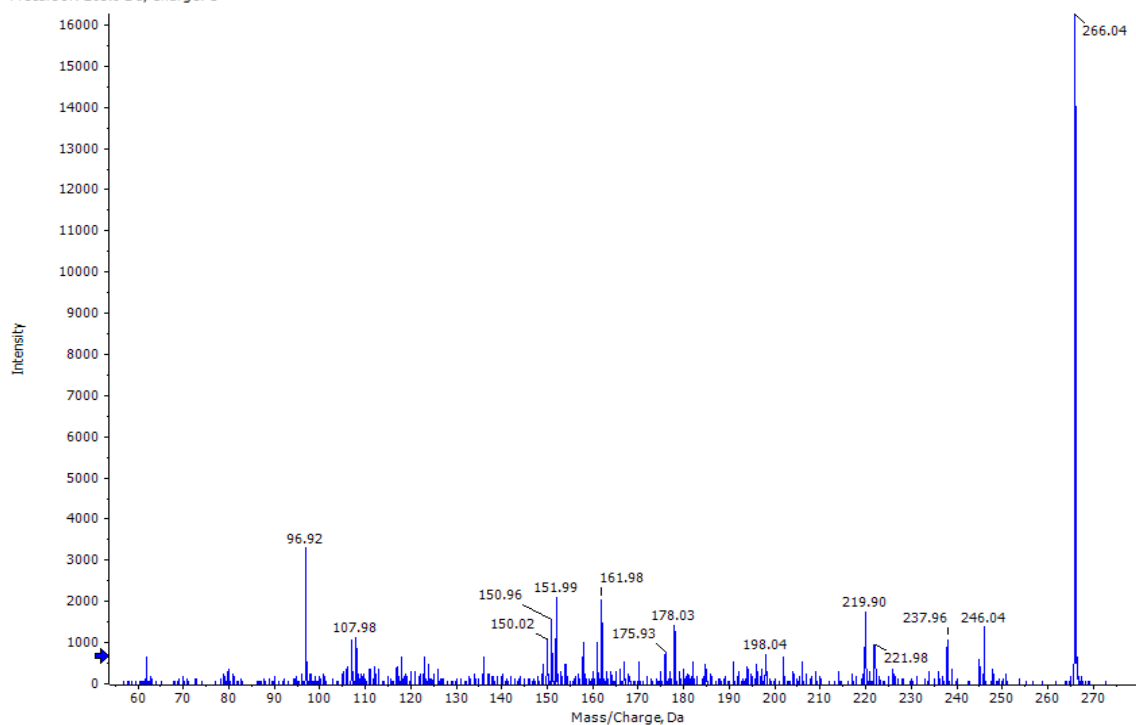


Figure S20. MS² mass chromatogram of Atransfusarin.

Spectrum from AT +ve 1-6-2022 .wiff (sample 1) - AT +ve, Experiment 2, +EPI (50 - 800) from 32.173 min
Precursor: 281.6 Da, Charge: 3, CE: 35.0

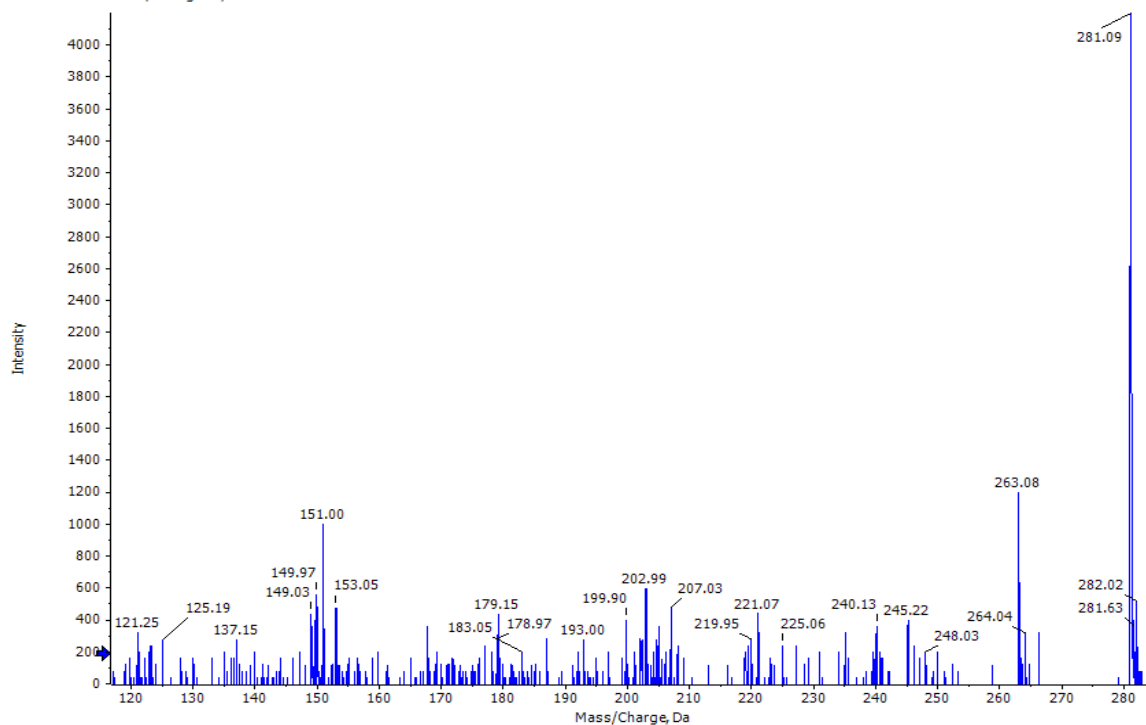


Figure S21. MS² mass chromatogram of Alternatain A.