Supplementary material

An integrated strategy of UHPLC-ESI-MS/MS combined with bioactivity-based molecular networking for identification of antitumoral withanolides from *Athenaea fasciculata* (Vell.) I.M.C. Rodrigues & Stehmann

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Figure S1. MS/MS spectrum of compound **1** at *m/z* 528.9 $[M-H]^-$ (virginol A)

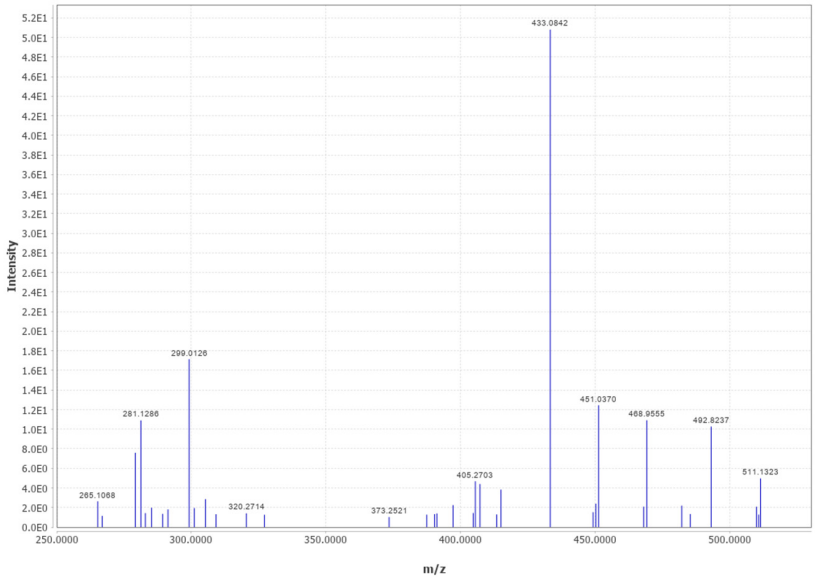


Figure S2. MS/MS spectrum of compound **2** at *m/z* 486.9 $[M-H]^-$ (16-deoxyphiladelphicalactone C)

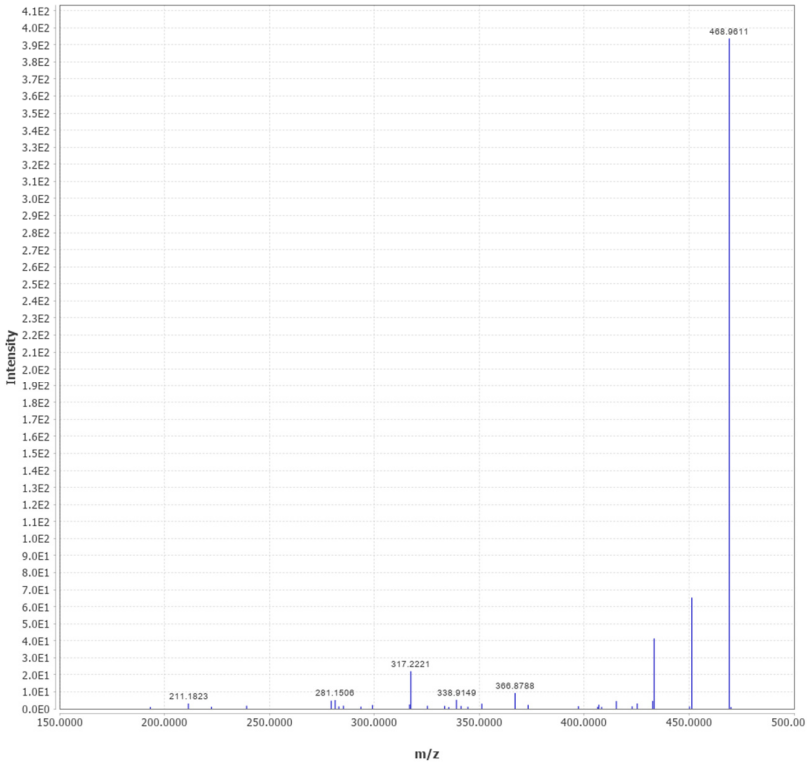


Figure S3. MS/MS spectrum of compound **3** at *m*/*z* 542.9 $[M-H]^-$ (withaneomexolide A).

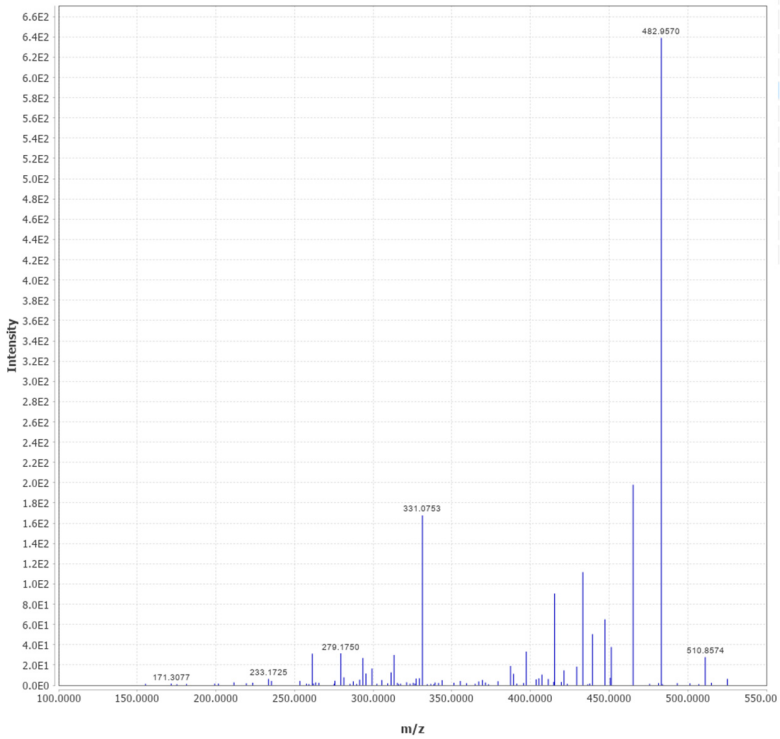


Figure S4. MS/MS spectrum of compound **4** at *m*/*z* 560.9 [M-H]$^-$ (20S,22R,24S,25S,26R/S)-15α-acetoxy-5,6β:22,26:diepoxy-24-methoxy-4β,25,26-trihydroxyergost-2-en-1-one).

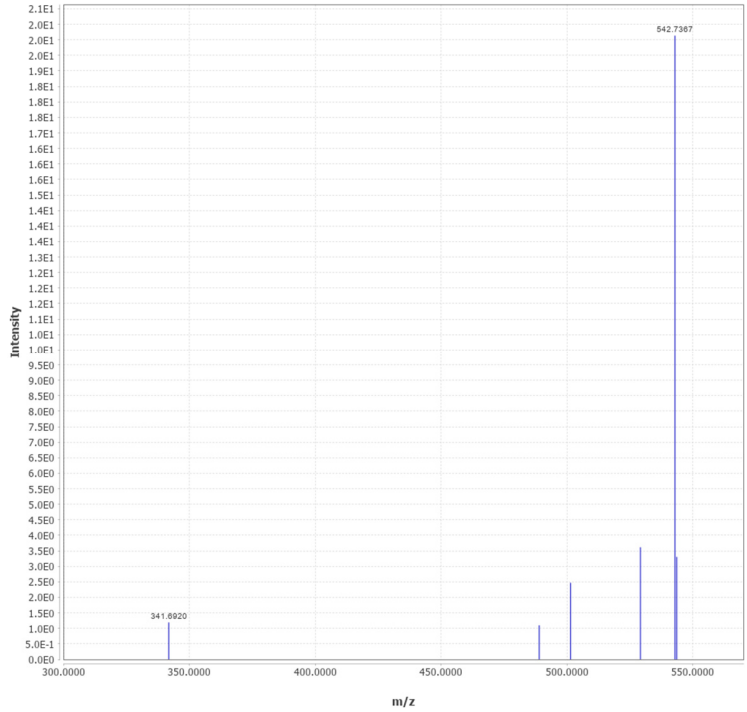


Figure S5. MS/MS spectrum of compound **5** at *m*/*z* 434.9 [M-H]$^-$ ((4S,20S,22R)-4-Hydroxy-1-oxo-witha-2,5,16,24-tetraenolide).

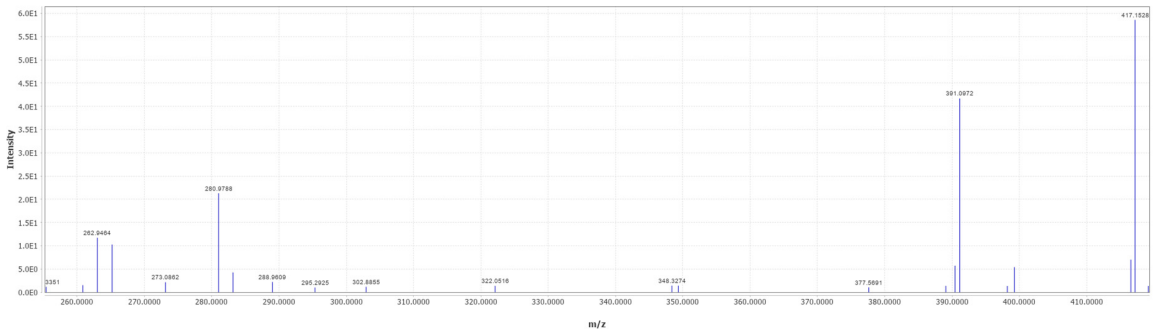


Figure S6. MS/MS spectrum of compound **6** at *m*/*z* 512.8 [M-H]$^-$ (physapubescin H).

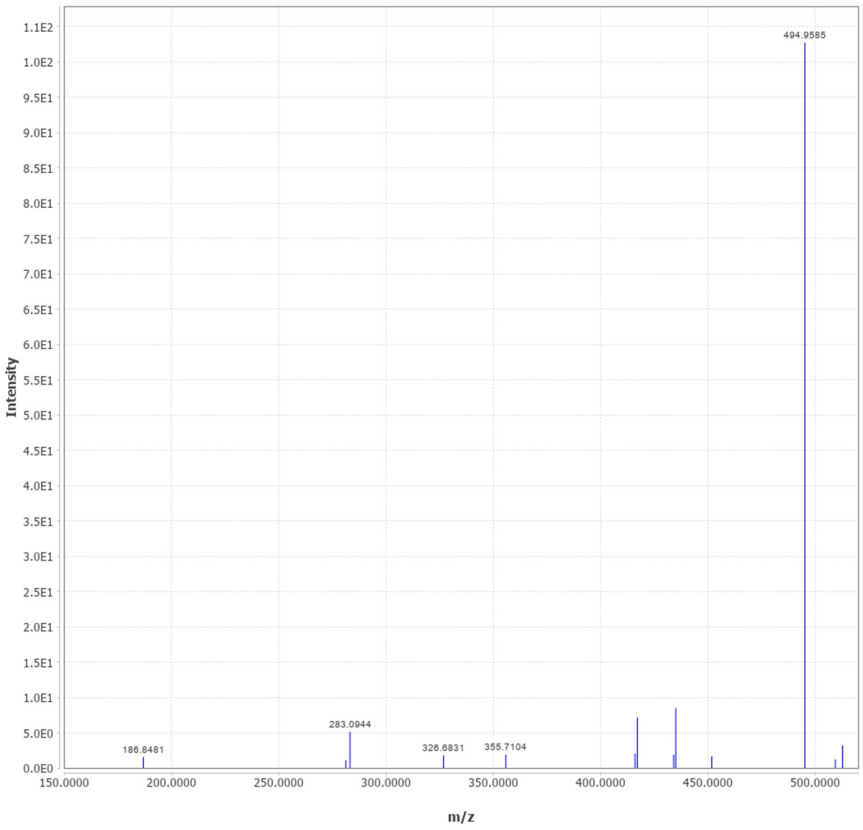

Intensity
1.1E2
1.0E2
9.5E1
9.0E1
8.5E1
8.0E1
7.5E1
7.0E1
6.5E1
6.0E1
5.5E1
5.0E1
4.5E1
4.0E1
3.5E1
3.0E1
2.5E1
2.0E1
1.5E1
1.0E1
5.0E0
0.0E0
494.9585
283.0944
186.8481
326.6831
355.7104
150.0000
200.0000
250.0000
300.0000
350.0000
400.0000
450.0000
500.0000
m/z

Figure S7. MS/MS spectrum of compound **7** at *m*/*z* 526.9 [M-H]$^-$ (aurelianolide A).

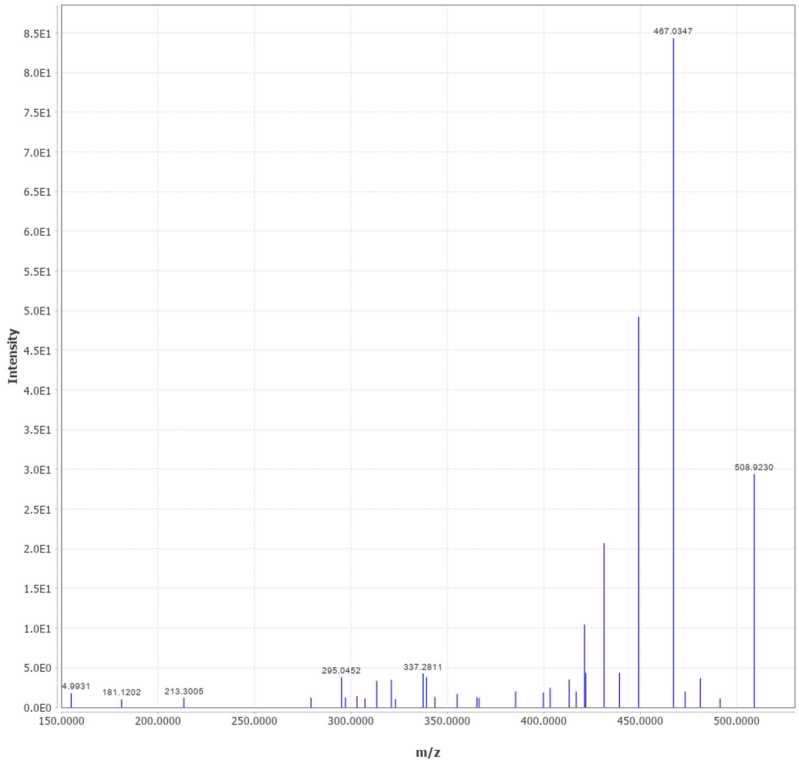


Figure S8. MS/MS spectrum of compound **8** at *m*/*z* 508.9 [M-H]$^-$ (physaminilide H).

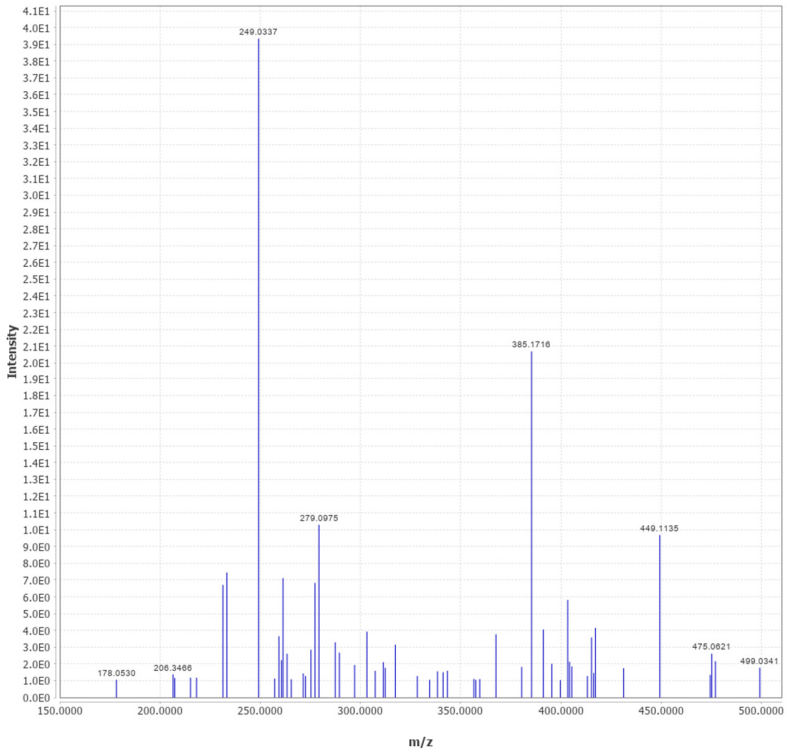


Figure S9. MS/MS spectrum of compound **8** at *m*/*z* 510.9 $[M+H]^+$ (physaminilide H).

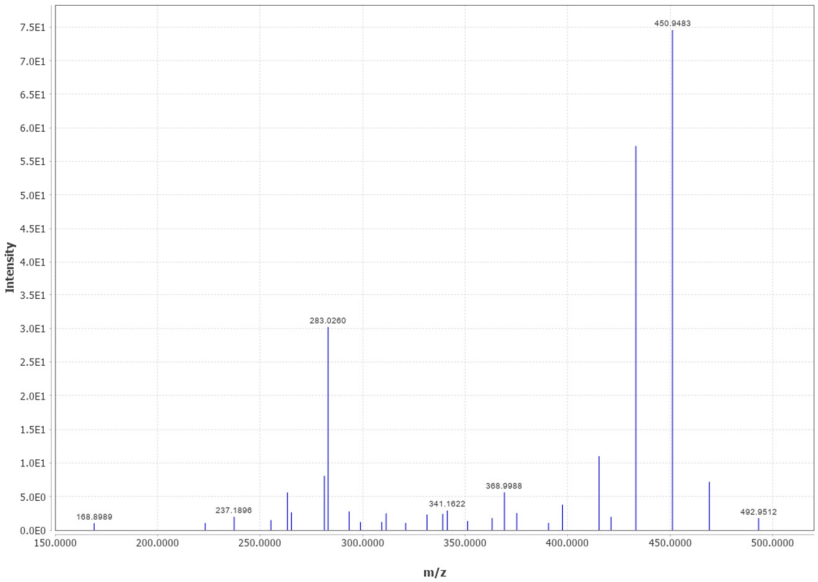


Figure S10. MS/MS spectrum of compound **9** at *m*/*z* 510.9 $[M-H]^-$ (aurelianolide B).

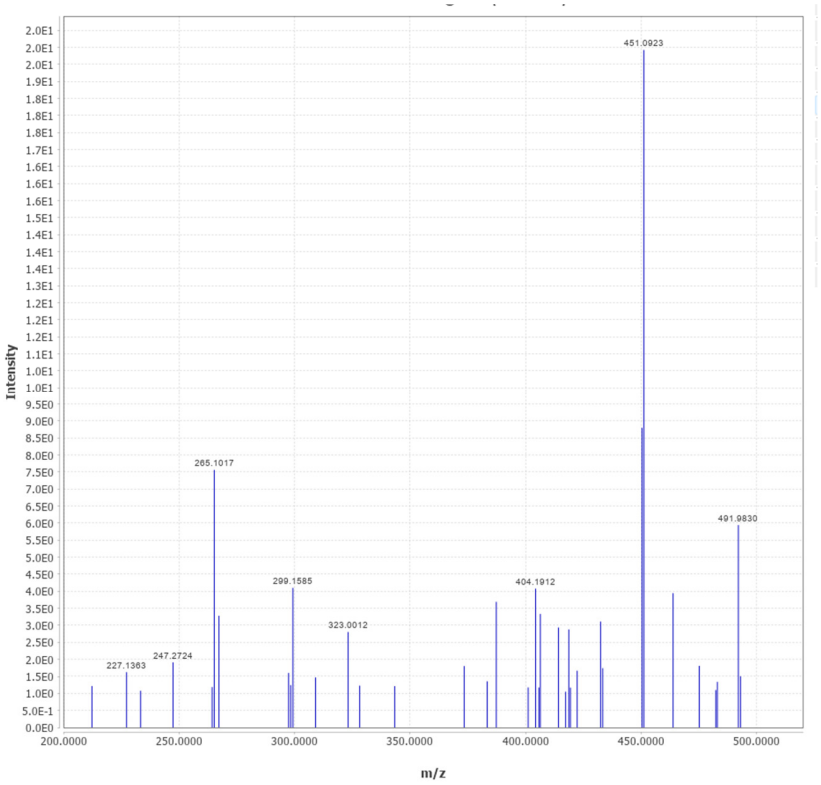


Figure S11. MS/MS spectrum of compound **9** at *m*/*z* 512.9 $[M+H]^+$ (aurelianolide B).

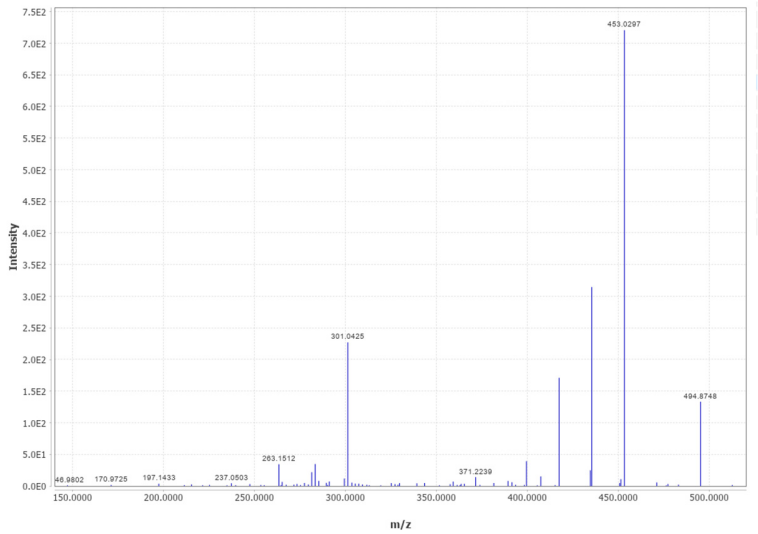


Figure S12. MS/MS spectrum of compound **10** at *m*/*z* 478.9 $[M-H]^-$ (nicanlode C).

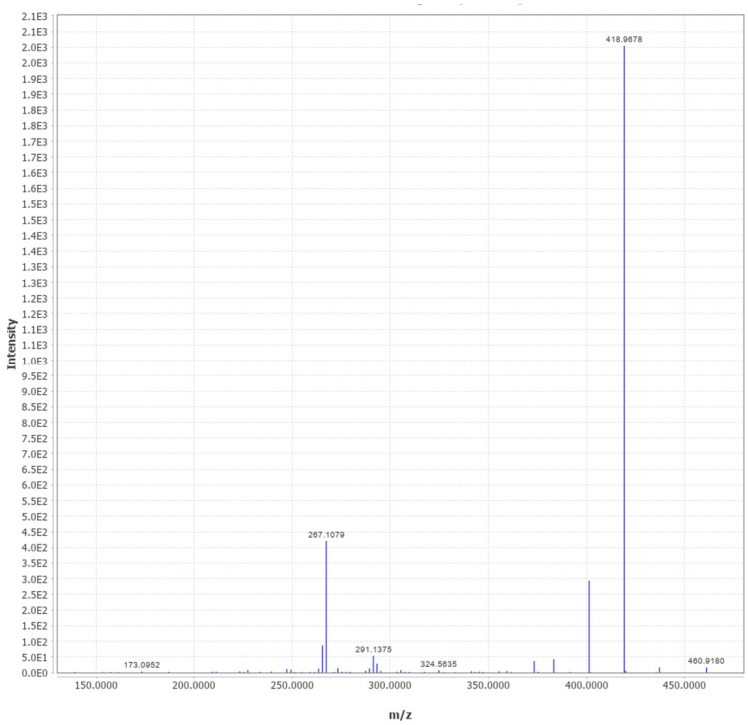


Figure S13. MS/MS spectrum of compound **11** at *m/z* 419.0 $[M-H]^-$ (phenowithanolide).

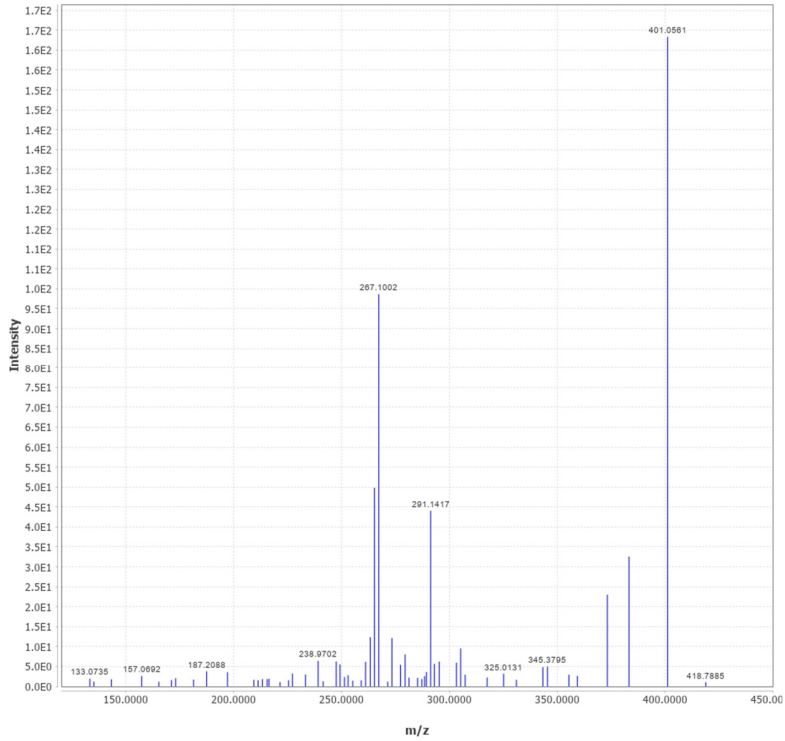


Figure S14. MS/MS spectrum of compound **12** at *m/z* 519.2 $[M-H]^-$ (withaperuvin N).

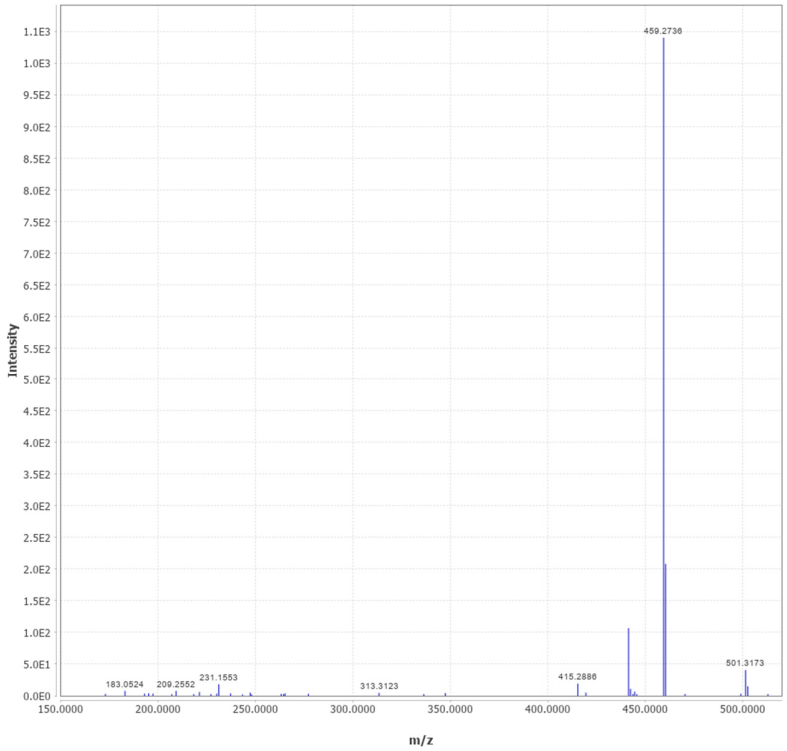


Figure S15. MS/MS spectrum of compound **13** at *m/z* 496.9 $[M-H]^-$ (baimantuoluoline).

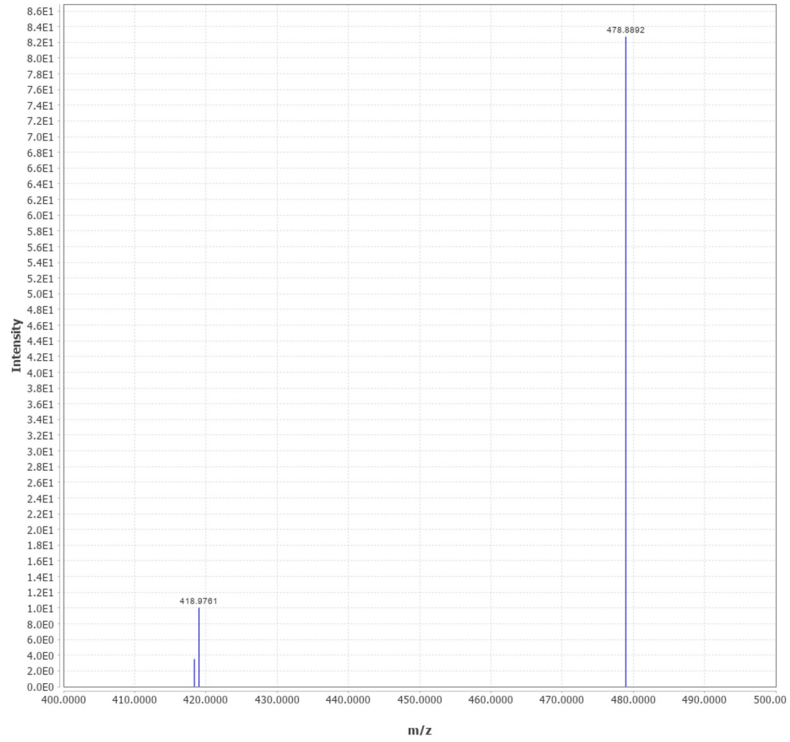


Figure S16. MS/MS spectrum of compound **14** at *m/z* 526.9 $[M+H]^+$ (physaminilide B).

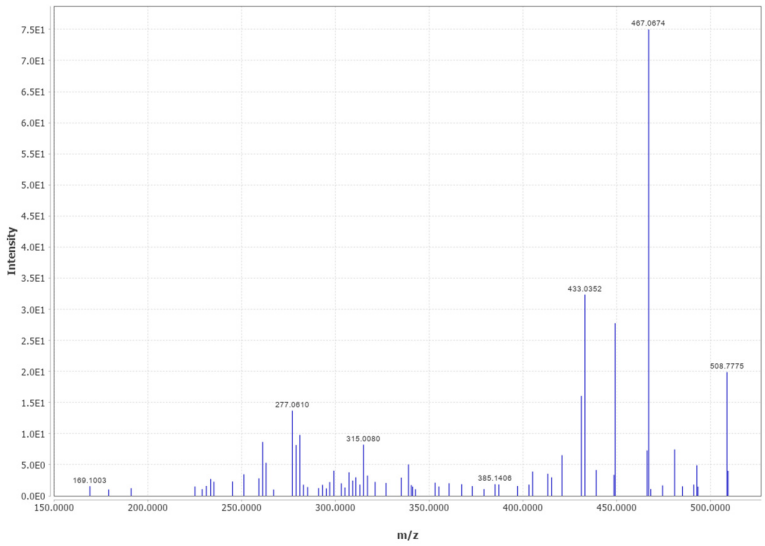


Figure S17. MS/MS spectrum of compound **15** at *m*/*z* 560.9 $[M+H]^+$ (physanicandrolide B).

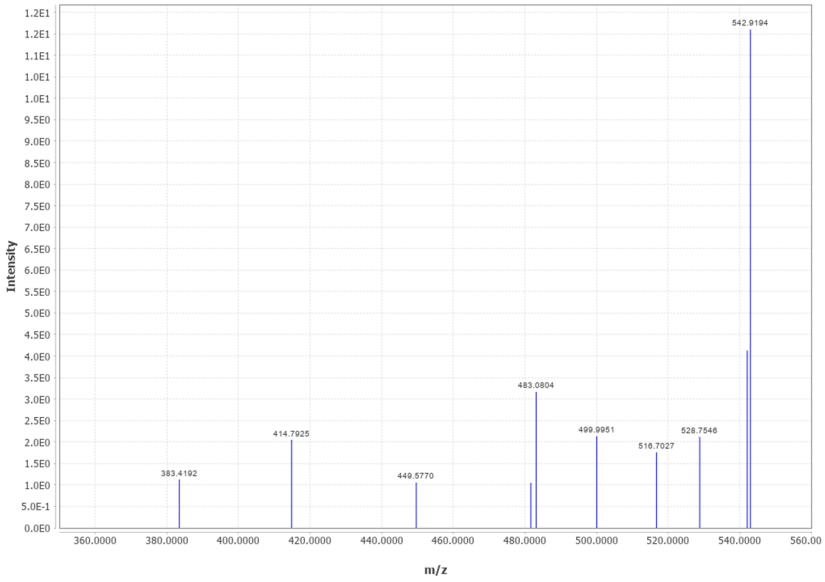


Figure S18. MS/MS spectrum of compound **16** at *m*/*z* 542.9 $[M+H]^+$ (physagulide C).

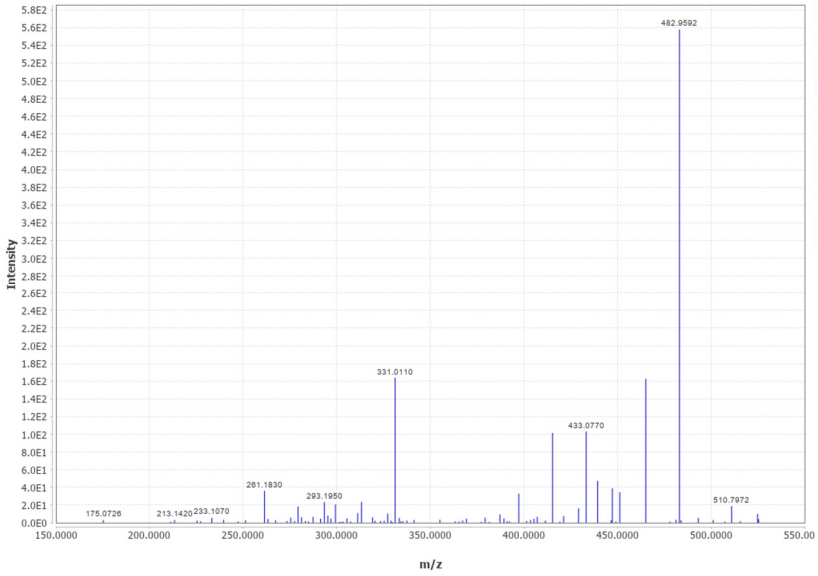


Figure S19. MS/MS spectrum of compound **17** at *m*/*z* 492.9 $[M+H]^+$ (capsisteroid G).

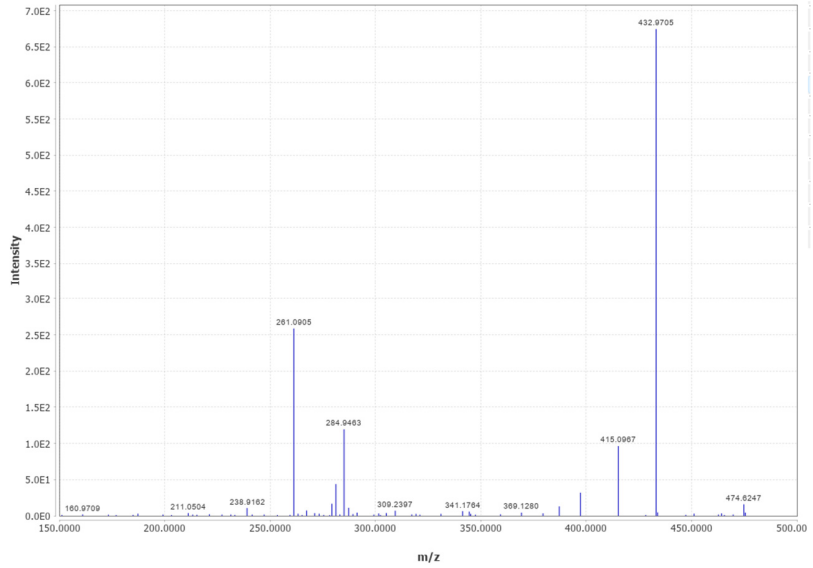


Figure S20. MS/MS spectrum of compound **18** at *m*/*z* 508.9 $[M+H]^+$ (capsisteroid D).

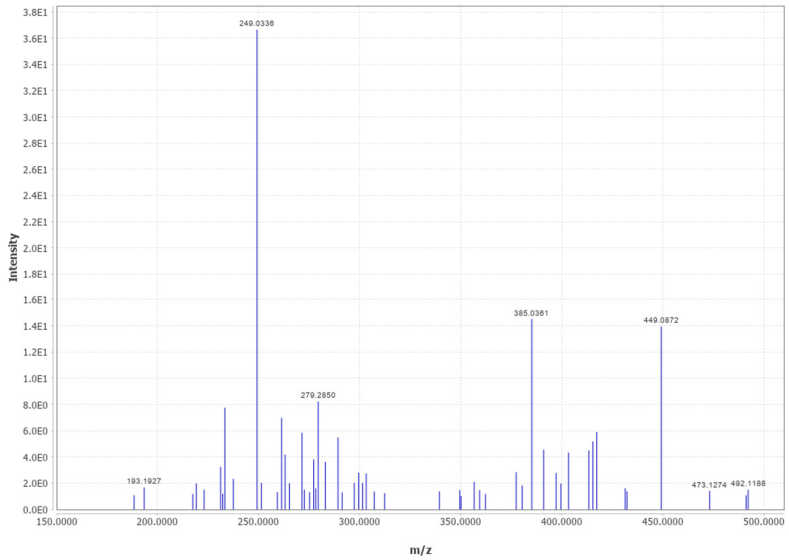


Figure S21. MS/MS spectrum of compound **19** at *m*/*z* 519.2 $[M+H]^+$ (withalongolide D).

