

Comparative Metabolic Profiling of *Raphanus sativus* Hybrid Varieties and Its Biological Properties

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Table S1. %RSA of *R. sativus* cultivars (RL1, RL2 and RL3).

Samples	% RSA
Positive control	91.18 ± 0.31 %
RL1	86.80 ± 0.55 %
RL2	84.79 ± 1.07 %
RL3	84.89 ± 0.73 %

Figure S1. Standard curve of positive control Gallic acid.

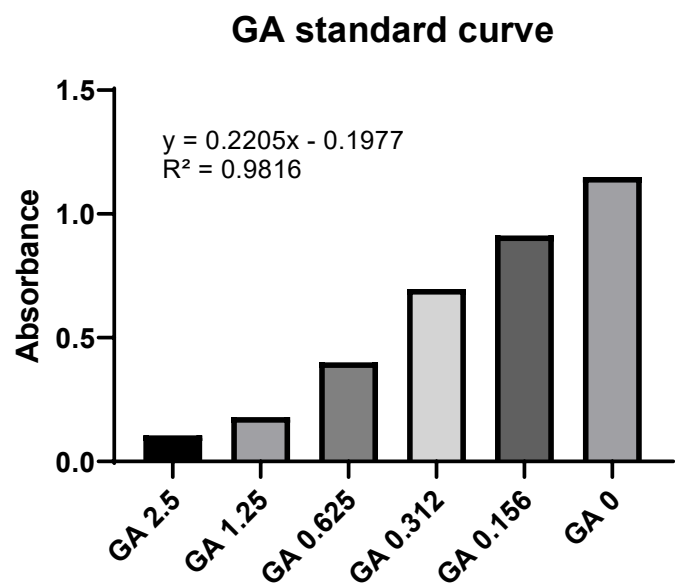
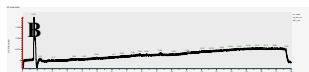
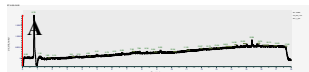


Figure S2. UV chromatograms of *Raphanus sativus* leaf extracts analyzed at λ_{max} 210 nm RL1 extract (**A**), RL2 extract (**B**), RL3 extract (**C**)



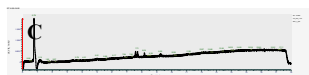
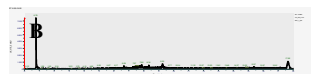
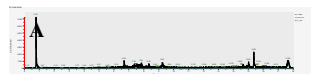


Figure S3. UV chromatograms of *Raphanus sativus* leaf extracts analyzed at λ_{max} 254 nm RL1 extract (**A**), RL2 extract (**B**), RL3 extract (**C**)



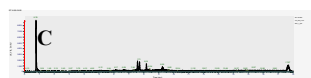
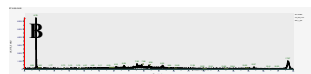
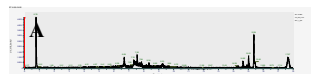


Figure S4. UV chromatograms of *Raphanus sativus* leaf extracts analysed in λ_{max} 315 nm RL1 extract (**A**), RL2 extract (**B**), RL3 extract (**C**)



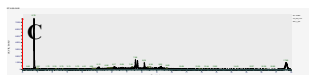
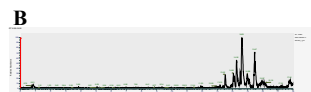


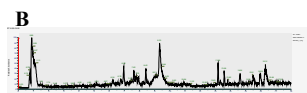
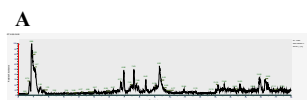
Figure S5. Mass spectra base peak of *Raphanus sativus* leaf extracts analyzed in positive ion mode RL1 extract (**A**), RL2 extract (**B**), RL3 extract (**C**)



C



Figure S6. Mass spectra base peak of *Raphanus sativus* leaf extracts analyzed in negative ion mode RL1 extract (**A**), RL2 extract (**B**), RL3 extract (**C**)



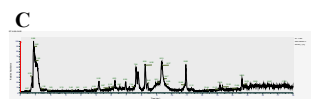


Figure S7. ESI-MS/MS spectrum of compound **1** in positive ion mode at m/z 287.0551 $[M+H]^+$

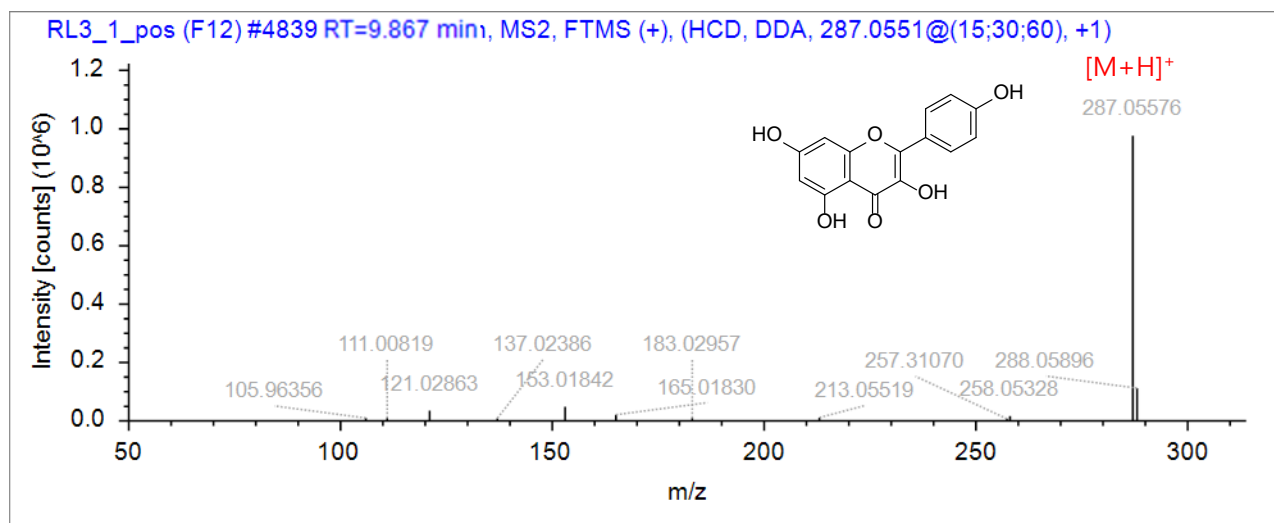


Figure S8. ESI-MS/MS spectrum of compound **2** in negative ion mode at m/z 285.0406 $[M-H]^-$

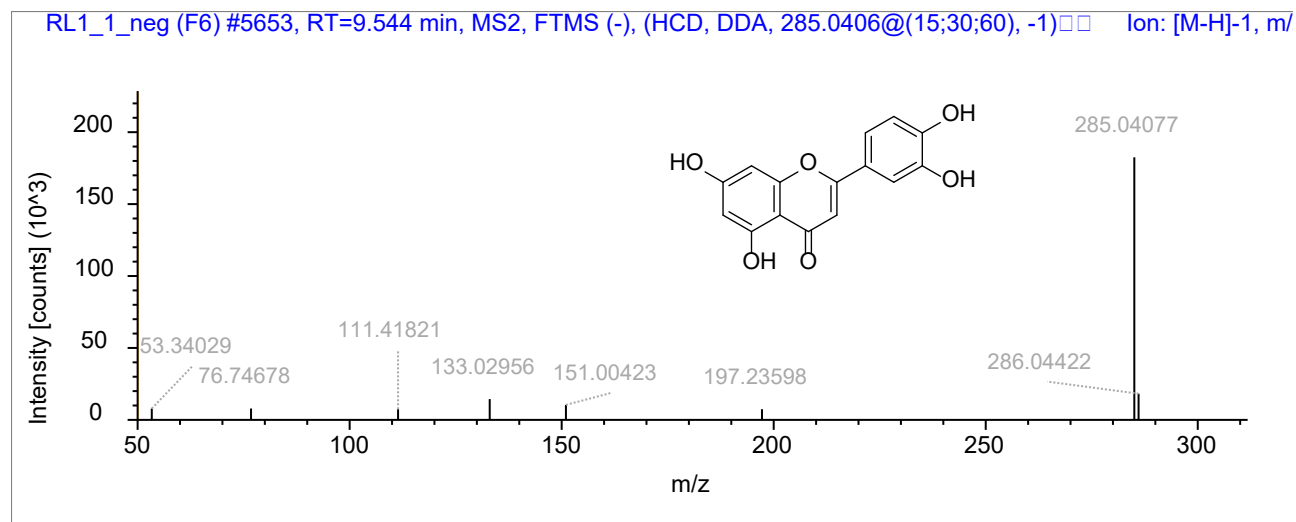


Figure S9. ESI-MS/MS spectrum of compound **3** in positive ion mode at m/z 341.0269 $[M+Na]^+$

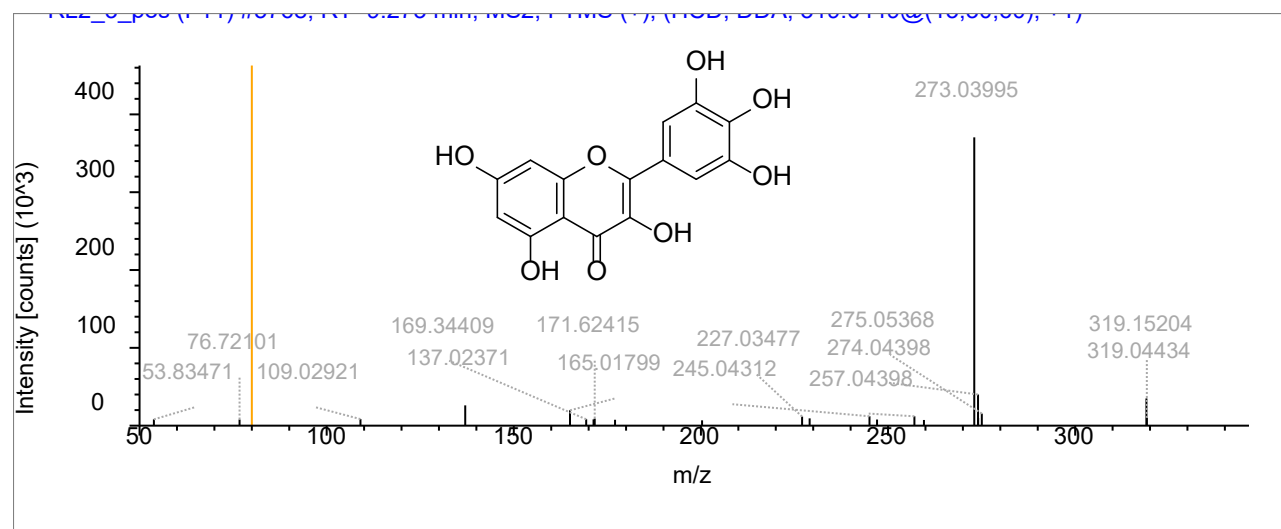


Figure S10. ESI-MS/MS spectrum of compound **4** in negative ion mode at m/z 331.0461 $[M-H]^-$

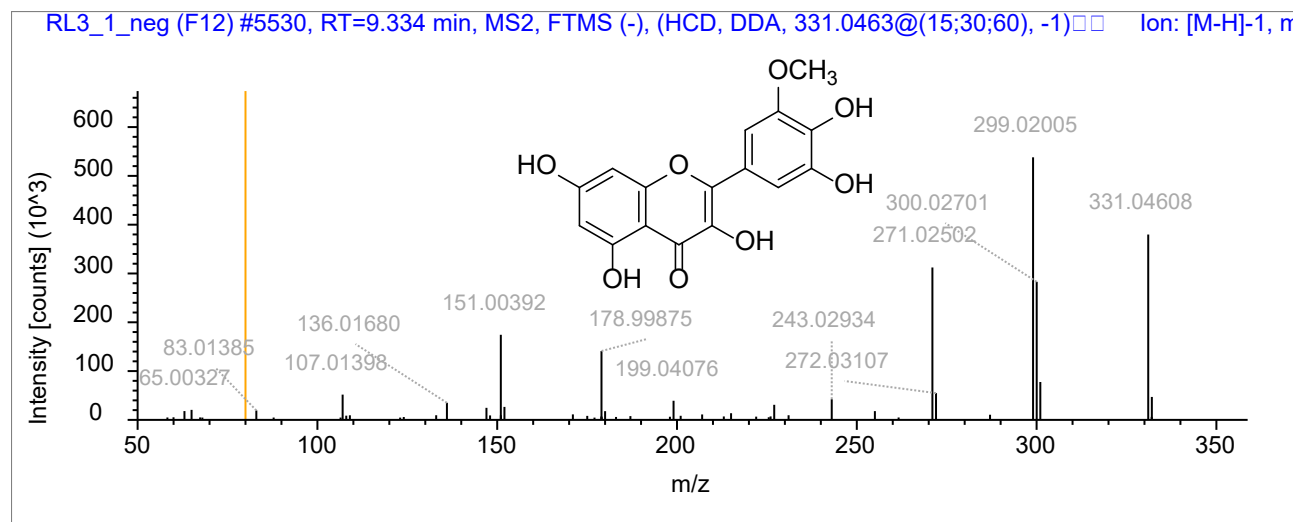


Figure S11. ESI-MS/MS spectrum of compound **5** in positive ion mode at m/z 273.1121 $[M+H]^+$

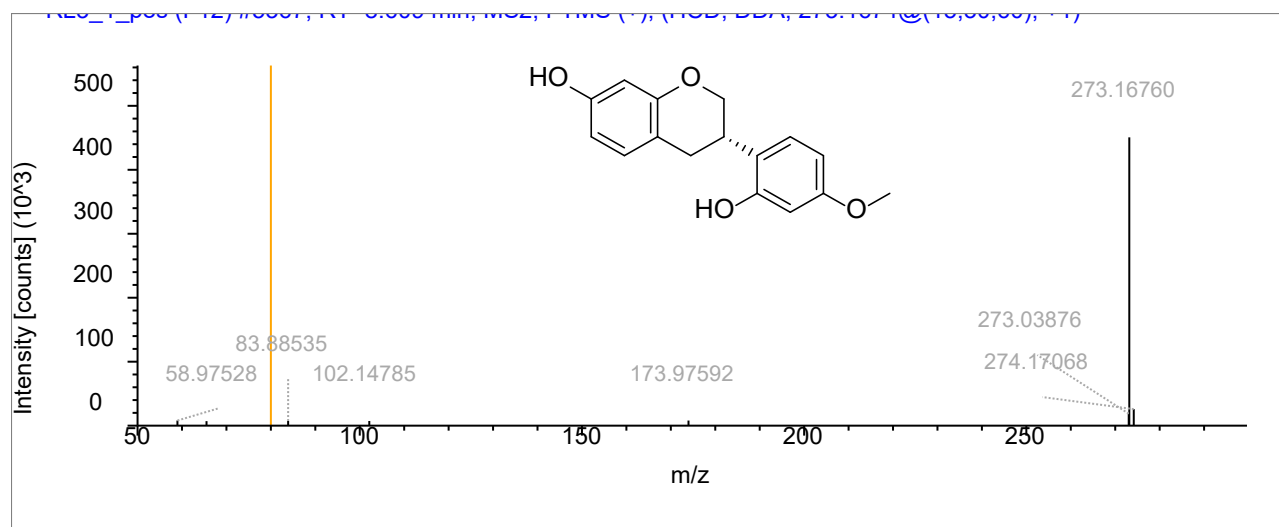


Figure S12. ESI-MS/MS spectrum of compound **6** in the negative ion mode at m/z 431.0984 $[M-H]^-$

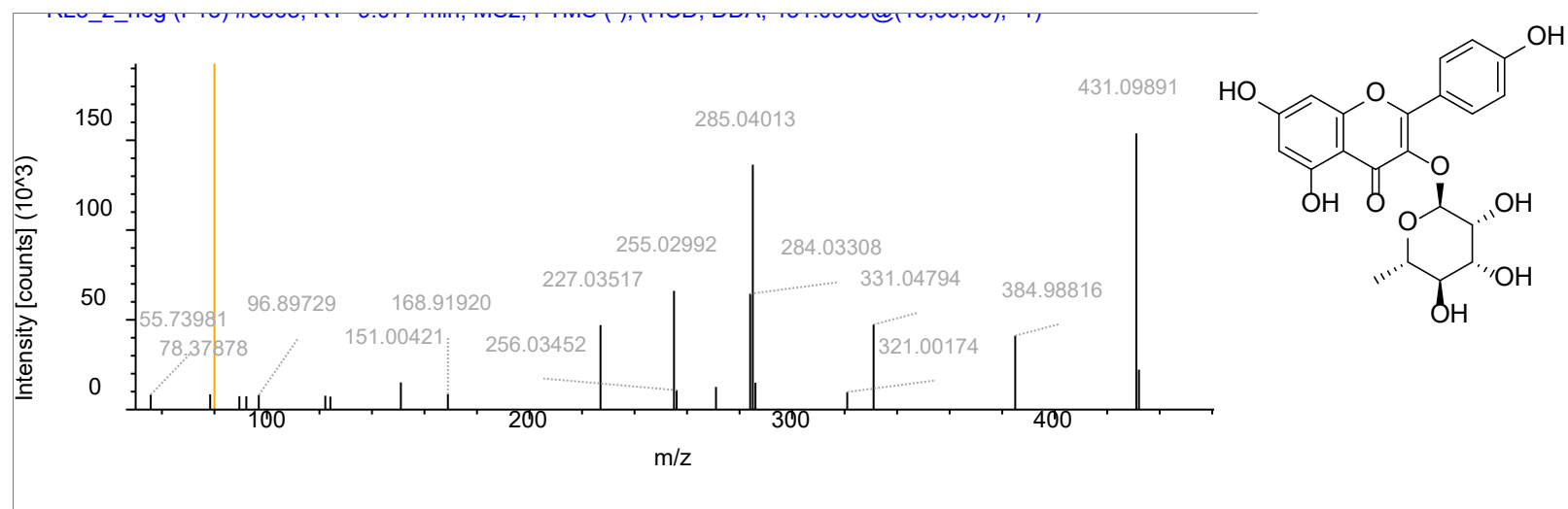


Figure S13. ESI-MS/MS spectrum of compound **7** in negative ion mode at m/z 447.0934 $[M-H]^-$

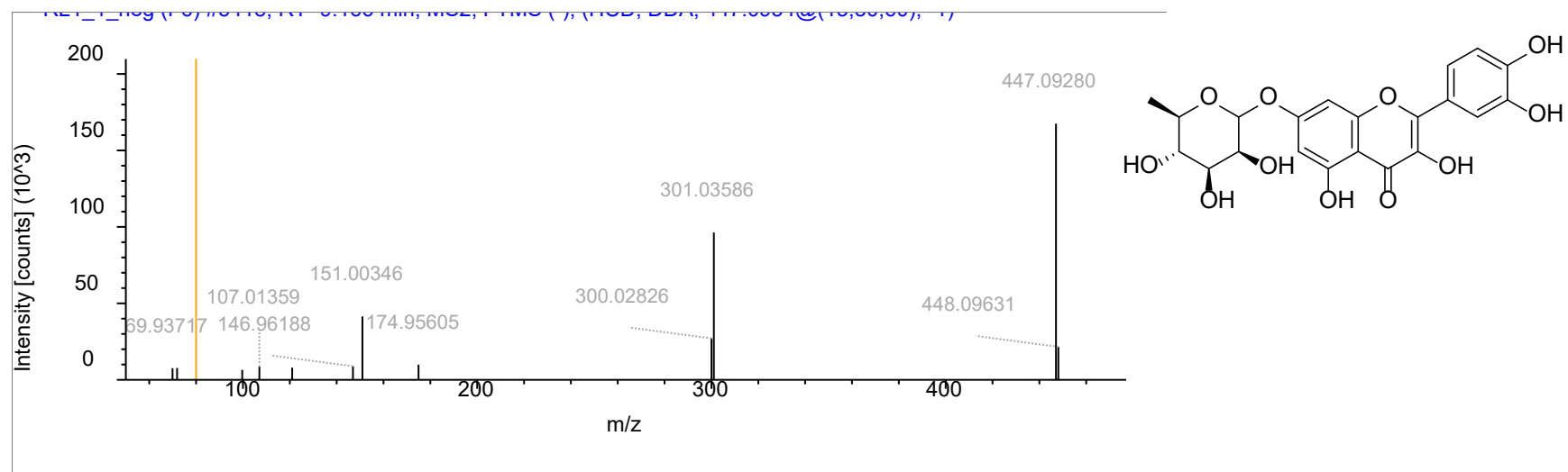


Figure S14. ESI-MS/MS spectrum of compound **8** in negative ion mode showing at m/z 447.0934 $[M-H]^-$

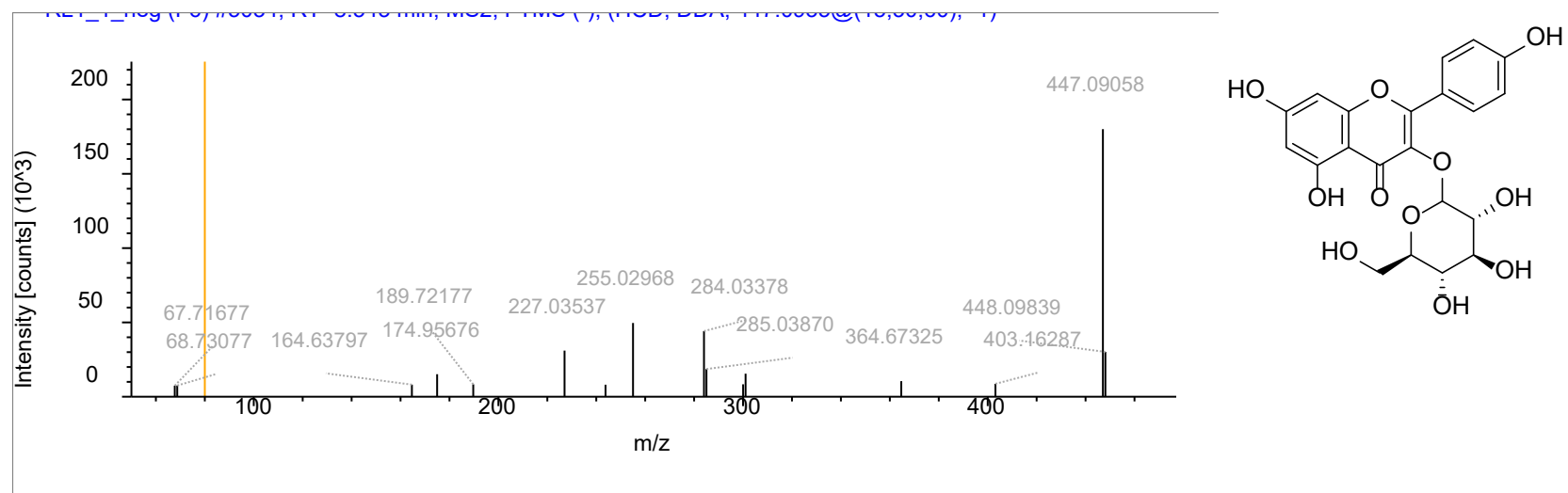


Figure S15. ESI-MS/MS spectrum of compound **9** in negative ion mode showing at m/z 463.0885 $[M-H]^-$

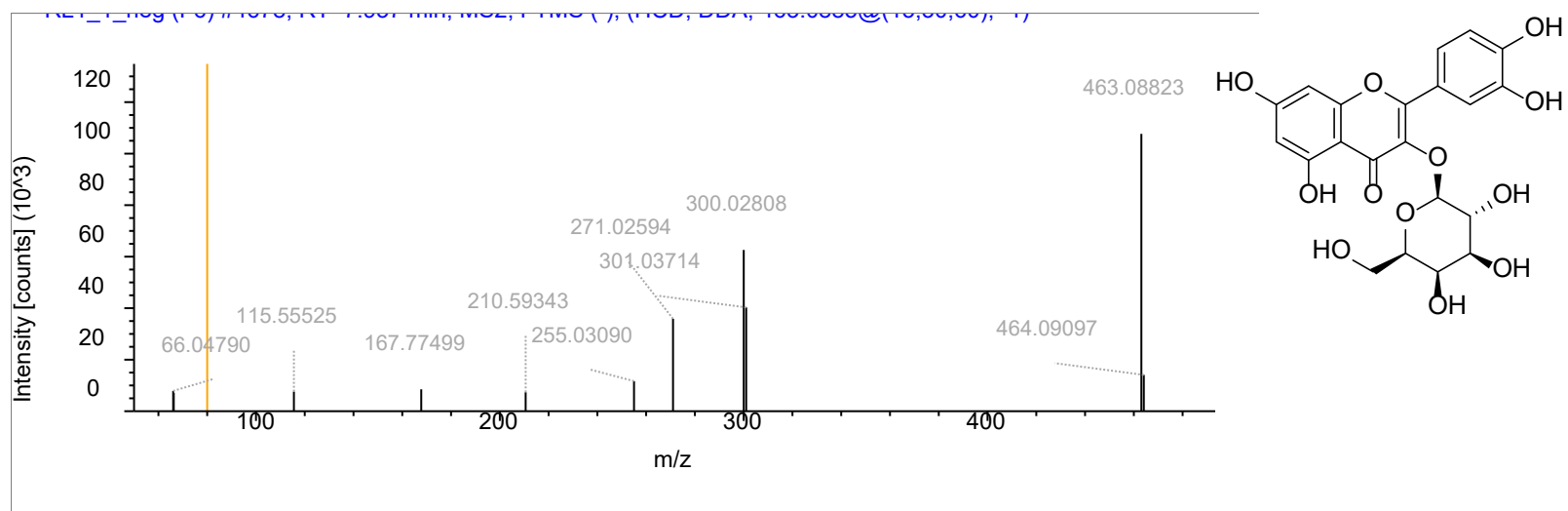


Figure S16. ESI-MS/MS spectrum of compound **10** in the negative ion mode showing at m/z 505.1355 $[M-H]^-$

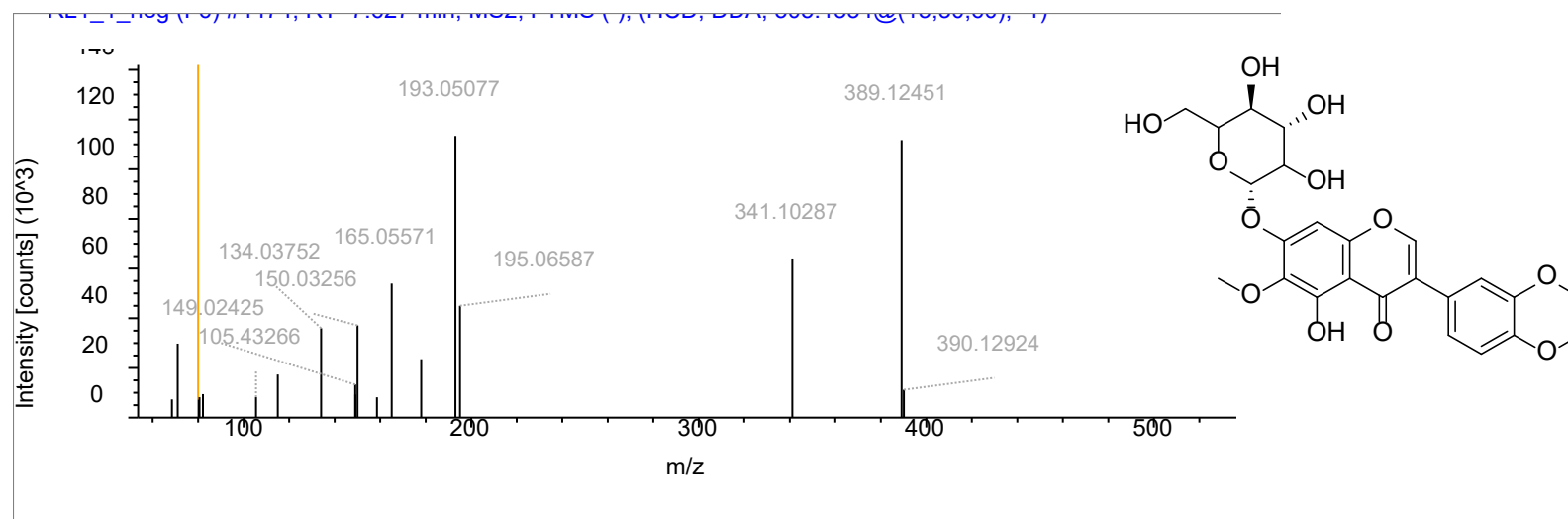


Figure S17. ESI-MS/MS spectrum of compound **11** in the negative ion mode showing at m/z 563.1410 $[M-H]^-$

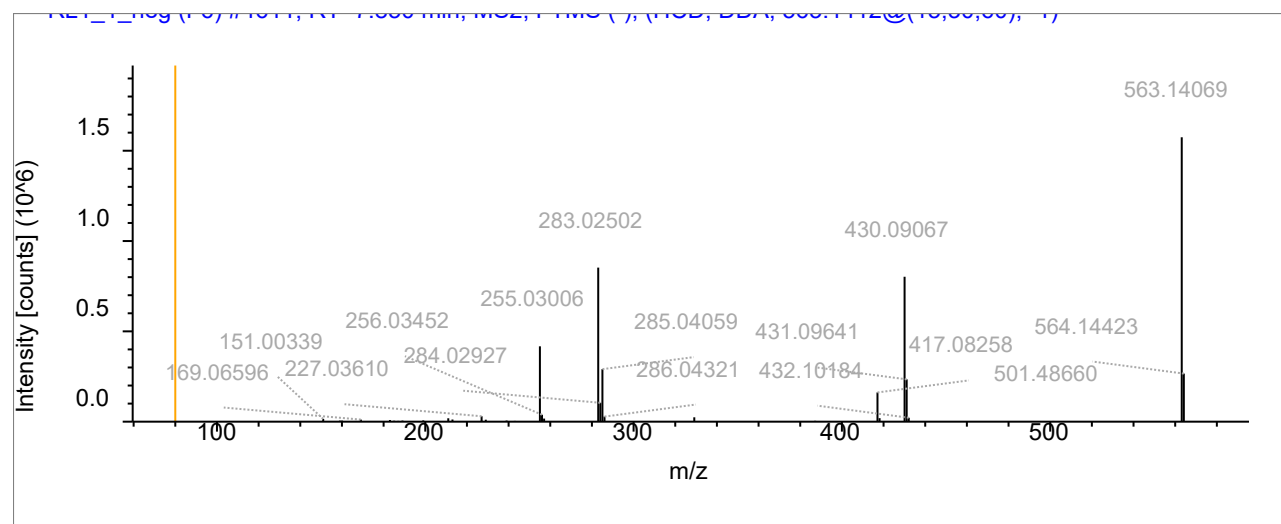


Figure S18. ESI-MS/MS spectrum of compound **12** in the positive ion mode showing at m/z 579.1711 $[M+H]^+$

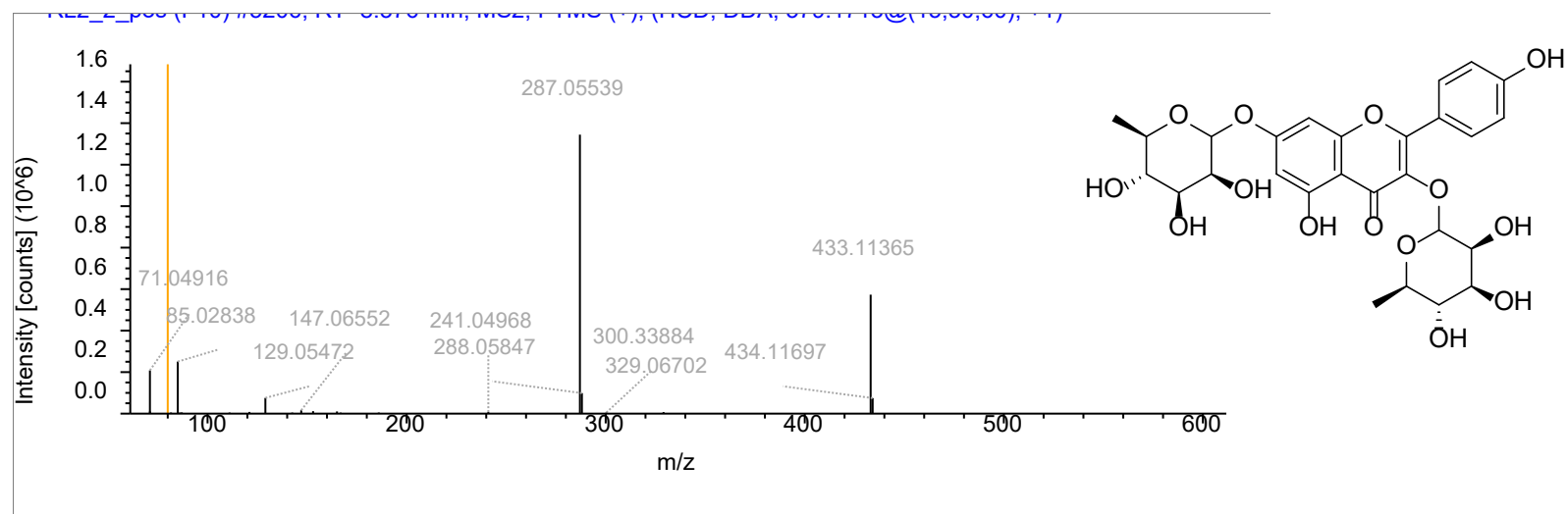


Figure S20. ESI-MS/MS spectrum of compound **13** in the positive ion mode showing at m/z 595.1663 $[M+H]^+$

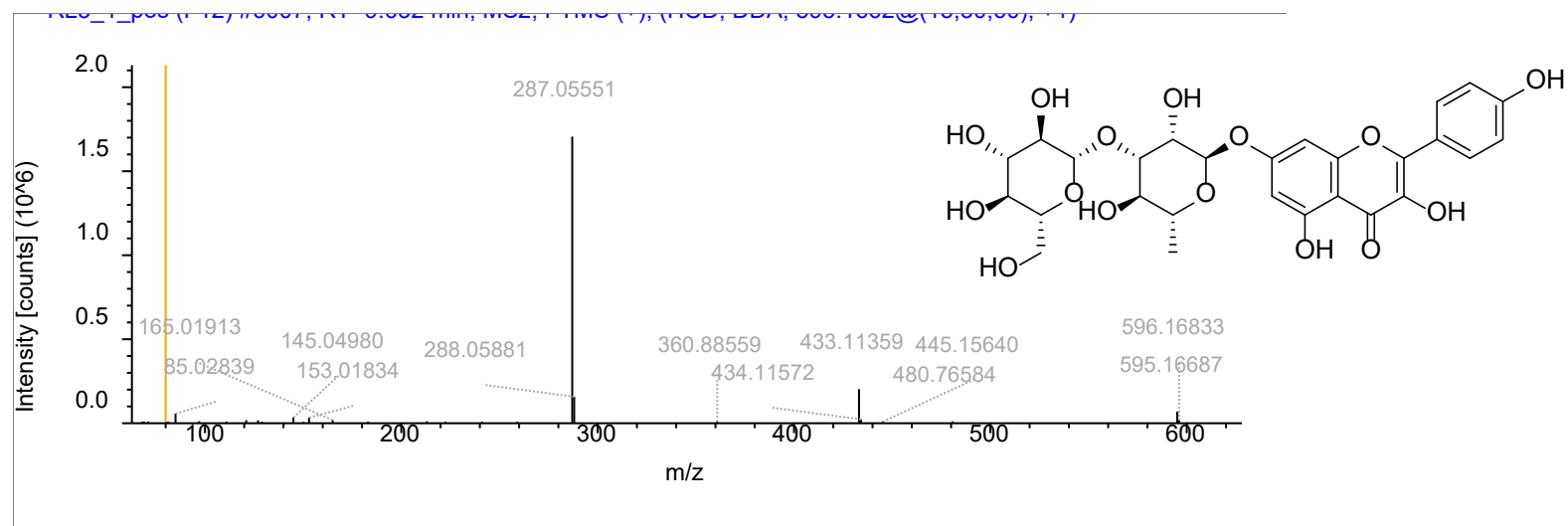


Figure S21. ESI-MS/MS spectrum of compound **14** in the positive ion mode showing at m/z 727.2083 $[M+H]^+$

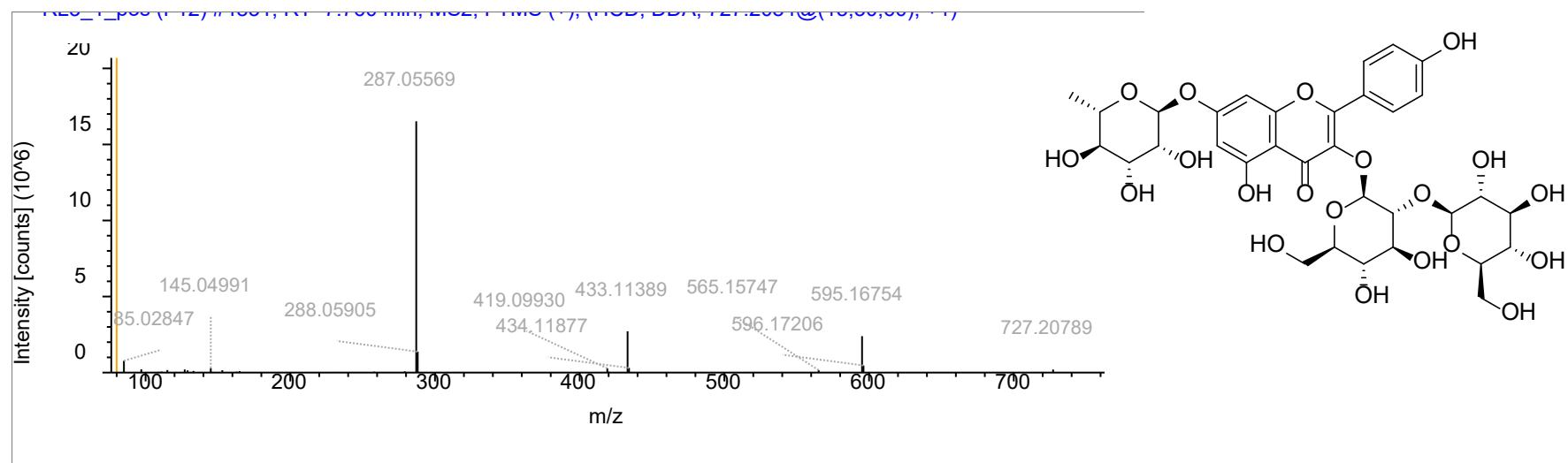


Figure S22. ESI-MS/MS spectrum compound **15** in the positive ion mode showing at m/z 741.2238 $[M+H]^+$

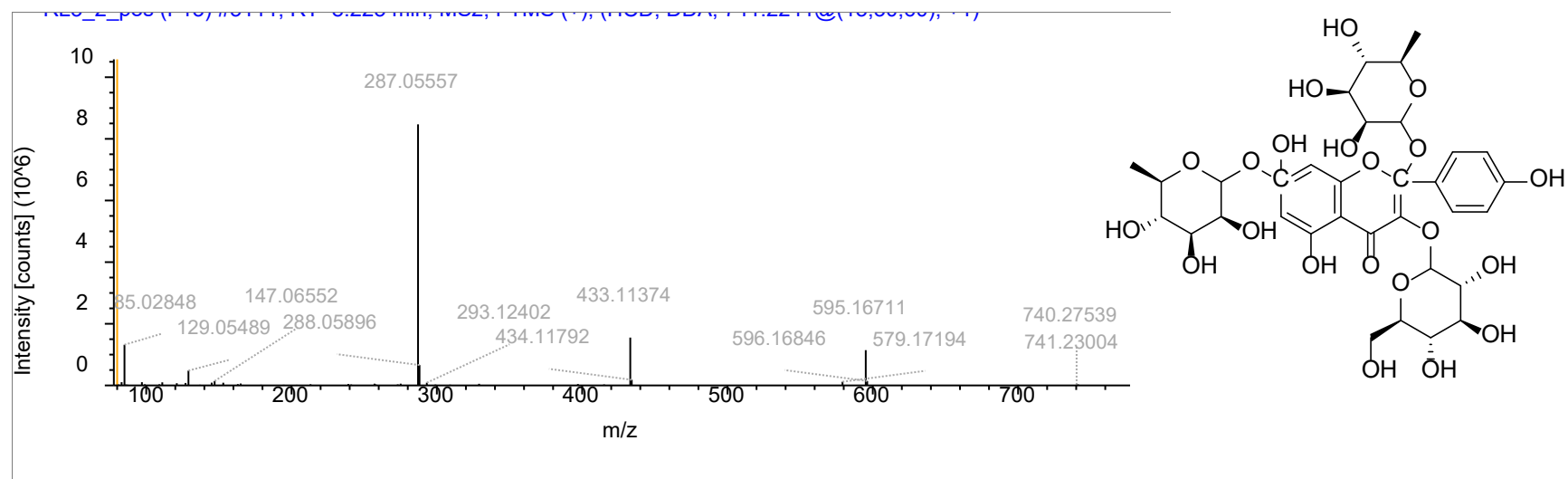


Figure S23. ESI-MS/MS spectrum of compound **16** in the negative ion mode showing at m/z 755.2051 $[M+H]^+$

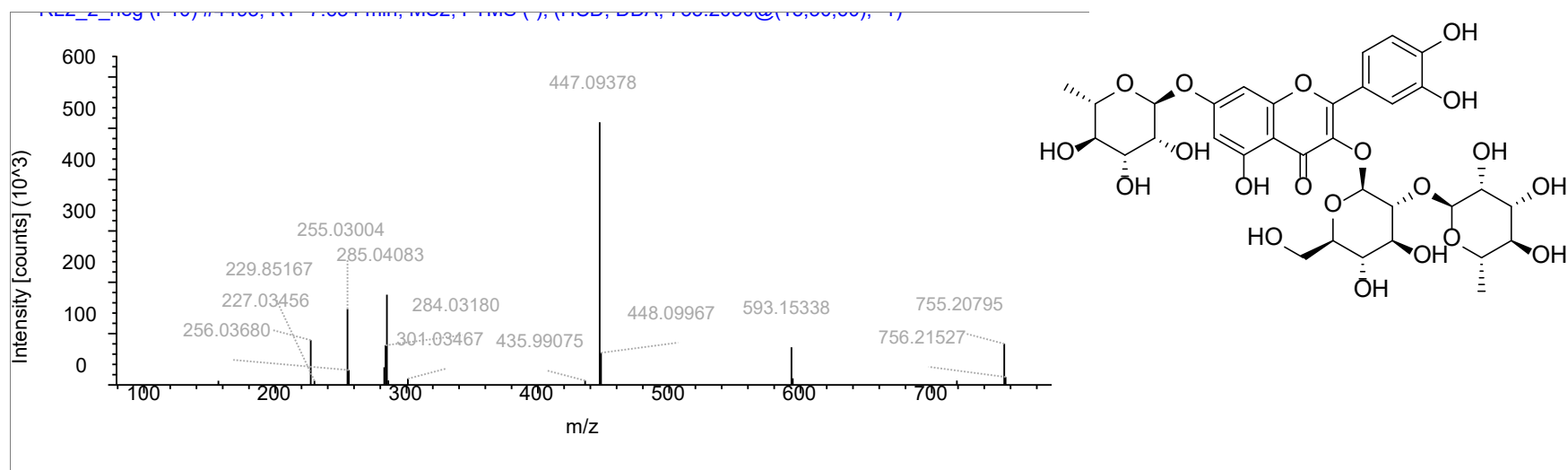


Figure S24. ESI-MS/MS spectrum of compound **17** in the negative ion mode showing at m/z 771.1999 $[M-H]^-$

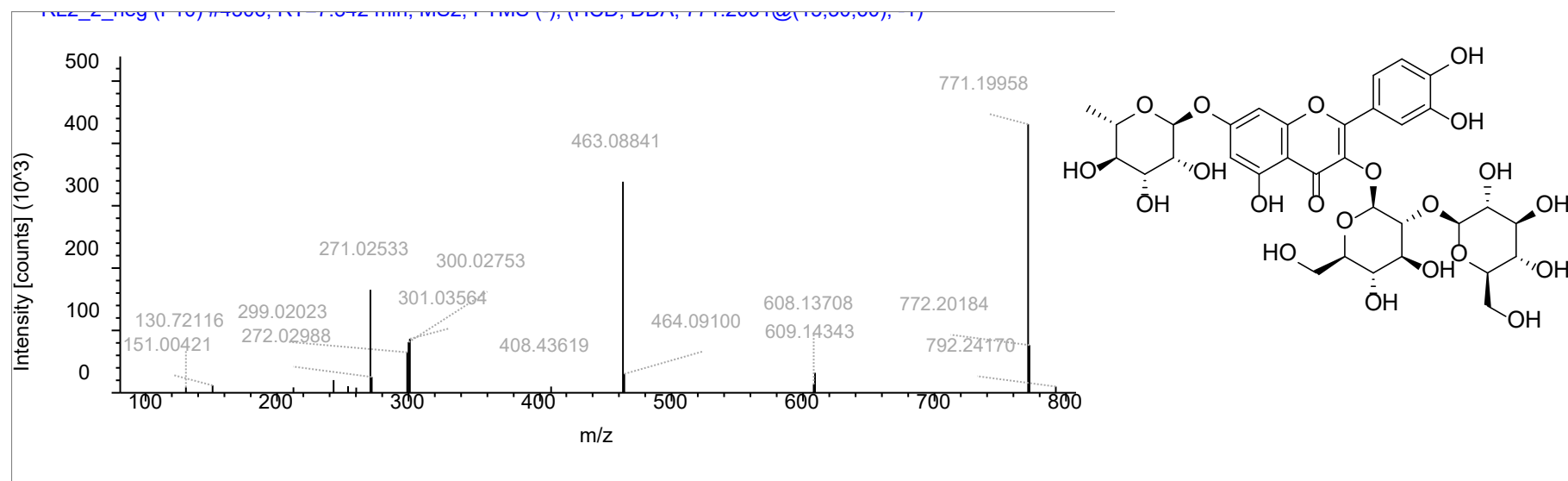


Figure S25. ESI-MS/MS spectrum of compound **18** in the positive ion mode showing at m/z 130.0862 $[M+H]^+$

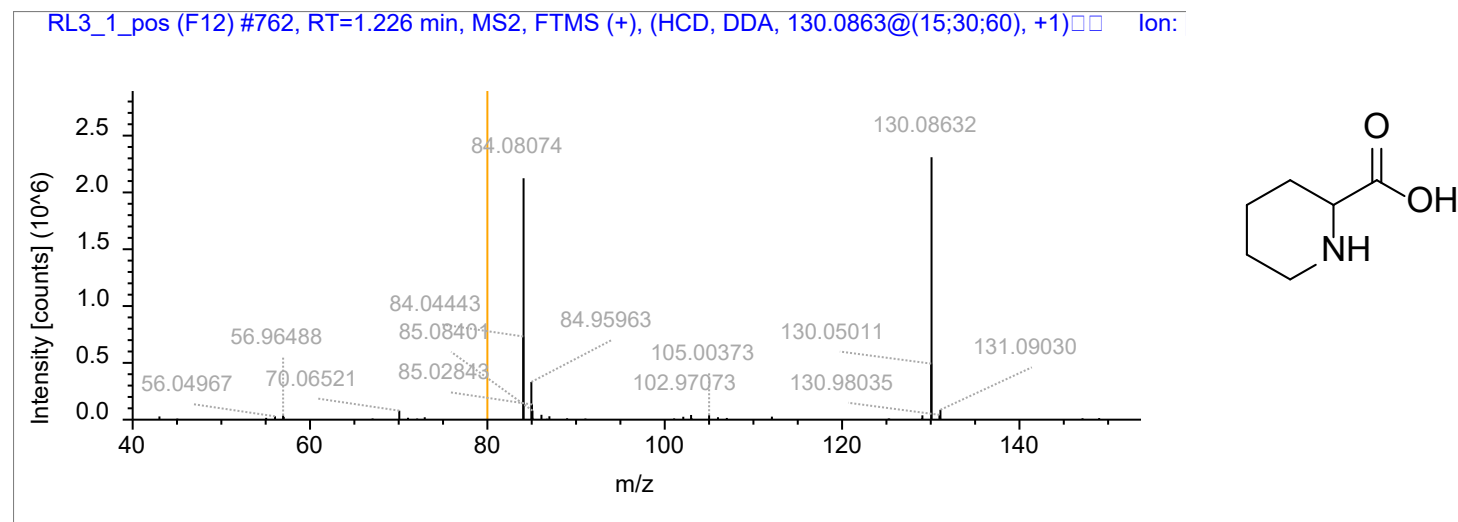


Figure S26. ESI-MS/MS spectrum of compound **19** in the positive ion mode showing at m/z 181.0495 $[M+H]^+$

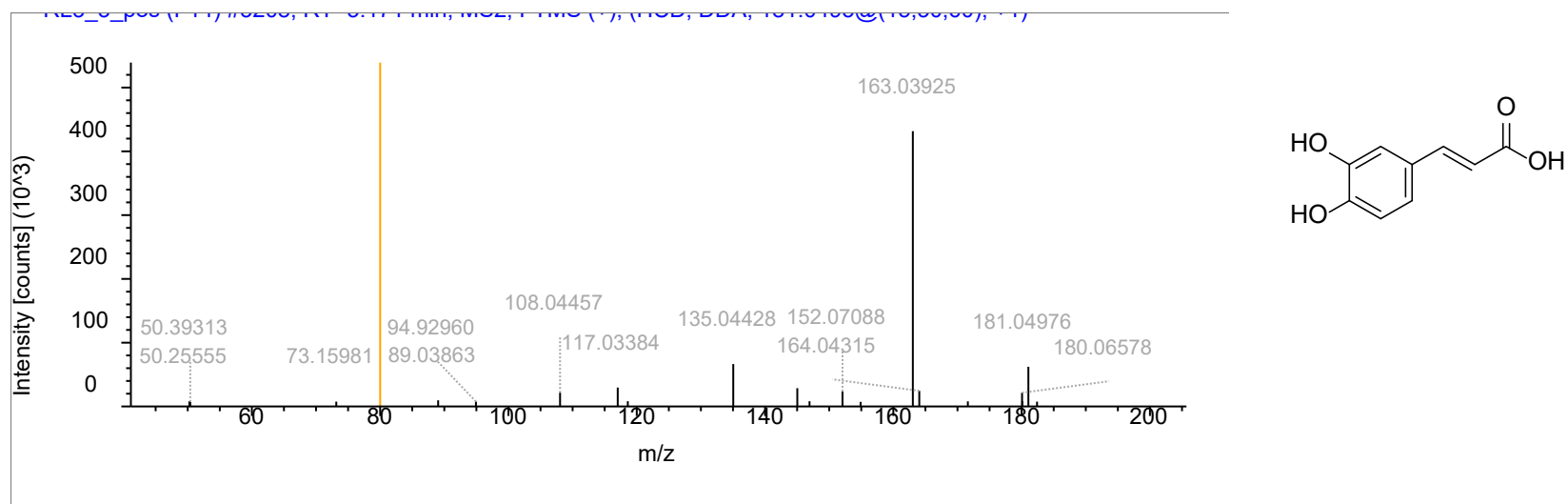
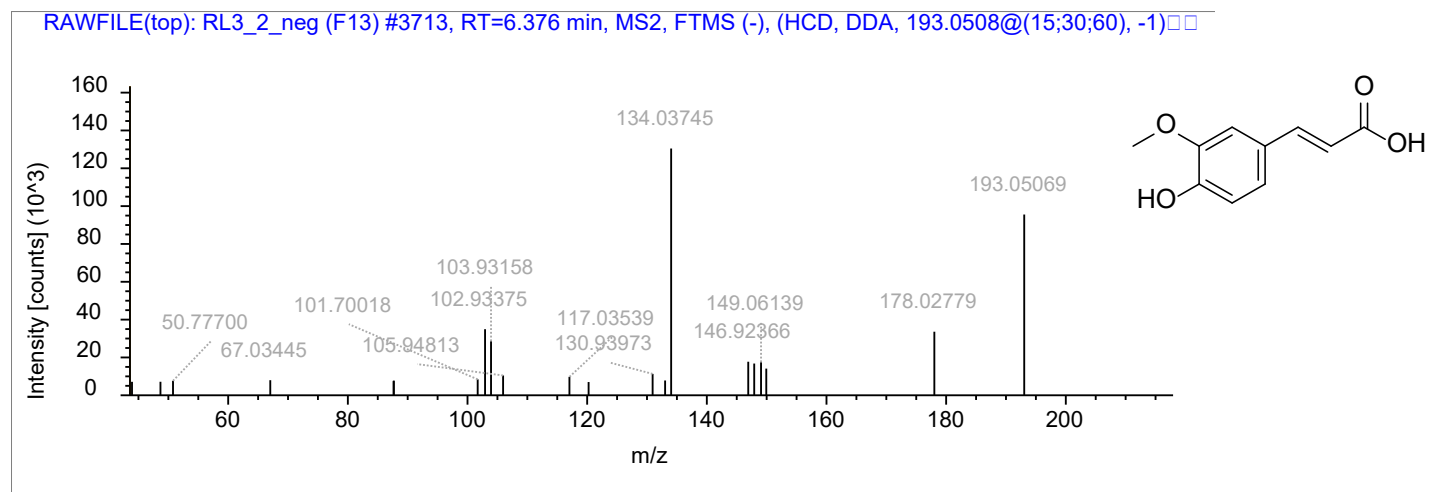


Figure S27. ESI-MS/MS spectrum of compound **20** in the positive ion mode showing at m/z at $[M-H]^+$ 193.0508



RAWFILE(top): RL3_3_pos (F14) #9024, RT=14.485 min, MS2, FTMS (+), (HCD, DDA, 300.2900@(15;30;60), +1)□□

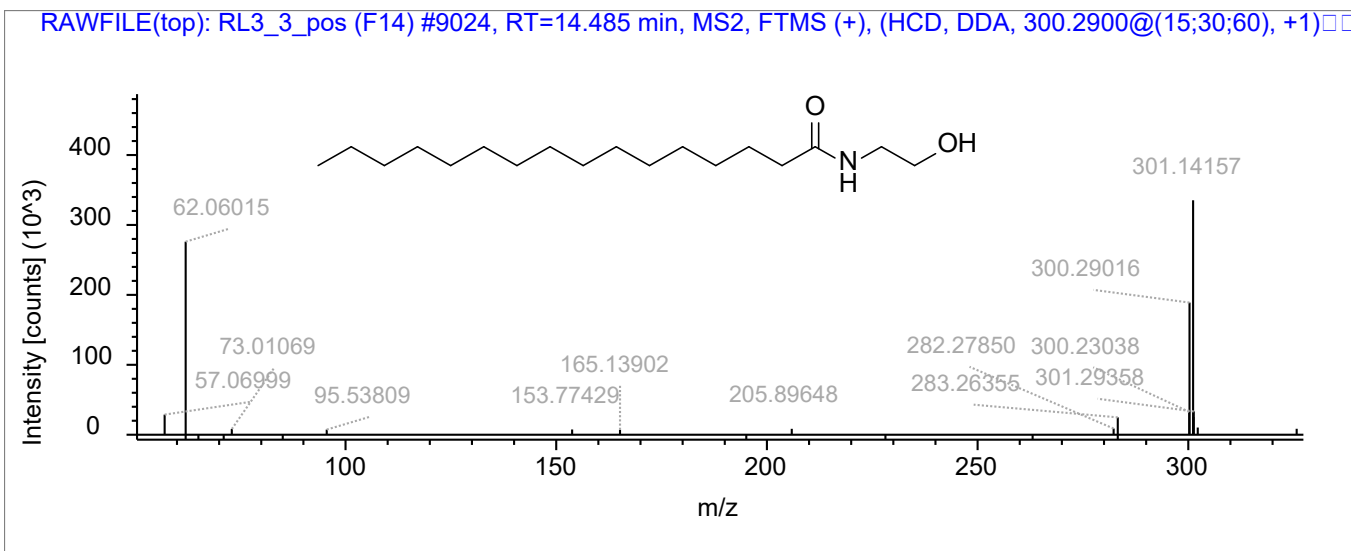


Figure S29. ESI-MS/MS spectrum of compound **22** in the positive ion mode showing at m/z 349.2738 $[M+H]^+$

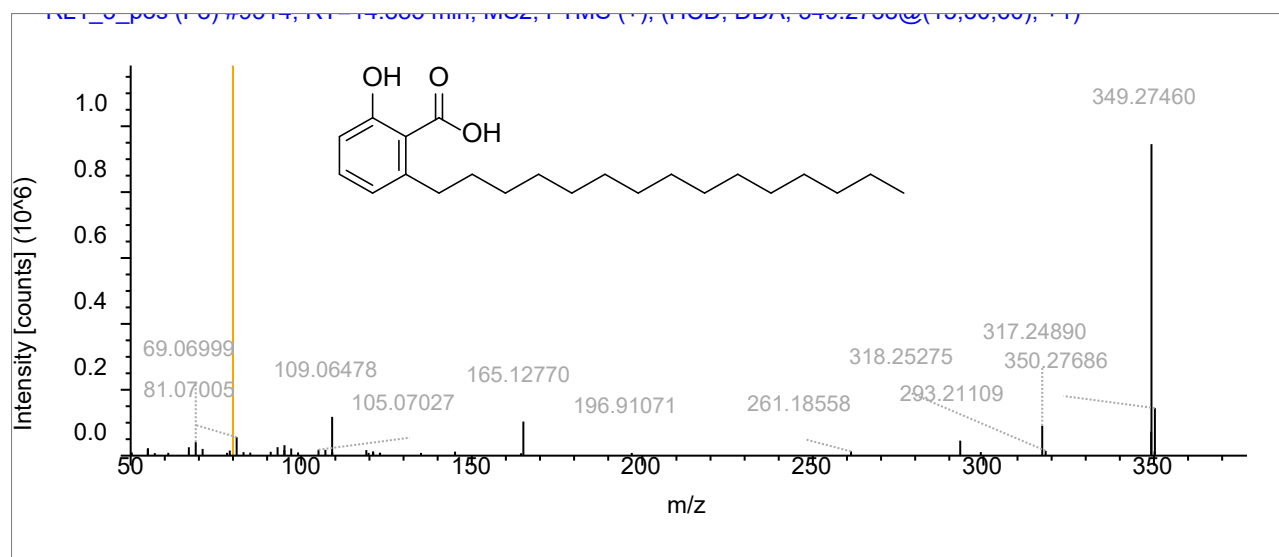


Figure S30. The principal component analysis (PCA) before normalization with QC samples showing: (a) correlation of phytochemical composition with RL1, 2, and 3, and (b) relationship of three *R. sativus* cultivars (RL1-3)

