Supporting Information

Comparative analysis of coumarin profiles in different parts of *Peucedanum japonicum* and their aldo-keto reductase inhibitory activities

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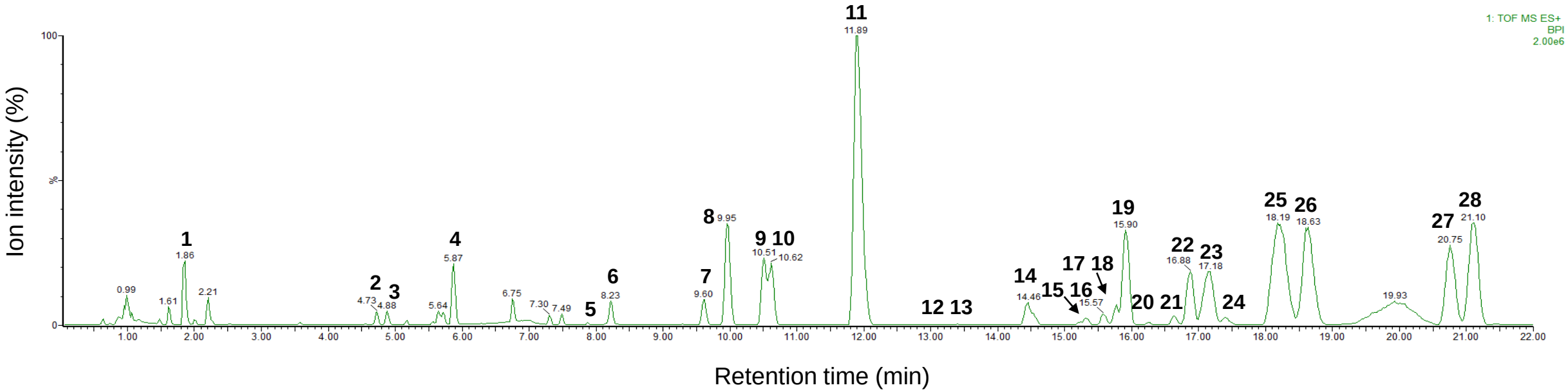


Figure S1. LC–MS base peak ion chromatograms of the dichloromethane fraction of the flowers of *P. japonicum* at positive ion mode (6 eV, ESI^+).

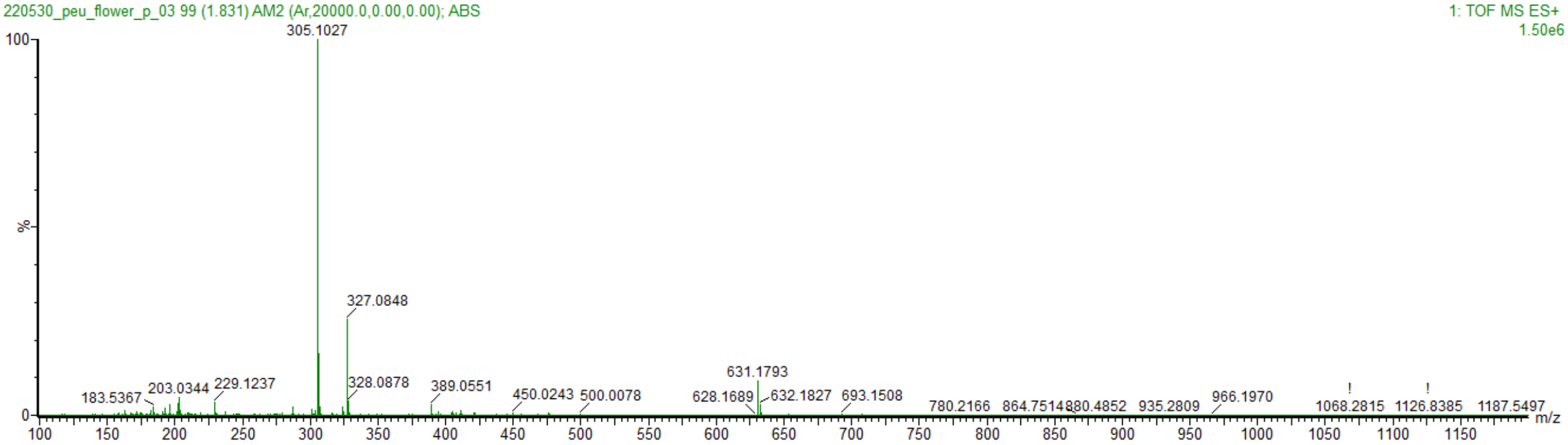


Figure S2. ESI-QTof-MS spectrum of oxypeucedanin hydrate (peak 1).

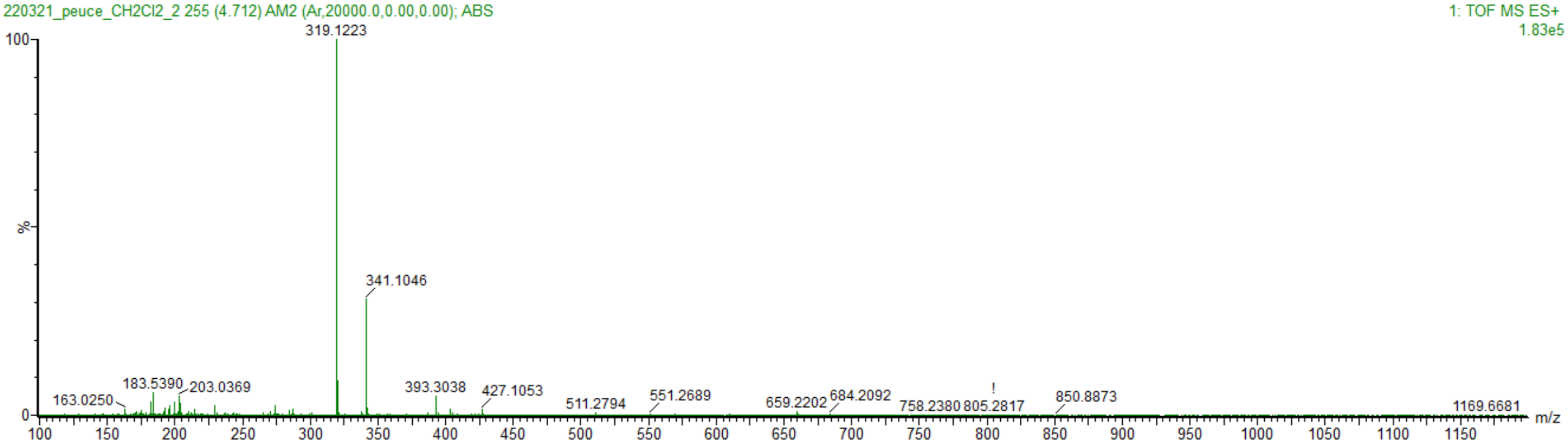


Figure S3. ESI-QTof-MS spectrum of oxypeucedanin methanolate (peak 2).

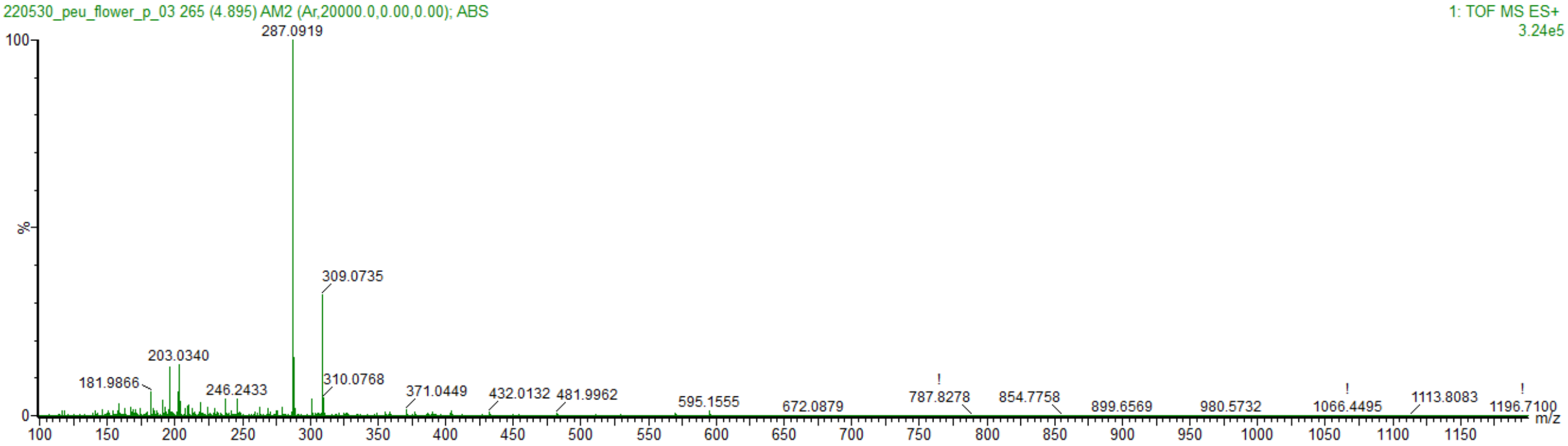


Figure S4. ESI-QTof-MS spectrum of pabulenol (peak 3).

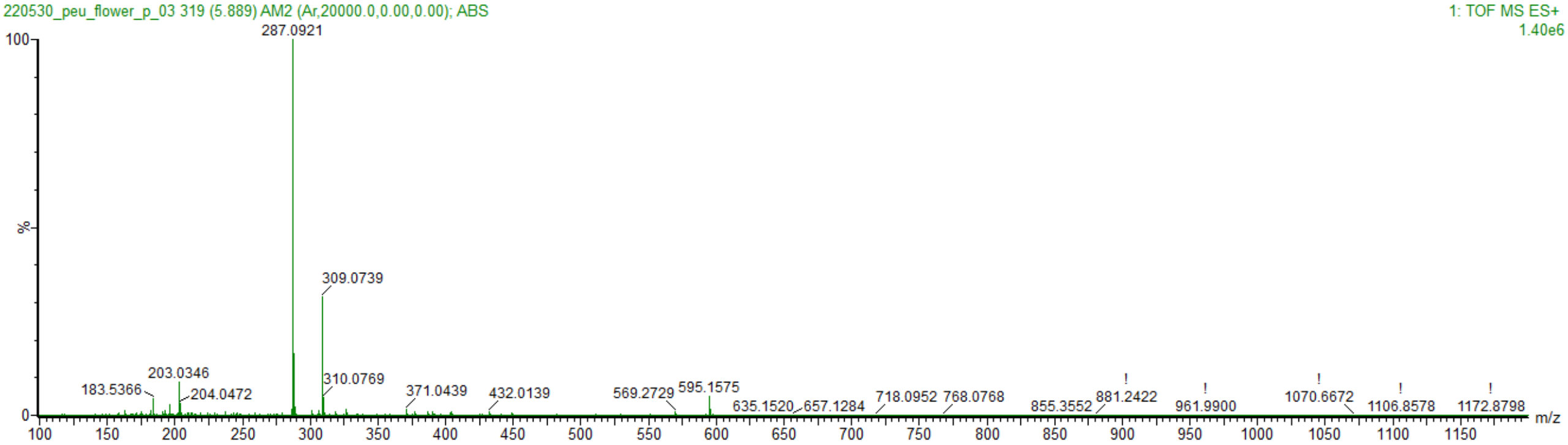


Figure S5. ESI-QTof-MS spectrum of 5-[(3-hydroxy-3-methyl-1-butenyl)oxy]psoralen (peak 4).

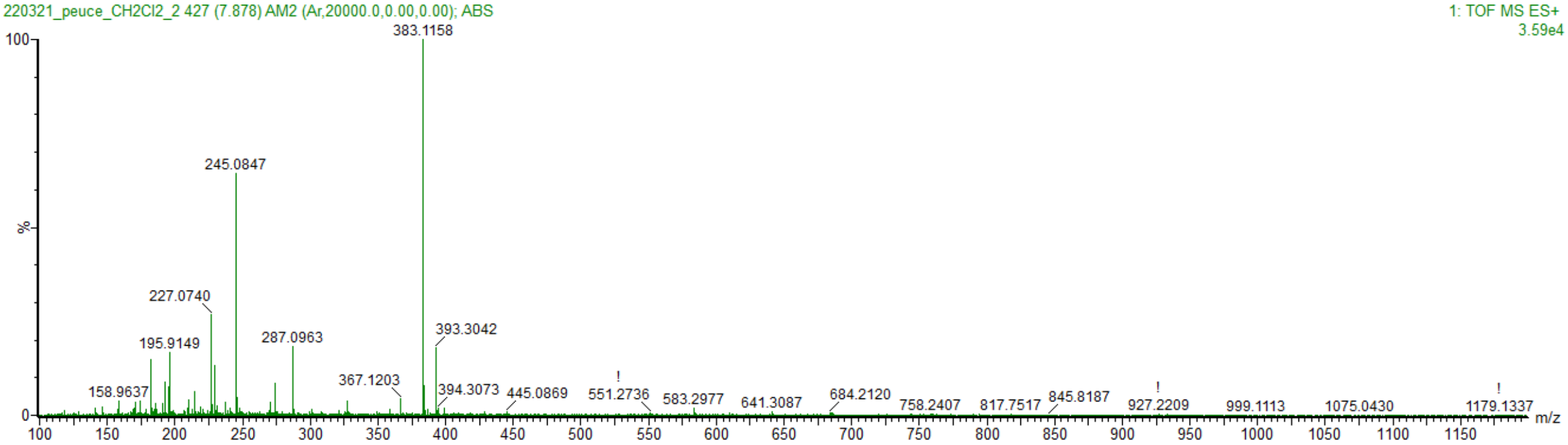


Figure S6. ESI-QTof-MS spectrum of 3'-O-acetyl-4'-O-propanoylkhellactone (peak 5).

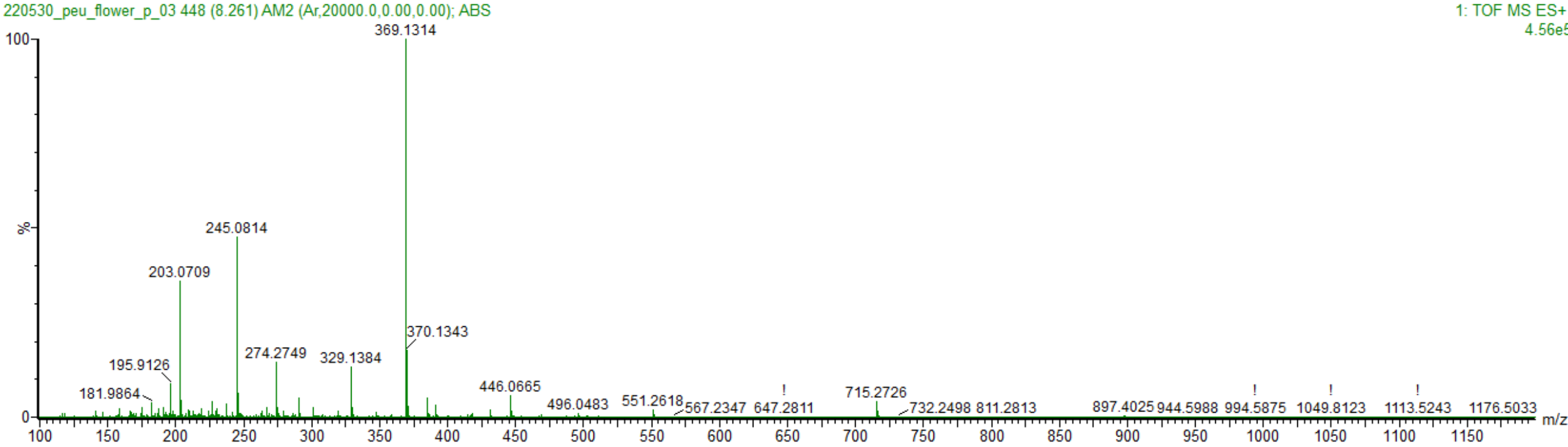


Figure S7. ESI-QTof-MS spectrum of 3'- O-(2-methyl-butyryl)-4'-hydroxy khellactone (or 3'-O-(isovaleryl)-4'-hydroxy khellactone) (peak 6)

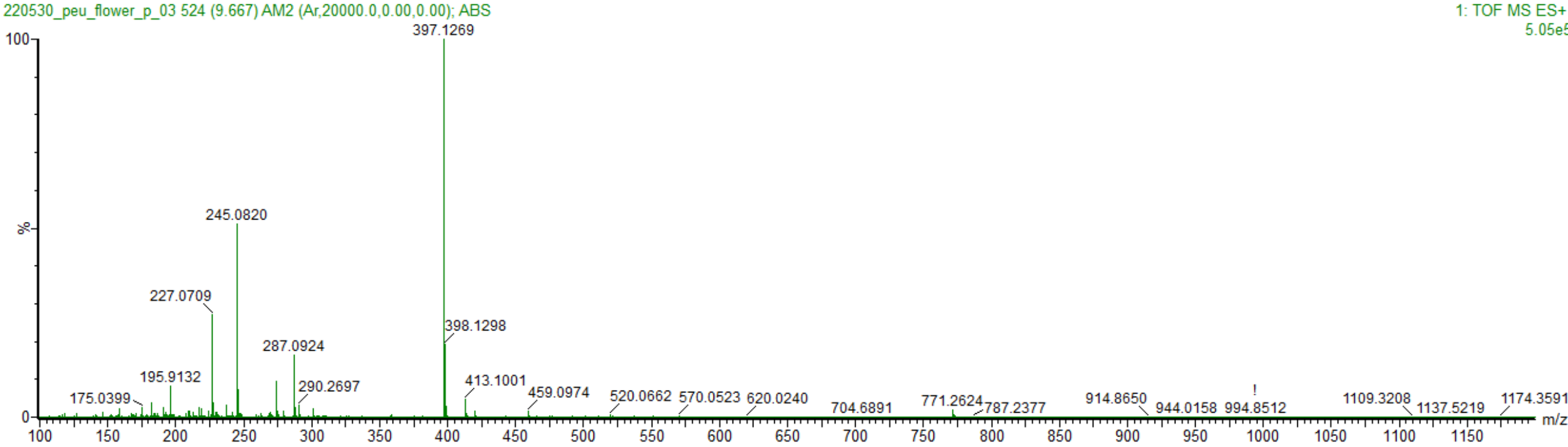


Figure S8. ESI-QTof-MS spectrum of 3'-O-acetyl-4'-O-isobutyryl khellactone (hyuganin D) (peak 7).

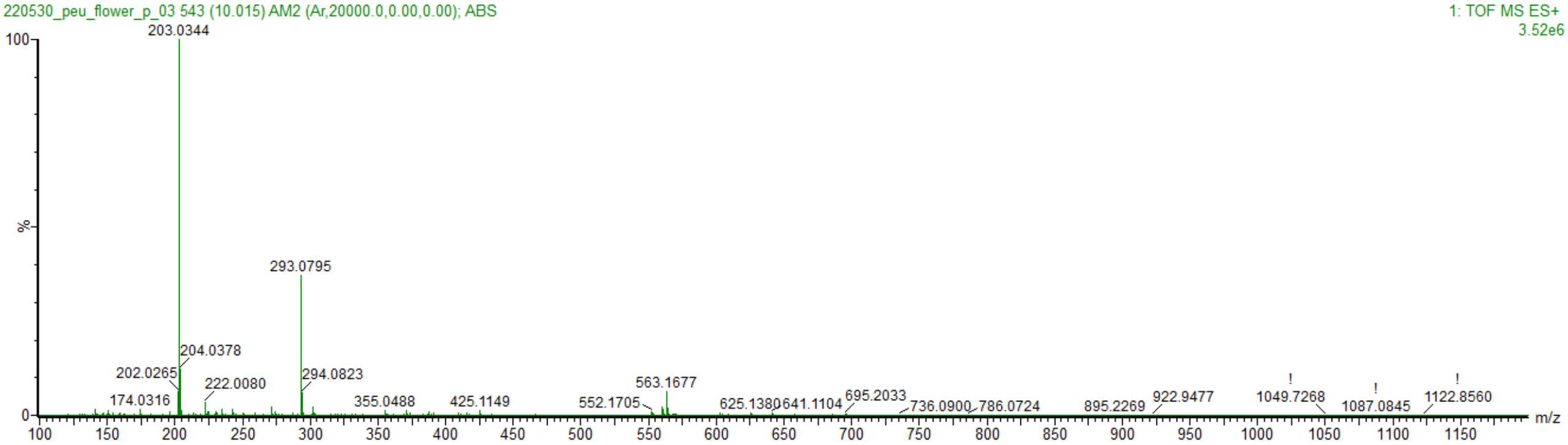


Figure S9. ESI-QTof-MS spectrum of isoimpertorin (peak 8).

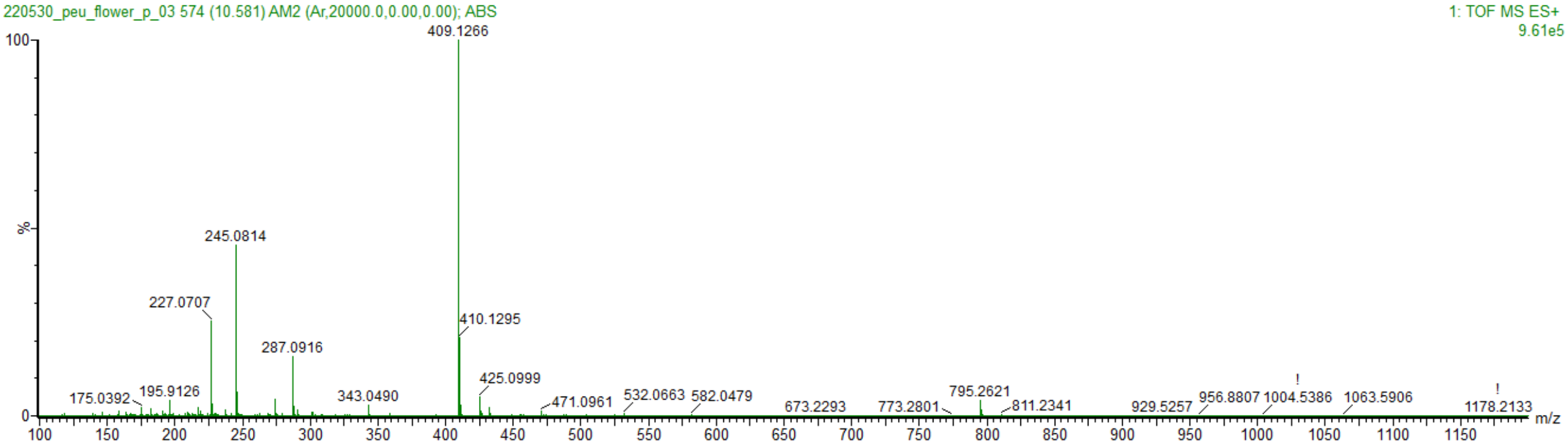


Figure S10. ESI-QTof-MS spectrum of 3'-O-acetyl-4'-O-angeloylkhellactone (pteryxin) (peak 9).

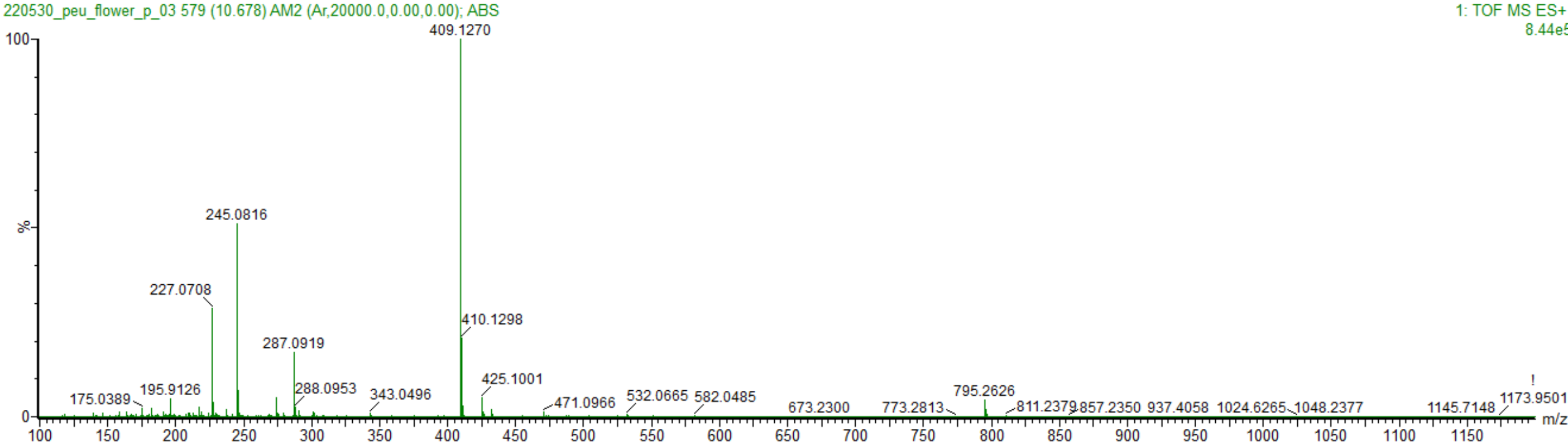


Figure S11. ESI-QTof-MS spectrum of 3'-O-acetyl-4'-O-senecioylkhellactone (peak 10).

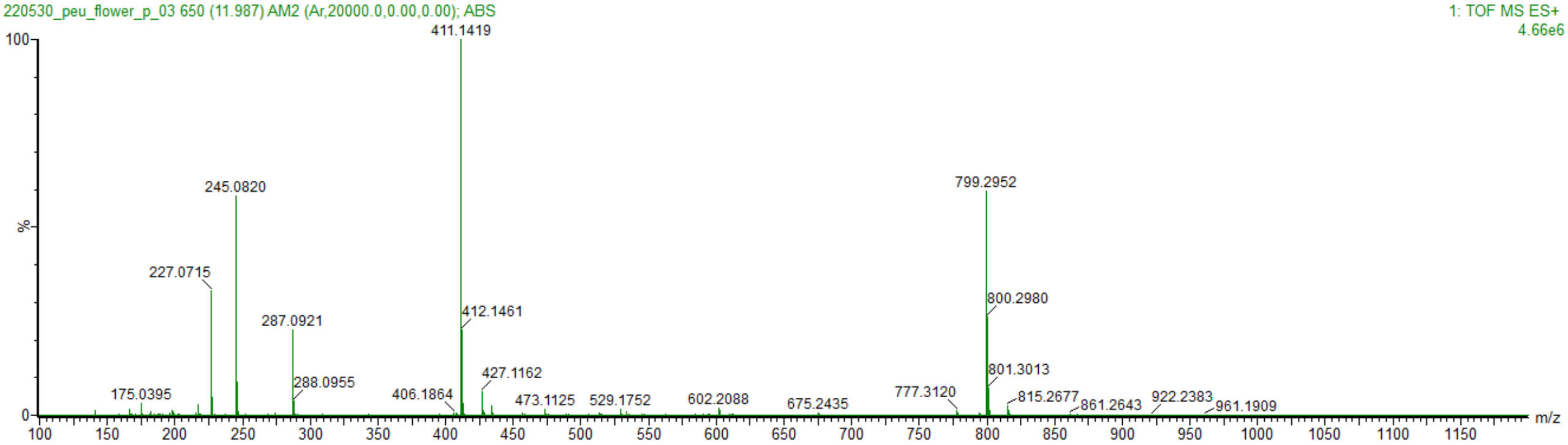


Figure S12. ESI-QTof-MS spectrum of 3'-O-acetyl-4'-O-(2-methyl butanoate)khellactone (or 3'-O-acetyl-4'-O-isovalerylkhellactone) (peak 11).

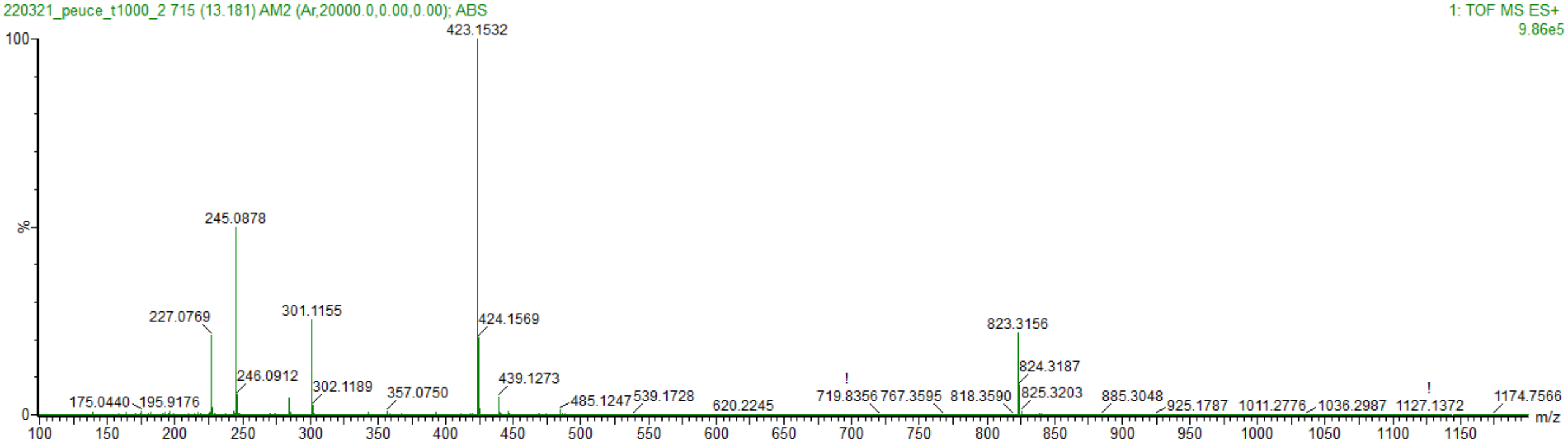


Figure S13. ESI-QTof-MS spectrum of 3'-O-propanoyl-4'-O-angeloyl khellactone (or 3'-O-propanoyl-4'-O-senecioylkhellactone) (peak 12).

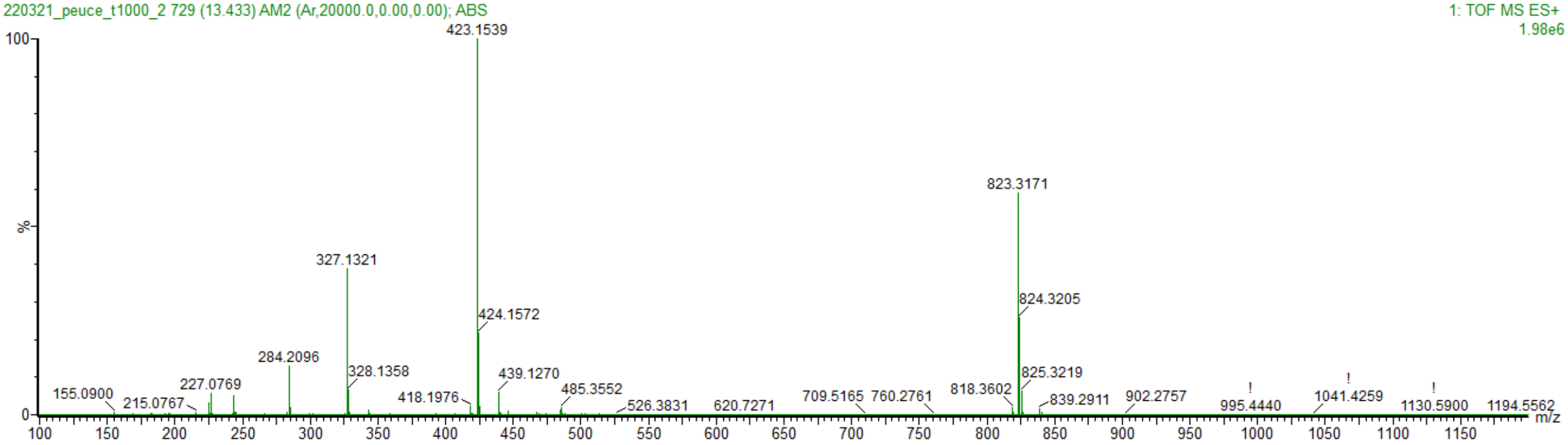


Figure S14. ESI-QTof-MS spectrum of 3'-O-angeloyl-4'-O-propanoylkhellactone (or 3'-O-senecioyl-4'-O-propanoylkhellactone) (peak 13).

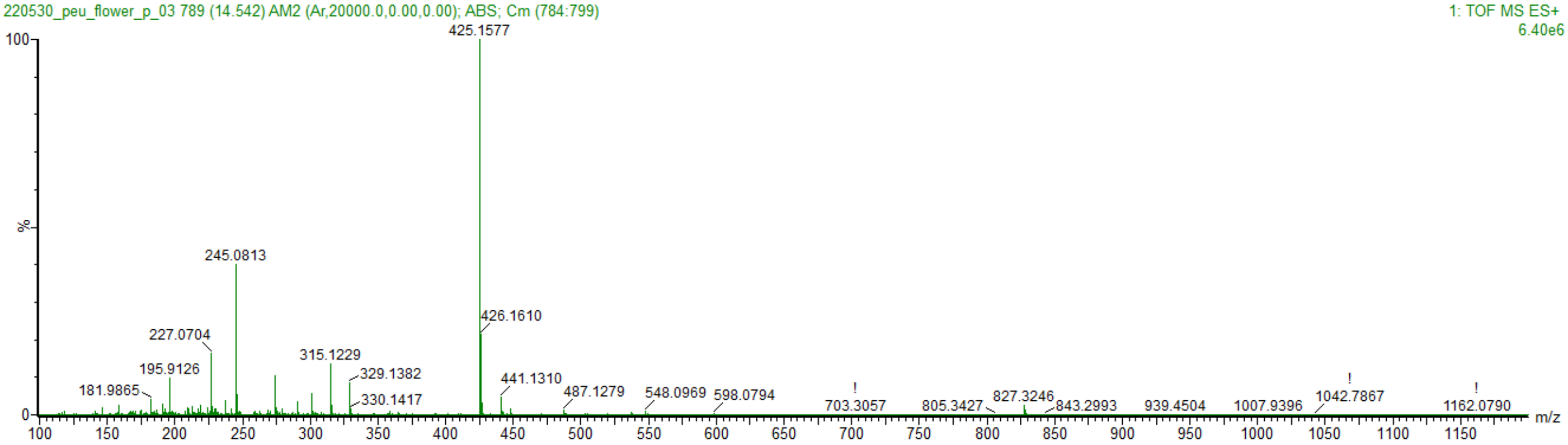


Figure S15. ESI-QTof-MS spectrum of 3'-O-isobutyryl-4'-O-isobutyrylkhellactone (peak 14).

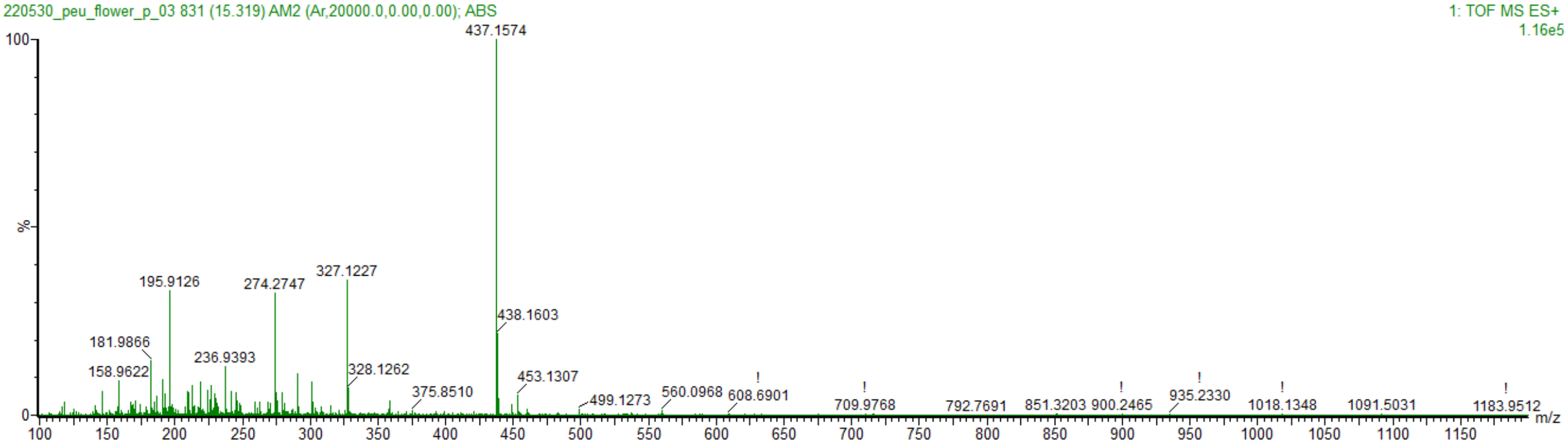


Figure S16. ESI-QTof-MS spectrum of 3'-O-angeloyl-4'-O-isobutyrylkhellactone (peak 15).

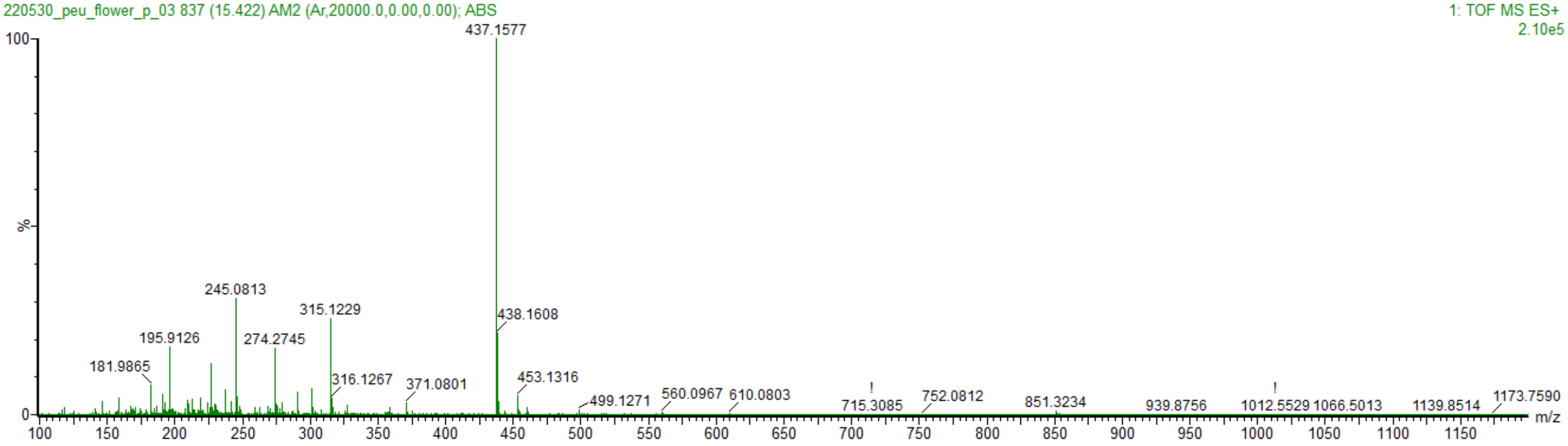


Figure S17. ESI-QTof-MS spectrum of 3'-O- isobutyryl-4'-O-angeloylkhellactone (peak 16).

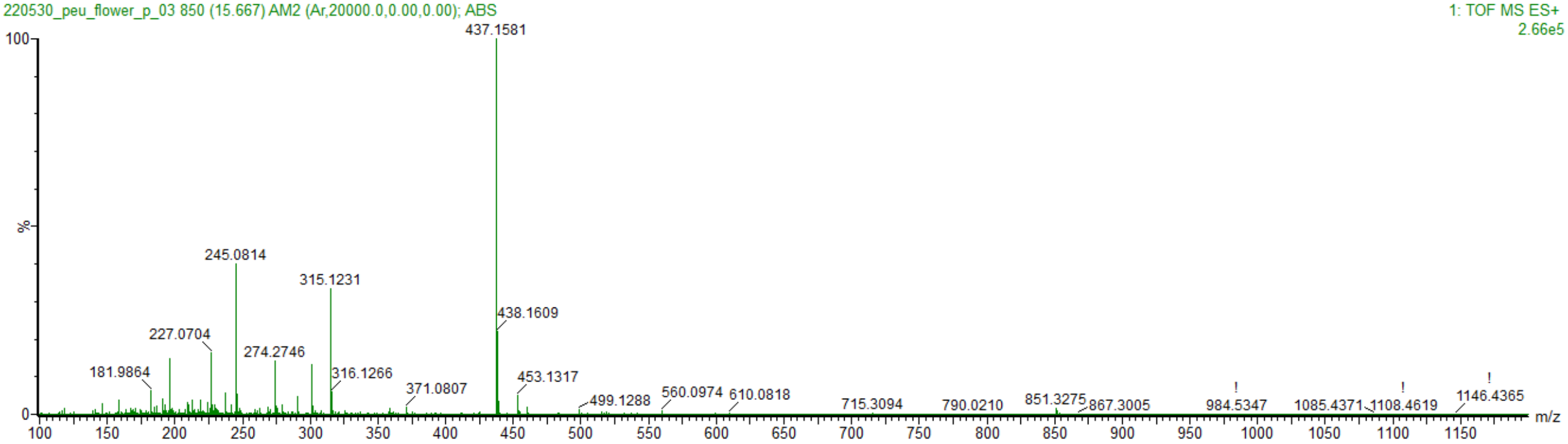


Figure S18. ESI-QTof-MS spectrum of 3'-O-isobutyryl-4'-O-senecioylkhellactone (peak 17).

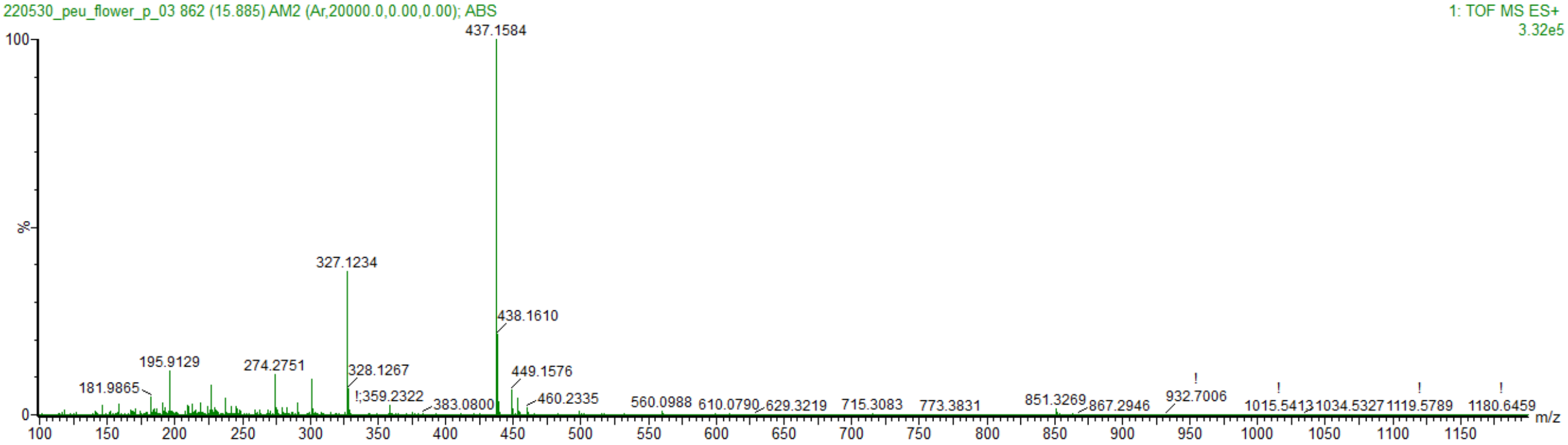


Figure S19. ESI-QTof-MS spectrum of 3'-O-senecioyl-4'-O-isobutyrylkhellactone (peak 18).

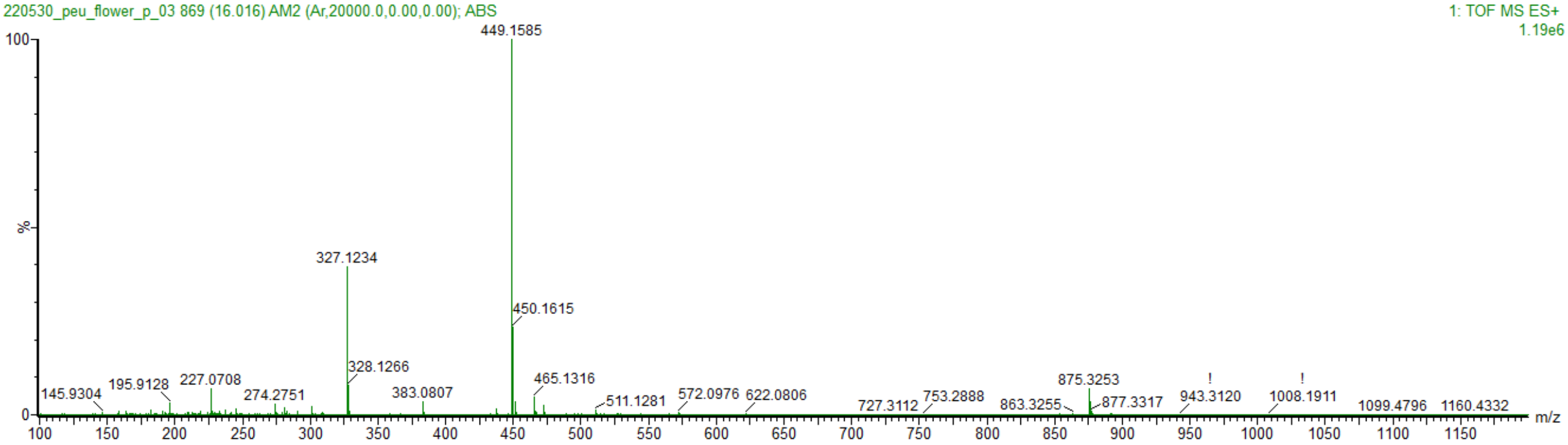


Figure S20. ESI-QTof-MS spectrum of 3'-O-angeloyl-4'-O-angeloylkhellactone (paeruptorin B) (peak 19).

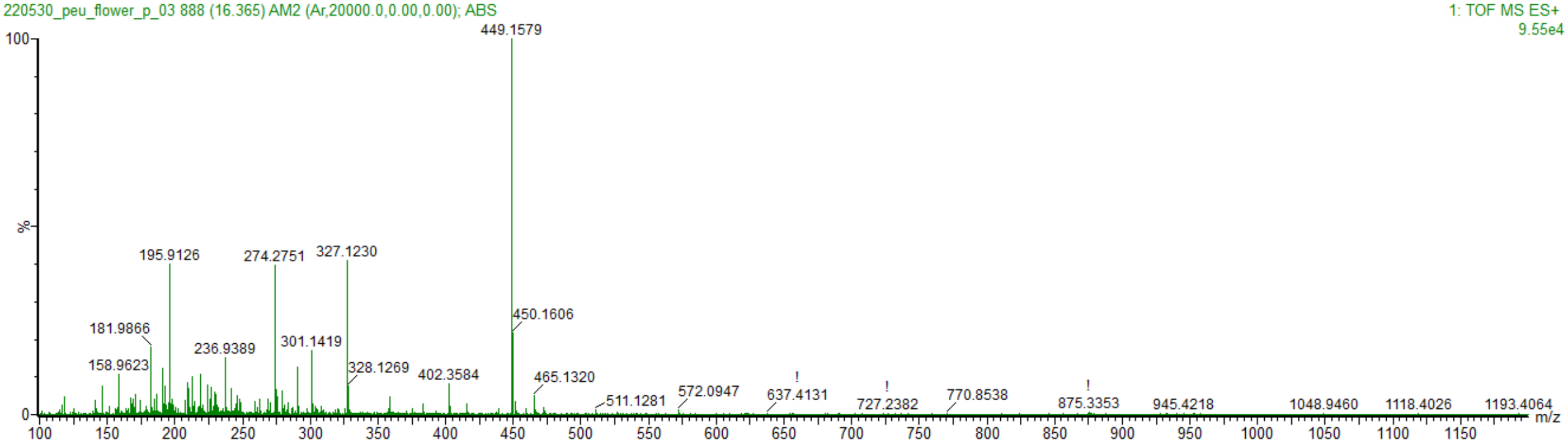


Figure S21. ESI-QTof-MS spectrum of 3'-O-angeloyl-4'-O-senecioylkhellactone (peak 20).

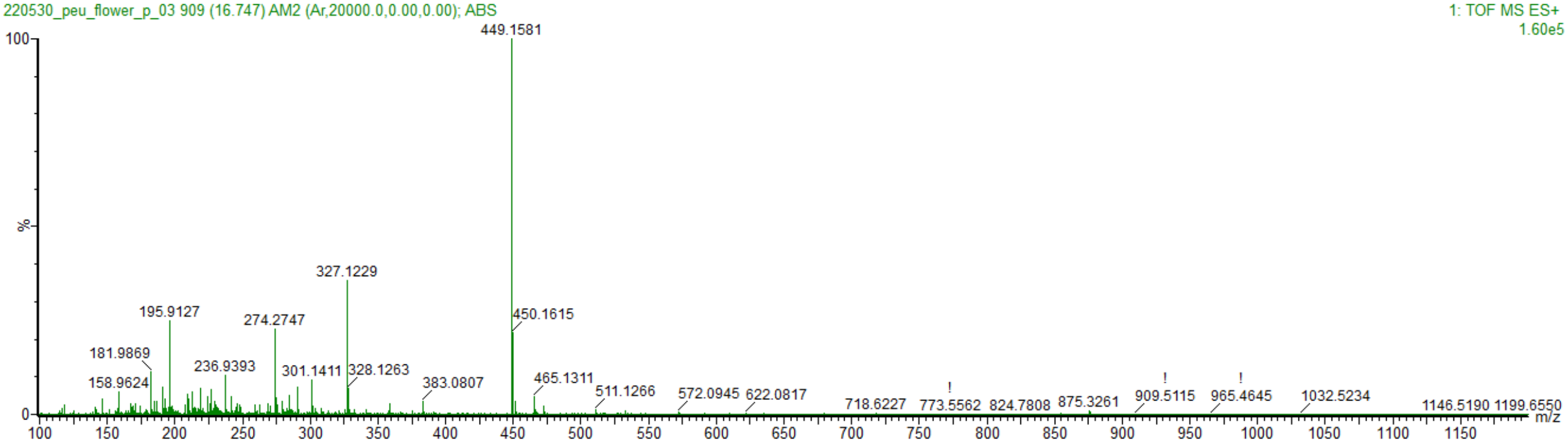


Figure S22. ESI-QTof-MS spectrum of 3'-O-senecioyl-4'-O-senecioylkhellactone (peak 21).

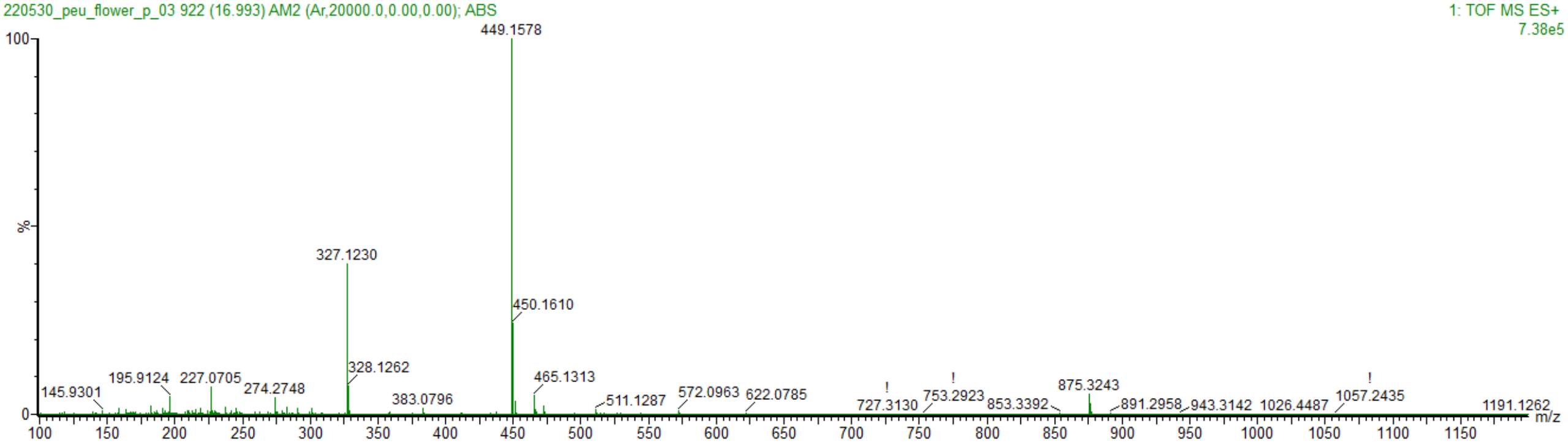


Figure S23. ESI-QTof-MS spectrum of 3'-O-senecioyl-4'-O-angeloylkhellactone (peak 22).

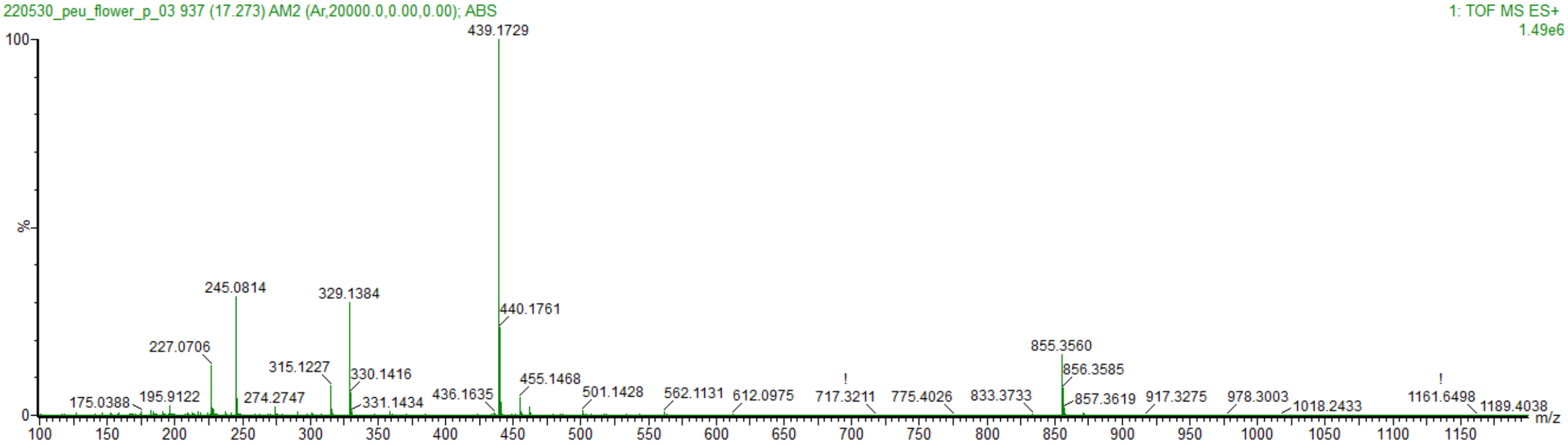


Figure S24. ESI-QTof-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-isobutyrylkhellactone (peak23).

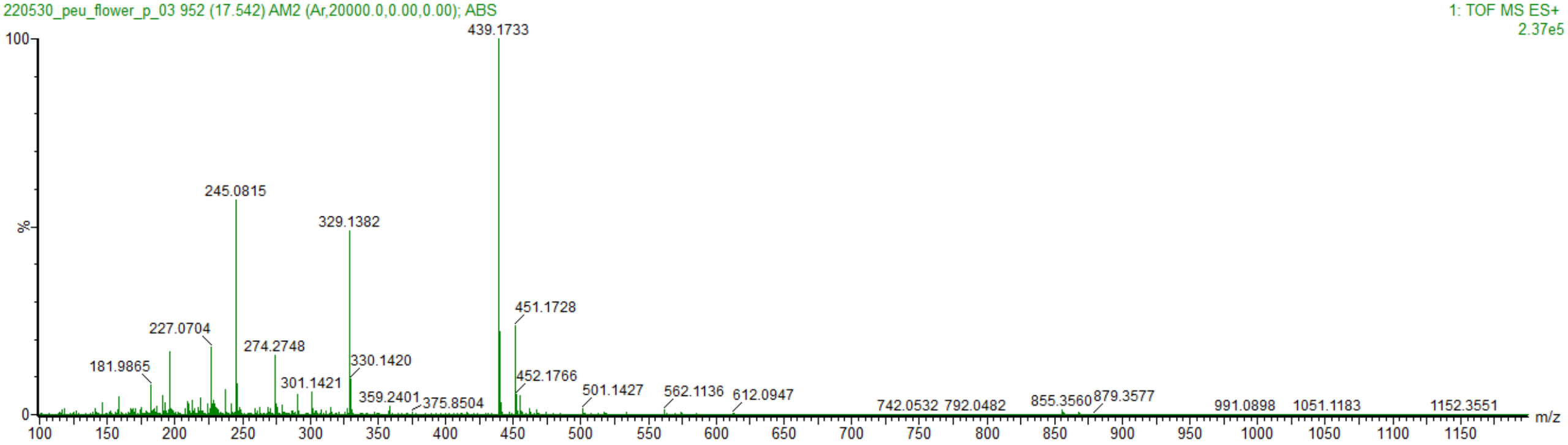


Figure S25. ESI-QTof-MS spectrum of 3'-O-isovaleryl-4'-O-isobutyrylkhellactone (peak 24).

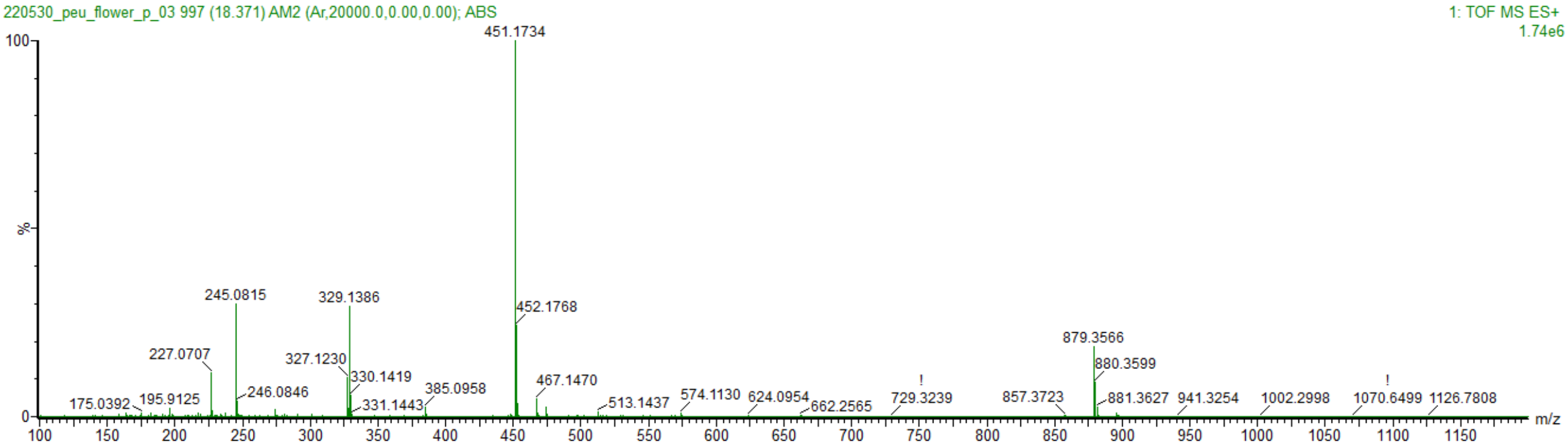


Figure S26. ESI-QTof-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-angeloylkhellactone [3'-O-(2-methyl butyryl)-4'-O-senecioyl khellactone, 3'-O-isovaleryl-4'-O-angeloylkhellactone (paeruptorin C), or 3'-O-isovaleryl-4'-O-senecioylkhellactone] (peak 25).

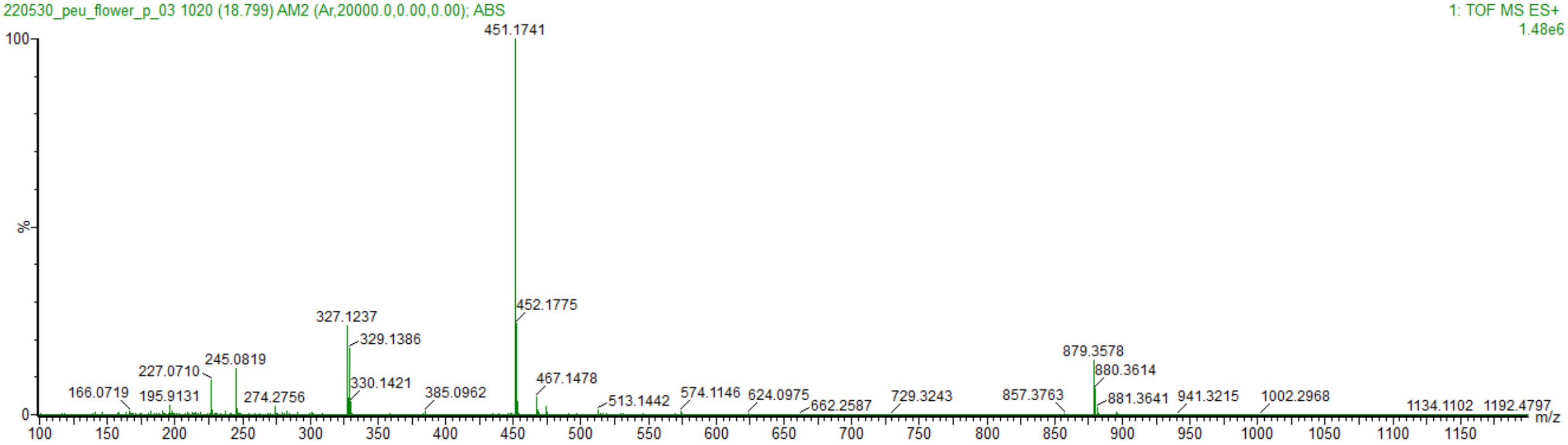


Figure S26. ESI-QTof-MS spectrum of 3'-O-angeloyl-4'-O-(2-methyl butyryl)khellactone [3'-O-angeloyl-4'-O-isovaleryl khellactone, 3'-O-senecioyl-4'-O-(2-methyl butyryl)khellactone, or 3'-O-senecioyl-4'-O-isovaleryl khellactone] (peak 26).

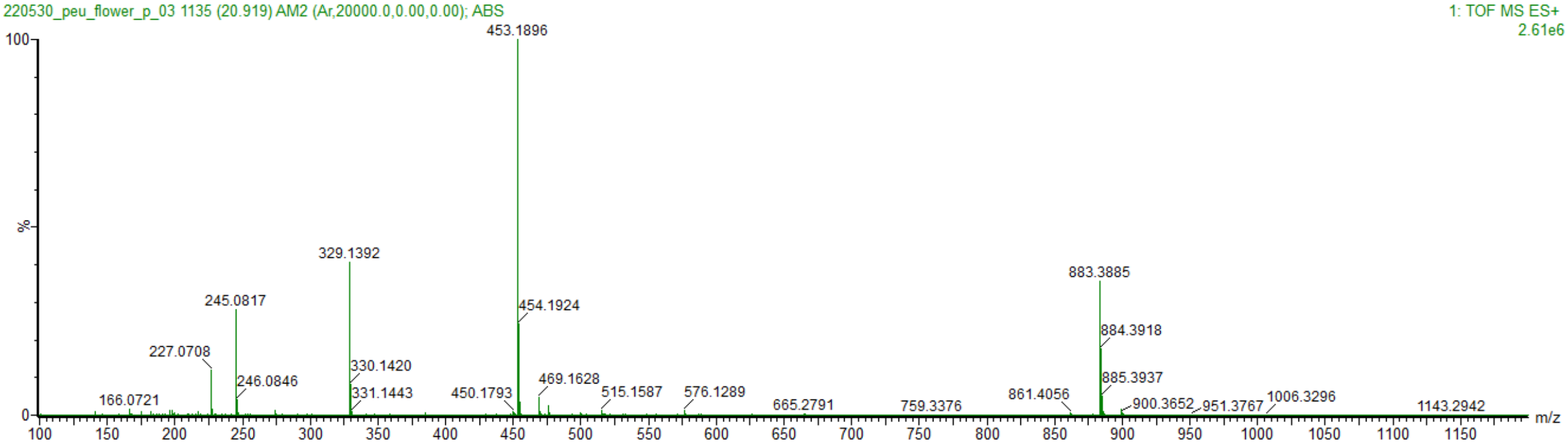


Figure S28. ESI-QTof-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-(2-methyl butyryl)khellactone (or 3'-O-(2-methyl butyryl)-4'-O-isovalerylkhellactone) (peak 27).

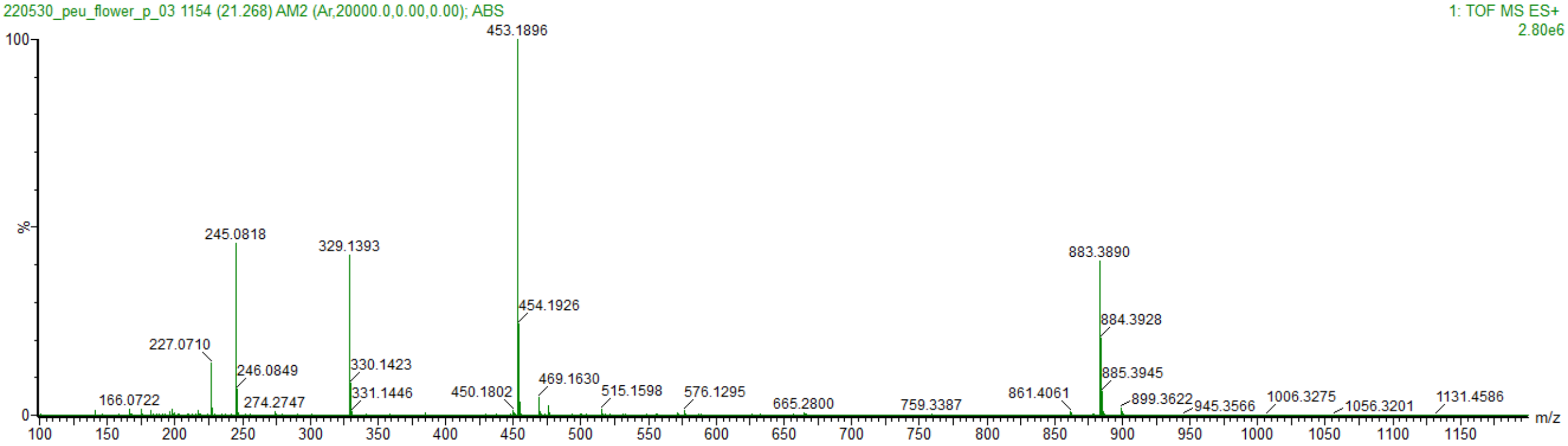


Figure S29. ESI-QTof-MS spectrum of 3'-O-isovaleryl-4'-O-(2-methyl butyryl)khellactone (or 3'-O-isovaleryl-4'-O-isovalerylkhellactone) (peak 28).

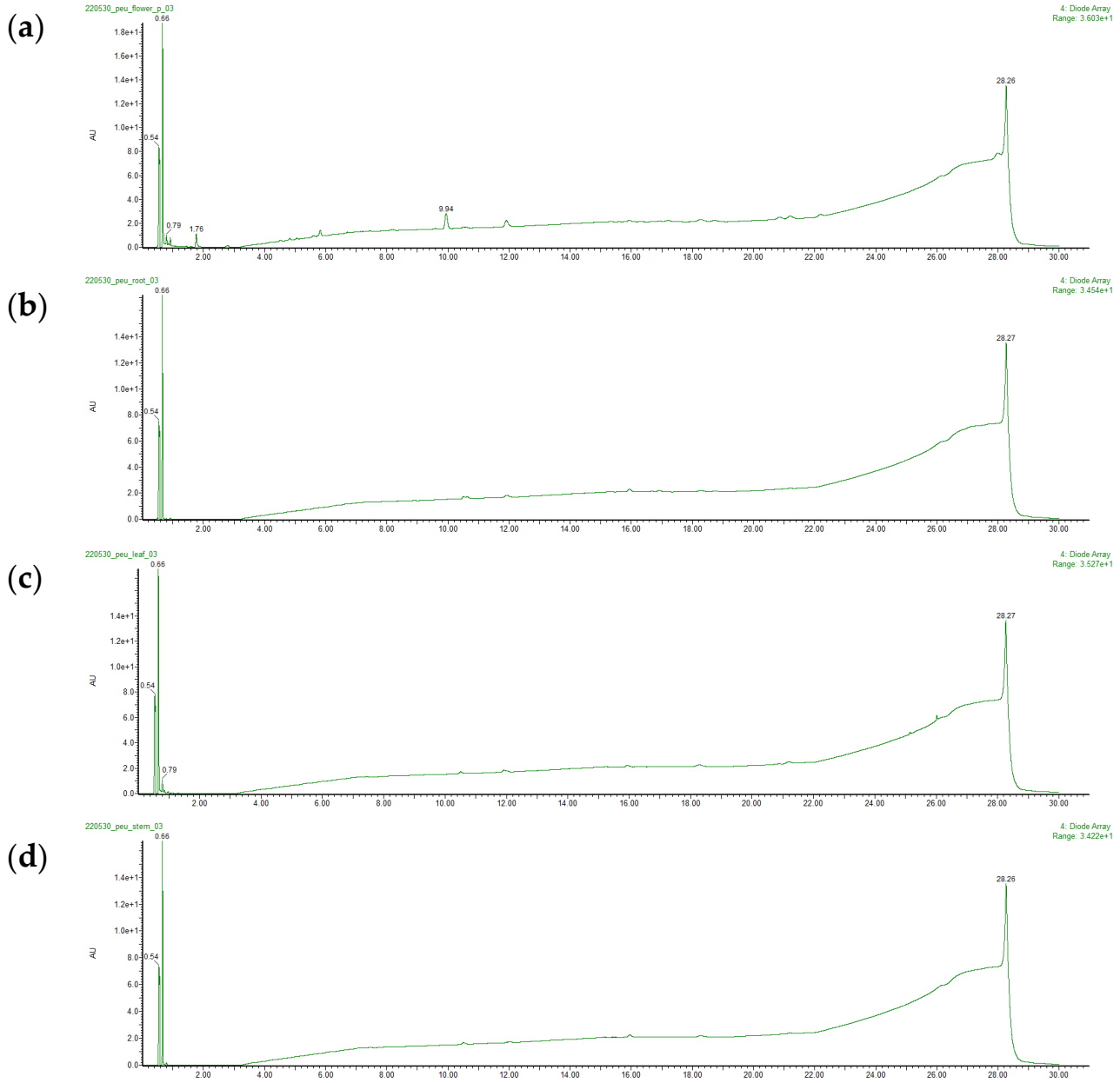


Figure S30. Total scan PDA chromatograms of (**a**) flowers (S3), (**b**) roots (S15), (**c**) leaves (S9), and (**d**) stems (S21) of *Peucedanum japonicum*

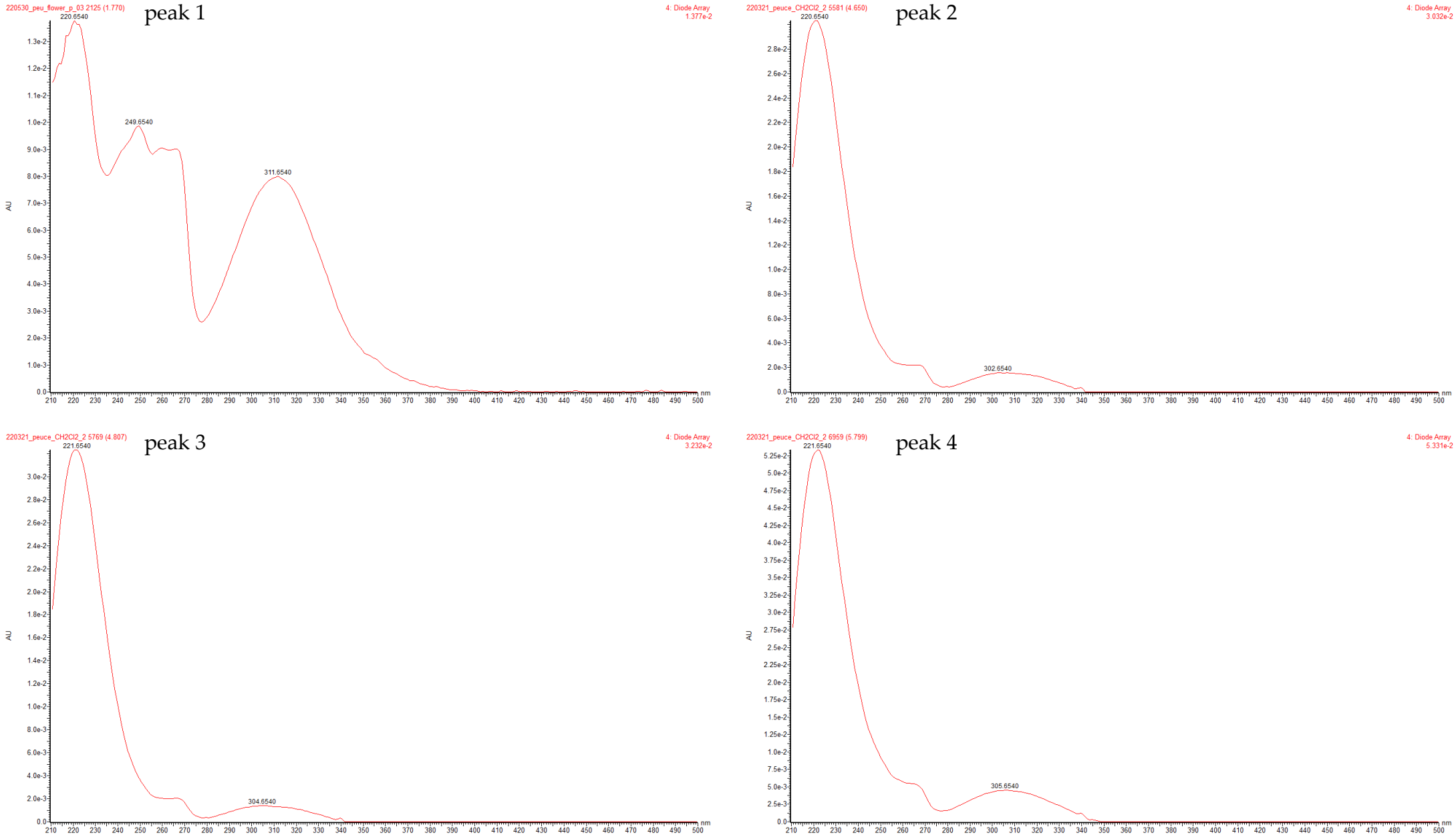


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm.

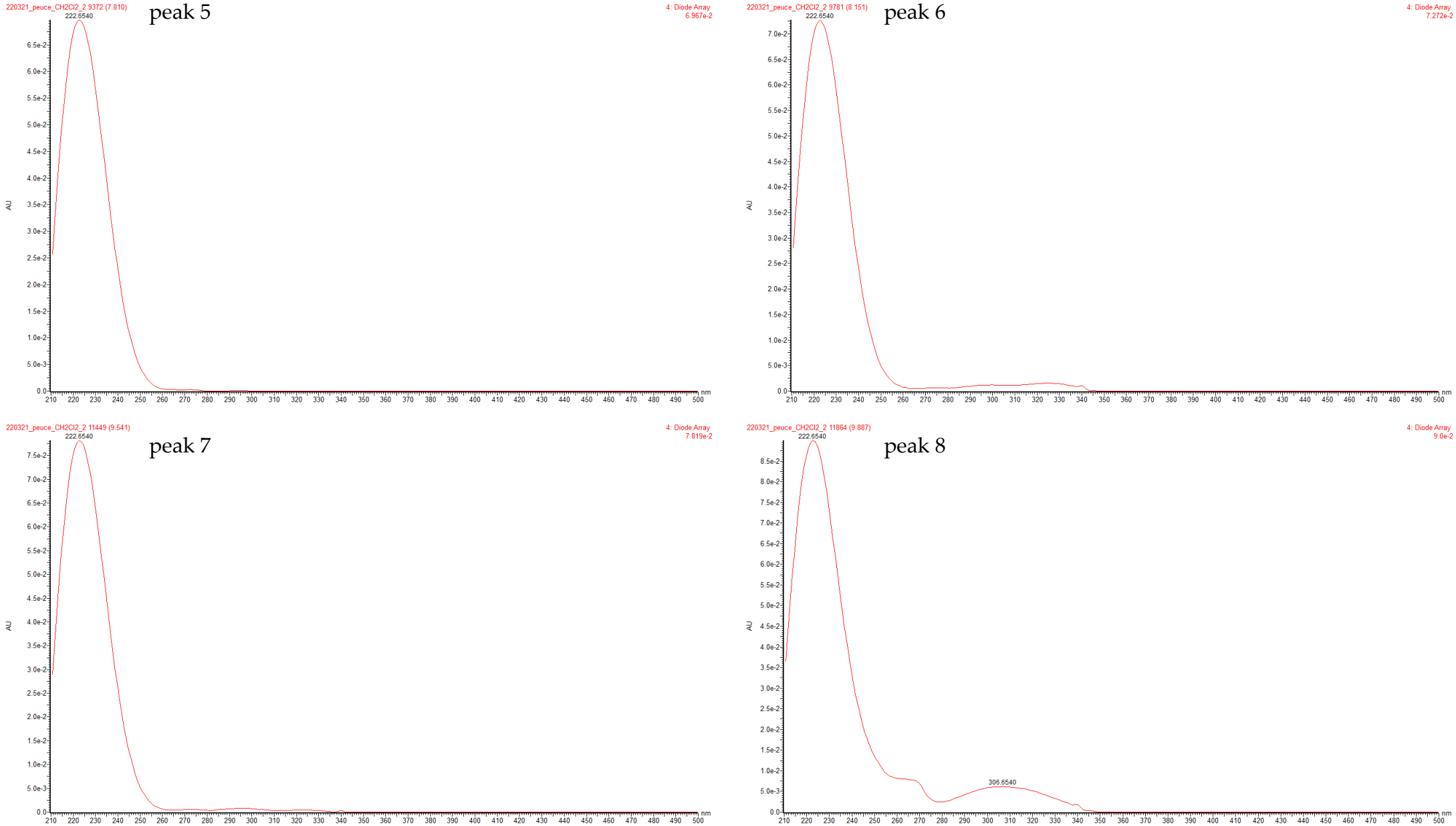
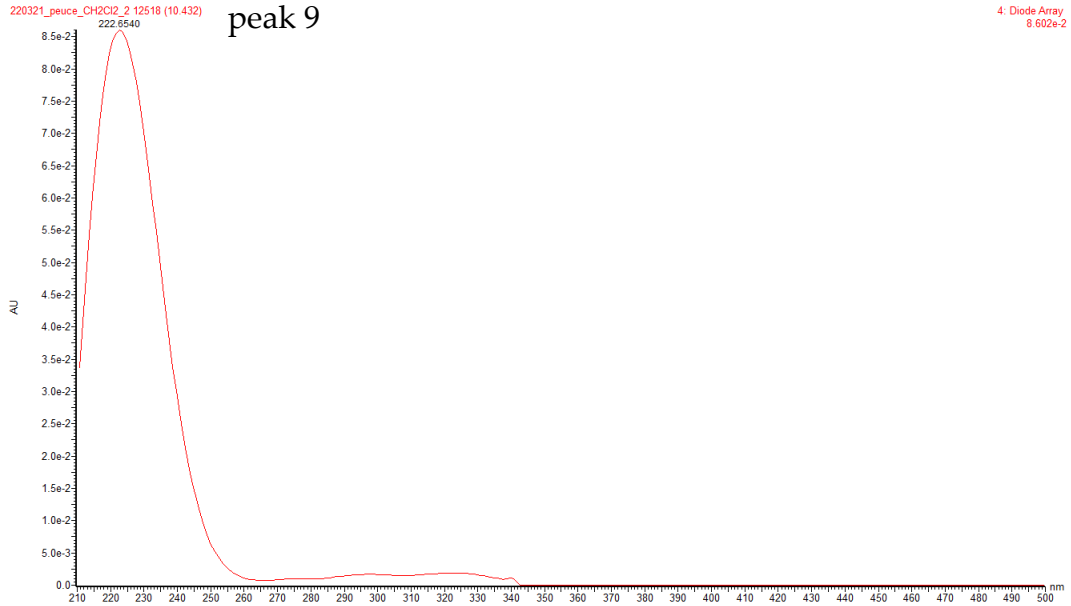
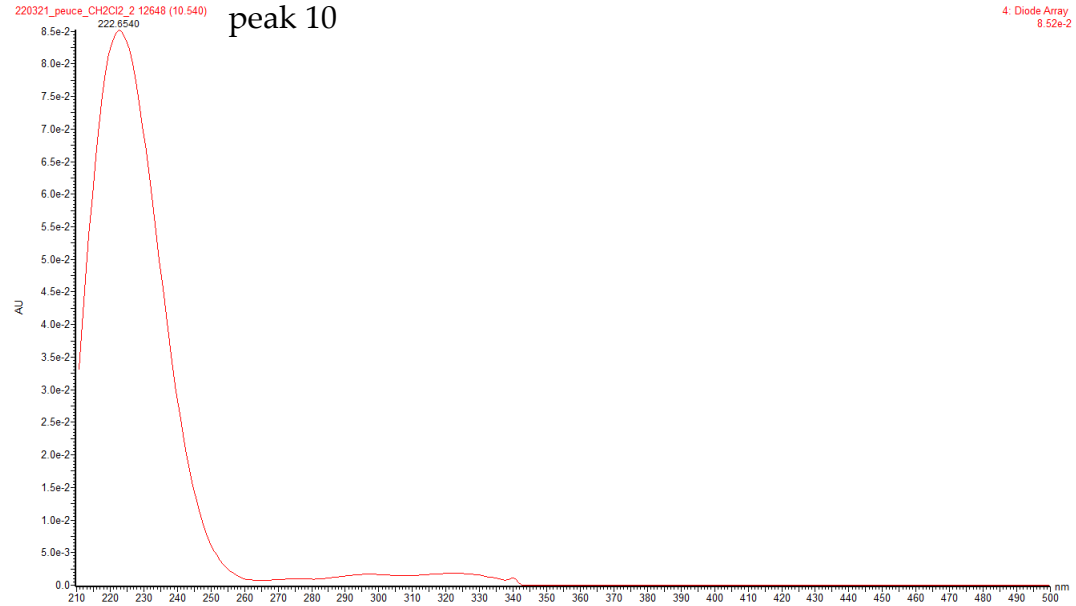
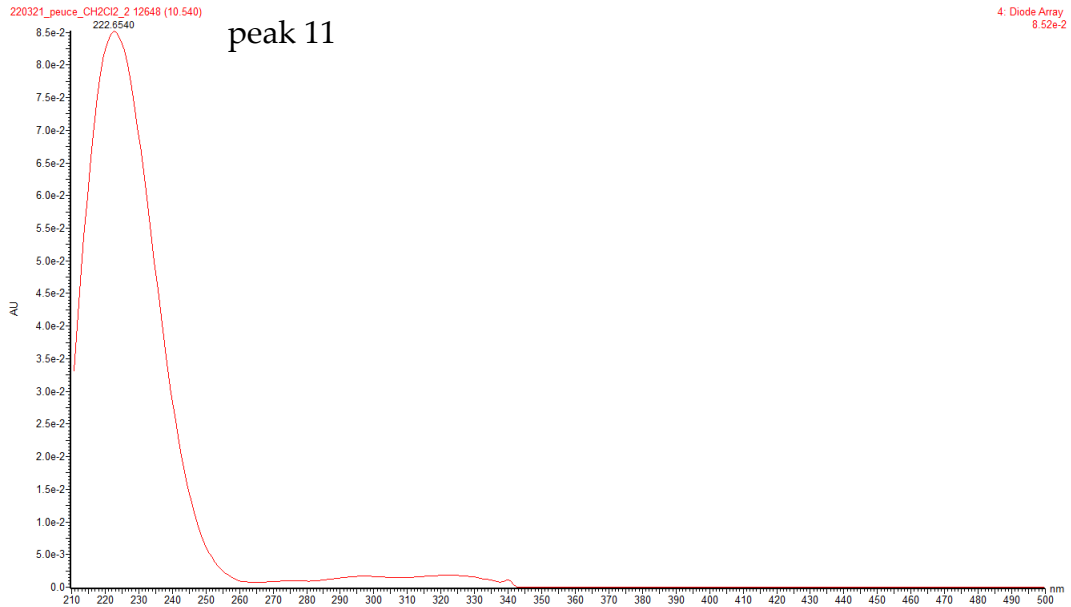


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)







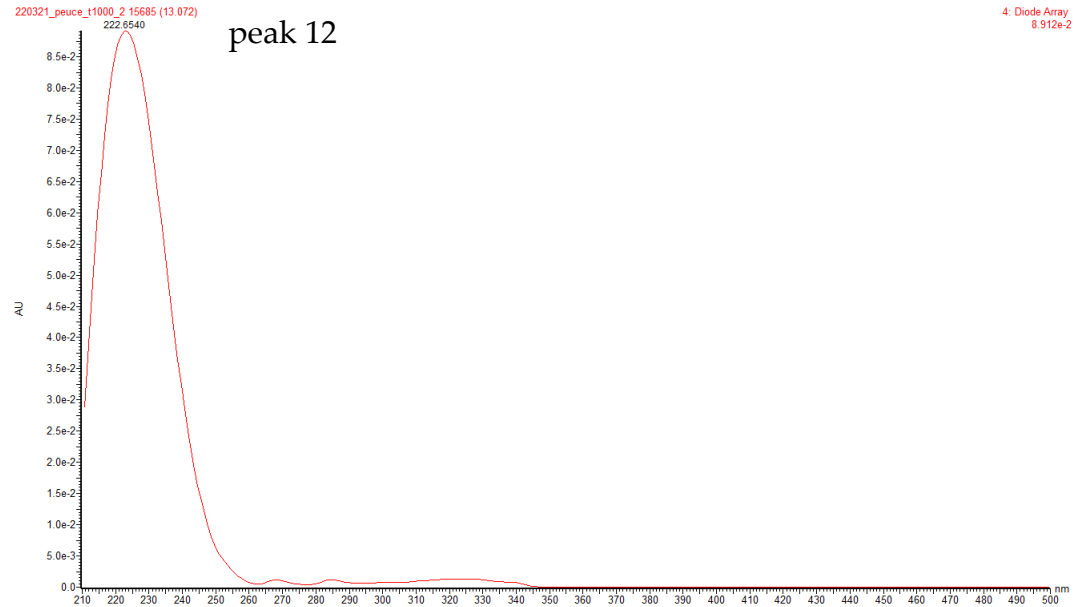
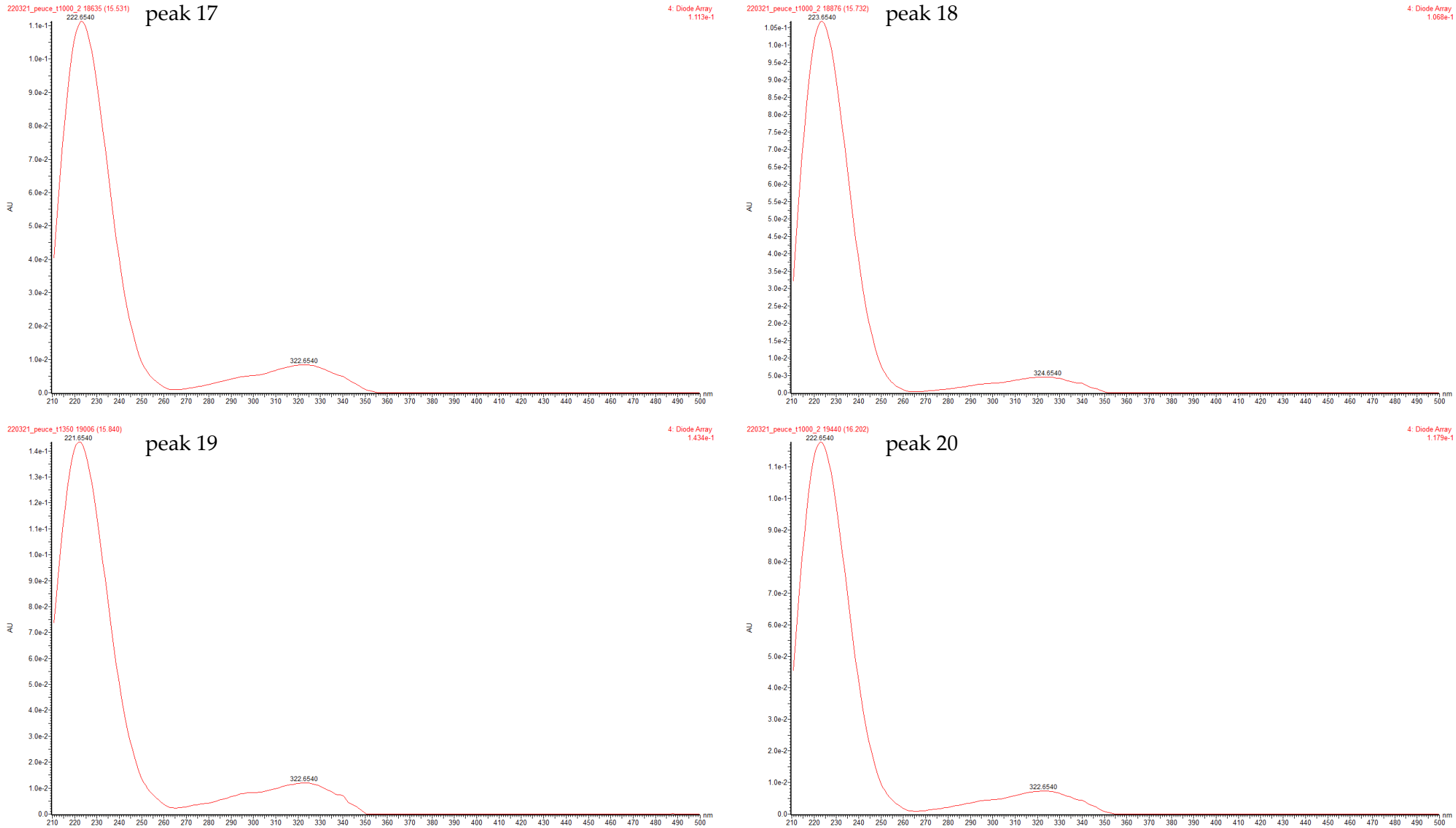


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)



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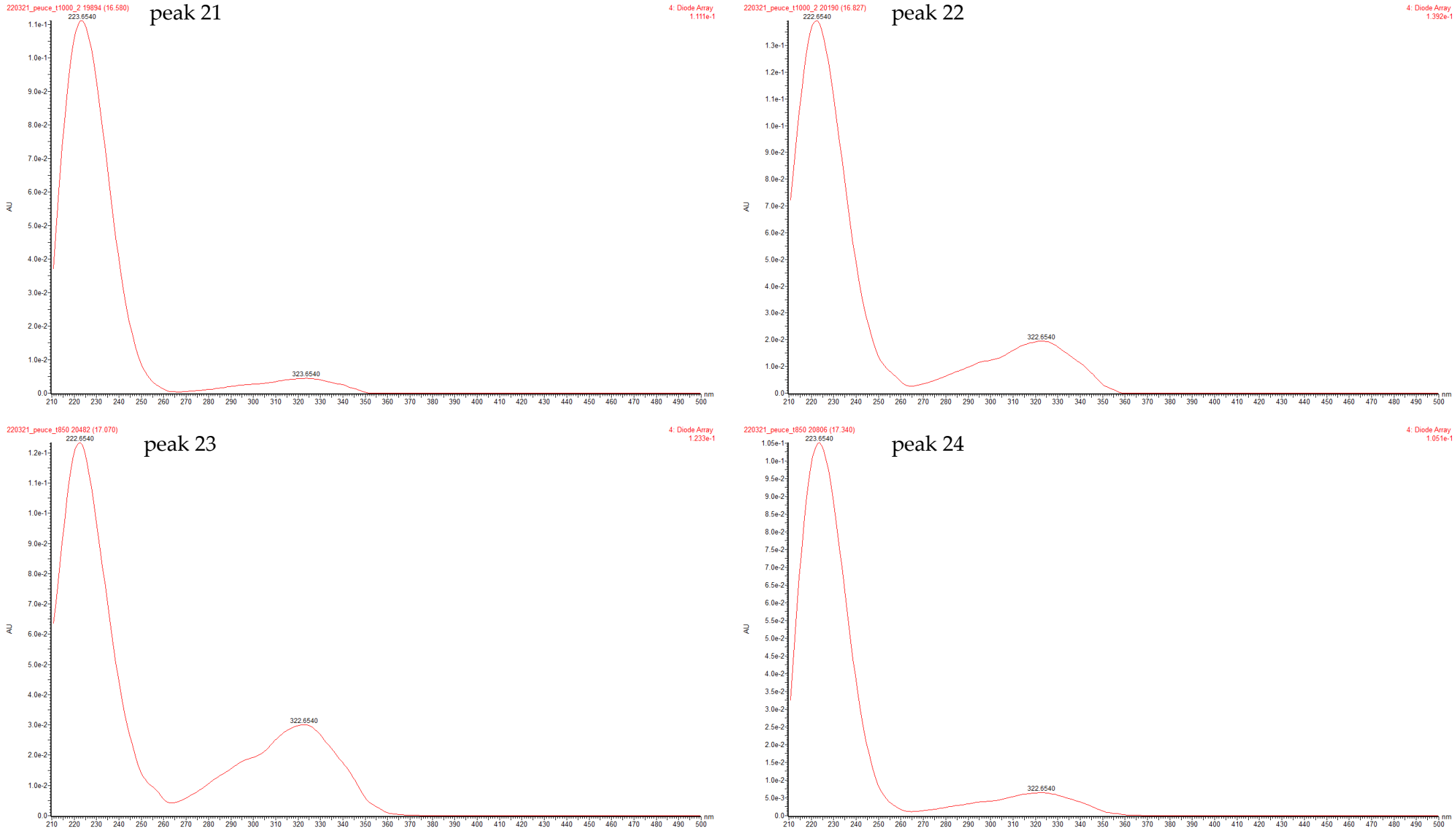

Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)

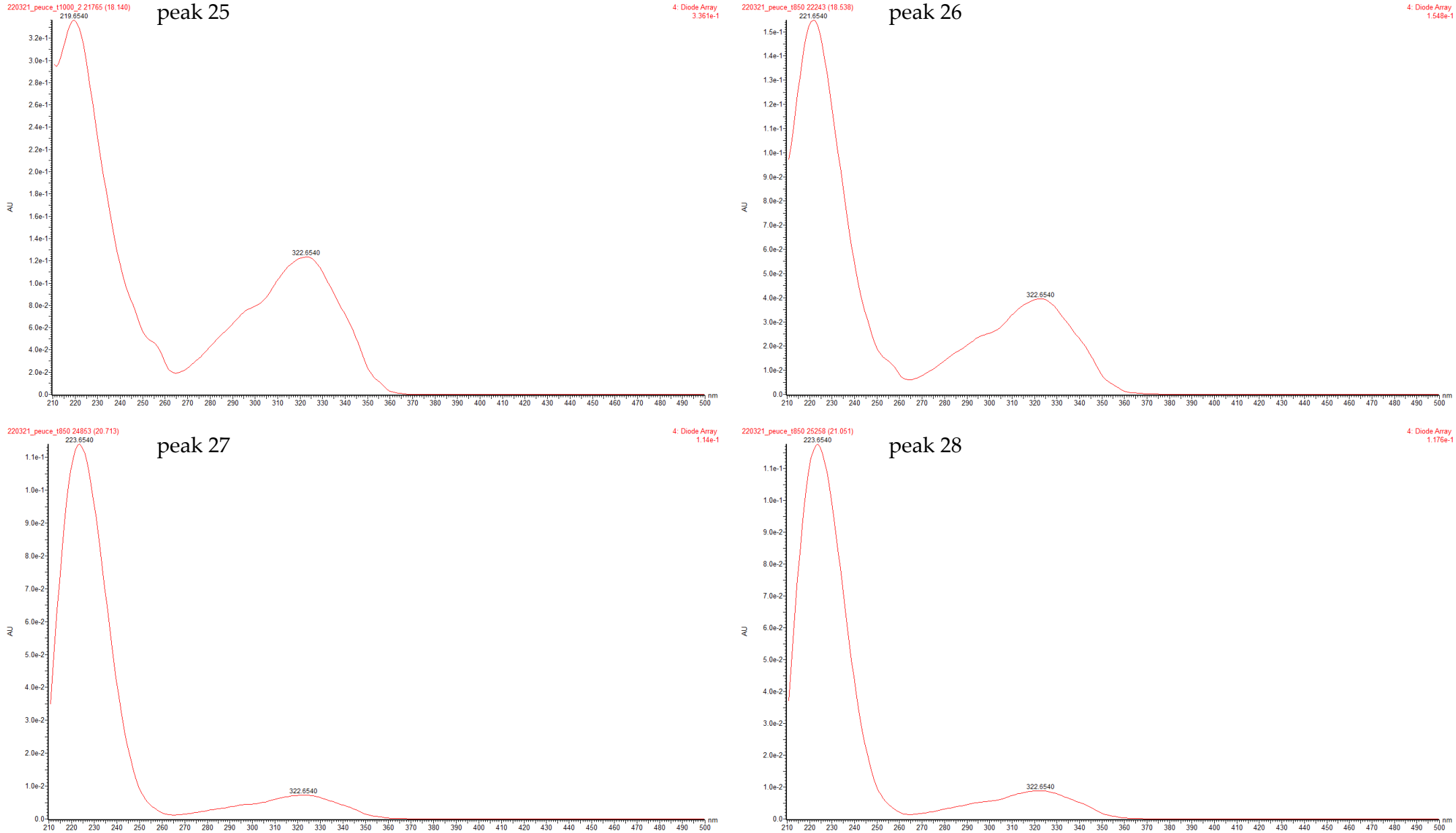

Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)

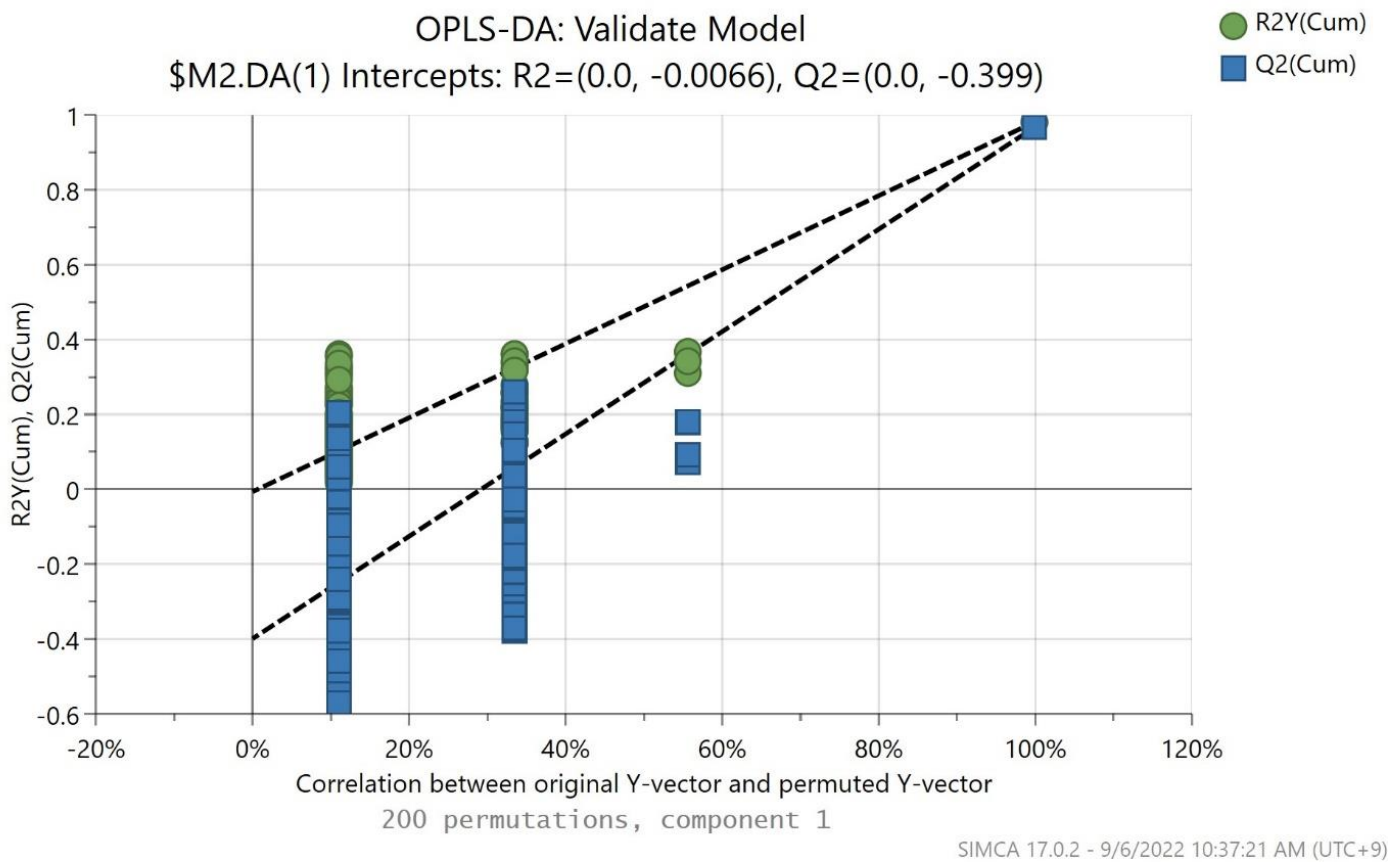

Figure S32. Permutation plot for validation of OPLS-DA obtained from 200 permutation test.