

Supporting Information

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

Jisu Park ^{1,2}, Sunil Babu Paudel ³, Chang Hyun Jin ¹, Gileung Lee ¹, Hong-Il Choi ¹, Ga-Hee Ryoo ¹, Yun-Seo Kil ³, Joo-Won Nam ³, Chan-Hun Jung ⁴, Bo-Ram Kim ⁵, MinKyun Na ², Ah-Reum Han ^{1,*}

- 1 Advanced Radiation Technology Institute, Korea Atomic Energy Research Institute, Jeongeup-si, Jeollabuk-do 56212, Republic of Korea; parkjs94@kaeri.re.kr (J.P.); chjin@kaeri.re.kr (C.H.J.); glee@kaeri.re.kr (G.L.); hichoi@kaeri.re.kr (H.-I.C.); ghryoo@kaeri.re.kr (G.H.R.)
 - 2 College of Pharmacy, Chungnam National University, Daejeon 34134, Republic of Korea; mkna@cnu.ac.kr (M.N)
 - 3 College of Pharmacy, Yeungnam University, Gyeongsan-si, Gyeongsangbukdo 38541, Republic of Korea; phrsunil@gmail.com (S.B.P.); yskil@yu.ac.kr (Y.-S.K.); jwnam@yu.ac.kr (J.-W.N.)
 - 4 Jeonju AgroBio-Materials Institute, Jeonju-si, Jeollabuk-do 54810, Republic of Korea; chjung@jami.re.kr (C.-H.J.)
 - 5 Natural Product Research Division, Honam National Institute of Biological Resources, Mokpo-si, Jeollanam-do 58762, Republic of Korea; boram0307@hnibr.re.kr (B.-R.K.)
- * Correspondence: arhan@kaeri.re.kr (A.-R.H.), Tel.: +82-63-570-3167 (A.-R.H.)

CONTENTS

Figure S1.	LC–MS base peak ion chromatograms of the flowers of <i>P. japonicum</i> 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 isoimperatorin (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-senecioidkhellactone (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-senecioidkhellactone) (peak 12)
Figure S14.	ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-propanoylkhellactone (or 3'-O-senecioid-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-senecioidkhellactone (peak 17)
Figure S19.	ESI-QToF-MS spectrum of 3'-O-senecioid-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-senecioidkhellactone (peak 20)
Figure S22.	ESI-QToF-MS spectrum of 3'-O-senecioid-4'-O-senecioidkhellactone (peak 21)
Figure S23.	ESI-QToF-MS spectrum of 3'-O-senecioid-4'-O-angeloylkhellactone (peak 22)
Figure S24.	ESI-QToF-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-isobutyrylkhellactone (peak 23)
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-senecioid khellactone, 3'-O-isovaleryl-4'-O-angeloylkhellactone (paeruptorin C), or 3'-O-isovaleryl-4'-O-senecioidkhellactone] (peak 25)
Figure S27.	ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-(2-methyl butyryl)khellactone [3'-O-angeloyl-4'-O-isovaleryl khellactone, 3'-O-senecioid-4'-O-(2-methyl butyryl)khellactone, or 3'-O-senecioid-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 S32.** Permutation plot for validation of OPLS-DA obtained from 200 permutation test.

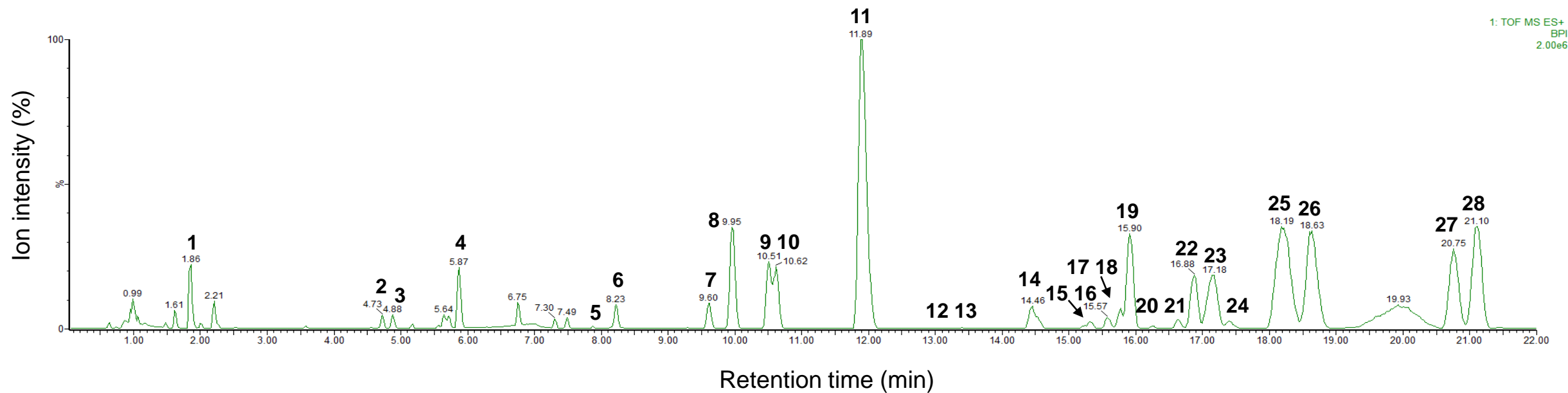


Figure S1. LC–MS base peak ion chromatograms of the dichloromethane fraction of the flowers of *P. japonicum* at positive ion mode (6 eV, ESI⁺).

220530_peu_flower_p_03 99 (1.831) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.50e6

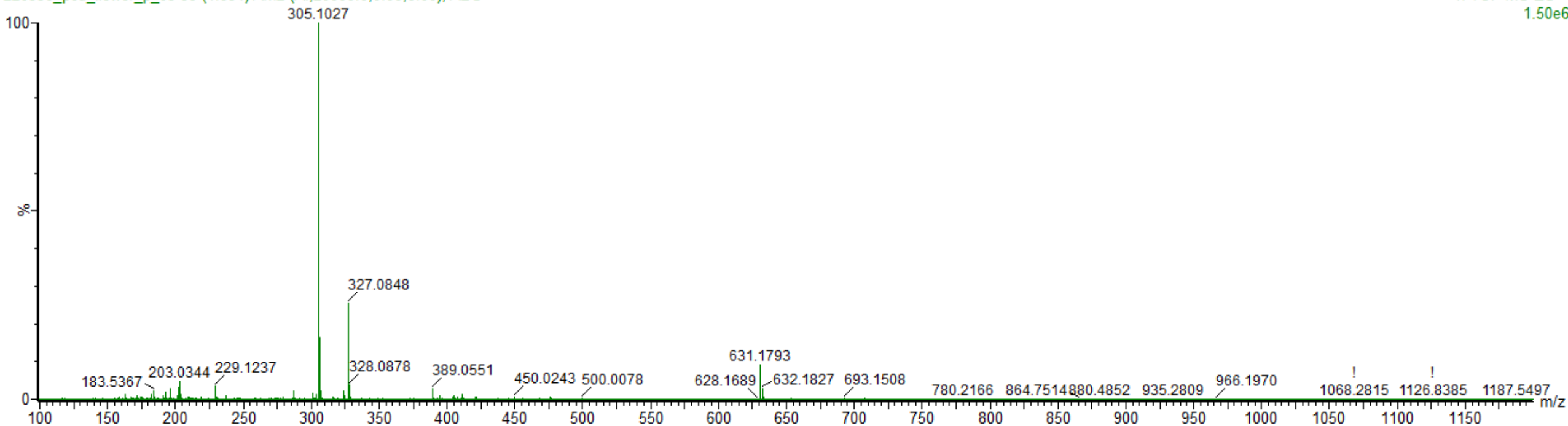


Figure S2. ESI-QToF-MS spectrum of oxypeucedanin hydrate (peak 1).

220321_peuce_CH2Cl2_2 255 (4.712) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.83e5

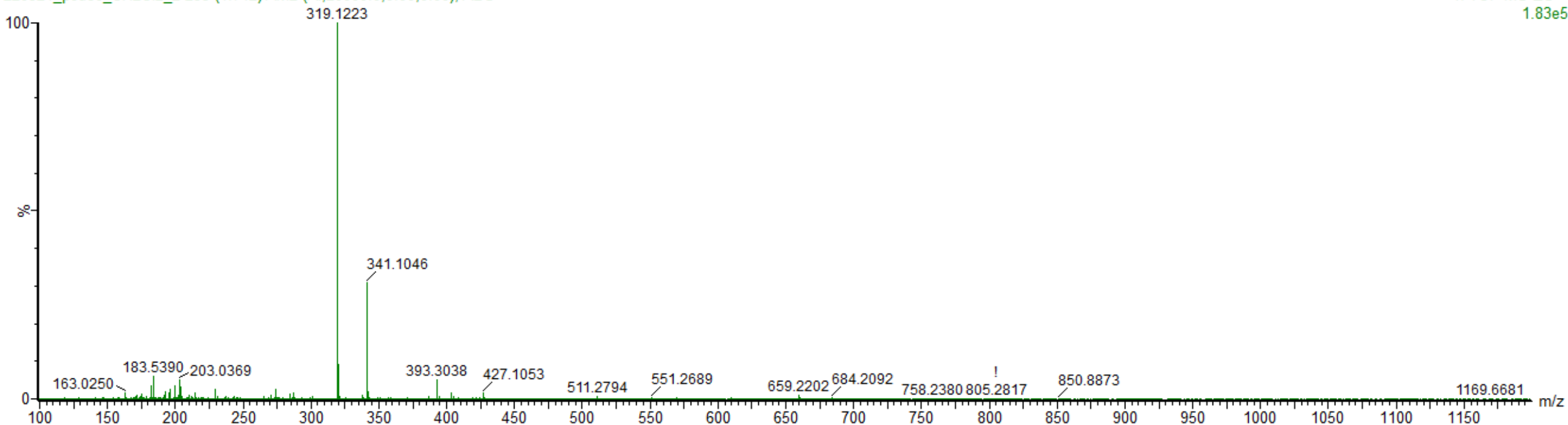


Figure S3. ESI-QToF-MS spectrum of oxypeucedanin methanolate (peak 2).

220530_peu_flower_p_03 265 (4.895) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
3.24e5

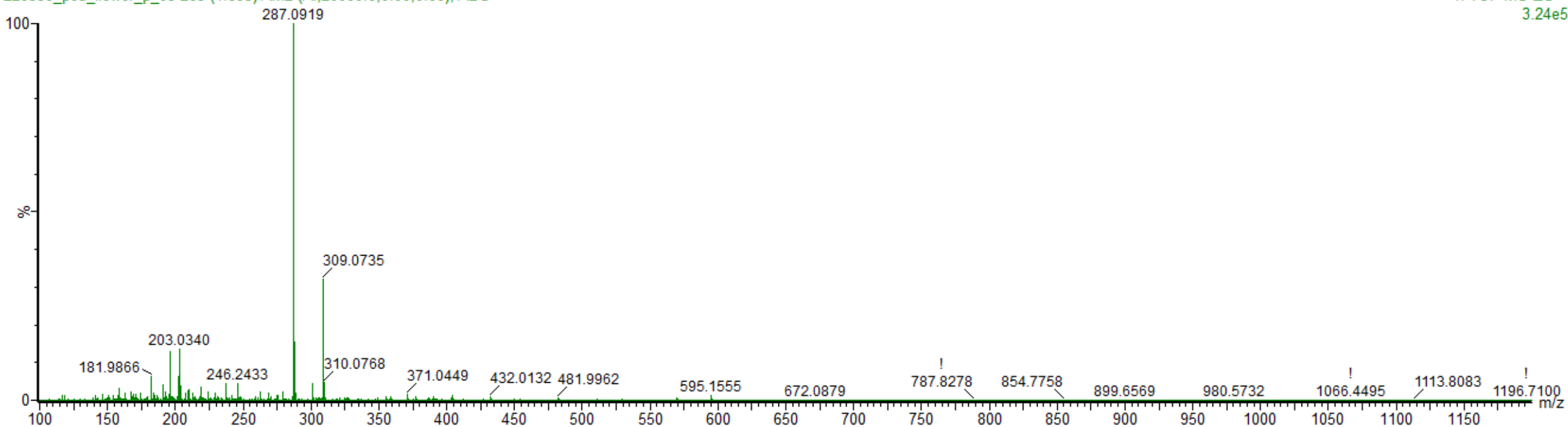


Figure S4. ESI-QToF-MS spectrum of pabulenol (peak 3).

220530_peu_flower_p_03 319 (5.889) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.40e6

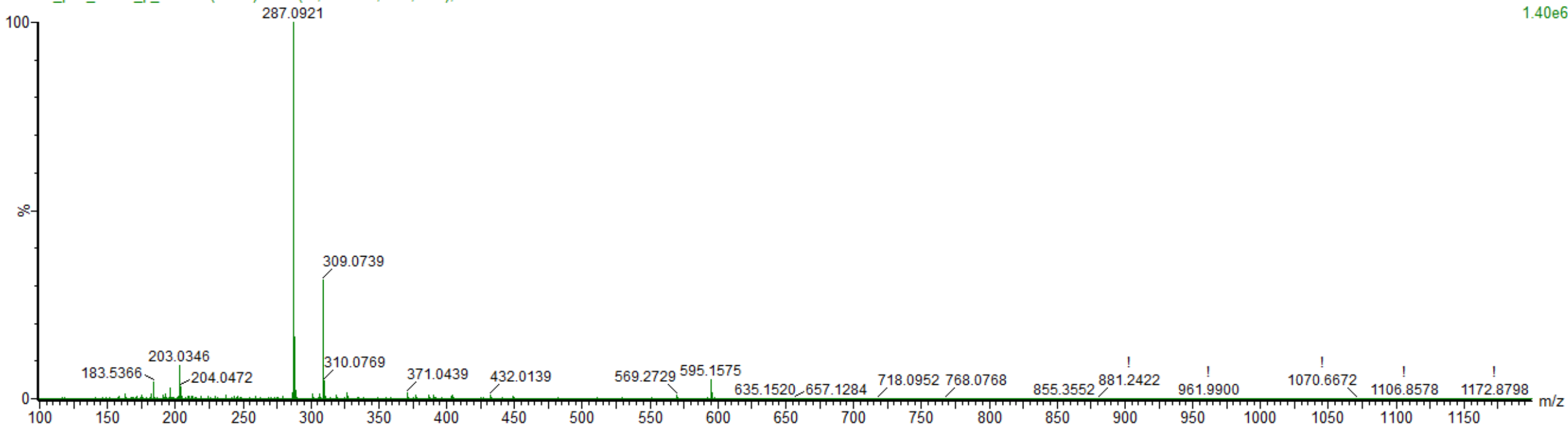


Figure S5. ESI-QToF-MS spectrum of 5-[(3-hydroxy-3-methyl-1-butenyl)oxy]psoralen (peak 4).

220321_peuce_CH2Cl2_2 427 (7.878) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
3.59e4

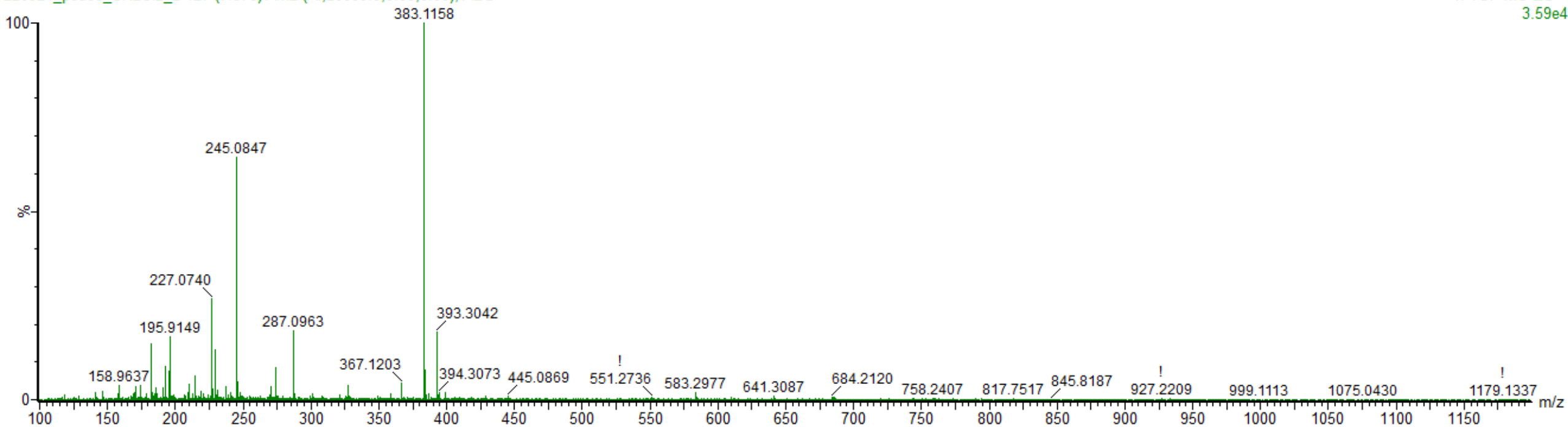


Figure S6. ESI-QToF-MS spectrum of 3'-O-acetyl-4'-O-propanoylkhellactone (peak 5).

220530_peu_flower_p_03 448 (8.261) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+

4.56e5



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

220530_peu_flower_p_03 524 (9.667) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+

5.05e5

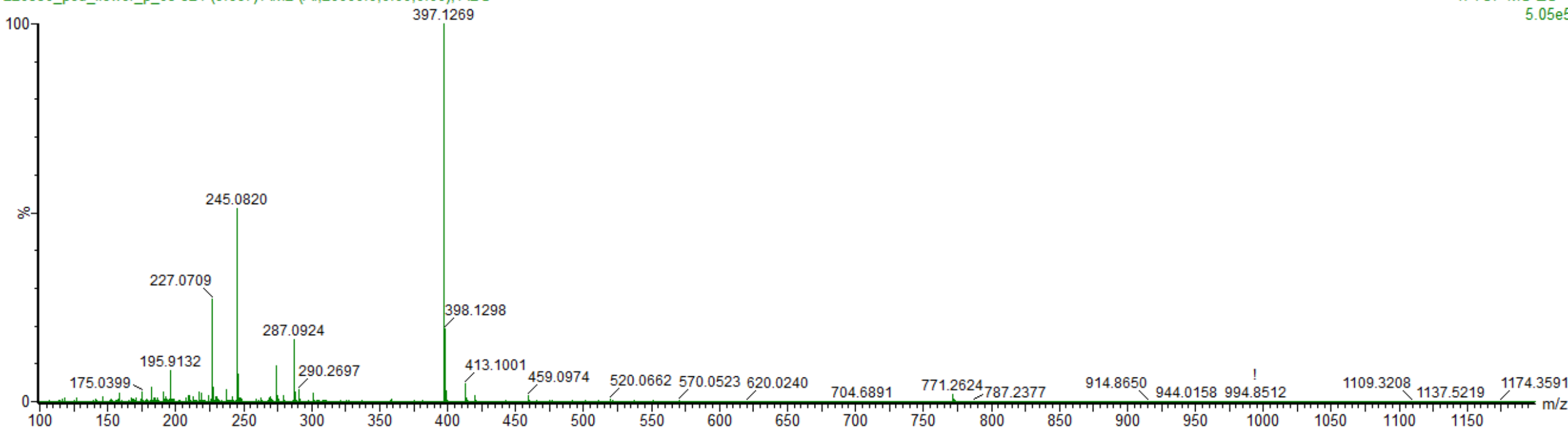


Figure S8. ESI-QToF-MS spectrum of 3'-O-acetyl-4'-O-isobutyryl khellactone (hyuganin D) (peak 7).

220530_peu_flower_p_03 543 (10.015) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
3.52e6

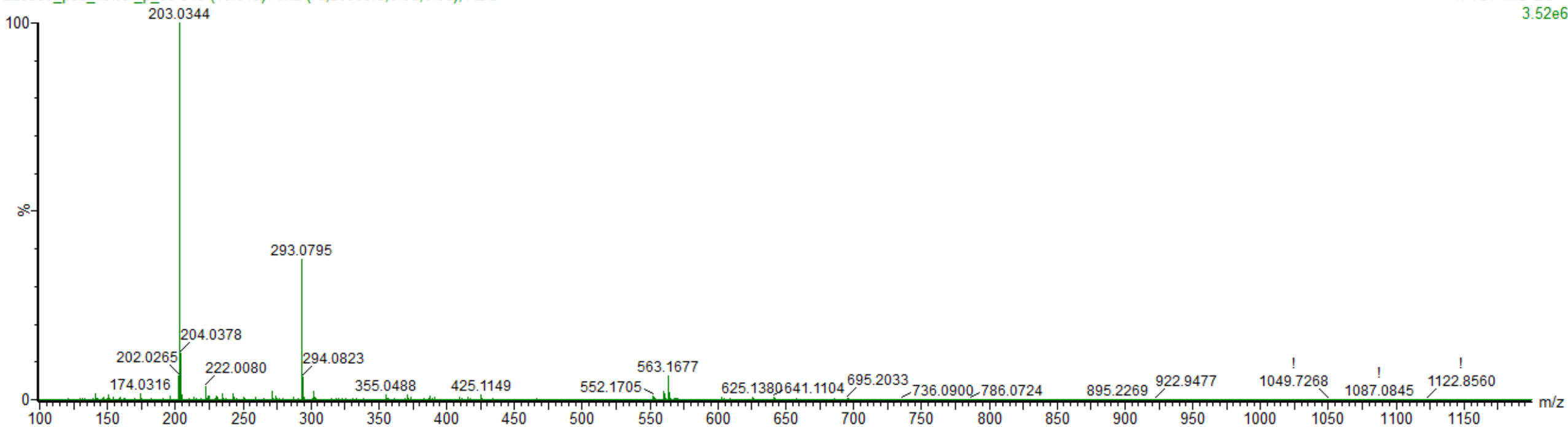


Figure S9. ESI-QToF-MS spectrum of isoimpertorin (peak 8).

220530_peu_flower_p_03 574 (10.581) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
9.61e5

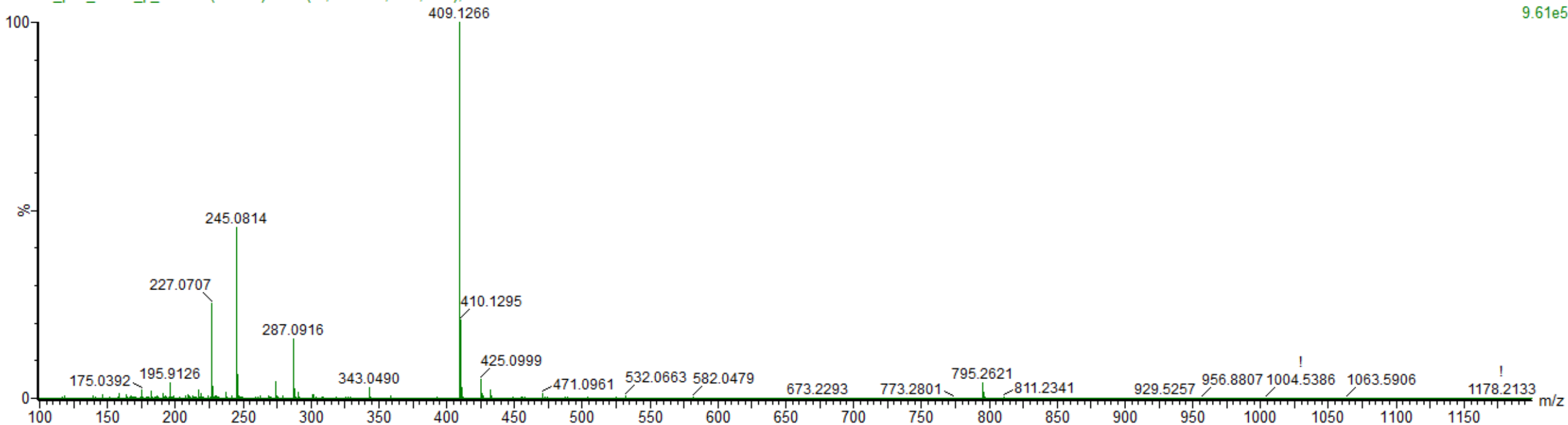


Figure S10. ESI-QToF-MS spectrum of 3'-O-acetyl-4'-O-angeloylkhellactone (pteryxin) (peak 9).

220530_peu_flower_p_03 579 (10.678) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
8.44e5

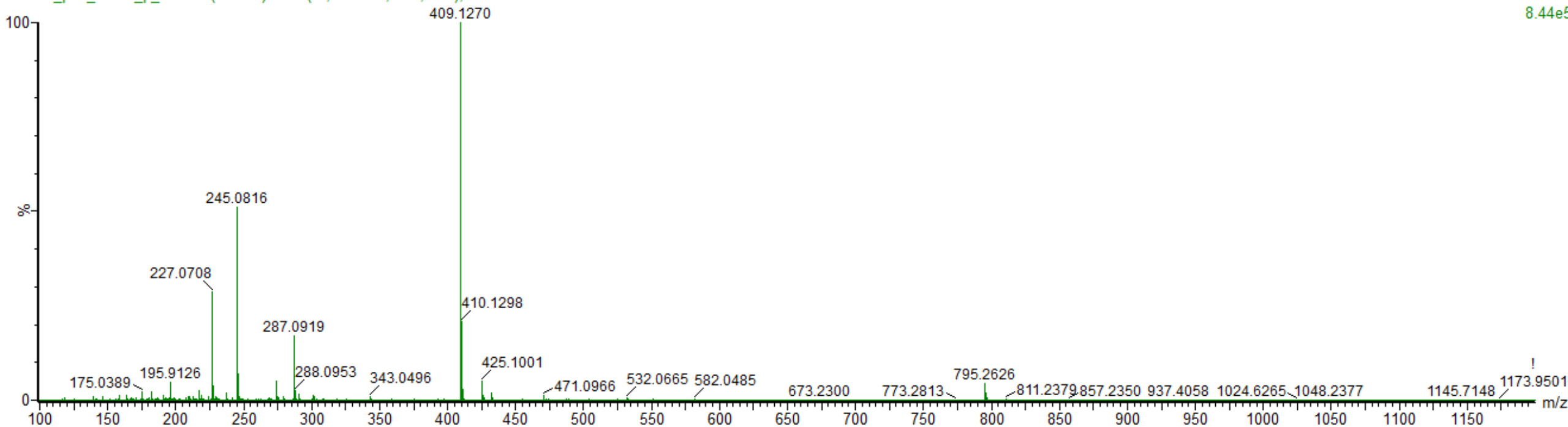


Figure S11. ESI-QToF-MS spectrum of 3'-O-acetyl-4'-O-seneciodylhellactone (peak 10).

220530_peu_flower_p_03 650 (11.987) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
4.66e6

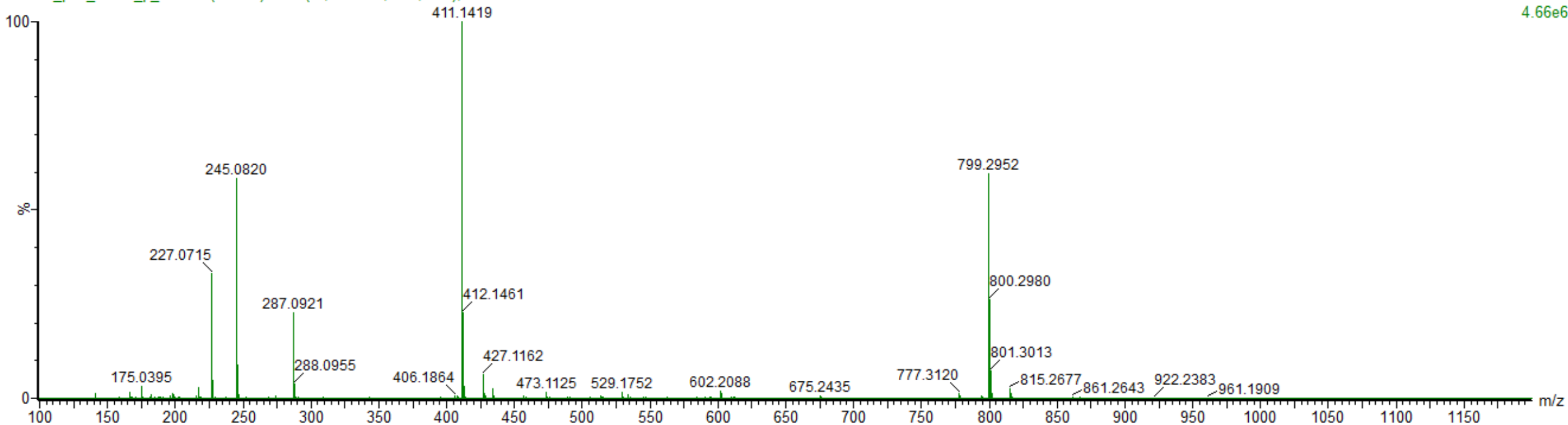


Figure S12. ESI-QToF-MS spectrum of 3'-O-acetyl-4'-O-(2-methyl butanoate)khellactone (or 3'-O-acetyl-4'-O-isovalerylkhellactone) (peak 11).

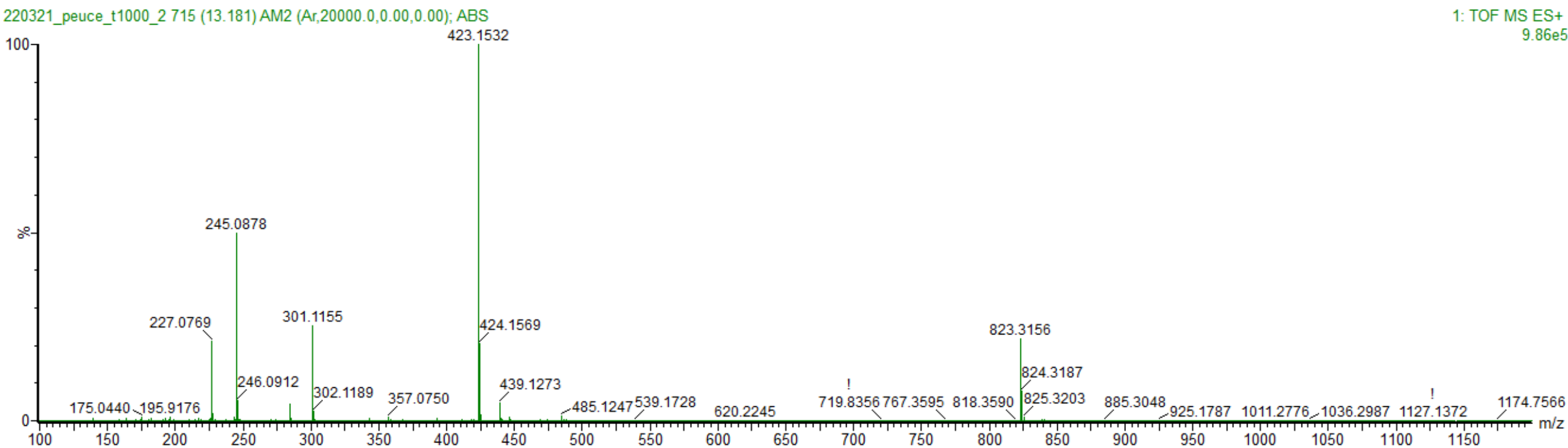


Figure S13. ESI-QToF-MS spectrum of 3'-O-propanoyl-4'-O-angeloyl khellactone (or 3'-O-propanoyl-4'-O-senecioylkhellactone) (peak 12).

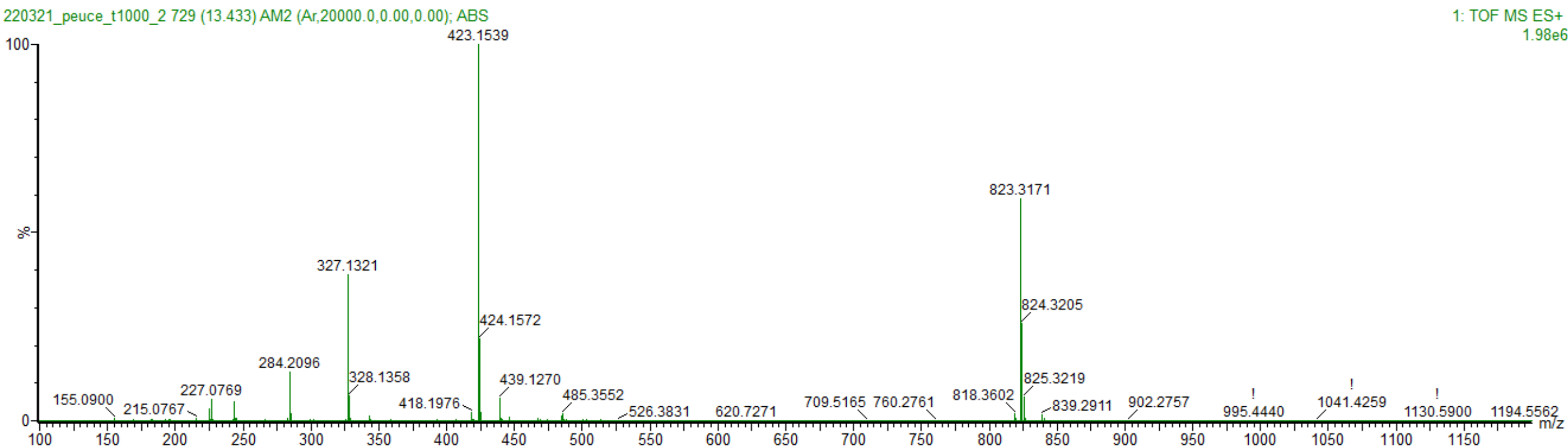


Figure S14. ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-propanoylkhellactone (or 3'-O-senecioid-4'-O-propanoylkhellactone) (peak 13).

220530_peu_flower_p_03 789 (14.542) AM2 (Ar,20000.0,0.00,0.00); ABS; Cm (784:799)

1: TOF MS ES+
6.40e6

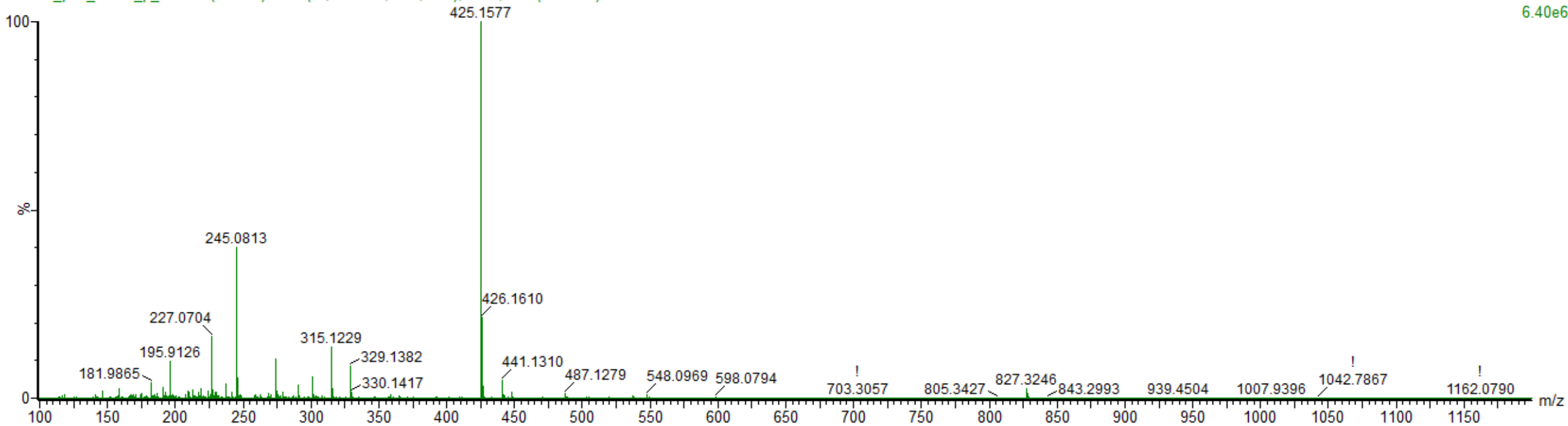


Figure S15. ESI-QToF-MS spectrum of 3'-O-isobutyryl-4'-O-isobutyrylhellactone (peak 14).

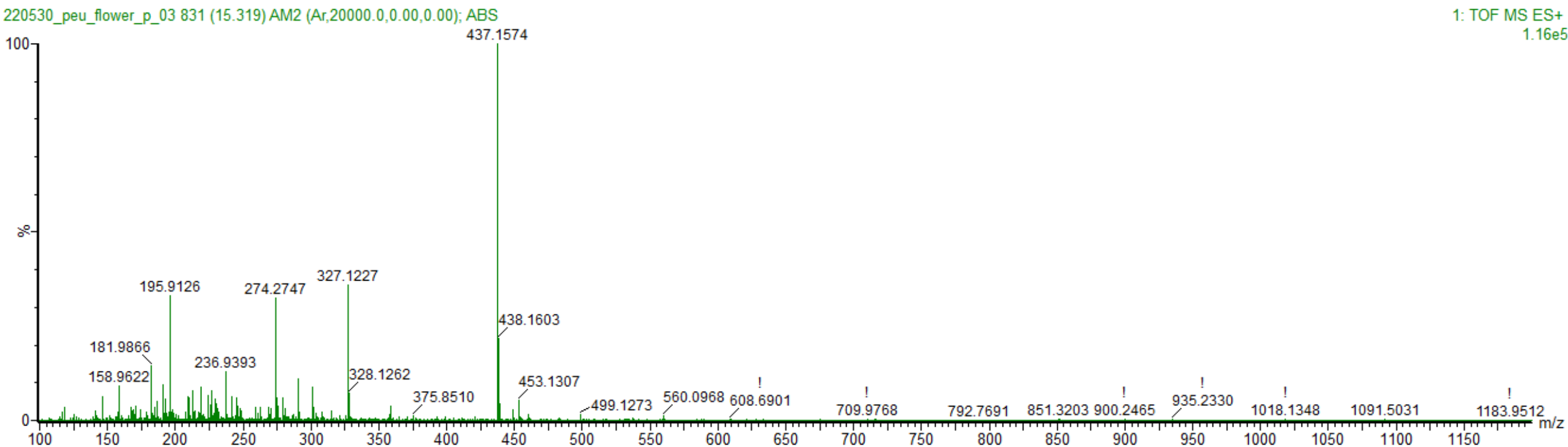


Figure S16. ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-isobutyrylhellactone (peak 15).

220530_peu_flower_p_03 837 (15.422) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
2.10e5

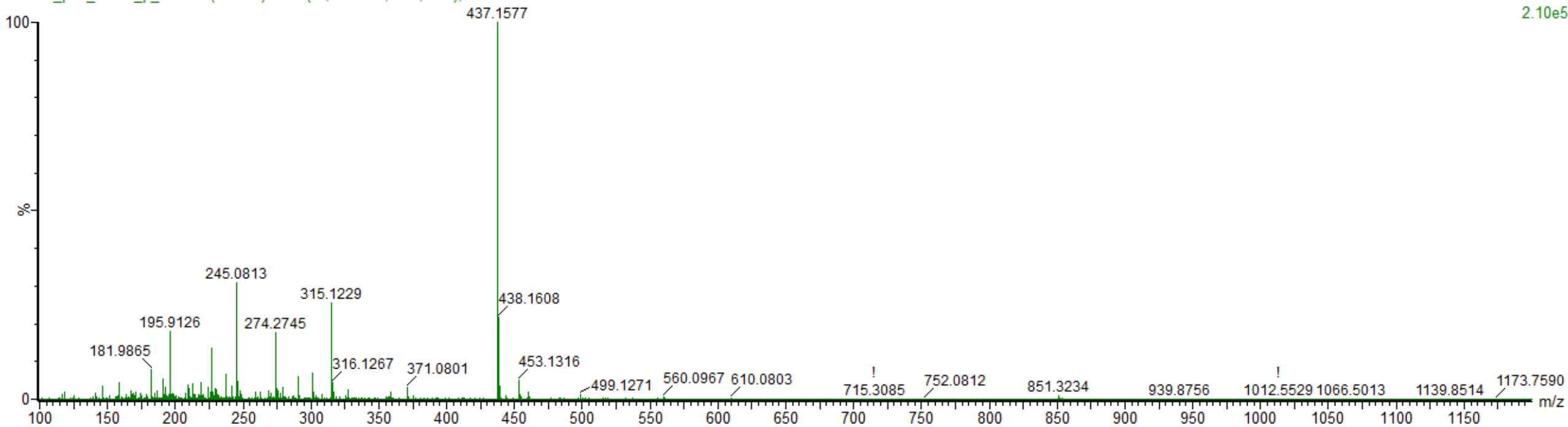


Figure S17. ESI-QToF-MS spectrum of 3'-O- isobutyryl-4'-O-angeloylkhellactone (peak 16).

220530_peu_flower_p_03 850 (15.667) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
2.66e5

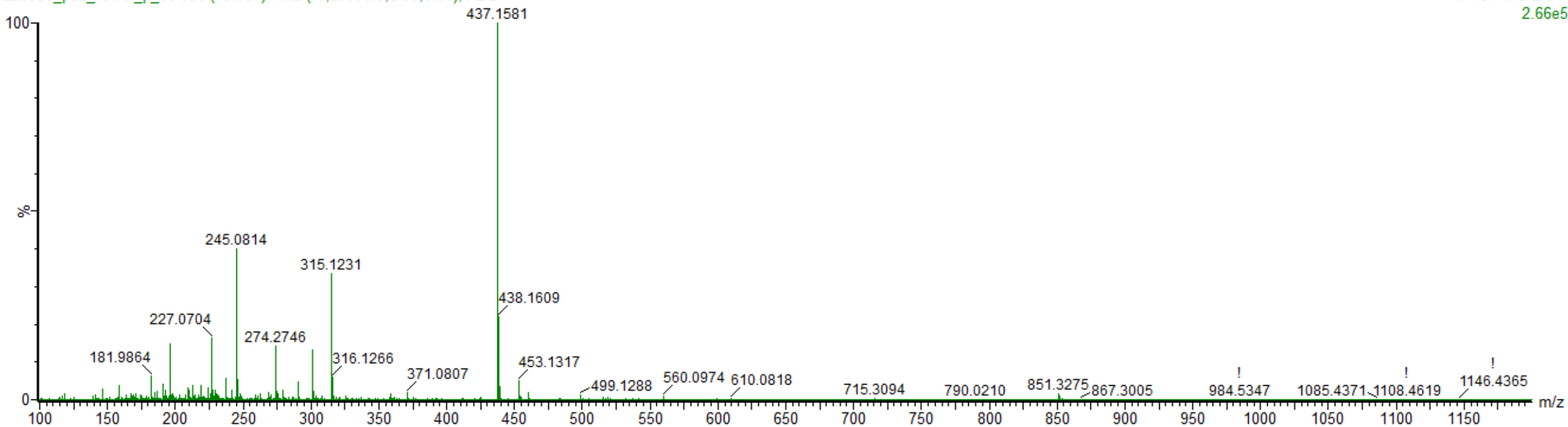


Figure S18. ESI-QToF-MS spectrum of 3'-O-isobutyryl-4'-O-senecioidhellactone (peak 17).

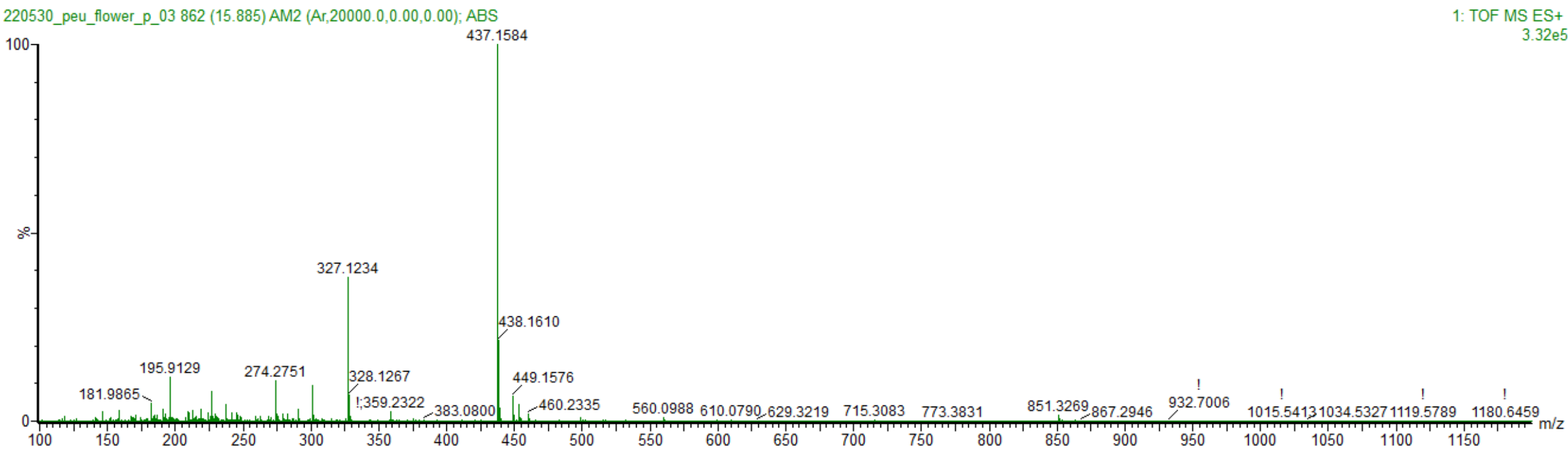


Figure S19. ESI-QToF-MS spectrum of 3'-O-senecioid-4'-O-isobutyrylhellactone (peak 18).

220530_peu_flower_p_03 869 (16.016) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.19e6

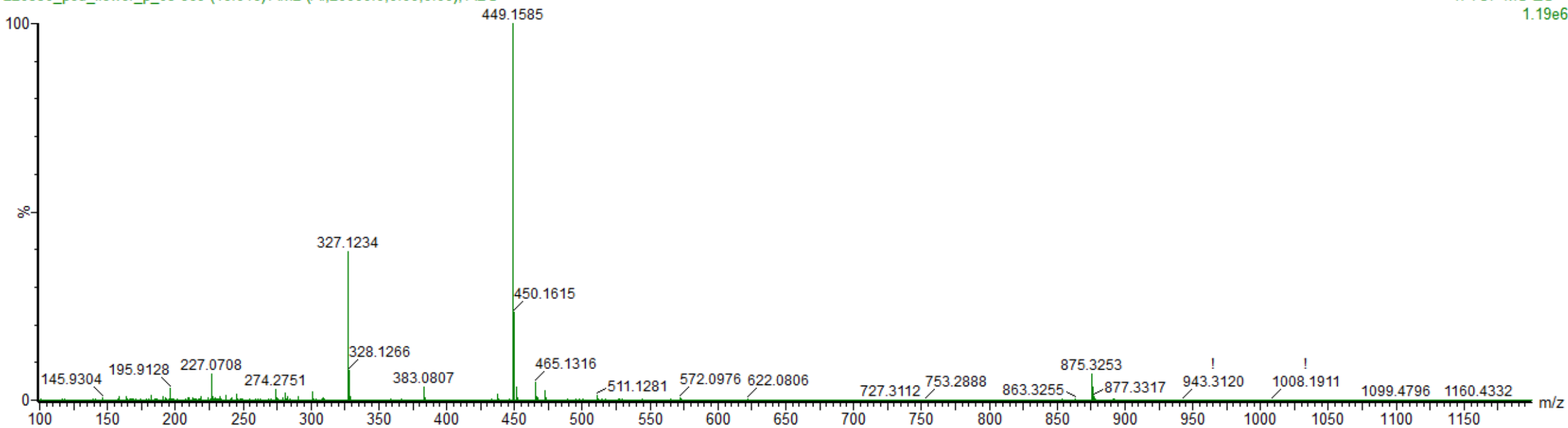


Figure S20. ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-angeloylkhellactone (paeruptorin B) (peak 19).

220530_peu_flower_p_03 888 (16.365) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
9.55e4

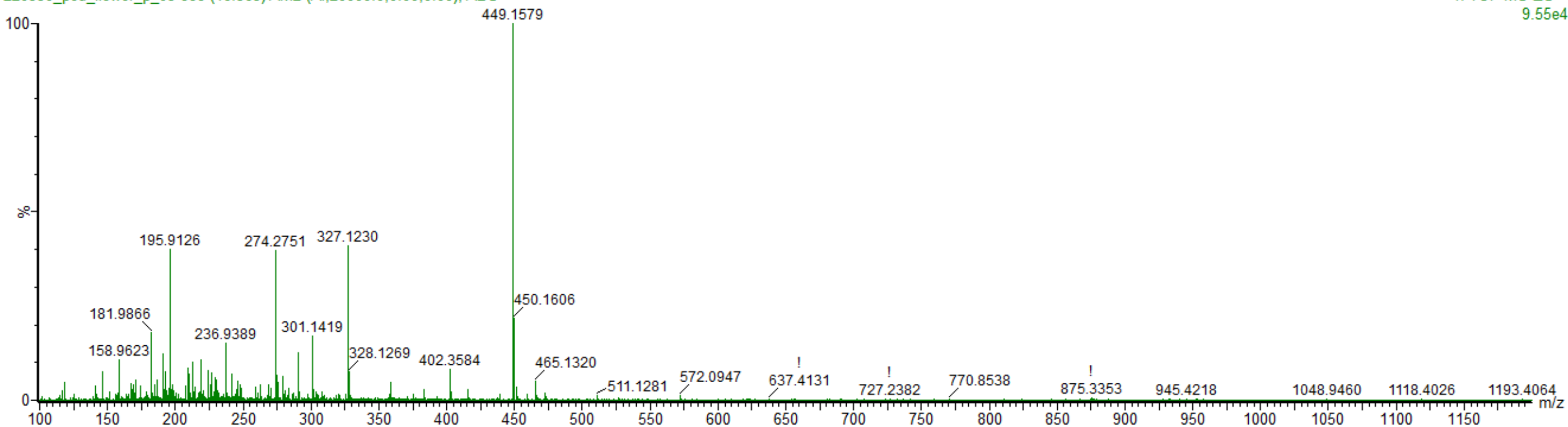


Figure S21. ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-seneciойlhellactone (peak 20).

220530_peu_flower_p_03 909 (16.747) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.60e5

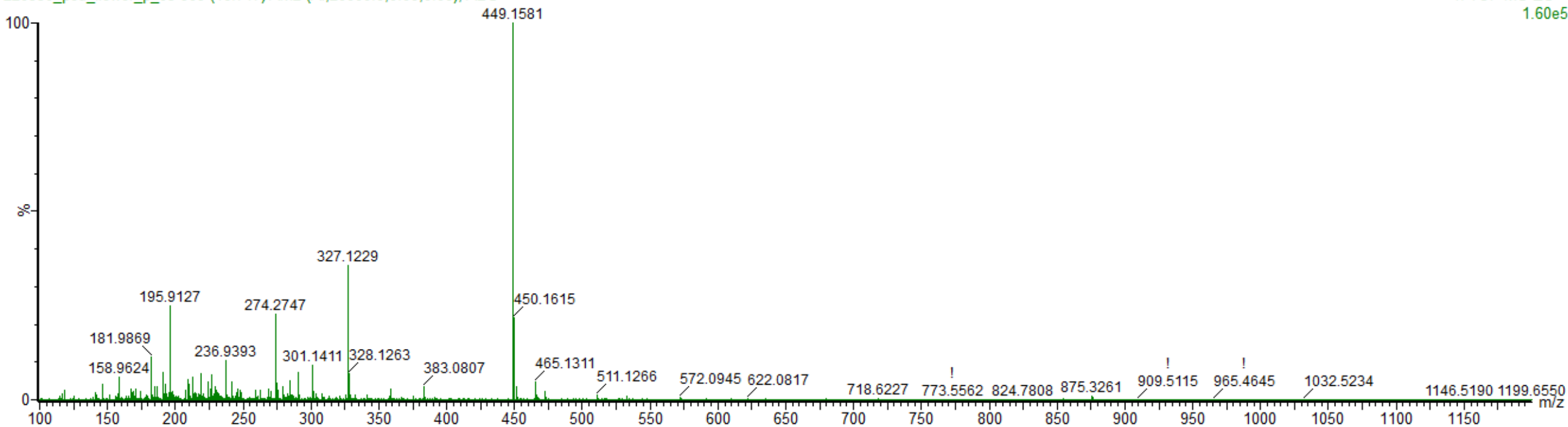


Figure S22. ESI-QToF-MS spectrum of 3'-O-senecieryl-4'-O-seneciylkhellactone (peak 21).

220530_peu_flower_p_03 922 (16.993) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
7.38e5

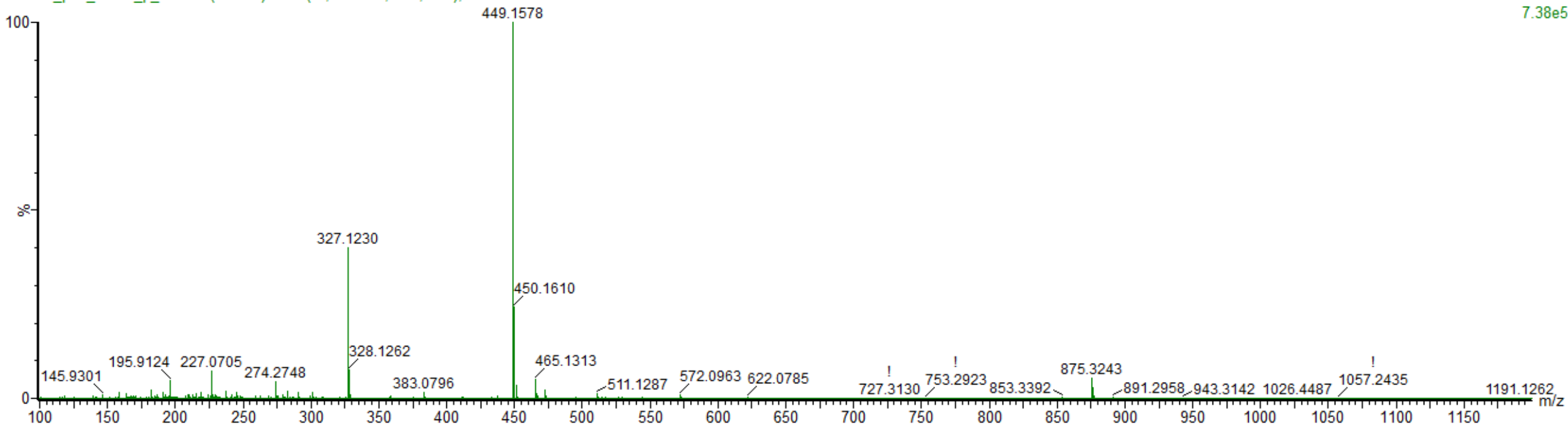


Figure S23. ESI-QToF-MS spectrum of 3'-O-senecieryl-4'-O-angeloylhellactone (peak 22).

220530_peu_flower_p_03 937 (17.273) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.49e6

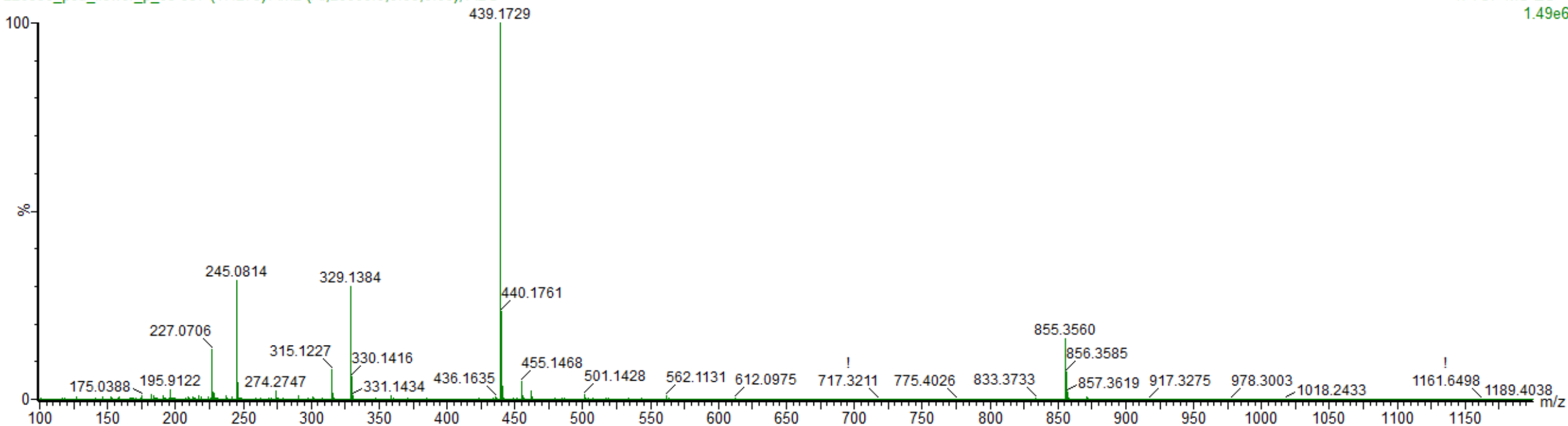


Figure S24. ESI-QToF-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-isobutyrylhellactone (peak23).

220530_peu_flower_p_03 952 (17.542) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
2.37e5

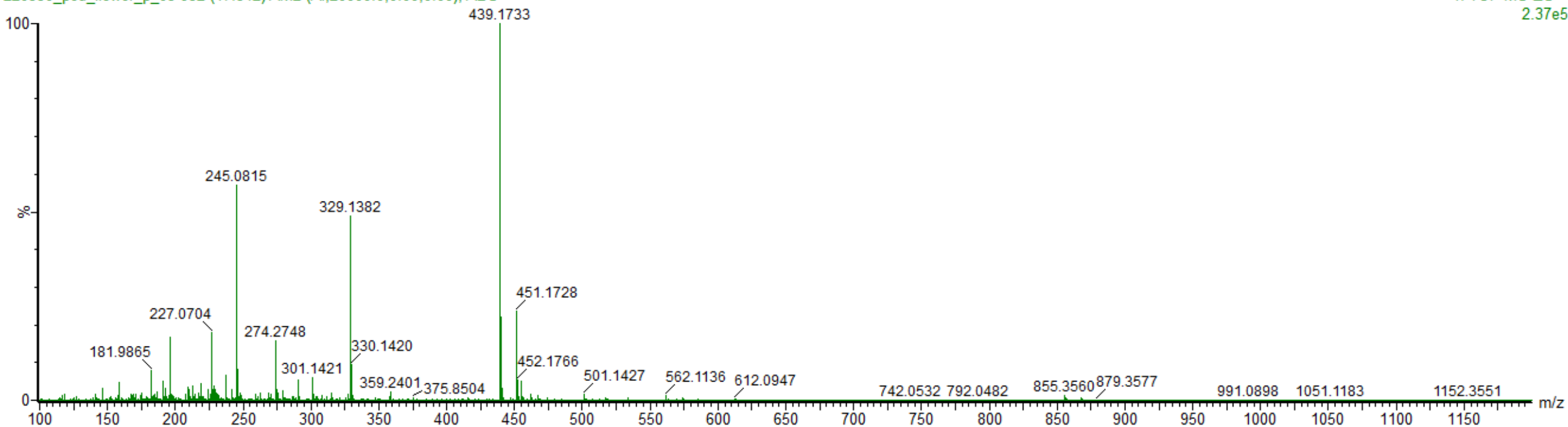


Figure S25. ESI-QToF-MS spectrum of 3'-O-isovaleryl-4'-O-isobutyrylkhellactone (peak 24).

220530_peu_flower_p_03 997 (18.371) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.74e6

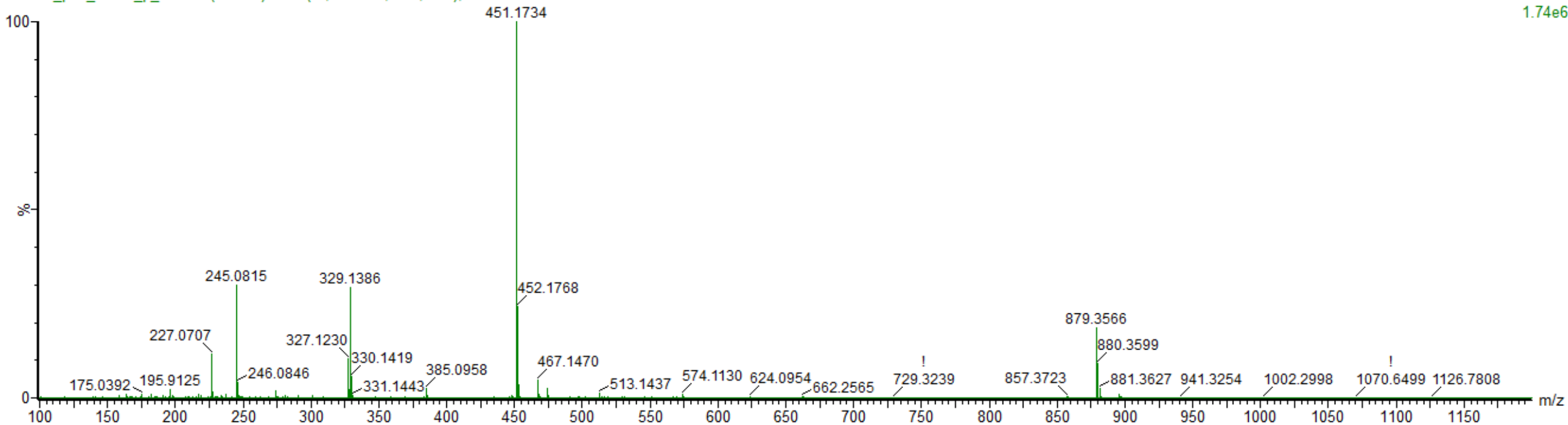


Figure S26. ESI-QToF-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-angeloylkhellactone [3'-O-(2-methyl butyryl)-4'-O-senecioyl khellactone, 3'-O-isovaleryl-4'-O-angeloylkhellactone (paeruptorin C), or 3'-O-isovaleryl-4'-O-senecioylkhellactone] (peak 25).

220530_peu_flower_p_03 1020 (18.799) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
1.48e6

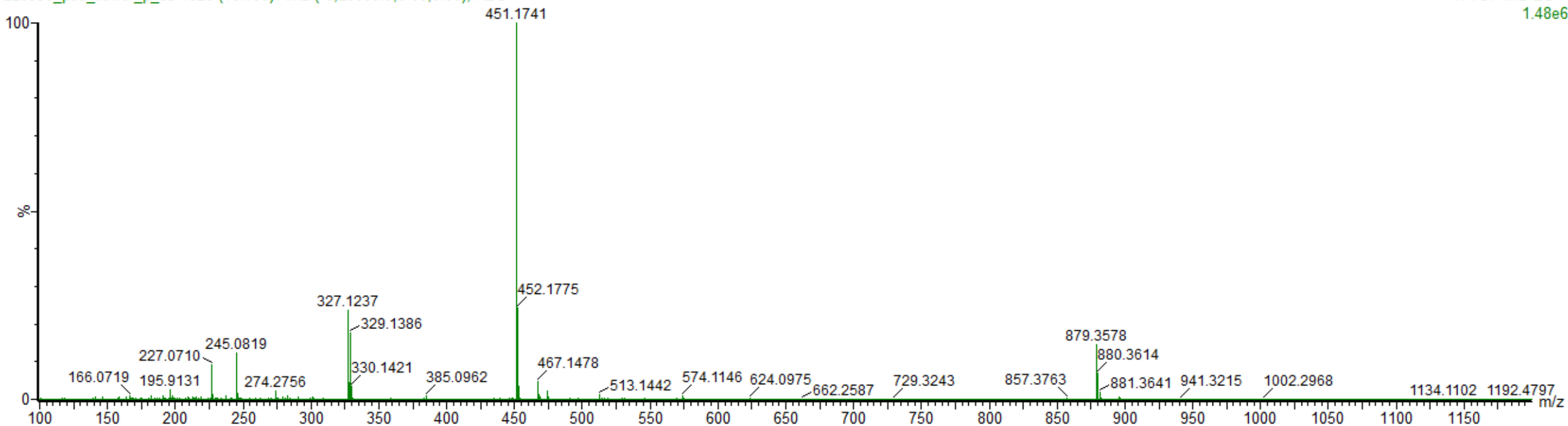


Figure S26. ESI-QToF-MS spectrum of 3'-O-angeloyl-4'-O-(2-methyl butyryl)khellactone [3'-O-angeloyl-4'-O-isovaleryl khellactone, 3'-O-senecieryl-4'-O-(2-methyl butyryl)khellactone, or 3'-O-senecieryl-4'-O-isovaleryl khellactone] (peak 26).

220530_peu_flower_p_03 1135 (20.919) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
2.61e6

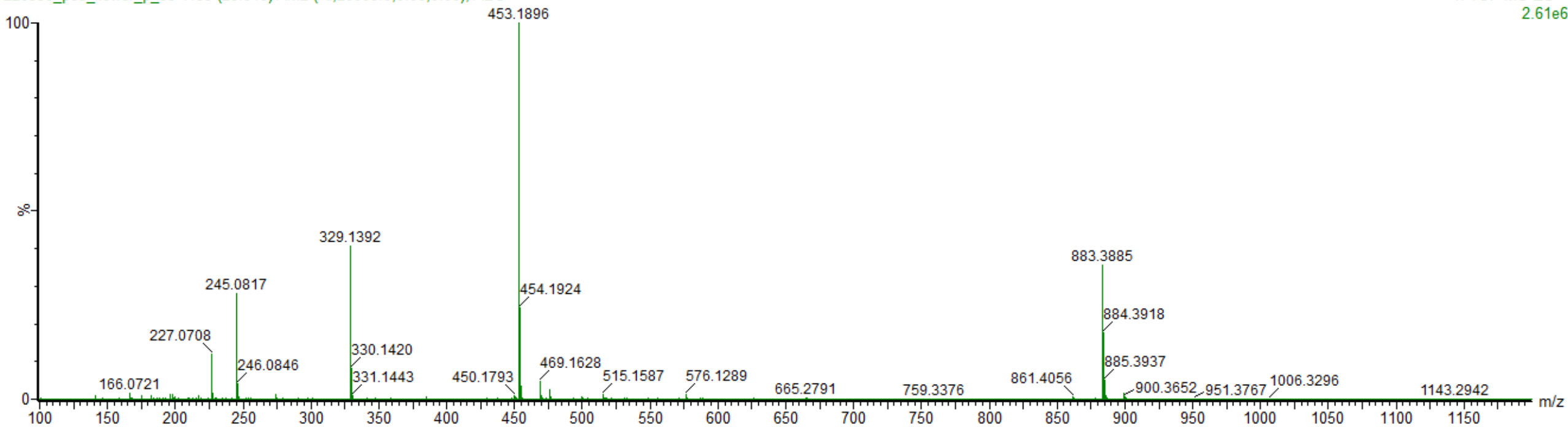


Figure S28. ESI-QToF-MS spectrum of 3'-O-(2-methyl butyryl)-4'-O-(2-methyl butyryl)khellactone (or 3'-O-(2-methyl butyryl)-4'-O-isovalerylkhellactone) (peak 27).

220530_peu_flower_p_03 1154 (21.268) AM2 (Ar,20000.0,0.00,0.00); ABS

1: TOF MS ES+
2.80e6

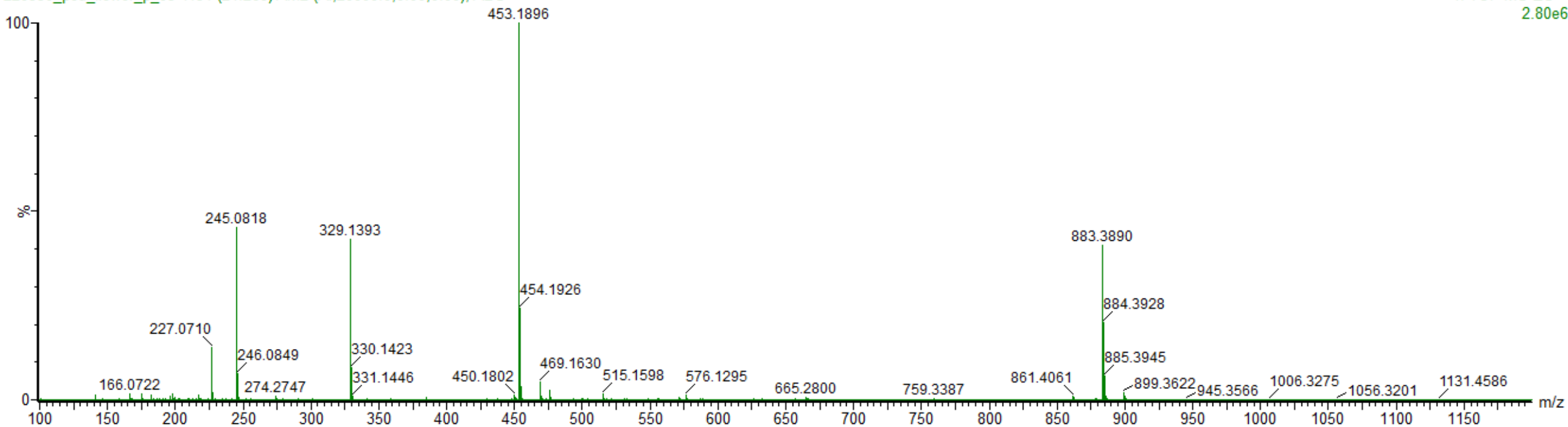


Figure S29. ESI-QToF-MS spectrum of 3'-O-isovaleryl-4'-O-(2-methyl butyryl)khellactone (or 3'-O-isovaleryl-4'-O-isovalerylkhellactone) (peak 28).

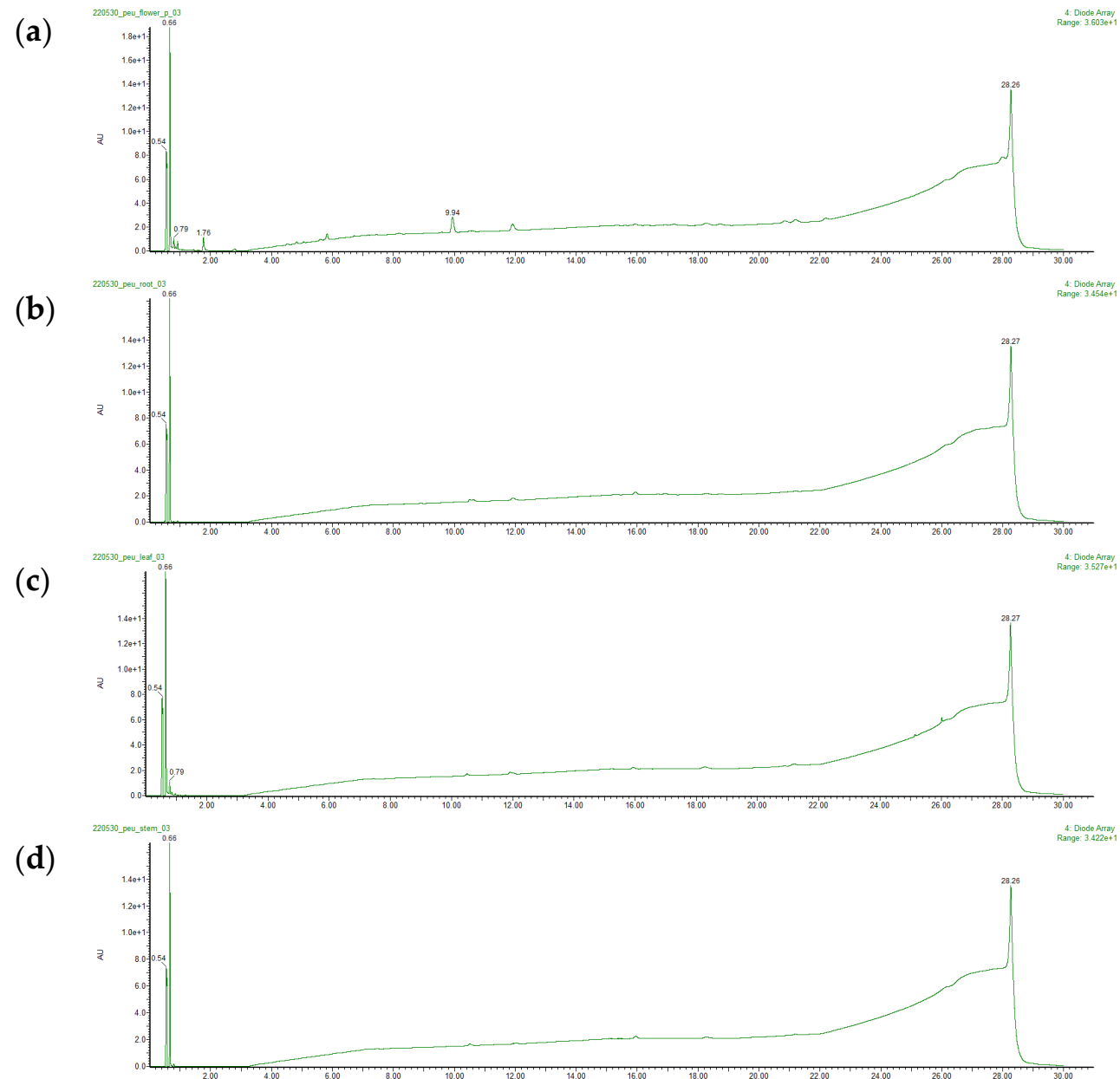


Figure S30. Total scan PDA chromatograms of (a) flowers (S3), (b) roots (S15), (c) leaves (S9), and (d) stems (S21) of *Peucedanum japonicum*

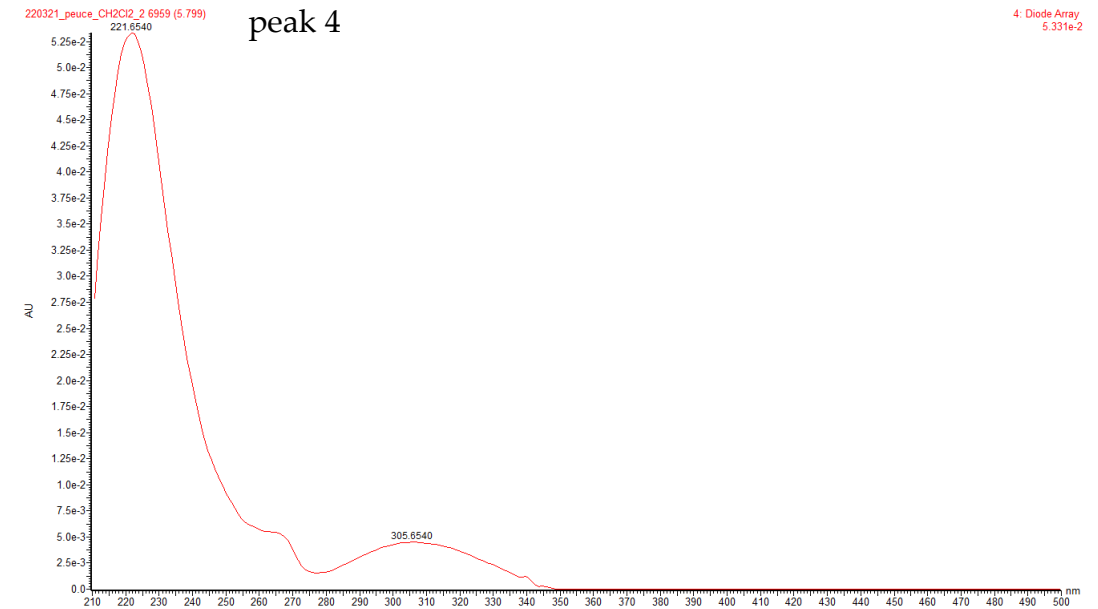
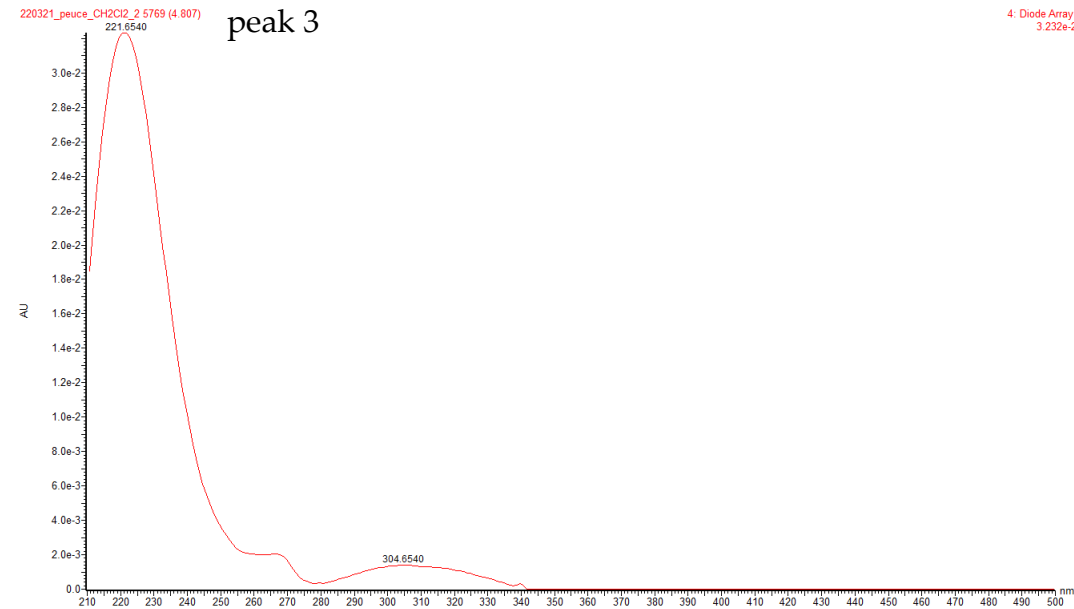
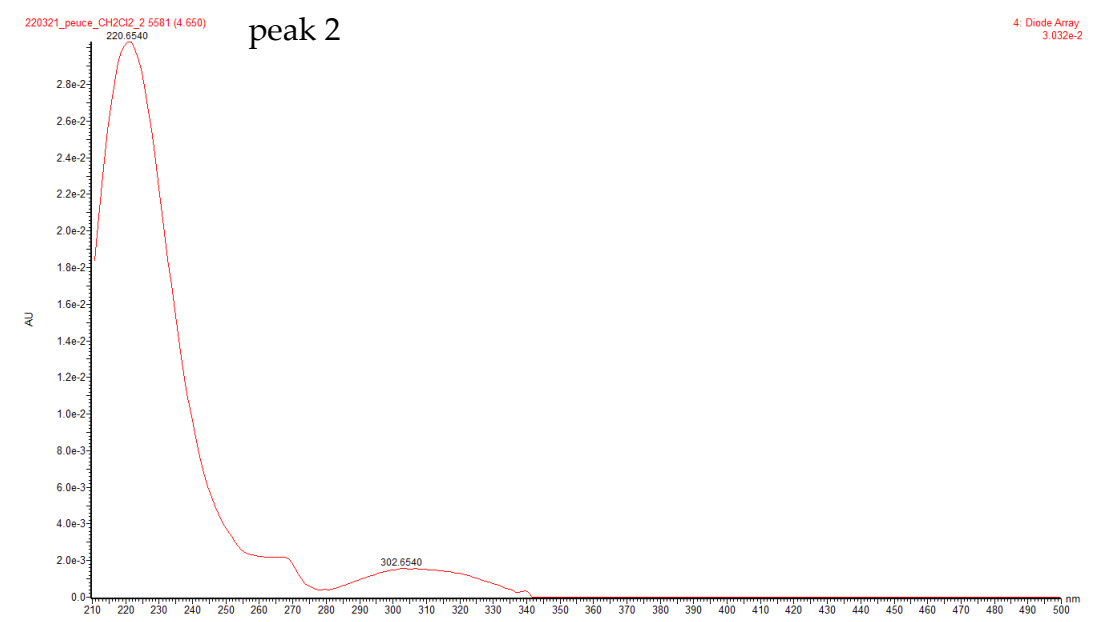
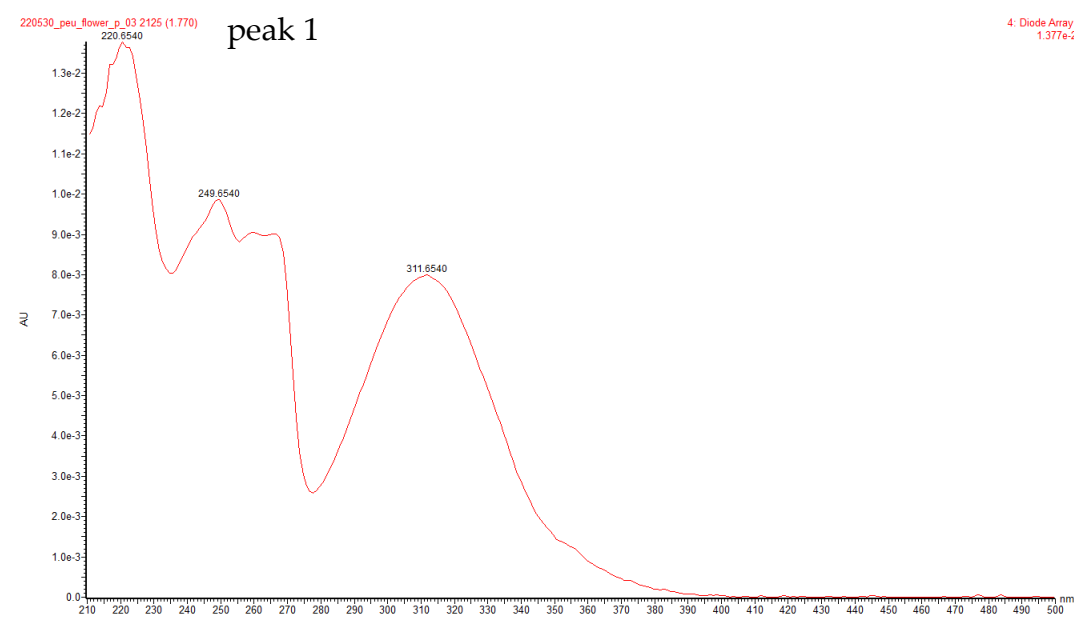


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm.

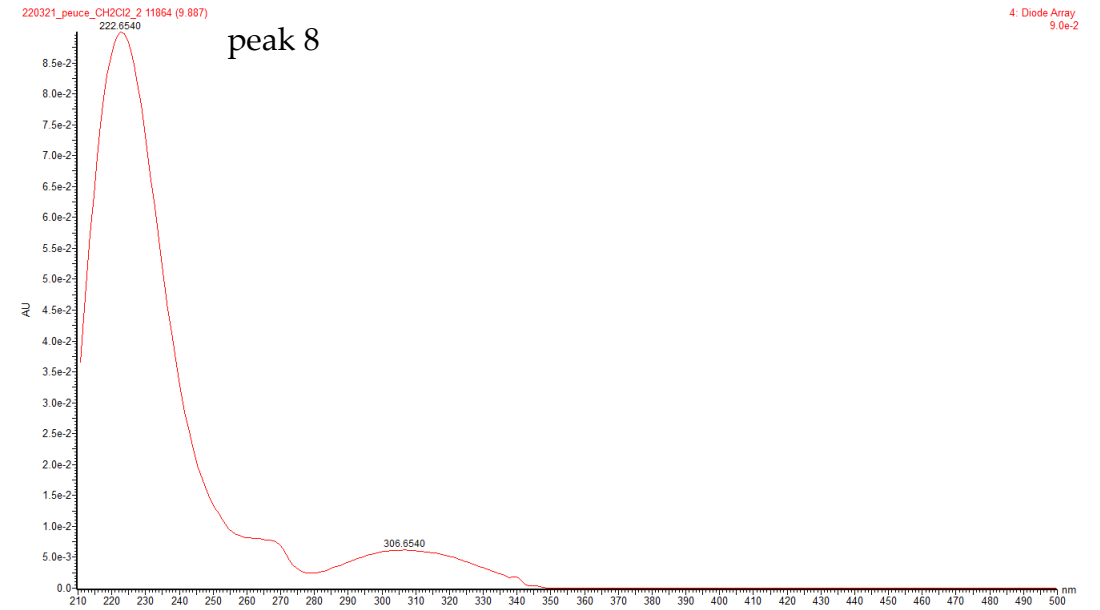
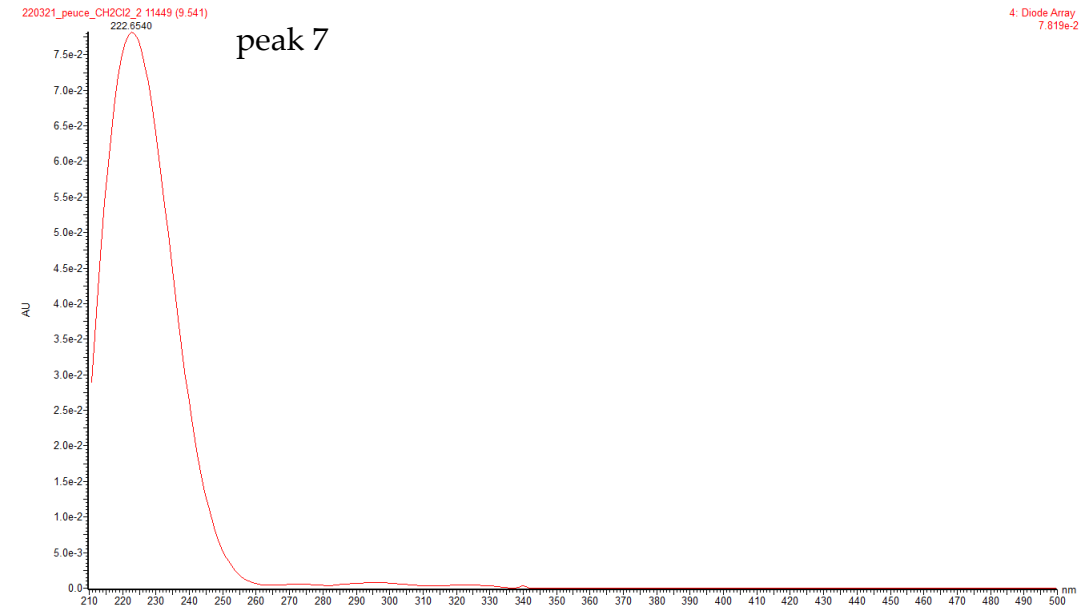
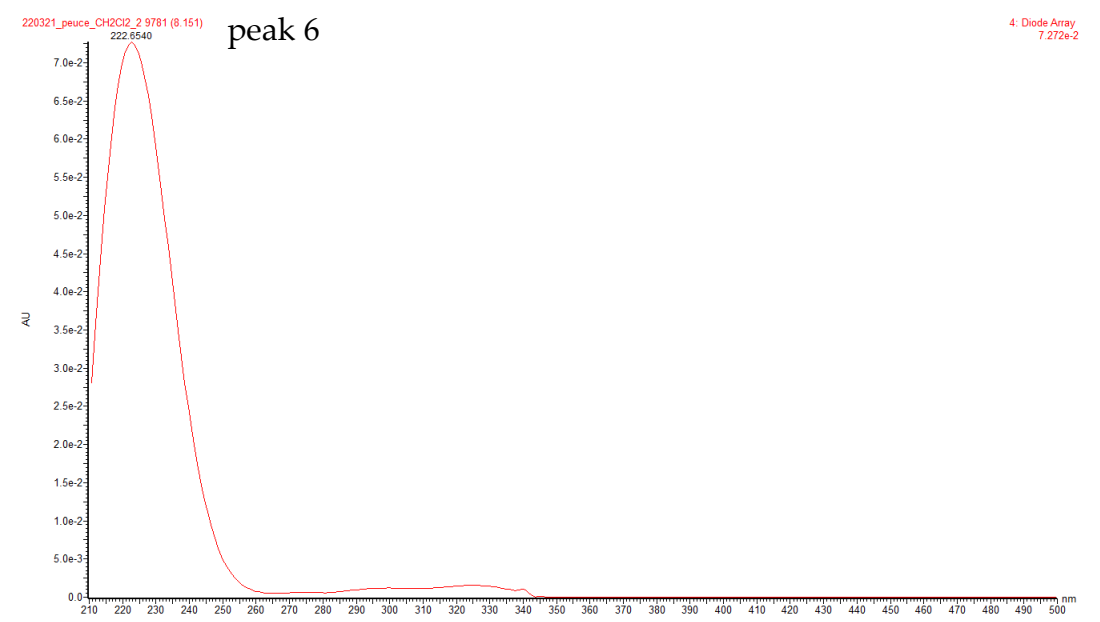
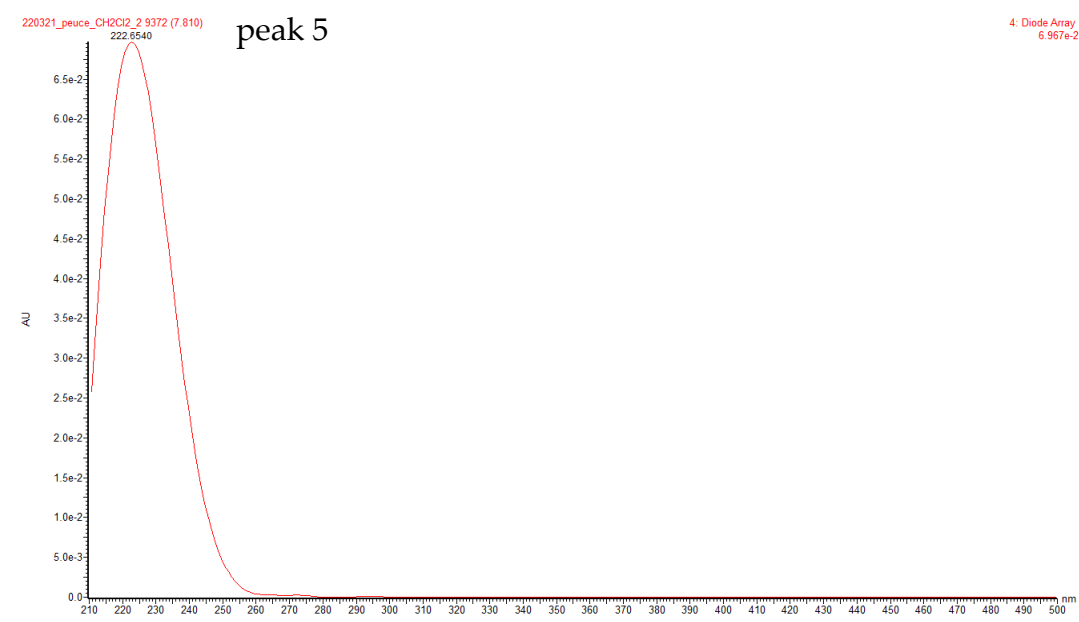


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)

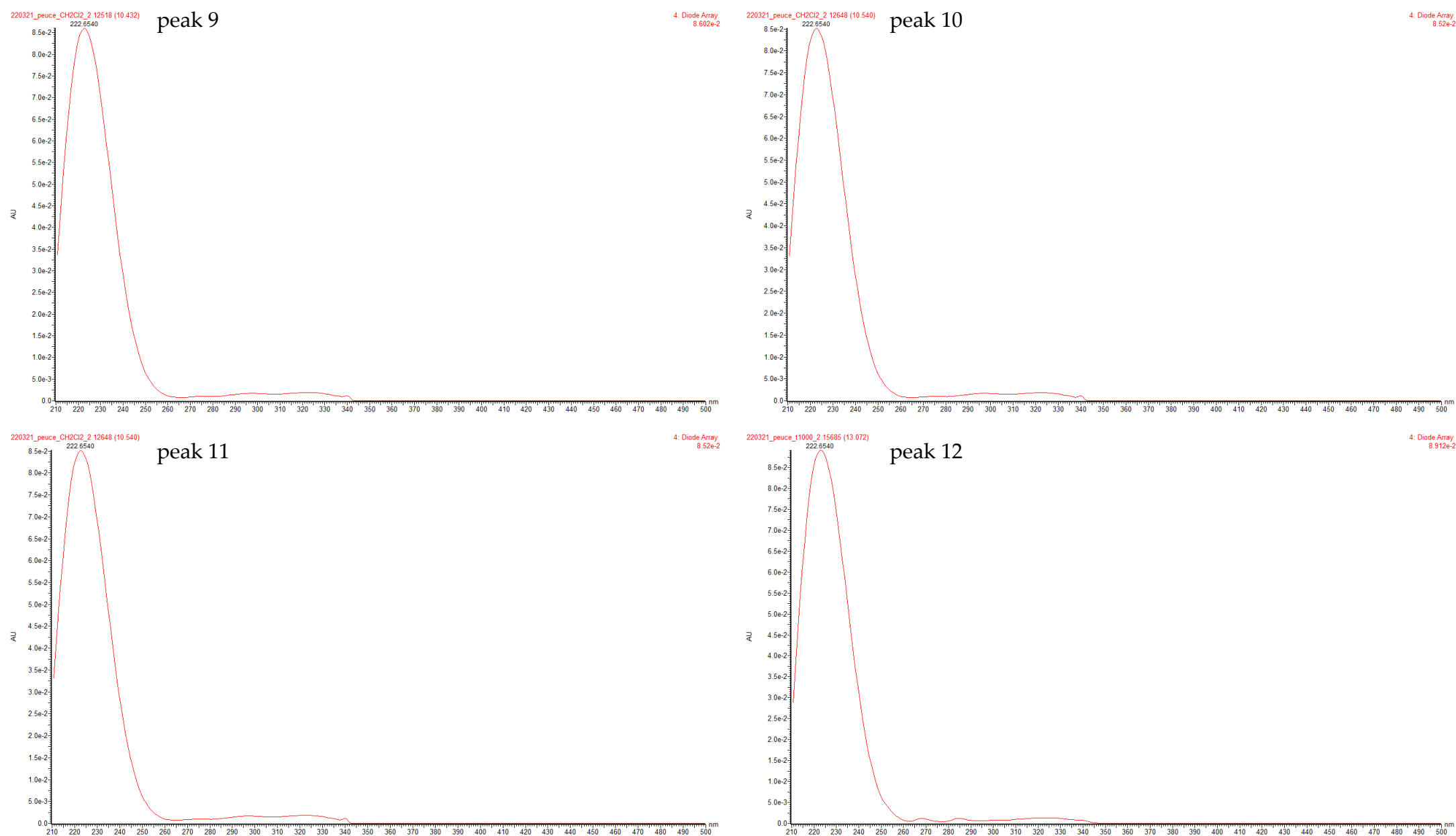


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)

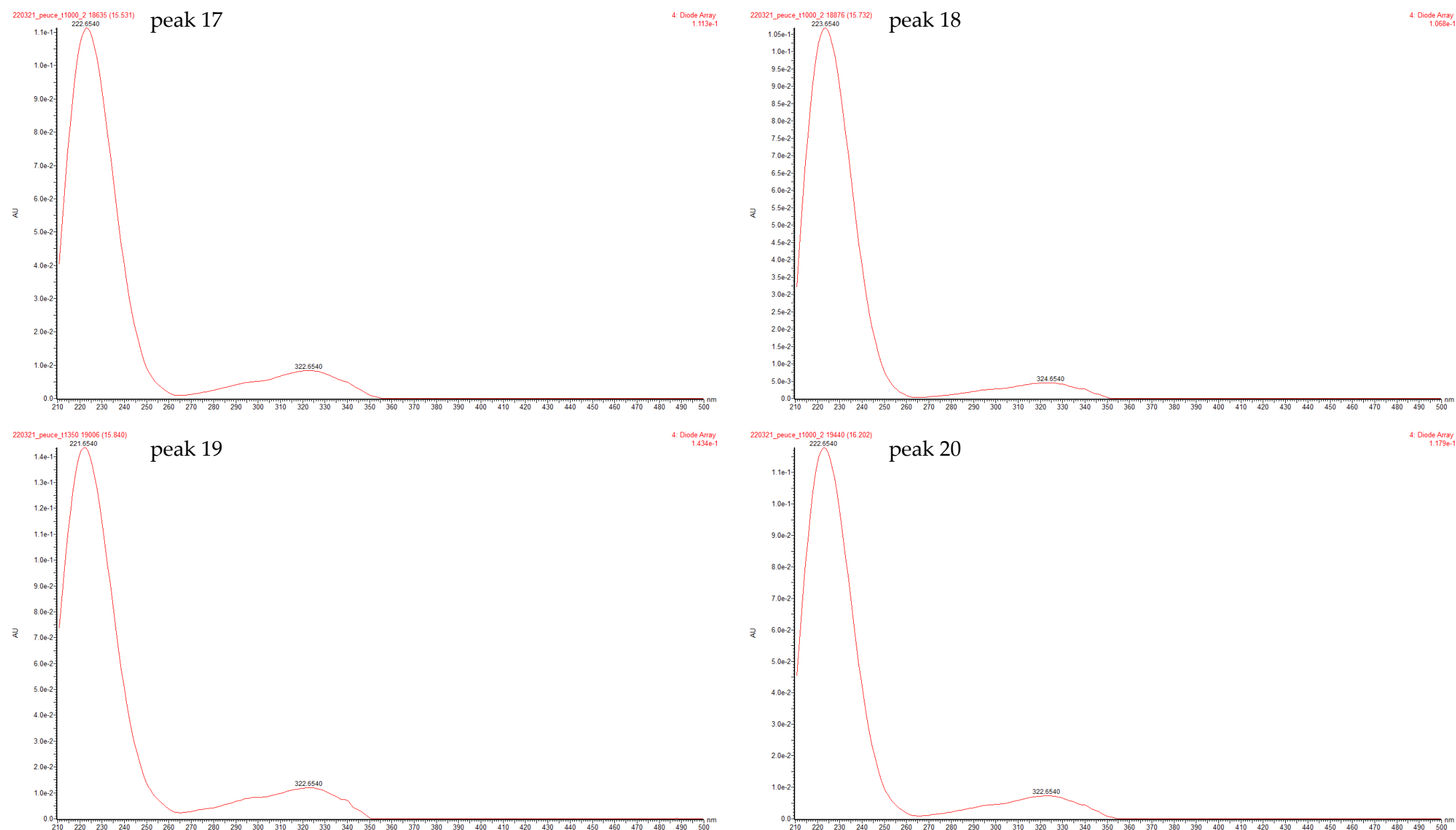


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)

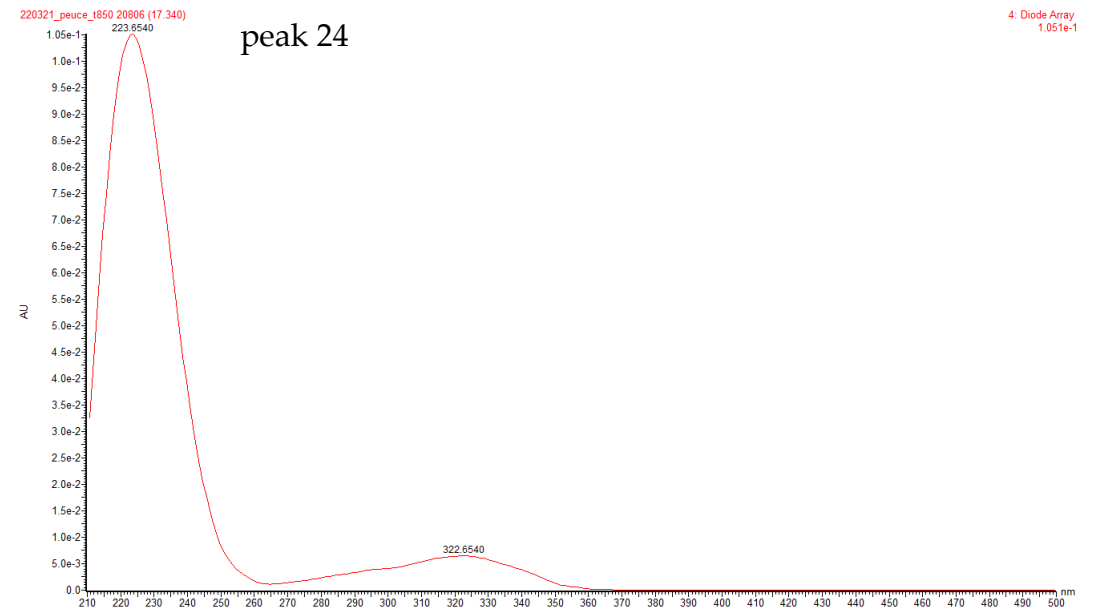
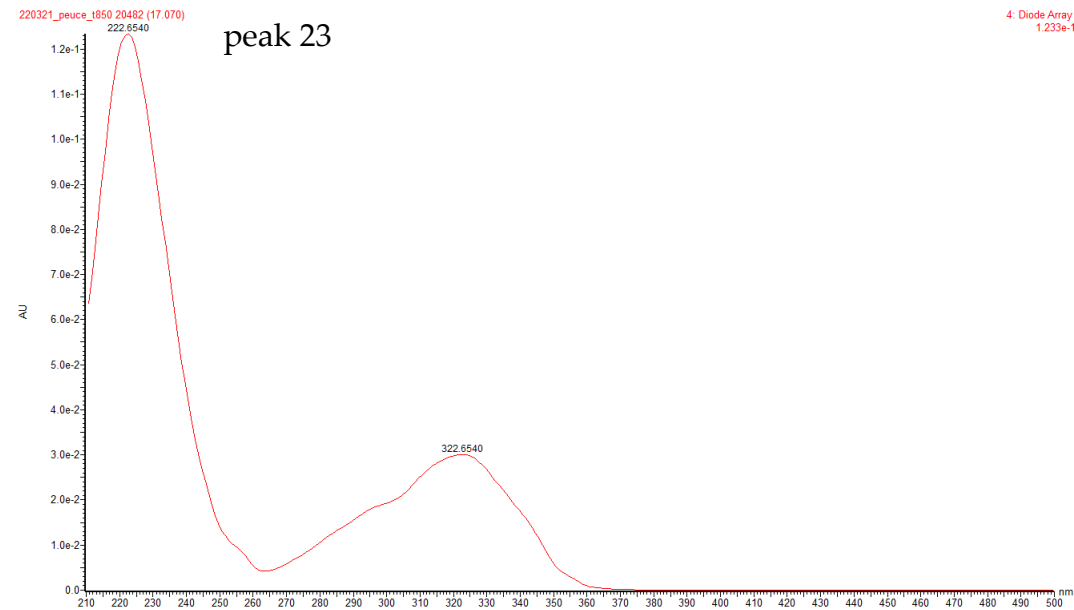
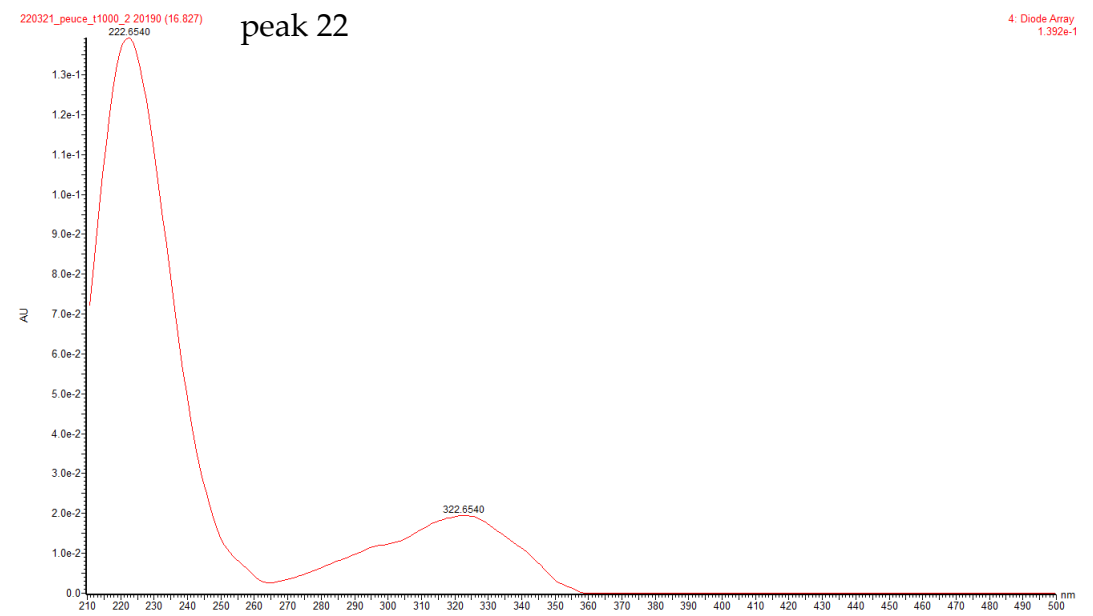
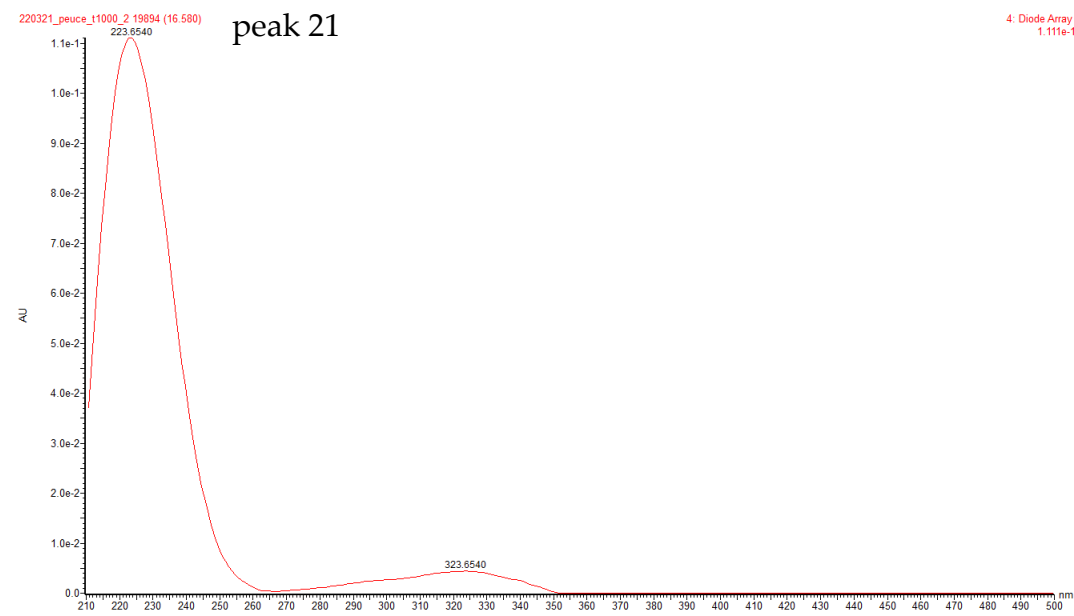


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (Cont)

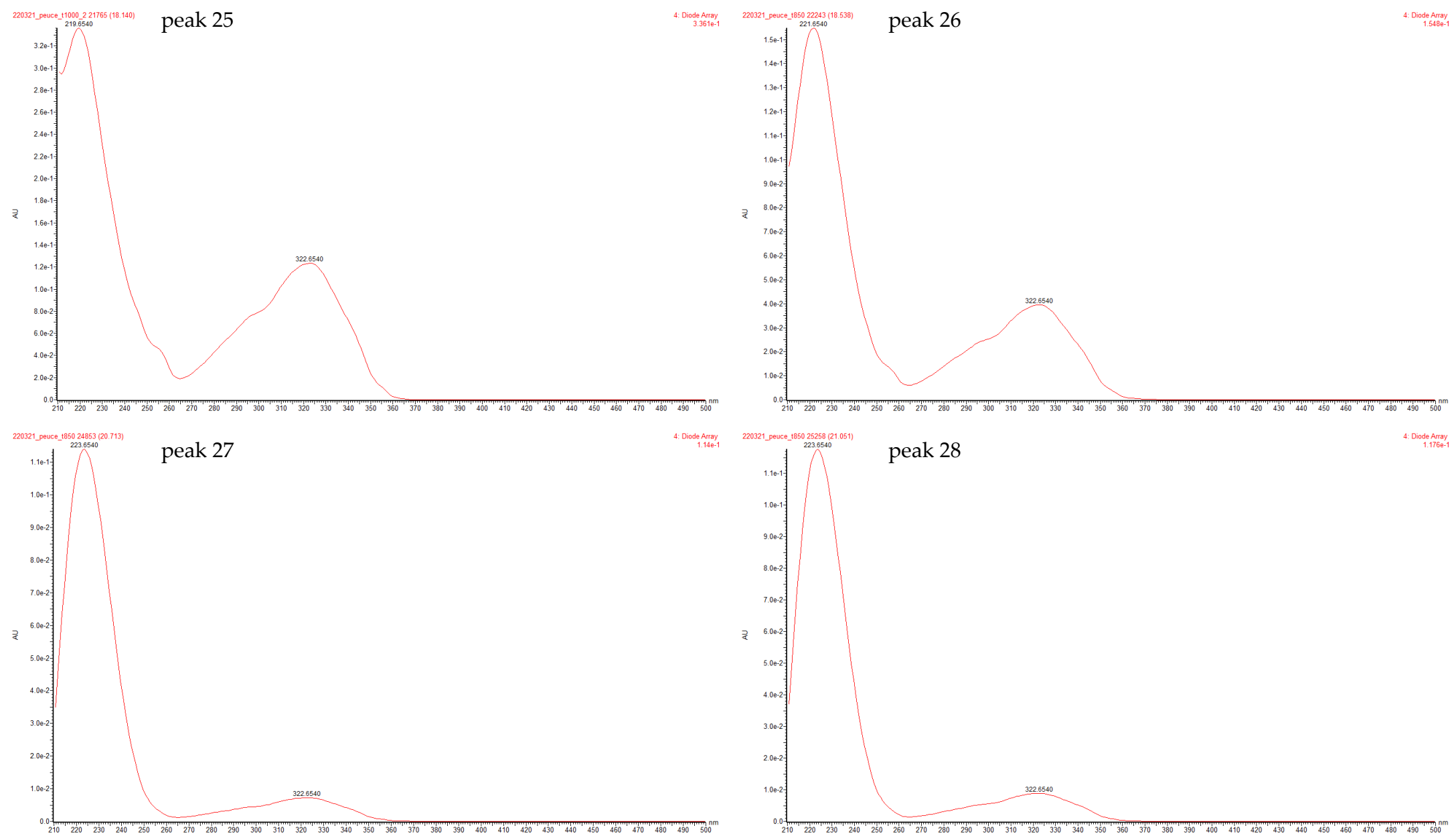


Figure S31. UV-Vis spectra of all the peaks present in PDA chromatograms of the methanol extract of four parts of *Peucedanum japonicum* between 200–500 nm. (*Cont*)

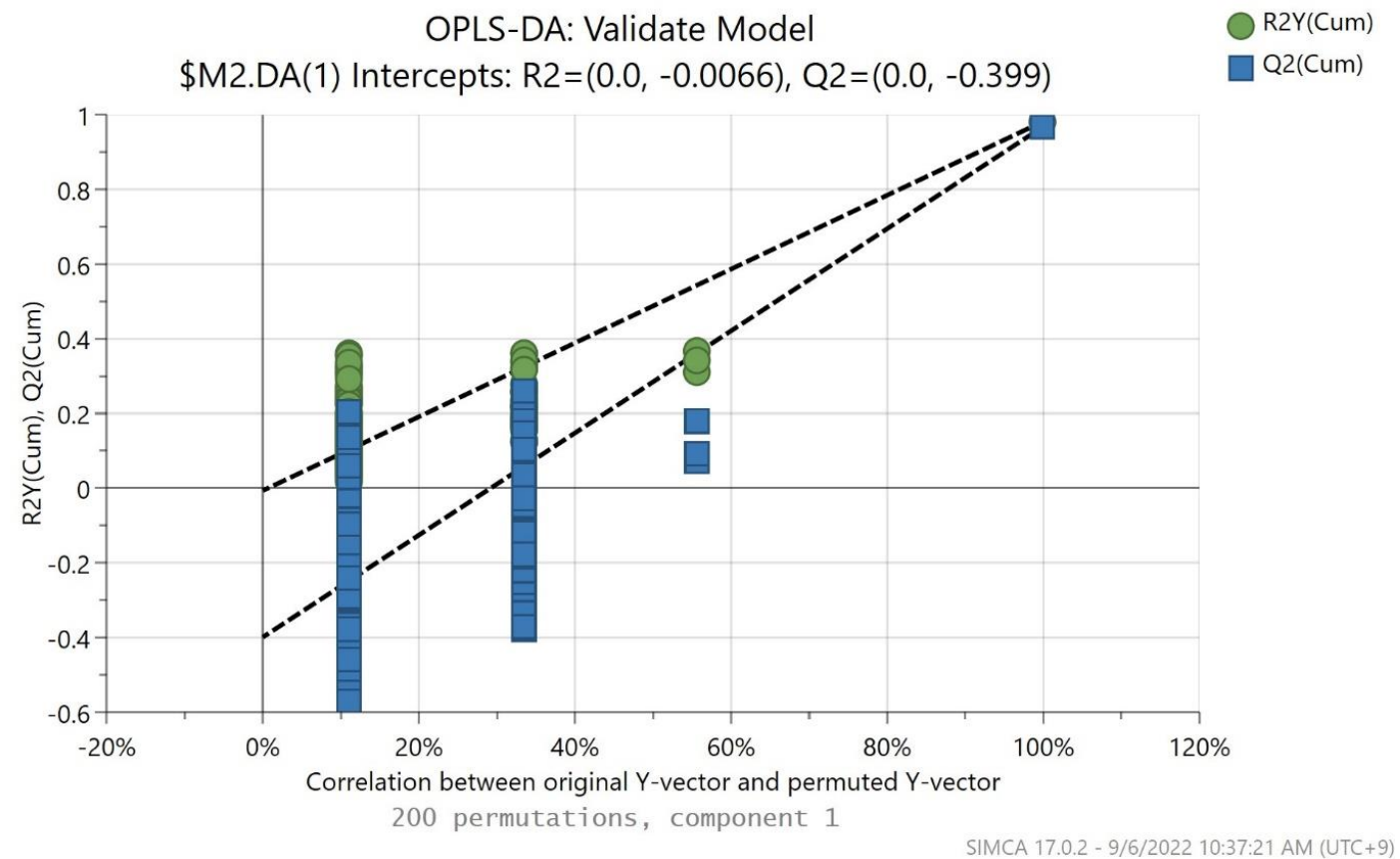


Figure S32. Permutation plot for validation of OPLS-DA obtained from 200 permutation test.