

LC-DAD-ESI-MS/MS and NMR analysis of conifer wood specialized metabolites

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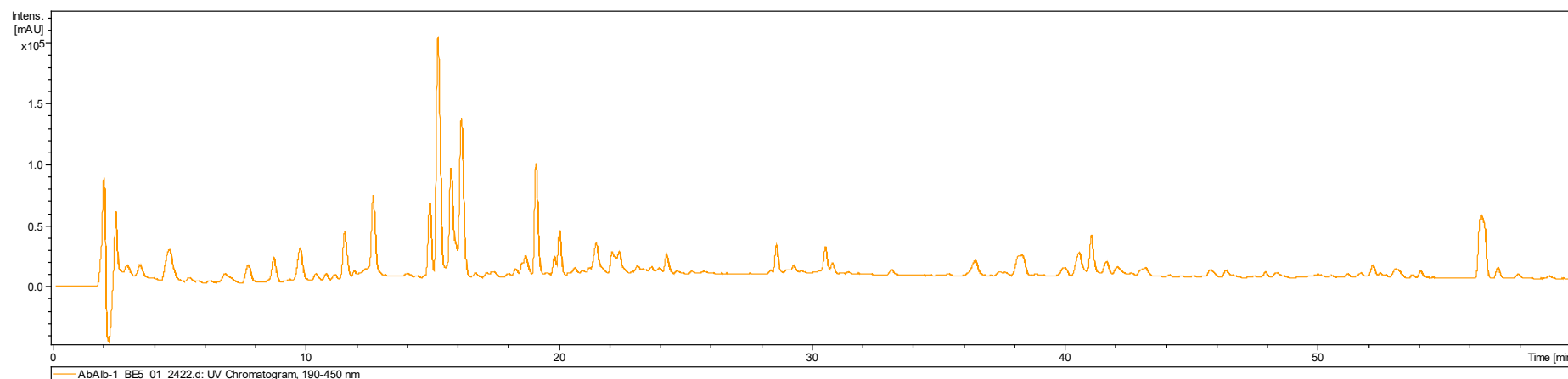


Figure S1. LC-DAD chromatogram of *Abies alba* Mill. branch wood methanolic extract taken at 190-450 nm.

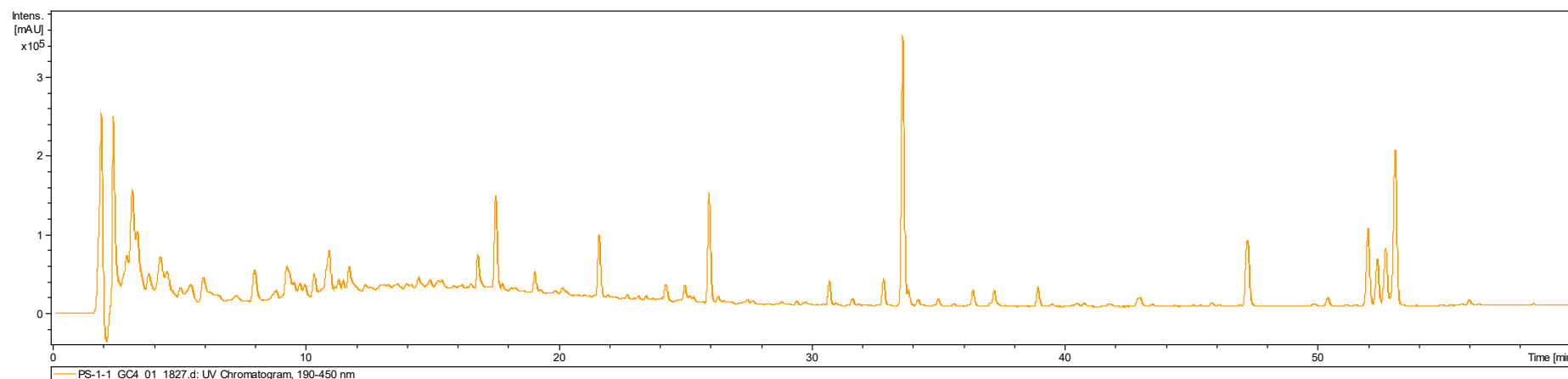


Figure S2. LC-DAD chromatogram of *Pinus sylvestris* L. branch wood methanolic extract taken at 190-450 nm.

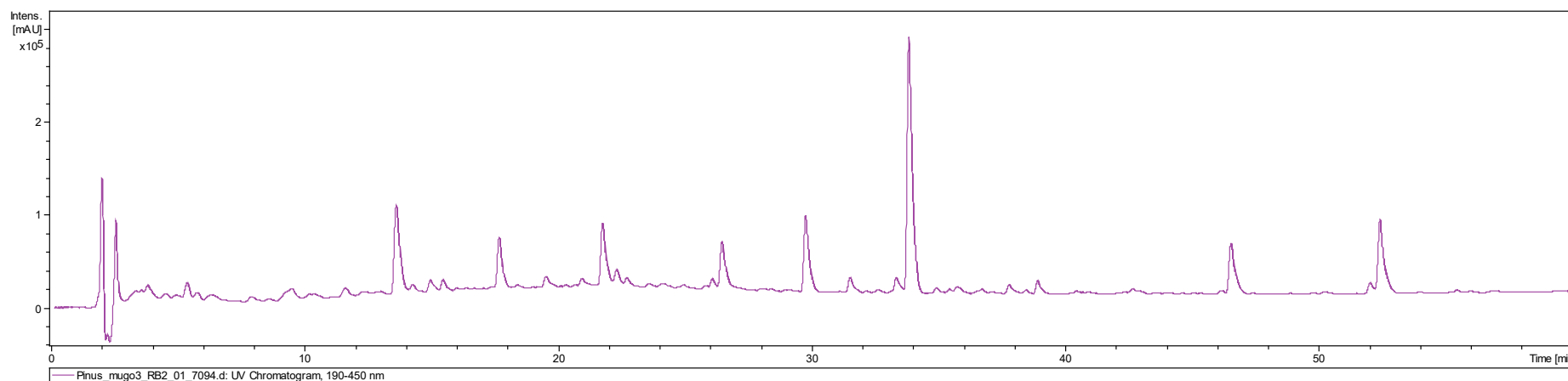


Figure S3. LC-DAD chromatogram of *Pinus mugo* Turra branch wood methanolic extract taken at 190-450 nm.

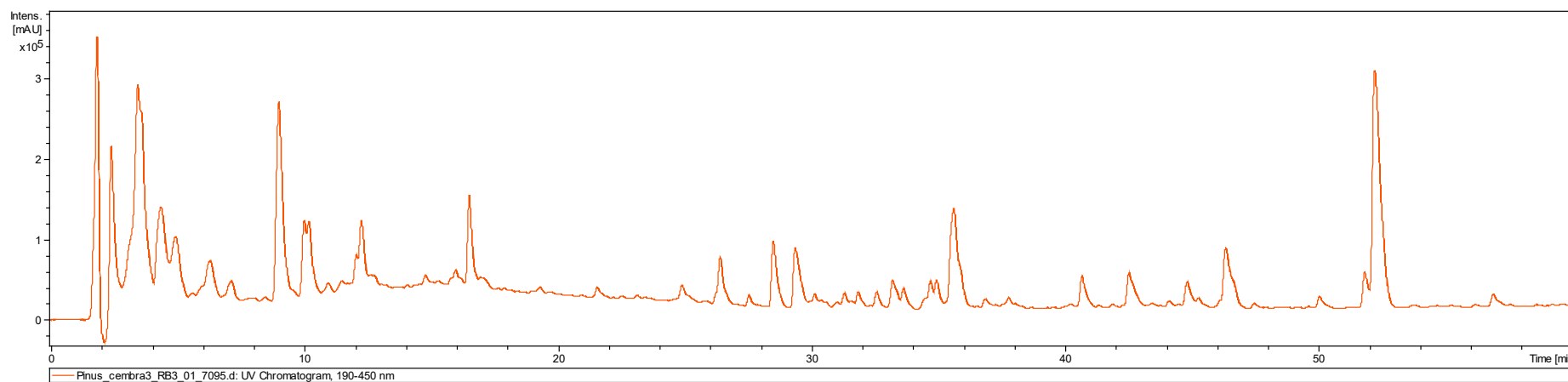


Figure S4. LC-DAD chromatogram of *Pinus cembra* L. branch wood methanolic extract taken at 190-450 nm.

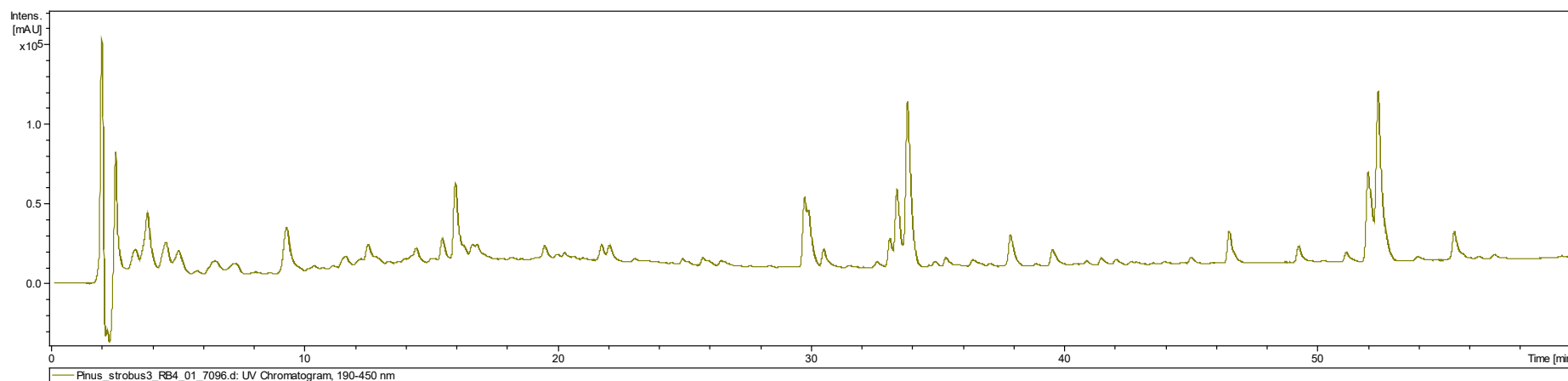


Figure S5. LC-DAD chromatogram of *Pinus strobus* L. branch wood methanolic extract taken at 190-450 nm.

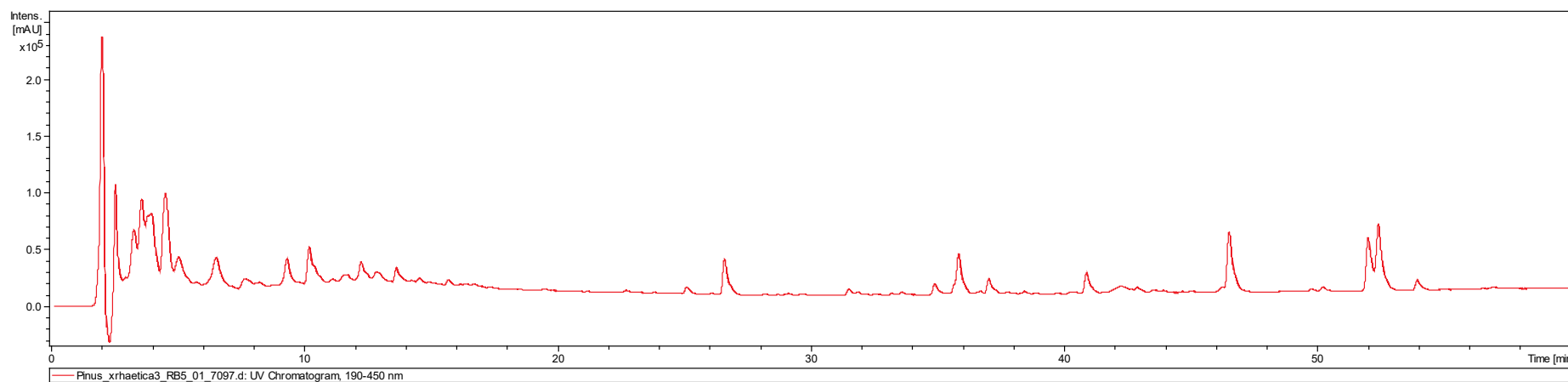


Figure S6. LC-DAD chromatogram of *Pinus x rhaetica* Brügger branch wood methanolic extract taken at 190-450 nm.

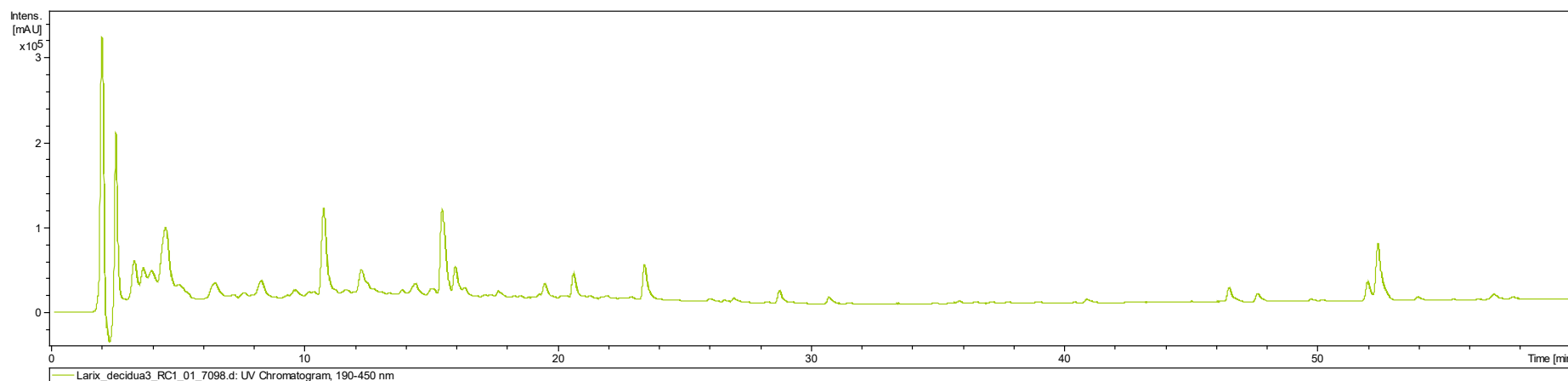


Figure S7. LC-DAD chromatogram of *Larix decidua* Mill. branch wood methanolic extract taken at 190-450 nm.

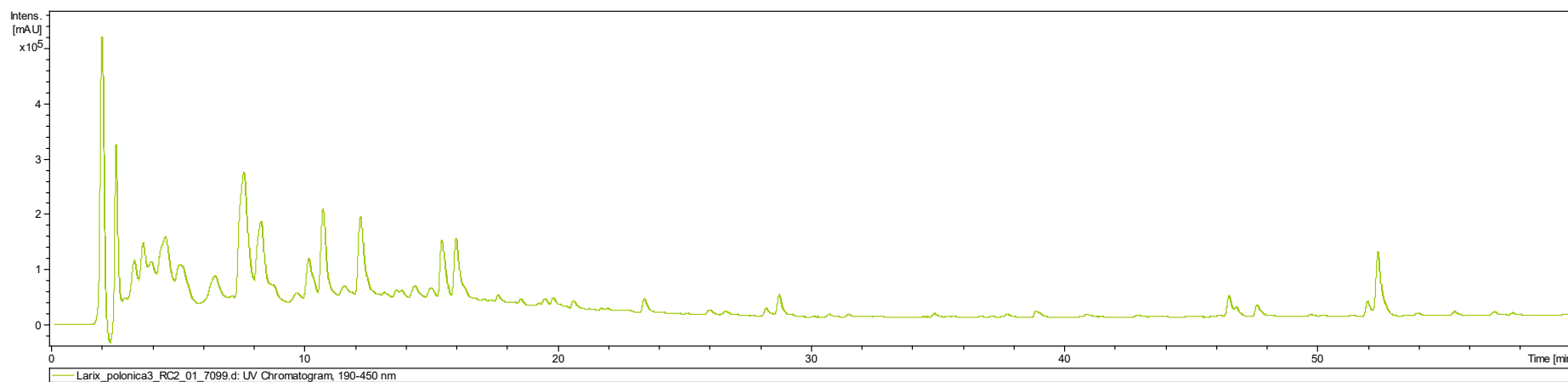


Figure S8. LC-DAD chromatogram of *Larix polonica* Rac. branch wood methanolic extract taken at 190-450 nm.

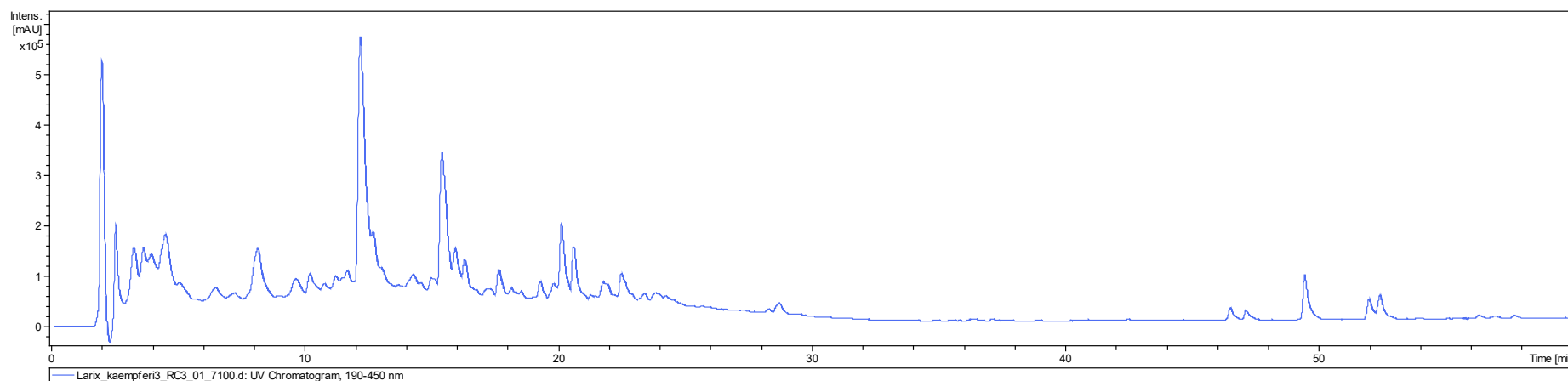


Figure S9. LC-DAD chromatogram of *Larix kaempferi* Lamb. branch wood methanolic extract taken at 190-450 nm.

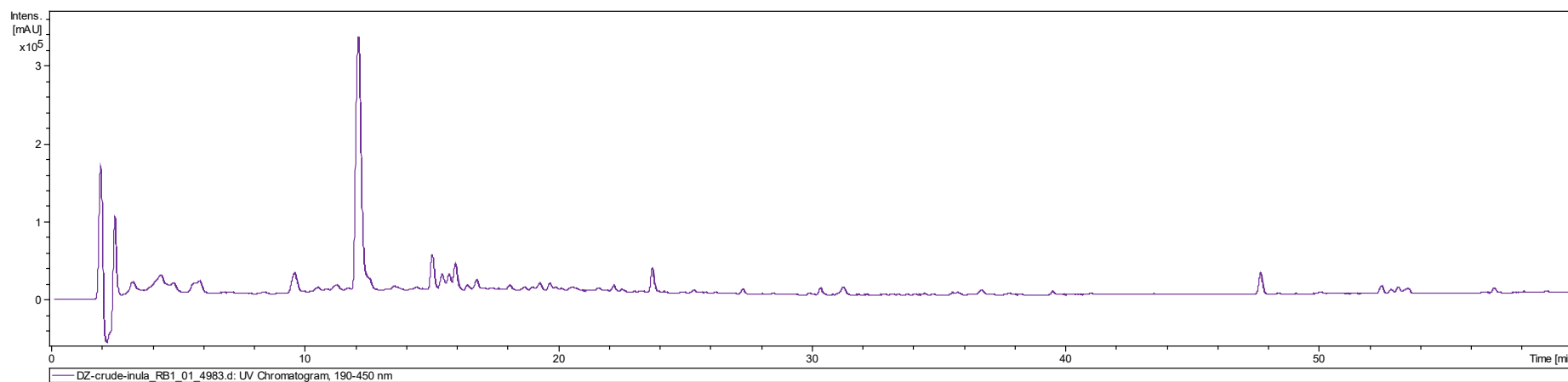


Figure S10. LC-DAD chromatogram of *Pseudotsuga menziesii* Mirb. branch wood methanolic extract taken at 190-450 nm.

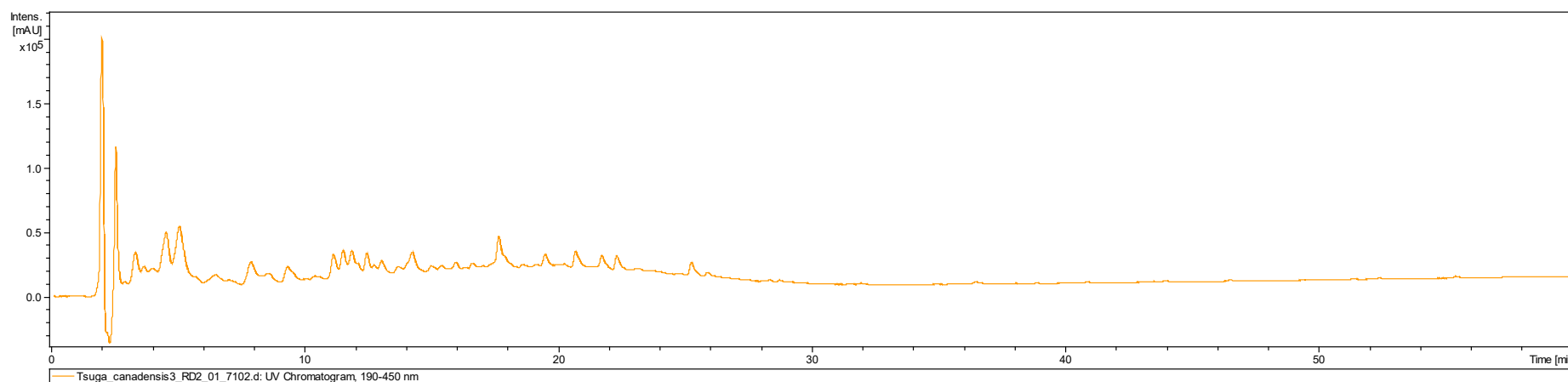


Figure S11. LC-DAD chromatogram of *Tsuga canadensis* Carrière branch wood methanolic extract taken at 190-450 nm.

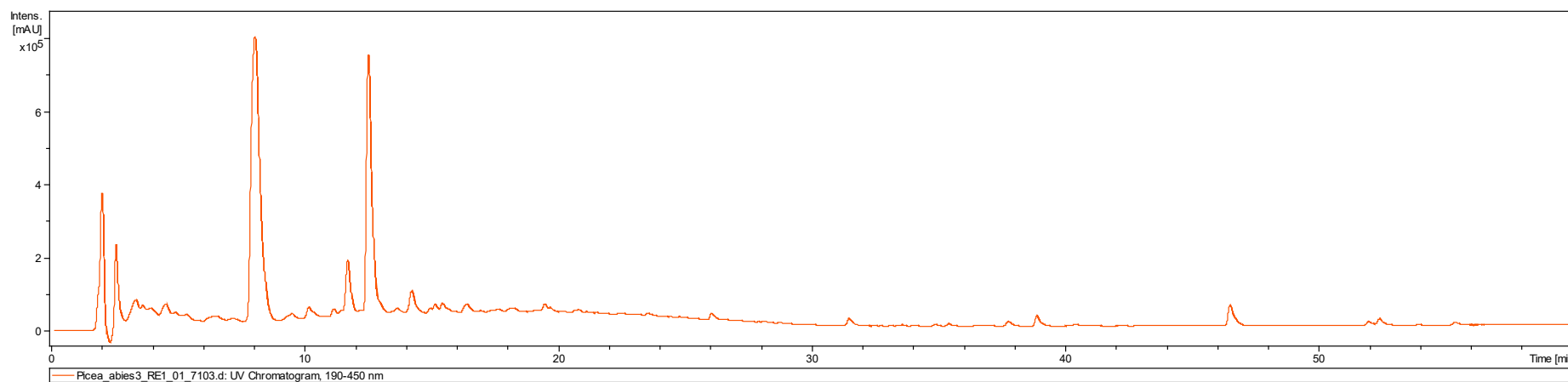


Figure S12. LC-DAD chromatogram of *Picea abies* L. branch wood methanolic extract taken at 190-450 nm.

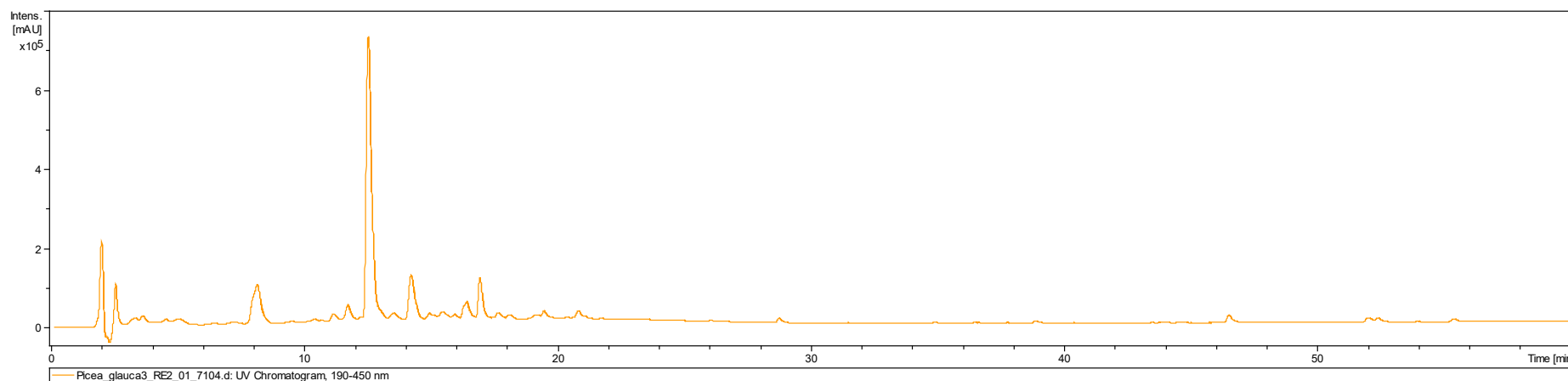


Figure S13. LC-DAD chromatogram of *Picea glauca* (Moench) Voss branch wood methanolic extract taken at 190-450 nm.

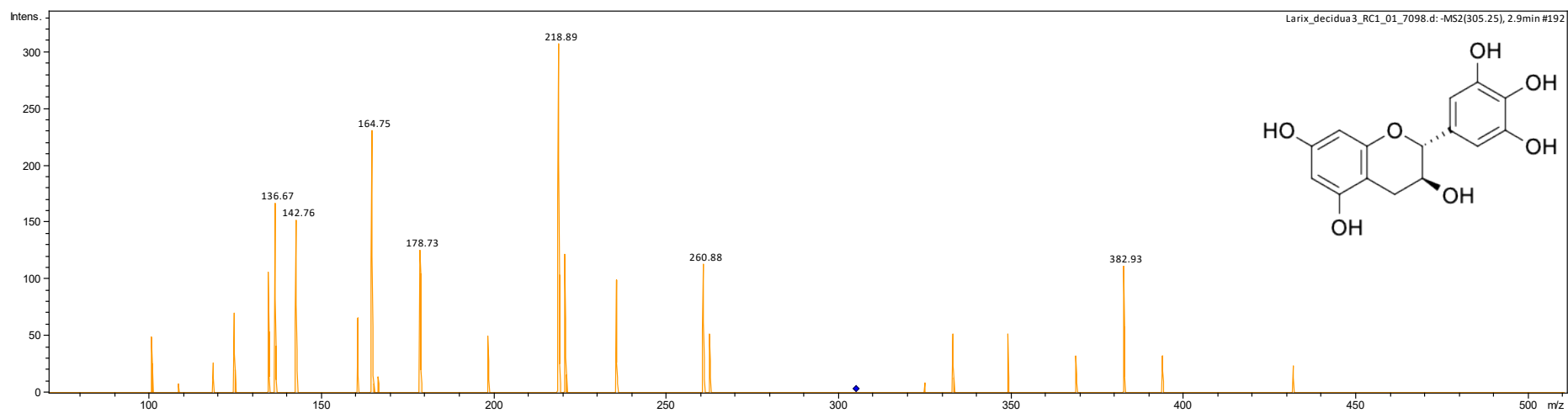


Figure S14. ESI-MS² spectrum of molecular ion at m/z 305 – compound (1).

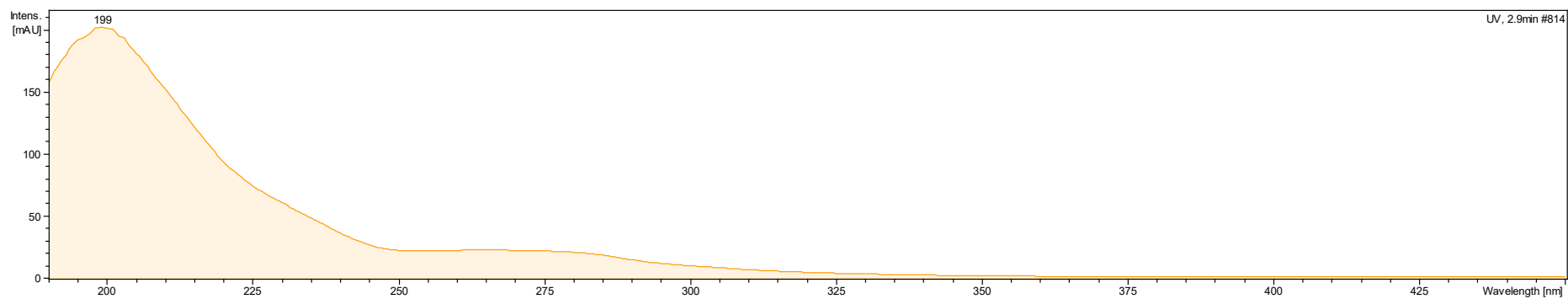


Figure S15. UV spectrum of compound (1).

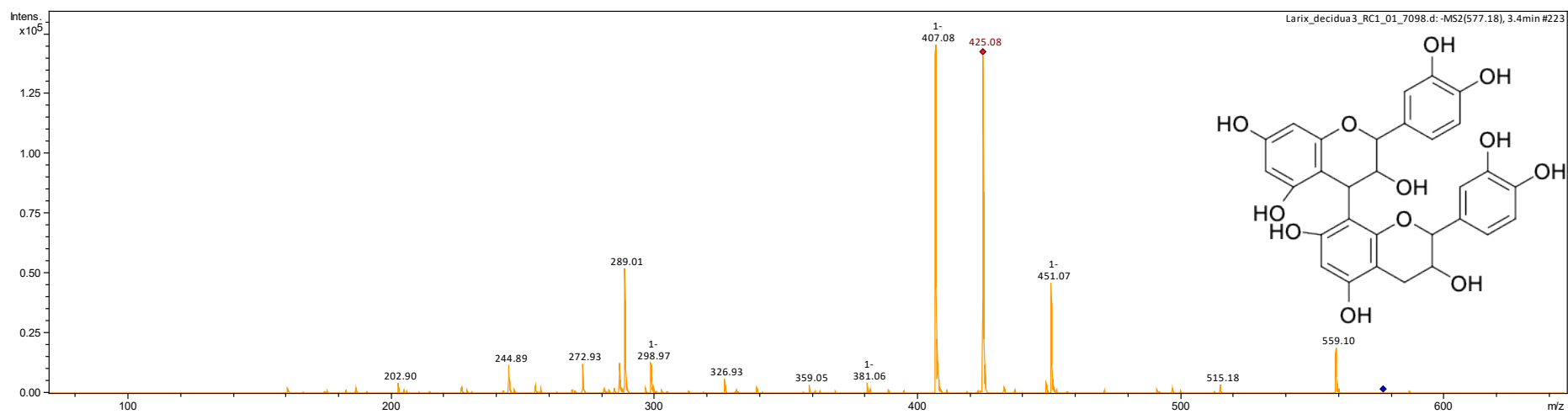


Figure S16. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 577 – compound (2).

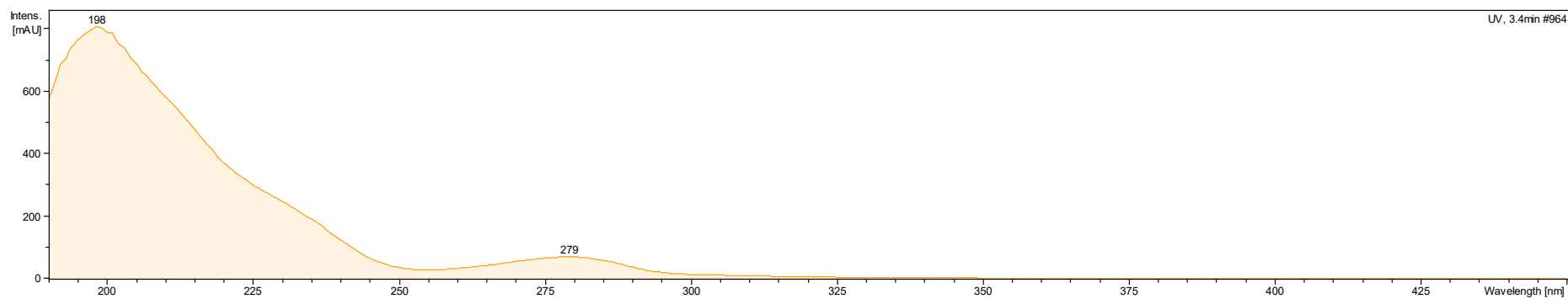


Figure S17. UV spectrum of compound (2).

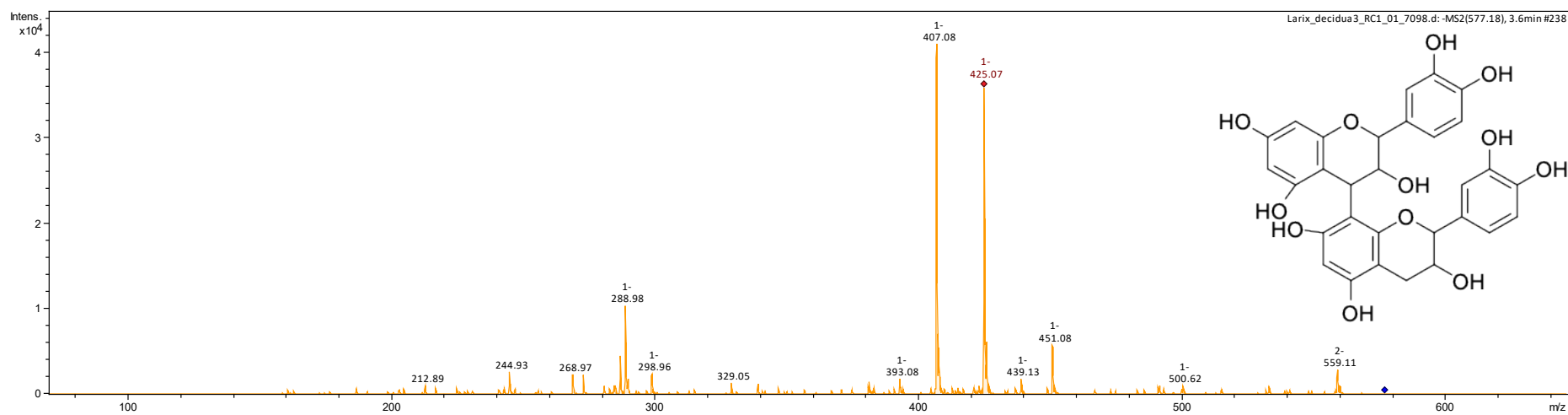


Figure S18. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 577 – compound (3).

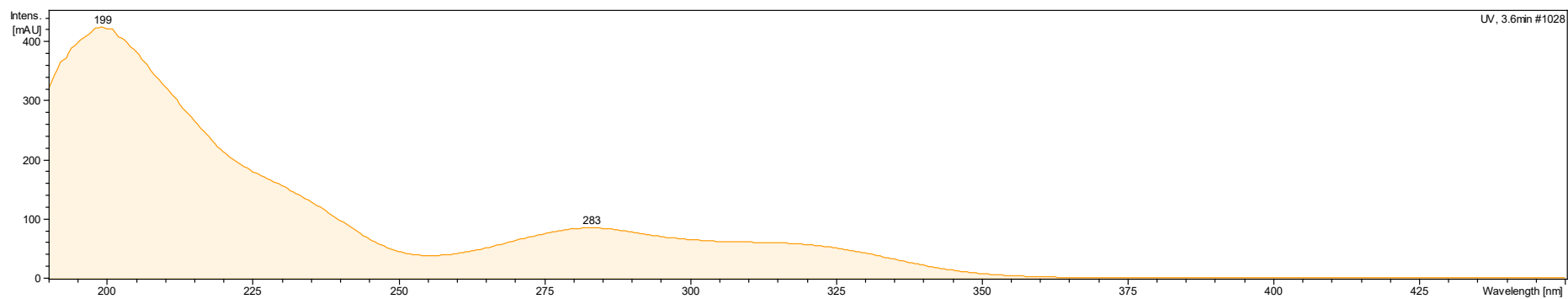


Figure S19. UV spectrum of compound (3).

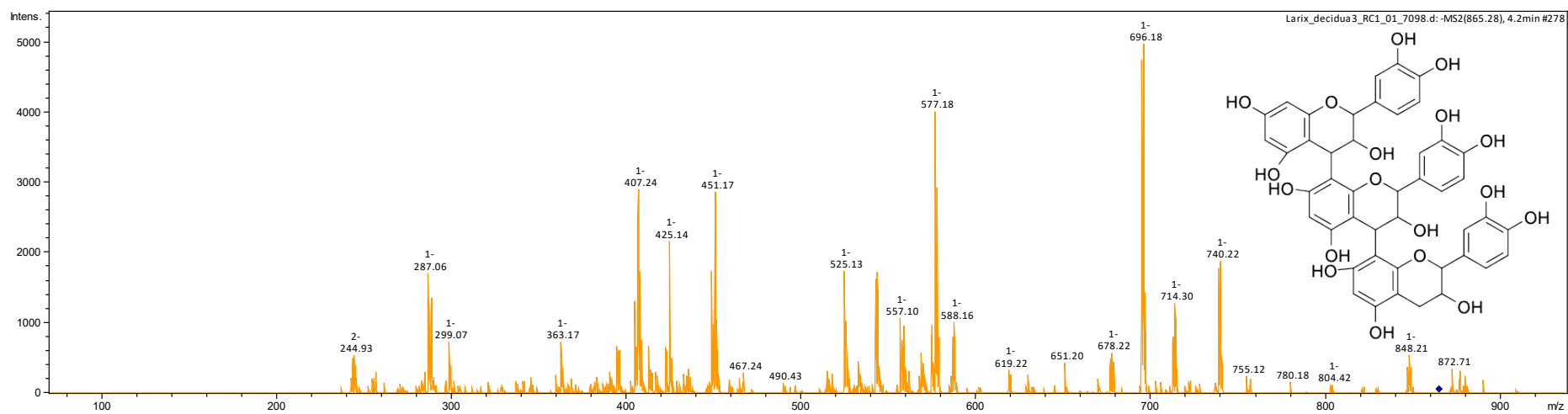


Figure S20. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 865 – compound (4).

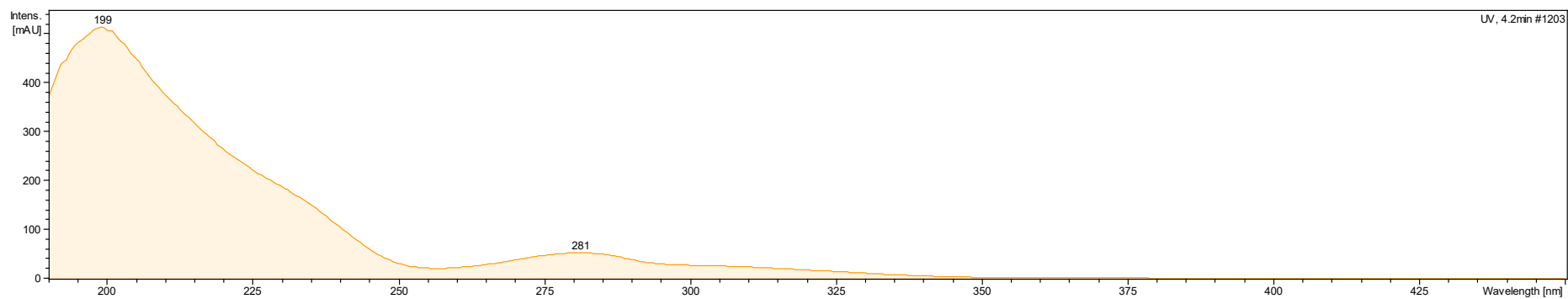


Figure S21. UV spectrum of compound (4).

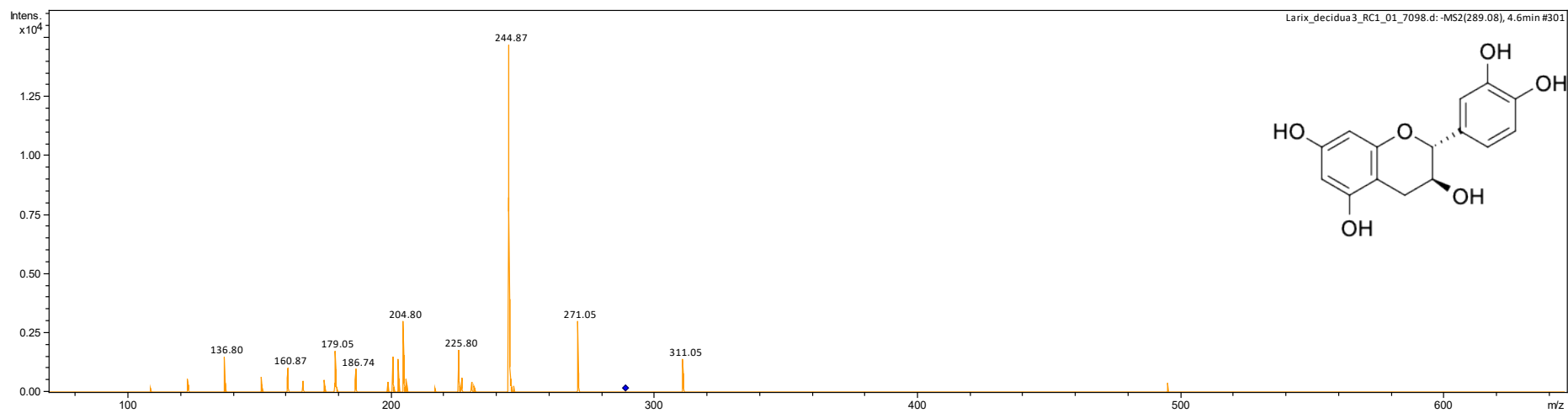


Figure S22. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 289 – compound (5).

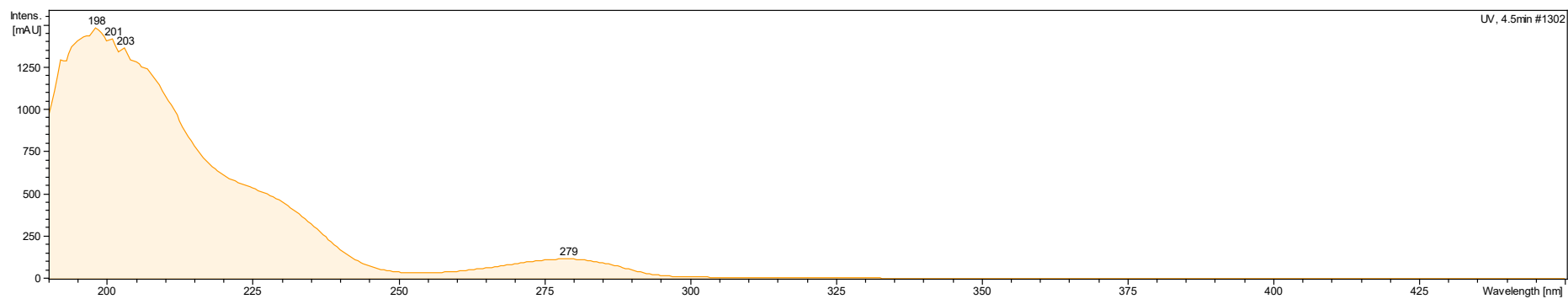


Figure S23. UV spectrum of compound (5).

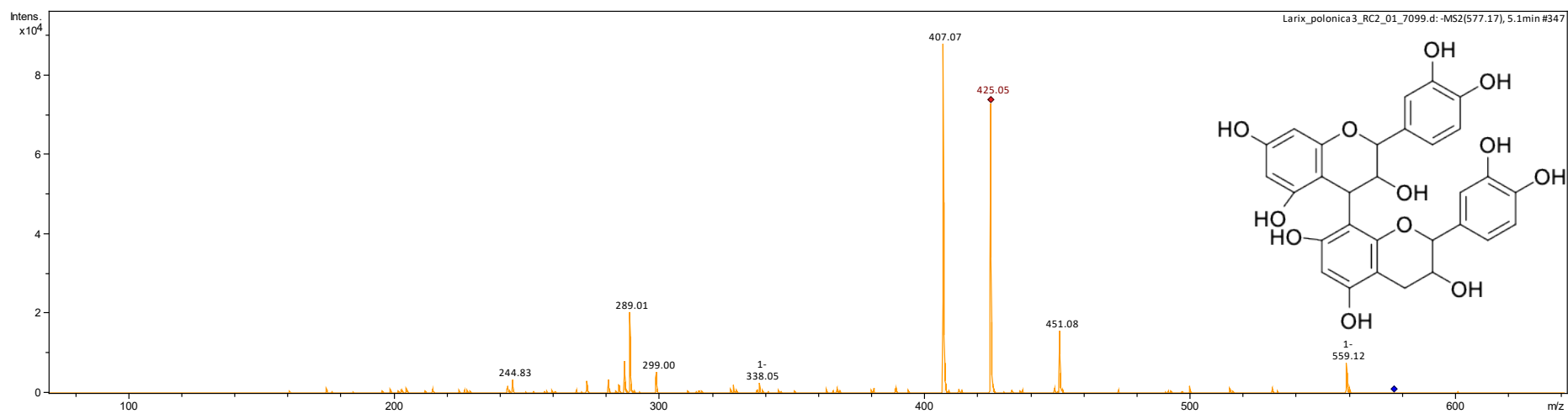


Figure S24. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 577 – compound (6).

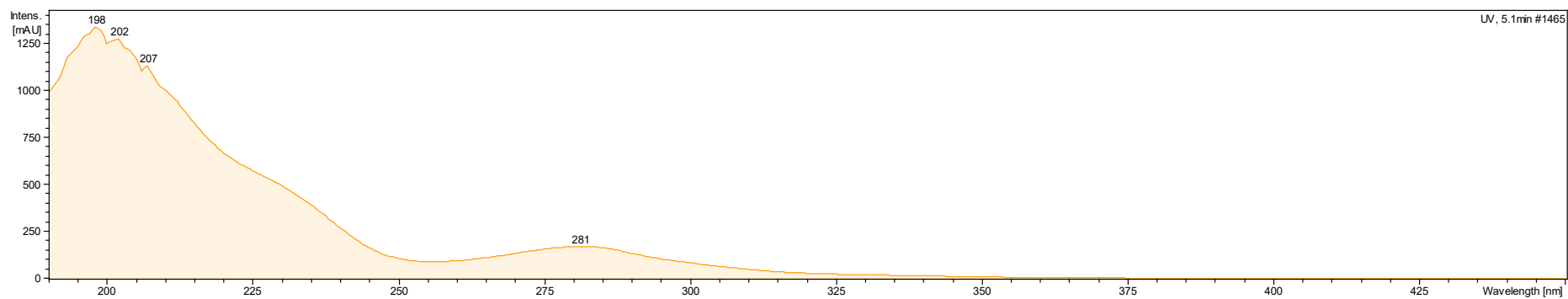


Figure S25. UV spectrum of compound (6).

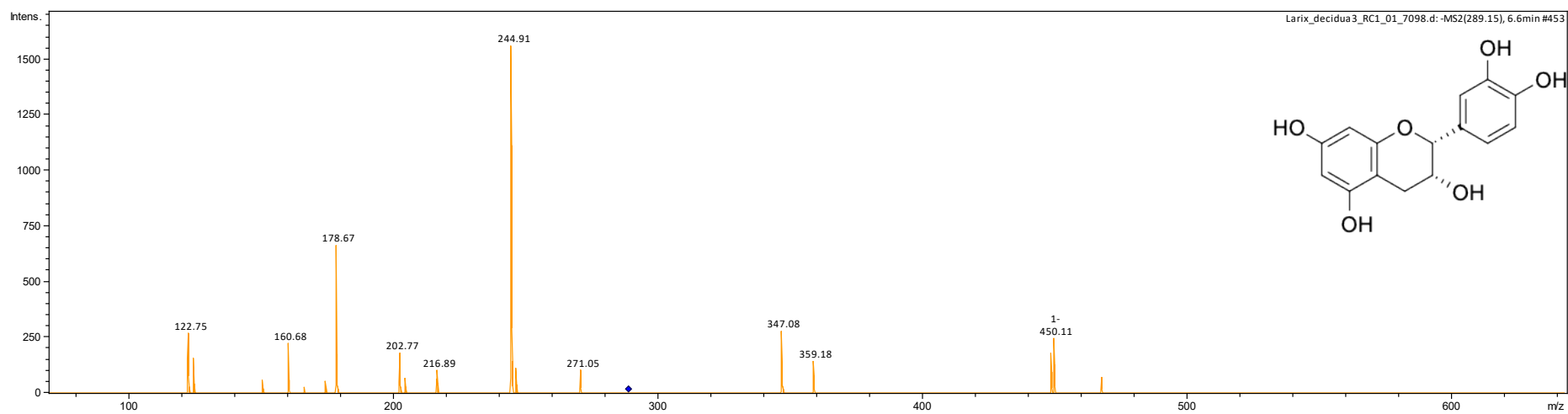


Figure S26. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 289 – compound (7).

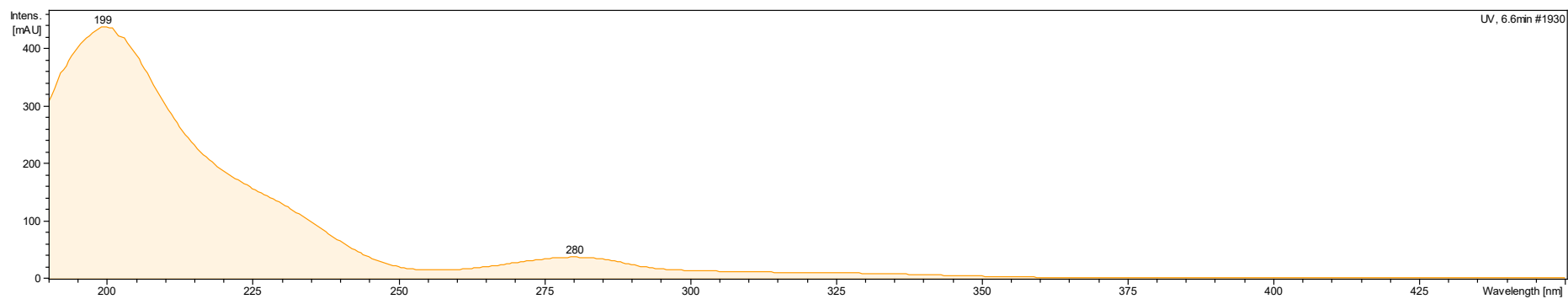


Figure S27. UV spectrum of compound (7).

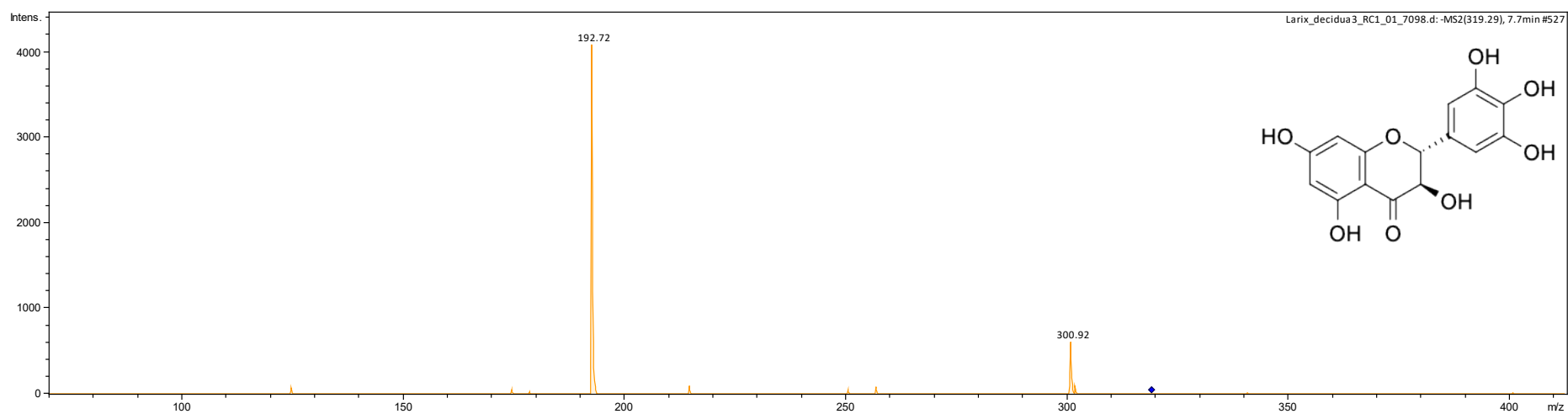


Figure S28. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 319 – compound (8).

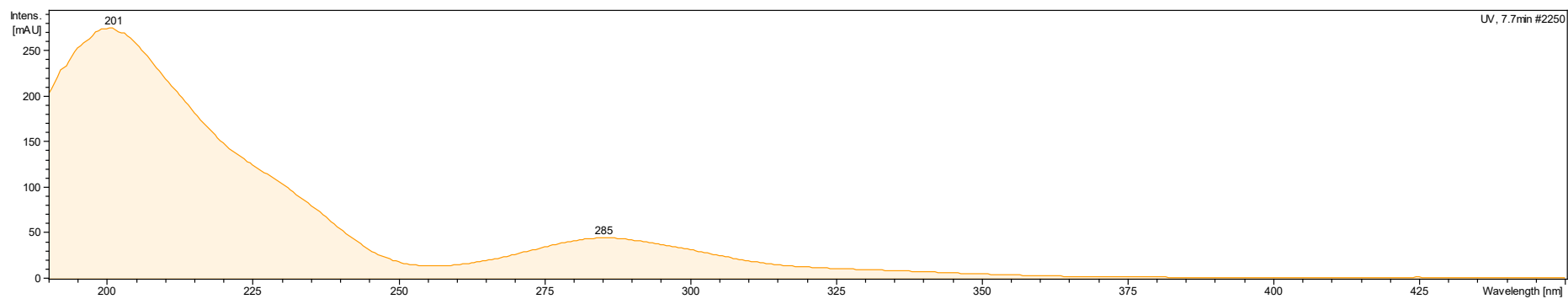


Figure S29. UV spectrum of compound (8).

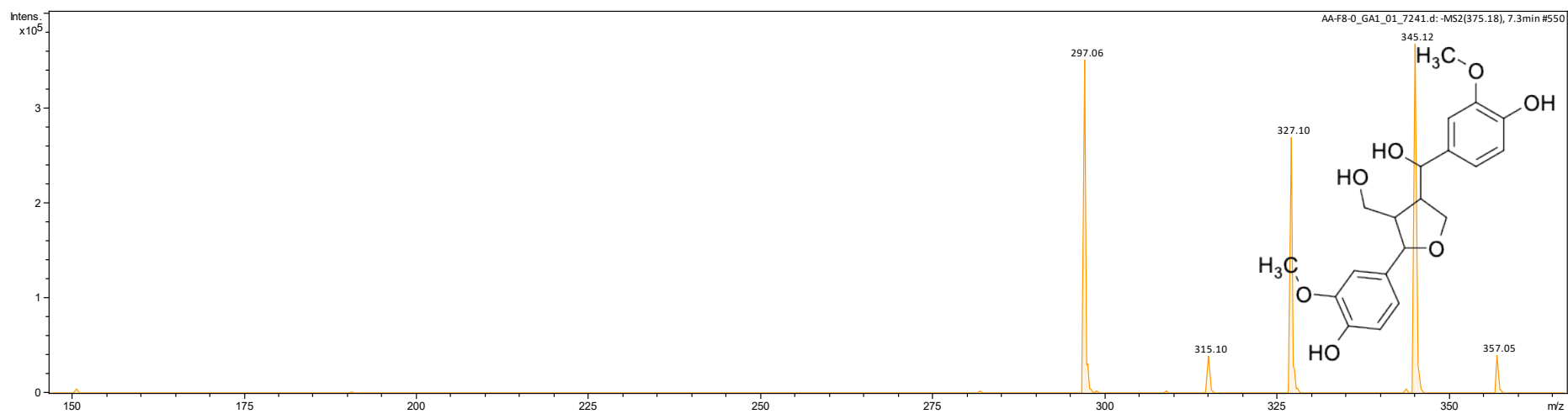


Figure S30. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 375 – compound (9).

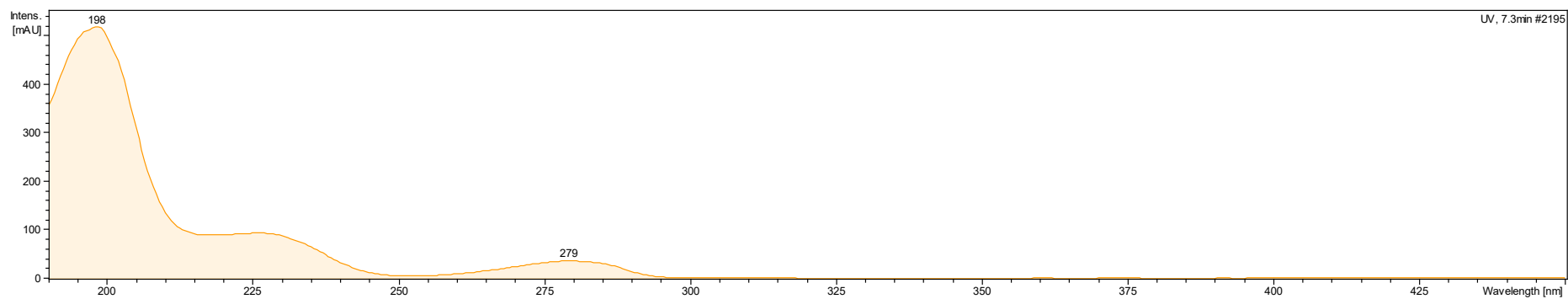


Figure S31. UV spectrum of compound (9).

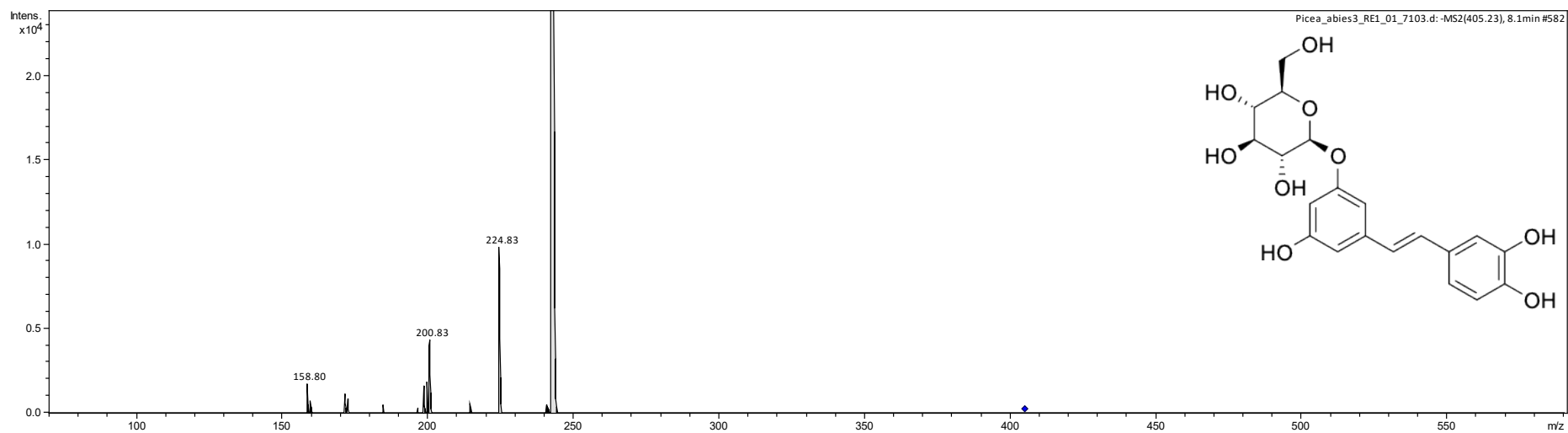


Figure S32. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 405 – compound (10).

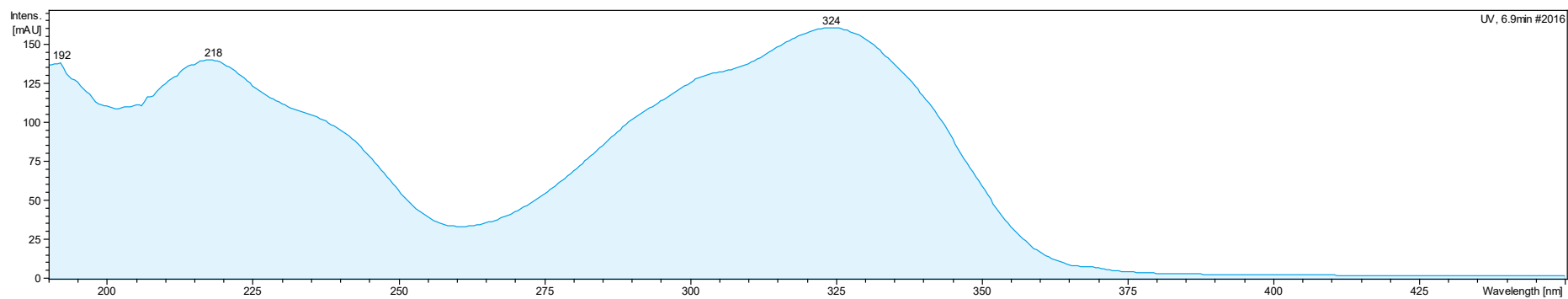


Figure S33. UV spectrum of compound (10).

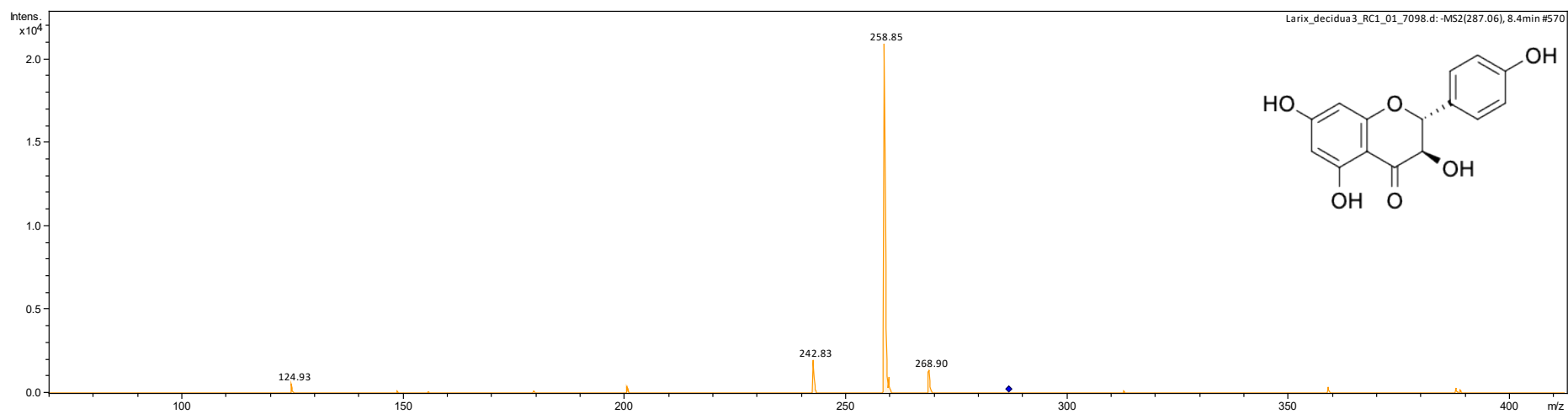


Figure S34. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 287 – compound (11).

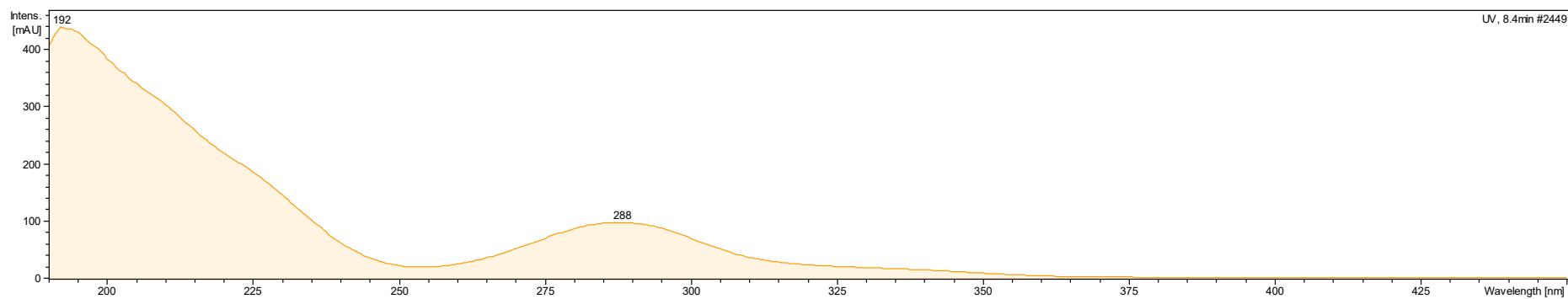


Figure S35. UV spectrum of compound (11).

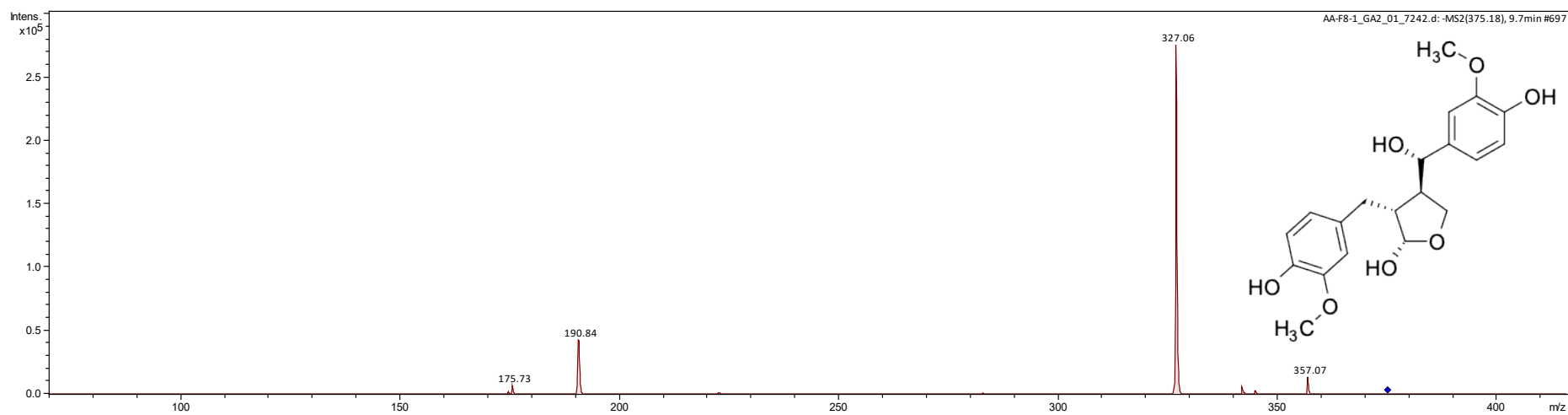


Figure S36. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 375 – compound (12).

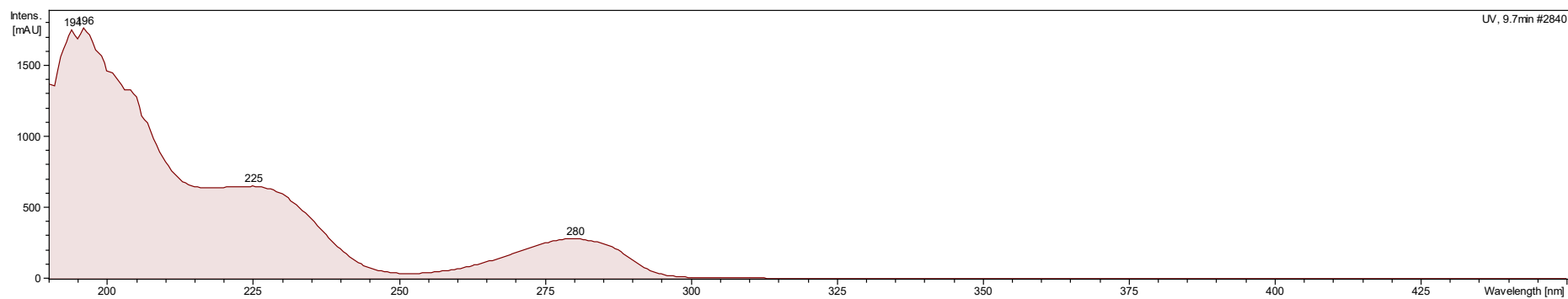


Figure S37. UV spectrum of compound (12).

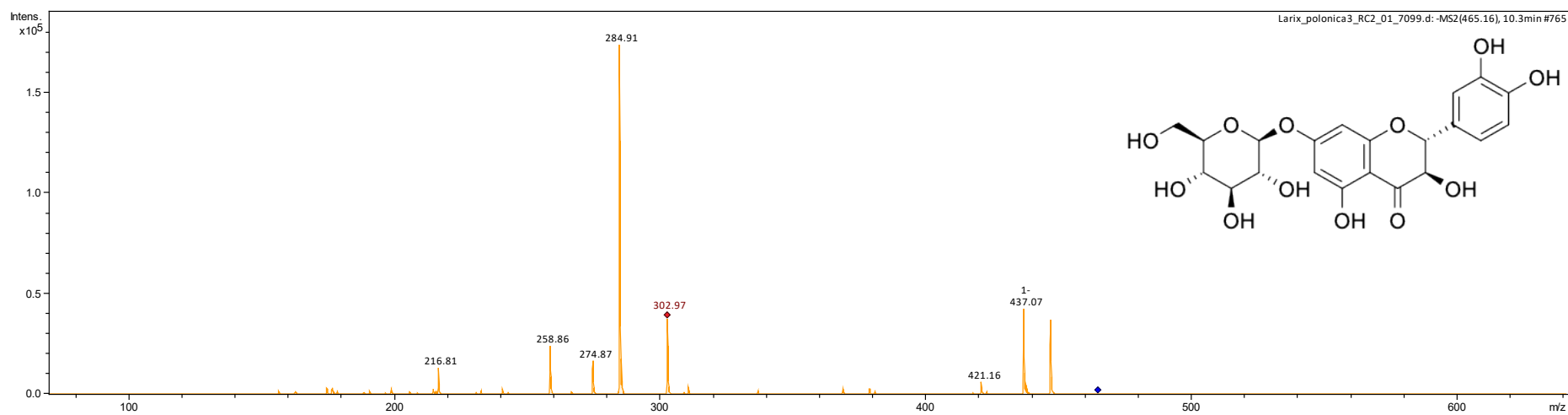


Figure S38. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 465 – compound (13).

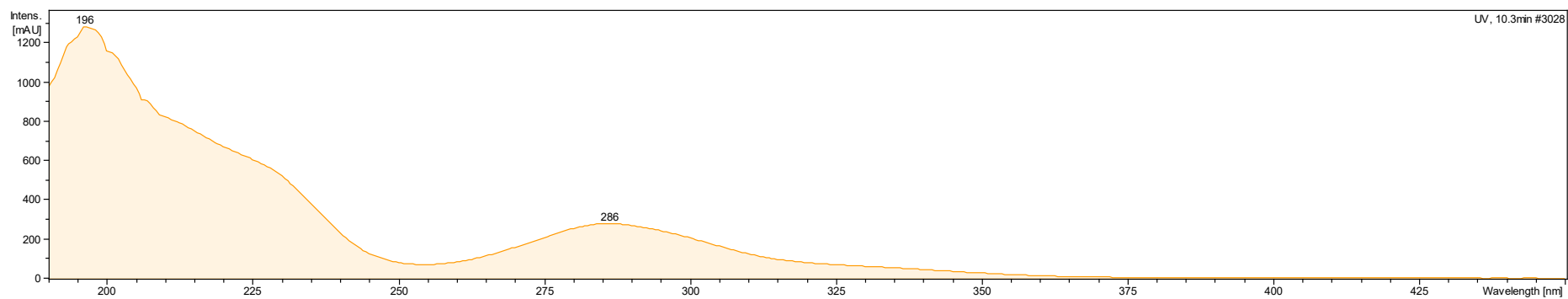


Figure S39. UV spectrum of compound (13).

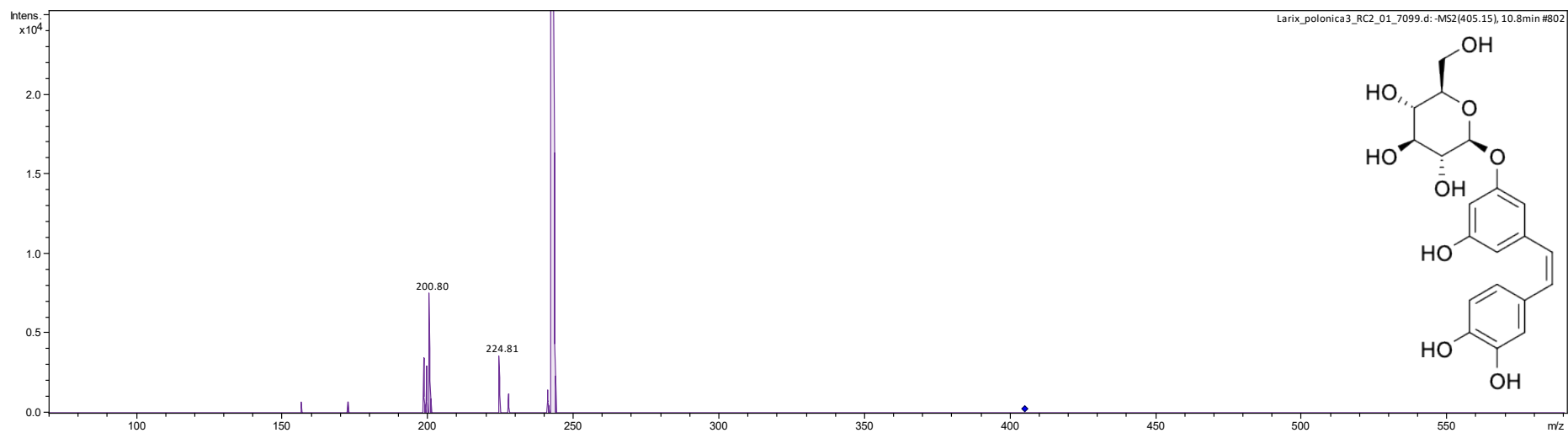


Figure S40. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 405 – compound (14).

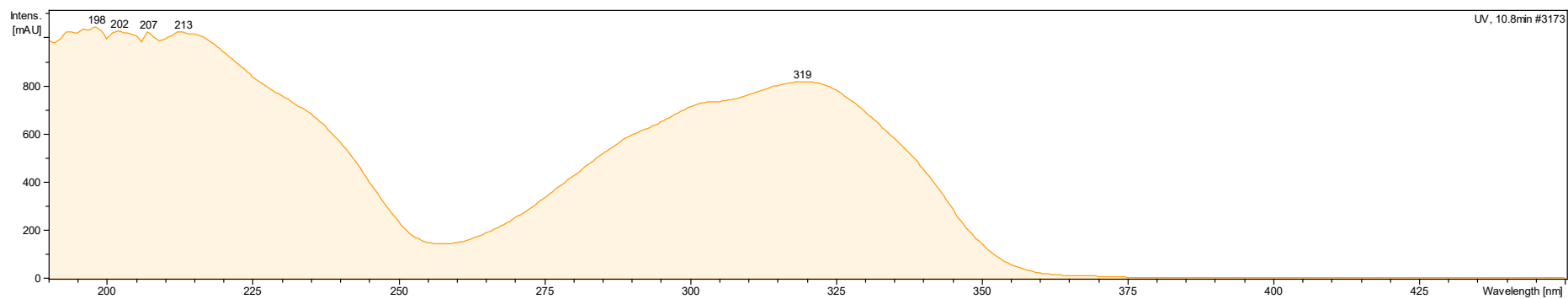


Figure S41. UV spectrum of compound (14).

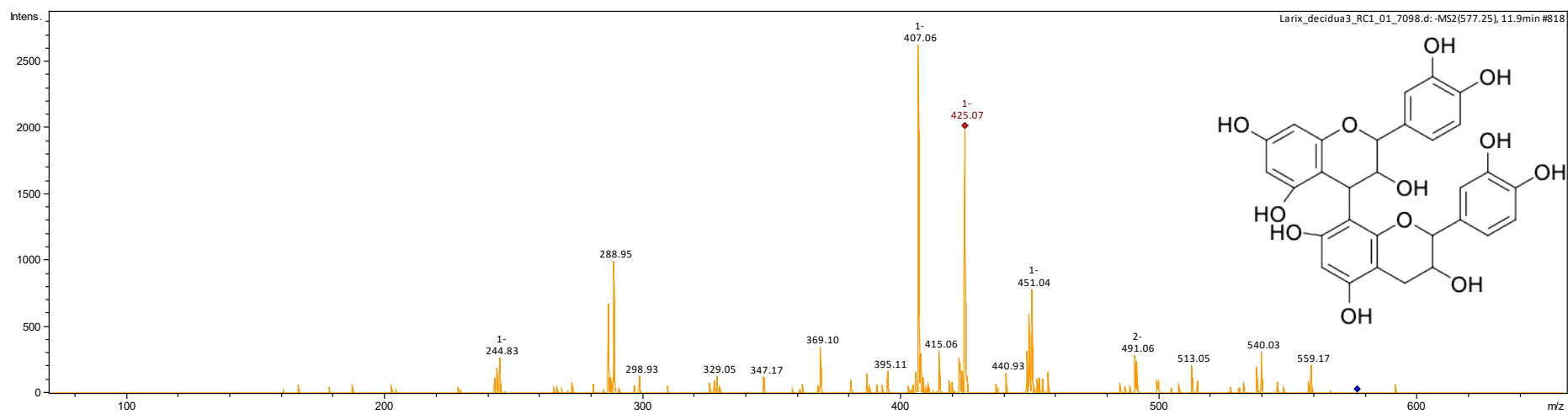


Figure S42. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 577 – compound (15).

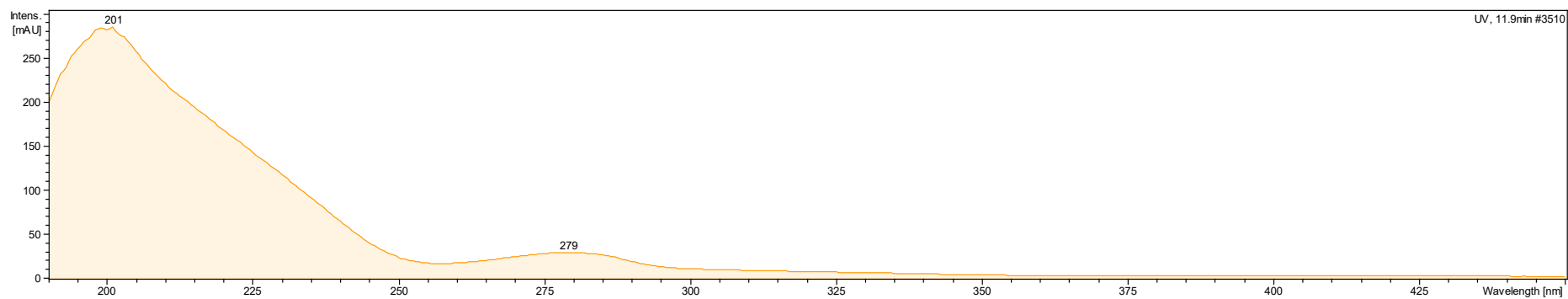


Figure S43. UV spectrum of compound (15).

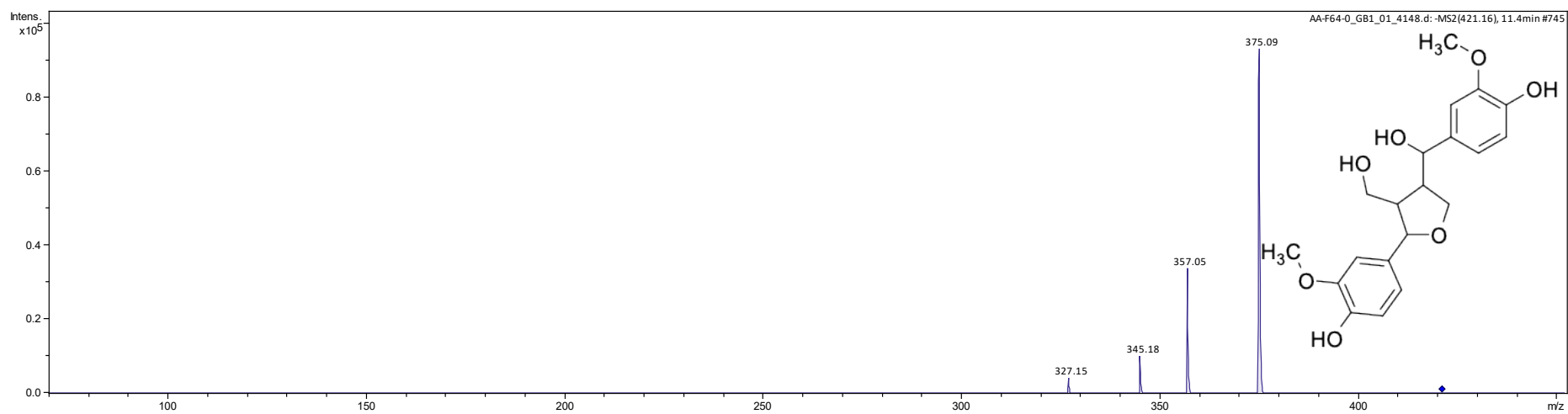


Figure S44. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 421 – compound (16).

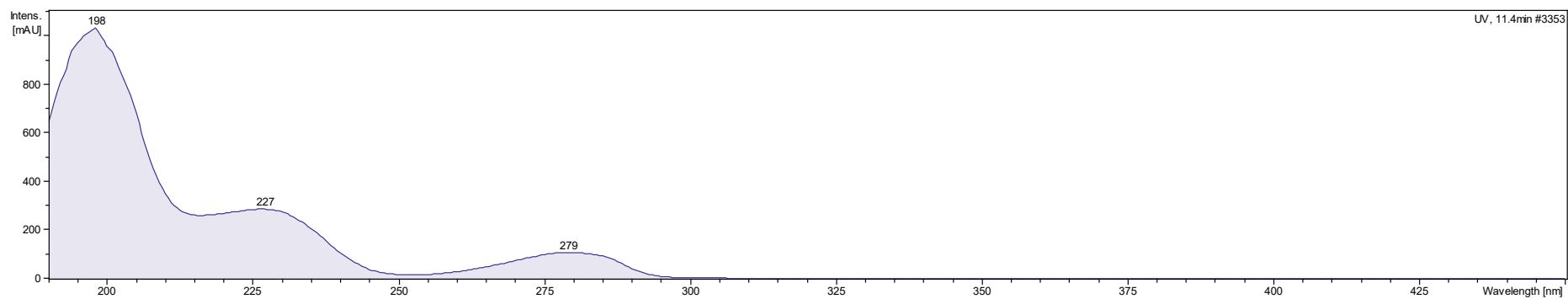


Figure S45. UV spectrum of compound (16).

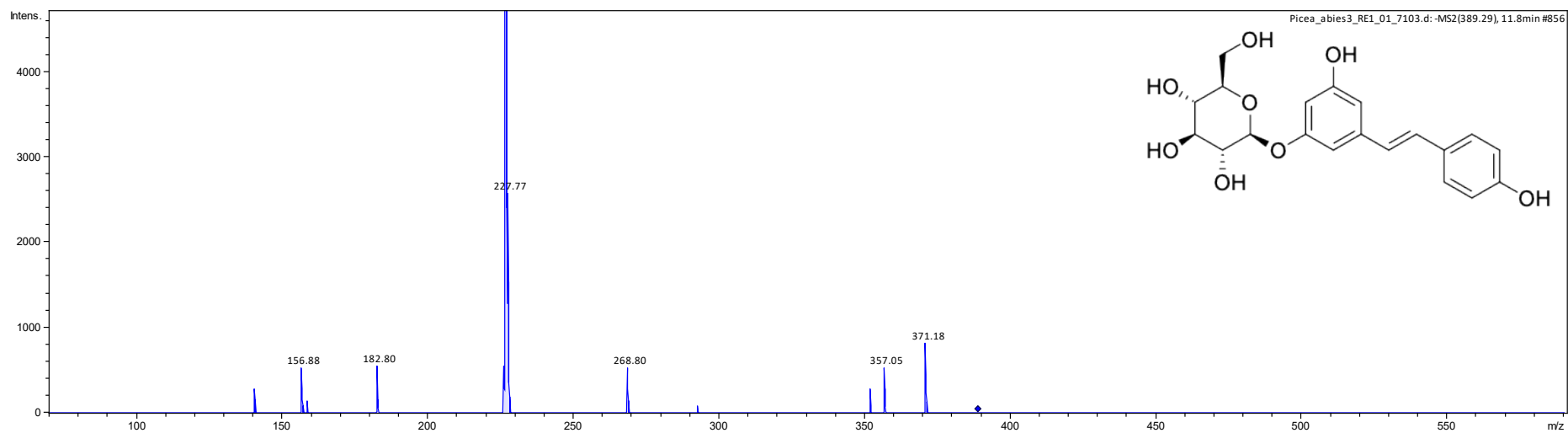


Figure S46. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 389 – compound (17).

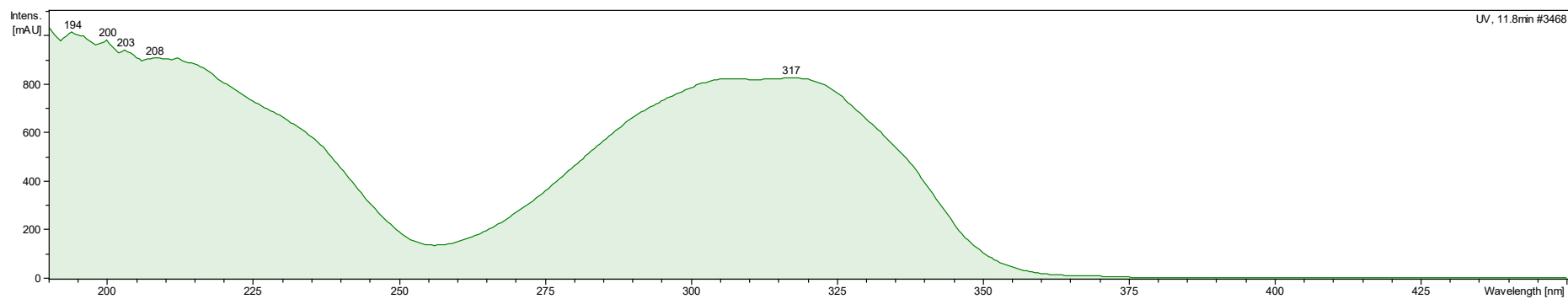


Figure S47. UV spectrum of compound (17).

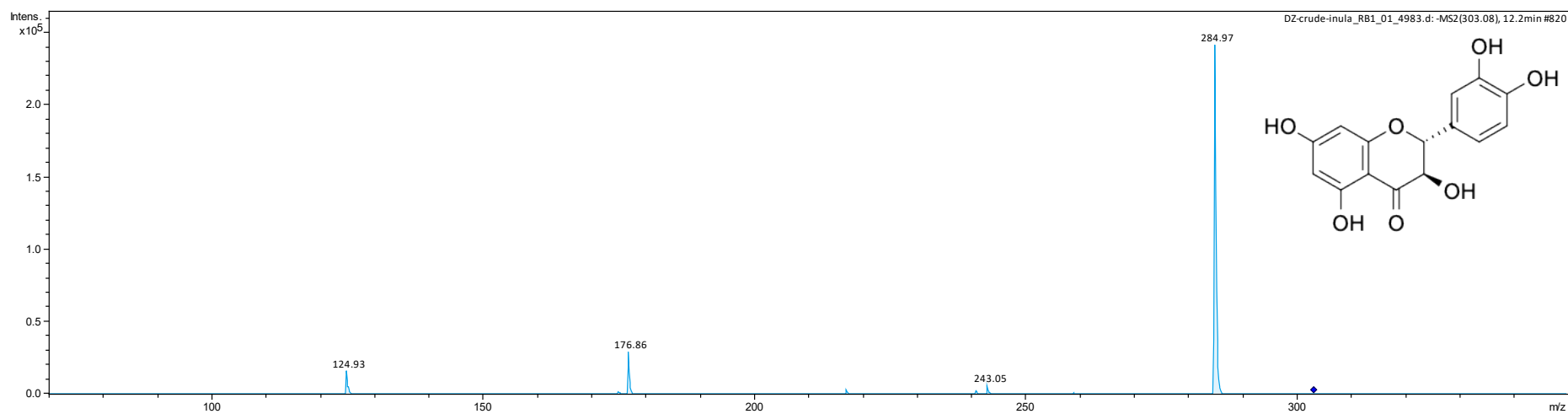


Figure S48. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 303 – compound (18).

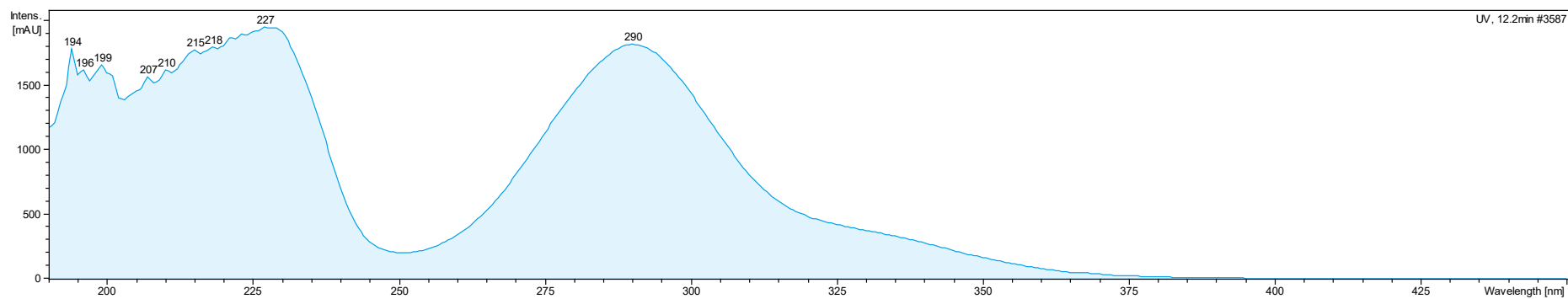


Figure S49. UV spectrum of compound (18).

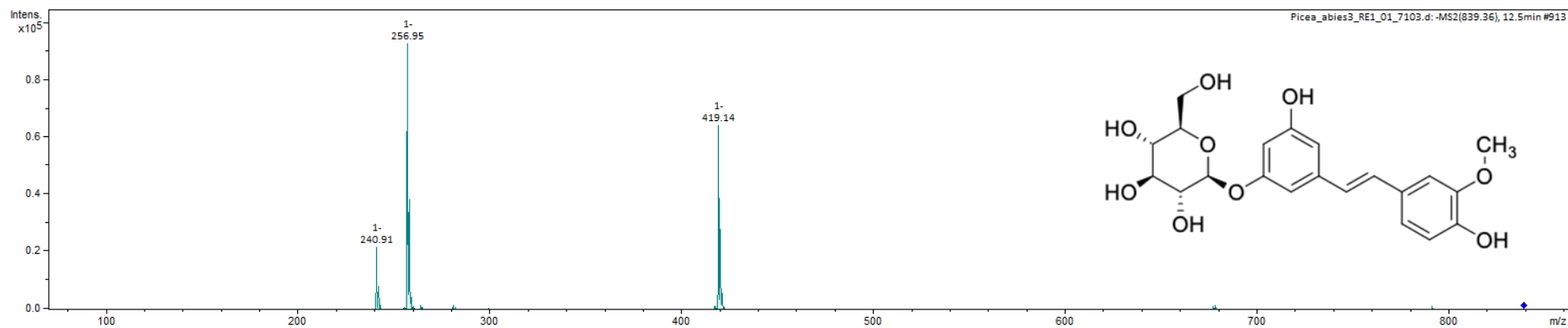


Figure S50. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 465 – compound (19).

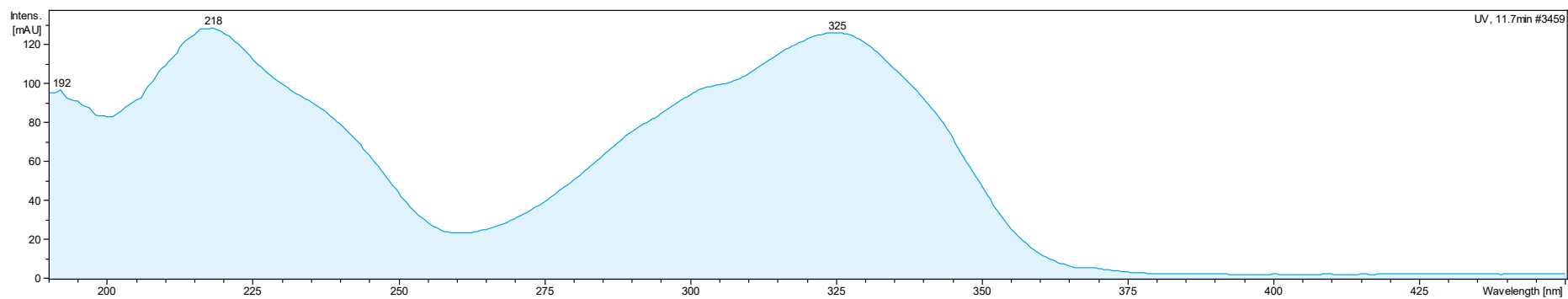


Figure S51. UV spectrum of compound (19).

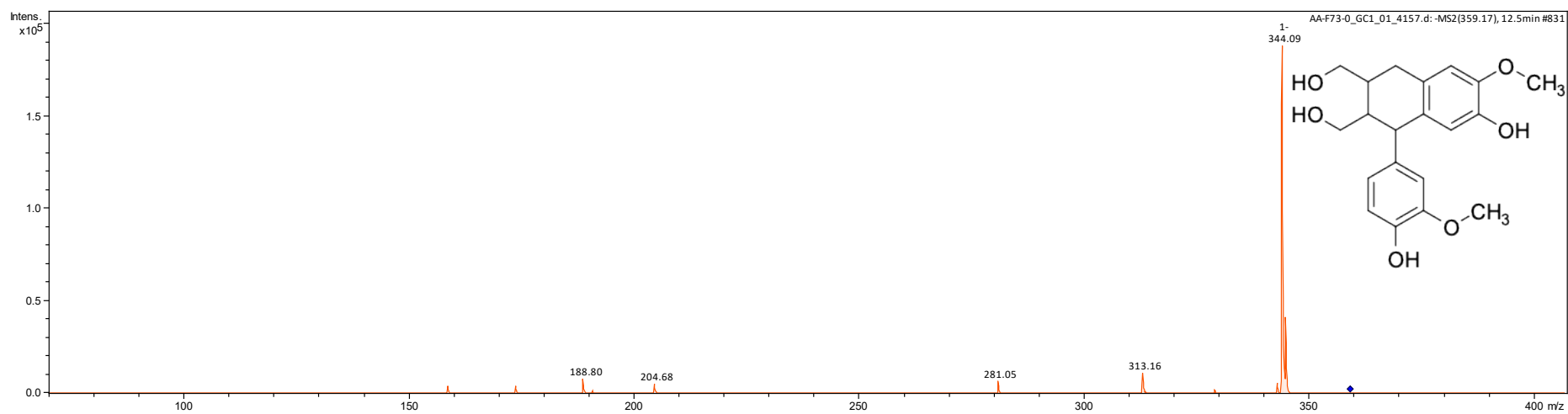


Figure S52. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 359 – compound (20).

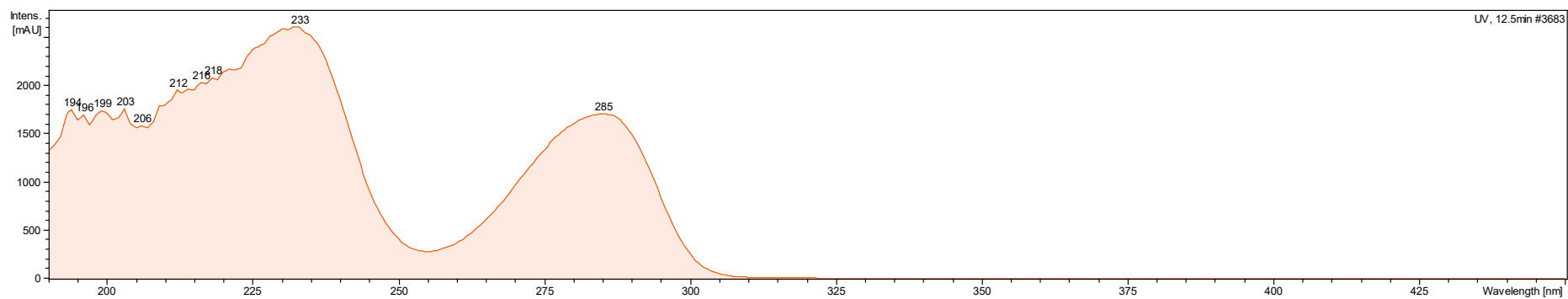


Figure S53. UV spectrum of compound (20).

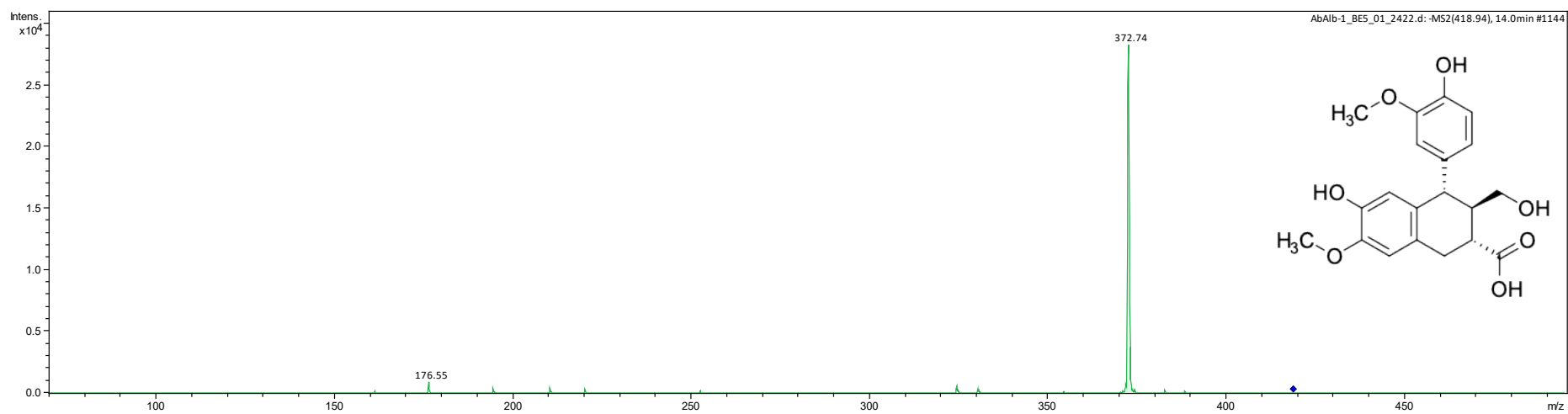


Figure S54. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 419 – compound (21).

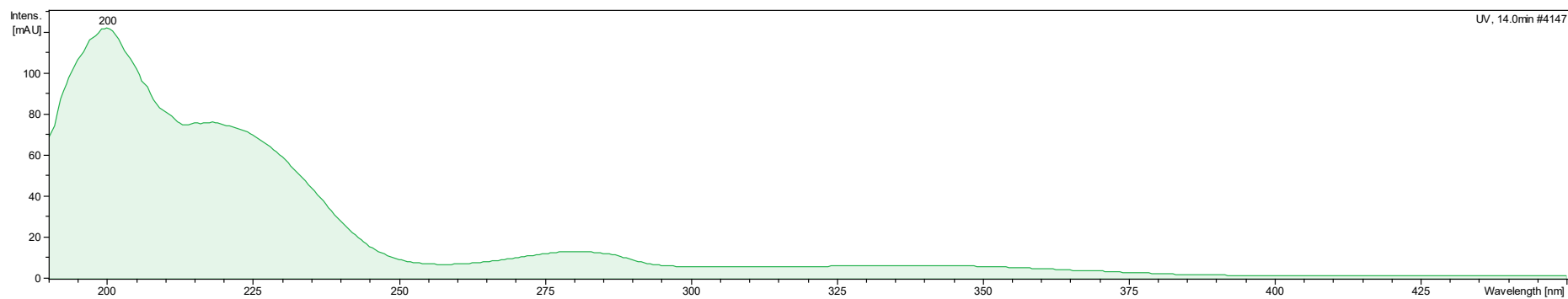


Figure S55. UV spectrum of compound (21).

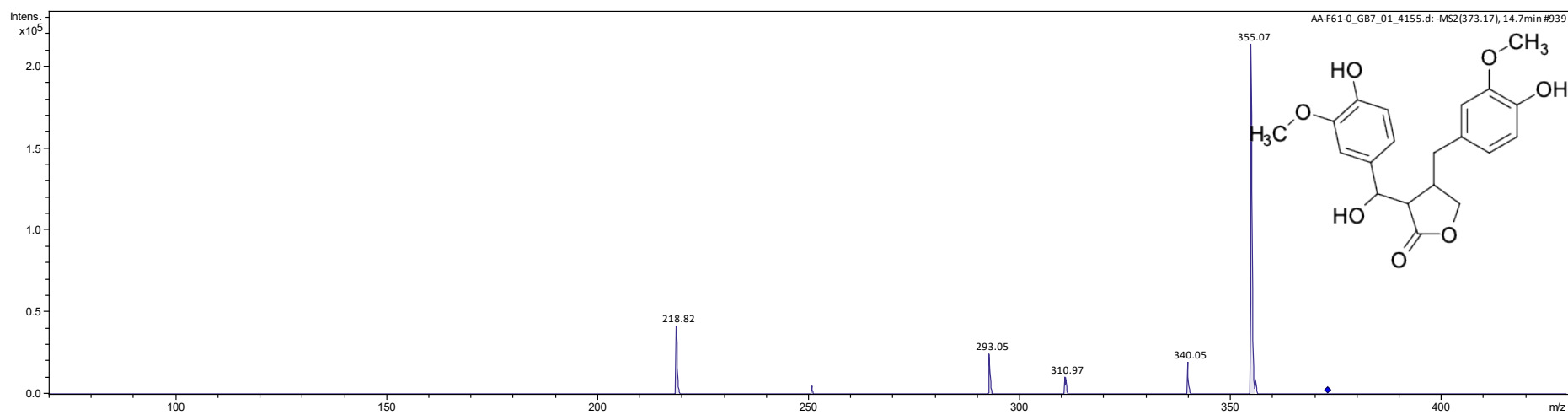


Figure S56. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 373 – compound (22).

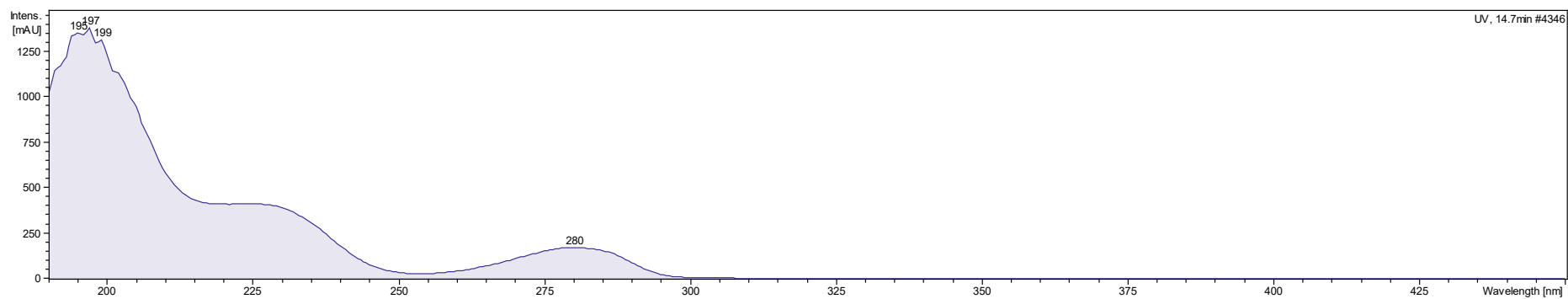


Figure S57. UV spectrum of compound (22).

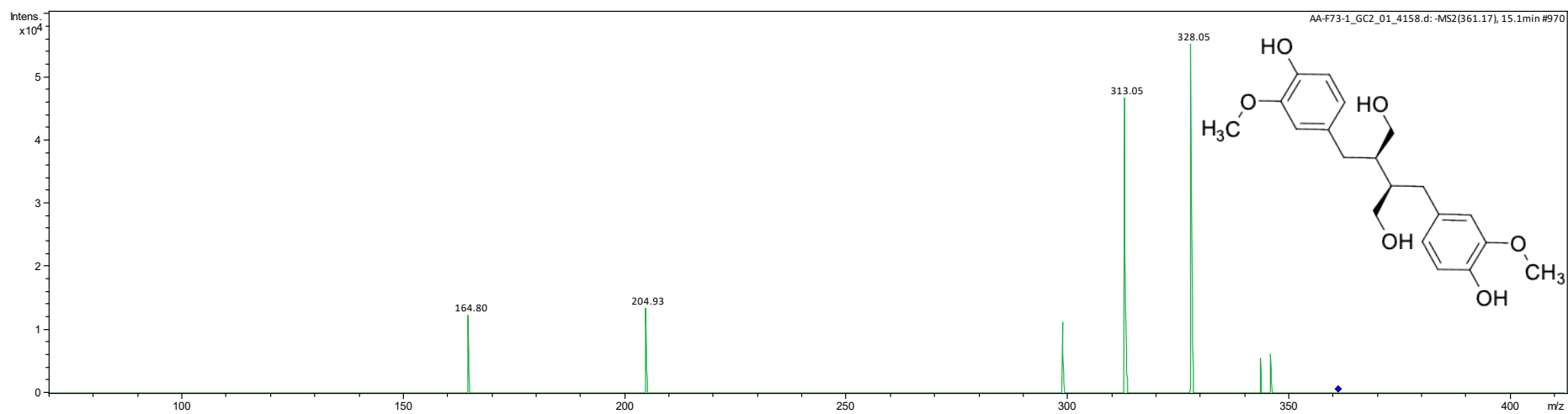


Figure S58. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 361 – compound (23).

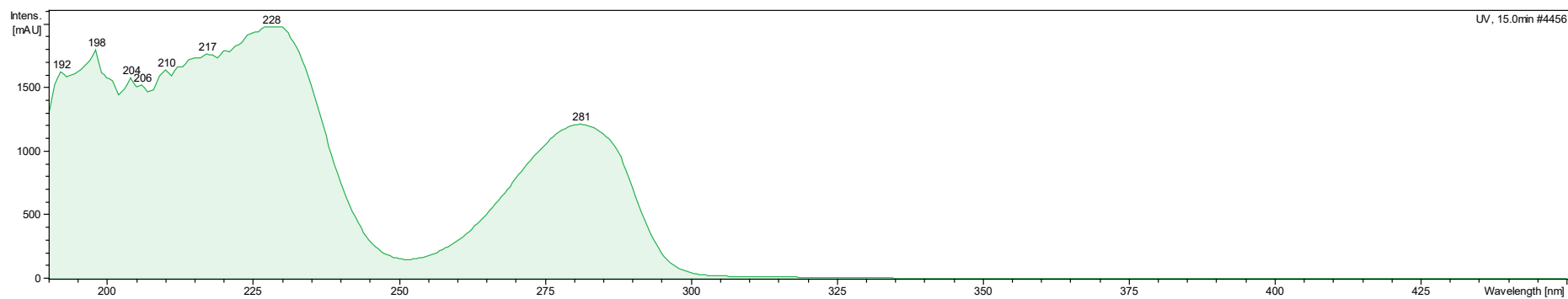


Figure S59. UV spectrum of compound (23).

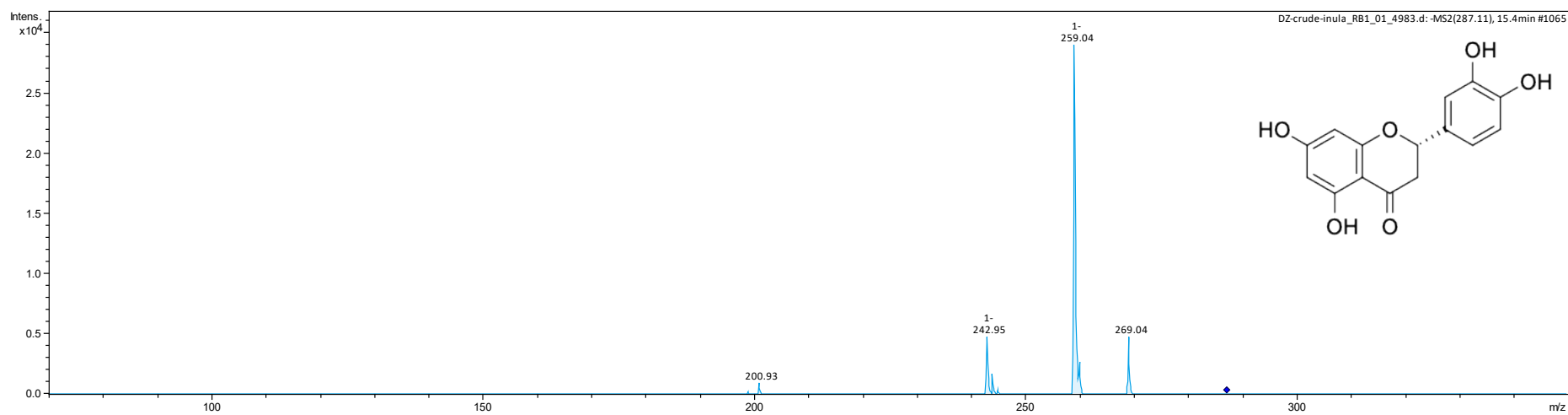


Figure S60. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 287 – compound (24).

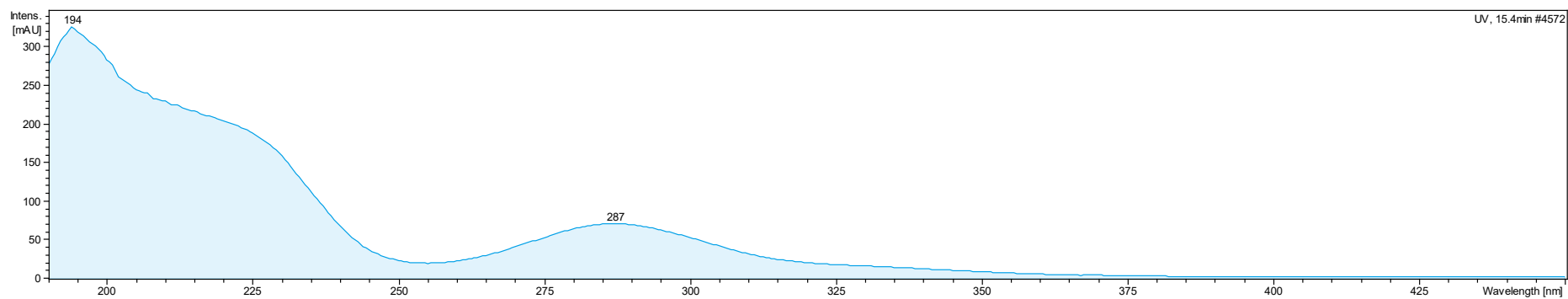


Figure S61. UV spectrum of compound (24).

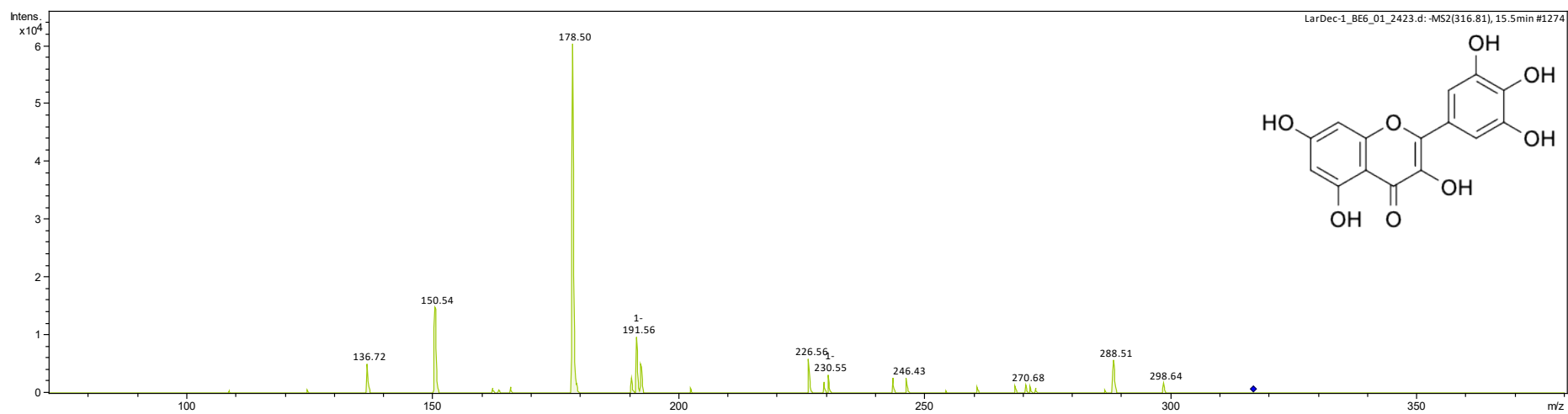
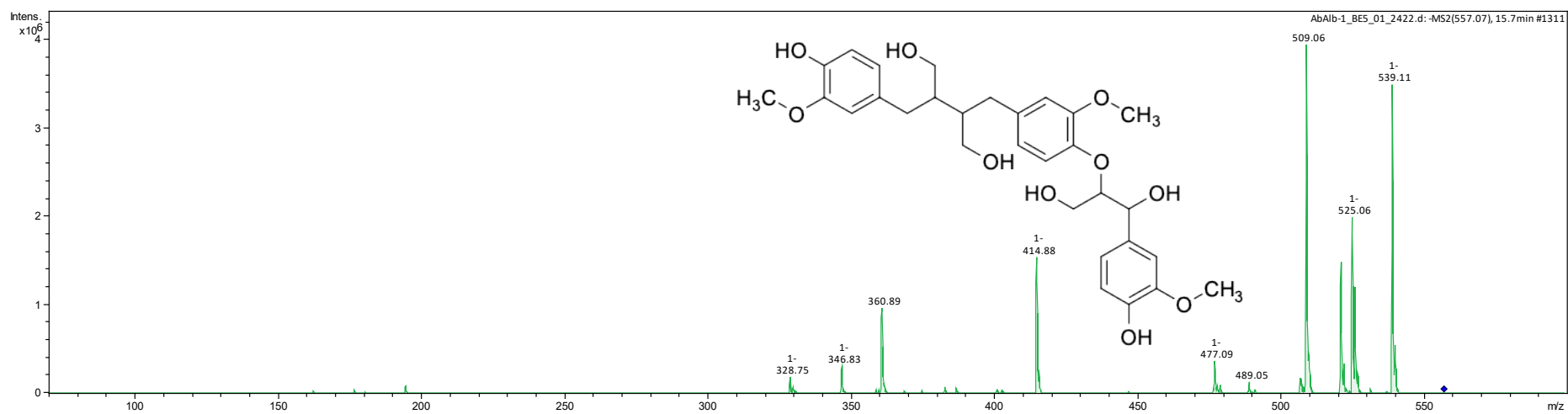
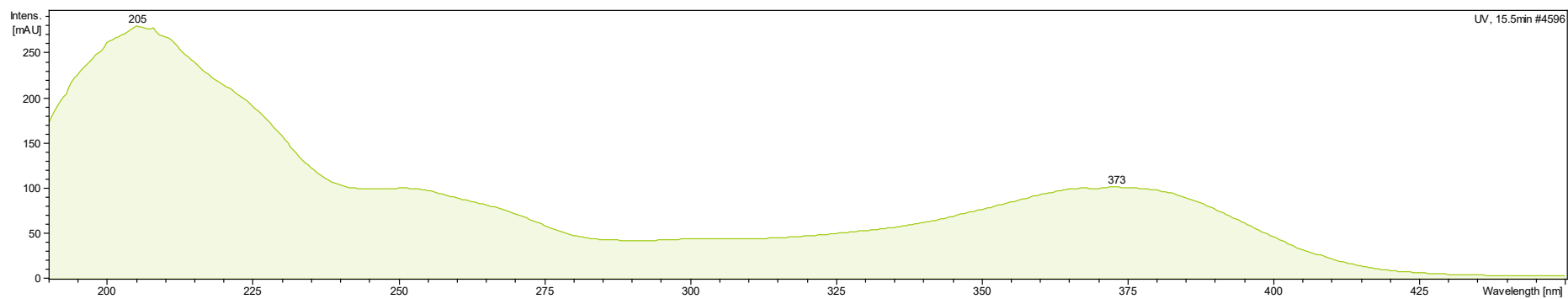


Figure S62. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 317 – compound (25).



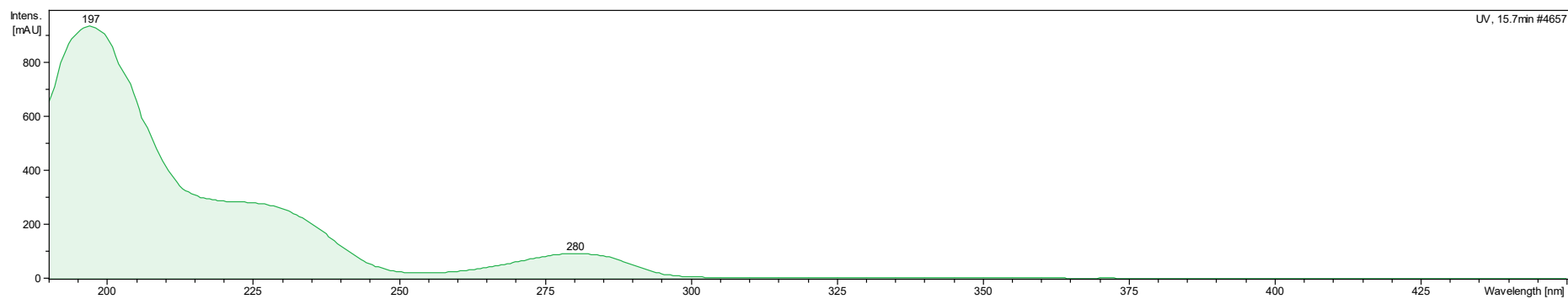


Figure S65. UV spectrum of compound (26).

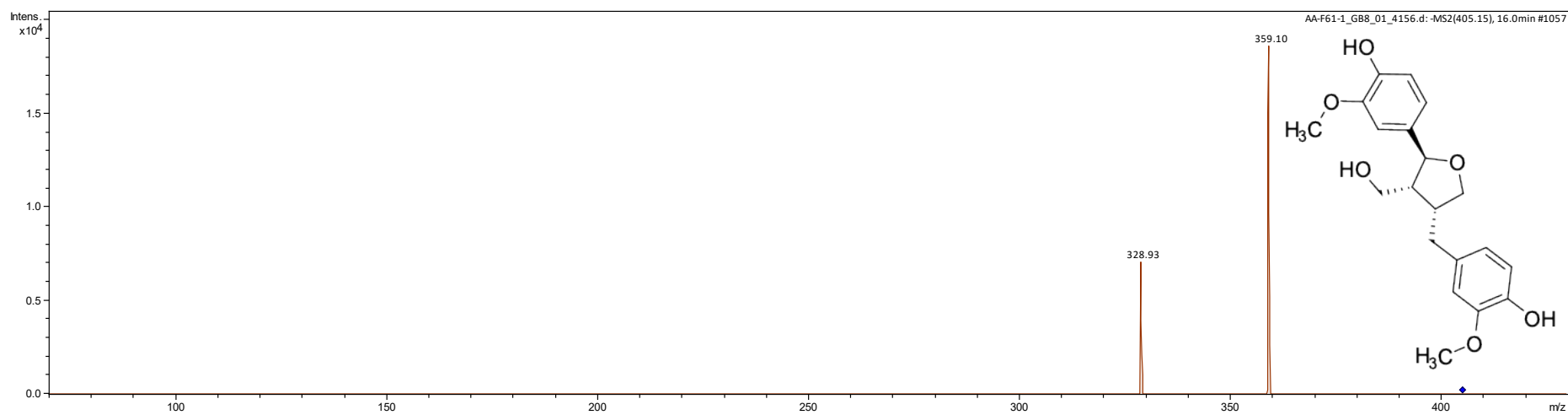


Figure S66. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 405 – compound (27).

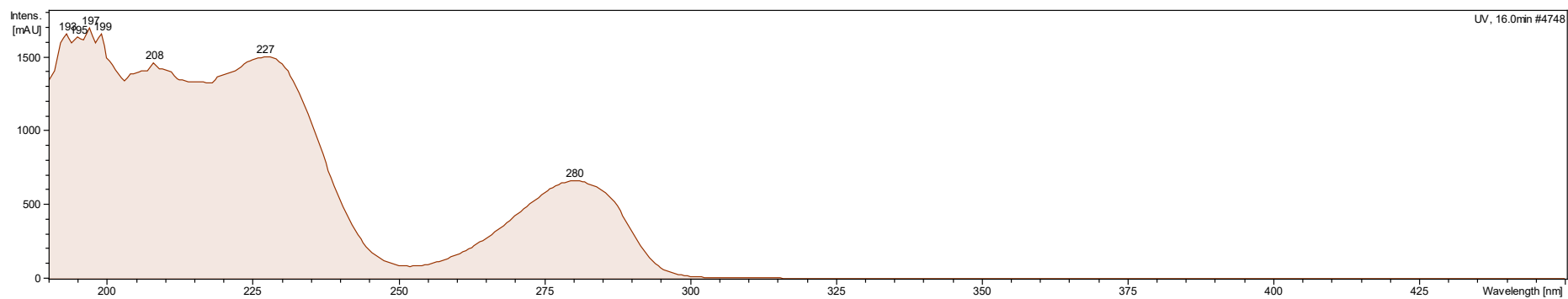


Figure S67. UV spectrum of compound (27).

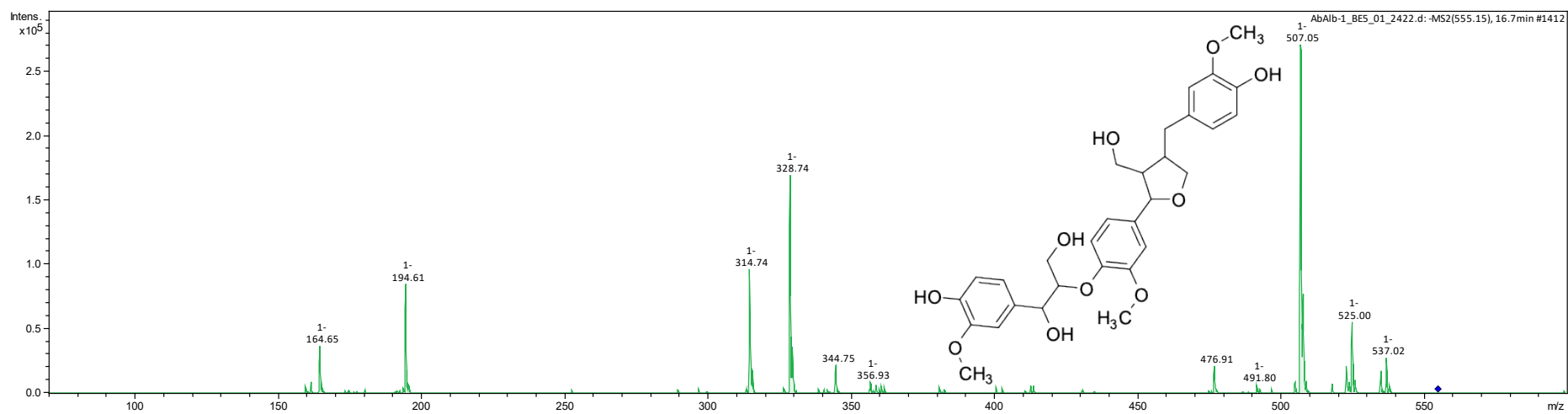


Figure S68. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 555 – compound (28).

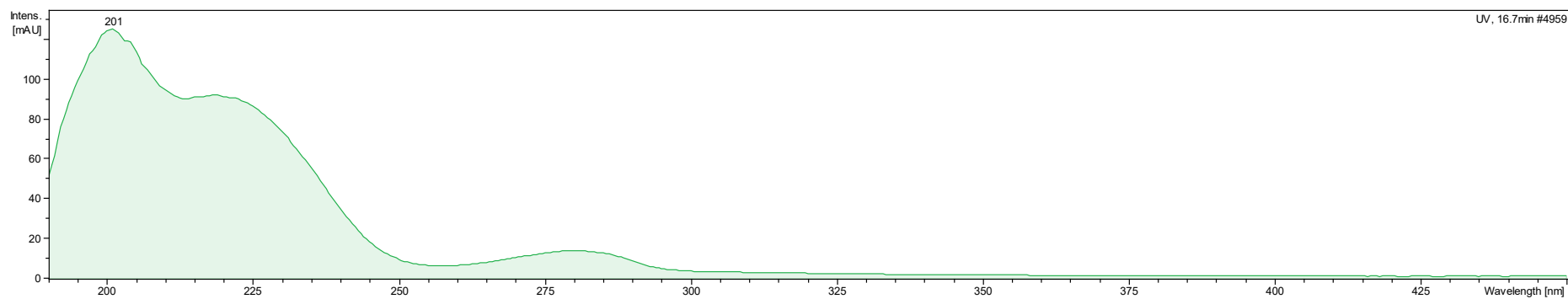


Figure S69. UV spectrum of compound (28).

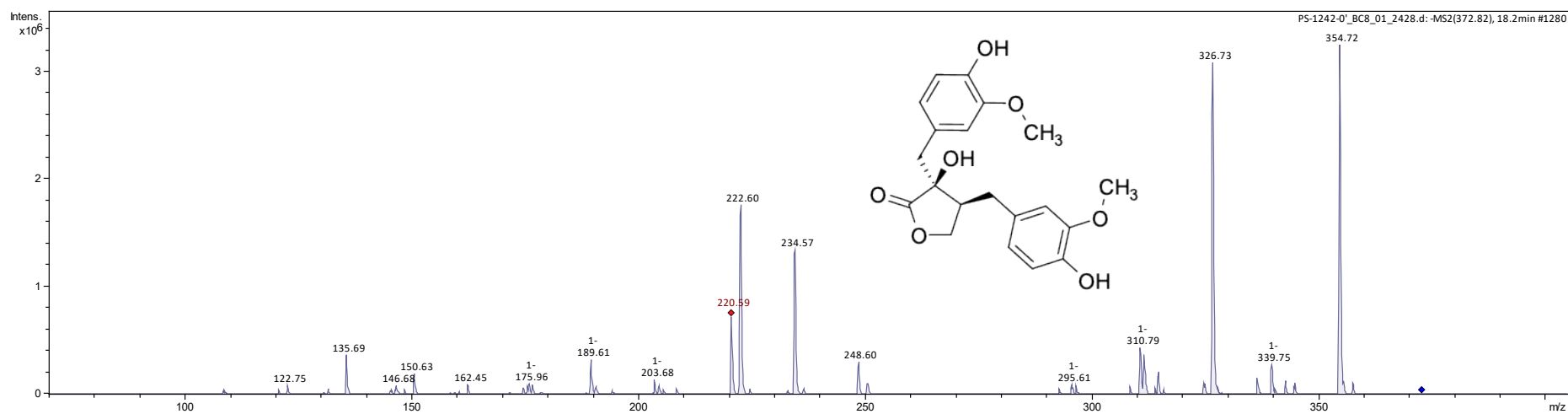


Figure S70. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 373 – compound (29).

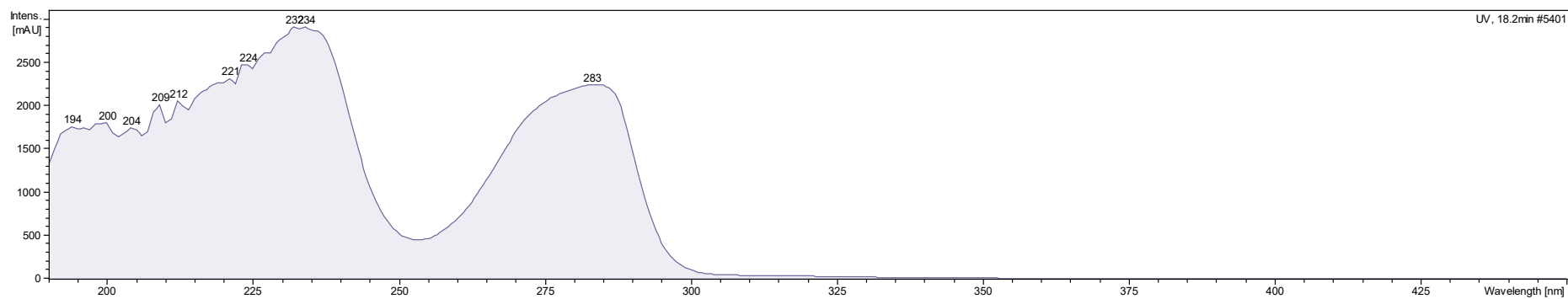


Figure S71. UV spectrum of compound (29).

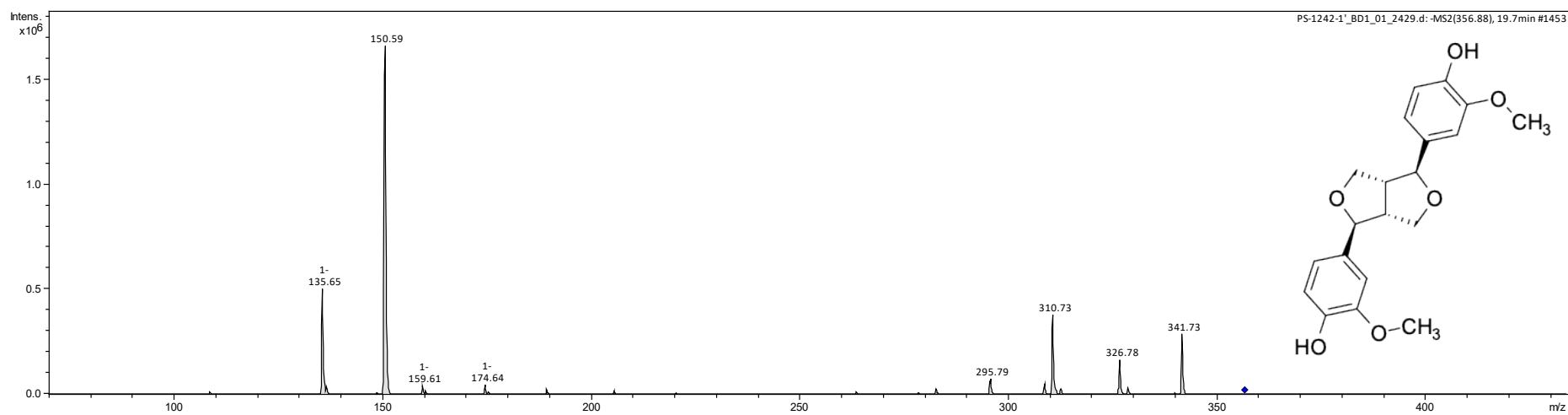


Figure S72. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 357 – compound (30).

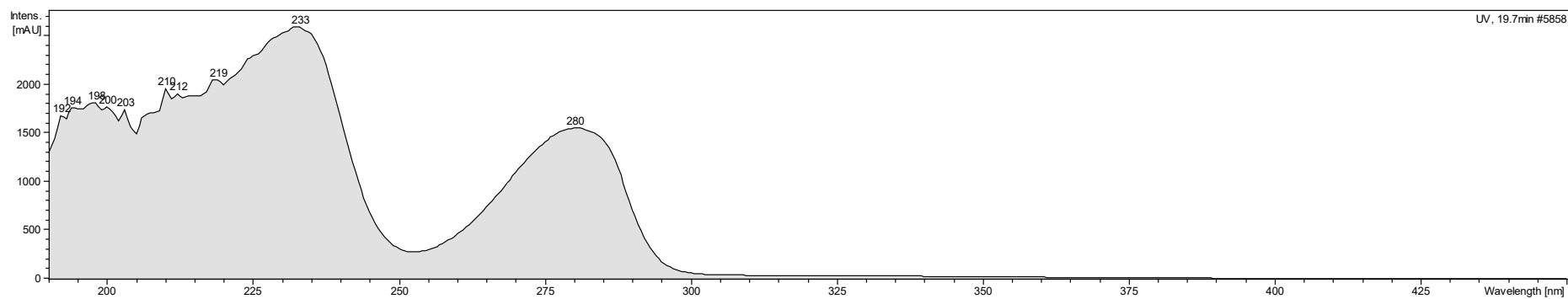


Figure S73. UV spectrum of compound (30).

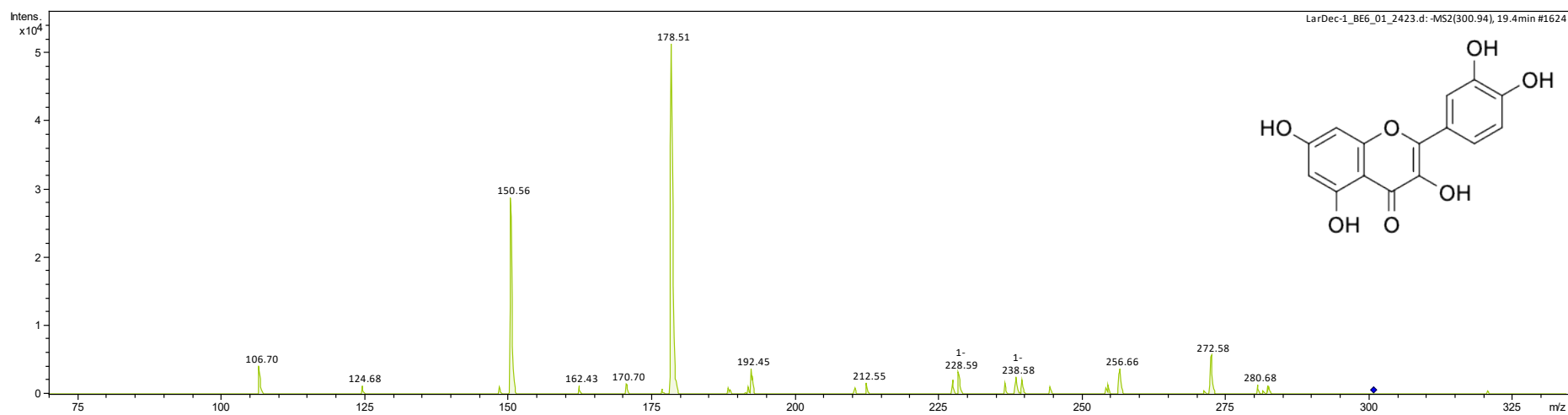


Figure S74. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 301 – compound (31).

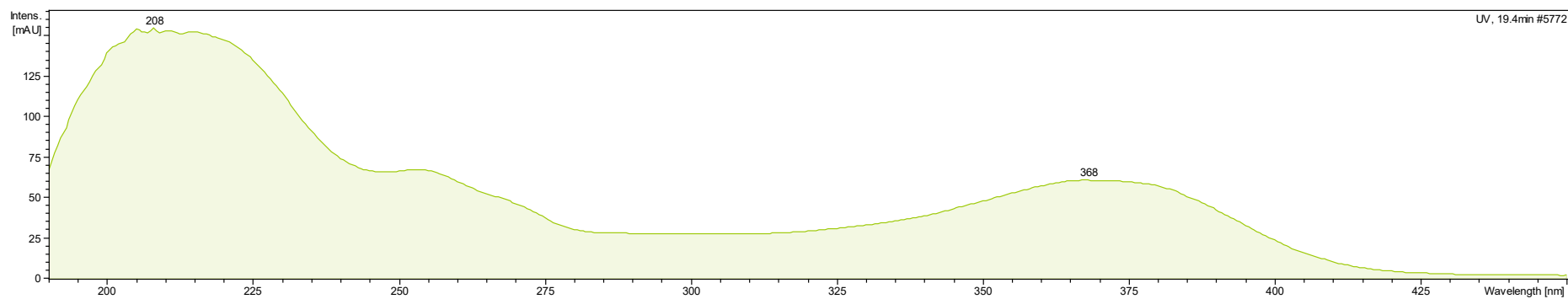


Figure S75. UV spectrum of compound (31).

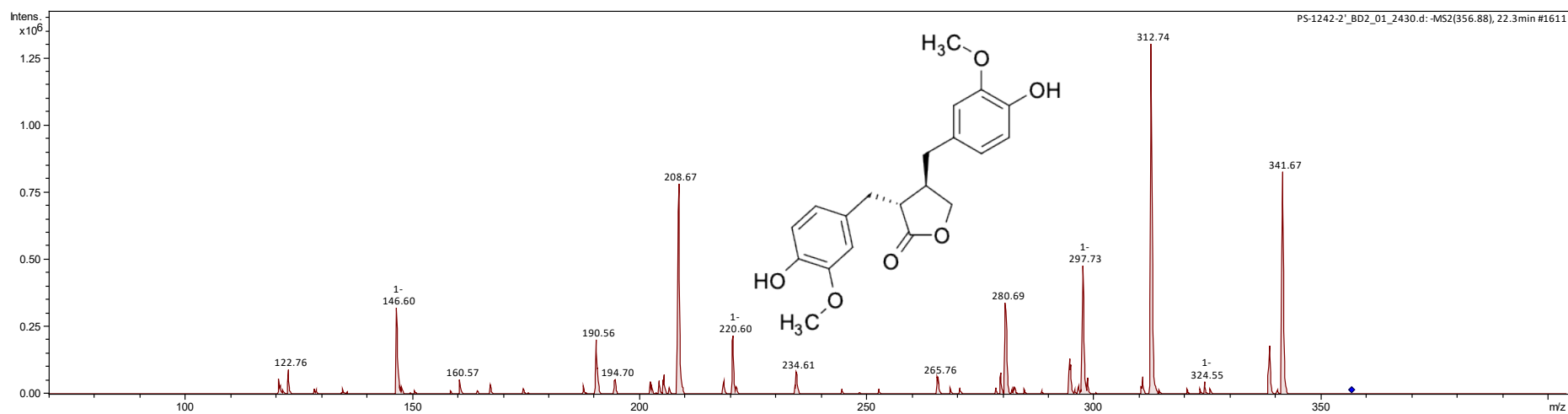


Figure S76. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 357 – compound (32).

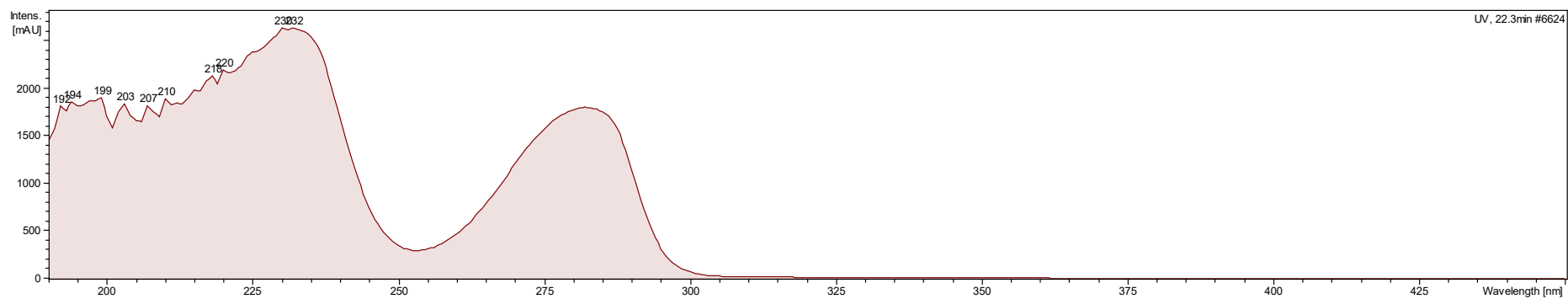


Figure S77. UV spectrum of compound (32).

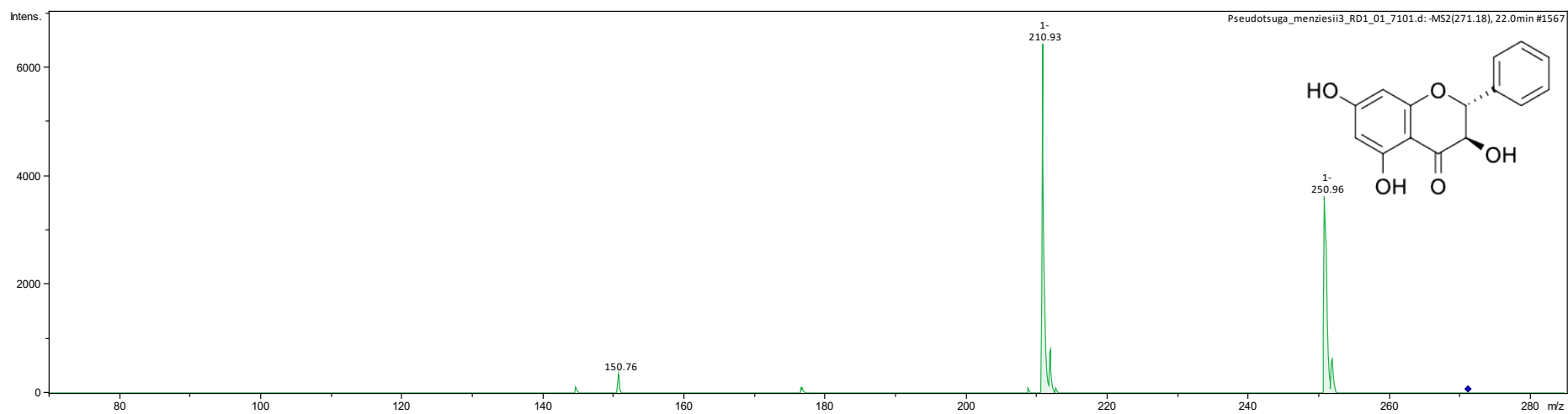


Figure S78. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 271 – compound (33).

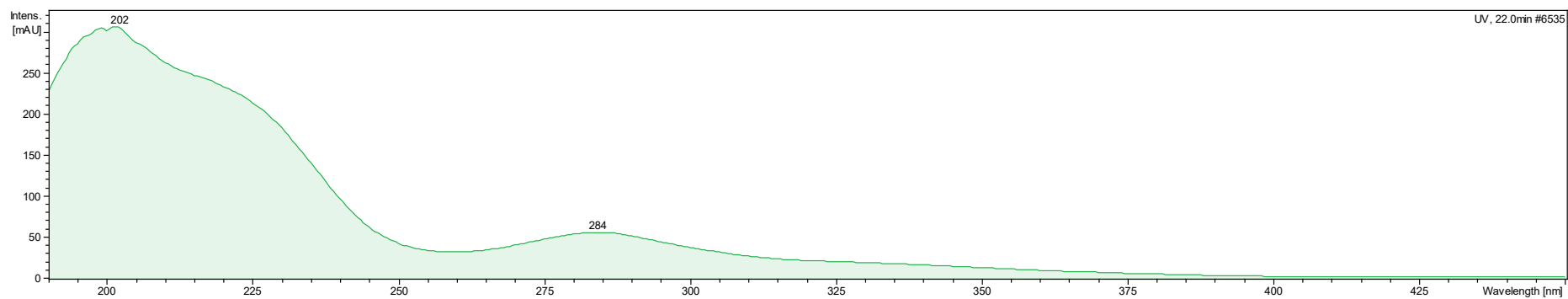


Figure S79. UV spectrum of compound (33).

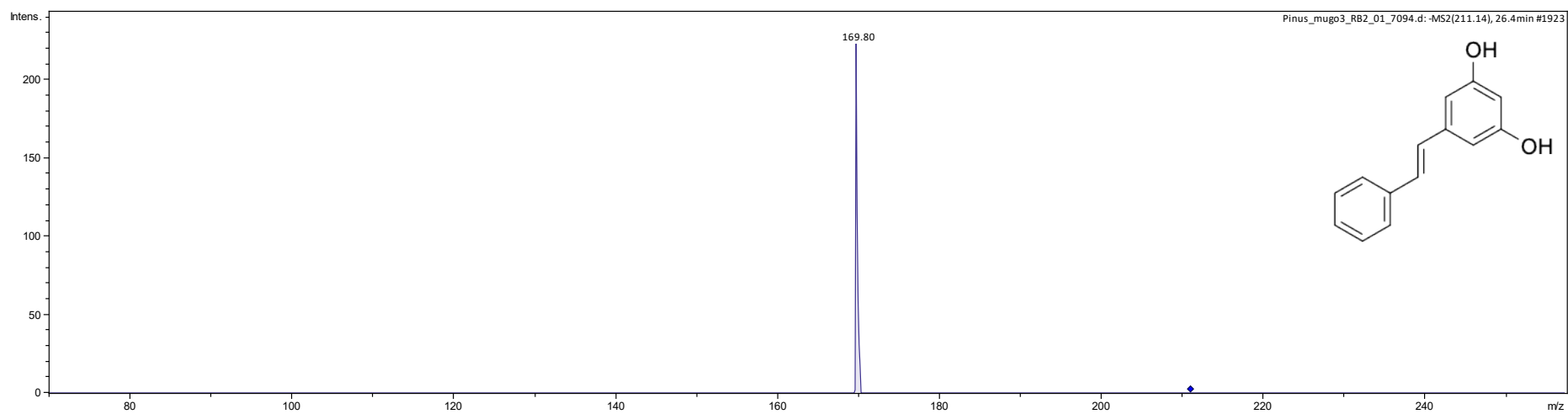


Figure S80. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 211 – compound (34).

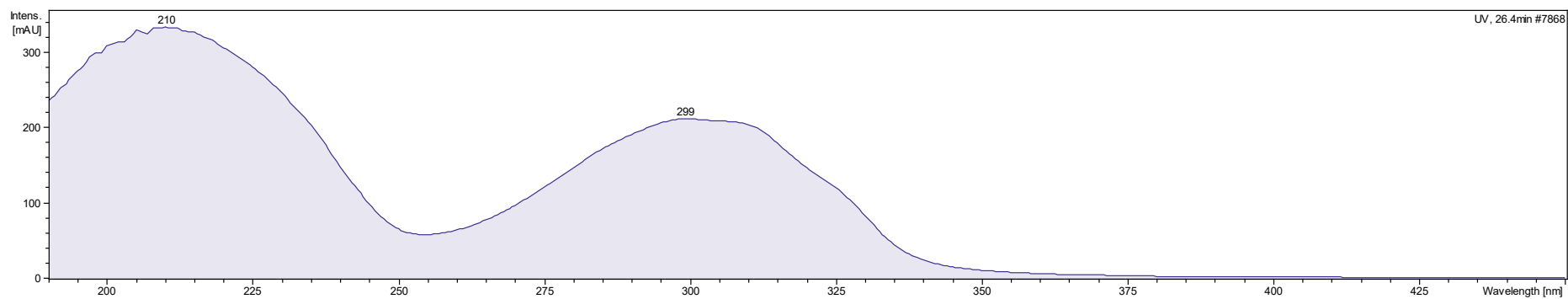


Figure S81. UV spectrum of compound (34).

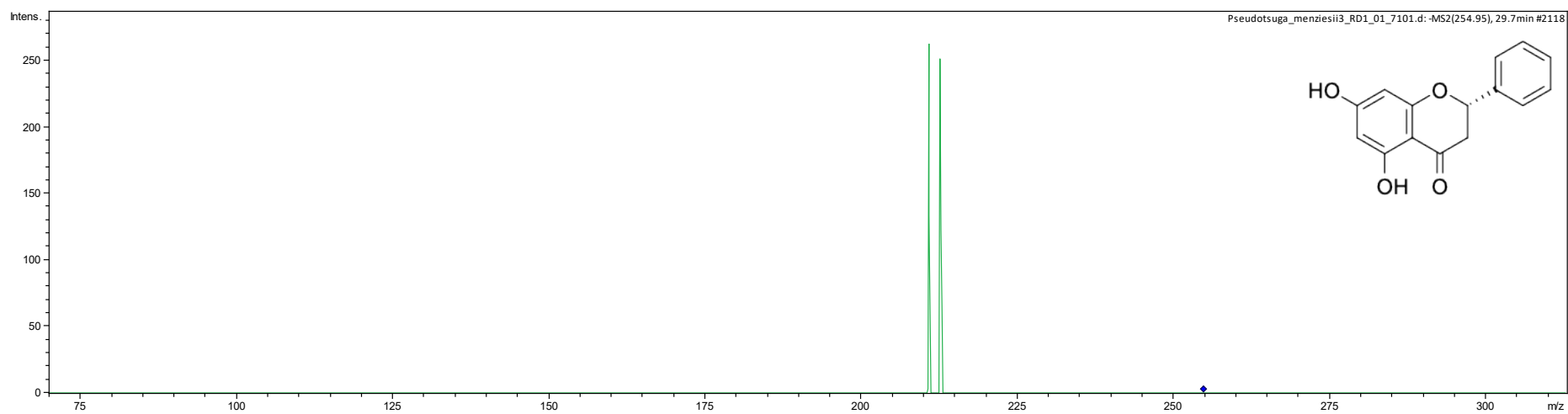


Figure S82. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 255 – compound (35).

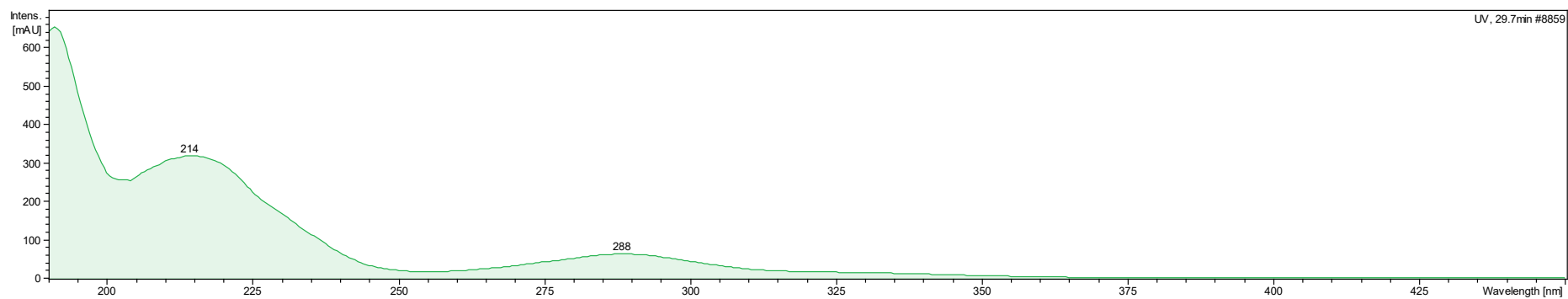


Figure S83. UV spectrum of compound (35).

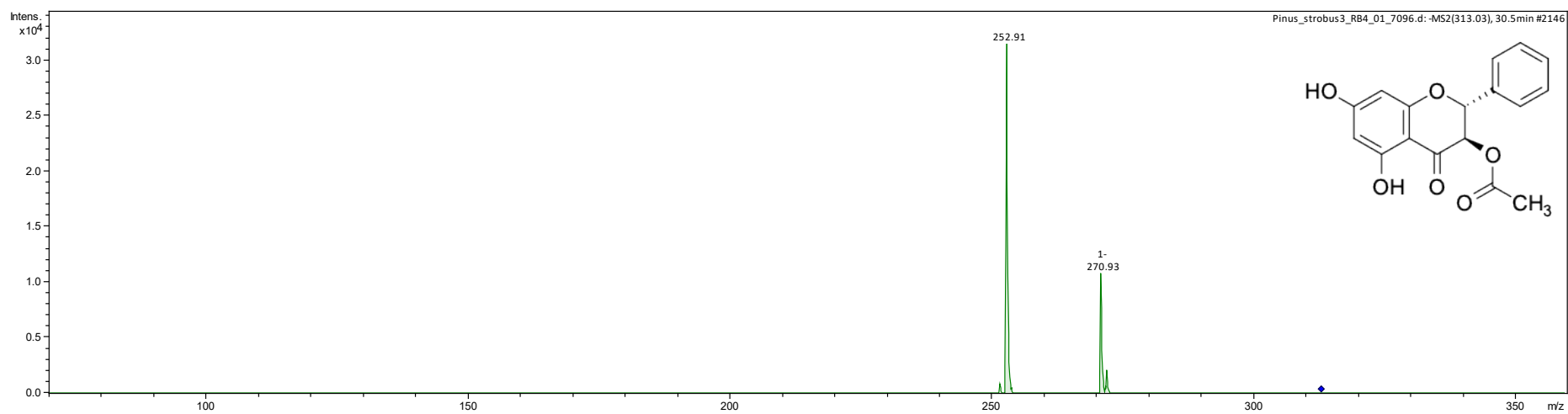


Figure S84. ESI-MS² spectrum (negative ion mode) of molecular ion at m/z 313 – compound (36).

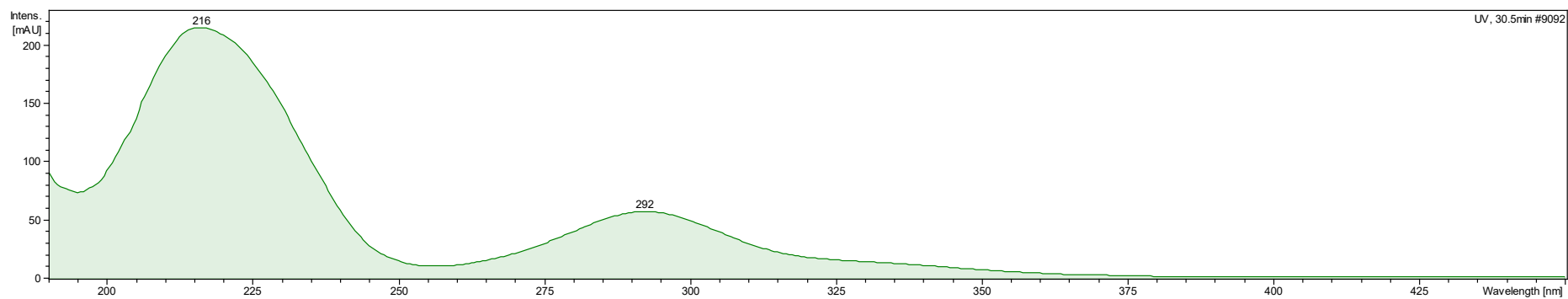


Figure S85. UV spectrum of compound (36).

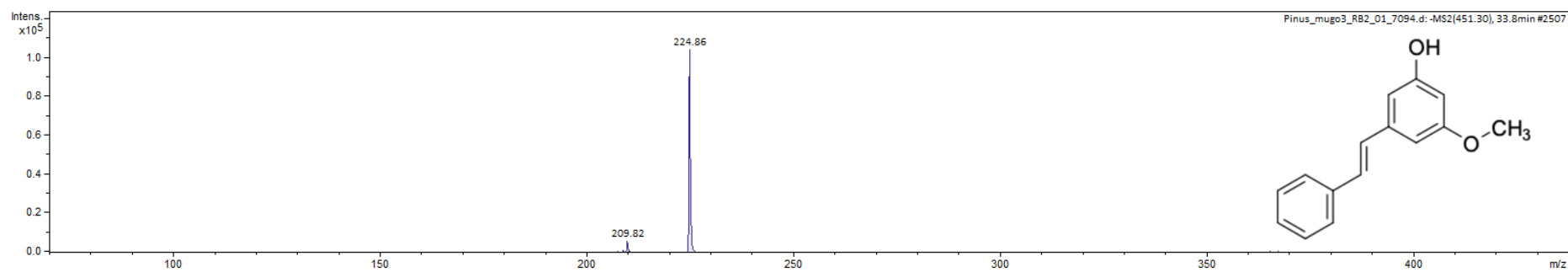


Figure S86. ESI-MS² spectrum (positive ion mode) of molecular ion at m/z 227 – compound (37).

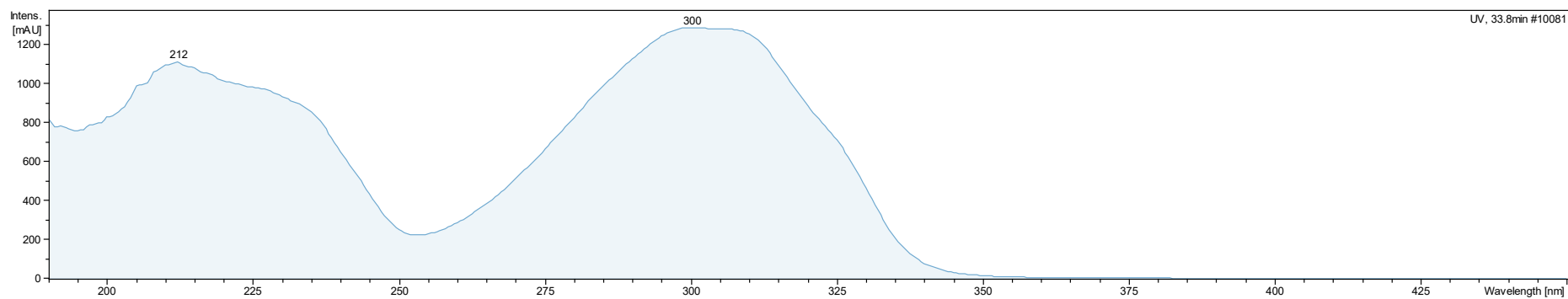


Figure S87. UV spectrum of compound (37).

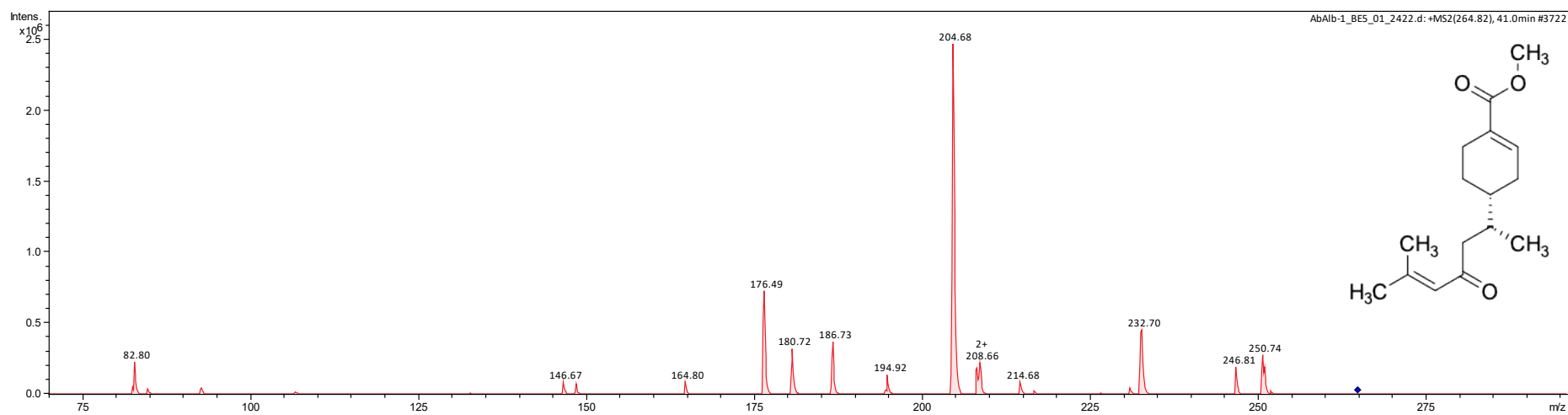


Figure S88. ESI-MS² spectrum (positive ion mode) of molecular ion at m/z 265 – compound (38).

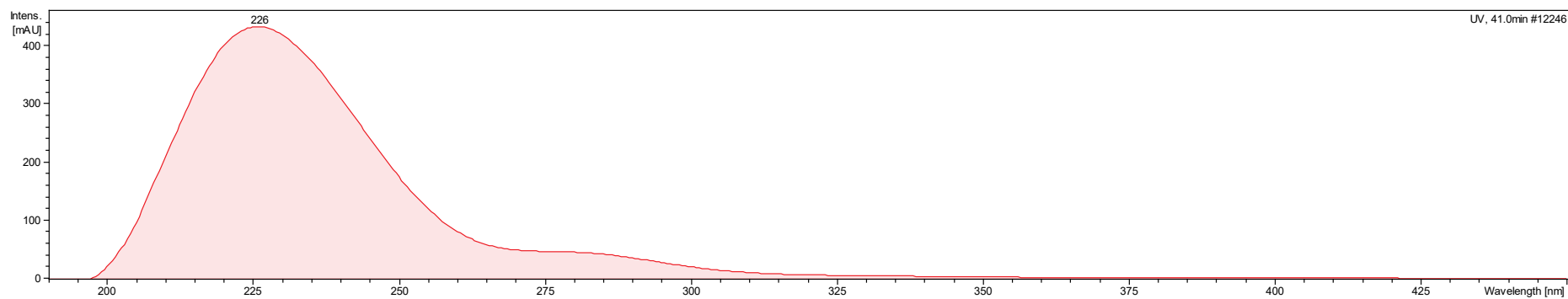


Figure S89. UV spectrum of compound (38).

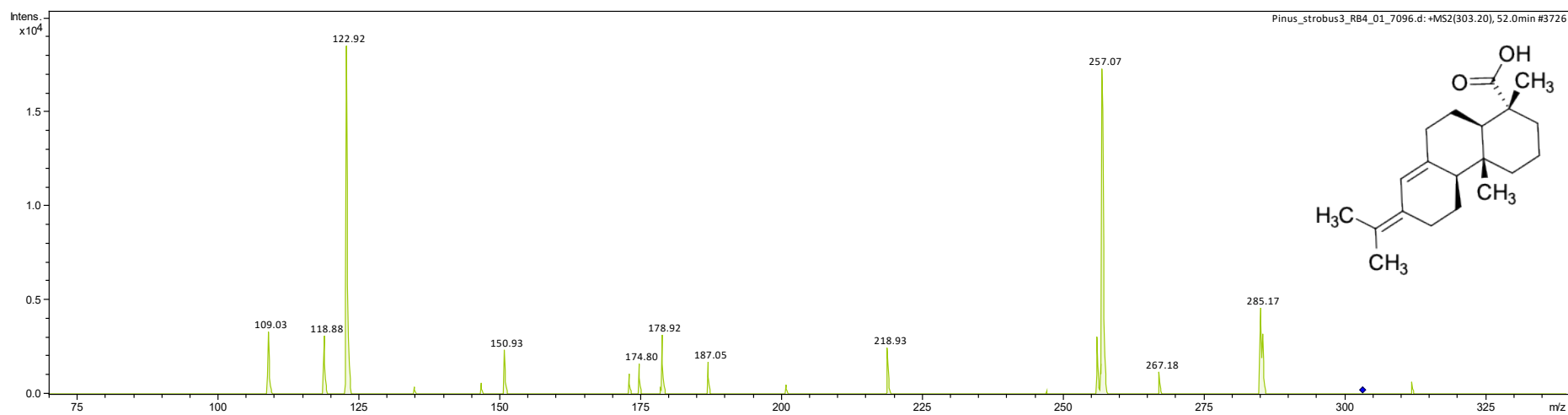


Figure S90. ESI-MS² spectrum (positive ion mode) of molecular ion at m/z 303 – compound (39).

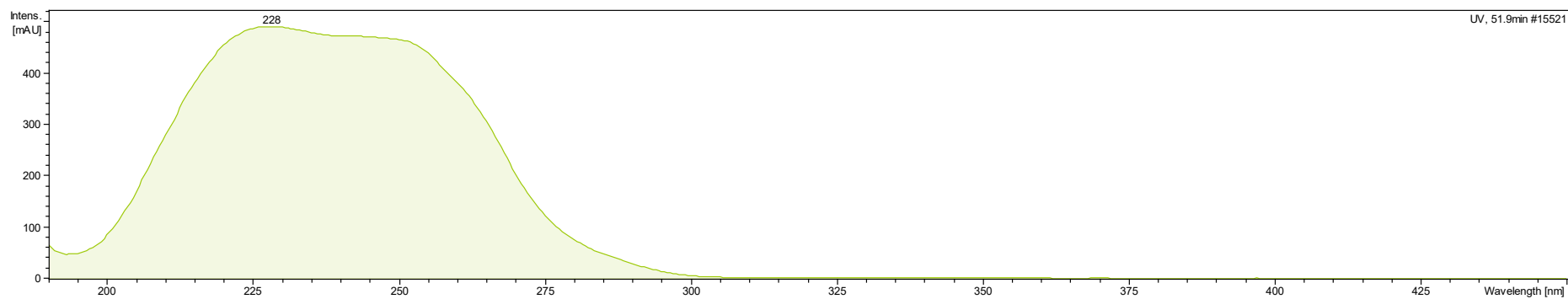


Figure S91. UV spectrum of compound (39).

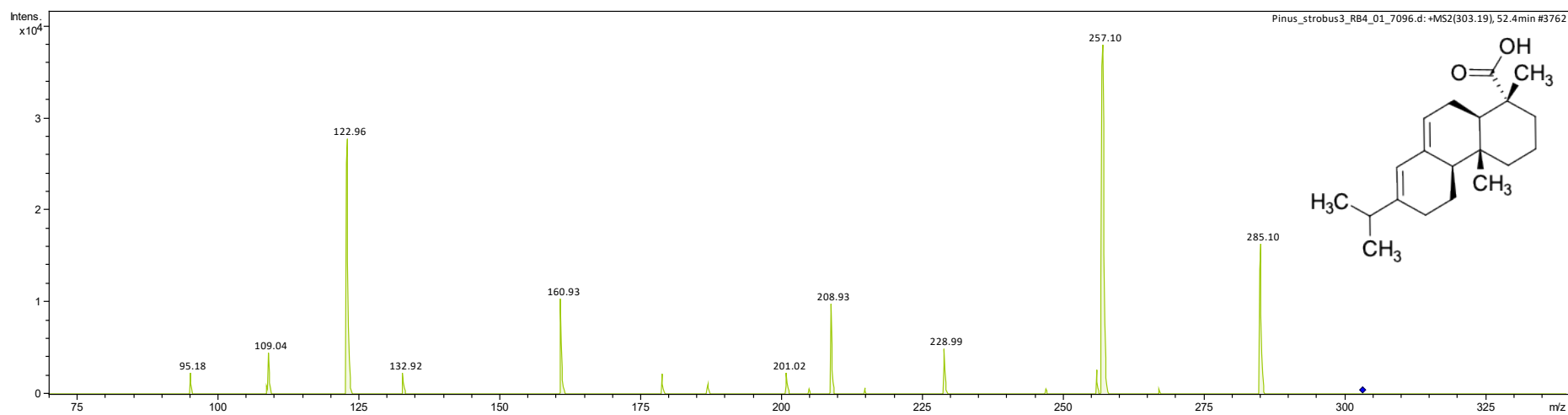


Figure S92. ESI-MS² spectrum (positive ion mode) of molecular ion at m/z 303 – compound (40).

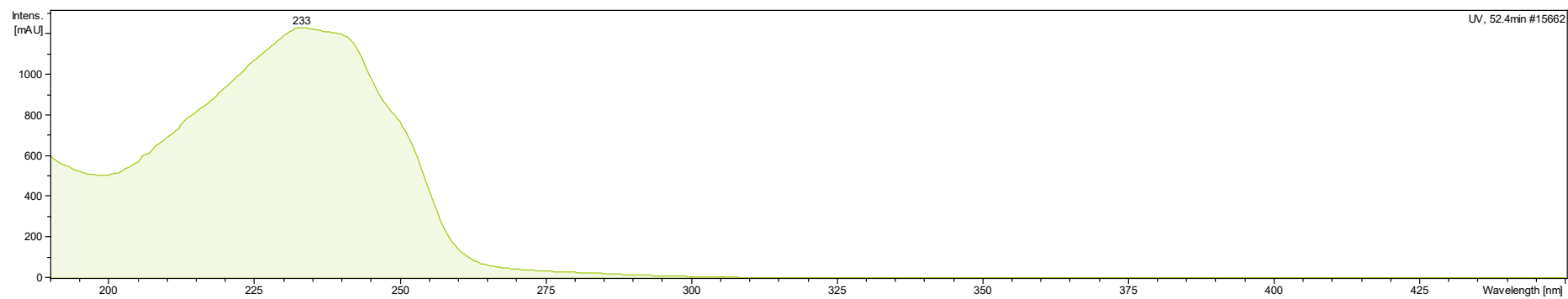


Figure S93. UV spectrum of compound (40).

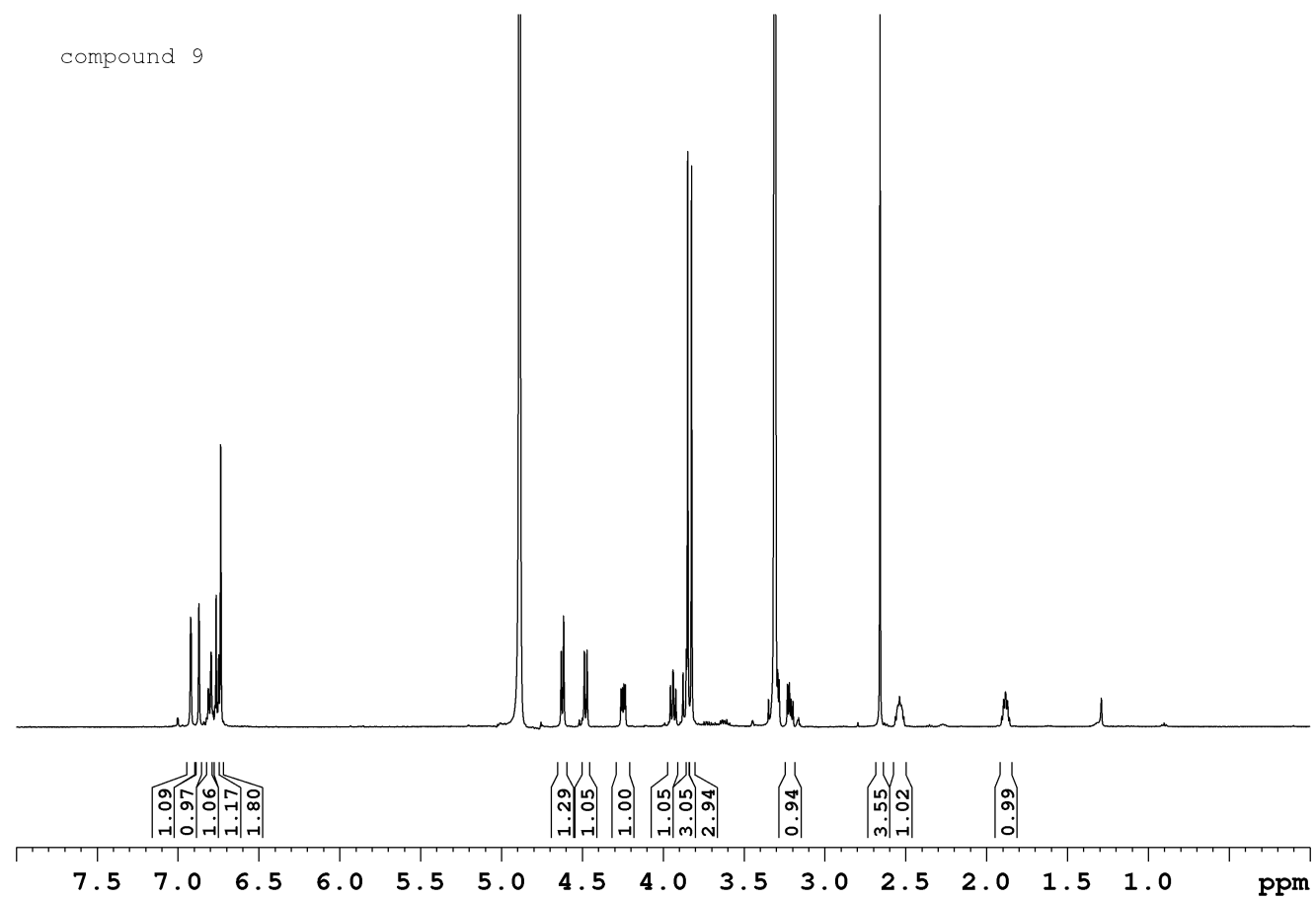


Figure S94. ^1H NMR spectrum of compound (9).

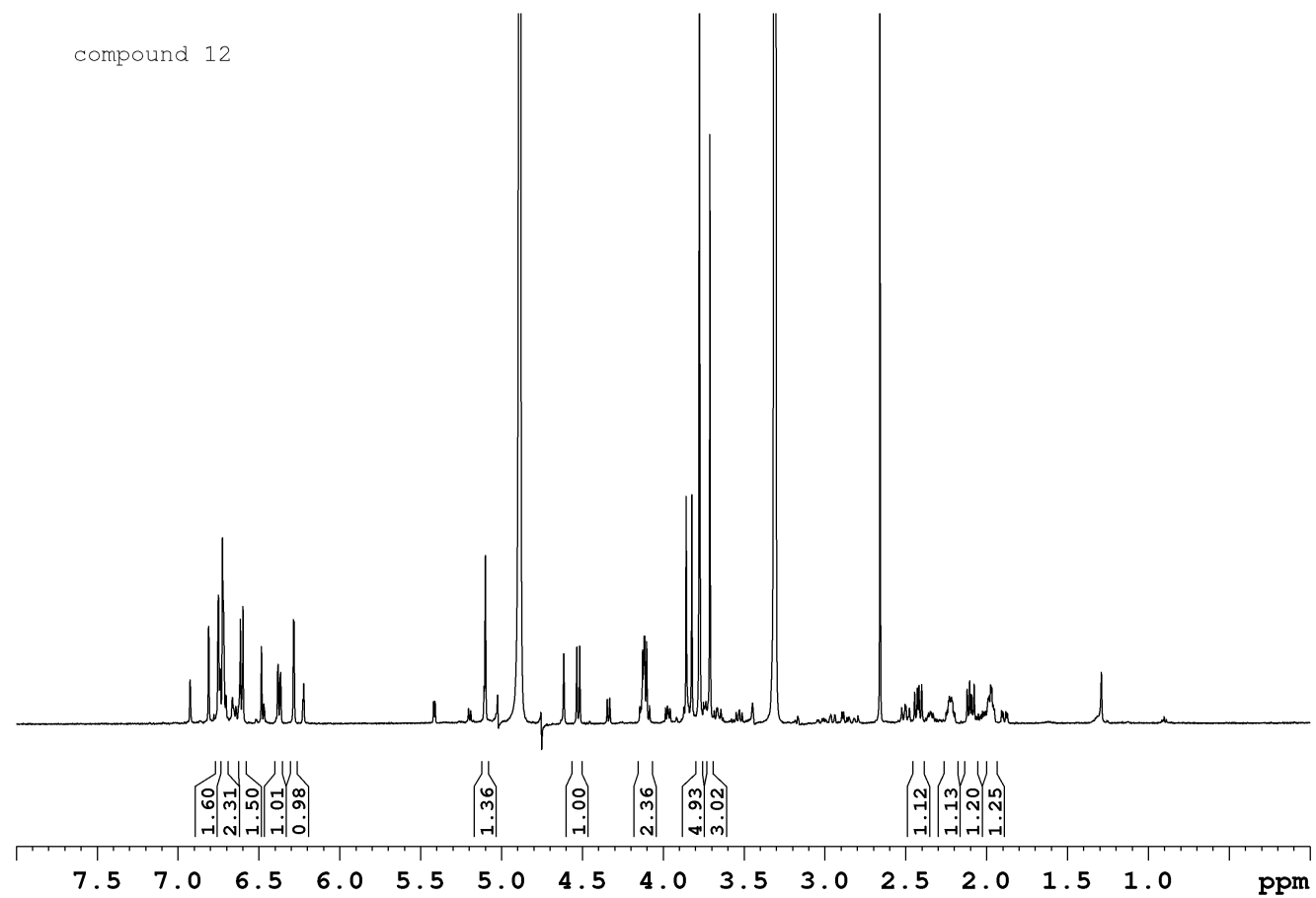


Figure S95. ^1H NMR spectrum of compound (12).

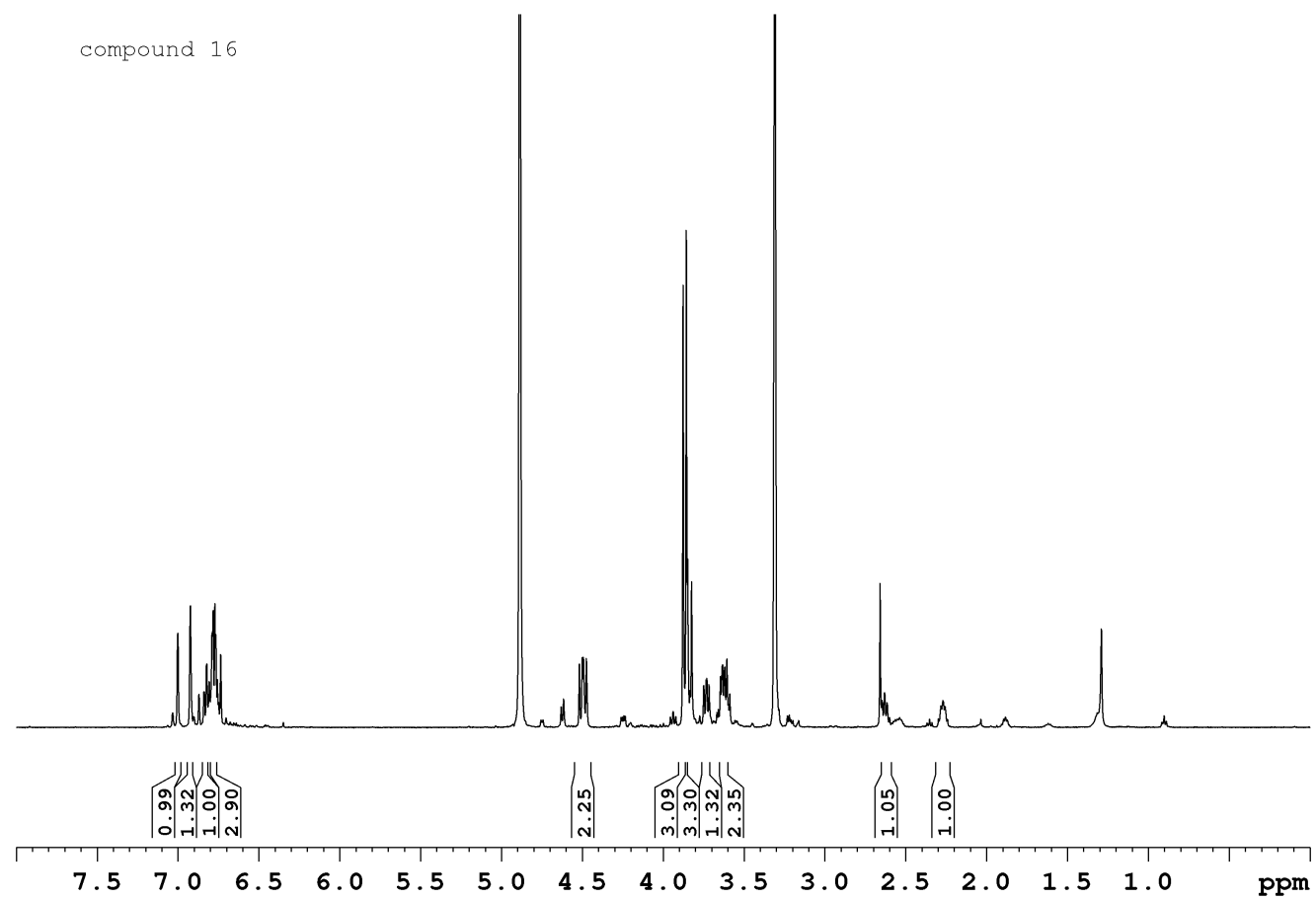


Figure S96. ^1H NMR spectrum of compound (16).

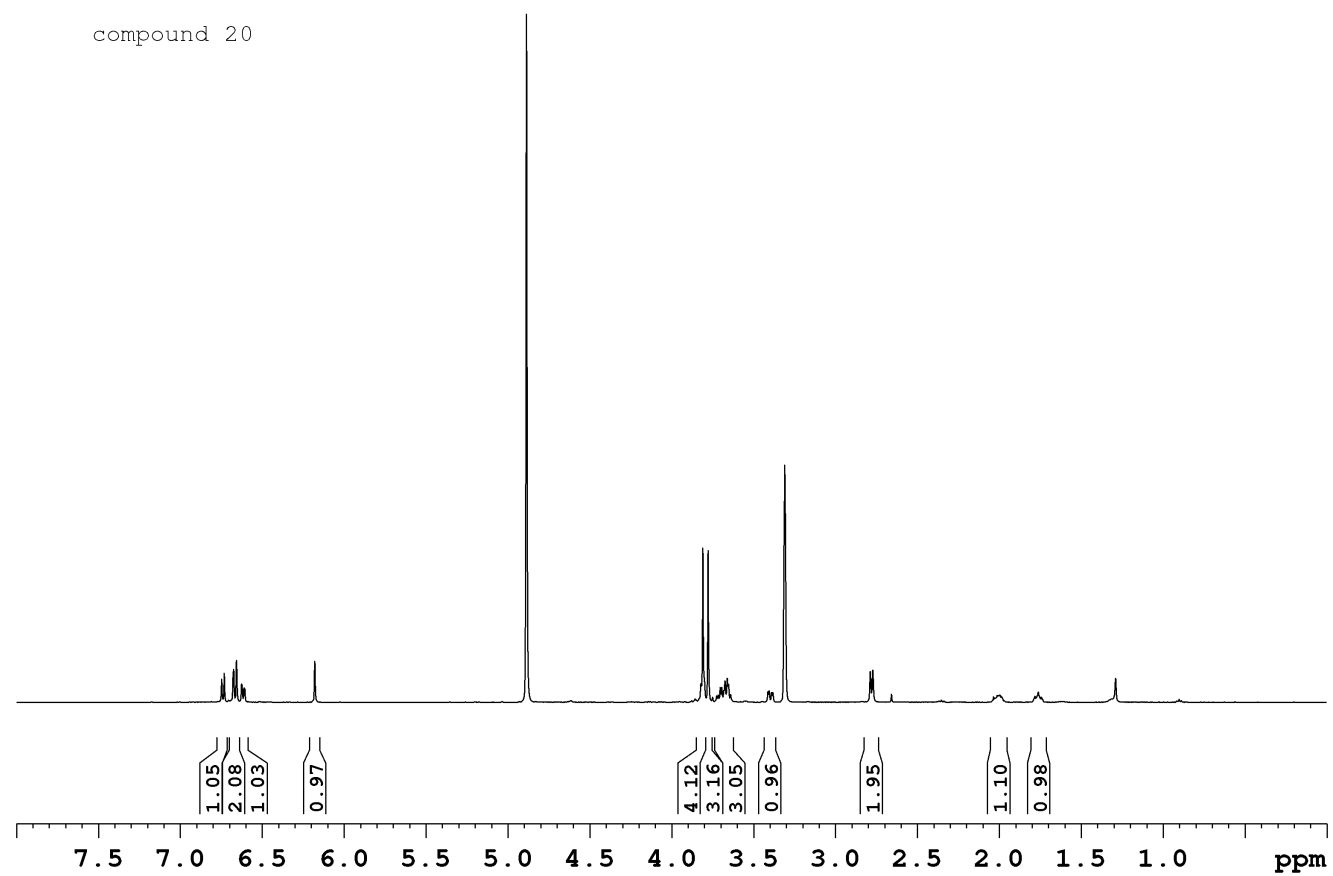


Figure S97. ^1H NMR spectrum of compound (20).

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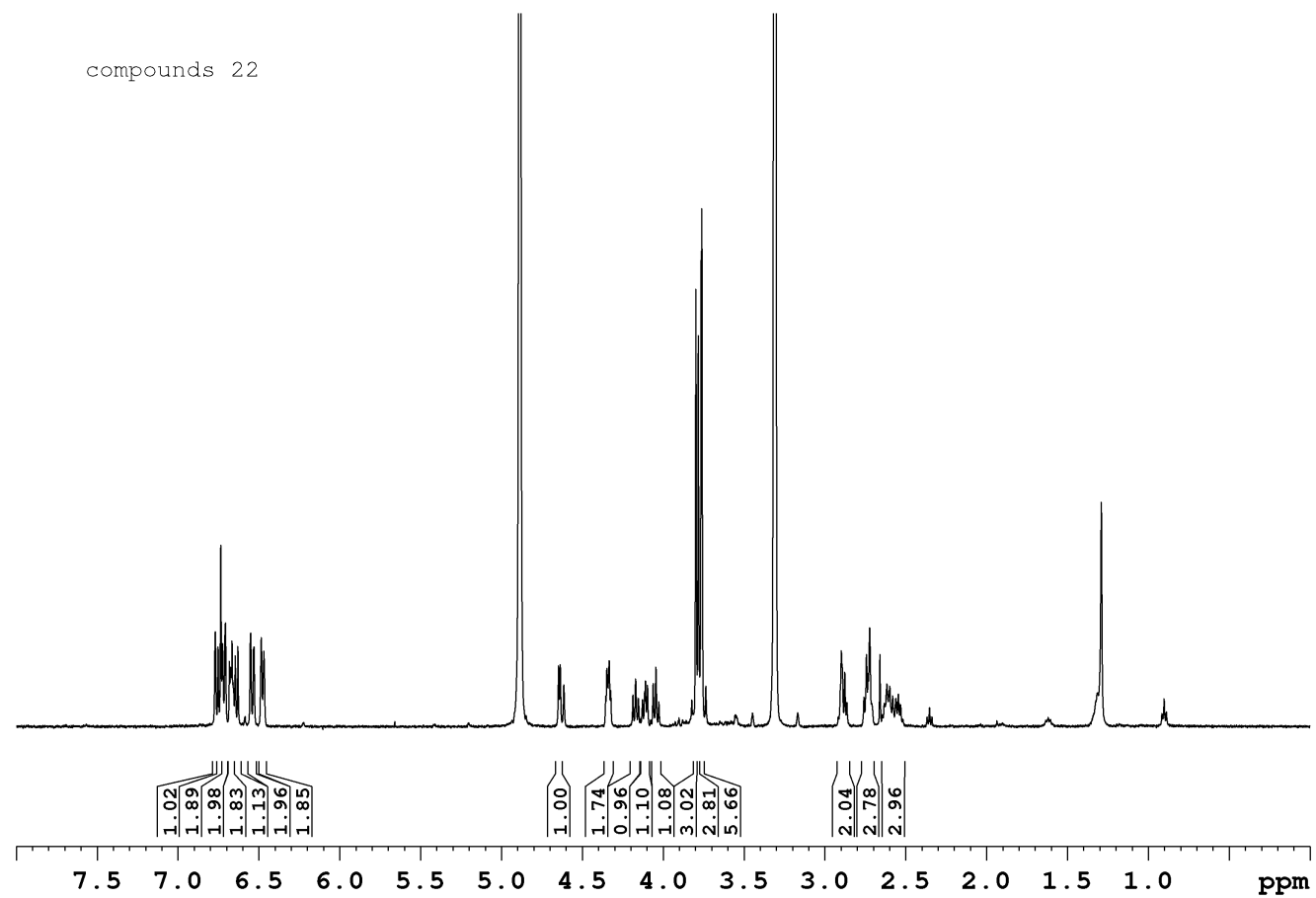


Figure S98. ^1H NMR spectrum of compound (22).

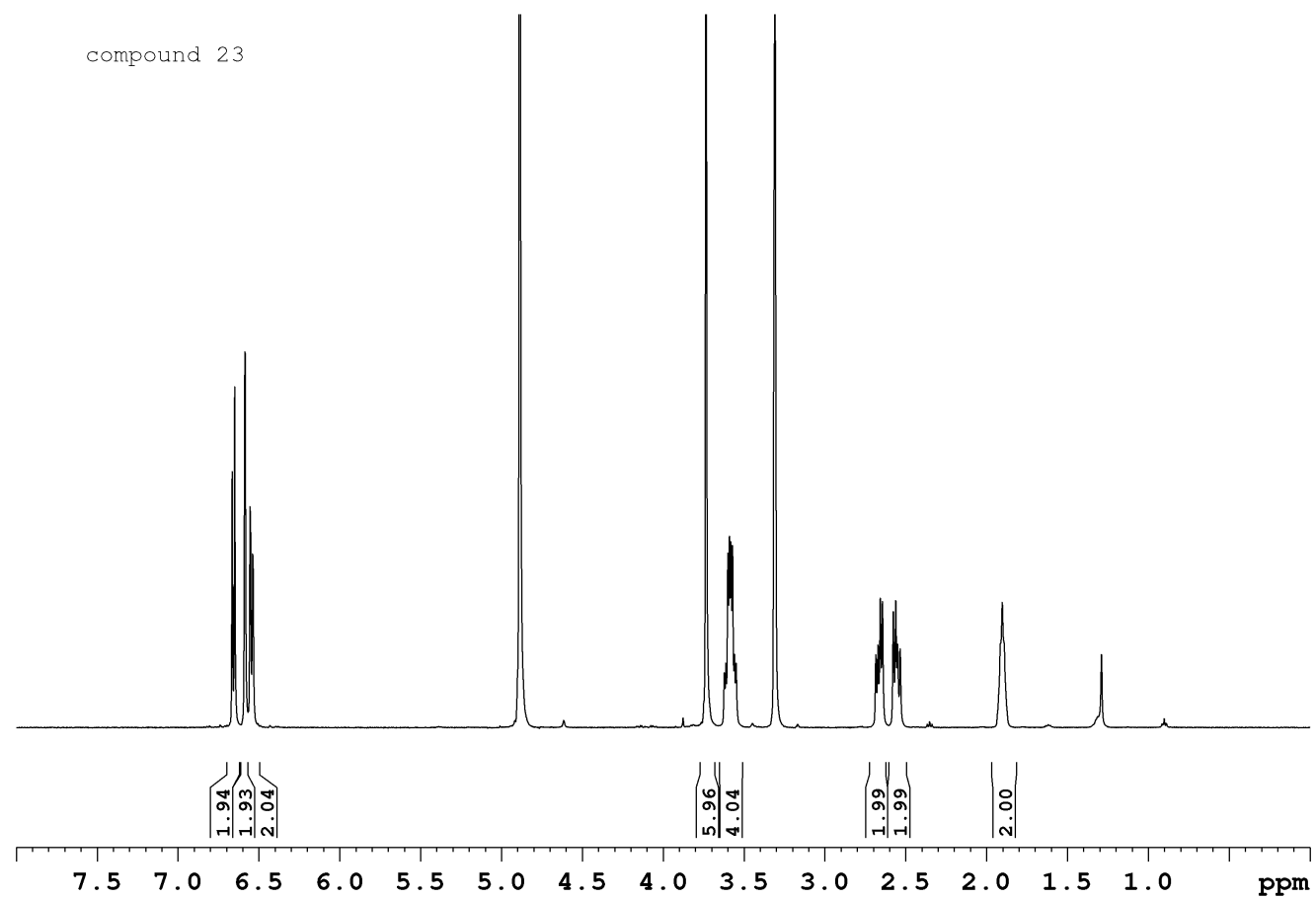


Figure S99. ¹H NMR spectrum of compound (23).

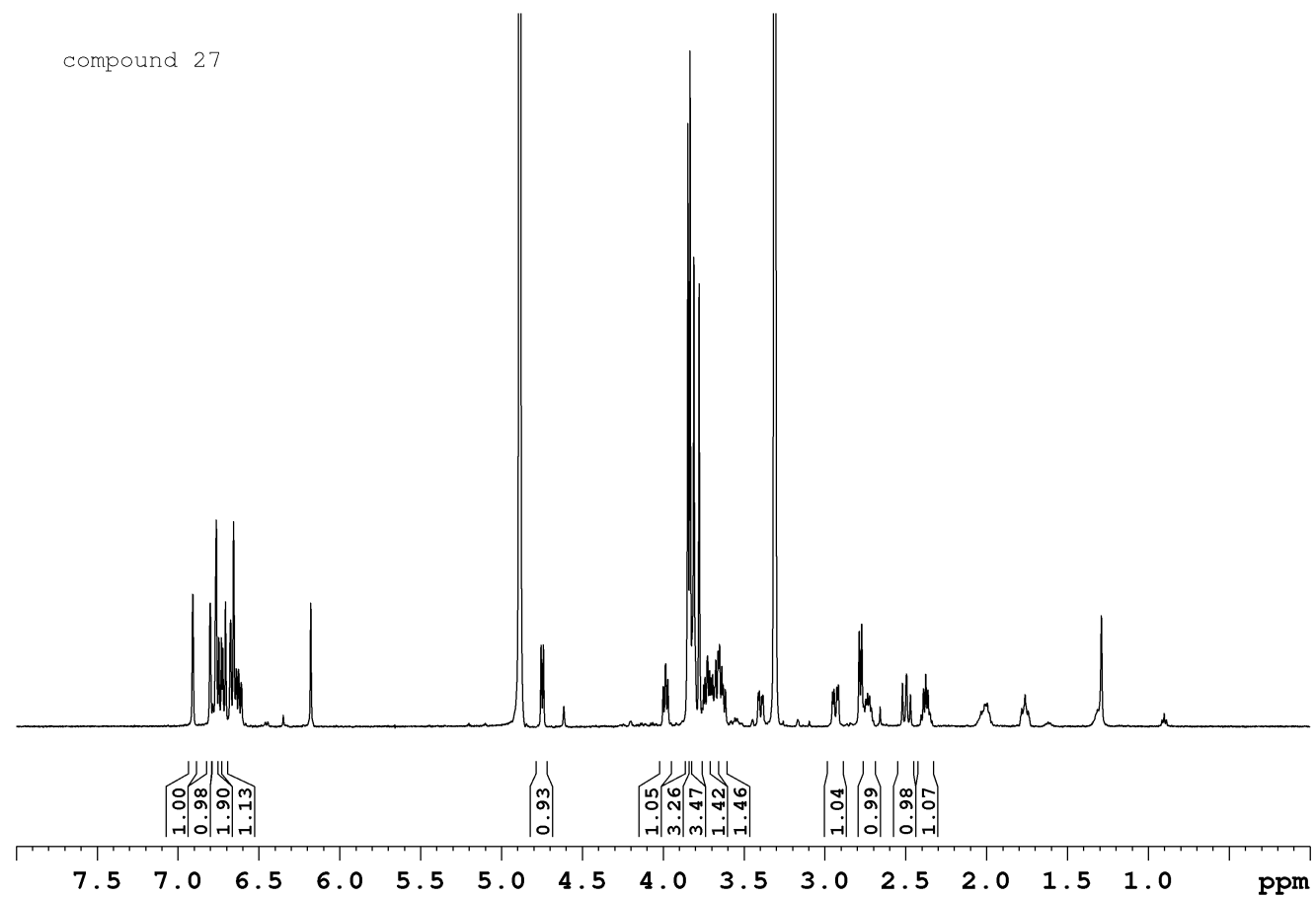


Figure S100. ¹H NMR spectrum of compound (27).

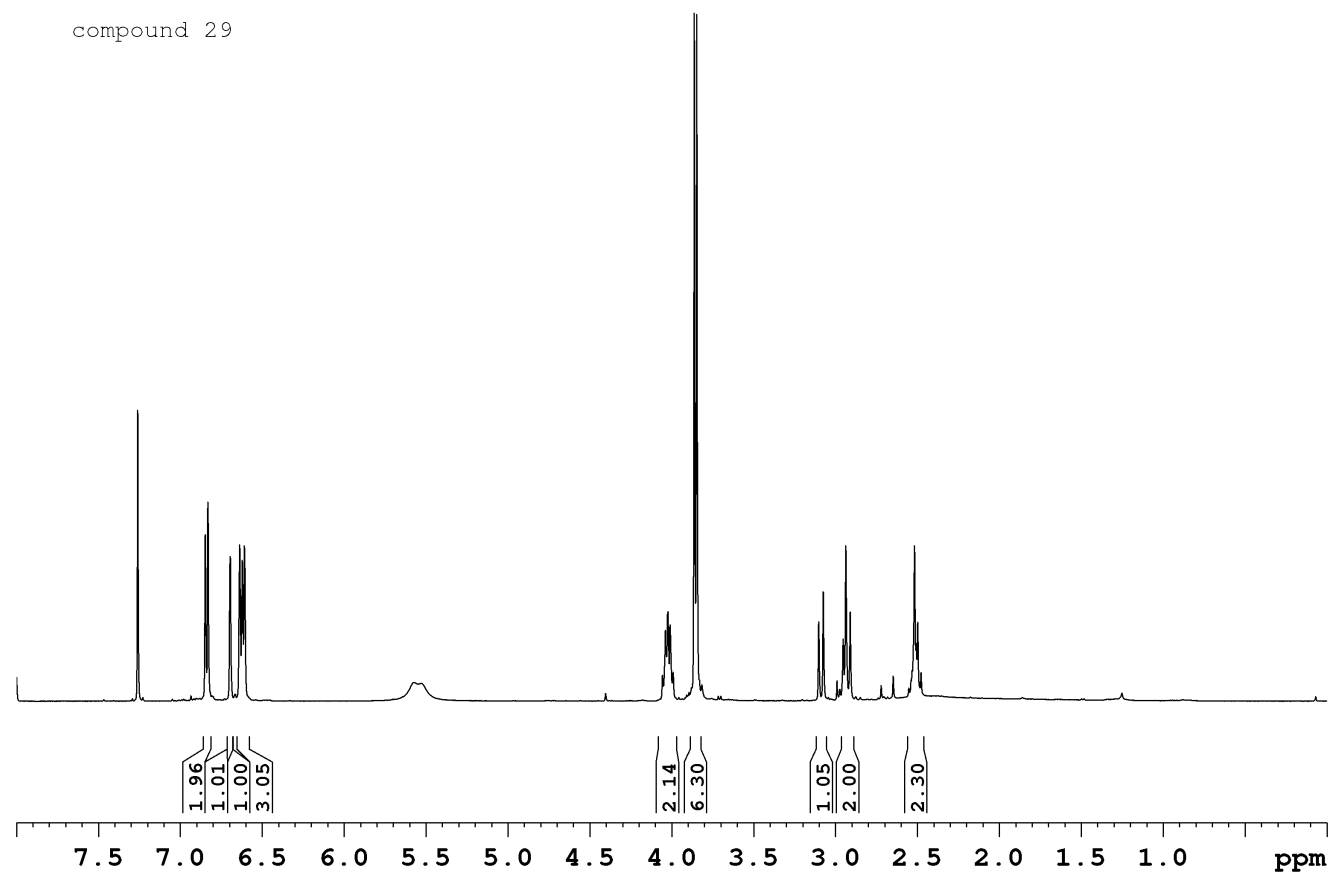


Figure S101. ^1H NMR spectrum of compound (29).

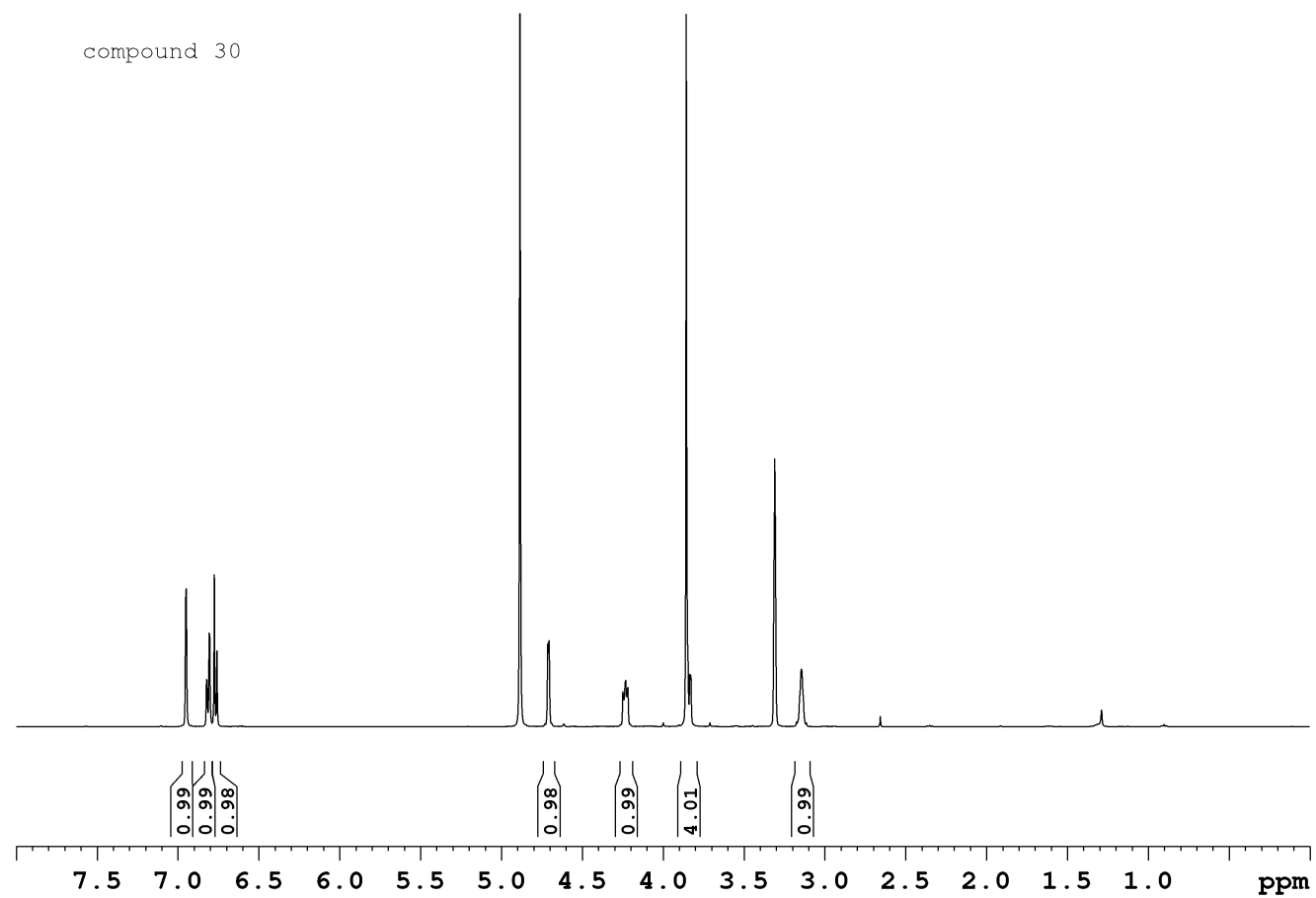


Figure S102. ^1H NMR spectrum of compound (30).

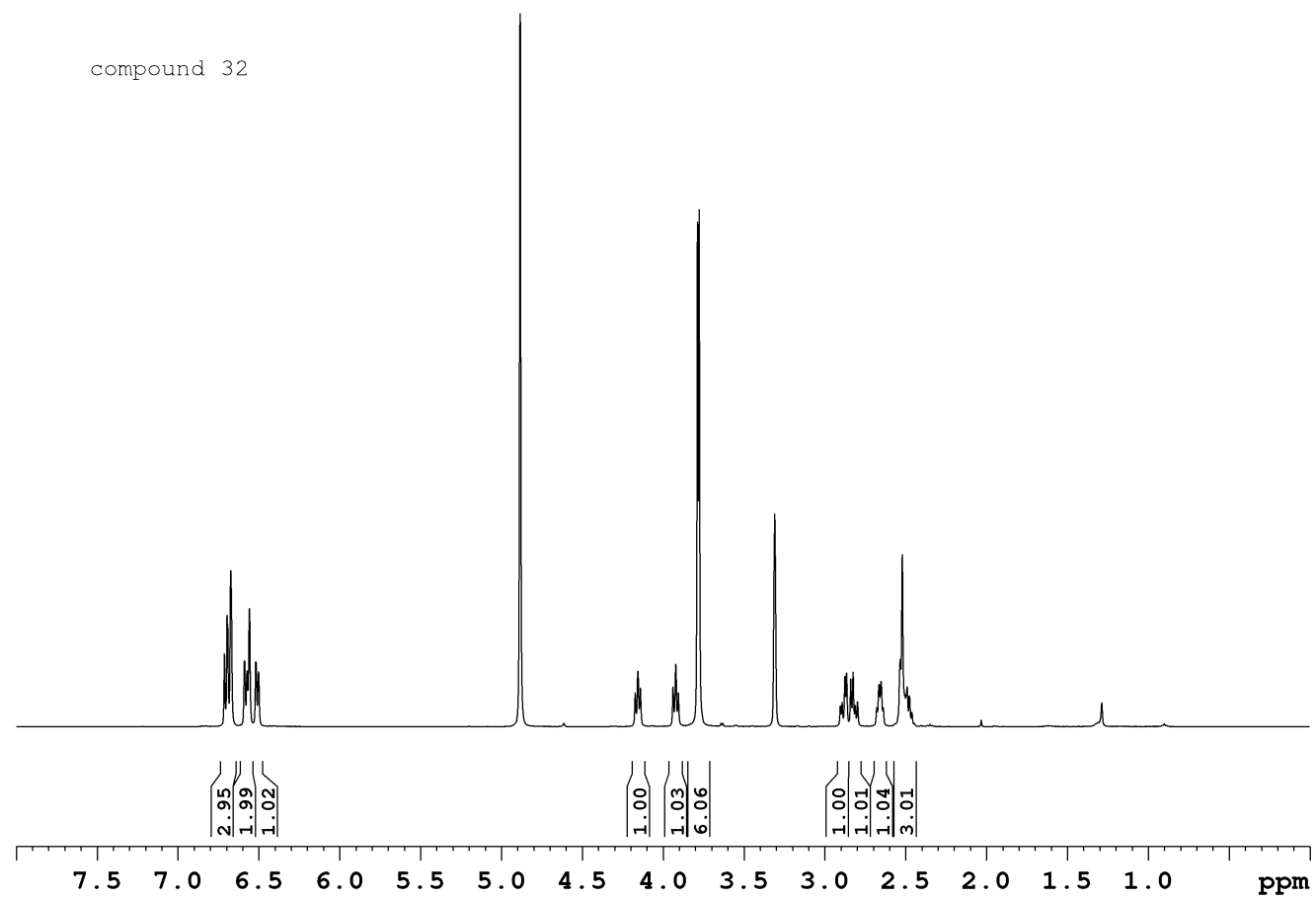


Figure S103. ^1H NMR spectrum of compound (32).

Table S1. ¹H chemical shifts in ppm for compounds **9**, **12**, **16**, **20**, **22**, **23**, **27**, **30** and **32** in methanol-d₄ and **29** in chloroform-d (500 MHz, 295 K).

atom	9	12	16	20	22*	23	27	29	30	32
H2	6.92	6.29	6.92	6.18	6.53; 6.55	6.59	6.91	6.70	6.95	6.67
H5	6.76	6.61	6.78	6.67	6.64; 6.67	6.66	6.77	6.84	6.76	6.71
H6	6.81	6.37	6.80		6.48; 6.48	6.55	6.77	6.63	6.81	6.58
H7a	4.62	2.10	4.51	2.78	2.59; 2.73	2.56	4.75	2.92	4.71	2.82
H7b	-	2.41	-	2.78	2.73; 2.88	2.67	-	3.09	-	2.89
H8	1.88	1.99	2.27	2.00	2.73; 2.90	1.90	2.38	-	3.15	2.66
H9a	3.21	5.10	3.61	3.67	-	3.56	3.63	-	3.84	-
H9b	3.30	-	3.73	3.67	-	3.61	3.83	-	4.23	-
OMe	3.85	3.72	3.86	3.81	3.76; 3.77	3.74	3.85	3.85	3.86	3.79
H2'	6.87	6.75	7.00	6.68	6.71; 6.77	6.59	6.80	6.61	6.95	6.56
H5'	6.74	6.73	6.78	6.74	6.74; 6.74	6.66	6.72	6.84	6.76	6.68
H6'	6.74	6.72	6.83	6.62	6.66; 6.73	6.55	6.65	6.63	6.81	6.51
H7'a	4.48	4.53	4.48	3.81	4.34; 4.64	2.56	2.50	2.51	4.71	2.53
H7'b	-	-	-	-	-	2.67	2.94	2.95	-	2.53
H8'	2.54	2.23	2.63	1.76	2.55; 2.62	1.90	2.74	2.51	3.15	2.49
H9'a	3.94	4.11	3.63	3.40	4.05; 4.17	3.56	3.72	4.01	3.84	3.92
H9'b	4.25	4.11	3.63	3.71	4.11; 4.34	3.61	3.99	4.04	4.23	4.16
OMe'	3.82	3.78	3.88	3.78	3.78; 3.80	3.74	3.83	3.86	3.86	3.78

* isolated as a mixture of diastereoisomers at C7'

Table S2. Canonical SMILES of identified compounds

Compounds	Canonical SMILES
1.	<chem>C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)O</chem>
2.	<chem>C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C(=C5)O)O)O)O)O)C6=CC(=C(C(=C6)O)O)O)O</chem>
3.	<chem>C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C(=C5)O)O)O)O)O)C6=CC(=C(C(=C6)O)O)O)O</chem>
4.	<chem>C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=C(C(=CC(=C34)O)O)C5C(C(OC6=CC(=CC(=C56)O)O)C7=CC(=C(C(=C7)O)O)O)C8=CC(=C(C(=C8)O)O)O)O)O)C9=CC(=C(C(=C9)O)O)O)O</chem>
5.	<chem>C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)O</chem>
6.	<chem>C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C(=C5)O)O)O)O)O)C6=CC(=C(C(=C6)O)O)O)O</chem>
7.	<chem>C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)O</chem>
8.	<chem>C1=C(C=C(C(=C1O)O)O)C2C(C(=O)C3=C(C=C(C(=C3O2)O)O)O)O</chem>
9.	<chem>COC1=C(C=CC(=C1)C2C(C(CO2)C(C3=CC(=C(C(=C3)O)OC)O)CO)O</chem>
10.	<chem>C1=CC(=C(C=C1C=CC2=CC(=CC(=C2)OC3C(C(C(C(O3)CO)O)O)O)O)O)O</chem>
11.	<chem>C1=CC(=CC=C1C2C(C(=O)C3=C(C=C(C(=C3O2)O)O)O)O)O</chem>
12.	<chem>COC1=C(C=CC(=C1)CC2C(COC2O)C(C3=CC(=C(C(=C3)O)OC)O)O</chem>
13.	<chem>C1=CC(=C(C=C1C2C(C(=O)C3=C(C=C(C(=C3O2)OC4C(C(C(C(O4)CO)O)O)O)O)O)O)O)O</chem>
14.	<chem>C1=CC(=C(C=C1C=CC2=CC(=CC(=C2)OC3C(C(C(C(O3)CO)O)O)O)O)O)O</chem>
15.	<chem>C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C(=C5)O)O)O)O)O)C6=CC(=C(C(=C6)O)O)O)O</chem>
16.	<chem>COC1=C(C=CC(=C1)C2C(C(CO2)C(C3=CC(=C(C(=C3)O)OC)O)CO)O</chem>
17.	<chem>C1=CC(=CC=C1C=CC2=CC(=CC(=C2)OC3C(C(C(C(O3)CO)O)O)O)O)O</chem>
18.	<chem>C1=CC(=C(C=C1C2C(C(=O)C3=C(C=C(C(=C3O2)O)O)O)O)O</chem>
19.	<chem>COC1=C(C=CC(=C1)C=CC2=CC(=CC(=C2)OC3C(C(C(C(O3)CO)O)O)O)O)O</chem>
20.	<chem>COC1=C(C=C2C(C(C(CC2=C1)CO)CO)C3=CC(=C(C(=C3)O)OC)O</chem>
21.	<chem>COC1=C(C=C2C(C(C(CC2=C1)C(=O)O)CO)C3=CC(=C(C(=C3)O)OC)O</chem>
22.	<chem>COC1=C(C=CC(=C1)CC2COC(=O)C2C(C3=CC(=C(C(=C3)O)OC)O)O</chem>
23.	<chem>COC1=C(C=CC(=C1)CC(CO)C(CC2=CC(=C(C(=C2)O)OC)CO)O</chem>
24.	<chem>C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC(=C(C(=C3)O)O</chem>
25.	<chem>C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C(=C3O2)O)O)O</chem>
26.	<chem>COC1=C(C=CC(=C1)CC(CO)C(CC2=CC(=C(C(=C2)OC(CO)C(C3=CC(=C(C(=C3)O)OC)O)OC)CO)O</chem>
27.	<chem>COC1=C(C=CC(=C1)CC2COC(C2CO)C3=CC(=C(C(=C3)O)OC)O</chem>
28.	<chem>COC1=C(C=CC(=C1)CC2COC(C2CO)C3=CC(=C(C(=C3)OC(CO)C(C4=CC(=C(C(=C4)O)OC)O)OC)O)O</chem>
29.	<chem>COC1=C(C=C(=C1)CC2COC(=O)C2(CC3=CC(=C(C(=C3)O)OC)O)O</chem>
30.	<chem>COC1=C(C=CC(=C1)C2C3COC(C3CO2)C4=CC(=C(C(=C4)O)OC)O</chem>
31.	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C(=C3O2)O)O)O)O)O</chem>
32.	<chem>COC1=C(C=CC(=C1)CC2COC(=O)C2CC3=CC(=C(C(=C3)O)OC)O</chem>
33.	<chem>C1=CC=C(C=C1)C2C(C(=O)C3=C(C=C(C(=C3O2)O)O)O)O</chem>
34.	<chem>C1=CC=C(C=C1)C=CC2=CC(=CC(=C2)O)O</chem>
35.	<chem>C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=CC=C3</chem>
36.	<chem>CC(=O)OC1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=CC=C3</chem>
37.	<chem>COC1=CC(=CC(=C1)C=CC2=CC=C(C(=C2)O)OC</chem>
38.	<chem>COC1=CC(=CC(=C1)O)C=CC2=CC=CC=C2</chem>

39.	<chem>CC(CC(=O)C=C(C)C)C1CCC(=CC1)C(=O)OC</chem>
40.	<chem>COC1=CC(=CC(=C1)C=CC2=CC=CC=C2)OC</chem>
41.	<chem>CC(=C1CCC2C(=C1)CCC3C2(CCCC3(C)C(=O)O)C)C</chem>
42.	<chem>CC(C)C1=CC2=CCC3C(C2CC1)(CCCC3(C)C(=O)O)C</chem>
