

Supporting Information

Retention time-independent strategy for screening pesticide residues in herbs based on a fingerprint database and all ion fragmentation acquisition with LC-QTOF MS

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Table S1. The fingerprint database of 150 pesticides

Number	Pesticide	CAS No.	Molecular Formula	Element Composition of Qualified Ions	Accurate <i>m/z</i> of Qualified Ions
1	Carbofuran-3-hydroxy	[16655-82-6]	C ₁₂ H ₁₃ NO ₄	C ₁₂ H ₁₅ NO ₄ Na, C ₁₂ H ₁₅ NO ₄ NH ₄ , C ₁₂ H ₁₆ NO ₄ , C ₁₂ H ₁₄ NO ₃ , C ₁₀ H ₁₃ O ₃ , C ₁₀ H ₁₁ O ₂ , C ₉ H ₁₁ O, C ₇ H ₇ O, C ₇ H ₇ , C ₂ H ₄ NO	260.0893, 255.1339, 238.1074, 220.0968, 181.0859, 163.0754, 135.0804, 107.0491, 91.0542, 58.0287
2	Aldicarb	[116-06-3]	C ₇ H ₁₄ N ₂ O ₂ S	C ₇ H ₁₄ N ₂ O ₂ SNa, C ₇ H ₁₄ N ₂ O ₂ SNH ₄ , C ₇ H ₁₅ N ₂ O ₂ S, C ₅ H ₁₀ NS, C ₂ H ₅ NO ₂ Na, C ₄ H ₉ S, C ₄ H ₆ N, C ₂ H ₅ S, C ₂ H ₃ S	213.0668, 208.1114, 191.0849, 116.0528, 98.0212, 89.0419, 68.0495, 61.0106, 58.9950
3	Aldicarb-sulfone	[1646-88-4]	C ₇ H ₁₄ N ₂ O ₄ S	C ₇ H ₁₄ N ₂ O ₄ SNa, C ₇ H ₁₄ N ₂ O ₄ SNH ₄ , C ₇ H ₁₅ N ₂ O ₄ S, C ₅ H ₁₀ NO ₂ S, C ₄ H ₈ NO, CH ₅ O ₂ S, C ₂ H ₆ NO ₂ , CH ₃ OS, C ₃ H ₇ O	245.0566, 240.1013, 223.0747, 148.0427, 86.0600, 81.0005, 76.0393, 62.9899, 59.0491
4	Aldicarb-sulfoxide	[1646-87-3]	C ₇ H ₁₄ N ₂ O ₃ S	C ₇ H ₁₄ N ₂ O ₃ SNa, C ₇ H ₁₄ N ₂ O ₃ SNH ₄ , C ₇ H ₁₅ N ₂ O ₃ S, C ₅ H ₁₀ NOS, C ₄ H ₉ S, C ₄ H ₇ N, CH ₅ O ₂ S, C ₂ H ₄ NO	229.0617, 224.1063, 207.0798, 132.0478, 89.0419, 69.0573, 65.0056, 58.0287
5	Cadusafos	[95465-99-9]	C ₁₀ H ₂₃ O ₂ PS ₂	C ₁₀ H ₂₃ O ₂ PS ₂ Na, C ₁₀ H ₂₃ O ₂ PS ₂ NH ₄ , C ₁₀ H ₂₄ O ₂ PS ₂ , C ₆ H ₁₆ O ₂ PS ₂ , C ₂ H ₈ O ₂ PS ₂ , H ₄ O ₂ PS ₂ , H ₂ O ₂ PS, OPS	293.0769, 288.1215, 271.0952, 215.0324, 158.9698, 130.9385, 96.9508, 78.9402
6	Carbofuran	[1563-66-2]	C ₁₂ H ₁₃ NO ₃	C ₁₂ H ₁₅ NO ₃ Na, C ₁₂ H ₁₅ NO ₃ NH ₄ , C ₁₂ H ₁₆ NO ₃ , C ₁₀ H ₁₃ O ₂ , C ₈ H ₉ O ₂ , C ₇ H ₇ O ₂ , C ₆ H ₅ , C ₄ H ₇	244.0944, 239.1392, 222.1125, 165.0911, 137.0597, 123.0441, 77.0386, 55.0542
7	Chlordimeform	[6164-98-3]	C ₁₀ H ₁₃ ClN ₂	C ₁₀ H ₁₃ ClN ₂ Na, C ₁₀ H ₁₃ ClN ₂ NH ₄ , C ₁₀ H ₁₄ [³⁷ Cl]N ₂ , C ₁₀ H ₁₄ ClN ₂ , C ₈ H ₇ [³⁷ Cl]N, C ₈ H ₇ ClN, C ₇ H ₆ [³⁷ Cl], C ₇ H ₆ Cl, C ₈ H ₇ N, C ₇ H ₆ , C ₇ H ₅	219.0659, 214.1106, 199.0812, 197.084, 154.0233, 152.0262, 127.0124, 125.0153, 117.0573, 90.0462, 89.0386
8	Chlorsulfuron	[64902-72-3]	C ₁₂ H ₁₂ ClN ₃ O ₄ S	C ₁₂ H ₁₂ ClN ₃ O ₄ SNa, C ₁₂ H ₁₂ ClN ₃ O ₄ SNH ₄ , C ₁₂ H ₁₃ [³⁷ Cl]N ₃ O ₄ S, C ₁₂ H ₁₃ ClN ₃ O ₄ S, C ₆ H ₇ N ₄ O ₂ , C ₅ H ₉ N ₄ O, C ₂ H ₄ NO, C ₃ H ₆ N	380.0191, 375.0637, 360.0344, 358.0371, 167.0564, 141.0771, 58.0287, 56.0495
9	Coumaphos	[56-72-4]	C ₁₄ H ₁₆ ClO ₃ PS	C ₁₄ H ₁₆ ClO ₃ PSNa, C ₁₄ H ₁₆ ClO ₃ PSNH ₄ , C ₁₄ H ₁₇ [³⁷ Cl]O ₃ PS, C ₁₄ H ₁₇ ClO ₃ PS, C ₁₀ H ₉ [³⁷ Cl]O ₃ PS, C ₁₀ H ₉ ClO ₃ PS, C ₁₀ H ₈ [³⁷ Cl]O ₂ S, C ₁₀ H ₈ ClO ₂ S, H ₂ O ₂ PS	385.0037, 380.0483, 365.0191, 363.0217, 308.9564, 306.9591, 228.9899, 226.9928, 96.9508
10	Demeton	8065-48-3	C ₈ H ₁₉ O ₃ PS ₂	C ₈ H ₁₉ O ₃ PS ₂ Na, C ₈ H ₁₉ O ₃ PS ₂ NH ₄ , C ₈ H ₂₀ O ₃ PS ₂ , C ₆ H ₁₅ O ₃ PS ₂ Na, C ₄ H ₉ S, C ₂ H ₅ S	281.0405, 276.0851, 259.0586, 253.0092, 89.0419, 61.0106
11	Ethametsulfuron-methyl	[97780-06-8]	C ₁₅ H ₁₈ N ₆ O ₆ S	C ₁₅ H ₁₈ N ₆ O ₆ SNa, C ₁₅ H ₁₈ N ₆ O ₆ SNH ₄ , C ₁₅ H ₁₉ N ₆ O ₆ S, C ₇ H ₁₀ N ₅ O ₂ , C ₅ H ₆ N ₅ O ₂ , C ₃ H ₃ N ₂ O	433.0901, 428.1347, 411.1081, 196.0829, 168.0516, 83.024
12	Ethoprophos	[13194-48-4]	C ₈ H ₁₉ O ₂ PS ₂	C ₈ H ₁₉ O ₂ PS ₂ Na, C ₈ H ₁₉ O ₂ PS ₂ NH ₄ , C ₈ H ₂₀ O ₂ PS ₂ , C ₆ H ₁₆ O ₂ PS ₂ , C ₃ H ₁₀ O ₂ PS ₂ , H ₄ O ₂ PS ₂ , H ₂ O ₂ PS, OPS	265.0456, 260.0902, 243.0637, 215.0324, 172.9854, 130.9385, 96.9508, 78.9402

13	Fenamiphos	[22224-92-6]	C ₁₃ H ₂₂ NO ₃ PS	C13H22NO3PSNa,C13H22NO3PSNH4,C13H23NO3PS,C11H19NO3PS,C8H13NO3PS, C8H10O3PS,C7H7O3PS,C7H6OS	326.095,321.1396,304.1131,276.0816,234.0348,217.0083,201.9848, 138.0134
14	Fenamiphos-sulfone	[31972-44-8]	C ₁₃ H ₂₂ NO ₃ PS	C13H22NO5PSNa,C13H22NO5PSNH4,C13H23NO5PS,C11H19NO5PS,C8H13NO5PS, C7H11NO3P,C7H8O,C7H7	358.0849,353.1296,336.1029,308.0716,266.0247,188.0471,108.057,91.0542
15	Fenamiphos-sulfoxide	[31972-43-7]	C ₁₃ H ₂₂ NO ₄ PS	C13H22NO4PSNa,C13H22NO4PSNH4,C13H23NO4PS,C11H19NO4PS,C8H10O4PS, C8H11O2S,C7H8O2S,C7H8O,H3NO2P	342.0899,337.1345,320.108,292.0767,233.0032,171.0474,156.024,108.057, 79.9896
16	Fonofos	[944-22-9]	C ₁₀ H ₁₅ OPS ₂	C10H15OPS2Na,C10H15OPS2NH4,C10H16OPS2,C4H10OPS,C2H6OPS,H2OPS,PS	269.0194,264.064,247.0375,137.0184,108.9871,80.9558,62.9453
17	Isazofos	[42509-80-8]	C ₉ H ₁₇ CIN ₃ O ₃ PS	C9H17CIN3O3PSNa,C9H17CIN3O3PSNH4,C9H18[37C1]N3O3PS,C9H18CIN3O3PS, C5H9[37C1]N3O,C5H9CIN3O,C2H3[37C1]N3O,C2H3CIN3O,H2O2PS	336.0309,331.0755,316.0461,314.049,164.04,162.0429,121.993,119.9959, 96.9508
18	Isocarbophos	[24353-61-5]	C ₁₁ H ₁₆ NO ₄ PS	C11H16NO4PSNa,C11H16NO4PSNH4,C11H17NO4PS,C8H10NO4PSNa,C8H8NO4PNa, C8H8O4PS,C7H5O2,H2O2PS	312.043,307.0876,290.061,269.996,236.0083,230.9875,121.0284,96.9508
19	Isofenphos-methyl	[99675-03-3]	C ₁₄ H ₂₂ NO ₄ PS	C14H22NO4PSNa,C14H22NO4PSNH4,C14H23NO4PS,C11H16NO4PSNa,C8H7O4PSNa, C8H8O4PS,C8H9NO4P,C7H8O3P,C7H5O2,C5H5	354.0899,349.1345,332.108,312.043,252.9695,230.9875,214.0264,171.0206, 121.0284,65.0386
20	Methamidophos	[10265-92-6]	C ₂ H ₈ NO ₂ PS	C2H8NO2PSNa,C2H8NO2PSNH4,C2H9NO2PS,C2H6O2PS,CH5NO2P,H3NO2P,CH4O2P, H3NOP	163.9906,159.0352,142.0086,124.9821,94.0052,79.9896,78.9943,63.9947
21	Metsulfuron-methyl	[74223-64-6]	C ₁₄ H ₁₅ N ₃ O ₆ S	C14H15N5O6SNa,C14H15N5O6SNH4,C14H16N5O6S,C8H7O4S,C6H7N4O2,C8H7O2,C6H5, C3H6N	404.0635,399.1071,382.0816,199.006,167.0564,135.0441,77.0386,56.0495
22	Monocrotophos	[6923-22-4]	C ₇ H ₁₄ NO ₃ P	C7H14NO5PNa,C7H14NO5PNH4,C7H15NO5P,C6H10O5P,C2H8O4P,C2H6O3P,C5H8NO, C2H4NO	246.0502,241.0948,224.0682,193.026,127.0155,109.0049,98.06,58.0287
23	Phorate	[298-02-2]	C ₇ H ₁₇ O ₂ PS ₃	C7H17O2PS3Na,C7H17O2PS3NH4,C7H18O2PS3,C4H10O2PS,CH4O2PS2,H2O2PS,C3H7S	283.002,278.0467,261.0201,153.0134,142.9385,96.9508,75.0263
24	Phorate-sulfone	[2588-04-7]	C ₇ H ₁₇ O ₄ PS ₃	C7H17O4PS3Na,C7H17O4PS3NH4,C7H18O4PS3,C6H16O4PS2,C4H12O3PS,C2H8O3PS, H4O3PS,H2O2PS	314.9919,310.0365,293.0099,247.0222,171.0239,142.9926,114.9613, 96.9508
25	Phorate-sulfoxide	[2588-03-6]	C ₇ H ₁₇ O ₃ PS ₃	C7H17O3PS3Na,C7H17O3PS3NH4,C7H18O3PS3,C5H12O2PS2,C3H8O2PS2,CH4O2PS2, H2O2PS,H2O2P	298.997,294.0416,277.015,199.0011,170.9698,142.9385,96.9508,64.9787

26	Phosfolan	[947-02-4]	C ₇ H ₁₄ NO ₃ PS ₂	C7H14NO3PS2Na,C7H14NO3PS2NH4,C7H15NO3PS2,C5H11NO3PS2,CH3NO3PS,C2H5S, CH2NS	278.0045,273.0491,256.0225,227.9912,139.9566,61.0106,59.9902,
27	Phosphamidon	[13171-21-6]	C ₁₀ H ₁₉ CINO ₃ P	C10H19CINO5PNa,C10H19CINO5PNH4,C10H20[37Cl]NO5P,C10H20CINO5P, C8H13[37Cl]NO,C8H13CINO,C2H8O4P,C2H6O3P,C5H10NO,C3H6NO	322.0582,317.1028,302.0737,300.0762,176.0652,174.068,127.0155, 109.0049,100.0757,72.0444
28	Sulfotep	[3689-24-5]	C ₈ H ₂₀ O ₃ P ₂ S ₂	C8H20O5P2S2Na,C8H20O5P2S2NH4,C8H21O5P2S2,C6H17O5P2S2,C4H12O3PS, C2H8O3PS,H4O3PS,H2O2PS	345.012,340.0566,323.03,294.9987,171.0239,142.9926,114.9613,96.9508
29	Terbufos-sulfone	[56070-16-7]	C ₉ H ₂₁ O ₄ PS ₃	C9H21O4PS3Na,C9H21O4PS3NH4,C9H22O4PS3,C4H12O3PS,C2H8O3PS,H4O3PS,H2O2PS	343.0232,338.0678,321.0412,171.0239,142.9926,114.9613,96.9508
30	Terbufos-sulfoxide	[10548-10-4]	C ₉ H ₂₁ O ₃ PS ₃	C9H21O3PS3Na,C9H21O3PS3NH4,C9H22O3PS3,C4H12O2PS2,C2H8O2PS2,H4O2PS2, H2O2PS,C4H9	327.0283,322.0729,305.0463,187.0011,158.9698,130.9385,96.9508,57.0699
31	Acetamidrid	[135410-20-7]	C ₁₀ H ₁₁ CIN ₄	C10H11CIN4Na,C10H11CIN4NH4,C10H12[37Cl]N4,C10H12CIN4,C6H5[37Cl]N,C6H5CIN, C5H4[37Cl],C5H4Cl,C6H4N,C3H6N	245.0564,240.101,225.0717,223.0745,128.0076,126.0105,100.9967,98.9996, 90.0338,56.0495
32	Bitertanol	[55179-31-2]	C ₂₀ H ₂₃ N ₃ O ₂	C20H23N3O2Na,C20H23N3O2NH4,C20H24N3O2,C18H21O2,C6H11O,C2H4N3,C4H9	360.1682,355.2129,338.1863,269.1536,99.0804,70.04,57.0699
33	Carbaryl	[63-25-2]	C ₁₂ H ₁₁ NO ₂	C12H11NO2Na,C12H11NO2NH4,C12H12NO2,C10H9O,C10H7,C9H9,C9H7,C6H5	224.0682,219.1128,202.0863,145.0648,127.0542,117.0699,115.0542, 77.0386
34	Carbendazim	[10605-21-7]	C ₉ H ₉ N ₃ O ₂	C9H9N3O2Na,C9H9N3O2NH4,C9H10N3O2,C8H6N3O,C7H6N3,C6H5N2,C5H5	214.0587,209.1033,192.0768,160.0505,132.0556,105.0447,65.0386
35	Clofentazine	[74115-24-5]	C ₁₄ H ₈ Cl ₂ N ₄	C14H8Cl2N4Na,C14H8Cl2N4NH4,C14H9Cl[37Cl]N4,C14H9Cl2N4,C7H5[37Cl]N,C7H5CIN, C7H4N,C6H3	325.0018,320.0464,305.0171,303.0199,140.0076,138.0105,102.0338, 75.0229
36	Diethofencarb	[87130-20-9]	C ₁₄ H ₂₁ NO ₄	C14H21NO4Na,C14H21NO4NH4,C14H22NO4,C11H16NO4,C10H14NO2,C8H10NO2, C6H6NO2,C5H5O2,C5H6N	290.1363,285.1809,268.1543,226.1074,180.1019,152.0706,124.0393, 97.0284,80.0496
37	Diflubenzuron	[35367-38-5]	C ₁₄ H ₉ ClF ₂ N ₂ O ₂	C14H9ClF2N2O2Na,C14H9ClF2N2O2NH4,C14H10[37Cl]F2N2O2,C14H10ClF2N2O2, C7H6F2NO,C7H3F2O,C6H3F2	333.0213,328.0659,313.0368,311.0393,158.0412,141.0146,113.0197
38	Dimethomorph	[110488-70-5]	C ₂₁ H ₂₂ CINO ₄	C21H22CINO4Na,C21H22CINO4NH4,C21H23[37Cl]NO4,C21H23CINO4,C17H14[37Cl]O3, C17H14ClO3,C9H9O3,C3H4NO	410.113,405.1576,390.1289,388.131,303.0602,301.0626,165.0546,70.0287
39	Flusilazole	[85509-19-9]	C ₁₆ H ₁₅ F ₂ N ₃ Si	C16H15F2N3SiNa,C16H15F2N3SiNH4,C16H16F2N3Si,C14H13F2Si,C12H9F2Si,C8H8FN3, C7H6F	338.0896,333.1342,316.1076,247.0749,219.0436,165.0697,109.0448

40	Forchlorfenuron	[68157-60-8]	C ₁₂ H ₁₀ ClN ₃ O	C12H10ClN3ONa,C12H10ClN3ONH4,C12H11[37Cl]N3O,C12H11ClN3O,C5H6[37Cl]N2, C5H6ClN2,C5H5N2,C4H4N	270.0405,265.0851,250.0559,248.0585,131.0185,129.0214,93.0447,66.0338
41	Haloxypop-methyl	[69806-40-2]	C ₁₆ H ₁₃ ClF ₃ NO ₄	C16H13ClF3NO4Na,C16H13ClF3NO4NH4,C16H14[37Cl]F3NO4,C16H14ClF3NO4, C14H10[37Cl]F3NO2,C14H10ClF3NO2,C13H10[37Cl]F3NO,C13H10ClF3NO, C12H6[37Cl]F3NO,C12H6ClF3NO,C7H7	398.0377,393.0823,378.0534,376.0558,318.0321,316.0347,290.0368, 288.0398,274.0055,272.0085,91.0542
42	Hexythiazox	[78587-05-0]	C ₁₇ H ₂₁ ClN ₂ O ₂ S	C17H21ClN2O2SNa,C17H21ClN2O2SNH4,C17H22[37Cl]N2O2S,C17H22ClN2O2S, C10H11[37Cl]NOS,C10H11ClNOS,C9H11[37Cl]N,C9H11ClN,C9H8,C9H7	375.0904,370.1351,355.1056,353.1085,230.0215,228.0244,170.0546, 168.0575,116.0621,115.0542
43	Imidacloprid	[138261-41-3]	C ₉ H ₁₀ ClN ₃ O ₂	C9H10ClN3O2Na,C9H10ClN3O2NH4,C9H11[37Cl]N3O2,C9H11ClN3O2,C9H10[37Cl]N4, C9H10ClN4,C9H11N4,C9H9N4,C6H5N2	278.0415,273.0861,258.0569,256.0596,211.0559,209.0589,175.0978, 173.0822,105.0447
44	Indoxacarb	[144171-61-9]	C ₂₂ H ₁₇ ClF ₃ N ₃ O ₇	C22H17[37Cl]F3N3O7Na,C22H17ClF3N3O7Na,C22H17ClF3N3O7NH4, C22H18[37Cl]F3N3O7,C22H18ClF3N3O7,C13H10[37Cl]N2O4,C13H10ClN2O4,C9H7F3NO2, C8H4F3NO2,C8H5[37Cl]N,C8H5ClN,C2H2NO	552.057,550.0599,545.1045,530.0761,528.078,295.0294,293.0324,218.0423, 203.0189,152.0076,150.0105,56.0131
45	Kresoxim-methyl	[143390-89-0]	C ₁₈ H ₁₉ NO ₄	C18H19NO4Na,C18H19NO4NH4,C18H20NO4,C17H16NO3,C17H15O3,C15H13NO, C15H12NO,C14H12N,C13H10N,C14H10,C8H6N	336.1206,331.1652,314.1387,282.1125,267.1016,223.0992,222.0913, 194.0964,180.0808,178.0777,116.0495,
46	Metalaxyl	[57837-19-1]	C ₁₅ H ₂₁ NO ₄	C15H21NO4Na,C15H21NO4NH4,C15H22NO4,C14H18NO3,C13H18NO2,C12H18NO, C11H14N,C10H14N,C9H12N,C9H10N	302.1363,297.1809,280.1543,248.1281,220.1332,192.1383,160.1121, 148.1121,134.0964,132.0808
47	Omethoate	[1113-02-6]	C ₃ H ₁₂ NO ₄ PS	C5H12NO4PSNa,C5H12NO4PSNH4,C5H13NO4PS,C4H8O4PS,C3H8O3PS,C2H6O2PS, C2H6O3P,CH4O2P	236.0117,231.0563,214.0297,182.9875,154.9926,124.9821,109.0049, 78.9943
48	Phoxim	[14816-18-3]	C ₁₂ H ₁₅ N ₂ O ₃ PS	C12H15N2O3PSNa,C12H15N2O3PSNH4,C12H16N2O3PS,C8H5N2,C2H6O2PS,H2O2PS, C6H5	321.0433,316.0879,299.0614,129.0447,124.9821,96.9508,77.0386
49	Prochloraz	[67747-09-5]	C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	C15H16Cl3N3O2Na,C15H16Cl3N3O2NH4,C15H17Cl2[37Cl]N3O2,C15H17Cl3N3O2, C12H13Cl2[37Cl]NO2,C12H13Cl3NO2,C5H11N,C3H4NO,C3H6N	398.02,393.0646,378.0353,376.0381,309.9978,308.0006,85.0886,70.0287, 56.0495
50	Prompamocarb	[24579-73-5]	C ₉ H ₂₀ N ₂ O ₂	C9H20N2O2Na,C9H20N2O2NH4,C9H21N2O2,C7H14NO2,C4H8NO2,C2H4NO2,C3H8N	211.1417,206.1863,189.1598,144.1019,102.055,74.0237,58.0651
51	Pymetrozine	[123312-89-0]	C ₁₀ H ₁₁ N ₃ O	C10H11N3ONa,C10H11N3ONH4,C10H12N3O,C6H5N2,C5H5N,C5H4N	240.0856,235.1302,218.1036,105.0447,79.0417,78.0338
52	Spinosad	[168316-95-8]	C ₄₁ H ₆₅ NO ₁₀	C41H65NO10Na,C41H65NO10NH4,C41H66NO10,C8H16NO,C6H12N,C3H7O2	754.4501,749.4947,732.4681,142.1226,98.0964,75.0441

53	Thiabendazole	[148-79-8]	C ₁₀ H ₇ N ₃ S	C10H7N3SNa,C10H7N3SNH4,C10H8N3S,C9H7N2S,C8H7N2,C5H5	224.0253,219.0699,202.0433,175.0324,131.0604,65.0386
54	Thiamethoxam	[153719-23-4]	C ₈ H ₁₀ ClN ₅ O ₃ S	C8H10ClN5O3SNa,C8H10ClN5O3SNH4,C8H11[37Cl]N5O3S,C8H11ClN5O3S,C8H11N4OS, C7H9N4S,C6H6N3S,C4H3ClNS,C5H6N3	314.0085,309.0531,294.0237,292.0266,211.0658,181.0542,152.0277, 131.9669,108.0556
55	Tolfenpyrad	[129558-76-5]	C ₂₁ H ₂₂ ClN ₅ O ₂	C21H22ClN5O2Na,C21H22ClN5O2NH4,C21H23[37Cl]N5O2,C21H23ClN5O2,C14H13O, C12H10,C6H10[37Cl]N2,C6H10ClN2,C7H7	406.1293,401.1739,386.1452,384.1473,197.0961,154.0777,147.0498, 145.0527,91.0542
56	Azoxystrobin	[131860-33-8]	C ₂₂ H ₁₇ N ₅ O ₅	C22H17N5O5Na,C22H17N5O5NH4,C22H18N3O5,C21H14N3O4,C20H14N3O3, C19H11N3O3,C11H7N2O,C10H6NO2,C10H6NO	426.106,421.1506,404.1241,372.0979,344.103,329.0795,183.0553,172.0393, 156.0444
57	Boscalid	[188425-85-6]	C ₁₈ H ₁₂ Cl ₂ N ₂ O	C18H12Cl2N2O2Na,C18H12Cl2N2ONH4,C18H13Cl[37Cl]N2O,C18H13Cl2N2O, C18H12[37Cl]N2O,C18H12ClN2O,C18H12N2O,C18H11N2O,C5H4N	365.0219,360.0665,345.0373,343.0399,309.0609,307.0633,272.0944, 271.0866,78.0338
58	Buprofezin	[69327-76-0]	C ₁₆ H ₂₃ N ₃ OS	C16H23N3OSNa,C16H23N3OSNH4,C16H24N3OS,C9H17N2OS,C7H8N,C4H9	328.1454,323.19,306.1635,201.1056,106.0651,57.0699
59	Carbosulfan	[55285-14-8]	C ₂₀ H ₃₂ N ₂ O ₃ S	C20H32N2O3SNa,C20H32N2O3SNH4,C20H33N2O3S,C8H18NS,C5H12NS,C2H6NS,C4H9	403.2026,398.2472,381.2206,160.1154,118.0685,76.0219,57.0699
60	Clothianidin	[210880-92-5]	C ₆ H ₈ ClN ₅ O ₂ S	C6H8ClN5O2SNa,C6H8ClN5O2SNH4,C6H9[37Cl]N5O2S,C6H9ClN5O2S,C6H9N4S, C4H3[37Cl]NS,C4H3ClNS,C4H5N2S,C3H3S	271.9979,267.0425,252.013,250.016,169.0542,133.9638,131.9669,113.0168, 70.995
61	Cymoxanil	[57966-95-7]	C ₇ H ₁₀ N ₄ O ₃	C7H10N4O3Na,C7H10N4O3NH4,C7H11N4O3,C4H6N3O2,C4H3N2O2,C3H3N2O,C2HN2	221.0645,216.1091,199.0826,128.0455,111.0189,83.024,53.0134
62	Cyromazine	[66215-27-8]	C ₆ H ₁₀ N ₆	C6H10N6Na,C6H10N6NH4,C6H11N6,C2H5N4,C2H2N3,CH6N3,C3H6N	189.0859,184.1305,167.104,85.0509,68.0243,60.0556,56.0495
63	Fenpropimorph	[67564-91-4]	C ₂₀ H ₃₃ NO	C20H33NONa,C20H33NONH4,C20H34NO,C11H15,C10H12,C9H9,C4H9	326.2454,321.29,304.2635,147.1168,132.0934,117.0699,57.0699
64	Flutriafol	[76674-21-0]	C ₁₆ H ₁₃ N ₃ OF ₂	C16H13N3OF2Na,C16H13N3OF2NH4,C16H14N3OF2,C7H4FO,C6H4F,C2H4N3	324.0919,319.1365,302.1099,123.0241,95.0292,70.04
65	Maleic hydrazide	[123-33-1]	C ₄ H ₄ N ₂ O ₂	C4H4N2O2Na,C4H4N2O2NH4,C4H5N2O2,C3H5N2O,C4H8N,C3H3N2,C2H5N2,C3HO	135.0165,130.0611,113.0346,85.0396,70.0651,67.0291,57.0447,53.0022
66	Novaluron	[116714-46-6]	C ₁₇ H ₉ ClF ₈ N ₂ O ₄	C17H9ClF8N2O4Na,C17H9ClF8N2O4NH4,C17H10[37Cl]F8N2O4,C17H10ClF8N2O4, C7H6F2NO,C7H3F2O	515.0015,510.0461,495.0173,493.0196,158.0412,141.0146
67	Spirodiclofen	[148477-71-8]	C ₂₁ H ₂₄ Cl ₂ O ₄	C21H24Cl2O4Na,C21H24Cl2O4NH4,C21H25Cl[37Cl]O4,C21H25Cl2O4,C15H15Cl[37Cl]O3, C15H15Cl2O3,C15H13Cl[37Cl]O2,C15H13Cl2O2,C9H3Cl[37Cl]O2,C9H3Cl2O2, C8H3Cl[37Cl]O,C8H3Cl2O,C5H11	433.0944,428.139,413.1099,411.1124,315.0366,313.0393,297.026,295.0287, 214.9476,212.9505,186.9527,184.9555,71.0855

68	Spirotetramat	[203313-25-1]	C ₂₁ H ₂₇ NO ₅	C21H27NO5Na,C21H27NO5NH4,C21H28NO5,C20H28NO3,C18H24NO3,C17H20NO2, C13H14NO2,C11H13	396.1781,391.2227,374.1962,330.2064,302.1751,270.1489,216.1019, 145.1012
69	Thiacloprid	[111988-49-9]	C ₁₀ H ₉ ClN ₄ S	C10H9ClN4SNa,C10H9ClN4SNH4,C10H10[37Cl]N4S,C10H10ClN4S,C6H5[37Cl]N, C6H5ClN,C5H4[37Cl],C5H4Cl,C6H4N	275.0129,270.0575,255.028,253.0309,128.0076,126.0105,100.9967,98.9996, 90.0338
70	Thiophanate-methyl	[23564-05-8]	C ₁₂ H ₁₄ N ₄ O ₄ S ₂	C12H14N4O4S2Na,C12H14N4O4S2NH4,C12H15N4O4S2,C11H11N4O3S2,C9H6N3OS2, C7H7N2S,C6H7N,C2H4NS	365.0349,360.0795,343.0529,311.0267,235.9947,151.0324,93.0573,74.0059
71	Trichlorfon	[52-68-6]	C ₄ H ₈ Cl ₃ O ₄ P	C4H8Cl3O4PNa,C4H8Cl3O4PNH4,C4H9Cl[37Cl]2O4P,C4H9Cl2[37Cl]O4P,C4H9Cl3O4P, C4H8Cl[37Cl]O4P,C4H8Cl2O4P,C2H6O3P,CHCl[37Cl],CHCl2,CH4O2P	278.9118,273.9564,260.9242,258.927,256.9299,222.9503,220.9532, 109.0049,84.942,82.945,78.9943
72	Zoxamide	[156052-68-5]	C ₁₄ H ₁₆ Cl ₃ NO ₂	C14H16Cl3NO2Na,C14H16Cl3NO2NH4,C14H17Cl[37Cl]2NO2,C14H17Cl2[37Cl]NO2, C14H17Cl3NO2,C8H5Cl[37Cl]O,C8H5Cl2O,C7H5Cl[37Cl],C7H5Cl2	358.0139,353.0585,340.0265,338.0291,336.0319,188.9683,186.9712, 160.9734,158.9763
73	Amidosulfuron	[120923-37-7]	C ₉ H ₁₃ N ₅ O ₇ S ₂	C9H15N5O7S2Na,C9H15N5O7S2NH4,C9H16N5O7S2,C7H9N4O5S,C6H8N3O4S,C5H5N3O2, C2HN2O	392.0305,387.0751,370.0486,261.0288,218.023,139.0376,69.0083
74	Benfuracarb	[82560-54-1]	C ₂₀ H ₃₀ N ₂ O ₅ S	C20H30N2O5SNa,C20H30N2O5SNH4,C20H31N2O5S,C12H14NO3S,C10H11O2S, C10H10O2,C8H16NO2	433.1768,428.2214,411.1948,252.0689,195.0474,162.0675,158.1176
75	Bensulfuron-methyl	[83055-99-6]	C ₁₆ H ₁₈ N ₄ O ₇ S	C16H18N4O7SNa,C16H18N4O7SNH4,C16H19N4O7S,C7H8N3O3,C9H9O2,C8H7O,C7H7	433.0788,428.1234,411.0969,182.056,149.0597,119.0491,91.0542
76	Bifenazate	[149877-41-8]	C ₁₇ H ₂₀ N ₂ O ₃	C17H20N2O3Na,C17H20N2O3NH4,C17H21N2O3,C13H12NO,C12H12N,C11H10N,C12H9, C12H8	323.1366,318.1812,301.1547,198.0913,170.0964,156.0808,153.0699, 152.0621
77	Chlorantraniliprole	[500008-45-7]	C ₁₈ H ₁₄ BrCl ₂ N ₃ O ₂	C18H14BrCl2N3O2Na,C18H14BrCl2N3O2NH4,C18H15[81Br]Cl[37Cl]N3O2, C18H15[81Br]Cl2N3O2,C18H15BrCl2N3O2,C17H10[81Br]Cl[37Cl]N4O2, C17H10[81Br]Cl2N4O2,C17H10BrCl2N4O2,C9H4[81Br][37Cl]N3O,C9H4[81Br]ClN3O, C9H4BrClN3O,C8H4[37Cl]N3,C8H4ClN3,C5H3[37Cl]N,C5H3ClN	503.96,499.0046,485.9734,483.9758,481.9781,454.9312,452.9336,450.9359, 287.9713,285.9199,283.9221,179.006,177.0088,113.9919,111.9949
78	Chlorimuron-ethyl	[90982-32-4]	C ₁₅ H ₁₅ ClN ₄ O ₆ S	C15H15ClN4O6SNa,C15H15ClN4O6SNH4,C15H16[37Cl]N4O6S,C15H16ClN4O6S, C6H5[37Cl]N3O2,C6H5ClN3O2,C7H5O4S,C7H5O2,C3H3N2O	437.0293,432.0739,417.0449,415.0474,188.0037,186.0065,184.9903, 121.0284,83.024
79	Chlorobenzuron	[57160-47-1]	C ₁₄ H ₁₀ N ₂ O ₂ Cl ₂	C14H10N2O2Cl2Na,C14H10N2O2Cl2NH4,C14H11N2O2Cl[37Cl],C14H11N2O2Cl2, C7H7[37Cl]NO,C7H7ClNO,C7H4[37Cl]O,C7H4ClO,C6H4[37Cl],C6H4Cl	331.0012,326.0458,311.0165,309.0192,158.0182,156.0211,140.9917, 138.9945,112.9967,110.9996

80	Chlorotoluron	[15545-48-9]	C ₁₀ H ₁₃ ClN ₂ O	C10H13ClN2ONa,C10H13ClN2ONH4,C10H14[37Cl]N2O,C10H14ClN2O,C7H7[37Cl]N, C7H7ClN,C6H5,C3H6NO,C2H2NO	235.0609,230.1055,215.0762,213.0789,142.0233,140.0262,77.0386,72.0444, 56.0131
81	Diafenthuron	[80060-09-9]	C ₂₃ H ₃₂ N ₂ OS	C23H32N2OSNa,C23H32N2OSNH4,C23H33N2OS,C19H25N2OS,C16H19N2OS,C19H20NO, C16H14NO	407.2128,402.2574,385.2308,329.1682,287.1213,278.1539,236.107
82	Fenpyroximate	[111812-58-9]	C ₂₄ H ₂₇ N ₃ O ₄	C24H27N3O4Na,C24H27N3O4NH4,C24H28N3O4,C20H20N3O4,C12H13N3O,C6H8N3O, C8H7O2,C7H7O	444.1894,439.234,422.2074,366.1448,215.1053,138.0662,135.0441, 107.0491
83	Imidaclothiz	[105843-36-5]	C ₇ H ₈ ClN ₃ O ₂ S	C7H8ClN3O2SNa,C7H8ClN3O2SNH4,C7H9[37Cl]N3O2S,C7H9ClN3O2S,C7H9N4S, C7H8N4S,C6H9N3,C6H8N3,C4H5N3	283.9979,279.0425,264.0131,262.016,181.0542,180.0464,123.0791, 122.0713,95.0478
84	Monosulfuron	[155860-63-2]	C ₁₂ H ₁₁ N ₃ O ₃ S	C12H11N3O3SNa,C12H11N3O3SNH4,C12H12N3O3S,C6H6N3O,C5H8N3,C5H5N2	360.0373,355.0819,338.0554,136.0505,110.0713,93.0447
85	Prothioconazole	[178928-70-6]	C ₁₄ H ₁₅ Cl ₂ N ₃ OS	C14H15Cl2N3OSNa,C14H15Cl2N3OSNH4,C14H16Cl[37Cl]N3OS,C14H16Cl2N3OS, C14H14Cl[37Cl]N3S,C14H14Cl2N3S,C12H10[37Cl],C12H10Cl,C12H10,C7H6[37Cl],C7H6Cl, C2H2N3S	366.0205,361.0651,346.0357,344.0386,328.0251,326.028,191.0438, 189.0466,154.0777,127.0124,125.0153,102.012
86	Pyraclostrobin	[175013-18-0]	C ₁₉ H ₁₈ N ₃ O ₄ Cl	C19H18N3O4ClNa,C19H18N3O4ClNH4,C19H19N3O4[37Cl],C19H19N3O4Cl,C10H12NO3, C9H10NO2,C9H9NO2,C8H7NO2,C8H7NO,C7H7N	410.0878,405.1324,390.1037,388.1059,194.0812,164.0706,163.0628, 149.0471,133.0522,105.0573
87	Acephate	[30560-19-1]	C ₄ H ₁₀ NO ₃ PS	C4H10NO3PSNa,C4H10NO3PSNH4,C4H11NO3PS,C2H8O3PS,C2H6O2PS,CH4O3P, CH5NO2P,CH4O2P,H2O2P,H3NOP	206.0011,201.0457,184.0192,142.9926,124.9821,94.9893,94.0052,78.9943, 64.9787,63.9947
88	Bupirimate	[41483-43-6]	C ₁₃ H ₂₄ N ₄ O ₃ S	C13H24N4O3SNa,C13H24N4O3SNH4,C13H25N4O3S,C11H20N3O,C8H12N3O,C2H6NO2S, C5H8NO,C5H6NO	339.1461,334.1907,317.1642,210.1601,166.0975,108.0114,98.0587,96.0444
89	Chlorpyrifos-methyl	[5598-13-0]	C ₇ H ₇ Cl ₃ NO ₃ PS	C7H7Cl3NO3PSNa,C7H7Cl3NO3PSNH4,C7H8Cl[37Cl]2NO3PS,C7H8Cl2[37Cl]NO3PS, C7H8Cl3NO3PS,C6H4Cl[37Cl]2NO2PS,C6H4Cl2[37Cl]NO2PS,C6H4Cl3NO2PS,C2H6O2PS, CH4O2P	343.8842,338.9288,325.8964,323.8993,321.9023,293.8701,291.8731, 289.876,124.9821,78.9943
90	Cyprodinil	[121552-61-2]	C ₁₄ H ₁₅ N ₃	C14H15N3Na,C14H15N3NH4,C14H16N3,C7H10N,C6H7N,C6H5	248.1158,243.1604,226.1339,108.0808,93.0573,77.0386
91	Diazinon	[333-41-5]	C ₁₂ H ₂₁ N ₂ O ₃ PS	C12H21N2O3PSNa,C12H21N2O3PSNH4,C12H22N2O3PS,C10H18N2O3PS,C8H13N2S, C8H13N2O,H2O2PS,C5H5N2	327.0903,322.1349,305.1083,277.077,169.0794,153.1022,96.9508,93.0447

92	Dichlorvos	[62-73-7]	C ₄ H ₇ Cl ₂ O ₄ P	C ₄ H ₇ Cl ₂ O ₄ PNa, C ₄ H ₇ Cl ₂ O ₄ PNH ₄ , C ₄ H ₈ Cl[37Cl]O ₄ P, C ₄ H ₈ Cl ₂ O ₄ P, C ₂ H ₈ O ₄ P, C ₂ H ₆ O ₃ P, C ₂ HCl[37Cl], C ₂ HCl ₂ , CH ₄ O ₂ P, C ₂ H[37Cl], C ₂ HCl	242.9351, 237.9797, 222.9503, 220.9532, 127.0155, 109.0049, 96.942, 94.945, 78.9943, 61.9732, 59.9761
93	Epoxiconazole	[133855-98-8]	C ₁₇ H ₁₃ ClFN ₃ O	C ₁₇ H ₁₃ ClFN ₃ ONa, C ₁₇ H ₁₃ ClFN ₃ ONH ₄ , C ₁₇ H ₁₄ [37Cl]FN ₃ O, C ₁₇ H ₁₄ ClFN ₃ O, C ₇ H ₄ FO, C ₈ H ₆ F, C ₈ H ₅	352.0623, 347.1069, 332.078, 330.0804, 123.0241, 121.0448, 101.0386
94	Imazalil	[35554-44-0]	C ₁₄ H ₁₄ Cl ₂ N ₂ O	C ₁₄ H ₁₄ Cl ₂ N ₂ ONa, C ₁₄ H ₁₄ Cl ₂ N ₂ ONH ₄ , C ₁₄ H ₁₅ Cl[37Cl]N ₂ O, C ₁₄ H ₁₅ Cl ₂ N ₂ O, C ₇ H ₅ Cl[37Cl], C ₇ H ₅ Cl ₂ , C ₃ H ₅ N ₂	319.0375, 314.0821, 299.0528, 297.0556, 160.9734, 158.9763, 69.0447
95	Malathion	[121-75-5]	C ₁₀ H ₁₉ O ₆ PS ₂	C ₁₀ H ₁₉ O ₆ PS ₂ Na, C ₁₀ H ₁₉ O ₆ PS ₂ NH ₄ , C ₁₀ H ₂₀ O ₆ PS ₂ , C ₈ H ₁₄ O ₅ PS ₂ , C ₆ H ₇ O ₃ , C ₂ H ₆ O ₂ PS, C ₄ H ₃ O ₃	353.0253, 348.0699, 331.0433, 285.0015, 127.039, 124.9821, 99.0077
96	Metolachlor	[51218-45-2]	C ₁₅ H ₂₂ ClNO ₂	C ₁₅ H ₂₂ ClNO ₂ Na, C ₁₅ H ₂₂ ClNO ₂ NH ₄ , C ₁₅ H ₂₃ [37Cl]NO ₂ , C ₁₅ H ₂₃ ClNO ₂ , C ₁₄ H ₁₉ [37Cl]NO, C ₁₄ H ₁₉ ClNO, C ₁₂ H ₁₈ N, C ₉ H ₁₂ N, C ₉ H ₁₁ N, C ₇ H ₇	306.1231, 301.1677, 286.1387, 284.1412, 254.1124, 252.115, 176.1434, 134.0964, 133.0886, 91.0542
97	Napropamide	[15299-99-7]	C ₁₇ H ₂₁ NO ₂	C ₁₇ H ₂₁ NO ₂ Na, C ₁₇ H ₂₁ NO ₂ NH ₄ , C ₁₇ H ₂₂ NO ₂ , C ₁₃ H ₁₁ O ₂ , C ₁₂ H ₁₁ O, C ₇ H ₁₅ NO, C ₄ H ₁₀ N, C ₃ H ₈ N, C ₃ H ₅ O	294.1465, 289.1911, 272.1645, 199.0754, 171.0804, 129.1148, 72.0808, 58.0651, 57.0335
98	Oxadixyl	[77732-09-3]	C ₁₄ H ₁₈ N ₂ O ₄	C ₁₄ H ₁₈ N ₂ O ₄ Na, C ₁₄ H ₁₈ N ₂ O ₄ NH ₄ , C ₁₄ H ₁₉ N ₂ O ₄ , C ₁₂ H ₁₅ N ₂ O ₂ , C ₉ H ₁₁ N, C ₉ H ₁₀ N, C ₈ H ₇ N, C ₄ H ₈ NO ₂	301.1159, 296.1605, 279.1339, 219.1128, 133.0886, 132.0808, 117.0573, 102.055
99	Phosalone	[2310-17-0]	C ₁₂ H ₁₅ ClNO ₄ PS ₂	C ₁₂ H ₁₅ ClNO ₄ PS ₂ Na, C ₁₂ H ₁₅ ClNO ₄ PS ₂ NH ₄ , C ₁₂ H ₁₆ [37Cl]NO ₄ PS ₂ , C ₁₂ H ₁₆ ClNO ₄ PS ₂ , C ₈ H ₅ [37Cl]NO ₂ , C ₈ H ₅ ClNO ₂ , C ₇ H ₅ [37Cl]N, C ₇ H ₅ ClN, C ₆ H ₄ [37Cl], C ₆ H ₄ Cl, C ₇ H ₄ N	389.9761, 385.0207, 369.9913, 367.9941, 183.9976, 182.0003, 140.0076, 138.0105, 112.9967, 110.9996, 102.0338
100	Pirimiphos-methyl	[29232-93-7]	C ₁₁ H ₂₀ N ₃ O ₃ PS	C ₁₁ H ₂₀ N ₃ O ₃ PSNa, C ₁₁ H ₂₀ N ₃ O ₃ PSNH ₄ , C ₁₁ H ₂₁ N ₃ O ₃ PS, C ₉ H ₁₄ N ₃ , C ₅ H ₆ N ₃ , C ₃ H ₃ N ₂	328.0855, 323.1301, 306.1036, 164.1182, 108.0556, 67.0291
101	Propanil	[709-98-8]	C ₉ H ₉ NOCl ₂	C ₉ H ₉ NOCl ₂ Na, C ₉ H ₉ NOCl ₂ NH ₄ , C ₉ H ₁₀ NOCl[37Cl], C ₉ H ₁₀ NOCl ₂ , C ₆ H ₆ Cl[37Cl]N, C ₆ H ₆ Cl ₂ N, C ₆ H ₆ [37Cl]N, C ₆ H ₆ ClN, C ₆ H ₆ N, C ₃ H ₅ O	239.9953, 235.0399, 220.0105, 218.0134, 163.9843, 161.9872, 129.0154, 127.0183, 92.0495, 57.0335
102	Propiconazole	[60207-90-1]	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂ Na, C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂ NH ₄ , C ₁₅ H ₁₈ Cl[37Cl]N ₃ O ₂ , C ₁₅ H ₁₈ Cl ₂ N ₃ O ₂ , C ₇ H ₅ Cl[37Cl], C ₇ H ₅ Cl ₂ , C ₅ H ₉	364.059, 359.1036, 344.0744, 342.0771, 160.9734, 158.9763, 69.0699
103	Triadimenol	[55219-65-3]	C ₁₄ H ₁₈ N ₃ O ₂ Cl	C ₁₄ H ₁₈ N ₃ O ₂ ClNa, C ₁₄ H ₁₈ N ₃ O ₂ ClNH ₄ , C ₁₄ H ₁₉ N ₃ O ₂ [37Cl], C ₁₄ H ₁₉ N ₃ O ₂ Cl, C ₆ H ₁₁ O, C ₆ H ₅ , C ₂ H ₄ N ₃	318.098, 313.1426, 298.1135, 296.116, 99.0804, 77.0386, 70.04
104	Triazophos	[24017-47-8]	C ₁₂ H ₁₆ N ₃ O ₃ PS	C ₁₂ H ₁₆ N ₃ O ₃ PSNa, C ₁₂ H ₁₆ N ₃ O ₃ PSNH ₄ , C ₁₂ H ₁₇ N ₃ O ₃ PS, C ₈ H ₈ N ₃ O, C ₇ H ₇ N ₂ , H ₂ O ₂ PS	336.0542, 331.0988, 314.0723, 162.0662, 119.0604, 96.9508
105	Benalaxyl	[71626-11-4]	C ₂₀ H ₂₃ NO ₃	C ₂₀ H ₂₃ NO ₃ Na, C ₂₀ H ₂₃ NO ₃ NH ₄ , C ₂₀ H ₂₄ NO ₃ , C ₁₉ H ₂₀ NO ₂ , C ₁₂ H ₁₈ NO ₂ , C ₁₀ H ₁₄ N, C ₇ H ₇	348.157, 343.2016, 326.1751, 294.1489, 208.1332, 148.1121, 91.0542

106	Cyproconazole	[94361-06-5]	C ₁₅ H ₁₈ ClN ₃ O	C15H18ClN3ONa,C15H18ClN3ONH4,C15H19[37Cl]N3O,C15H19ClN3O,C7H6[37Cl], C7H6Cl,C2H4N3	314.1031,309.1477,294.1186,292.1211,127.0124,125.0153,70.04
107	Difenoconazole	[119446-68-3]	C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	C19H17Cl2N3O3Na,C19H17Cl2N3O3NH4,C19H18Cl[37Cl]N3O3,C19H18Cl2N3O3, C13H9Cl[37Cl]O,C13H9Cl2O,C12H9[37Cl],C12H9Cl	428.0539,423.0985,408.0694,406.072,252.9997,251.0025,190.036,188.0387
108	Etoxadole	[153233-91-1]	C ₂₁ H ₂₃ F ₂ N ₂ O ₂	C21H23F2NO2Na,C21H23F2NO2NH4,C21H24F2NO2,C17H16F2NO2,C7H3F2O,C6H3F2, C4H9	382.1589,377.2035,360.177,304.1144,141.0146,113.0197,57.0699
109	Fenamidone	[161326-34-7]	C ₁₇ H ₁₇ N ₃ OS	C17H17N3OSNa,C17H17N3OSNH4,C17H18N3OS,C16H14N3O,C15H14N3,C6H6N,C5H5	334.0985,329.1431,312.1165,264.1131,236.1182,92.0495,65.0386
110	Fenobucarb	[3766-81-2]	C ₁₂ H ₁₇ NO ₂	C12H17NO2Na,C12H17NO2NH4,C12H18NO2,C8H9NO2Na,C8H10NO2,C6H7O,C6H5,C4H9	230.1151,225.1598,208.1332,174.0525,152.0706,95.0491,77.0386,57.0699
111	Fenthion-sulfone	[3761-42-0]	C ₁₀ H ₁₅ O ₅ PS ₂	C10H15O5PS2Na,C10H15O5PS2NH4,C10H16O5PS2,C9H12O4PS2,C2H6O2PS,C2H6O3P, CH4O2P	332.9991,328.0437,311.0171,278.9909,124.9821,109.0049,78.9943
112	Fenthion-sulfoxide	[3761-41-9]	C ₁₀ H ₁₅ O ₄ PS ₂	C10H15O4PS2Na,C10H15O4PS2NH4,C10H16O4PS2,C9H13O4PS2,C2H6O2PS,C2H6O3P, CH4O2P	317.0042,312.0488,295.0222,279.9987,124.9821,109.0049,78.9943
113	Flutolanil	[66332-96-5]	C ₁₇ H ₁₆ F ₃ N ₂ O ₂	C17H16F3NO2Na,C17H16F3NO2NH4,C17H17F3NO2,C14H11F3NO2,C14H10F2NO2, C14H9FNO2,C6H5O,C5H5	346.1025,341.1471,324.1206,282.0736,262.0674,242.0612,93.0335,65.0386
114	Fluazifop-butyl	[69806-50-4]	C ₁₉ H ₂₀ F ₃ NO ₄	C19H20F3NO4Na,C19H20F3NO4NH4,C19H21F3NO4,C15H13F3NO4,C14H11F3NO2, C12H7F3NO,C7H7	406.1237,401.1683,384.1417,328.0791,282.0736,238.0474,91.0543
115	Oxadiazon	[19666-30-9]	C ₁₅ H ₁₈ Cl ₂ N ₂ O ₃	C15H18Cl2N2O3Na,C15H18Cl2N2O3NH4,C15H19Cl[37Cl]N2O3,C15H19Cl2N2O3, C12H13Cl[37Cl]N2O3,C12H13Cl2N2O3,C7H4Cl[37Cl]NO3,C7H4Cl2NO3,C7H4[37Cl]NO3, C7H4ClNO3,C6H9O2	367.0587,362.1033,347.074,345.0767,305.027,303.0298,221.9534,219.9563, 186.9847,184.9874,113.0597
116	Pyriproxyfen	[95737-68-1]	C ₂₀ H ₁₉ NO ₃	C20H19NO3Na,C20H19NO3NH4,C20H20NO3,C12H9O2,C5H6NO,C5H4N,C6H5	344.1257,339.1703,322.1438,185.0597,96.0444,78.0338,77.0386
117	Quinoxifen	[124495-18-7]	C ₁₅ H ₈ NOFCl ₂	C15H8NOFCl2Na,C15H8NOFCl2NH4,C15H9NOFCl[37Cl],C15H9NOFCl2,C9H5Cl[37Cl]N, C9H5Cl2N,C9H5[37Cl]N,C9H5ClN,C6H4F	329.9859,325.0305,310.0012,308.004,198.9765,196.9794,164.0077, 162.0105,95.0292
118	Simazine	[122-34-9]	C ₇ H ₁₂ ClN ₃	C7H12ClN3Na,C7H12ClN3NH4,C7H13[37Cl]N3,C7H13ClN3,C6H10N3,C2H3[37Cl]N3, C2H3ClN3,C2H2N3,CH[37Cl]N,CHClN	224.0673,219.1119,204.0825,202.0854,124.0869,105.9981,104.001,68.0243, 63.9763,61.9792

119	Terbutylazine	[5915-41-3]	C ₉ H ₁₆ ClN ₅	C ₉ H ₁₆ ClN ₅ Na,C ₉ H ₁₆ ClN ₅ NH ₄ ,C ₉ H ₁₇ [37Cl]N ₅ ,C ₉ H ₁₇ ClN ₅ ,C ₅ H ₉ [37Cl]N ₅ ,C ₅ H ₉ ClN ₅ , C ₂ H ₃ [37Cl]N ₃ ,C ₂ H ₃ ClN ₃ ,C ₄ H ₆ N ₃ ,C ₂ H ₂ N ₃	252.0986,247.1432,232.1139,230.1167,176.0512,174.0541,105.9981, 104.001,96.0556,68.0243
120	Tetraconazole	[112281-77-3]	C ₁₃ H ₁₁ Cl ₂ F ₄ N ₃ O	C ₁₃ H ₁₁ Cl ₂ F ₄ N ₃ ONa,C ₁₃ H ₁₁ Cl ₂ F ₄ N ₃ ONH ₄ ,C ₁₃ H ₁₂ Cl[37Cl]F ₄ N ₃ O,C ₁₃ H ₁₂ Cl ₂ F ₄ N ₃ O, C ₇ H ₅ Cl[37Cl],C ₇ H ₅ Cl ₂ ,C ₂ H ₄ N ₃	394.0108,389.0554,374.026,372.0288,160.9734,158.9763,70.04
121	Thiobencarb	[28249-77-6]	C ₁₂ H ₁₆ ClNOS	C ₁₂ H ₁₆ ClNOSNa,C ₁₂ H ₁₆ ClNOSNH ₄ ,C ₁₂ H ₁₇ [37Cl]NOS,C ₁₂ H ₁₇ ClNOS,C ₇ H ₆ [37Cl], C ₇ H ₆ Cl,C ₇ H ₅	280.0533,275.0979,260.0686,258.0714,127.0124,125.0153,89.0386
122	Acetochlor	[34256-82-1]	C ₁₄ H ₂₀ ClNO ₂	C ₁₄ H ₂₀ ClNO ₂ Na,C ₁₄ H ₂₀ [37Cl]NO ₂ NH ₄ ,C ₁₄ H ₂₀ ClNO ₂ NH ₄ ,C ₁₄ H ₂₁ [37Cl]NO ₂ , C ₁₄ H ₂₁ ClNO ₂ ,C ₁₂ H ₁₅ [37Cl]NO,C ₁₂ H ₁₅ ClNO,C ₁₀ H ₁₄ N,C ₉ H ₁₁ N,C ₉ H ₁₀ N,C ₃ H ₇ O	292.1075,289.1496,287.1521,272.123,270.1255,226.081,224.0837,148.1121, 133.0886,132.0808,59.0491
123	Alachlor	[15972-60-8]	C ₁₄ H ₂₀ ClNO ₂	C ₁₄ H ₂₀ ClNO ₂ Na,C ₁₄ H ₂₀ [37Cl]NO ₂ NH ₄ ,C ₁₄ H ₂₀ ClNO ₂ NH ₄ ,C ₁₄ H ₂₁ [37Cl]NO ₂ , C ₁₄ H ₂₁ ClNO ₂ ,C ₁₃ H ₁₇ [37Cl]NO,C ₁₃ H ₁₇ ClNO,C ₁₁ H ₁₆ N,C ₁₀ H ₁₃ N,C ₉ H ₁₀ N	292.1075,289.1496,287.1521,272.123,270.1255,240.0967,238.0993, 162.1277,147.1043,132.0808
124	Ametryn	[834-12-8]	C ₉ H ₁₇ N ₅ S	C ₉ H ₁₇ N ₅ SNa,C ₉ H ₁₇ N ₅ NH ₄ ,C ₉ H ₁₈ N ₅ S,C ₆ H ₁₂ N ₅ S,C ₄ H ₆ N ₃ ,C ₂ H ₄ N ₃ ,C ₃ H ₇ N ₂ ,C ₂ H ₂ N ₃	250.1097,245.1543,228.1277,186.0808,96.0556,74.0059,71.0604,68.0243
125	Atrazine	[1912-24-9]	C ₆ H ₁₄ ClN ₅	C ₈ H ₁₄ ClN ₅ Na,C ₈ H ₁₄ ClN ₅ NH ₄ ,C ₈ H ₁₅ [37Cl]N ₅ ,C ₈ H ₁₅ ClN ₅ ,C ₅ H ₉ [37Cl]N ₅ ,C ₅ H ₉ ClN ₅ , C ₂ H ₃ [37Cl]N ₃ ,C ₂ H ₃ ClN ₃ ,C ₄ H ₆ N ₃ ,C ₂ H ₂ N ₃ ,CH[37Cl]N,CHClN	238.083,233.1276,218.0982,216.101,176.0512,174.0541,105.9981,104.001, 96.0556,68.0243,63.9763,61.9792
126	Butachlor	[23184-66-9]	C ₁₇ H ₂₆ ClNO ₂	C ₁₇ H ₂₆ ClNO ₂ Na,C ₁₇ H ₂₆ ClNO ₂ NH ₄ ,C ₁₇ H ₂₇ [37Cl]NO ₂ ,C ₁₇ H ₂₇ ClNO ₂ ,C ₁₃ H ₁₇ [37Cl]NO, C ₁₃ H ₁₇ ClNO,C ₁₁ H ₁₆ N,C ₁₀ H ₁₃ N,C ₉ H ₁₀ N,C ₄ H ₉	334.1544,329.199,314.1701,312.1725,240.0967,238.0993,162.1277, 147.1043,132.0808,57.0699
127	Edifenphos	[17109-49-8]	C ₁₄ H ₁₅ O ₂ PS ₂	C ₁₄ H ₁₅ O ₂ PS ₂ Na,C ₁₄ H ₁₅ O ₂ PS ₂ NH ₄ ,C ₁₄ H ₁₆ O ₂ PS ₂ ,C ₁₂ H ₁₂ O ₂ PS ₂ ,C ₆ H ₆ O ₂ PS,C ₆ H ₇ S, C ₆ H ₅ S,C ₆ H ₅	333.0143,328.0589,311.0324,283.0011,172.9821,111.0263,109.0106, 77.0386
128	Ethion	[563-12-2]	C ₉ H ₂₂ O ₄ P ₂ S ₄	C ₉ H ₂₂ O ₄ P ₂ S ₄ Na,C ₉ H ₂₂ O ₄ P ₂ S ₄ NH ₄ ,C ₉ H ₂₃ O ₄ P ₂ S ₄ ,C ₅ H ₁₂ O ₂ PS ₂ ,C ₃ H ₈ O ₂ PS ₂ ,CH ₄ O ₂ PS ₂ , H ₂ O ₂ PS	406.9768,402.0214,384.9949,199.0011,170.9698,142.9385,96.9509
129	Fenothiocarb	[62850-32-2]	C ₁₃ H ₁₉ NO ₂ S	C ₁₃ H ₁₉ NO ₂ SNa,C ₁₃ H ₁₉ NO ₂ SNH ₄ ,C ₁₃ H ₂₀ NO ₂ S,C ₇ H ₁₄ NOS,C ₇ H ₇ O,C ₆ H ₅ ,C ₃ H ₆ NO	276.1029,271.1475,254.1209,160.0791,107.0491,77.0386,72.0444
130	Fenthion	[55-38-9]	C ₁₀ H ₁₅ O ₃ PS ₂	C ₁₀ H ₁₅ O ₃ PS ₂ Na,C ₁₀ H ₁₅ O ₃ PS ₂ NH ₄ ,C ₁₀ H ₁₆ O ₃ PS ₂ ,C ₉ H ₁₂ O ₂ PS ₂ ,C ₈ H ₉ S ₂ ,C ₂ H ₆ O ₂ PS, C ₈ H ₉ ,C ₇ H ₇ ,CH ₄ O ₂ P	301.0092,296.0538,279.0273,247.0011,169.014,124.9821,105.0699,91.0542, 78.9943
131	Iprobenfos	[26087-47-8]	C ₁₃ H ₂₁ O ₃ PS	C ₁₃ H ₂₁ O ₃ PSNa,C ₁₃ H ₂₁ O ₃ PSNH ₄ ,C ₁₃ H ₂₂ O ₃ PS,C ₁₀ H ₁₆ O ₃ PS,C ₇ H ₁₀ O ₃ PS,C ₇ H ₇ ,C ₅ H ₅	311.0841,306.1287,289.1022,247.0552,205.0083,91.0542,65.0386
132	Isoprothiolane	[50512-35-1]	C ₁₂ H ₁₈ O ₄ S ₂	C ₁₂ H ₁₈ O ₄ S ₂ Na,C ₁₂ H ₁₈ O ₄ S ₂ NH ₄ ,C ₁₂ H ₁₉ O ₄ S ₂ ,C ₉ H ₁₁ O ₃ S ₂ ,C ₆ H ₅ O ₃ S ₂ ,C ₅ H ₅ O ₃ S ₂ ,C ₂ H ₅ S ₂	313.0539,308.0985,291.0719,231.0144,188.9675,144.9776,88.9514
133	Mefenacet	[73250-68-7]	C ₁₆ H ₁₄ N ₂ O ₂ S	C ₁₆ H ₁₄ N ₂ O ₂ SNa,C ₁₆ H ₁₄ N ₂ O ₂ SNH ₄ ,C ₁₆ H ₁₅ N ₂ O ₂ S,C ₉ H ₆ NO ₂ S,C ₉ H ₁₀ NO,C ₈ H ₁₀ N,C ₇ H ₇	321.0668,316.1114,299.0849,192.0114,148.0757,120.0808,91.0542

134	Metribuzin	[21087-64-9]	C ₈ H ₁₄ N ₄ OS	C8H14N4OSNa,C8H14N4OSNH4,C8H15N4OS,C7H15N4S,C5H10N,C2H4NS,CH2NS,C4H9	237.0781,232.1227,215.0961,187.1012,84.0808,74.0059,59.9902,57.0699
135	Molinate	[2212-67-1]	C ₉ H ₁₇ NOS	C9H17NOSNa,C9H17NOSNH4,C9H18NOS,C7H12NO,C6H12N,C6H11,C4H7	210.0923,205.1369,188.1104,126.0913,98.0964,83.0855,55.0542
136	Paclbutrazol	[76738-62-0]	C ₁₅ H ₂₀ ClN ₃ O	C15H20ClN3ONa,C15H20ClN3ONH4,C15H21[37Cl]N3O,C15H21ClN3O,C7H6[37Cl], C7H6Cl,C2H4N3	316.1187,311.1633,296.1342,294.1368,127.0124,125.0153,70.04
137	Parathion	[56-38-2]	C ₁₀ H ₁₄ NO ₃ PS	C10H14NO5PSNa,C10H14NO5PSNH4,C10H15NO5PS,C8H11NO5PS,C6H7NO5PS, C6H6NO3,C6H5NO2,H2O2PS,C6H6O	314.0223,309.0669,292.0403,264.009,235.9777,140.0342,123.0315,96.9508, 94.0413
138	Pendimethalin	[40487-42-1]	C ₁₃ H ₁₈ N ₂ O ₄	C13H19N3O4Na,C13H19N3O4NH4,C13H20N3O4,C8H10N3O4,C8H8N3O3,C8H8N2O, C7H7N2,C5H5	304.1268,299.1714,282.1448,212.0666,194.056,148.0631,119.0604,65.0386
139	Phosmet	[732-11-6]	C ₁₁ H ₁₂ NO ₄ PS ₂	C11H12NO4PS2Na,C11H12NO4PS2NH4,C11H13NO4PS2,C10H11NO4PS,C9H6NO2, C8H5O2,C2H8NP	339.9838,335.0284,318.0018,272.0141,160.0393,133.0284,77.0389
140	Pretilachlor	[51218-49-6]	C ₁₇ H ₂₆ ClNO ₂	C17H26ClNO2Na,C17H26ClNO2NH4,C17H27[37Cl]NO2,C17H27ClNO2,C14H19[37Cl]NO, C14H19ClNO,C12H18N,C10H13N,C9H10N	334.1544,329.199,314.1701,312.1725,254.1124,252.115,176.1434,147.1043, 132.0808
141	Profenofos	[41198-08-7]	C ₁₁ H ₁₅ BrClO ₃ PS	C11H15BrClO3PSNa,C11H15BrClO3PSNH4,C11H16[81Br][37Cl]O3PS, C11H16[81Br]ClO3PS,C11H16BrClO3PS,C9H12[81Br][37Cl]O3PS,C9H12[81Br]ClO3PS, C9H12BrClO3PS,C6H6[81Br][37Cl]O3PS,C6H6[81Br]ClO3PS,C6H6BrClO3PS,C6H5[37Cl]O, C6H5ClO,H2O2PS	394.9244,389.969,376.9376,374.9402,372.9424,348.9062,346.9088, 344.9111,306.8592,304.8619,302.8642,129.9995,128.0023,96.9508
142	Prometryn	[7287-19-6]	C ₁₀ H ₁₉ N ₃ S	C10H19N5SNa,C10H19N5SNH4,C10H20N5S,C7H14N5S,C4H8N5S,C2H4NS,C2H2N3	264.1253,259.1699,242.1434,200.0964,158.0495,74.0059,68.0243
143	Pyridaphenthion	[119-12-0]	C ₁₄ H ₁₇ N ₂ O ₄ PS	C14H17N2O4PSNa,C14H17N2O4PSNH4,C14H18N2O4PS,C10H9N2OS,C10H9N2O2, H2O2PS,C6H6N	363.0539,358.0985,341.0719,205.043,189.0659,96.9508,92.0495
144	Quinalphos	[13593-03-8]	C ₁₂ H ₁₅ N ₂ O ₃ PS	C12H15N2O3PSNa,C12H15N2O3PSNH4,C12H16N2O3PS,C10H12N2O3PS,C8H7N2S, C8H7N2O,C8H5N2,H2O2PS	321.0433,316.0879,299.0614,271.0301,163.0324,147.0553,129.0447, 96.9508
145	tau-Fluvalinate	[102851-06-9]	C ₂₆ H ₂₂ ClF ₃ N ₂ O ₃	C26H22ClF3N2O3Na,C26H22ClF3N2O3NH4,C26H23[37Cl]F3N2O3,C26H23ClF3N2O3, C14H10NO,C13H9O	525.1163,520.1609,505.1326,503.1344,208.0757,181.0648
146	Triadimefon	[43121-43-3]	C ₁₄ H ₁₆ ClN ₃ O ₂	C14H16ClN3O2Na,C14H16ClN3O2NH4,C14H17[37Cl]N3O2,C14H17ClN3O2, C9H12[37Cl]N3,C9H12ClN3,C5H9,C4H9,C4H7	316.0823,311.1269,296.0979,294.1004,199.0686,197.0714,69.0699,57.0699, 55.0542

147	Dimethoate	[60-51-5]	C ₅ H ₁₂ NO ₃ PS ₂	C ₅ H ₁₂ NO ₃ PS ₂ Na, C ₅ H ₁₂ NO ₃ PS ₂ NH ₄ , C ₅ H ₁₃ NO ₃ PS ₂ , C ₄ H ₈ O ₃ PS ₂ , C ₃ H ₈ O ₂ PS ₂ , C ₂ H ₆ O ₂ PS, C ₃ H ₆ NS, CH ₄ O ₂ P	251.9888, 247.0334, 230.0069, 198.9647, 170.9698, 124.9821, 88.0215, 78.9943
148	Pirimicarb	[23103-98-2]	C ₁₁ H ₁₈ N ₄ O ₂	C ₁₁ H ₁₈ N ₄ O ₂ Na, C ₁₁ H ₁₈ N ₄ O ₂ NH ₄ , C ₁₁ H ₁₉ N ₄ O ₂ , C ₉ H ₁₆ N ₃ O, C ₄ H ₉ N ₂ , C ₃ H ₆ NO, C ₂ H ₂ NO	261.1322, 256.1768, 239.1503, 182.1288, 85.076, 72.0444, 56.0131
149	Anilofos	[64249-01-0]	C ₁₃ H ₁₉ ClNO ₃ PS ₂	C ₁₃ H ₁₉ ClNO ₃ PS ₂ Na, C ₁₃ H ₁₉ ClNO ₃ PS ₂ NH ₄ , C ₁₃ H ₂₀ [³⁷ Cl]NO ₃ PS ₂ , C ₁₃ H ₂₀ ClNO ₃ PS ₂ , C ₄ H ₈ O ₃ PS ₂ , C ₃ H ₈ O ₂ PS ₂ , C ₂ H ₆ O ₂ PS ₂ , C ₂ H ₆ O ₂ PS, CH ₄ O ₂ P	390.0125, 385.0571, 370.0277, 368.0305, 198.9647, 170.9698, 156.9541, 124.9821, 78.9943
150	Chlorpyrifos	[2921-88-2]	C ₉ H ₁₁ Cl ₃ NO ₃ PS	C ₉ H ₁₁ Cl ₃ NO ₃ PSNa, C ₉ H ₁₁ Cl ₃ NO ₃ PSNH ₄ , C ₉ H ₁₂ Cl[³⁷ Cl]NO ₃ PS, C ₉ H ₁₂ Cl ₂ [³⁷ Cl]NO ₃ PS, C ₉ H ₁₂ Cl ₃ NO ₃ PS, C ₅ H ₃ Cl[³⁷ Cl] ₂ NO, C ₅ H ₃ Cl ₂ [³⁷ Cl]NO, C ₅ H ₃ Cl ₃ NO, C ₂ H ₆ O ₂ PS, H ₂ O ₂ PS	371.9155, 366.9601, 353.9278, 351.9306, 349.9336, 201.9217, 199.9246, 197.9275, 124.9821, 96.9508

30 banned pesticides in standard solutions and *Isatidis Folium* were used to evaluate the anti-interference capability of SWATH and AIF. The results showed that lower signal intensity and less fragment ions can be achieved for pesticides in *Isatidis Folium* regardless of the acquisition mode being SWATH or AIF. What's more, the signal intensity and the number of fragment ions decreased more significantly for SWATH. Taking ethoprophos at 1 ng/mL as an example to explain the different matrix effect for the two acquisition modes. For SWATH, when the $[M+H]^+$ of ethoprophos ($C_8H_{20}O_2PS_2$, the accurate m/z is 243.0637) was used as a precursor ion, five fragment ions with m/z 96.9510, 130.9389, 172.9854, 215.0332, 243.0640 (which may correspond to H_2O_2PS , $H_4O_2PS_2$, $C_3H_{10}O_2PS_2$, $C_6H_{16}O_2PS_2$, and $C_8H_{20}O_2PS_2$ of ethoprophos) can be found in MS/MS spectra of standard solutions, but only one fragment ion with m/z 172.9854 (which may refer to $C_3H_{10}O_2PS_2$ of ethoprophos) can be found in MS/MS spectra of the spiked *Isatidis Folium* (Figure S1). In addition, the peak of $[M+H]^+$ in MS spectra and the peaks of potential fragment ions in MS/MS spectra were much lower for ethoprophos in *Isatidis Folium*. Similarly, three fragment ions, corresponding to H_2O_2PS , $H_4O_2PS_2$, $C_3H_{10}O_2PS_2$ of ethoprophos, were filtered out in standard solutions using AIF (Figure S2). But there were still two fragment ions of ethoprophos can be found in the spiked *Isatidis Folium*. Compared with AIF, the spectra of SWATH are influenced more seriously by coeluting matrix. Therefore, the AIF exhibits more significantly anti-interference capability.

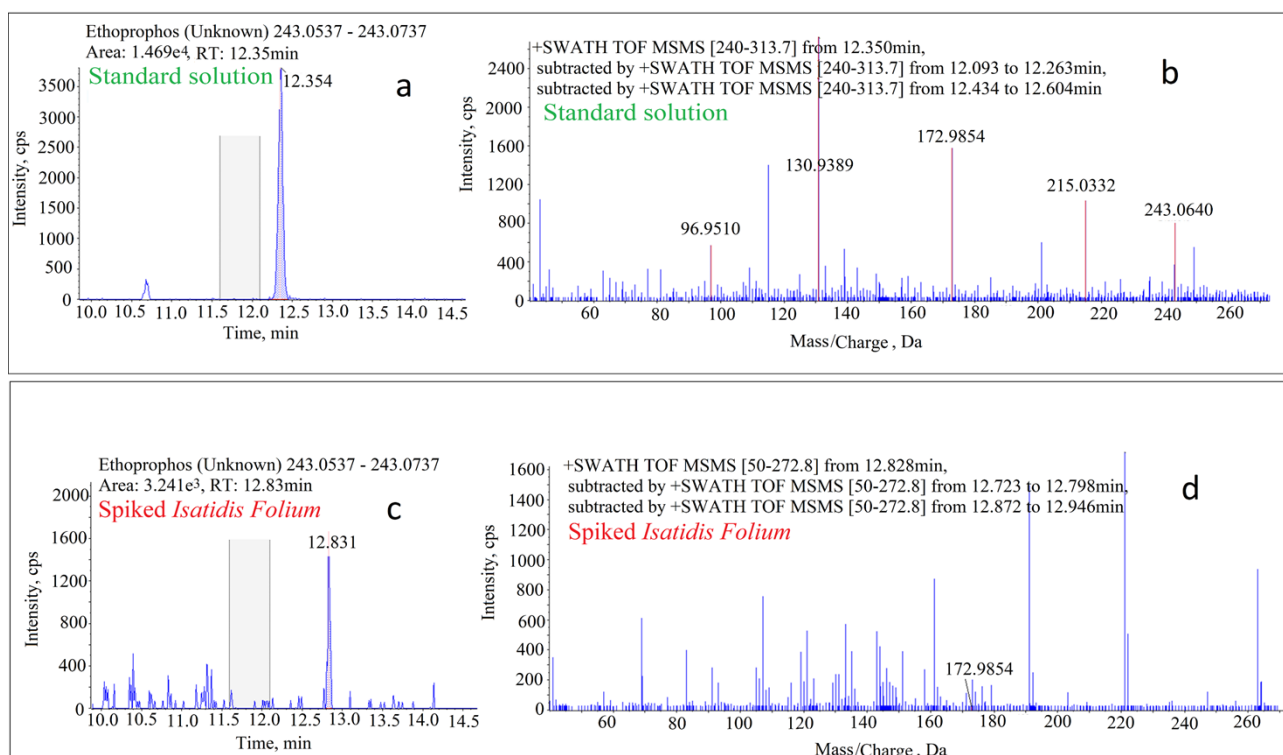


Figure S1 The MS and MS/MS results of ethoprophos using the acquisition mode of SWATH. (a) is the EIC of the $[M+H]^+$ of ethoprophos in the standard solution. (b) is the MS/MS spectrum of the $[M+H]^+$ of ethoprophos in standard solution. (c) is the EIC of the $[M+H]^+$ of ethoprophos in the spiked *Isatidis Folium*. (d) is the MS/MS spectrum of the $[M+H]^+$ of ethoprophos in the spiked *Isatidis Folium*.

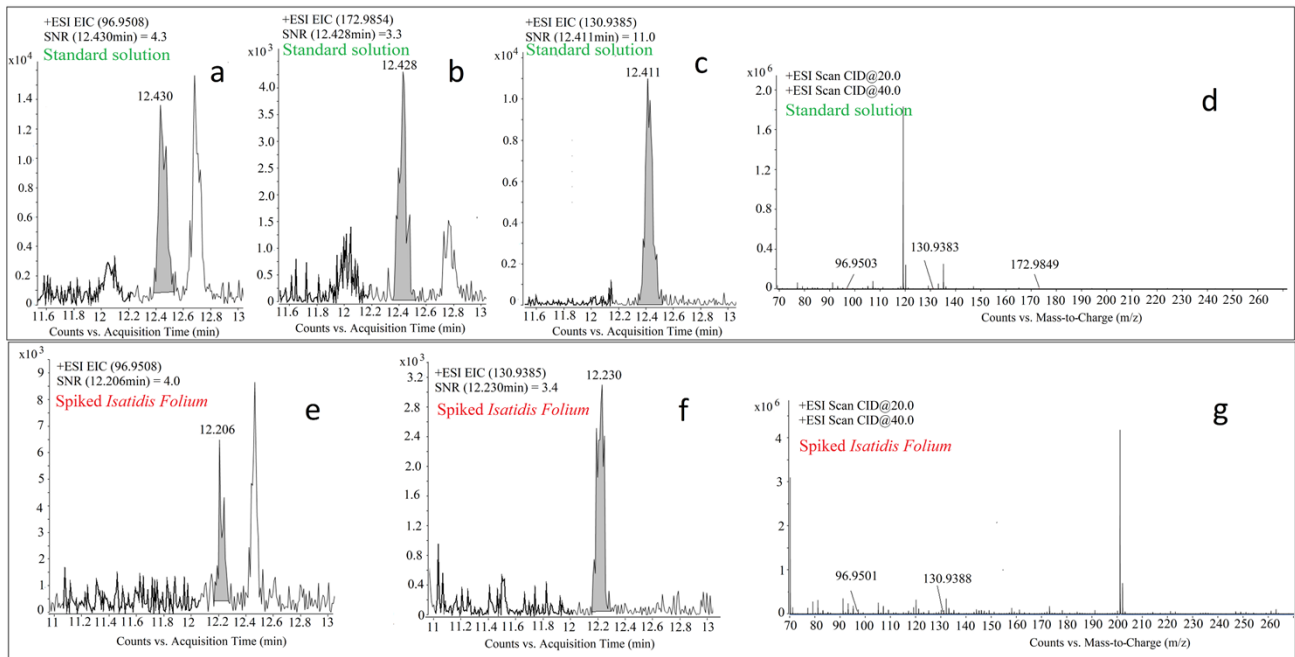


Figure S2 The MS and MS/MS results of ethoprophos using the acquisition mode of AIF. (a-c) is the EICs of the qualified ions of ethoprophos in the standard solution. (d) is the MS/MS spectrum of ethoprophos in standard solution. (e-f) is the EICs of the qualified ions of Ethoprophos in the spiked *Isatidis Folium*. (g) is the MS/MS spectrum of ethoprophos in the spiked *Isatidis Folium*.

To confirm phorate-sulfoxide in *Ganoderma* using targeted-MSMS, the $[M+H]^+$ of phorate-sulfoxide (m/z 277.0150) was used as a precursor ion. Five fragment ions with m/z 64.9790, 96.9509, 142.9380, 170.9696, 199.0002, corresponding to H₂O₂P, H₂O₂PS, CH₄O₂PS₂, C₃H₈O₂PS₂, C₅H₁₂O₂PS₂ of phorate-sulfoxide, were found at 8.779 min.

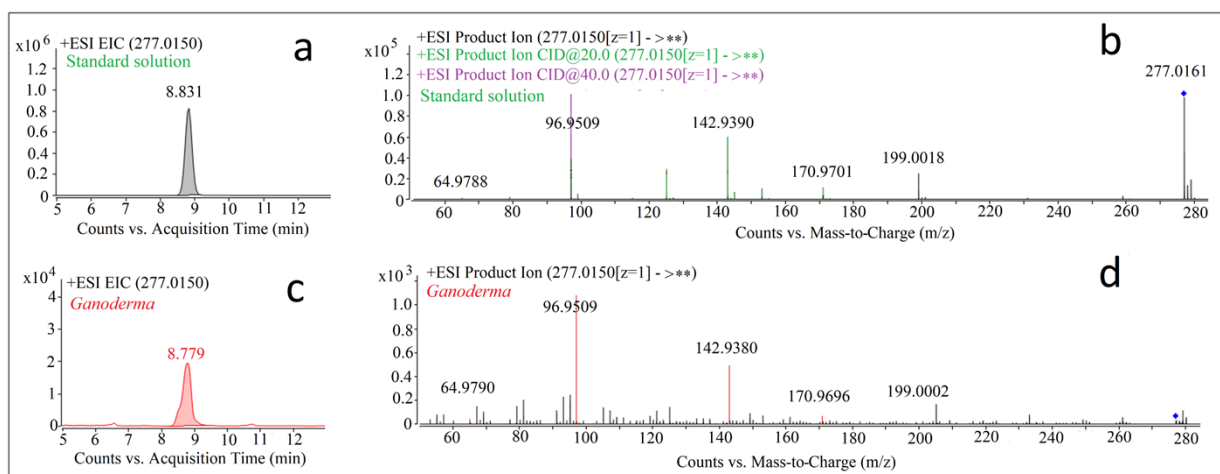


Figure S3 (a) is the EIC of the $[M+H]^+$ of phorate-sulfoxide in standard solution. (b) is the overlaid fragmentation spectra of the $[M+H]^+$ of phorate-sulfoxide in the standard solution. (c) is the EIC of the $[M+H]^+$ of phorate-sulfoxide in *Ganoderma*. (d) is the overlaid fragmentation spectra of the $[M+H]^+$ of phorate-sulfoxide in *Ganoderma*.

To confirm phorate-sulfone in *Ganoderma* using targeted-MSMS, the $[M+H]^+$ of phorate-sulfone (m/z 293.0099) was used as a precursor ion. Four fragment ions with m/z 96.9502, 114.9612, 142.9920, 171.0257, corresponding to H₂O₂PS, H₄O₃PS, C₂H₈O₃PS, C₄H₁₂O₃PS of phorate-sulfone, were found at 10.889 min.

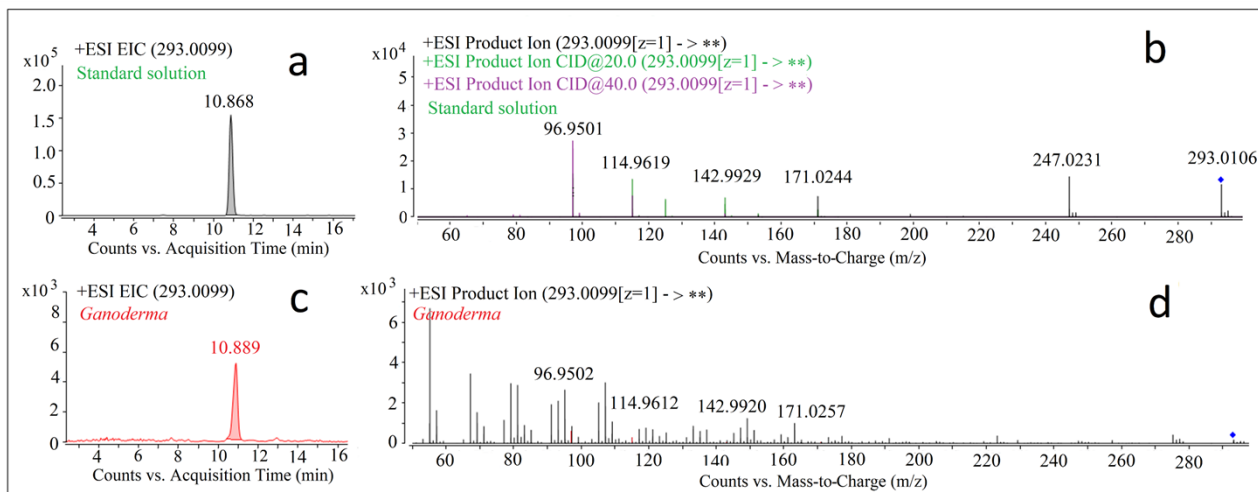


Figure S4 (a) is the EIC of the $[M+H]^+$ of phorate-sulfone in standard solution. (b) is the overlaid fragmentation spectra of the $[M+H]^+$ of phorate-sulfone in standard solution. (c) is the EIC of the $[M+H]^+$ of phorate-sulfone in *Ganoderma*. (d) is the overlaid fragmentation spectra of the $[M+H]^+$ of phorate-sulfone in *Ganoderma*.

To confirm terbufos-sulfoxide in *Foeniculi Fructus* using targeted-MSMS, the $[M+H]^+$ of terbufos-sulfoxide (m/z 305.0463) was used as a precursor ion. Five fragment ions with m/z 57.0702, 96.9507, 130.9384, 158.9695, 187.0007, corresponding to C₄H₉, H₂O₂PS, H₄O₂PS₂, C₂H₈O₂PS₂, C₄H₁₂O₂PS₂ of terbufos-sulfoxid, were found at 10.577 min.

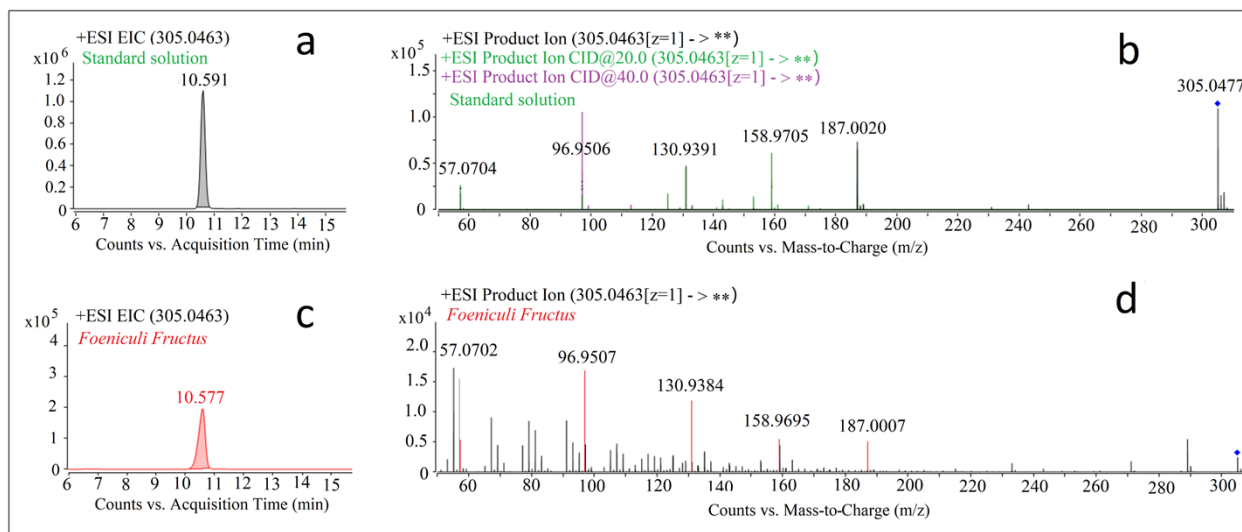


Figure S5 (a) is the EIC of the $[M+H]^+$ of terbufos-sulfoxide in standard solution. (b) is the overlaid fragmentation spectra of the $[M+H]^+$ of terbufos-sulfoxide in standard solution. (c) is the EIC of the $[M+H]^+$ of terbufos-sulfoxide in *Foeniculi Fructus*. (d) is the overlaid fragmentation spectra of the $[M+H]^+$ of terbufos-sulfoxide in *Foeniculi Fructus*.

To confirm terbufos-sulfone in *Foeniculi Fructus* using targeted-MSMS, the $[M+H]^+$ of terbufos-sulfone (m/z 321.0412) was used as a precursor ion. Four fragment ions with m/z 96.9506, 114.9610, 142.9914, 171.0232, corresponding to H₂O₂PS, H₄O₃PS, C₂H₈O₃PS, C₄H₁₂O₃PS₂ of terbufos-sulfone, were found at 12.486 min.

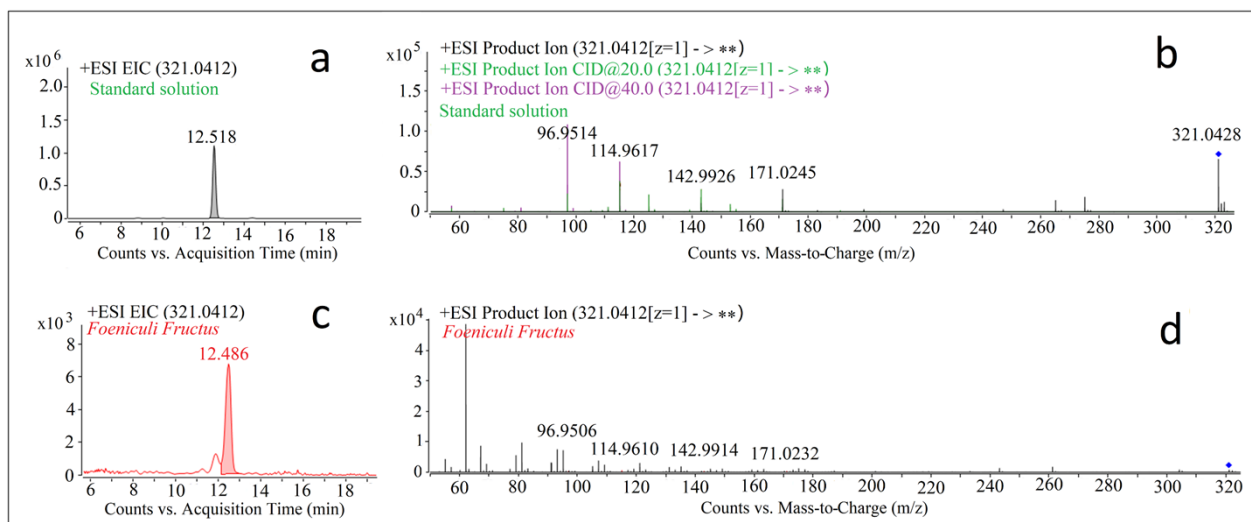


Figure S6 (a) is the EIC of the $[M+H]^+$ of terbufos-sulfone in standard solution. (b) is the overlaid fragmentation spectra of the $[M+H]^+$ of terbufos-sulfone in standard solution. (c) is the EIC of the $[M+H]^+$ of terbufos-sulfone in *Foeniculi Fructus*. (d) is the overlaid fragmentation spectra of the $[M+H]^+$ of terbufos-sulfone in *Foeniculi Fructus*.