

Electronic supplementary information

**Simultaneous combination of MS2 workflows for pesticides multiresidue
analysis with LC-QOrbitrap**

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Supplementary Table 1 Non-target pesticides

Pesticide	Precursor	Fragments						
Acetochlor	270.1255	224.0837	148.1121	90.0105	59.0494			
Alachlor	270.1255	238.0993	224.0837	220.0888	208.0888	162.1278	90.0105	
Ametryn	228.1277	186.0808	96.0556	91.0324				
Anilofos	368.0305	198.9649	188.9805	170.9699	142.9928			
Atrazine	216.1011	174.0542	132.0324	104.0010	96.0556			
Atrazine-Desethyl	188.0698	146.0229	110.0462	104.0010	79.0058	68.0244		
Azamethiphos	324.9809	182.9958	170.9957	139.0059	127.9899			
Azinphos-ethyl	346.0444	232.9491	137.0056	132.0444	114.9614			
Bensulfuron-methyl	411.0969	213.0331	182.0563	156.0770	149.0599	119.0493		
Bromacil	261.0233	204.9608	187.9342	161.9549				
Buturon	237.0789	84.0807	58.0654	53.0389				
Cambendazole	303.0910	214.0542	261.0441					
Carbetamide	237.1234	192.0656	120.0445	118.0863	72.0808			
Chlorbromuron	292.9687	203.9211	182.0242	62.0603				
Chloridazon	222.0429	146.0116	104.0495	92.0494				
Chloroxuron	291.0895	218.0369	164.0946	72.0444				
Chromafenozide	395.2329	175.0754	133.0648					
Cinosulfuron	414.1078	215.0373	183.0514	157.0721	141.0005	121.0285	59.0494	
Clethodim	360.1395	206.1178	166.0865	164.0707	129.0385			
Cyanazine	241.0963	214.0855	205.1198	174.0542	104.0010	96.0556		
Diafenthiuron	385.2308	329.1685	312.1419	287.1215	278.1542	270.1854	228.1386	
Dialifos	394.0098	208.0159	187.0010	158.9698	130.9385	114.9613		
Diclobutrazol	328.0978	199.0077	158.9763	70.0400	59.0494			

Difenoxyuron	287.1390	214.0863	123.0441	95.0492	72.0444			
Diflufenican	395.0814	284.0532	266.0426	246.0364				
Dimefuron	339.1218	295.1321	256.0484	167.0008	72.0444			
Dimethylvinphos, Z-	330.9455	204.9375	169.9686	145.0262	127.0156	98.9842		
Dodemorph	282.2791	116.1070	98.0965	83.0855	69.0700			
Edifenphos	311.0324	283.0011	219.9926	190.9927	140.9828	111.0263		
Ethiofencarb	226.0896	164.0704	107.0490	91.0541	79.0541			
Ethiprole	396.9899	350.9483	319.9840	254.9698				
Etrimfos	293.0719	265.0406	233.0144	142.9927				
Fenbendazole	300.0801	268.0536	190.0068	159.0426	109.0106			
Fenfuram	202.0863	120.0444	109.0285	94.0651	92.0495	83.0491		
Fenoxaprop-ethyl	362.0790	288.0424	244.0526	238.0501	119.0493			
Fenpropidin	274.2529	147.1169	86.0964	57.0700				
Fenuron	165.1022	120.0444	95.0491	92.0494	72.0444			
Flamprop-methyl	336.0797	105.0336	95.0492	53.0390				
Flazasulfuron	408.0584	301.0909	227.0098	182.0562	156.0770			
Fluacrypyrim	427.1475	205.0859	145.0648					
Fluazifop-Butyl	384.1417	328.0789	282.0735	254.0785				
Fluometuron	233.0896	168.0257	72.0445					
Fluridone	330.1100	310.1038	309.0963					
Fonofos	247.0375	200.9955	155.0290	137.0185	126.9977	108.9872		
Forchlorfenuron	248.0585	155.0007	129.0214	111.0553	94.0651			
Fuberidazole	185.0709	157.0761	156.0683	92.0494				
Furathiocarb	383.1635	326.1423	252.0691	195.0477	177.0371	180.0691	167.0528	
Heptenophos	251.0235	215.0470	127.0156	125.0155	89.0386			
Imazapyr	262.1186	220.0716	217.0971	202.0611	86.0964			
Imazaquin	312.1343	284.1396	270.0874	267.1129	199.0504	86.0964		
Isazofos	314.0490	272.0024	171.0242	162.0432	119.9961			
Isofenphos	346.1236	245.0036	234.9828	216.9723	137.0058	121.0285		
Isofenphos-oxon	330.1465	229.0261	219.0053	200.9948	121.0283			
Isoproturon	207.1492	165.1027	162.0917	72.0446				
Lenacil	235.1441	153.0660	136.0395	83.0855				
Mebendazole	296.1030	264.0765	105.0331	77.0381				
Mecarbam	330.0593	226.9960	199.0012	170.9698	116.0343	114.9614		
Metamitron	203.0927	175.0979	104.0495					
Metazachlor	278.1055	210.0680	134.0964	105.0699	76.9788			
Metolachlor	284.1412	252.1150	212.0837	176.1434	73.0648			
Metosulam	418.0138	354.0521	228.0313	189.9822	174.9952	140.0262		
Metoxuron	229.0738	184.0161	156.0211	72.0444				
Metribuzin	215.0961	187.1013	148.0632	131.0388	89.0168	84.0808		
Metsulfuron-methyl	382.0816	313.9920	209.9858	199.0062	167.0566	141.0772	127.0156	
Mevinphos	225.0523	193.0262	127.0155	99.0441	67.0180			
Monolinuron	215.0582	148.0632	126.0106	62.0603				
Monuron	199.0633	171.0805	154.0055	126.0106	72.0444			
Naled	378.7899	314.9000	252.7816	173.8634	144.9816	127.0155	91.6972	

Napropamide	272.1645	199.0757	171.0807	129.1151	100.1123	74.0965	72.0809	
Nuarimol	315.0695	252.0819	243.0372	138.9945	81.0447			
Ofurace	282.0892	254.0942	236.0837	224.0837	160.1121			
Oxycarboxin	268.0638	193.0166	175.0060	164.9853	120.0444	146.9747		
Paraoxon ethyl	276.0632	220.0002	248.0318	238.0111				
Paraoxon methyl	248.0319	127.0155	202.0388	89.0391	90.0469			
Phosphamidon	300.0762	226.9871	174.0682	127.0155	100.0757			
Picolinafen	377.0908	359.0804	284.0531	256.0582				
Picoxystrobin	368.1104	205.0863	177.0913	173.0600	117.0700	115.0543		
Promecarb	208.1332	151.1119	119.0605	109.0649	91.0543			
Prometryn	242.1434	200.0966	158.0497					
Propachlor	212.0837	170.0371	152.0265	106.0653	94.0653	91.0544		
Propaphos	305.0971	263.0496	239.0132	221.0027	202.9922	141.0367		56.0498
Propaquizafop	444.1321	444.1321	371.0794	299.0583	144.1020	100.0757	70.0652	
Propazine	230.1167	188.0699	146.0229	104.0010	79.0058			
Prosulfocarb	252.1417	128.1072	91.0542	86.0602	65.0389			
Pyrazophos	374.0934	346.0623	238.0646	222.0874	194.0563	176.0457	114.9614	
Pyridaphenthion	341.0719	313.0405	205.0431	189.0658	114.9613			
Pyrifenox	295.0399	263.0138	93.0573					
Pyrimidifen	378.1943	184.0636	157.0401	150.1025				
Quinalphos	299.0614	242.9988	163.0325	147.0553	114.9613			
Sulfosulfuron	471.0751	261.0287	236.0334	211.0535	156.0768			125.0420
Sulprofos	323.0358	295.0044	265.0116	236.9803	218.9698	157.0141	154.9983	
Terbumeton	226.1662	170.1036	142.0724	114.0662	100.0505	75.0553		
Terbutylazine-desethyl	202.0854	146.0228	104.0010	110.0461	79.0057	68.0243		
Tetrachlorvinphos	364.9065	238.8985	203.9297	127.0156				
Thifensulfuron-methyl	388.0380	222.9731	204.9626	167.0565	141.0772			
Thiophanate	371.0842	282.0363	235.9945	206.0923	160.0505	151.0324	59.9905	
Tolfenpyrad	384.1473	197.0965	171.0323	145.0530				
Triasulfuron	402.0633	236.9984	167.0565	141.0772	137.0057	121.0285		
Tribenuron-methyl	396.0972	364.0712	350.0162	181.0721	155.0928	135.0442		
Tricyclazole	190.0433	163.0313	136.0216	109.0106				
Vamidotion	288.0488	146.0634	118.0321	86.0600	58.0654			

Supplementary Table 2 Target pesticides

Pesticide	Precursor	Fragments							RT
Acephate	184.0192	142.9927	128.9770	112.9998					3.07
Acetamidrid	223.0745	149.0235	126.0106	56.0498					4.54
Aldicarb	213.0668	116.0529	101.0295	89.0426	70.0659	68.0497	61.0110		4.92
Aldicarb-sulfone	223.0747	148.0427	86.0607	81.0012	76.0401	62.9908	59.0501		3.65
Aldicarb-sulfoxide	207.0798	132.0479	89.0426	73.0649	69.0582	65.0056			3.53
Azinphos-methyl	318.0131	167.0162	142.9927	132.0445	105.0336	104.0495			6.9
Azoxystrobin	404.1241	372.0980	344.1031	329.0795	172.0393				7.01

Bifenazate	301.1547	198.0918	170.0968	153.0702					7.72
Bitertanol	338.1863	269.1536	251.1431	171.0805	99.0804	70.0400	57.0702		8.86
Boscalid	343.0399	307.0634	272.0935	271.0867	139.9899				7.3
Bromuconazole	375.9414	306.9286	227.0024	172.9556	158.9763	70.0400			7.70,8.42
Bupirimate	317.1642	272.1068	237.2077	210.1604	166.0978				7.79
Buprofezin	306.1635	201.1058	116.0529	106.0652	57.0702				9.63
Carbaryl	145.0648	155.0606	127.0543	122.0194	117.0700	115.0544	103.0543		5.82
Carbendazim	192.0768	160.0506	132.0557						4.01
Carbofuran	222.1125	165.0912	137.0599	123.0441	119.0857	55.0546			5.42
Chlorantraniliprole	481.9781	450.9361	283.9222	279.0087	194.0004	190.9451			6.66
Chlorfenvinphos, B-	358.9768	204.9375	155.0469	127.0156	98.9842	349.9336			8.62
Chlorpyrifos	349.9336	293.8709	197.9276	171.0240	114.9614				10.15
Chlorpyrifos-methyl	321.9023	289.8761	142.9928	127.0155					9.21
Clofentezine	303.0199	256.8833	156.0210	138.0105	130.0400				9.29
Clomazone	240.0786	128.0708	125.0155	89.0386					6.83
Clothianidin	250.016	169.0543	131.9670	113.0168					4.3
Coumaphos	363.0217	334.9906	306.9593	288.9487	226.9929	211.0158			8.79
Cyazofamid	325.0521	261.0903	225.1136	217.0403	108.0114				8.08
Cymoxanil	199.0826	147.0400	129.0294	111.0189	83.0245				4.6
Cyproconazole	292.1211	138.9947	125.0155	70.0402					7.42,7.69
Cyprodinil	226.1339	210.1025	108.0808	93.0573					8.42
Cyromazine	167.104	125.0824	85.0510	83.0605	60.0560				2.32
Demeton-S-Methyl-Sulfone	263.0171	230.9910	169.0084	142.9927	127.0155	121.0318			3.89
Demeton-S-methylsulfoxide	247.0222	169.0083	142.9927	127.0155	105.0369				3.83
Diazinon	305.1083	169.0797	153.1025	114.9616					8.62
Dichlorvos	220.9532	127.0149							5.42
Dicrotophos	238.0839	193.0264	127.0157	112.0759	72.0445				4.12
Diethofencarb	268.1543	198.0761	180.1019	152.0706	124.0393				6.88
Difenoconazole	406.072	337.0394	264.9817	251.0026					9.2
Diffubenzuron	311.0393	159.9692	158.0413	141.0147	114.9614				8.32
Dimethoate	230.0069	198.9649	170.9699	142.9928	124.9822	88.0216			4.45
Dimethomorph	388.131	301.0629	165.0549	114.0551					7.15,7.43
Diniconazole	326.0821	308.0715	252.0090	158.9763	70.0399				9.05
Diuron	233.0243	187.9664	159.9715	72.0444					6.65
Dodine	228.2434	186.2217	71.0863	60.0566	57.0708				9.17
Emamectin B1a	886.5311	302.1966	158.1178	126.0915	82.0652				10.14
Epoxiconazole	330.0804	141.0103	123.0242	121.0449	70.0401				8.05
Ethion	384.9949	199.0013	170.9699	142.9387	114.9614				9.97
Ethirimol	210.1601	193.1336	182.1289	140.1070	98.0600				4.89
Ethoprophos	243.0637	215.0324	201.0167	172.9855	130.9385	114.9614			7.89
Etofenprox	394.2377	359.2005	305.1535	183.0805	177.1274	135.0804	107.0491		11.53
Famoxadone	392.1605	331.1440	238.1100	195.0805	146.0601	93.0573			8.76
Fenamidone	312.1165	264.1132	236.1183	165.0482	103.0542	92.0495			7.11
Fenamiphos	304.1131	276.0819	262.0662	234.0349	217.0084				8.16
Fenamiphos-sulfone	336.1029	308.0718	266.0249	188.0473					5.61

Fenamiphos-sulfoxide	320.108	292.0767	251.0138	171.0475					5.48
Fenarimol	331.0399	304.0294	268.0527	259.0079	81.0448				7.85
Fenazaquin	307.1805	161.1325	147.0553	57.0702					11.33
Fenbuconazole	337.1215	194.0481	136.0482	125.0153	70.0400				8.14
Fenhexamid	302.0709	142.0057	97.1013	55.0546					7.71
Fenoxycarb	302.1387	256.0968	211.0754	116.0706	88.0393				8.3
Fenpropathrin	350.1751	134.0965	129.0170	125.0962	97.1012				10.49
Fenpropimorph	304.2635	147.1170	130.1229	116.1072	57.0703				7.00
Fenpyrazamine	290.09574	272.1757	231.1367	230.1289	216.1131	189.0896	131.0730	225.0426	7.57
Fenpyroximate	422.2074	422.2074	366.1451	231.1004	215.1055	214.0976	138.0663		10.69
Fenthion	279.0273	247.0011	231.0240	169.0141	149.0234	142.9927			8.65
Fenthion-sulfone	311.0171	142.9928	137.0421						5.9
Fenthion-sulfoxide	295.0222	279.9987	278.0194	264.0038	232.0317				5.76
Flonicamid	230.0536	203.0430	176.0321	174.0164	148.0371				3.83
Flufenacet	364.0737	152.0505	124.0558	109.0451					7.84
Flufenoxuron	489.0435	487.0290	141.0146	158.0412					10.44
Fluopyram	397.0537	208.0137	190.0475	173.0210	170.0413				7.71
Fluquinconazole	376.0163	349.0057	324.9943	306.9838	272.0150	123.9950	108.0243		7.78
Flusilazole	316.1076	187.0585	165.0699	95.0491					8.27
Flutriafol	302.11	233.0775	137.0399	123.0242	109.0450	70.0401			6.19
Formetanate	222.1237	165.1024	120.0445						3.43
Fosthiazate	284.0539	227.9915	199.9602	119.9938	104.0165				5.93
Haloxypop	362.0402	316.0347	288.0371	91.0542	272.0073				8.24
Hexaconazole	314.0821	184.9923	158.9766	70.0401					8.73
Hexythiazox	353.1085	271.0305	228.0246	194.0370	168.0577				10.13
Imazalil	297.0556	255.0086	200.9869	158.9764	69.0448				6.17
Imidacloprid	256.0596	212.0585	209.0588	175.0979	84.0556				4.28
Indoxacarb	528.078	496.0530	293.0329	249.0429	218.0428	190.0058	168.0214	150.0109	9.25
Iprovalicarb	321.2173	203.1392	186.1126	144.0656	119.0856	116.0707	91.0542	72.0808	7.7
Isocarbophos	230.9875	216.9722	137.0058	121.0285					8.35
Isofenfos methyl	332.108	273.0345	230.9868	121.0248	198.9601	171.0205			8.35
Isoprocab	194.1176	162.0573	152.0707	137.0962	95.0496				6.17
Isoxaflutole	360.0512	250.9985	69.0336	159.0427	278.0434	78.9859	108.0455		6.39
Kresoxim-methyl	314.1387	282.1124	267.1015	235.0752	222.0912	132.0807	131.0729	116.0494	8.35
Linuron	249.0192	182.0245	159.9719	132.9608	62.0604	60.0448			7.23
Lufenuron	510.9857	327.9725	236.0117	158.0413	141.0147	87.0441			10.12
Malaoxon	315.0662	99.0077	127.0390	142.9926	173.0808	269.0243			5.46
Malathion	331.0433	285.0015	257.0065	210.9648	142.9927	127.0390	99.0077		7.4
Mandipropamid	412.131	356.1050	328.1101	204.1022	189.0912	125.0154			7.34
Mepanipyrim	224.1182	209.0948	167.0703	123.0440					8.06
Metalaxyl	280.1543	248.1281	220.1332	192.1383	160.1121	148.1121			6.28
Metconazole	320.1524	177.0466	125.0153	70.0400					8.8
Methidathion	145.0066	122.0194	103.0508	85.0397	71.0249	58.0297			6.65
Methiocarb	226.0896	169.0683	121.0648	91.0542					7.15
Methiocarb-sulfone	258.0795	201.0584	137.0600	122.0728	107.0493				4.56

Methiocarb-sulfoxide	242.0845	185.0631	170.0396	168.0603	153.0369	122.0726			4.36
Methomyl	163.0536	106.0322	88.0216	72.9981	65.0058	58.0291			6.06
Methoxyfenozide	369.2173	149.0597	133.0648	93.0699	91.0542				7.54
Metobromuron	259.0077	169.9600	148.0631	62.0603					6.31
Monocrotophos	224.0682	193.0263	127.0156	98.0601	58.0291				4
Myclobutanil	289.1215	220.0888	151.0310	125.0153	70.0400				7.55
Nitenpyram	271.0956	225.1027	196.0637	190.1339	130.0975	99.0917	86.0838	56.0498	3.74
Omethoate	214.0297	196.0192	182.9876	154.9926	142.9926	61.0109			3.41
Oxadixyl	279.1339	219.1129	133.0887	132.0809	119.0856	88.0393			5.05
Oxamyl	237.1016	192.1384	90.0550	72.0452	56.0134				3.7
Paclobutrazol	294.1368	207.0936	139.0309	125.0153	87.0804	70.0400	57.0702		7.33
Paraoxon methyl	248.0319	127.0155	202.0388	89.0391	90.0469				5.13
Penconazole	284.0716	172.9921	158.9764	70.0401					8.53
Pencycuron	329.1415	261.0790	218.0732	125.0153					9.07
Pendimethalin	282.1448	194.0560	149.0584	118.0528	71.0862				10.28
Phenthoate	321.0379	247.0013	163.0755	142.9929	135.0442	107.0492	91.0543		8.35
Phosalone	367.9941	322.0064	181.9998	138.0103	110.9994				8.94
Phosmet	318.0018	248.8919	160.0395	70.0401	133.0284	105.0335	77.0386		6.93
Phoxim	299.0614	129.0447	114.9614	105.0448	95.0492				8.88
Pirimicarb	239.1503	195.1608	182.1291	72.0445					5.12
Pirimicarb, desmethyl-	225.1346	180.0767	168.1131	72.0444					4.2
Pirimiphos-methyl	306.1036	278.0726	164.1185	142.9929	136.0872	108.0557			8.74
Prochloraz	376.0381	308.0008	265.9538	194.9168	85.0886	70.0288			8.83
Profenofos	372.9424	344.9114	302.8644	222.8980	206.9209	143.9797	128.0024	114.9614	9.58
Propamocarb	189.1598	147.1129	144.1020	86.0964	74.0236	102.0549			3.47
Propaquizafop	444.1321	371.0794	299.0583	144.1020	100.0757	70.0652	56.0498		9.76
Propargite	368.189	231.1745	175.1119	107.0492	81.0699	57.0702			10.29
Propiconazole	342.0771	204.9820	186.9714	158.9765	69.0700				8.68
Propoxur	210.1125	168.0656	153.0911	111.0441	93.0335	65.0387	58.0291		5.36
Propyzamide	256.0291	189.9822	172.9558	67.0544	65.0388				7.41
Proquinazid	373.0408	330.9940	288.9470	271.9204	215.9308	162.0426			10.8
Prothioconazole	344.0386	326.0282	189.0467	114.0122	102.0121				8.68
Pymetrozine	218.1036	105.0448	79.0416						3.54
Pyraclostrobin	388.1059	194.0813	163.0628	149.0473	133.0522				8.88
Pyrethrini	329.2111	161.0960	143.0855	133.1011	69.0335				10.47
Pyrethrini	373.201	161.0960	143.0855	133.1011	105.0698	69.0335			9.3
Pyridaben	365.1449	309.0826	147.1170	132.0935	117.0699				10.95
Pyridate	379.1242	351.1294	319.1573	207.0321	71.0856	57.0702			11.38
Pyrimethanil	200.1182	183.0918	107.0604	82.0651					7.2
Pyriproxyfen	322.1438	227.1066	185.0598	134.0726	96.0444				10.04
Quinoclamine	208.016	180.0211	172.0392	137.0153	105.0335				5.46
Quinoxifen	308.004	272.0272	213.9820	196.9793					10.37
Rotenone	395.1489	213.0911	203.0704	192.0782					8.23
Spinosyn A	732.4681	142.1226	98.0964						9.08
Spinosyn D	746.4838	142.1226	98.0964						9.47

Spirodiclofen	411.1124	313.0391	295.0286	230.9610	71.0856				10.58
Spiromesifen	371.2217	255.1379	227.1430	187.0754					10.29
Spirotetramat	374.1962	330.2064	302.1752	298.1803	270.1489	244.1333			7.73
Spiroxamine	298.2741	144.1384	100.1120	72.0808	58.0654				7.32
Tebuconazole	308.1524	125.0155	70.0402						8.5
Tebufenozide	353.2224	297.1600	203.1546	133.0650	123.0806	72.0809			8.27
Tebufenpyrad	334.1681	171.0321	147.1169	145.0528					9.71
Terbuthylazine	230.1167	174.0543	96.0557	79.0058					7.22
Tetraconazole	372.0288	184.9922	176.9670	158.9764	70.0401				7.94
Thiabendazole	202.0433	175.0324	131.0604	65.0386					4.5
Thiacloprid	253.0309	211.0092	186.0140	126.0106					4.8
Thiamethoxam	292.0266	246.0339	211.0650	181.0544	131.9671				3.95
Thiobencarb	258.0714	125.0153	100.0757	72.0444					9.02
Thiodicarb	355.0563	107.9937	88.0216	78.9671	72.9981	62.0062			6.06
Thiophanate-methyl	343.0529	311.0268	268.0210	235.9948	226.0646	160.0507	151.0326		5.36
Tolclofos-methyl	300.9616	286.9458	174.9712	142.9926	127.0154				9.03
Triadimefon	294.1004	225.0676	197.0728	115.0754	69.0700	57.0702			7.5
Triadimenol	296.116	209.0713	99.0811	70.0408	57.0709	156.0811	183.0920	227.0819	7.65
Triazophos	314.0723	286.0409	178.0434	162.0662	114.9614				7.76
Trichlorfon	256.9299	220.9534	144.9818	127.0156	93.0101	78.9944			4.36
Trifloxystrobin	409.137	206.0814	186.0527	134.0601	131.0731	116.0496			9.24
Triflumuron	359.0405	178.0476	156.0212	138.9947	113.0153				8.9
Triticonazole	318.1368	191.0625	125.0155	70.0401					7.81
Zoxamide	336.0319	203.9981	186.9715	132.0577					8.67