Electronic Supplementary Material (ESI) for Analytical Methods.

Support information

Multi-pesticide residue analysis by High Resolution Mass Spectrometry in complementary matrices: wheat flour, lettuce and apple samples

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Table S1. HRMS parameters used for identification of the target compounds.

Pesticides	RT (min)	Elemental composition	Class[c]	Selected ion	m/z experimental	m/z calculated	Mass error (ppm)
2,4 –D[a]	9.7	$C_8H_6Cl_2O_3$	H	$[M + H]^-$	218.9610	218.9666	2.6
Acetamiprid [a]	7.8	$C_{10}H_{11}ClN_4$	I	$[M + H]^+$	223.0745	223.0746	0.3
Ametryn[a]	9.9	$C_9H_{17}N_5S$	H	$[M + H]^+$	228.1277	228.1284	3.0
Azoxystrobin[b]	12.6	$C_{22}H_{17}N_3O_5$	F	$[M + H]^+$	404.1240	404.1242	0.2
Benalaxyl [a]	11.3	$C_{20}H_{23}NO_3$	F	$[M + H]^+$	326.1750	326.1753	0.8
Bendiocarb [a]	9.1	$C_{11}H_{13}NO_4$	I	$[M + H]^+$	224.0917	224.0917	0.2
Bentazon [a]	10.1	$C_{10}H_{12}N_2O_3S$	H	$[M + H]^-$	239.0484	239.0493	3.8
Bioallethrin [a]	13.9	$C_{19}H_{26}O_3$	I	$[M + H]^+$	303.1954	303.1985	5.0
Bitertanol [a]	15.2	$C_{20}H_{23}N_3O_2$	F	$[M + H]^+$	338.1863	338.1863	0.0
Boscalid [a]	12.8	$C_{18}H_{12}Cl_2N_2O$	F	$[M + H]^+$	343.0399	343.0399	0.2
Bromoxynil [a]	9.6	$C_7H_3Br_2NO$	H	$[M + H]^-$	273.8497	273.8500	5.0
Carbaryl [a]	11.7	$C_{12}H_{11}NO_2$	I	$[M + H]^+$	202.0862	202.0861	1.0
Carbendazin [a]	8.3	$C_9H_9N_3O_2$	F	$[M + H]^+$	192.0767	192.0760	3.7
Carbofuran[b]	9.1	$C_{12}H_{15}NO_3$	I	$[M + H]^+$	222.1124	222.1126	0.5
Carboxine [a]	9.2	$C_{12}H_{13}NO_2S$	F	$[M + H]^+$	236.0739	236.0748	3.4
Chlorantraniliprole [a]	10.7	$C_{18}H_{14}BrCl_2N_5O_2$	I	$[M + H]^+$	483.9757	483.9770	5.0

Cyproconazol [a]	13.6	$C_{15}H_{18}ClN_3O$	F	$[M + H]^+$	292.1211	292.1206	1.7
Chlorpyriphos [a]	15.8	$C_9H_{11}Cl_3NO_3PS$	I	$[M + H]^+$	349.9335	349.9324	3.2
Clothianidin [a]	7.7	$C_6H_8ClN_5O_2S$	F	$[M + H]^+$	250.0159	250.0178	2.6
Cymoxanil [a]	8.2	$C_7H_{10}N_4O_3$	F	$[M + Na]^+$	221.0645	221.0666	2.1
Cyprodinil [a]	11.1	$C_{14}H_{13}N_3$	F	$[M + H]^-$	226.1338	226.1371	3.4
Dazomet [a]	8.4	$C_5H_{10}N_2S_2$	F	$[M + H]^+$	163.0358	163.0336	4.1
Diazinon [a]	11.4	$C_{12}H_{21}N_2O_3PS$	I	$[M + H]^+$	305.1083	305.1088	1.6
Diclofop-methyl [a]	12.8	$C_{16}H_{14}Cl_2O_4$	H	$[M + NH_4]^+$	358.0607	358.0604	1.0
Dichlorvos[b]	9.1	$C_4H_7Cl_2O_4P$	I	$[M + H]^+$	220.9531	220.9542	4.5
Difenoconazol [a]	15.6	$C_{19}H_{17}Cl_2N_3O_3$	F	$[M + H]^+$	406.0719	406.0707	3.2
Dimethoate [a]	10.0	$C_5H_{12}NO_3PS_2$	I	$[M + H]^+$	230.0068	230.0069	0.1
Dimethomorph [a]	9.9	$C_{21}H_{22}ClNO_4$	F	$[M + H]^+$	388.1310	388.1303	1.8
Diuron [a]	12.4	$C_9H_{10}Cl_2N_2O$	H	$[M + H]^+$	233.0242	233.0246	1.2
Ethion [a]	13.5	$C_9H_{22}O_4P_2S_4$	I	$[M + H]^+$	384.9948	384.9945	0.9
Etoxazole [a]	15.9	$C_{21}H_{23}F_2NO_2$	Ac	$[M + H]^+$	360.1769	360.1760	2.6
Fenamidone [a]	9.9	$C_{17}H_{17}N_3OS$	F	$[M + H]^+$	312.1165	312.1165	0.2
Fenarimol [a]	10.2	$C_{17}H_{12}Cl_2N_2O$	F	$[M + H]^+$	331.0399	331.0386	4.2
Fenitrothion[b]	10.4	$C_9H_{12}NO_5PS$	I	$[M + H]^+$	278.0246	278.0255	4.4
Fenpropathrin [a]	16.8	$C_{22}H_{23}NO_3$	I	$[M + H]^+$	350.1751	350.1743	2.3
Fluazinam [a]	13.2	$C_{13}H_4Cl_2F_6N_4O_4$	F	$[M + H]^-$	462.9430	462.9490	3.9

Flufenoxuron [a]	13.8	$C_{21}H_{11}ClF_6N_2O_3$	Ac	$[M + H]^+$	489.0435	489.0459	4.9
Fenpyroximate [a]	12.9	$C_{24}H_{27}N_3O_4$	Ac	$[M + H]^+$	422.2074	422.2062	3.0
Fenthion [a]	15.1	$C_{10}H_{15}O_3PS_2$	I	$[M + H]^+$	279.0220	279.0270	4.6
Fipronil [a]	13.5	$C_{12}H_4Cl_2F_6N_4OS$	I	$[M + NH_4]^+$	453.9725	453.9718	1.6
Fluopicolide [a]	10.1	$C_{14}H_8Cl_3F_3N_2O$	F	$[M + H]^+$	382.9727	382.9758	4.1
Fluquinconazole [a]	11.4	$C_{16}H_8Cl_2FN_5O$	F	$[M + H]^+$	376.0162	376.0153	2.6
Fluxapyroxad [a]	10.0	$C_{18}H_{12}F_5N_3O$	F	$[M + H]^+$	382.0973	382.0973	0.0
Flutriafol [a]	11.9	$C_{16}H_{13}F_2N_3O$	F	$[M + H]^+$	302.1099	302.1103	1.2
Hexaconazol [a]	11.8	$C_{14}H_{17}Cl_2N_3O$	F	$[M + H]^+$	314.0821	314.0852	4.9
Imazalil [a]	11.2	$C_{14}H_{14}Cl_2N_2O$	F	$[M + H]^+$	297.0555	297.0561	1.7
Imidacloprid [b]	9.3	$C_9H_{10}ClN_5O_2$	I	$[M + H]^+$	256.0595	256.0597	0.6
Iprovalicarb [a]	13.3	$C_{18}H_{28}N_2O_3$	F	$[M + H]^+$	321.2172	321.2199	2.1
Imibenconazole [a]	13.7	$C_{17}H_{13}Cl_3N_4S$	F	$[M + H]^+$	412.9970	412.9993	4.4
Indoxacarb [a]	15.2	$C_{22}H_{17}ClF_3N_3O_7$	I	$[M + H]^+$	528.0779	528.0765	2.8
kresoxim-methyl [a]	10.9	$C_{18}H_{19}NO_4$	F	$[M + H]^+$	314.1386	314.1384	0.8
Lufenuron [a]	12.5	$C_{17}H_8Cl_2F_8N_2O_3$	I	$[M + H]^-$	508.9700	508.9711	2.2
ʎ-Cyhalothrin [a]	15.5	$C_{23}H_{19}ClF_3NO_3$	I	$[M + NH4]^+$	467.1344	467.1327	3.6
Metalaxyl-M [a]	9.6	$C_{15}H_{21}NO_4$	F	$[M + H]^+$	280.1509	280.1546	2.1
Methamidophos [a]	4.8	$C_2H_8NO_2PS$	I	$[M + H]^+$	142.0086	142.0099	1.7
Metconazol [a]	15.5	$C_{17}H_{22}ClN_3O$	F	$[M + H]^+$	320.1524	320.1522	0.8

Methidathion [a]	9.8	$C_6H_{11}N_2O_4PS_3$	I	$[M + H]^+$	302.9691	302.9696	1.6
Methomyl[b]	8.3	$C_5H_{10}N_2O_2S$	I	$[M + H]^+$	163.0536	163.0538	1.2
Metribuzin[b]	9.3	$C_8H_{14}N_4OS$	H	$[M + H]^+$	215.0961	215.0980	4.4
Myclobutanil [a]	10.4	$C_{15}H_{17}ClN_4$	F	$[M + H]^+$	289.1214	289.1238	4.7
Novaluron [a]	11.4	$C_{17}H_9ClF_8N_2O_4$	I	$[M + H]^-$	491.0039	491.0063	4.3
Parathion methyl[b]	10.0	$C_8H_{10}NO_5PS$	I	$[M + H]^+$	264.0090	264.0085	1.9
Pedimentalina [a]	14.5	$C_{13}H_{19}N_3O_4$	H	$[M + H]^+$	282.1448	282.1490	4.2
Phosmet [a]	9.7	$C_{11}H_{12}NO_4PS_2$	I	$[M + H]^+$	318.0018	318.0023	3.9
Phorate [a]	10.0	$C_7H_{17}O_2PS_3$	I	$[M + H]^+$	261.0201	261.0214	4.9
Phoxim [a]	15.0	$C_{12}H_{15}N_2O_3PS$	I	$[M + H]^+$	299.0614	299.0613	0.4
Pyraclostrobin [a]	11.0	$C_{19}H_{18}ClN_3O_4$	F	$[M + H]^+$	388.1058	388.1055	1.0
Pyrazophos[b]	15.8	$C_{14}H_{20}N_3O_5PS$	F	$[M + H]^+$	374.0934	374.0928	1.6
Pirimicarb [b]	9.1	$C_{11}H_{18}N_4O_2$	I	$[M + H]^+$	239.1502	239.1506	1.5
Pirimiphos-methyl [a]	15.6	$C_{11}H_{20}N_3O_3PS$	I	$[M + H]^+$	306.1035	306.1037	0.5
Pyriproxifen [a]	13.1	$C_{20}H_{19}NO_3$	I	$[M + H]^+$	322.1437	322.1467	4.5
Prochloraz [a]	11.4	$C_{15}H_{16}Cl_3N_3O_2$	H	$[M + H]^+$	376.0380	376.0369	3.1
Propargite [a]	16.1	$C_{19}H_{26}O_4S$	H	$[M + NH_4]^+$	368.1890	368.1876	3.8
Pyridaben [a]	9.5	$C_{19}H_{25}ClN_2OS$	H	$[M + H]^+$	365.1468	365.1470	0.8
Pyrimethanil [a]	12.9	$C_{12}H_{13}N_3$	I	$[M + H]^+$	200.1182	200.1185	1.2
Simazin [a]	9.2	$C_7H_{12}ClN_5$	H	$[M + H]^+$	202.0854	202.0870	4.8

Spinosad A [a]	13.7	$C_{41}H_{65}NO_{10}$	I	$[M + H]^+$	732.4681	732.4694	1.7
Spinosad D [a]	10.1	$C_{42}H_{67}NO_{10}$	I	$[M + H]^+$	746.4838	746.4852	1.9
Spiromesifen [a]	14.9	$C_{23}H_{30}O_4$	I	$[M + H]^+$	371.2216	371.2212	1.2
Tebuconazol [b]	11.2	$C_{16}H_{22}ClN_3O$	H	$[M + H]^+$	308.1524	308.1523	0.5
Tebufenozide [a]	10.9	$C_{22}H_{28}N_2O_2$	I	$[M + H]^-$	353.2223	353.2224	0.7
Tetraconazole [a]	10.4	$C_{13}H_{11}Cl_2F_4N_3O$	I	$[M + H]^+$	372.0288	372.0286	0.5
Thiabendazole [a]	8.9	$C_{10}H_7N_3S$	F	$[M + H]^+$	202.0433	202.0435	0.9
Thiophanate- methyl [a]	11.5	$C_{12}H_{14}N_4O_4S_2$	F	$[M + H]^+$	343.0529	343.0536	2.0
Thiamethoxam [a]	6.9	$C_8H_{10}ClN_5O_3S$	I	$[M + H]^+$	292.0265	292.0261	1.7
Triadimefon [b]	10.3	$C_{14}H_{16}ClN_3O_2$	I	$[M + H]^+$	294.1004	294.1004	0.0
Triadimenol [b]	10.5	$C_{14}H_{18}ClN_3O_2$	I	$[M + H]^+$	296.1160	296.1170	3.2
Trichlorfon [a]	8.0	$C_4H_8Cl_3O_4P$	I	$[M + H]^+$	256.9298	256.9301	0.8
Trifloxystrobin [a]	11.7	$C_{20}H_{19}F_3N_2O_4$	F	$[M + H]^+$	409.1369	409.1371	0.4
Triflumizole [a]	11.8	$C_{15}H_{15}ClF_3N_3O$	F	$[M + H]^+$	346.0928	346.0925	1.0
Triforin [a]	9.7	$C_{10}H_{14}Cl_6N_4O_2$	F	$[M + H]^-$	432.9135	432.9153	4.1
Zoxamide [a]	16.9	$C_{14}H_{16}Cl_3NO_2$	F	$[M + H]^+$	336.0319	336.0322	0.8

Table 2: Validation parameters of the optimized method.

	R^2	Matrix effect	Recovery (%)		Inter-day precision (% RSD)	Intra-day precision (% RSD)	LOD (μg kg^{-1})	LOQ (μg kg^{-1})
			10 (μg kg^{-1})	200 (μg kg^{-1})				
Apple samples								
2,4 –D	0.991	-45.4	83.0	74.1	3.6	3.9	5	10
Acetamiprid	0.999	-11.9	93.6	100.9	10.2	4.6	1	5
Ametryn	0.997	-4.4	102.4	98.8	4.8	3.9	1	5
Azoxystrobin	0.999	-5.1	100.4	102.3	4.6	2.2	1	5
Benalaxyl	0.990	-7.1	99.4	100.8	6.7	5.5	1	5
Bendiocarb	0.999	-2.5	104.4	101.0	6.1	3.4	5	10
Bentazon	0.993	-17.5	89.7	104.0	12.4	2.9	1	5
Bioallethrin	0.999	-8.4	106.5	101.1	4.7	4.5	5	10
Bitertanol	0.998	-7.2	111.1	104.3	11.9	9.2	7	10
Boscalid	0.999	-10.5	92.5	99.6	18.5	6.1	2	5
Bromoxynil	0.999	3.5	108.0	104.1	1.5	1.6	7	10
Carbaryl	0.998	-7.6	100.3	97.4	10.4	2.1	2	5
Carbendazin	0.999	17.8	91.6	103.5	14.9	5.8	2	5
Carbofuran	0.999	-3.1	101.3	99.4	6.1	3.4	2	5
Carboxine	0.998	-8.4	103.6	97.4	8.6	6.3	3	5
Chlorantraniliprole	0.999	-5.4	97.7	102.7	15.5	6.0	1	5
Cyproconazol	0.998	1.8	115.4	101.3	9.8	3.0	7	10
Chlorpyriphos	0.992	-9.3	92.1	102.5	8.5	5.0	1	5

Clothianidin	0.999	-24.1	85.1	89.1	10.2	7.1	1	5
Cymoxanil	0.999	-11.4	95.2	90.0	8.9	5.8	3	5
Cyprodinil	0.999	-18.6	98.7	97.0	3.0	2.9	1	5
Dazomet	0.999	-63.5	73.8	77.1	16.3	18.7	8	10
Diazinon	0.999	-15.9	93.1	98.6	2.8	3.5	1	5
Diclofop-methyl	0.998	-21.0	86.5	97.9	10.1	4.2	3	5
Dichlorvos	0.997	3.1	102.4	100.6	7.3	4.5	3	5
Difenoconazol	0.995	-2.5	98.2	100.7	10.7	5.4	2	5
Dimethoate	0.999	-5.7	95.9	95.6	8.6	1.9	1	5
Dimethomorph	0.999	11.6	105.7	108.9	17.9	5.7	2	5
Diuron	0.998	7.0	106.5	101.2	4.9	3.3	3	5
Ethion	0.998	-7.6	99.1	101.4	5.5	4.4	3	5
Etoxazole	0.999	-7.2	101.6	100.2	8.2	6.9	3	5
Fenamidone	0.992	8.3	96.4	105.7	18.7	8.9	5	10
Fenarimol	0.999	-10.9	99.9	101.9	10.7	2.0	3	5
Fenitrothion	0.997	-25.7	102.9	97.1	9.2	9.1	3	5
Fenpropathrin	0.998	-3.7	87.5	99.2	15.8	12.6	2	5
Fluazinam	0.999	11.1	107.0	106.6	6.3	2.2	3	5
Flufenoxuron	0.999	-6.0	106.9	98.2	12.5	8.8	5	10
Fenpyroximate	0.999	-8.4	91.2	97.9	17.4	13.3	3	5
Fenthion	0.998	-20.8	100.2	100.9	8.8	3.2	5	10
Fipronil	0.994	-9.3	92.8	101.7	19.0	3.6	8	10
Fluopicolide	0.999	-7.2	100.1	104.4	9.6	3.0	3	5
Fluquinconazole	0.995	-16.2	99.5	93.9	8.3	11.4	5	10

Fluxapyroxad	0.999	-4.3	100.5	101.1	8.0	5.1	5	10
Flutriafol	0.999	-7.1	87.1	97.3	18.7	6.8	5	10
Hexaconazol	0.999	-3.7	90.8	99.8	10.2	4.0	5	10
Imazalil	0.999	-4.7	100.3	99.9	5.2	3.6	3	5
Imidacloprid	0.991	12.9	73.3	96.4	14.0	10.5	5	10
Iprovalicarb	0.999	-5.9	111.6	118.1	9.1	1.7	3	5
Imibenconazole	0.997	-12.9	112.8	113.8	7.7	4.1	8	10
Indoxacarb	0.999	6.8	100.8	102.9	11.1	1.9	5	10
kresoxim-methyl	0.998	-7.7	106.9	101.7	3.7	4.8	5	10
Lufenuron	0.999	60.3	115.1	112.0	13.7	2.4	3	5
ƛ-Cyhalothrin	0.998	7.2	102.6	95.5	7.6	6.8	3	5
Metalaxyl-M	0.990	-3.2	103.6	102.6	4.4	1.8	5	10
Methamidophos	0.999	-67.0	110.2	101.2	14.9	10.5	5	10
Metconazol	0.999	-2.3	105.4	105.8	6.9	3.3	2	5
Methidathion	0.999	-8.5	103.9	101.2	6.8	2.6	5	10
Methomyl	0.995	13.5	93.3	90.9	8.6	4.5	10	20
Metribuzin	0.999	-11.6	89.7	93.2	7.6	2.8	3	5
Myclobutanil	0.993	-5.4	101.8	106.3	6.0	2.5	5	10
Novaluron	0.999	5.2	101.9	81.4	14.3	1.6	5	10
Parathion methyl	0.997	-33.6	102.0	91.6	7.0	5.5	8	10
Pedimentalina	0.997	-11.4	107.4	97.9	4.8	6.3	8	10
Phosmet	0.999	-11.1	113.0	104.8	7.1	1.6	5	10
Phorate	0.999	-42.9	94.8	101.1	13.4	5.1	8	10
Phoxim	0.993	-4.5	104.2	98.2	6.0	2.1	8	10

Pyraclostrobin	0.999	-7.4	101.3	101.8	4.5	2.3	3	5
Pyrazophos	0.999	3.6	108.3	110.1	11.7	5.3	5	10
Pirimicarb	0.996	-7.5	106.5	98.9	6.0	3.7	3	5
Pirimiphos-methyl	0.999	-8.5	97.6	100.9	7.1	4.1	8	10
Pyriproxifen	0.999	-9.7	95.0	99.0	9.0	6.1	8	10
Prochloraz	0.998	-11.5	99.3	106.2	9.2	3.6	5	10
Propargite	0.998	-16.4	97.6	102.4	12.1	3.8	8	10
Pyridaben	0.997	-41.9	108.9	88.3	17.5	14.3	10	20
Pyrimethanil	0.999	-6.2	101.3	98.5	3.4	4.8	5	10
Simazin	0.998	-7.6	101.9	97.6	6.1	3.0	5	10
Spinosad A	0.999	-7.9	99.4	100.6	3.9	5.1	8	10
Spinosad D	0.998	-8.8	109.1	101.8	4.4	2.9	8	10
Spiromesifen	0.998	-10.8	99.5	101.1	8.7	2.9	5	10
Tebuconazol	0.999	-1.7	107.6	103.5	6.7	3.7	8	10
Tebufenozide	0.999	0.5	110.3	105.7	2.9	1.3	5	10
Tetraconazole	0.998	-12.5	100.9	104.4	8.3	1.0	8	10
Thiabendazole	0.999	-14.7	88.7	90.7	6.4	2.2	5	10
Thiophanate- methyl	0.999	-13.7	97.2	98.3	11.5	3.5	8	10
Thiamethoxam	0.999	-6.3	102.6	101.0	7.4	1.5	10	20
Triadimefon	0.992	4.8	97.5	98.5	12.8	12.0	10	20
Triadimenol	0.998	9.0	99.2	104.1	15.5	17.9	5	10
Trichlorfon	0.998	-23.2	85.4	86.6	15.9	4.4	8	10
Trifloxystrobin	0.999	-10.1	99.2	104.1	10.5	2.3	5	10
Triflumizole	0.999	-4.4	100.1	101.7	8.6	3.8	8	10

Triforin	0.997	-22.6	101.0	94.6	7.5	5.9	5	10
Zoxamide	0.996	-6.8	102.2	102.9	8.0	3.4	5	10
Lettuce samples								
2,4 –D	0.993	11.8	103.9	91.3	9.1	14.0	5	10
Acetamiprid	0.999	-3.7	94.8	96.3	9.7	6.1	1	5
Ametryn	0.997	-11.6	94.5	93.7	6.9	3.4	5	10
Azoxystrobin	0.999	-15.1	85.2	87.2	8.8	5.2	1	5
Benalaxyl	0.994	-0.8	102.3	99.7	7.4	6.4	1	5
Bendiocarb	0.999	-4.7	103.6	97.7	9.9	5.4	5	10
Bentazon	0.992	34.2	113.8	92.8	1.6	3.2	1	5
Bioallethrin	0.999	-2.1	100.8	103.4	14.4	6.9	5	10
Bitertanol	0.998	8.1	107.7	106.2	12.2	3.3	7	10
Boscalid	0.999	2.4	99.8	110.9	17.9	8.0	2	5
Bromoxynil	0.995	4.8	117.6	112.7	6.5	5.9	7	10
Carbaryl	0.998	-7.9	96.4	97.4	10.2	4.3	5	10
Carbendazin	0.999	11.6	102.5	114.0	16.2	5.7	2	5
Carbofuran	0.999	-1.2	100.7	101.3	8.7	1.9	5	10
Carboxine	0.998	-10.9	88.8	92.8	14.3	10.0	3	5
Chlorantraniliprole	0.993	-15.3	83.1	91.4	15.4	10.0	1	5
Cyproconazol	0.998	17.1	113.3	101.7	19.2	8.3	7	10
Chlorpyriphos	0.999	-11.1	84.3	92.0	9.4	8.8	5	10
Clothianidin	0.999	4.2	98.7	100.9	10.2	1.9	1	5
Cymoxanil	0.999	-16.0	96.9	93.8	11.7	9.4	5	10
Cyprodinil	0.999	-5.3	98.4	95.8	8.4	6.9	1	5

Dazomet	0.999	-47.8	72.9	101.7	13.5	4.6	2	5
Diazinon	0.996	-11.4	91.9	96.1	9.6	6.2	1	5
Diclofop-methyl	0.998	1.5	88.8	99.6	17.0	11.0	3	5
Dichlorvos	0.997	2.6	108.4	103.4	10.0	6.2	3	5
Difenoconazol	0.999	5.1	92.2	99.7	11.6	7.1	2	5
Dimethoate	0.999	1.1	101.8	100.5	10.7	1.9	1	5
Dimethomorph	0.992	21.3	110.9	115.9	10.2	15.6	2	5
Diuron	0.998	-41.9	75.3	70.3	13.0	10.5	5	10
Ethion	0.998	3.0	97.4	98.9	12.6	6.5	3	5
Etoxazole	0.999	0.7	100.5	96.9	14.0	8.4	3	5
Fenamidone	0.999	19.5	82.4	114.7	13.9	1.7	5	10
Fenarimol	0.999	-5.5	89.2	96.8	19.0	6.0	3	5
Fenitrothion	0.997	-15.7	96.4	93.9	11.0	7.5	3	5
Fenpropathrin	0.998	16.1	112.2	115.8	18.1	11.2	2	5
Fluazinam	0.992	-1.6	104.9	109.4	11.2	2.5	3	5
Flufenoxuron	0.999	0.3	106.7	103.6	18.1	14.9	5	10
Fenpyroximate	0.999	19.2	113.7	117.9	18.6	12.4	6	10
Fenthion	0.998	-15.0	92.0	96.6	11.4	10.3	5	10
Fipronil	0.994	15.1	102.7	115.8	8.6	4.7	8	10
Fluopicolide	0.999	-1.3	101.3	107.9	9.3	7.9	3	5
Fluquinconazole	0.995	4.6	97.8	109.0	13.1	9.9	5	10
Fluxapyroxad	0.992	1.7	103.9	104.6	6.9	5.2	5	10
Flutriafol	0.999	-2.3	96.6	112.4	16.2	11.7	5	10
Hexaconazol	0.999	-5.4	84.5	99.4	18.3	4.9	5	10

Imazalil	0.999	-12.8	84.2	86.9	19.0	14.2	3	5
Imidacloprid	0.994	11.1	97.5	105.5	19.3	12.9	5	10
Iprovalicarb	0.999	1.3	105.6	110.0	10.8	3.6	3	5
Imibenconazole	0.997	17.4	107.4	108.0	8.4	3.9	8	10
Indoxacarb	0.991	6.6	109.4	102.5	5.4	5.1	5	10
kresoxim-methyl	0.998	-4.2	98.2	98.8	15.7	5.8	5	10
Lufenuron	0.999	-14.5	118.8	94.0	16.1	6.5	3	5
ʎ-Cyhalothrin	0.998	-8.4	99.4	106.0	6.0	5.7	3	5
Metalaxyl-M	0.993	-22.1	78.3	79.9	9.1	6.6	5	10
Methamidophos	0.999	-93.1	116.5	118.3	18.5	15.7	3	5
Metconazol	0.999	3.8	94.9	102.8	14.9	7.1	2	5
Methidathion	0.992	-14.1	73.9	72.4	11.6	5.8	5	10
Methomyl	0.995	12.1	96.6	92.7	11.7	7.7	10	20
Metribuzin	0.999	-7.7	111.2	114.7	19.0	10.5	3	5
Myclobutanil	0.992	20.6	91.1	85.0	11.4	11.3	3	5
Novaluron	0.999	2.3	92.8	93.2	12.9	2.8	5	10
Parathion methyl	0.997	-45.3	91.1	85.0	11.4	11.3	8	10
Pedimentalina	0.996	-4.4	87.6	105.8	10.6	7.1	8	10
Phosmet	0.999	-20.5	101.7	92.8	9.3	4.0	5	10
Phorate	0.999	-19.5	88.0	91.2	14.3	11.1	8	10
Phoxim	0.999	-10.5	93.5	105.0	7.9	3.7	8	10
Pyraclostrobin	0.999	-3.6	97.1	100.6	7.1	2.3	5	10
Pyrazophos	0.999	1.1	116.3	108.1	7.6	6.0	2	5
Pirimicarb	0.999	-1.2	95.3	96.8	12.3	5.1	3	5

Pirimiphos-methyl	0.999	-0.6	97.1	97.8	9.1	6.8	8	10
Pyriproxifen	0.992	-6.3	90.1	94.5	13.6	7.7	8	10
Prochloraz	0.999	-8.4	94.1	94.4	19.6	14.6	5	10
Propargite	0.998	-4.7	98.4	100.3	9.4	7.4	8	10
Pyridaben	0.997	-37.4	94.1	96.7	13.5	10.5	8	10
Pyrimethanil	0.999	-12.9	90.9	80.5	13.0	10.5	5	10
Simazin	0.998	-7.9	99.8	97.7	6.5	4.5	5	10
Spinosad A	0.993	-2.5	105.8	98.3	9.8	4.8	8	10
Spinosad D	0.998	-3.9	101.2	109.3	6.3	4.1	8	10
Spiromesifen	0.992	-7.8	112.3	92.6	16.2	11.6	5	10
Tebuconazol	0.999	2.7	99.5	101.3	11.6	5.6	8	10
Tebufenozide	0.999	10.1	97.0	105.7	2.5	1.4	10	20
Tetraconazole	0.998	6.1	112.5	109.9	6.6	6.4	8	10
Thiabendazole	0.993	-9.9	85.8	91.2	11.8	5.3	5	10
Thiophanate- methyl	0.999	-21.4	85.5	83.6	15.3	11.0	8	10
Thiamethoxam	0.999	-3.1	106.4	98.7	8.6	3.2	10	20
Triadimefon	0.999	23.8	117.3	113.7	13.4	13.3	10	20
Triadimenol	0.998	37.8	114.5	101.5	8.6	6.6	5	10
Trichlorfon	0.998	-10.8	106.9	97.7	11.3	2.5	8	10
Trifloxystrobin	0.992	-2.0	96.3	97.5	12.3	7.2	5	10
Triflumizole	0.999	-2.9	98.2	96.3	14.8	9.6	8	10
Triforin	0.997	-13.2	107.7	101.0	16.3	11.0	5	10
Zoxamide	0.996	4.6	98.6	108.6	6.7	3.4	5	10
Wheat flour samples								

2,4 –D	0.999	-4.6	97.7	96.7	8.2	3.7	5	10
Acetamiprid	0.999	-15.1	83.7	95.1	15.8	3.6	1	5
Ametryn	0.997	-5.5	98.7	92.0	7.5	6.8	1	5
Azoxystrobin	0.999	-4.8	101.1	98.9	6.5	4.6	5	10
Benalaxyl	0.999	-3.2	94.3	102.1	12.3	6.9	1	5
Bendiocarb	0.992	-2.9	96.6	102.9	7.3	6.1	5	10
Bentazon	0.999	-17.5	108.7	102.2	10.6	3.2	1	5
Bioallethrin	0.999	-4.1	108.0	111.7	5.9	5.0	5	10
Bitertanol	0.998	10.3	95.8	93.4	11.1	4.9	7	10
Boscalid	0.993	-14.8	93.4	6.6	103.3	3.2	2	5
Bromoxynil	0.999	4.1	80.3	88.3	11.2	2.1	7	10
Carbaryl	0.998	-11.3	100.5	92.0	10.0	5.7	5	10
Carbendazin	0.999	-2.8	72.5	92.3	16.1	5.4	2	5
Carbofuran	0.999	1.7	101.9	98.8	8.6	4.9	2	5
Carboxine	0.998	-7.6	98.3	92.5	7.1	6.6	3	5
Chlorantraniliprole	0.996	10.5	115.1	112.5	10.9	9.4	1	5
Cyproconazol	0.998	9.4	111.6	93.2	12.8	7.7	7	10
Chlorpyriphos	0.999	-43.3	80.5	74.7	17.3	3.7	5	10
Clothianidin	0.999	0.2	96.8	100.4	9.5	4.8	1	5
Cymoxanil	0.995	-14.9	82.6	86.7	9.6	9.5	3	5
Cyprodinil	0.999	-37.5	88.2	80.4	8.5	6.2	1	5
Dazomet	0.999	-24.3	92.2	85.7	12.9	7.1	2	5
Diazinon	0.999	-14.8	89.6	85.0	8.9	6.8	1	5
Diclofop-methyl	0.998	-18.4	79.3	70.1	19.2	15.1	3	5

Dichlorvos	0.997	9.4	94.0	99.8	12.9	8.8	3	5
Difenoconazol	0.993	-30.4	83.7	83.9	11.4	10.4	5	10
Dimethoate	0.999	-1.7	94.1	95.3	8.7	3.1	1	5
Dimethomorph	0.999	18.9	113.4	118.4	19.0	8.2	2	5
Diuron	0.998	-78.1	77.3	83.9	10.4	3.7	3	5
Ethion	0.998	-7.4	84.2	82.0	6.2	5.0	5	10
Etoxazole	0.999	-2.8	96.3	94.0	19.5	16.2	3	5
Fenamidone	0.999	8.3	108.2	10.6	117.1	3.1	5	10
Fenarimol	0.992	-12.9	99.5	91.6	4.7	3.9	3	5
Fenitrothion	0.997	-33.3	91.7	81.2	17.9	8.8	3	5
Fenpropathrin	0.998	-7.8	96.1	98.4	19.4	15.5	2	5
Fluazinam	0.999	-1.6	119.9	108.9	3.4	1.6	3	5
Flufenoxuron	0.999	-12.5	111.5	117.2	9.4	3.8	5	10
Fenpyroximate	0.999	9.2	110.4	112.8	16.7	14.9	3	5
Fenthion	0.998	-21.2	82.4	87.2	15.1	5.9	5	10
Fipronil	0.999	4.8	99.7	108.8	18.6	14.9	8	10
Fluopicolide	0.996	-6.6	97.7	109.2	18.7	8.6	3	5
Fluquinconazole	0.995	-8.9	95.7	100.8	12.8	3.3	5	10
Fluxapyroxad	0.999	-5.6	85.3	96.0	13.9	12.9	5	10
Flutriafol	0.999	-7.8	102.8	100.4	7.7	4.3	5	10
Hexaconazol	0.993	-25.1	110.6	17.2	112.9	10.8	5	10
Imazalil	0.999	-4.2	99.3	97.2	8.7	6.5	3	5
Imidacloprid	0.999	15.1	118.0	114.3	15.0	3.2	5	10
Iprovalicarb	0.999	1.6	103.8	112.6	8.8	4.4	3	5

Imibenconazole	0.997	-5.1	85.0	102.2	14.9	3.1	8	10
Indoxacarb	0.999	6.4	117.3	118.5	17.2	2.5	5	10
kresoxim-methyl	0.998	-14.6	70.1	89.2	16.9	2.9	5	10
Lufenuron	0.999	60.3	103.7	91.2	10.7	5.5	5	10
ʎ-Cyhalothrin	0.998	-19.8	94.7	93.1	21.6	14.5	3	5
Metalaxyl-M	0.999	-2.4	100.5	93.7	7.6	5.7	5	10
Methamidophos	0.999	-57.6	119.2	115.9	7.7	4.0	5	10
Metconazol	0.999	-21.2	80.4	86.2	18.0	10.1	2	5
Methidathion	0.999	-38.6	72.1	80.1	11.4	3.8	5	10
Methomyl	0.995	16.2	89.5	92.3	11.6	11.7	10	20
Metribuzin	0.999	-11.6	88.7	94.4	13.2	5.2	3	5
Myclobutanil	0.993	18.4	115.2	112.5	10.8	9.9	3	5
Novaluron	0.999	5.2	89.0	115.1	13.9	5.4	5	10
Parathion methyl	0.997	-49.6	81.0	89.6	7.3	5.2	8	10
Pedimentalina	0.997	-13.4	76.2	97.7	17.4	3.8	8	10
Phosmet	0.999	-39.7	84.3	76.2	9.9	4.2	5	10
Phorate	0.999	-51.0	71.9	83.0	13.4	10.8	5	10
Phoxim	0.999	-16.1	84.9	98.4	14.0	6.4	8	10
Pyraclostrobin	0.999	-8.3	98.4	95.3	14.7	3.8	3	5
Pyrazophos	0.999	11.0	114.9	111.3	17.9	12.8	2	5
Pirimicarb	0.992	-1.9	97.2	104.1	7.2	4.4	3	5
Pirimiphos-methyl	0.999	-6.8	92.5	80.9	9.2	6.2	8	10
Pyriproxifen	0.999	-8.9	76.6	78.6	7.8	4.5	8	10
Prochloraz	0.999	-2.5	108.3	103.7	5.0	4.9	5	10

Propargite	0.998	-8.4	85.7	95.5	10.9	5.8	8	10
Pyridaben	0.997	-47.7	77.0	112.9	14.1	13.8	8	10
Pyrimethanil	0.999	-5.2	78.8	88.8	16.0	10.7	5	10
Simazin	0.998	-12.7	100.5	91.7	9.8	5.9	5	10
Spinosad A	0.999	-4.0	102.9	97.7	3.9	3.8	8	10
Spinosad D	0.998	-10.2	102.9	96.4	9.4	6.5	5	10
Spiromesifen	0.998	-13.7	89.5	97.6	13.1	8.0	5	10
Tebuconazol	0.992	3.4	109.5	107.4	19.1	16.2	8	10
Tebufenozide	0.999	9.6	88.0	94.8	26.8	14.0	10	20
Tetraconazole	0.998	-1.5	96.0	100.9	13.8	12.2	8	10
Thiabendazole	0.999	-22.6	76.2	82.4	6.4	4.3	5	10
Thiophanate- methyl	0.999	1.2	117.6	113.6	15.0	13.3	8	10
Thiamethoxam	0.991	-11.8	93.0	98.8	9.0	4.0	10	20
Triadimefon	0.999	-1.1	115.1	114.1	17.4	13.4	10	20
Triadimenol	0.998	-4.6	110.2	110.6	12.2	8.2	5	10
Trichlorfon	0.998	-3.6	104.7	103.5	10.3	5.0	8	10
Trifloxystrobin	0.999	-6.9	77.5	82.2	5.4	2.7	5	10
Triflumizole	0.999	9.3	97.9	97.5	14.8	11.2	8	10
Triforin	0.997	-11.2	92.8	100.9	12.6	8.5	5	10
Zoxamide	0.996	-10.5	83.1	109.6	7.6	6.0	5	10