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Supplementary Information

Development of a Multiresidue Method for Pesticide Analysis in Drinking Water by Solid Phase Extraction and Determination by Gas and Liquid Chromatography with Triple Quadrupole Tandem Mass Spectrometry

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Table S1. Optimized parameters for the analyzed pesticides by LC-MS/MS

Compound	t_R / min	ESI (+/-)	Precursor ion / (*m/z*)	1st Transition (quantification)		2nd Transition (confirmation)	
				Product ion / (*m/z*)	Collision energy / eV	Product ion / (*m/z*)	Collision energy / eV
Methamidophos	5.60	+	142.0	93.8	12.5	124.8	12.5
Imazapyr	7.13	+	262.0	217.0	19.0	220.0	17.0
Aldicarb sulfoxide	7.41	+	207.0	105.0	10.0	132.0	5.0
Aldicarb sulfone	7.45	+	240.0	223.0	7.5	166.0	11.0
Imazapic	7.47	+	276.0	231.0	18.0	234.0	16.5
Metsulfurom-methyl	7.65	+	382.0	167.5	12.0	198.9	19.5
Imazethapyr	7.76	+	290.0	245.0	19.0	248.0	17.0
Thiamethoxam	7.79	+	292.0	210.0	11.0	181.0	19.5
Bentazone	7.83	–	239.0	131.7	25.5	196.6	19.0
Quincloraque	7.92	+	242.0	223.8	13.0	160.9	37.0
Azinssulfuron	7.97	+	425.0	182.0	12.5	156.0	40.0
Imidacloprid	8.05	+	256.1	209.0	14.0	175.0	17.0
Tricyclazole	8.72	+	190.0	136.0	25.5	109.0	31.5
Carbendazin	8.84	+	192.0	160.0	15.0	131.9	27.0
Pyrazossulfuron	8.95	+	415.0	182.0	15.5	139.0	39.0
2,4-D	8.99	–	219.0	160.6	11.5	–	–
Aldicarb	8.99	+	208.0	116.0	5.0	89.0	15.0
Thiophanate-methyl	9.15	+	243.0	151.0	15.5	160.0	23.0
Etoxissulfuron	9.16	+	399.0	261.0	12.5	218.0	21.0
Thiabendazole	9.27	+	202.0	175.0	19.5	131.0	27.0
Carbofuran	9.44	+	222.0	165.0	7.5	122.9	16.5
Bispyribac sodium	9.55	+	453.0	296.6	18.5	179.0	18.5
2,4,5-T	9.56	–	252.8	158.6	28.0	194.5	11.0
Simazine	9.57	+	202.0	131.9	19.5	123.9	18.0
Carbaryl	9.59	+	202.0	114.9	8.0	126.9	26.5
Azoxystrobin	9.89	+	404.0	372.0	14.5	328.9	30.0

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Table S1. Optimized parameters for the analyzed pesticides by LC-MS/MS (cont.)

Compound	t_R / min	ESI (+/-)	Precursor ion / (*m/z*)	1st Transition (quantification)		2nd Transition (confirmation)	
				Product ion / (*m/z*)	Collision energy / eV	Product ion / (*m/z*)	Collision energy / eV
Pendimethalin	9.98	+	282.0	194.0	15.5	–	–
Atrazine	9.99	+	216.0	173.0	13.5	103.8	24.5
Diuron	10.10	–	231.0	150.0	24.0	186.0	16.0
Clomazone	10.28	+	240.0	124.9	18.0	88.9	39.5
Malationa	10.48	+	331.0	284.9	8.0	126.9	9.0
Propanil	10.54	+	218.0	162.0	15.0	127.0	25.0
Linuron d-6[a]	10.59	+	255.0	159.9	15.5	185.0	15.5
Tetraconazol	10.79	+	372.0	158.9	24.0	–	–
Fipronil	10.80	–	435.0	329.7	15.5	249.6	26.5
Molinate	10.99	+	188.0	126.0	20.0	160.0	12.0
Triphenylphosphate[b]	11.10	+	327.0	152.0	29.0	214.9	20.5
Tebuconazole	11.19	+	308.0	69.9	14.0	124.9	33.0
Propiconazole	11.35	+	342.0	158.9	25.5	69.0	14.0
Chlorpyrifos oxon	11.36	+	334.5	306.0	10.0	278.0	15.0
Cyhalofop-butyl	11.47	+	375.0	256.0	15.0	358.0	6.5
Trifloxystrobin	11.50	+	409.0	186.0	14.0	206.0	11.0
Difenoconazole	11.59	+	406.0	250.9	24.0	336.9	15.5
Benfuracarb	11.83	+	411.0	252.0	12.0	158.0	7.0
Chlorpyrifos-ethyl	11.93	+	322.0	124.8	15.0	289.7	14.5
Profenofos	12.12	+	375.0	304.7	19.5	346.7	12.0
Terbufos	12.33	+	288.9	102.9	5.0	232.9	5.0
Benomyl	12.34	+	293.0	219.0	6.5	101.0	16.0
Chlorpyrifos-ethyl	13.14	+	349.9	197.8	16.0	321.7	10.5

[a]Surrogate standard; [b]internal standard.

Table S2. Optimized parameters for the analyzed pesticides by GC-MS/MS

Compound	t_R / min	Segment	Precursor ion / (*m/z*)	1st Transition (quantification)		2nd Transition (confirmation)	
				Product ion / (*m/z*)	Collision energy / eV	Product ion / (*m/z*)	Collision energy /eV
Trifluralin d-14[a]	7.05	1	315.0	267.0	8	209.0	10
Trifluralin	7.08		306.0	264.0	10	159.0	30
Lindane	7.64	2	219.0	147.0	20	183.0	10
Metolachlor	7.95	3	162.0	132.5	20	118.0	20
Alachlor	8.02		188.0	130.0	40	160.0	10
Parathion-methyl	8.04		263.0	109.0	25	136.0	10
Fenitrothion	8.19	4	277.0	109.0	25	260.0	10
Aldrin	8.41		263.0	193.0	30	191.0	30
Chlordano	8.82	5	375.0	266.0	10	303.0	10
Endosulfan-alpha	8.92		241.0	170.0	15	172.0	15
Oxifluorfen	8.95		300.0	223.0	20	132.0	40
2.4 DDE	9.95	6	246.0	176.0	25	246.0	25
2.4 DDD	9.05		235.0	199.0	20	165.0	20
Dieldrin	9.11		277.0	170.0	40	206.0	15
Endrin	9.30	7	263.0	193.0	30	191.0	30
DDT	9.32		235.0	165.0	20	199.0	20
Endosulfan-beta	9.38		241.0	206.0	10	170.0	20
Endosulfan-sulfate	9.69	8	272.0	237.0	15	235.0	10
Triphenylphosphate[b]	9.77		325.0	169.0	18	226.0	18
Bifenthrin	9.81		181.0	165.0	20	166.0	10
Permethrin	10.30	9	165.0	91.0	10	127.0	5
Cyhalothrin-lambda	10.43		197.0	141.0	10	161.0	5
Cyfluthrin	11.79	10	164.0	91.0	15	127.0	5
Cypermethrin	12.29		164.0	91.0	15	127.0	5
Deltamethrin	14.22	11	253.0	174.0	10	172.0	5

[a]Surrogate standard; [b]internal standard.

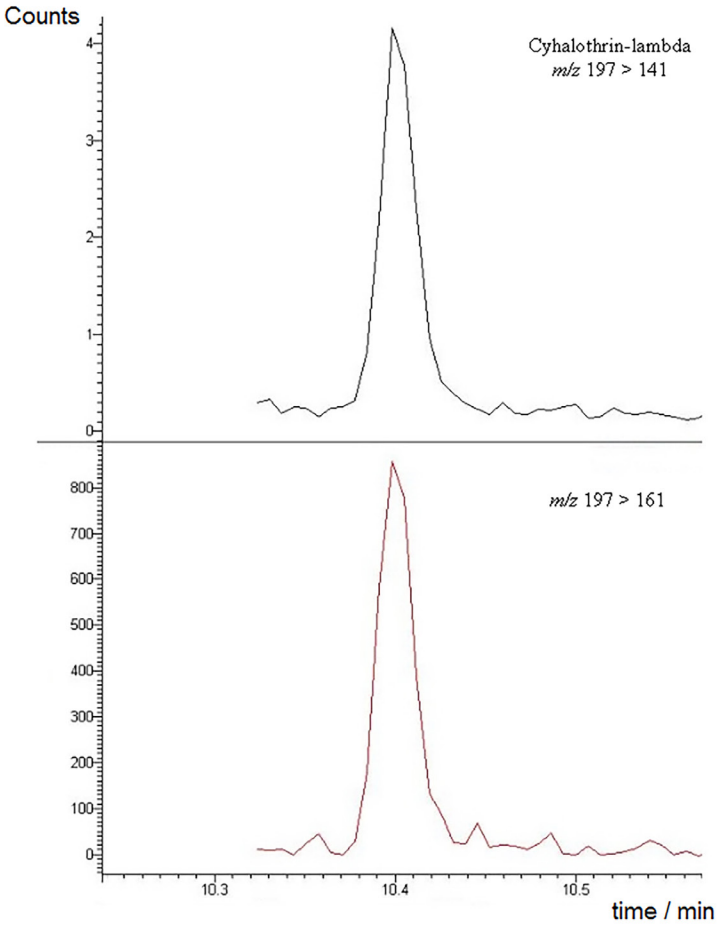

Figure S1. GC-MS/MS SRM chromatograms of a sample containing 0.65 μg L^{-1} of cyhalothrin-lambda.