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BSI Standards Publication

Food analysis — Determination of pesticide residues by GC-MS — Retention times, mass spectrometric parameters and detector response information

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Food analysis - Determination of pesticide residues by GC-MS - Retention times, mass spectrometric parameters and detector response information

Analyse des produits alimentaires - Détermination des résidus de pesticides par CG-SM - Temps de rétention, paramètres de spectrométrie de masse et information sur la réponse des détecteurs

Lebensmitteluntersuchung - Bestimmung von Pestizidrückständen mit GC-MS - Retentionszeiten, Parameter für die Massenspektrometrie und Detektionsempfindlichkeit

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Contents

Page

Foreword

This document (CEN/TR 16468:2013) has been prepared by Technical Committee CEN/TC 275 “Food analysis - Horizontal methods”, the secretariat of which is held by DIN.

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Introduction

Pesticide residue analysis employs multiple methods involving extraction of residues from foods and clean-up of the extract to obtain as many analytes as possible in the purified extracts. Afterwards the extracts can be analysed by different kinds of instruments.

The hyphenation of gas chromatography (GC) and mass spectrometry (MS) is one of the most often used universal and selective analysis techniques for identification and quantification of pesticide residues in food extracts.

For the ionisation of the analytes (pesticides and/or their metabolites) in GC-MS, electron impact ionisation (EI) is most commonly used. If the typical electron energy of 70 eV is used, very often molecular ions (cation radicals) and several fragment ions are formed simultaneously.

The selective determination of each target analyte is performed by simultaneous aquisition of typically three ions formed by the analyte in the selected ion monitoring (SIM) mode. The diagnostic value of an ion depends on its mass. Usually even-numbered, high mass ions are less frequently formed and their recording results in more specific chromatograms. A reduction of selectivity may be caused by background ions formed during ‘column bleeding’ or by sample matrix (e.g. typical ions from fatty of fruit acids or hydrocarbons).

1 Scope

This Technical Report lists mass spectrometric parameters which are useful for the application of European Standards for the determination of pesticide residues in foods that use GC-MS, such as the following standards:

— EN 1528 (all parts), *Fatty food — Determination of pesticides and polychlorinated biphenyls (PCBs)*;

— EN 12393 (all parts), *Foods of plant origin — Multiresidue methods for the gas chromatographic determination of pesticide residues*;

— EN 15662, *Foods of plant origin — Determination of pesticide residues using GC-MS and/or LC-MS/MS following acetonitrile extraction/partitioning and clean-up by dispersive SPE — QuEChERS-method*.

To facilitate the determination of pesticides and/or metabolites using GC-MS, Table 1 specifies the diagnostic ions suitable for quantification, which can be used.

2 Analyte specific parameters for gas chromatographic determination of pesticides

2.1 General

All values indicated in Table 1 were acquired using GC-MS, GC-ECD or GC-NPD systems under the experimental conditions as outlined in 2.2. Comparative investigations showed that these parameters can be transferred simply on instruments of other types of the same or other manufacturers [1].

2.2 GC-MS, GC-ECD and GC-NPD Parameters

The following GC operating conditions have been proven to be satisfactory. This is an example for appropriate experimental conditions. Equivalent conditions may be used if they can be shown to lead to the same results.

Gas chromatograph	Agilent model 6890
Carrier gas	Helium, constant flow 1,0 ml/min (typical pressure at 70 °C is 61 kPa)
Injection technique	Pulsed splitless, 200 kPa; Pulse time 1,0 min
Injector temperature	240 °C
Injection liner	single taper, splitless (Agilent 5181-3316)
Injection volume	1 µl or 2 µl
Purge Gas	Helium; purge flow to split vent 50 ml/min; Purge time 1,5 min
Column	Fused silica capillary column HP-5MS, length 30 m, inner diameter 0,25 mm, film thickness 0,25 µm (Agilent Nr. 19091S-433)
Temperature programme	2 min 70 °C, programmed to rise at 25 °C/min to 170 °C, at 3 °C/min to 210 °C, at 30 °C/min to 290 °C, then isothermal for 9 min
Transfer Line Temperatur	280 °C
Mass spectrometer	Agilent MSD 5973N inert
MS temperatures	Quadrupole 150 °C; Source 230 °C;
Ionisation	Electron impact 70 eV
Solvent Delay	4,0 min
Retention time of parathion	15,85 min (parathion is used for calculation of relative retention times)

As an alternative to the abovementioned fused silica capillary column HP-5MS a column DB-35MS can be used. This column requires some slightly changed conditions.

Column	Fused silica capillary column DB-35MS, length 30 m, inner diameter 0,25 mm, film thickness 0,25 µm (Agilent Nr. 122-3832)
Carrier gas/MS detection	Hydrogen, constant flow 1,1 ml/min (typical pressure at 80 °C is 15,9 kPa)
Carrier gas/NPD and ECD detection	Hydrogen, constant flow 1,9 ml/min (typical pressure at 80 °C is 88,3 kPa)
Temperature programme	1,8 min 80 °C, programmed to rise at 30 °C/min to 190 °C, at 6 °C/min to 240 °C, at 30 °C/min to 290 °C, then isothermal for 12 min
Injection technique/MS detection	Pulsed splitless, 80 kPa; Pulse time 1,5 min
Injection technique/NPD and ECD, parallel detection	Pulsed splitless, 172 kPa; Pulse time 1,5 min
Injector temperature	240 °C
Injection liner	single taper, splitless (Agilent 5181-3316)
Injection volume	2 µl
Purge Gas	nitrogen; purge flow to split vent 35 ml/min; Purge time 2,0 min
Detector split ratio	1:5 (ECD:NPD; post column)
Detector temperature (NPD)	280 °C
Detector temperature (ECD)	300 °C
Transfer line temperature (MS)	280 °C
Mass spectrometer	Agilent MSD 5973N
MS temperatures	Quadrupole 150 °C; Source 230 °C;
Ionisation	Electron impact 70 eV
Solvent Delay/MS	4,0 min
Retention time of parathion	14,69 min (RT parathion with GC NPD/ECD is used for calculation of relative retention times)

As slight fluctuations in the measurement conditions influence the retention time, usually relative retention times (RRT), related to a standard substance, are compared. The standard substance for the calculation of the RRT values in the tables was parathion (RRT = 1,000).

2.3 Analyte specific retention times and MS parameters

The analyte specific parameters for selected ion monitoring (SIM) of pesticides by GC-MS with EI ionisation are listed in Table 1. These data are completed by some indications about the sensitivity of detection, which can be expected if GC-MS with the most intense ion and GC-ECD or GC-NPD are used. The names of the individual active substances are supplemented by the CAS number (Chemical Abstracts Service), which is useful for the search in data bases. It is usually taken from [2], but there can be several numbers in individual cases, e.g. for isomers and racemates.

The RRT data for columns HP-5MS and DB-35MS in Table 1 are relative retention times compared to parathion (RRT = 1,00). The units for numbers presented in columns Ion 1 to Ion 4 are Da (or m/z). Three crosses in the columns MSD, ECD or NPD indicate a better sensitivity compared to two or one crosses.

Table 1 — Parameters of 691 analytes

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Acephate	30560-19-1	0,47	0,58	136	94	95	96	xx	x	xx
Aclonifen	74070-46-5	1,40	1,34	264	266	212	77	xxx	x	x
Acrinathrin, 1	101007-06-1	1,57	1,41	207	181	281	208	xx	xxx	xx
Acrinathrin, 2	101007-06-1	1,58	1,46	181	208	207	93	xxx	xxx	xx
Alachlor	15972-60-8	0,89	0,88	160	188	146	237	xxx	xxx	x
Aldicarb, -sulfone	1646-88-4	0,33	0,43	68	80	65	69	xx	x	x
Aldrin	309-00-2	0,97	0,93	263	66	265	261	xxx	xxx	
Allidochlor	93-71-0	0,40	0,47	56	138	132	70	xxx	xx	xx
Ametryn	834-12-8	0,89	0,93	227	212	170	185	xxx		xx
Amidithion	919-76-6	0,96	1,03	125	131	93	143	x	x	x
Aminocarb	2032-59-9	0,73	0,79	151	150	136	208	xx		xx
Amitraz	33089-61-1	1,56	1,46	121	162	132	293	xx		x
Amitraz hydrolysis product (Dimethylaniline, 2,4,-	95-68-1	0,35	0,41	121	120	106	77	xxx		x
Amitraz-metabolite (BTS 27271)	33089-74-6	0,55	0,61	162	132	120	106	x		xx
Ancymidol	12771-68-5	1,36	1,30	228	107	121	215	xx		xxx
Anilazine	101-05-3	1,09	1,11	239	241	178	143	x	xx	x
Anilofos	64249-01-0	1,53	1,46	226	125	184	334	xx	xx	xx
Aramite, 1	140-57-8	1,32	1,20	185	175	319	334	x	x	
Aramite, 2	140-57-8	1,35	1,22	185	175	319	334	x	x	
Aspon	3244-90-4	0,99	0,90	211	210	253	378	xxx	xx	xxx
Atraton	1610-17-9	0,69	0,74	196	211	169	154	xx		x
Atrazine	1912-24-9	0,71	0,76	200	215	202	173	xxx	x	xxx
Atrazine, -desethyl	6190-65-4	0,63	0,71	172	174	187	145	xx	x	x
Atrazine, -desethyl-desisopropyl	3397-62-4	0,56	0,66	145	110	68	147	x	x	xx
Atrazine, -desisopropyl	1007-28-9	0,61	0,72	173	158	145	68	x	x	x
Azaconazole	60207-31-0	1,32	1,30	217	219	173	175	xx	x	xx
Azamethiphos	35575-96-3	1,44	1,39	215	155	125	109	x	x	xx
Azinphos-ethyl	2642-71-9	1,55	1,59	132	160	77	105	x	xx	xxx
Azinphos-methyl	86-50-0	1,55	1,55	160	132	77	105	xx	xx	xxx
Azobenzene	103-33-3	0,60	0,66	77	182	105	51	x	x	xxx
Azoxystrobin	131860-33-8	1,82	2,28	344	388	345	372	xx	xx	x
Beflubutamid	113614-08-7	1,13	1,03	91	176	221	193	xx	x	x
Benalaxyl	71626-11-4	1,45	1,35	148	91	206	204	xxx		x
Benazolin-ethyl	25059-80-7	1,09	1,13	170	271	198	134	xxx	xxx	x
Benfluralin	1861-40-1	0,64	0,61	292	264	276	335	xx	xxx	xx
Benfuracarb	82560-54-1	1,58	1,50	190	163	164	102	xx	x	xx
Benfuresate	68505-69-1	0,84	0,90	163	256	121	164	xxx	x	x
Benodanil	15310-01-7	1,43	1,38	231	323	203	76	xxx	xx	x
Benoxacor	98730-04-2	0,82	0,87	120	259	261	176	xx	xxx	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Bentazone-methyl	61592-45-8	0,89	0,94	212	105	254	133	xxx	x	xx
Benzoylprop-ethyl	22212-55-1	1,50	1,39	105	77	292	294	xxx	xx	x
Bifenazate	149877-41-8	1,52	1,44	300	258	199	196	xx		x
Bifenazate-metabolite (5-Phenyl-o-anisidine)	39811-17-1	0,95	1,01	184	156	199		x	x	x
Bifenox	42576-02-3	1,53	1,46	341	343	310	173	xx	xxx	x
Bifenthrin	82657-04-3	1,52	1,36	181	165	166	182	xxx	xxx	
Binapacryl	485-31-4	1,37	1,22	83	55	84	53	x	x	x
Bioallethrin S-cyclopentyl (Esbiol)	28434-00-6	1,12	1,00	123	136	79	107	xx	xxx	
Bioallethrin, cis- (Allethrin)	584-79-2	1,11	1,00	123	136	79	91	x	xxx	
Bioallethrin, trans- (Allethrin)	584-79-2	1,12	1,00	123	136	79	91	xx	xxx	
Bioresmethrin	28434-01-7	1,49	1,35	123	171	143	128	xxx	x	
Biphenyl	92-52-4	0,45	0,51	154	153	152	155	xxx		
Bitertanol, 1	70585-36-3	1,60	1,55	170	168	171	112	xx	x	x
Bitertanol, 2	70585-38-5	1,61	1,57	170	168	171	112	xx	x	x
Boscalid	188425-85-6	1,67	1,78	140	342	142	344	xx	xxx	xx
Bromacil	314-40-9	0,96	1,05	205	207	206	188	x	xx	xx
Metobromuron-metabolite (4-Bromoaniline)	106-40-1	0,41	0,49	171	173	92	65	xxx	x	x
Bromfenvinfos, (E)-	58580-14-6	1,24	1,13	267	269	323	325	xx	xx	x
Bromfenvinfos, (Z)-	58580-13-5	1,20	1,19	267	269	323	325	x	xx	x
Bromocyclen	1715-40-8	0,81	0,80	357	359	361	355	xxx	xxx	
Bromophos	2104-96-3	1,04	1,03	331	329	125	333	xxx	xxx	xxx
Bromophos-ethyl	4824-78-6	1,17	1,09	359	303	357	97	xxx	xxx	xxx
Bromopropylate	18181-80-1	1,51	1,40	341	343	339	183	xxx	xxx	
Bromuconazole, cis-	116255-48-2	1,51	1,44	173	295	175	293	xxx	x	xx
Bromuconazole, trans-	116255-48-2	1,53	1,48	173	175	295	293	xxx	x	xx
Bupirimate	41483-43-6	1,34	1,24	273	208	316	166	xxx	xx	xx
Buprofezin	69327-76-0	1,31	1,20	105	172	106	175	xxx	x	x
Butachlor	23184-66-9	1,21	1,08	176	160	57	188	xxx	xxx	xc
Butafenacil	134605-64-4	1,63	1,58	331	333	180	332	xx	xx	x
Butamifos	36335-67-8	1,24	1,17	286	200	232	202	x	xxx	xxx
Butralin	33629-47-9	1,05	0,95	266	224	295	267	xx	xx	x
Butylate	2008-41-5	0,47	0,50	57	146	156	174	xx		xx
Cadusafos	95465-99-9	0,65	0,67	159	158	88	97	xxx	xxx	xxx
Cafenstrole	125306-83-4	1,64	1,68	100	188	72	119	xx	xx	x
Captafol	2425-06-1	1,48	1,43	79	80	77	183	xx	x	x
Captan	133-06-2	1,11	1,19	79	149	77	80	xx	xx	x
Captan-metabolite (Tetrahydrophthalimide)	1469-48-3	0,50	0,62	79	151	80	77	xxx	x	x
Carbaryl-GC-artifact (1-Naphthol)	90-15-3	0,52	0,53	144	115	116	145	xx		
Carbetamide	16118-49-3	1,03	1,04	119	120	91	64	x		
Carbofuran	1563-66-2	0,70	0,80	164	149	131	122	xx		x
Carbofuran, -phenol	1563-38-8	0,42	0,46	164	149	131	122	xx	x	
Carbophenothion	786-19-6	1,45	1,34	157	342	121	153	xxx	xx	xxx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Carbosulfan	55285-14-8	1,51	1,37	160	118	163	164	xx	x	xx
Carboxin	5234-68-4	1,30	1,30	143	235	87	236	xx	x	x
Carfentrazone-ethyl	128639-02-1	1,46	1,32	312	340	330	290	x	xx	xx
Carvone	99-49-0	0,39	0,44	82	108	93	54	xxx		
Chinomethionat	2439-01-2	1,15	1,20	206	234	116	148	x	xxx	xxx
Chlorbicyclen	2550-75-6	1,09	1,04	229	272	237	273	xx	xxx	
Chlordimeform-metabolite (Chloro-2-methyl-aniline)	95-69-2	0,41	0,48	141	106	140	143	xx	x	xx
Metoxuron-metabolite (3-Chlor-4-methoxyaniline)	5345-54-0	0,48	0,57	142	157	114	144	xx	x	xx
Chloroaniline, 3- (Carbamate-hydrolysis product)	108-42-9	0,36	0,44	127	129	65	92	xx	xx	x
Chloroaniline, 4- (Monuron-hydrolysis product)	106-47-8	0,37	0,44	127	129	65	92	xxx	xx	x
Chlorbenside	103-17-3	1,14	1,14	125	127	268	270	xx	xx	
Chlorbenside, -sulfone	7082-99-7	1,44	1,39	125	127	89	126	xx	xxx	
Chlorobenzilate	510-15-6	1,39	1,26	251	253	139	111	xx	xx	
Chlorbufam	1967-16-4	0,70	0,75	223	127	164	225	xx	x	x
Chlordane, cis-	5103-71-9	1,20	1,13	375	373	377	371	xxx	xxx	
Chlordane, oxy-	27304-13-8	1,09	1,02	115	185	387	187	xxx	xxx	
Chlordane, trans-	5103-74-2	1,15	1,11	373	375	377	371	xxx	xxx	
Chlordene, trans-	3734-48-3	0,77	0,77	66	237	101	232	xxx	xxx	
Chlordimeform	6164-98-3	0,63	0,68	196	181	117	152	xxx		xx
Chlorethoxyfos	54593-83-8	0,59	0,61	153	97	301	299	xxx	xxx	xx
Chlorfenapyr	122453-73-0	1,37	1,24	59	247	328	408	xx	xx	xx
Chlorfenethol (BCPE)	80-06-8	1,10	1,10	251	139	253	111	x	x	
Chlorfenprop-methyl	14437-17-3	0,57	0,63	125	165	196	197	xx	xxx	
Chlorfenson	80-33-1	1,23	1,24	175	111	302	177	xx	xxx	
Chlorfenvinphos, (E)-	18708-86-6	1,08	1,03	267	269	323	325	xxx	xx	x
Chlorfenvinphos, (Z)-	18708-87-7	1,12	1,09	267	323	269	325	xxx	xx	x
Chlorflurenol-methyl	2536-31-4	1,15	1,18	215	152	217	274	xxx	xxx	
Chloridazon (Pyrazon)	1698-60-8	1,46	1,45	221	77	220	223	x	x	x
Chlormephos	24934-91-6	0,48	0,54	121	97	234	154	xx	xx	xxx
Chlornitrofen	1836-77-7	1,44	1,34	317	319	287	289	x	xxx	x
Chloroneb	2675-77-6	0,52	0,58	191	193	206	208	xxx	xx	
Chlorpropham	101-21-3	0,62	0,66	127	213	171	154	xx	x	x
Chloropropylate	5836-10-2	1,38	1,24	251	253	139	111	xxx	xx	
Chlorpyrifos	2921-88-2	1,00	0,97	197	199	314	97	xxx	xxx	xxx
Chlorpyrifos-methyl	5598-13-0	0,87	0,89	286	288	125	290	xxx	xxx	xxx
Chlorthal-dimethyl	1861-32-1	1,02	0,97	301	299	303	332	xxx	xxx	
Chlorothalonil	1897-45-6	0,79	0,91	266	264	268	270	xx	xxx	x
Chlorthiamide	1918-13-4	0,85	1,00	170	172	205	171	x	x	x
Chlorthion	500-28-7	1,02	1,04	109	125	297	299	x	xxx	xxx
Chlorthiophos, 1	21923-23-9	1,38	1,26	222	224	257	97	x	xxx	xx
Chlorthiophos, 2	77503-29-8	1,40	1,28	269	325	271	97	xx	xxx	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Chlorthiophos, 3	77503-28-7	1,42	1,30	269	325	97	271	xx	xxx	xx
Chlorotoluron	15545-48-9	0,38	0,42	132	167	169	166	xxx	x	x
Chlozolinate	72391-46-9	1,11	1,04	259	188	331	186	xx	xxx	x
Cinerin I (Pyrethrins compound)	25402-06-6	1,34	1,14	123	121	150	93	xx	x	
Cinerin II (Pyrethrins compound)	121-20-0	1,55	1,42	107	121	93	91	xx	x	
Cinidon-ethyl	142891-20-1	1,91	2,33	330	332	358	331	xx	xx	x
Clodinafop-propargyl	105512-06-9	1,47	1,36	349	238	266	351	x	x	x
Clomazone	81777-89-1	0,71	0,77	125	204	127	205	xx	x	xx
Cloquintocet-mexyl	99607-70-2	1,52	1,42	192	194	193	163	x	xx	x
Coumaphos	56-72-4	1,62	1,62	362	226	109	364	xx	xx	xxx
Crimidine	535-89-7	0,52	0,61	142	156	171	144	xx	x	xx
Crotoxyphos	7700-17-6	1,15	1,12	127	105	193	166	x	xx	xx
Crufomate	299-86-5	1,03	1,04	256	182	276	169	xx	x	xx
Cyanazine	21725-46-2	1,01	1,08	225	172	198	212	xx	xx	xxx
Cyanofenphos	13067-93-1	1,45	1,37	157	169	141	185	xxx	xx	xxx
Cyanophos	2636-26-2	0,74	0,82	243	109	125	79	xx	x	xxx
Cycloate	1134-23-2	0,61	0,64	83	154	55	72	xxx		x
Cyflufenamid	180409-60-3	1,37	1,23	91	55	412	294	xxx	xxx	xx
Cyfluthrin, beta-1	68359-37-5	1,64	1,59	163	165	206	226	xx	xx	x
Cyfluthrin, beta-2	68359-37-5	1,64	1,60	163	165	206	226	xx	xx	x
Cyfluthrin, beta-3	68359-37-5	1,65	1,61	163	165	206	226	xx	xx	x
Cyfluthrin, beta-4	68359-37-5	1,65	1,61	163	165	206	226	xx	xx	x
Cyhalofop-butyl	122008-85-9	1,56	1,47	256	357	229	228	xx	x	x
Cyhalothrin, lambda-	91465-08-6	1,57	1,44	181	197	208	209	xxx	xxx	xx
Cyhalothrin, cis-	68085-85-8	1,57	1,42	181	197	208	209	xxx	xx	x
Cymiazole	61676-87-7	0,88	0,94	144	218	115	119	xxx	x	x
Cymoxanil	57966-95-7	0,59	0,65	111	167	70	183	x		x
Cypermethrin, zeta-1	52315-07-8	1,66	1,64	163	181	165	209	xx	xx	x
Cypermethrin, zeta-2	52315-07-8	1,66	1,65	163	181	165	209	xx	xx	x
Cypermethrin, zeta-3	52315-07-8	1,67	1,66	163	181	165	209	xx	xx	x
Cypermethrin, zeta-4	52315-07-8	1,67	1,66	163	181	165	209	xx	xx	x
Cypermethrin, alpha-	67375-30-8	1,67	1,66	163	181	165	209	xx	xx	x
Cyphenothrin, cis-	39515-40-7	1,59	1,49	123	181	375	167	xx	xx	x
Cyphenothrin, trans-	39515-40-7	1,59	1,50	123	181	375	167	xx	xx	x
Cyproconazole, (2RS + 3RS)	94361-06-5	1,35	1,28	222	139	224	125	xx	xx	xx
Cyproconazole, (2RS + 3SR)	94361-07-6	1,35	1,29	222	139	224	125	xx	xx	xx
Cyprodinil	121552-61-2	1,07	1,06	224	225	210	226	xxx		xxx
Cyprofuram	69581-33-5	1,40	1,35	69	211	213	279	xx	xxx	xxx
DDD, -ethyl (Perthane)	72-56-0	1,37	1,25	223	224	165	178	xxx	x	
DDD, 2,4-	53-19-0	1,30	1,24	235	237	165	236	xxx	xxx	
DDD, 4,4-	72-54-8	1,40	1,31	235	237	165	236	xxx	xxx	
DDE, 2,4-	3424-82-6	1,17	1,11	246	248	318	316	xxx	xxx	
DDE, 4,4-	72-55-9	1,27	1,19	246	318	316	248	xxx	xxx	

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
DDT, 2,4-	789-02-6	1,41	1,29	235	237	165	236	xxx	xxx	
DDT, 4,4-	50-29-3	1,46	1,35	235	237	165	236	xxx	xxx	
Diethyltoluamide (DEET)	134-62-3	0,56	0,62	119	190	191	91	xxx		xx
Deltamethrin	52918-63-5	1,79	1,91	181	253	251	255	xx	xxx	x
Demeton-S-methyl	919-86-8	0,59	0,67	88	60	109	142	xx	x	xxx
Demeton-S-methyl, -sulfone	17040-19-6	0,92	1,06	169	109	125	142	xx	xx	xx
Desmetryn	1014-69-3	0,84	0,90	213	198	171	82	xxx		xxx
Dialifos	10311-84-9	1,59	1,56	208	210	357	209	xx	xx	xx
Di-allate, cis-	2303-16-4	0,66	0,67	86	234	128	236	xxx	xx	x
Di-allate, trans-	2303-16-4	0,67	0,69	234	86	236	128	xxx	xx	x
Diazinon	333-41-5	0,76	0,75	179	137	304	152	xxx	xxx	xxx
Diazinon, -oxon	962-58-3	0,73	0,75	273	137	288	151	x	x	xx
Brompropylate-metabolite (Dibromobenzophenone, 4,4-)	3988-03-2	1,33	1,29	183	185	340	338	xx	xx	
Dichlobenil	1194-65-6	0,43	0,51	171	173	136	100	xxx	xxx	x
Dichlofenthion	97-17-6	0,85	0,84	279	223	97	281	xxx	xx	xxx
Dichlofluanid	1085-98-9	0,96	0,99	123	224	167	226	xxx	xxx	x
Dichlofluanid-metabolite (DMSA)	2418-14-6	0,62	0,74	200	92	65	93	x		x
Dichlone	117-80-6	0,77	0,87	228	191	163	230	x	x	
Dichlobenil-metabolite (2,6-Dichlorbenzamide)	2008-58-4	0,63	0,76	173	175	189	191	xxx	xxx	x
Dichloraniline, 3,5-	626-43-7	0,47	0,54	161	163	90	99	xxx	xx	x
Dichlormid	37764-25-3	0,43	0,49	172	124	166	174	xxx	xxx	xx
Dichlorprop-methyl	57153-17-0	0,63	0,63	162	164	189	248	xx	x	
Dichlorvos	62-73-7	0,38	0,45	109	185	79	145	xx	x	xxx
Diclobutrazol, cis-	66345-62-8	1,31	1,22	270	272	159	161	xx	xx	xx
Diclobutrazol, trans-	66345-62-8	1,37	1,26	270	272	159	161	xx	xx	xx
Diclofop-methyl	51338-27-3	1,48	1,37	253	340	255	342	xx	x	
Dicloran	99-30-9	0,69	0,79	206	124	176	208	x	xxx	x
Dicofol, 2,4-	10606-46-9	1,54	1,38	139	251	253	141	xx	x	
Dicofol, 4,4-	115-32-2	1,52	1,38	139	251	253	111	xx	x	
Dicofol-2.4-metabolite (2,4-Dichlorobenzophenone)	85-29-0	0,92	0,96	139	250	141	111	xxx	xxx	
Dicofol-4.4-metabolite (4,4-Dichlorobenzophenone)	90-98-2	1,00	1,03	139	250	111	141	xxx	xxx	
Dicrotophos, -(E)	141-66-2	0,63	0,72	127	67	193	237	xx	x	x
Dicrotophos, -(Z)	18250-63-0	0,59	0,72	127	67	193	237	xx	x	x
Dieldrin	60-57-1	1,27	1,21	79	263	277	279	xxx	xxx	
Dienochlor	2227-17-0	0,42	0,42	203	201	205	238	xx	x	
Diethofencarb	87130-20-9	0,98	0,96	267	225	124	151	xx		xx
Difenoconazole, cis-	119446-68-3	1,76	1,97	323	265	325	267	x	xx	x
Difenoconazole, trans-	119446-68-3	1,77	1,98	323	265	325	267	x	xx	x
Diflufenican	83164-33-4	1,49	1,35	266	394	267	246	x	xxx	x
Dimefox	115-26-4	0,27	0,33	110	154	153	111	xxx		xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Dimepiperate	61432-55-1	1,12	1,13	119	118	117	91	xx	x	x
Dimethachlor	50563-36-5	0,85	0,88	134	197	132	210	xxx	xx	x
Dimethenamid-P	163515-14-8	0,85	0,86	154	230	203	232	xxx	xx	xx
Dimethipin	55290-64-7	0,71	0,90	54	53	118	76	xx	xxx	x
Dimethoate	60-51-5	0,69	0,81	87	93	125	143	xx	x	xxx
Dimethomorph, (E)-	110488-70-5	1,83	2,26	301	387	303	165	x	xx	x
Dimethomorph, (Z)-	110488-70-5	1,82	2,17	301	303	387	165	x	xx	x
Dimoxystrobin	149961-52-4	1,52	1,42	116	205	58	295	xx	x	xx
Diniconazole	83657-24-3	1,39	1,29	268	270	70	269	xx	xx	x
Dinobuton	973-21-7	1,14	1,04	211	205	163	240	xx	xx	x
Dinocap, 4-ethyl-hexyl-	39300-45-3	1,52	1,37	69	--	--	--	x	x	x
Dinocap, 4-methyl-heptyl-	39300-45-3	1,52	1,37	69	--	--	--	x	x	x
Dinocap, 4-propyl-pentyl-	39300-45-3	1,51	1,35	69		--	--	xxx	x	x
Dinocap, 6-ethyl-hexyl-	39300-45-3	1,49	1,31	69	--	--	--	x	x	x
Dinocap, 6-methyl-heptyl-	39300-45-3	1,49	1,31	69	--	--	--	x	x	x
Dinocap, 6-propyl-pentyl-	39300-45-3	1,50	1,33	69	--	--	--	x	x	x
Dinoseb acetate	2813-95-8	0,91	0,89	240	211	163	89	x	xxx	x
Diofenolan, cis-	63837-33-2	1,45	1,33	186	300	225	301	xx		
Diofenolan, trans-	63837-33-2	1,46	1,34	186	300	225	301	xx		
Dioxacarb	6988-21-2	0,46	0,95	121	166	165	122	xx		
Dioxacarb-metabolite (-phenol)	6988-19-8	0,46	0,55	121	166	165	122	x		
Dioxathion	78-34-2	0,73	0,80	97	125	270	73	xx	xx	xxx
Diphenylamine	122-39-4	0,60	0,67	169	168	167	170	xxx		xxx
Dipropetryn	4147-51-7	0,97	0,95	255	240	184	222	xxx		xx
Di-n-propyl isocinchomeronate	136-45-8	0,87	0,86	165	179	192	164	xx	xx	xx
Disulfoton	298-04-4	0,77	0,79	88	89	97	142	xx	x	xxx
Disulfoton, -oxon	126-75-0	0,68	0,73	88	60	170	126	xx	xxx	xxx
Disulfoton, -sulfone	2497-06-5	1,20	1,23	213	153	97	125	x	x	x
Disulfoton, -sulfoxide	2497-07-6	0,42	0,48	97	125	212	153	xx		x
Ditalimfos	5131-24-8	1,22	1,23	130	148	299	209	xx	xx	xxx
DNOC	534-52-1	1,26	0,69	198	105	121	168	x		x
Dodemorph, cis-	1593-77-7	1,04	0,90	154	281	238	141	xxx		xx
Dodemorph, trans-	1593-77-7	1,08	0,94	154	281	238	141	xxx		xx
Edifenphos	17109-49-8	1,45	1,40	109	173	310	201	xx	x	xx
Empenthrin, 1	54406-48-3	0,66	0,60	123	91	81	79	xx	x	
Empenthrin, 2	54406-48-3	0,67	0,61	123	91	81	79	xx	x	
Empenthrin, 3	54406-48-3	0,67	0,64	123	91	81	79	xx	x	
Empenthrin, 4	54406-48-3	0,68	0,64	123	91	81	79	xx	x	
Empenthrin, 5	54406-48-3	0,68	0,64	123	91	81	79	xx	x	
Endosulfan, alpha-	33213-66-0	1,19	1,14	241	237	195	239	xx	xxx	
Endosulfan, beta-	33213-65-9	1,37	1,32	195	237	241	207	xx	xxx	
Endosulfan, -sulfate	1031-07-8	1,45	1,38	272	274	387	237	xx	xxx	
Endrin	72-20-8	1,34	1,28	263	265	281	261	xxx	xxx	

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Endrin-metabolite (Endrin-aldehyde)	7421-93-4	1,41	1,35	345	67	250	347	xx	xx	
Endrin-metabolite (Endrin-keton)	53494-70-5	1,50	1,31	317	315	319	281	xx	x	
EPN	2104-64-5	1,52	1,43	157	169	185	141	xx	xx	x
Epoxiconazole, cis-	106325-08-0	1,45	1,36	192	194	138	165	xx	xx	xx
Epoxiconazole, trans-	106325-08-0	1,49	1,41	192	194	138	165	xx	xx	xx
EPTC	759-94-4	0,43	0,48	128	86	132	189	xx	x	xx
Esfenvalerate	66230-04-4	1,74	1,82	125	167	181	152	xx	xx	x
Esprocarb	85785-20-2	0,95	0,93	91	222	162	71	xx		xx
Etaconazole, cis-	60207-93-4	1,40	1,31	245	173	247	175	xx		
Etaconazole, trans-	60207-93-4	1,41	1,31	245	173	247	55	xx		
Ethiofencarb	29973-13-5	0,82	0,90	107	168	77	108	x		xx
Ethiofencarb-metabolite (2-Ethylthiomethylphenol)	65370-06-1	0,47	0,54	107	168	77	78	xxx	x	xx
Ethion	563-12-2	1,42	1,30	231	153	97	125	xxx	xxx	xxx
Ethirimol	23947-60-6	0,91	0,96	166	96	209	167	x		
Ethofumesate	26225-79-6	0,95	0,97	207	161	286	137	xx	x	
Ethofumesate-metabolite (2-Oxo-ethofumesate)	26244-33-7	0,85	0,96	149	177	256	77	xx	xx	xx
Ethoprophos	13194-48-4	0,60	0,65	158	97	139	126	xxx	xx	xx
Ethoxyfen-ethyl	131086-42-5	1,51	1,36	333	335	450	452	xxx	xxx	
Ethoxyquin	91-53-2	0,69	0,72	202	174	203	145	xx		x
Etofenprox	80844-07-1	1,68	1,69	163	135	164	107	xxx		
Etoxazole	153233-91-1	1,53	1,40	204	141	300	187	xx		xx
Etridiazole	2593-15-9	0,49	0,54	211	183	213	185	xxx	xx	xx
Etridiazole-metabolite (Etridiazole, -deschloro)	A-108	0,43	0,49	149	184	141	186	xx	x	xx
Etrimfos	38260-54-7	0,80	0,79	292	181	153	277	xx	x	xxx
Famoxadone	131807-57-3	1,83	2,22	330	329	196	197	x	xx	x
Famphur (Famophos)	52-85-7	1,45	1,37	218	125	217	93	x	xxx	xxx
Fenamidone	161326-34-7	1,53	1,47	238	268	237	206	xx	xxx	xxx
Fenamiphos	22224-92-6	1,24	1,20	303	154	288	217	x		xxx
Fenamiphos, -sulfone	31972-44-8	1,51	1,44	320	292	321	335	xx		x
Fenamiphos, -sulfoxide	31972-43-7	1,50	1,44	304	122	303	319	xxx	xx	xx
Fenarimol	60168-88-9	1,57	1,54	139	219	251	107	xx	xx	xx
Fenazaquin	120928-09-8	1,53	1,43	145	160	207	146	xx		xx
Fenazox	495-48-7	0,81	0,87	77	198	91	169	xxx		x
Fenbuconazole, cis-	146887-38-9	1,64	1,70	129	198	125	127	x	xx	xx
Fenbuconazole, trans-	146887-37-8	1,64	1,70	129	198	125	127	x	xx	xx
Fenchlorazole-ethyl	103112-35-2	1,53	1,36	212	297	124	331	xx	x	x
Fenchlorphos	299-84-3	0,91	0,90	285	287	125	289	xx	xx	xxx
Fenchlorphos, -oxon	3983-45-7	0,83	0,86	269	271	109	304	xxx	xxx	xx
Fenclorim	3740-92-9	0,67	0,72	224	189	226	191	xx	xxx	xx
Fenfuram	24691-80-3	0,78	0,84	109	201	110	202	xx		xx
Fenhexamid	126833-17-8	1,46	1,35	97	177	55	179	x	xx	x

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Fenitrothion	122-14-5	0,94	0,98	277	125	109	260	xx	xx	xxx
Fenitrothion, -oxon	2255-17-6	0,85	1,18	244	109	261	231	x	xx	xx
Fenobucarb	3766-81-2	0,58	0,64	121	150	91	122	xxx		xx
Fenoprop-methylester (2,4,5-TP-methyl)	4841-20-7	0,74	0,75	196	198	223	282	xx	xxx	
Fenoxanil	115852-48-7	1,37	1,27	189	191	293	140	xx	xxx	x
Fenoxaprop, -P-ethyl	71283-80-2	1,59	1,54	288	361	290	363	xxx	x	x
Fenoxycarb	79127-80-3	1,52	1,43	116	88	186	255	x		x
Fenpiclonil	74738-17-3	1,50	1,49	236	238	174	201	xx	xxx	x
Fenpropathrin	64257-84-7	1,52	1,40	97	181	125	265	xx	xx	xx
Fenpropidin	67306-00-7	0,92	0,81	98	99	273	117	xxx		x
Fenpropimorph 1	67306-03-0	0,94	0,81	128	184	84	70	xxx		xx
Fenpropimorph 2	67564-91-4	1,00	0,86	128	129	303	117	xxx		xx
Fenpyroximate	134098-61-6	0,70	0,78	213	212	77	142	xx		x
Fenson	80-38-6	1,03	1,08	77	141	268	270	xxx	xx	
Fensulfothion	115-90-2	1,39	1,33	292	293	97	156	x	x	xx
Fensulfothion, -oxon	6552-21-2	1,29	1,30	276	277	140	220	x		x
Fensulfothion, -sulfone-oxon	6132-17-8	1,35	1,32	109	201	265	308	x	xx	xx
Fensulfothione, -sulfone	14255-72-2	1,43	1,35	324	188	109	97	xx	xxx	xxx
Fenthion	55-38-9	0,99	1,02	278	125	109	169	xxx	x	xxx
Fenthion, -oxon	6552-12-1	0,91	0,97	262	247	109	263	x	xx	xx
Fenthion, -sulfone-oxon	14086-35-2	1,32	1,32	294	215	109	230	x	xx	xx
Fenthion, -sulfone	3761-42-0	1,41	1,35	310	125	109	136	x	xx	xx
Fenthion, -sulfoxide	3761-41-9	1,40	1,35	279	125	294	109	x	xx	xx
Fenvalerate, (RS+SR)	51630-58-1	1,72	1,79	167	125	181	152	xx	xx	x
Fenvalerate, (RR+SS)	51630-58-1	1,74	1,82	125	167	181	152	xx	xx	x
Fipronil	120068-37-3	1,12	1,01	367	369	213	368	xxx	xxx	xx
Fipronil, -desulfinyl	111246-15-2	0,90	0,84	388	333	390	335	xxx	xxx	xx
Fipronil, -sulfide	120067-83-6	1,11	1,00	351	353	420	422	xxx	xxx	xx
Fipronil, -sulfone	120068-36-2	1,33	1,17	383	385	255	213	xx	xxx	xxx
Flamprop-M-isopropyl	57973-67-8	1,41	1,26	105	276	77	363	xxx	xxx	xx
Flamprop-M-methyl	52756-22-6	1,31	1,23	105	77	276	106	xxx	xx	x
Fluacrypyrim	229977-93-9	1,45	1,29	145	189	204	320	xxx	xxx	x
Fluazifop-butyl	69806-50-4	1,38	1,19	282	383	254	255	xxx	x	x
Fluazifop-P-butyl	79241-46-6	1,38	1,19	282	383	254	255	xxx	xx	x
Fluazinam	79622-59-6	1,11	0,95	418	420	372	337	x	xxx	x
Fluazolate	174514-07-9	1,26	1,10	385	383	402	400	xxx	xx	x
Flubenzimine	37893-02-0	1,29	1,10	416	186	135	77	xx	xxx	xxx
Fluchloralin	33245-39-5	0,77	0,72	306	326	264	328	xxx	xx	x
Fluconazol	86386-73-4	1,21	1,24	224	127	82	225	xx	xx	xx
Flucythrinate, 1	70124-77-5	1,67	1,65	199	157	451	181	xx	xx	x
Flucythrinate, 2	70124-77-5	1,69	1,68	199	157	451	181	xx	xx	x
Fludioxonil	131341-86-1	1,27	1,28	248	127	154	182	x	x	x
Flufenacet	142459-58-3	1,01	0,96	151	211	123	122	xx	x	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Flumiclorac-pentyl	87546-18-7	1,80	2,03	423	308	425	424	xx	xx	
Flumioxazin	103361-09-7	1,73	2,02	354	287	355	259	x	xx	x
Fluorodifen	15457-05-3	1,25	1,20	190	126	328	162	x	xx	x
Fluoroglycofen-ethyl	77501-90-7	1,58	1,49	344	447	345	223	x	xxx	x
Fluoroimide	41205-21-4	0,68	0,75	259	261	180	137	x	x	
Fluotrimazole	31251-03-3	1,50	1,36	311	379	165	233	xxx	xxx	xx
Fluquinconazole	136426-54-5	1,62	1,63	340	342	298	286	xxx	xxx	xx
Flurenol-butyl	2314-09-2	1,16	1,15	181	152	182	282	xx	xx	
Fluridone	59756-60-4	1,71	1,90	328	329	330	207	x		x
Flurochloridone	61213-25-0	1,03	1,05	311	187	313	174	x	xxx	x
Fluroxypyr-meptyl	81406-37-3	1,49	1,35	57	209	71	181	x	xx	xx
Flurprimidol	56425-91-3	0,85	0,83	269	107	270		x	xxx	xx
Flurtamone	96525-23-4	1,55	1,48	120	333	123	207	x	xx	x
Flusilazole	85509-19-9	1,32	1,24	233	206	234	315	xx	x	x
Fluthiacet-methyl	117337-19-6	1,92	2,61	403	405	56	207	x	xx	x
Flutolanil	66332-96-5	1,26	1,18	173	145	281	323	xx	xx	x
Flutriafol	76674-21-0	1,21	1,23	123	219	164	83	xx	xx	xx
Fluvalinate, tau-	69409-94-6	1,72	1,74	250	252	181	251	xxx	xx	x
Folpet	133-07-3	1,13	1,20	260	262	104	130	x	xx	x
Folpet-metabolite (Phthalimid)	85-41-6	0,51	0,60	147	76	104	103	xxx	xx	x
Fonofos	944-22-9	0,75	0,79	109	246	137	110	xxx	xx	xxx
Formothion	2540-82-1	0,82	0,93	125	93	126	170	x	x	xxx
Fosthiazate, cis-	98886-44-3	1,05	1,11	195	97	126	166	x	xx	x
Fosthiazate, trans-	98886-44-3	1,06	1,12	195	97	126	166	x	xx	xx
Fuberidazole	3878-19-1	0,87	0,98	184	155	156	129	x		x
Furathiocarb	65907-30-4	1,54	1,44	163	135	194	325	xx	x	xx
Genite	97-16-5	1,20	1,19	141	77	302	304	x	xx	x
Halfenprox	111872-58-3	1,66	1,62	263	265	183	185	xx	xx	
Haloxyfop-etotyl	87237-48-7	1,50	1,34	302	316	288	433	x	xxx	xx
Haloxyfop-methyl	72619-32-0	1,18	1,06	316	288	375	289	xxx	xx	x
HCH, alpha-	319-84-6	0,67	0,73	181	219	183	217	xxx	xxx	
HCH, beta-	319-85-7	0,72	0,85	181	219	183	217	xxx	xxx	
HCH, delta-	319-86-8	0,78	0,90	219	181	183	217	xxx	xxx	
HCH, epsilon-	6108-10-7	0,80	0,93	181	183	219	217	xxx	xxx	
HCH, gamma- (Lindane)	58-89-9	0,73	0,80	183	181	219	217	xxx	xxx	
Heptachlor	76-44-8	0,89	0,87	272	274	100	270	xx	xxx	
Heptachlor epoxide, cis-	28044-83-9	1,08	1,05	353	355	351	81	xxx	xxx	
Heptachlor epoxide, trans-	1024-57-3	1,10	1,07	351	353	355	81	xx	xxx	
Heptenophos	23560-59-0	0,56	0,63	124	89	109	126	xx	xx	xxx
Hexachlorobenzene (HCB)	118-74-1	0,68	0,71	284	286	282	287	xxx	xxx	
Hexaconazole	79983-71-4	1,24	1,18	83	214	216	82	xx	xx	xx
Hexazinone	51235-04-2	1,47	1,42	171	83	128	71	xxx		xxx
Hexythiazox	78587-05-0	1,16	1,26	156	155	227	157	x	x	x
Hydroprene, (S)	65733-18-8	0,93	0,73	139	111	81	266	xx		

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Imazalil	35554-44-0	1,25	1,21	215	173	217	175	x	x	x
Imazamethabenz-methyl	81405-85-8	1,33	1,27	144	187	256	245	x		
Imibenconazole	86598-92-7	1,88	2,36	207	125	44	82	xx	xx	xx
Imibenconazole-metabolite (Imibenconazole, desbenzyl-)	199338-48-2	1,30	1,31	88	87	235	270	x	xx	x
Indoxacarb	173584-44-6	1,78	1,91	150	218	59	203	xxx	xx	x
Ioxynil octanoate	3861-47-0	1,57	1,50	127	57	128	55	x	xx	x
Ipconazole	125225-28-7	1,57	1,50	125	83	70	249	xx	x	x
Iprobenfos	26087-47-8	0,81	0,82	91	204	123	122	xx	x	xx
Iprodione	36734-19-7	1,51	1,41	314	316	187	189	x	xx	x
Ipronidazole	14885-29-1	0,48	0,56	123	169	154	81	x	x	xxx
Iprovalicarb, (SR)	140923-25-7	1,31	1,18	119	134	116	72	xx		x
Iprovalicarb, (SS)	140923-25-7	1,35	1,21	119	134	116	72	xx		x
Isazofos	42509-80-8	0,79	0,82	161	119	162	97	xxx	x	xx
Isobenzan	297-78-9	1,02	0,95	311	103	313	309	xxx	xxx	
Isocarbamid	30979-48-7	0,73	0,85	142	130	113	71	x	x	xx
Isocarbophos	24353-61-5	1,02	1,05	136	121	120	110	xx	xx	xx
Isodrin	465-73-6	1,05	1,02	193	195	263	66	xxx	xxx	
Isofenphos	25311-71-1	1,12	1,05	213	58	121	255	xxx	xx	xxx
Isofenphos, -oxon	106848-93-5	1,02	0,99	229	201	120	58	xx	x	xx
Isomethiozin	57052-04-7	1,00	0,98	225	198	57	82	xxx	xx	x
Isoprocarb	2631-40-5	0,53	0,60	121	136	91	122	xxx		xx
Isopropalin	33820-53-0	1,07	0,98	280	238	281	264	xxx	xx	xx
Isoproturon-metabolite (Isopropylaniline, 4-)	99-88-7	0,38	0,44	120	135	103	91	xxx	x	x
Isoprothiolane	50512-35-1	1,24	1,27	118	162	189	290	xx	xxx	x
Isoxadifen-ethyl	163520-33-0	1,44	1,35	204	165	180	222	xx	xx	x
Isoxathion	18854-01-8	1,35	1,27	105	177	313	77	x	x	xx
Jasmolin I (Pyrethrins-compound)	4466-14-2	1,43	1,22	123	164	93	81	xx	x	
Jasmolin II (Pyrethrins-compound)	1172-63-0	1,58	1,45	107	133	91	167	xx	x	
Jodfenphos	18181-70-9	1,24	1,21	377	379	125	378	xx	xxx	xxx
Kresoxim-methyl	143390-89-0	1,34	1,27	116	206	131	132	xx	xx	x
Lactofen	77501-63-4	1,57	1,46	344	345	346	223	xx	xx	x
Lenacil	2164-08-1	1,47	1,40	153	154			x		x
Leptophos	21609-90-5	1,55	1,47	377	171	375	379	xx	x	x
Lindane (HCH, gamma-)	58-89-9	0,73	0,80	183	181	219	217	xxx	xxx	
Linuron	330-55-2	0,96	0,97	61	149	248	187	x	x	x
Malaoxon	1634-78-2	0,88	0,91	127	99	109	125	x	x	x
Malathion	121-75-5	0,97	0,97	173	125	127	93	xx	xx	xxx
Malathion, iso-	3344-12-5	1,14	1,14	127	99	283	173	xx	xx	xx
MCPA-butolyl	19480-43-4	1,13	1,05	300	200	57	155	xx	x	
Mecarbam	2595-54-2	1,12	1,09	131	97	159	125	x	xxx	xxx
Mefenacet	73250-68-7	1,56	1,54	192	120	136	77	x	x	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Mefenpyr-diethyl	135590-91-9	1,50	1,39	253	255	299	301	xx	xxx	xx
Mepanipyrim	110235-47-7	1,21	1,22	222	223	221	224	xx		xx
Mephosfolan	950-10-7	1,11	1,24	196	140	227	168	x	xx	xxx
Mepronil	55814-41-0	1,43	1,33	119	269	91	120	xx		xx
Methiocarb	2032-65-7	0,94	0,98	168	153	109	91	x		x
Metalaxyl	57837-19-1	0,90	0,92	206	160	249	132	xxx		xx
Metazachlor	67129-08-2	1,08	1,10	133	81	209	132	xxx	xx	x
Metconazole, cis-	125116-23-6	1,53	1,45	125	70	83	138	x	x	xxx
Metconazole, trans-	125116-23-6	1,55	1,48	125	70	83	138	x	x	xxx
Methabenzthiazuron-metabolite (Methylaminobenzthiazol)	16954-69-1	0,63	0,74	164	136	135	163	x		xx
Methacrifos	62610-77-9	0,51	0,56	125	208	180	240	xxx	xx	xxx
Methamidophos	10265-92-6	0,38	0,47	94	95	141	64	x		xx
Methidathion	950-37-8	1,16	1,20	145	85	93	125	x	xx	xxx
Methomyl	16752-77-5	0,55	0,35	105	58	88	59	xx		x
Methoprotryne	841-06-5	1,33	1,26	256	213	226	240	xx		xx
Methoxychlor, 2,4-	30667-99-3	1,48	1,39	227	121	228	258	xxx	xx	
Methoxychlor, -olefin	2132-70-9	1,45	1,35	308	310	238	223	xxx	xxx	
Methoxychlor	72-43-5	1,52	1,44	227	228	212	113	xxx	xxx	
Bromoxynil-metabolite (4-Bromphenylisocyanate)	2493-02-9	0,36	0,43	197	199	90	171	x	xx	xx
Metolachlor	51218-45-2	0,98	0,95	162	238	240	146	xxx	xx	x
Metominostrobin, (E)-	133408-50-1	1,27	1,27	191	196	238	238	xx	x	
Metominostrobin, (Z)-	133408-51-2	1,34	1,30	191	196	165	238	xx	x	
Metrafenone	220899-03-6	1,59	1,54	395	393	377	379	xx	xxx	
Metribuzin	21087-64-9	0,85	0,94	198	199	57	103	xx	xxx	xx
Mevinphos, (E)-	338-45-4	0,47	0,54	127	192	109	67	xx	x	xxx
Mevinphos, (Z)-	298-01-1	0,47	0,55	127	192	109	67	xx	x	xxx
Mirex	2385-85-5	1,56	1,47	272	274	270	237	xxx	xxx	
Molinate	2212-67-1	0,54	0,60	126	55	187	83	xx		xx
Monocrotophos	6923-22-4	0,64	0,76	127	192	67	97	x		xxx
Monolinuron	1746-81-2	0,72	0,78	61	214	126	153	x	x	x
Myclobutanil	88671-89-0	1,31	1,27	179	150	181	288	x	xx	xx
Naled	300-76-5	0,63	0,46	109	145	185	79	x	xx	xxx
Naphthyloxyacetic acid, -methylester, 2-	1929-87-9	0,82	0,88	216	115	127	157	xx	x	
Naproanilide	52570-16-8	1,57	1,53	291	171	144	120	x		x
Napropamide	15299-99-7	1,23	1,20	72	128	271	100	xxx		xx
Nicotine	54-11-5	0,43	0,49	84	133	161	162	xxx		xx
Nitralin	4726-14-1	1,50	1,39	316	274	300	258	xx	xxx	xxx
Nitrapyrin	1929-82-4	0,49	0,55	194	196	198	91	xx	xx	x
Nitrofen	1836-75-5	1,35	1,29	283	285	202	139	xx	xxx	x
Nitrothal-isopropyl	10552-74-6	1,02	0,93	236	194	212	254	xx	xx	x
Nonachlor, cis-	5103-73-1	1,40	1,29	409	407	411	405	xxx	x	
Nonachlor, trans-	39765-80-5	1,21	1,12	409	407	411	405	xxx	xxx	

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Norflurazon-metabolite (Norflurazon, -desmethyl)	23576-24-1	1,44	1,37	145	289	288	291	x	xx	x
Nuarimol	63284-71-9	1,48	1,38	235	203	107	314	xx	xxx	xx
S421	127-90-2	0,91	0,88	130	132	79	83	xx	x	
Octachlorostyrene	29082-74-4	1,07	0,99	308	380	343	379	xxx	xx	
Ofurace	58810-48-3	1,44	1,40	132	160	232	281	x	xxx	xx
Omethoate	1113-02-6	0,57	0,69	156	110	109	79	x	x	xx
Orbencarb	34622-58-7	0,93	0,95	100	222	72	125	xxx	x	xx
Oryzalin	19044-88-3	1,61	1,57	317	275	406	301	xx		
Oxadiazon	19666-30-9	1,30	1,16	175	177	258	302	xxx	xxx	x
Oxadixyl	77732-09-3	1,41	1,37	163	105	132	120	xx	x	x
Oxydemeton-methyl (Demeton-methyl-sulfoxid)	301-12-2	0,34	0,40	109	110	168	79	xx		x
Oxyfluorfen	42874-03-3	1,32	1,19	252	361	300	302	x	xxx	x
Paclobutrazol	76738-62-0	1,18	1,14	236	125	238	167	xxx	x	xx
Paraoxon-ethyl	311-45-5	0,90	0,94	109	149	81	139	x	x	x
Paraoxon-methyl	950-35-6	0,77	0,86	109	230	96	247	x	x	x
Parathion	56-38-2	1,00	1,00	291	109	97	125	xx	xx	xxx
Parathion-methyl	298-00-0	0,87	0,93	263	109	125	233	xx	xx	xxx
Parlar 26	142534-71-2	1,34	1,21	329	331	231	305	xx	xxx	
Parlar 32	51775-36-1	1,40	1,33	233	235	159	247	xx	xxx	
Parlar 50	66860-80-8	1,49	1,37	83	195	279	159	xx	xxx	
Parlar 62	164159-06-5	1,54	1,48	340	177	161	164	x	xx	
PCB 3 (PCB-4)	2051-62-9	0,57	0,63	188	152	190	153	xxx	x	
PCB 15 (PCB-4,4´)	2050-68-2	0,76	0,80	222	224	152	223	xxx	xxx	
PCB 28 (PCB-2,4,4´)	7012-37-5	0,85	0,87	258	256	186	260	xx	xxx	
PCB 30 (PCB-2,4´,5)	35693-92-6	0,72	0,74	256	258	186	260	xx	xxx	
PCB 31 (PCB-2,4,5)	16606-02-3	0,85	0,87	258	256	186	260	xxx	xxx	
PCB 49 (PCB-2,2´,4,5´)	41464-40-8	0,95	0,94	292	290	294	220	xxx	xxx	
PCB 52 (PCB-2,2´,5,5´)	35693-99-3	0,94	0,93	292	290	294	220	xxx	xxx	
PCB 77 (PCB-3,3´,4,4´)	32598-13-3	1,30	1,24	292	290	294	220	xxx	xxx	
PCB 101 (PCB-2,2´,4,5,5´)	37680-73-2	1,18	1,11	326	328	324	254	xxx	xxx	
PCB 118 (PCB-2,3´,4,4´,5)	31508-00-6	1,38	1,27	326	328	324	254	xxx	xxx	
PCB 127 (PCB-3,3´,4,5,5´)	39635-33-1	1,43	1,31	326	328	207	324	xxx	xxx	
PCB 131 (PCB-2,2´,3,3´,4,6)	61798-70-7	1,46	1,32	360	362	288	290	xxx	xxx	
PCB 136 (PCB-2,2´,3,3´,5,6´)	38411-22-2	1,29	1,22	360	362	358	290	xxx	xxx	
PCB 138 (PCB-2,2´,3,4,4´,5´)	35065-28-2	1,47	1,34	360	362	358	290	xxx	xxx	
PCB 153 (PCB-2,2´,4,4´,5,5´)	35065-27-1	1,43	1,29	360	362	358	290	xxx	xxx	
PCB 169 (PCB-3,3´,4,4´,5,5´)	32774-16-6	1,55	1,46	360	362	358	364	xxx	xxx	
PCB 170 (PCB-2,2´,3,3´,4,4´,5)	35065-30-6	1,56	1,47	394	396	324	398	xxx	xxx	
PCB 180 (PCB-2,2´,3,4,4´,5,5´)	35065-29-3	1,53	1,42	394	396	324	392	xxx	xxx	
PCB 209 (PCB-2,2´,3,3´,4,4´,5,5´,6,6´)	2051-24-3	1,70	1,67	498	500	496	502	xxx	xxx	
Pebulate	1114-71-2	0,48	0,52	128	57	72	203	xx		x
Penconazole	66246-88-6	1,09	1,07	248	159	161	250	xxx	xxx	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Pendimethalin	40487-42-1	1,09	1,05	252	162	281	253	xxx	xxx	xx
Quintozene-metabolite (Pentachloroaniline)	527-20-8	0,83	0,88	265	267	263	269	xxx	xxx	x
Pentachlorophenol-metabolite (Pentachloroanisole)	1825-21-4	0,69	0,73	265	280	237	263	xxx	xxx	
Pentachlorobenzene	608-93-5	0,53	0,58	250	252	248	254	xxx	xxx	
Pentachlorophenol (PCP)	87-86-5	0,72	0,77	266	268	264	165	xx	x	
Pentachlorophenol-metabolite (Pentachlorophenol-acetate)	1441-02-7	0,78	0,79	266	268	264	270	xxx	xxx	
Pentanochlor	2307-68-8	0,95	0,93	141	143	71	239	xx	x	x
Permethrin, cis-	52645-53-1	1,61	1,54	183	207	163	165	xx	xx	
Permethrin, trans-	51877-74-8	1,61	1,55	183	163	165	184	xx	xx	
Phenkapton	2275-14-1	1,52	1,43	121	153	191	97	xx	x	xx
Phenothrin, cis-	51186-88-0	1,53	1,42	123	183	184	81	xxx	xx	
Phenothrin, trans-	26046-85-5	1,54	1,45	123	183	184	81	xx	xx	
Phenthoate	2597-03-7	1,13	1,11	274	121	125	93	xx	xx	xx
Phorate	298-02-2	0,66	0,70	75	121	260	231	xx	xx	xxx
Phorate, -oxon	2600-69-3	0,59	0,65	171	75	74	111	xx	x	xx
Phorate, -sulfone	2588-04-7	0,98	1,04	153	199	97	125	xx	xxx	xxx
Phorate, -sulfoxide	2588-03-6	0,96	1,03	153	199	97	125	xx	x	xxx
Phosalone	2310-17-0	1,55	1,49	182	121	184	367	xx	xx	xxx
Phosfolan	947-02-4	1,11	1,26	140	92	196	255	xx	xx	xxx
Phosmet	732-11-6	1,51	1,48	160	161	77	93	xx	x	xxx
Phosphamidon, (E)-	297-99-4	0,77	0,81	127	264	72	138	xx	x	xxx
Phosphamidon, (Z)-	23783-98-4	0,85	0,89	127	264	72	138	xx	x	xxx
Phosphorothioic acid,O-(3-bromo-4-methyl-2-oxo-2H-1-benzopyran-7-yl) O,O-diethyl ester	121227-99-4	1,67	1,76	406	408	270	272	x	x	xx
Picloram-methyl	14143-55-6	0,95	1,03	196	198	223	282	xx	xx	xx
Picolinafen	137641-05-5	1,52	1,40	238	376	239	377	xx	xx	xx
Picoxystrobin	117428-22-5	1,25	1,18	145	335	146	173	xxx	xxx	xx
Pindone	83-26-1	0,76	0,79	173	174	230	146	xx	xx	
Piperalin	3478-94-2	1,47	1,32	112	314	316	173	xx	xx	xx
Piperonyl butoxide	51-03-6	1,49	1,35	176	177	149	207	xx		
Piperophos	24151-93-7	1,52	1,42	320	140	122	97	xx	xxx	xxx
Pirimicarb	23103-98-2	0,82	0,86	166	72	238	167	xx		xx
Pirimicarb-metabolite (Pirimicarb, -desmethyl)	30614-22-3	0,84	0,92	152	72	224	153	xx		x
Pirimiphos-ethyl	23505-41-1	1,07	0,99	333	318	304	168	xx	x	xxx
Pirimiphos-methyl	29232-93-7	0,95	0,92	290	276	305	233	xx	x	xxx
Plifenate (Benzethazet)	21757-82-4	0,87	0,84	175	217	219	177	xx	xx	
Potasan	299-45-6	1,55	1,50	328	192	148	176	xxx	x	xxx
Prallethrin, cis-	23031-36-9	1,16	1,00	123	81	79	105	xx	xxx	
Prallethrin, trans-	23031-36-9	1,17	1,06	123	81	79	105	xxx	xxx	
Probenazole	27605-76-1	0,97	0,84	130	159	104	76	xx	xx	x

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Prochloraz	67747-09-5	1,62	1,59	180	308	310	70	x	x	xxx
Procymidone	32809-16-8	1,14	1,10	96	283	285	67	xxx	xxx	x
Prodiamine	29091-21-2	0,95	0,87	321	279	333	274	xx	xxx	xx
Profenofos	41198-08-7	1,26	1,21	208	139	339	337	xx	xxx	xxx
Profenofos-metabolite (4-Bromo-2-chlorophenol)	3964-56-5	0,39	0,46	208	206	63	210	xx	xxx	x
Profluralin	26399-36-0	0,74	0,68	55	318	330	264	xxx	xxx	xx
Promecarb	2631-37-0	0,65	0,71	135	150	91	136	xxx		x
Promecarb-metabolite (m-Thymol)	3228-03-3	0,41	0,46	135	150	91	136	xxx		
Prometon	1610-18-0	0,70	0,74	210	225	168	183	xxx		xx
Prometryn	7287-19-6	0,90	0,91	241	184	226	105	xxx		xx
Propachlor	1918-16-7	0,59	0,65	120	176	93	77	xx	xxx	x
Propamocarb	24579-73-5	0,45	0,50	58	59	56	129	xx		x
Propaphos	7292-16-2	1,17	1,13	220	304	140	262	xx		xx
Propargite	2312-35-8	1,48	1,35	135	173	81	201	xxx	x	
Propazine	139-40-2	0,72	0,75	214	229	172	58	xxx	x	xxx
Propetamphos	31218-83-4	0,74	0,75	138	194	236	222	xx	x	x
Propham	122-42-9	0,48	0,54	93	179	137	120	xx		x
Propiconazole, cis-	60207-90-1	1,46	1,35	259	173	69	261	xx	xx	xx
Propiconazole, trans-	60207-90-1	1,47	1,34	259	173	69	261	xx	xx	xx
Propisochlor	86763-47-5	0,90	0,86	162	223	224	211	xx	xx	xx
Propoxur	114-26-1	0,59	0,66	110	152	111	81	xxx		xxx
Propoxur-metabolite (2-Isopropoxyphenol)	4812-20-8	0,35	0,39	110	152	111	81	xxx	x	
Propyzamide	23950-58-5	0,74	0,75	173	175	145	255	xxx	xxx	x
Prosulfocarb	52888-80-9	0,91	0,91	128	91	251	86	xx		x
Prothioconazole	178928-70-6	1,30	1,28	274	125	276	275	x	x	x
Prothioconazole-metabolite (Prothioconazole, -desthio)	A-399	1,32	1,26	186	188	125	83	xxx	xx	xx
Prothiofos	34643-46-4	1,25	1,16	309	267	162	113	xxx	xx	x
Prothoate	2275-18-5	0,86	0,88	115	97	73	121	xx	xxx	xxx
Pyracarbolid	24691-76-7	1,04	1,09	125	217	97	107	x		x
Pyraclofos	89784-60-1	1,59	1,54	360	194	138	362	x	xxx	xxx
Pyraclostrobin	175013-18-0	1,60	1,58	132	325	111	133	xx	x	x
Pyraflufen-ethyl	129630-19-9	1,47	1,35	412	414	349	339	xx	xx	x
Pyrazophos	13457-18-6	1,58	1,51	221	232	373	237	xx	xx	xxx
Pyrethrin I (Pyrethrins-compound)	121-21-1	1,43	1,25	123	105	91	81	x	x	
Pyrethrin II (Pyrethrins-compound)	121-29-9	1,45	1,48	123	133	162	91	x	x	
Pyributicarb	88678-67-5	1,50	1,40	165	108	181	166	xx	xxx	xx
Pyridaben	96489-71-3	1,61	1,57	147	117	148	132	xx	xx	x
Pyridaphenthion	119-12-0	1,51	1,44	340	97	199	188	x	x	xx
Pyridate	55512-33-9	1,72	1,73	207	205	206	57	x	xx	x
Pyridinitril	1086-02-8	1,12	1,19	273	275	237	202	x	xx	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Pyrifenox, (Z)-	88283-41-4	1,10	1,09	262	264	92	187	xx	xx	x
Pyrifenox, (E)-	88283-41-4	1,18	1,15	262	264	92	187	xx	xx	x
Pyriftalid	135186-78-6	1,58	1,60	318	274	317	273	xx	x	xx
Pyrimethanil	53112-28-0	0,75	0,81	198	199	200	77	xxx		xxx
Pyrimidifen	105779-78-0	1,71	1,73	184	186	185	161	xxx	xxx	xx
Pyriminobac-methyl, (E)-	136191-64-5	1,47	1,31	302	256	330	303	xxx	xxx	xxx
Pyriminobac-methyl, (Z)-	136191-64-5	1,41	1,31	302	330	256	303	xxx	xxx	xxx
Pyriproxyfen	95737-68-1	1,55	1,48	136	96	78	226	xx		xx
Pyroquilon	57369-32-1	0,74	0,87	173	130	172	144	xx		xx
Quinalphos	13593-03-8	1,12	1,11	146	157	156	118	xx	xx	xxx
Quinoclamine	2797-51-5	0,95	1,09	207	172	209	89	x	xxx	x
Quinoxyfen	124495-18-7	1,45	1,35	237	272	307	309	xxx	xxx	x
Quintozene	82-68-8	0,74	0,78	237	249	295	239	xxx	xxx	x
Quintozene-metabolite (Pentachlorophenylmethylsulfide)	1825-19-0	0,95	0,95	296	298	294	246	xx	xxx	x
Quizalofop-P-ethyl	100646-51-3	1,67	1,70	299	372	374	301	x	x	x
Quizalofop-P-tefuryl	119738-06-6	2,07	2,84	285	428	299	287	x	x	x
Rabenzazole	40341-04-6	1,00	1,03	212	197	199	314	x		x
Resmethrin, cis-	10453-86-8	1,49	1,35	123	171	143	128	xx	x	
Resmethrin, trans-	10453-86-8	1,49	1,35	123	171	143	128	xxx	x	
Salithion (Dioxabenzofos)	3811-49-2	0,64	0,74	216	183	78	201	xx	x	x
Schradan	152-16-9	0,70	0,76	135	199	153	286	xx		xx
Sebuthylazine	7286-69-3	0,81	0,84	200	202	214	229	xx	x	xx
Sebuthylazine-metabolite (Sebuthylazine, desethyl-)	37019-18-4	0,72	0,78	172	174	186	201	xx	x	xx
Secbumeton	26259-45-0	0,78	0,81	196	210	169	225	xxx		xx
Silafluofen	105024-66-6	1,69	1,67	179	286	258	151	xxx	x	
Silthiofam	175217-20-6	0,83	0,81	252	253	75	254	xxx	x	xx
Simazine	122-34-9	0,70	0,78	201	186	173	203	xx	x	xxx
Simeconazole	149508-90-7	0,88	0,86	121	73	211	195	x	x	x
Simetryn	1014-70-6	0,88	0,94	213	170	155	198	xxx		xx
Spirodiclofen	148477-71-8	1,61	1,52	71	312	99	157	xxx	xxx	
Spiromesifen	283594-90-1	1,50	1,37	272	57	99	273	xxx	xxx	
Spiroxamine-metabolite (Cyclohexanone, 4-tert.-butyl-)	98-53-3	0,38	0,43	57	98	154	83	xxx		
Spiroxamine, A	118134-30-8	0,86	0,76	100	101	126	198	xxx		xx
Spiroxamine, B	118134-30-8	0,93	0,80	100	101	126	198	xxx		xx
Sulfallate	95-06-7	0,65	0,72	188	88	72	189	xxx	xxx	xx
Sulfentrazone	122836-35-5	1,53	1,47	307	388	387	351	xx	xx	
Sulfotep	3689-24-5	0,65	0,68	322	202	97	238	xxx	x	xxx
Sulprofos	35400-43-2	1,44	1,33	322	156	140	138	xx	xxx	xxx
SWEP	1918-18-9	0,71	0,77	187	189	219	221	xx	xx	x
Tebuconazole	107534-96-3	1,48	1,37	250	125	70	83	xx	x	xxx
Tebufenpyrad	119168-77-3	1,53	1,41	318	333	171	276	xxx	x	xx

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Tebupirimfos	96182-53-5	0,81	0,75	318	261	234	152	xxx	xxx	xxx
Tebutam	35256-85-0	0,65	0,67	91	57	190	233	xxx		x
Tebuthiuron	34014-18-1	0,52	0,61	156	171	74	88	x	x	x
Tecnazene	117-18-0	0,59	0,64	203	215	261	201	xxx	xxx	x
Tecnazene-Isomer (Tetrachloronitrobenzene, 1,2,3,4-)	879-39-0	0,64	0,70	203	215	261	201	xxx	xxx	
Tefluthrin	79538-32-2	0,79	0,71	177	197	178	199	xxx	x	
Temephos	3383-96-8	2,00	2,70	466	125	467	203	x	xx	
TEPP	107-49-3	0,55	0,63	263	161	179	235	xx		xxx
Terbacil	5902-51-2	0,78	0,87	161	160	117	163	xx	x	x
Terbufos	13071-79-9	0,74	0,74	231	57	153	103	xxx	xx	xxx
Terbufos, -oxon	A-233	0,67	0,70	171	215	170	57	xx	xx	xx
Terbufos, -sulfoxide-oxon	56165-57-2	0,97	1,38	109	140	57	183	x		
Terbufos, -sulfone	56070-16-7	1,09	1,11	153	199	97	125	xx		
Terbufos, -sulfoxide	10548-10-4	0,74	0,74	231	57	97	103	x		x
Terbumeton	33693-04-8	0,72	0,76	210	169	225	154	xxx		xx
Terbuthylazine	5915-41-3	0,74	0,78	214	173	229	216	xxx	x	xx
Terbutylazine-metabolite (Terbuthylazine, -desethyl)	30125-63-4	0,64	0,71	186	188	145	201	xxx	x	x
Terbutryn	886-50-0	0,93	0,94	226	185	241	170	xx		xx
Tetrachlorvinphos	22350-76-1	1,20	1,17	329	331	109	333	xxx	xxx	xxx
Tetraconazole	112281-77-3	1,02	0,99	336	338	337	171	xx	xx	x
Tetradifon	116-29-0	1,54	1,48	159	356	111	229	xxx	xxx	
Tetramethrin, cis-	51384-90-4	1,51	1,42	164	123	207	165	xx	xx	
Tetramethrin, trans-	1166-46-7	1,52	1,42	164	123	207	165	xx	xx	
Tetrasul	2227-13-6	1,42	1,31	252	324	254	322	xxx	xxx	
Thiabendazole	148-79-8	1,10	1,22	201	174	202	175	x		xx
Thiamethoxam	153719-23-4	1,05	1,15	212	182	247	132	x	x	x
Thiazopyr	117718-60-2	0,99	0,89	327	363	349	306	xxx	xxx	xx
Thifluzamide	130000-40-7	1,34	1,17	194	166	449	447	xx	xxx	x
Thionazin	297-97-2	0,58	0,65	97	96	107	143	xx	xx	xxx
Tiocarbazil, 1	36756-79-3	1,02	0,96	91	100	156	57	xx	x	x
Tiocarbazil, 2	36756-79-3	1,02	0,97	91	100	156	57	xx	x	x
Tolclofos-methyl	57018-04-9	0,88	0,92	265	267	125	266	xxx	xx	xx
Tolfenpyrad	129558-76-5	1,83	2,07	383	171	197	211	xx		
Tolylfluanid	731-27-1	1,11	1,09	137	238	240	181	xxx	xx	x
Tolylfluanid-metabolite (DMST)	66840-71-9	0,72	0,82	106	214	79	77	x		x
Transfluthrin	118712-89-3	0,88	0,82	163	165	91	127	xxx	xxx	
Triadimefon	43121-43-3	1,01	0,97	57	208	85	210	xx	xx	xxx
Triadimenol, Erythro-	70585-37-4	1,14	1,10	112	168	128	57	x	xx	xx
Triadimenol, Threo-	70585-35-2	1,13	1,08	112	168	128	57	x	xx	xx
Triallate	2303-17-5	0,79	0,78	86	268	270	128	xxx	xxx	x

Table 1 *(continued)*

Pesticide name	CAS-Nr.	RRT HP5MS	RRT DB35MS	Ion1	Ion2	Ion3	Ion4	MSD	ECD	NPD
Triamiphos	1031-47-6	1,41	1,34	160	294	135	161	x		xxx
Triapenthenol	76608-88-3	0,95	0,91	206	70	207	124	xxx		xx
Triazamate	112143-82-5	1,20	1,14	72	227	314	242	xx	xx	xxx
Triazophos	24017-47-8	1,44	1,37	161	162	172	257	x		xxx
Triazoxide	72459-58-6	1,49	1,28	247	203	231	176	xx	x	x
Tribufos (DEF)	78-48-8	1,28	1,17	169	57	202	170	xx	xxx	xxx
Trichlamide	70193-21-4	1,19	1,07	148	121	120	92	x	xx	
Trichlorfon	52-68-6	0,49	0,44	109	79	110	145	xx	xx	xx
Trichloronat	327-98-0	1,03	0,97	269	297	271	109	xxx	xxx	xxx
Tricyclazole	41814-78-2	1,25	1,35	189	162	161	135	x		xxx
Tridemorph , 4-tridecyl-	24602-86-6	0,81	0,68	128	129	297	268	x		x
Tridiphane	58138-08-2	0,90	0,89	173	187	189	175	xx	xxx	x
Trietazine	1912-26-1	0,74	0,77	200	229	214	186	xx	xx	xxx
Trifenmorph	1420-06-0	1,57	1,23	243	165	244	252	xx		
Trifenmorph metabolite, (Tritane)	519-73-3	1,02	1,02	244	165	167	166	xx		
Trifloxystrobin	141517-21-7	1,47	1,33	116	131	222	132	xx	xx	x
Triflumizole	99387-89-0	1,16	1,05	278	73	206	287	xx	xxx	xx
Trifluralin	1582-09-8	0,63	0,61	306	264	290	335	xxx	xxx	x
Trimethacarb, 2,3,5-	2655-15-4	0,62	0,69	136	121	91	137	xx		x
Trimethacarb, 3,4,5-	2686-99-9	0,70	0,77	136	121	135	91	xx		x
Triticonazole	131983-72-7	1,54	1,48	235	83	237	217	xxx	xx	xx
Uniconazole-P	83657-17-4	1,27	1,23	234	236	70	235	xx	xx	xx
Vamidothion	2275-23-2	1,19	1,25	87	145	109	58	x	x	xx
Vernolate	1929-77-7	0,48	0,51	128	86	146	203	xx		xxx
Vinclozolin	50471-44-8	0,87	0,86	212	285	198	187	xx	xxx	x
Zoxamide	156052-68-5	1,49	1,17	187	189	258	260	x	xx	x

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[1] Methode L 00.00-73 Untersuchung von Lebensmitteln - Rückstandsanalyse von Pflanzenschutzmitteln in Lebensmitteln (Tabellarische Auflistung der relativen Retentionszeiten von Pflanzenschutzmittel-Wirkstoffen bei der gaschromatographischen Bestimmung), Amtliche Sammlung von Untersuchungsverfahren nach § 64 Lebensmittel-, Bedarfsgegenstände- und Futtermittelgesetzbuch LFGB (Method L 00.00-73 Food analysis – Analysis of pesticide residues in food (Table listing relative retention times for GC analysis of pesticides), Collection of Official Methods under Article 64 of the German Federal Food and Feed Code LFGB).

[2] Pesticide Manual, 13th edition 2004, C.D.S. Tomlin (Ed.), British Crop Protection Council, Farnham, Surrey, UK.

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