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Foodstuffs — Determination of pesticide residues by GC-MS/MS — Tandem mass spectrometric parameters

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National foreword

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Foodstuffs - Determination of pesticide residues by GC-MS/MS - Tandem mass spectrometric parameters

Produits alimentaires - Détermination des résidus de pesticides par CG-SM/SM - Paramètres pour la spectrométrie de masse en tandem

Lebensmittel - Bestimmung von Pestizidrückständen mit GC-MS/MS - Parameter für die Tandem-Massenspektrometrie

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Foreword

This document (CEN/TR 16699:2014) 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 residues analysis employs multi methods involving extraction of residues from the homogenized sample and clean-up of the extract in order to determine as many components as possible in the extracts. Afterwards the extracts can be analysed by different kind of instruments. The hyphenation of gas chromatography (GC) and tandem mass spectrometry (MS/MS) is a highly selective technique for identification and quantification of pesticide residues in extracts of plant and animal origin. This technique may be used to replace GC-MS detection in existing methods without the need for additional validation provided that calibration was successful and has demonstrated the required sensitivity and precision.

For the ionization of the analytes (pesticides and/or their metabolites) in GC-MS/MS, electron impact ionization (EI) is widely used because it offers sufficient ionization of most compound classes. However, very often molecular ions (cation radicals) and several fragment ions are formed simultaneously. For that reason, a rich variety of potential parent ions for MS/MS transitions exists compared to the soft ionization techniques applied in LC-MS/MS. This results in a greater freedom for the selection of an appropriate transition for a given situation. Such freedom is useful and often necessary in GC-MS/MS because a higher number of (fragment) ions are often produced by the matrix, which may interfere with the signal of the target analyte. On the other hand, this higher number of options may be a bit confusing for less experienced analysts.

To simplify the selection of suitable GC-MS/MS transitions in that situation, this Technical Report lists those MS/MS transitions, which have been reported most often in the scientific literature or are most often proposed by suppliers of GC-MS/MS instruments.

1 Scope

This Technical Report lists the mass spectrometric parameters which are useful for the application of European Standards for the determination of pesticide residues in foods of plant origin that use GC-MS. These European Standards are as follows:

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 — QuEChERS-method*

To facilitate the determination of pesticides and/or metabolites using GC-MS/MS, Table 2 specifies the diagnostic ion transitions suitable for identification and quantification, which can be used.

2 Normative References

None.

3 Parameters for GC-MS/MS determination of pesticides following electron impact ionization

3.1 General

All parameters given in Table 2 were carefully selected from different sources (open literature, application notes of instrument providers or tested by experts of CEN/TC 275/WG 4). Only transitions that were applicable on instruments of at least two different manufacturers (e.g. Agilent Technologies, Bruker Daltonics, Thermo Scientific, former Varian Inc., Waters Corporation) were selected.

GC parameters and retention times are not described in this Technical Report. If needed, this information can be taken from CEN/TR 16468 "Food analysis - Determination of pesticide residues by GC-MS - Retention times, mass spectrometric parameters and detector response information".

3.2 General MS/MS Parameters

All listed MS/MS transitions were obtained from measurements with electron impact ionization at 70 eV. Other parameters (e.g. ion source temperature, ion source voltages, source pressure and the type of carrier gas) were not identical. It is well recognized that variations of these parameters may influence the intensity of selected precursor ions and individual optimization may be necessary. However, despite these differences very often the same preferred precursor ions were reported. This demonstrates that in many cases parameters can be transferred between instruments of other types of the same or other manufacturers, even if these instruments are operated under slightly different conditions.

3.3 Analyte specific MS/MS Parameters

The most often reported analyte specific ion transitions of pesticides are listed in Table 2. Transitions applicable for instruments of three suppliers are reported first and those transitions reported for instruments of two suppliers are written in italics. If available, at least two precursor ions with their transitions have been selected for each analyte. In general, transitions starting from ions with higher mass were preferred to transitions from low mass precursor ions.

Pesticide names (and those of some metabolites) are supplemented by the molecular mass and the CAS number (Chemical Abstracts Service), which is useful for searches in databases. The CAS number is usually taken from [1], but in various cases more than one number exists, e.g. for isomers and racemates.

In addition to the above mentioned parameters, an indication on the appropriate collision energy for each transition is given. Instead of definitive voltages, a classification into low, medium and high collision energies was chosen, because transitions are based on data from different instruments, which do not require identical voltages to obtain the optimal intensity for a given transition. Therefore, from each reference (application note, article, etc.) all parameter sets were sorted by the collision energy in order to obtain the categories. Afterwards, the sorted list was divided in three groups of equal size. The resulting meaning of low, medium and high collision energy is listed in Table 1.

Table 1 — Categories of collision energy (CE)

Instrument	Voltage corresponding to low CE [V]	Voltage corresponding to medium CE [V]	Voltage corresponding to high CE [V]
Agilent 7000 Series	< 13	13 to 21	> 21
Bruker SCION TQ	< 8	8 to 16	> 16
Thermo Quantum	< 15	15 to 19	> 19
Varian 1200 (L)	< 13	13 to 20	> 20
Waters Quattro micro	< 9	9 to 17	> 17

Table 2 — MS/MS Parameters

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Acephate	305-19-1	136 → 94	m	136 → 42	l						
Acetochlor	34256-82-1	146 → 130	h	223 → 132	h	223 → 146	l	*224 → 148*	*l*		
Aclonifen	74070-46-5	212 → 182	l	264 → 194	m	*264 → 211*	*l*	*264 → 182*	*h*	*264 → 212*	*l*
Acrinathrin	101007-06-1	181 → 152	m	208 → 181	l	289 → 93	l	*181 → 127*	*h*	*208 → 152*	*h*
Alachlor	15972-60-8	188 → 130	h	188 → 160	l						
Aldrin	309-00-2	263 → 191	h	263 → 193	h	263 → 228	m	*265 → 193*	*h*	*293 → 258*	*h*
Allethrin	584-79-2	123 → 81	l	*123 → 79*	*m*	*136 → 108*	*l*				
Atrazine	1912-24-9	200 → 94	m	200 → 104	m	200 → 122	l	215 → 173	l	215 → 200	l
Azinphos-ethyl	2642-71-9	132 → 77	l	160 → 77	m	160 → 104	l	160 → 132	l	132 → 104	l
Azinphos-methyl	86-50-0	132 → 77	m	160 → 77	m	160 → 104	l	160 → 132	l		
Azoxystrobin	131860-33-8	344 → 156	h	344 → 329	m	388 → 345	m	*388 → 300*	*m*		
Benfluralin	1861-40-1	292 → 160	m	292 → 206	m	292 → 264	l				
Bifenthrin	82657-04-3	181 → 115	h	181 → 165	h	181 → 166	m	*165 → 115*	*h*	*166 → 165*	*m*
Biphenyl	92-52-4	154 → 152	h	154 → 153	m	*153 → 152*	*m*	*154 → 128*	*m*		
Bitertanol	70585-36-3	141 → 115	m	170 → 115	h	170 → 141	m				
Boscalid (Nicobifen)	188425-85-6	140 → 76	h	140 → 112	l	342 → 140	m	*342 → 112*	*m*		
Bromophos	2104-96-3	329 → 314	m	331 → 286	h	331 → 316	m	*331 → 93*	*h*		
Bromophos-ethyl	4824-78-6	303 → 285	m	359 → 303	m	359 → 331	l	*357 → 301*	*m*	*358 → 303*	*m*
Bromopropylate	18181-80-1	185 → 157	h	341 → 155	h	341 → 157	h	341 → 183	m	341 → 185	m
Bupirimate	41483-43-6	273 → 108	m	273 → 193	l	316 → 208	l				
Buprofezin	69327-76-0	172 → 57	l	175 → 132	l	*105 → 77*	*m*	*105 → 104*	*l*		
Cadusafos	95465-99-9	159 → 97	m	159 → 131	l	*158 → 114*	*m*				
Captafol	2425-06-1	79 → 51	h	79 → 77	l	313 → 79	m	*150 → 79*	*m*	*151 → 79*	m
Captan	133-06-2	79 → 77	l	149 → 70	m	149 → 79	m	149 → 105	l		

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Captan metabolite (Tetrahydrophthalimide)	1469-48-3	151 → 79	l	151 → 80	l	151 → 122	l				
Carbaryl	63-25-2	144 → 115	h	144 → 116	m						
Carbaryl metabolite (1-Naphthol)	90-15-3	144 → 115	h	*115 → 63*	*h*	*115 → 89*	*m*				
Carbofuran	1563-66-2	164 → 131	m	164 → 149	l						
Carboxin	5234-68-4	235 → 87	h	235 → 143	l						
Chinomethionat	2439-01-2	206 → 148	m	234 → 206	l	*234 → 148*	*h*				
Chlorbenside	103-17-3	125 → 89	m	268 → 125	l						
Chlordane	5103-71-9	373 → 266	h	373 → 301	m	*272 → 237*	*m*	*410 → 375*	*l*		
Chlorfenapyr	122453-73-0	59 → 31	l	247 → 200	h	247 → 227	m	*247 → 197*	*m*	*408 → 59*	*l*
Chlorfenson	80-33-1	175 → 111	l	302 → 175	l	*302 → 111*	*h*				
Chlorfenvinphos	18708-86-6	267 → 159	m	323 → 267	m	*267 → 81*	*h*	*269 → 161*	*m*	*325 → 269*	*m*
Chlormephos	24934-91-6	154 → 121	l	234 → 121	m						
Chlorobenzilate	510-15-6	139 → 111	m	251 → 139	m	*251 → 111*	*h*	253 → 141	m		
Chloroneb	2675-77-6	206 → 191	l	191 → 141	l	*191 → 113*	*m*				
Chloropropylate	5836-10-2	139 → 111	l	251 → 111	h	251 → 139	m	253 → 141	m		
Chlorothalonil	1897-45-6	264 → 133	h	264 → 168	h	264 → 229	m	266 → 133	h	266 → 231	m
Chlorpropham	101-21-3	127 → 65	h	171 → 127	l	213 → 127	m	213 → 171	l		
Chlorpyrifos (ethyl)	2921-88-2	197 → 169	m	199 → 171	m	314 → 258	m	314 → 286	l	316 → 260	l
Chlorpyrifos-methyl	5598-13-0	286 → 93	m	286 → 271	m	288 → 93	h				
Chlorthal-dimethyl	1861-32-1	299 → 221	h	301 → 223	h	301 → 273	m	332 → 301	l		
Chlozolinate	84332-86-5	188 → 147	m	259 → 188	m	331 → 259	l				
Clomazone	81777-89-1	125 → 89	m	125 → 99	m	204 → 107	m				
Coumaphos	56-72-4	226 → 163	m	362 → 109	m	362 → 226	m	362 → 334	l		
Cyanazine	21725-46-2	198 → 91	l	225 → 189	l	240 → 225	l	*212 → 123*	*m*		
Cyanofenphos	13067-93-1	157 → 110	l	303 → 169	l	*169 → 141*	*l*	*303 → 141*	*m*		
Cyanophos	2636-26-2	243 → 79	h	243 → 109	m	243 → 127	m	*109 → 79*	*l*	*125 → 79*	*l*

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Cyfluthrin, beta-	86560-93-2	163 → 91	m	163 → 127	l	206 → 151	h	226 → 206	l	*227 → 199*	*l*
Cyhalothrin, lambda-	91465-08-6	181 → 152	h	197 → 141	m	197 → 161	l	*197 → 91*	*m*		
Cypermethrin	67375-30-8	163 → 91	m	163 → 127	l	181 → 152	h	*165 → 127*	*l*		
Cyproconazole	94361-06-5	139 → 111	m	222 → 82	l	222 → 125	m	*222 → 153*	*l*		
Cyprodinil	121552-61-2	224 → 197	h	224 → 208	m	225 → 224	l	*225 → 208*	*m*	*225 → 210*	*m*
DDD, o,p-	53-19-0	235 → 165	h	235 → 199	m	*237 → 165*	*h*				
DDD, p,p-	72-54-8	235 → 165	h	235 → 199	m	237 → 165	h				
DDE, o,p-	3424-82-6	246 → 176	h	318 → 248	m	*248 → 176*	*h*	*318 → 176*	*h*		
DDE, p,p-	72-55-9	246 → 176	h	248 → 176	h	318 → 246	h	318 → 248	h		
DDT, o,p-	789-02-6	235 → 165	h	237 → 165	m						
DDT, p,p-	50-29-3	235 → 165	h	235 → 199	m	237 → 165	h				
DEET	134-62-3	119 → 91	l	190 → 91	m	190 → 145	l	*190 → 117*	*m*	*190 → 119*	*m*
Deltamethrin	52918-63-5	181 → 152	h	253 → 93	m	253 → 172	l	253 → 174	l	*181 → 127*	*h*
Di-allate	2303-16-4	234 → 150	m	234 → 192	m						
Diazinon	333-41-5	179 → 122	h	179 → 137	m	304 → 179	m				
Dichlobenil	1194-65-6	171 → 100	h	171 → 136	m	*173 → 138*	*m*				
Dichlofenthion	97-17-6	223 → 205	l	279 → 205	h	279 → 223	m				
Dichlofluanid	1085-98-9	167 → 124	l	224 → 123	m	226 → 123	m	*123 → 77*	*m*	*167 → 97*	*m*
Dichlorbenzophenone, p,p-	90-98-2	139 → 75	h	139 → 111	m	250 → 139	l	250 → 215	l		
Dichloroaniline, 3,4-	95-76-1	161 → 99	h	161 → 126	m	*161 → 90*	*m*				
Dichlorvos	62-73-7	109 → 79	l	185 → 93	m	185 → 109	m				
Dicloran	99-30-9	176 → 148	m	206 → 124	h	206 → 148	m	206 → 176	l	208 → 178	l
Dicofol, p,p	115-32-2	139 → 111	m	251 → 139	m	253 → 141	m				
Dicrotophos	3735-78-3	127 → 95	m	127 → 109	l	193 → 127	l				
Dieldrin	60-57-1	263 → 191	h	263 → 193	h	279 → 243	m	*277 → 241*	*l*		
Difenoconazole	119446-68-3	323 → 265	m	325 → 267	m	*265 → 139*	*h*				

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Dimethoate	60-51-5	125 → 79	l	*125 → 93*	*m*	*143 → 111*	*l*	*229 → 87*	*l*		
Dimoxystrobin	149961-52-4	116 → 89	m	205 → 116	l	*205 → 89*	*h*				
Dioxathion	78-34-2	125 → 97	l	197 → 141	l	270 → 97	h	270 → 141	m	*270 → 169*	*l*
Diphenylamine	122-39-4	168 → 167	m	169 → 167	m	169 → 168	m	*168 → 140*	*h*	*169 → 141*	*h*
Disulfoton	298-04-4	186 → 142	l	274 → 88	l	*88 → 60*	*l*	*142 → 109*	*l*		
Edifenphos	17109-49-8	173 → 109	m	310 → 173	l						
Endosulfan sulfate	1031-07-8	272 → 237	m	274 → 239	m	*241 → 206*	*m*	*387 → 206*	*h*	*387 → 241*	*m*
Endosulfan, alpha-	33213-66-0	195 → 159	l	241 → 206	m	*239 → 204*	*m*	*241 → 170*	*h*	*265 → 193*	*h*
Endosulfan, beta-	33213-65-9	195 → 125	h	195 → 159	l	241 → 206	m	*241 → 170*	*h*	*277 → 241*	*l*
Endrin	72-20-8	263 → 191	h	263 → 193	h	*263 → 228*	*m*	*281 → 211*	*h*	*281 → 245*	*m*
EPN	2104-64-5	157 → 110	m	169 → 77	h	169 → 141	l	*157 → 77*	*h*	*157 → 139*	*l*
Epoxiconazol	133855-98-8	192 → 111	h	192 → 138	l	*194 → 140*	*l*				
Ethalfluralin	55283-68-6	276 → 202	m	316 → 276	l	*276 → 105*	*m*	*316 → 202*	*h*		
Ethion	563-12-2	231 → 129	h	231 → 175	m	231 → 185	m	*231 → 203*	*m*	*384 → 231*	*l*
Ethofumesate	26225-79-6	207 → 161	l	286 → 207	l	*207 → 137*	*m*				
Ethoxyquin	91-53-2	202 → 145	h	202 → 174	m	*202 → 159*	*h*	*203 → 175*	*m*	*217 → 174*	*h*
Etofenprox	80844-07-1	163 → 107	m	163 → 135	l						
Etridiazol	2593-15-9	211 → 140	m	211 → 183	l	*213 → 142*	*m*	*213 → 185*	*l*		
Etrimfos	38260-54-7	181 → 153	l	292 → 153	m	292 → 181	l				
Fenarimol	60168-88-9	219 → 107	m	251 → 139	m	330 → 139	m	*139 → 75*	*h*	*251 → 111*	*h*
Fenazaquin	120928-09-8	145 → 117	m	160 → 117	h	160 → 145	l				
Fenbuconazole	114369-43-6	129 → 102	m	198 → 129	l	*198 → 102*	*h*				
Fenchlorphos	299-84-3	287 → 272	m	285 → 270	m	*285 → 240*	*h*				
Fenitrothion	122-14-5	260 → 125	l	277 → 109	m	277 → 125	m	277 → 260	l	*125 → 79*	*l*
Fenpiclonil	74738-17-3	236 → 174	h	236 → 201	m	*201 → 166*	*m*				
Fenpropathrin	64257-84-7	181 → 127	h	181 → 152	h	265 → 89	h	265 → 210	m	*265 → 181*	*h*

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Fenpropidin	67306-00-7	98 → 55	m	98 → 70	m	*273 → 98*	*m*				
Fenpropimorph	67306-03-0	128 → 70	m	128 → 110	l						
Fenson	80-38-6	268 → 77	h	268 → 141	l	141 → 77	l				
Fensulfothion	115-90-2	293 → 97	h	293 → 125	m						
Fenthion	55-38-9	278 → 109	m	278 → 169	m						
Fenvalerate	51630-58-1	125 → 89	m	167 → 125	l	225 → 119	m	*125 → 99*	*h*	*167 → 89*	*h*
Fipronil	120068-37-3	367 → 213	h	367 → 255	h	369 → 215	h	*213 → 143*	*h*	*351 → 255*	*m*
Flucythrinate	70124-77-5	157 → 107	m	199 → 107	h	199 → 157	l				
Fludioxonil	131341-86-1	248 → 127	h	248 → 154	m	248 → 182	m	*154 → 127*	*l*		
Flufenacet	142459-58-3	151 → 95	h	151 → 136	m	211 → 123	l				
Fluquinconazole	136426-54-5	340 → 286	h	340 → 298	m	*340 → 108*	*h*				
Flusilazole	85509-19-9	233 → 152	m	233 → 165	m	*206 → 151*	*m*				
Flutriafol	76674-21-0	219 → 95	h	219 → 123	m	*123 → 75*	*m*	*164 → 109*	*m*		
Fluvalinate		250 → 200	m	252 → 200	m	250 → 55	m	*181 → 152*	*h*		
Fluvalinate, tau-	102851-06-9	250 → 55	m	250 → 200	m	*250 → 208*	*m*				
Folpet	133-07-3	260 → 130	m	262 → 130	m	*147 → 103*	*l*	*260 → 102*	*h*	*262 → 234*	*l*
Folpet metabolite (Phthalimide)	85-41-6	147 → 76	h	147 → 103	l	*147 → 104*	*l*				
Fonofos	944-22-9	137 → 109	l	246 → 109	m	246 → 137	l				
Formothion	2540-82-1	125 → 79	l	170 → 93	l	*93 → 63*	*l*	*198 → 170*	*l*	*224 → 125*	*m*
Halfenprox	111872-58-3	263 → 235	m	*183 → 153*	*h*	*263 → 117*	*l*	*265 → 117*	*l*	*265 → 237*	*m*
HCH, alpha-	319-84-6	181 → 145	m	219 → 145	m	219 → 183	l	*181 → 109*	*h*		
HCH, beta-	319-85-7	181 → 146	m	219 → 183	l	*219 → 147*	*h*				
HCH, delta-	58-89-9	181 → 145	m	219 → 183	l	*181 → 109*	*h*	*183 → 147*	*m*	*217 → 145*	*m*
HCH, gamma (Lindan)	608-72-1	181 → 145	l	219 → 183	l	*181 → 109*	*h*	*219 → 147*	*h*		
Heptachlor	76-44-8	272 → 237	m	274 → 239	m	*337 → 302*	*m*	*339 → 266*	*m*		
Heptachlor epoxide, cis-	28044-83-9	353 → 263	m	355 → 265	m	353 → 282	m	*217 → 182*	*m*		

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Hexachlorobenzene (HCB)	118-74-1	284 → 214	h	284 → 249	h	286 → 251	h	*249 → 214*	*m*		
Hexaconazole	79983-71-4	214 → 159	m	214 → 172	h	214 → 187	m	256 → 159	m		
Iprodione	36734-19-7	314 → 245	l	314 → 271	l	*187 → 124*	*m*	*314 → 56*	*m*		
Iprovalicarb	140923-25-7	158 → 116	l	*116 → 98*	*m*	*119 → 91*	*m*	*119 → 117*	*l*	*158 → 98*	*l*
Isazophos	42509-80-8	161 → 119	l	213 → 121	m	*213 → 185*	*l*				
Isofenphos	25311-71-1	213 → 121	m	213 → 185	l	*255 → 185*	*l*	*255 → 213*	*l*		
Isofenphos-methyl	99675-03-3	199 → 121	m	241 → 121	m						
Kresoxim-methyl	143390-89-0	206 → 116	l	206 → 131	m	*131 → 89*	*h*	*131 → 116*	*m*	*131 → 130*	*m*
Leptophos	21609-90-5	171 → 77	m	377 → 362	h	*171 → 124*	*m*	*377 → 269*	*h*		
Malathion	121-75-5	127 → 99	m	173 → 99	m	173 → 127	l	*158 → 125*	*l*		
Mecarbam	2595-54-2	159 → 86	m	159 → 131	l	*329 → 131*	*l*	*329 → 159*	*l*		
Mefenpyr-diethyl	135590-91-9	253 → 189	h	299 → 253	l	*253 → 190*	*m*	*299 → 189*	*h*		
Mepanipyrim	110235-47-7	222 → 207	m	*222 → 220*	*m*	*223 → 208*	*m*	*223 → 221*	*h*	*223 → 222*	*m*
Mepronil	55814-41-0	269 → 91	h	269 → 119	m	269 → 210	l	*119 → 91*	*m*		
Metalaxyl	57837-19-1	206 → 105	m	206 → 132	m						
Metazachlor	67129-08-2	133 → 117	h	209 → 117	h	*209 → 132*	*m*	*209 → 133*	*l*		
Methacrifos	62610-77-9	208 → 180	l	240 → 180	l	240 → 208	l	*125 → 79*	*l*	*180 → 93*	*m*
Methidathion	950-37-8	145 → 58	m	145 → 85	l						
Methiocarb	2032-65-7	168 → 109	m	168 → 153	l	*153 → 109*	*l*				
Methoxychlor, o,p-	30667-99-3	227 → 141	h	227 → 169	h	*227 → 212*	*m*				
Methoxychlor, p,p-	72-43-5	227 → 169	h	227 → 212	m	*227 → 115*	*h*	*227 → 141*	*h*	*227 → 184*	*h*
Metolachlor	51218-45-2	162 → 133	m	238 → 133	h	238 → 162	l				
Metribuzin	21087-64-9	198 → 82	m	198 → 110	l	*198 → 89*	*m*				
Mevinphos	338-45-4	127 → 95	m	127 → 109	l	192 → 127	l	192 → 164	l	*192 → 109*	*m*
Mirex	2385-85-5	272 → 143	h	272 → 237	m	*270 → 235*	*m*	*272 → 167*	*h*		
Monocrotophos	6923-22-4	127 → 109	m	192 → 127	m	*127 → 95*	*m*	*192 → 164*	*l*		

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Myclobutanil	88671-89-0	179 → 90	h	179 → 125	m	179 → 152	l				
Nitrapyrin	1929-82-4	194 → 133	m	194 → 158	m						
Nitrofen	1836-75-5	202 → 139	h	283 → 253	m	*283 → 162*	*h*	*285 → 255*	*m*		
Nuarimol	63284-71-9	235 → 139	m	314 → 139	m	*203 → 107*	*m*				
Omethoate	1113-02-6	110 → 79	m	156 → 110	m	*156 → 79*	*m*				
Oxadiazon	19666-30-9	175 → 112	m	258 → 175	l	*304 → 260*	*l*	*344 → 302*	*m*		
Oxadixyl	77732-09-3	163 → 117	h	163 → 132	l	233 → 146	m				
Oxyfluorfen	42874-03-3	252 → 196	m	252 → 224	m	300 → 223	m	361 → 300	l	*252 → 146*	*h*
Paraoxon-ethyl	311-45-5	149 → 119	l	*149 → 102*	*m*	*220 → 174*	*l*	*275 → 149*	*l*		
Paraoxon-methyl	950-35-6	230 → 136	l	*230 → 106*	*m*	*230 → 200*	*l*	*247 → 200*	*l*	*247 → 230*	*l*
Parathion	56-38-2	291 → 81	h	291 → 109	m	*109 → 81*	*l*	*125 → 97*	*l*	*291 → 137*	*l*
Parathion-methyl	298-00-0	263 → 79	h	263 → 109	m	263 → 127	m	263 → 246	l	*125 → 79*	*m*
PCB 28	7012-37-5	256 → 186	h	258 → 186	h						
PCB 52	35693-99-3	292 → 220	h	*290 → 220*	*m*	*292 → 222*	*h*	*292 → 257*	*l*		
PCB 101	37680-73-2	326 → 256	h	326 → 291	m	*324 → 254*	*h*				
PCB 138	35065-28-2	360 → 290	h	360 → 325	m	*358 → 288*	*h*				
PCB 153	35065-27-1	360 → 290	h	360 → 325	m	*358 → 288*	*h*	*362 → 290*	*h*		
PCB 180	35065-29-3	392 → 322	h	394 → 324	h	*396 → 361*	*m*				
Penconazole	66246-88-6	248 → 157	h	248 → 192	m	*159 → 123*	*m*				
Pendimethalin	40487-42-1	252 → 162	l	252 → 191	l	*252 → 208*	*l*				
Pentachloranilin	527-20-8	263 → 192	h	263 → 227	m	265 → 194	h	*265 → 158*	*h*	*265 → 192*	*h*
Permethrin	52645-53-1	163 → 127	l	183 → 153	m	183 → 168	m				
Pethoxamid	106700-29-2	260 → 119	h	260 → 147	m						
Phenothrin	51186-88-0	123 → 81	l	183 → 153	m	183 → 168	m				
Phenylphenol, 2-	90-43-7	170 → 115	h	170 → 141	h	*141 → 115*	*m*	*170 → 169*	*m*		
Phorate	298-02-2	121 → 65	l	231 → 203	l	*75 → 47*	*l*	*121 → 93*	*l*	*231 → 129*	*h*

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Phosalone	2310-17-0	182 → 75	h	182 → 111	m	182 → 138	l	367 → 182	l		
Phosmet	732-11-6	160 → 77	h	160 → 105	m	160 → 133	m	*317 → 160*	*m*		
Phosphamidon	297-99-4	127 → 109	m	227 → 127	l	264 → 127	m	*264 → 193*	*l*		
Picolinafen	137641-05-5	376 → 238	m	376 → 239	m	*238 → 145*	*h*				
Picoxystrobin	117428-22-5	303 → 157	m	335 → 173	l	*335 → 115*	*h*	*335 → 303*	*l*	*367 → 303*	*m*
Piperonyl-butoxid	51-03-6	176 → 117	m	176 → 131	l	*176 → 103*	*m*	*176 → 145*	*m*	*176 → 161*	*l*
Pirimiphos-ethyl	23505-41-1	304 → 168	m	318 → 166	m	333 → 168	h	*318 → 182*	*m*	*333 → 318*	*l*
Pirimiphos-methyl	29232-93-7	290 → 125	m	290 → 151	m	305 → 180	l	305 → 276	m	305 → 290	m
Prochloraz	67747-09-5	308 → 70	m	310 → 70	m						
Procymidone	32809-16-8	283 → 67	h	283 → 96	l	283 → 255	l	285 → 96	l	*285 → 257*	*l*
Profenofos	41198-08-7	337 → 188	h	337 → 267	m	339 → 188	h	339 → 269	m	*139 → 97*	*l*
Prometryn	7287-19-6	226 → 184	l	241 → 184	l	*241 → 199*	*l*				
Propachlor	1918-16-7	176 → 120	l	196 → 120	l	*120 → 77*	*m*	*120 → 92*	*l*	*176 → 77*	*m*
Propargite	2312-35-8	135 → 107	m	173 → 135	m	*135 → 77*	*h*	*173 → 105*	*m*	*173 → 107*	*h*
Propazine	139-40-2	214 → 172	l	229 → 187	l	229 → 214	l	*214 → 104*	*m*	*229 → 58*	*m*
Propetamphos	31218-83-4	138 → 110	l	194 → 166	l	236 → 166	m	236 → 194	l		
Propham	122-42-9	137 → 93	l	179 → 93	m	179 → 137	l				
Propiconazole	60207-90-1	259 → 69	l	259 → 173	m	*173 → 145*	*m*	*259 → 191*	*m*	*261 → 175*	*h*
Propoxur	114-26-1	110 → 64	m	152 → 110	l						
Propyzamide	23950-58-5	173 → 109	h	173 → 145	m	175 → 147	m	*254 → 226*	*m*		
Prothiofos	34643-46-4	267 → 221	h	267 → 239	l	309 → 221	h	309 → 239	m	*309 → 281*	*m*
Pyraclofos	77458-01-6	221 → 193	l	360 → 139	m	360 → 194	l	*194 → 138*	*m*	*221 → 149*	*m*
Pyraclostrobin	175013-18-0	132 → 77	m	164 → 132	m	*164 → 77*	*h*				
Pyrazophos	13457-18-6	221 → 149	m	221 → 177	m	221 → 193	l	232 → 204	l		
Pyridaben	96489-71-3	147 → 117	h	147 → 132	m	309 → 147	m				
Pyridaphenthion	119-12-0	340 → 109	m	340 → 199	l	*340 → 97*	*h*	*340 → 203*	*m*		

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Pyrimethanil	53112-28-0	198 → 118	h	198 → 183	m	199 → 198	l	*198 → 156*	*h*		
Pyriproxyfen	95737-68-1	136 → 78	m	136 → 96	l	*226 → 186*	*m*				
Quinalphos	13593-03-8	146 → 91	h	146 → 118	m	157 → 102	h	157 → 129	m	298 → 156	l
Quinoxyfen	124495-18-7	237 → 208	h	272 → 237	h	307 → 237	h	307 → 272	l	*309 → 237*	*m*
Quintozene (PCNB)	82-68-8	237 → 119	h	237 → 143	h	295 → 237	m	*214 → 179*	*l*	*249 → 214*	*m*
Resmethrin	10453-86-8	123 → 81	l	143 → 128	m	171 → 128	m	171 → 143	l		
Simazine	122-34-9	201 → 138	l	201 → 173	l	*201 → 158*	*l*	*201 → 186*	*l*		
Spirodiclofen	148477-71-8	312 → 109	m	312 → 259	l						
Spiroxamine	118134-30-8	100 → 58	l	100 → 72	l						
Sulfotep (ethyl)	3689-24-5	322 → 146	h	322 → 202	l	322 → 294	l	*322 → 174*	*m*	*202 → 146*	*l*
Tebuconazole	107534-96-3	125 → 89	m	250 → 125	h	252 → 127	h				
Tebufenpyrad	119168-77-3	276 → 171	m	318 → 131	m	333 → 171	m	333 → 276	l	*171 → 88*	*m*
Tecnazene	117-18-0	203 → 143	h	215 → 179	l	*203 → 83*	*h*	*215 → 144*	*m*	*215 → 180*	*l*
Tefluthrin	79538-32-2	177 → 127	m	177 → 137	m	197 → 141	m	*197 → 161*	*l*		
Terbufos	13071-79-9	231 → 175	l	*153 → 97*	*l*	*231 → 129*	*h*	*231 → 203*	*l*	*288 → 231*	*l*
Terbuthylazine	5915-41-3	214 → 104	m	214 → 132	l	229 → 138	m	229 → 173	l	*214 → 71*	*m*
Tetrachlorvinphos (E,Z)	961-11-5	329 → 109	h	331 → 109	h	*331 → 127*	*m*	*331 → 316*	*m*		
Tetraconazole	112281-77-3	336 → 204	h	336 → 218	m	*336 → 191*	*m*	*338 → 220*	*m*		
Tetradifon	116-29-0	159 → 131	m	227 → 199	m	229 → 201	m	*354 → 159*	*l*		
Tetramethrin	51384-90-4	164 → 77	h	164 → 107	m	164 → 135	l				
Thiometon	640-15-3	88 → 60	l	125 → 79	l	*158 → 125*	*l*	*246 → 88*	*l*		
Tolclofos-methyl	57018-04-9	250 → 220	l	265 → 93	h	265 → 220	h	265 → 250	m	267 → 252	m
Tolylfluanid	731-27-1	137 → 91	m	238 → 137	l	240 → 137	m	*137 → 65*	*h*		
Transfluthrin	118712-89-3	163 → 143	m	335 → 163	m						
Triadimefon	43121-43-3	208 → 111	m	208 → 127	m	208 → 181	l				
Triadimenol	70585-37-4	128 → 65	m	128 → 100	l	168 → 70	l	*168 → 112*	*l*		

Pesticide name	CAS-Nr.	MRM No. 1	CE	MRM No. 2	CE	MRM No. 3	CE	MRM No. 4	CE	MRM No. 5	CE
Tri-allate	2303-17-5	268 → 184	m	270 → 186	m	*143 → 83*	*m*	*268 → 226*	*m*		
Triazophos	24017-47-8	161 → 134	l	257 → 162	l	*161 → 77*	*h*	*161 → 106*	*m*		
Trifloxystrobin	141517-21-7	131 → 116	h	190 → 130	l	222 → 130	l	222 → 162	m	*116 → 89*	*m*
Triflumizole	68694-11-1	179 → 144	m	206 → 179	m	278 → 73	l	*206 → 144*	*h*	*287 → 218*	*m*
Trifluralin	1582-09-8	264 → 160	m	306 → 160	h	306 → 264	l	*264 → 206*	*l*		
Triphenyl phosphate	115-86-6	326 → 169	h	*326 → 215*	*h*	*326 → 233*	*l*				
Triticonazole	131983-72-7	235 → 182	l	235 → 217	l						
Vinclozolin	50471-44-8	212 → 145	h	212 → 172	m	285 → 212	l	*198 → 145*	*m*		

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