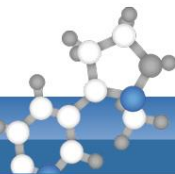
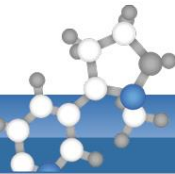


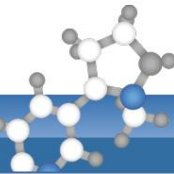
Method name	LC-ToF-ESI(-)-Screening		
Instrument	LC-ToF		
Chromatographic method	LC		
Extraction method	QuEChERS		
Clean-up	no		
Use of AP (analyte protectant)	no		
Internal standard(s)	Chlorpyrifos D ₁₀ ; Propyzamid D ₃		
Instrument parameters			
Ionisation mode	ESI(-)		
Column	Acquity UPLC BEH C18 1,7 µm 2,1 x 100 mm		
Pre-column	Acquity UPLC BEH C18 Van Guard 2,1 x 5mm		
Column temperature (°C)	40 °C		
Eluent A2	1 mmol NH ₄ -formiate + 0.002% formic acid in Wasser		
Eluent B2	1 mmol NH ₄ -formiate + 0.002% formic acid in MeOH		
Gradient	%A	Flow [mL/min]	Time [min]
	95	0.2	initial
	40	0.2	2.0
	35	0.2	3.0
	30	0.4	4.0
	10	0.4	8.0
	10	0.4	15.0
	95	0.4	15.1
	95	0.4	18.0
	95	0.2	18.1
95	0.2	18.5	
Injection volume (µL)	2		
Dilution	no		
Compounds in screening list			
1.4-Dimethylnaphthalene: M23			
1.3-Diphenylurea			
1-Naphtylacetic acid			
2-Chlorobenzoic acid			
2-(Trifluoromethyl)benzoic acid			
2.3.5-Triiodobenzoic acid # fragment 454.7			
2.4.5-T # fragment 195			
2.4.6-Trichlorophenol			
2.4-D # fragment 160			
2.4-DB # fragment 160			
2.4-D-glucoside # fragment 218.9 Peak 1			
2.4-Dichlorobenzoic acid			
2.4-Dichlorophenol			
2.5-Dichlorobenzoic acid			
2-Naphthyloxyacetic acid # fragment 143			
3-Chloro-5-(trifluoromethyl)picolinic acid			
3-(Trifluoromethyl)benzoic acid			
3.5-Dibromo-4-hydroxybenzoic acid			
4-Bromo-2-chlorophenol			



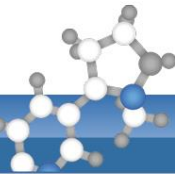
4-Chloro-2-methylphenol
4-Chlorobenzoic acid
4-CPA
4-Fluoro-3-phenoxybenzoic acid
4-Iodophenoxyacetic acid
4-Nitrophenol
5-Nitroguaiacol # fragment 153
6-Benzyladenine
Acephate
Acifluorfen # fragment 316
Ametoctradin
Ametoctradin: M650F01
Ametoctradin: M650F04
Ametoctradin: M650F06
Amidosulfuron
Aminopyralid # fragment 160.9
Amisulbrom: IT-4
Ampicillin # fragment 207
Asulam
Asulam: Acetyl sulfanilamide
Asulam: Sulfanilamide
Asulam-malonyl # fragment 229
Azimsulfuron
Azoxystrobin: 2-Hydroxybenzonitrile
Azoxystrobin: R401553
Azoxystrobin acid
Benazolin # fragment 170
Bensulfuron-methyl
Bentazone
Bentazone-6-hydroxy
Benthiavalicarb-isopropyl
Benzoic acid
Benzovindiflupyr
Benzthiazuron
Bicyclopyrone
BIT
Bixafen-desmethyl
Boscalid
Boscalid: M510F01
Boscalid-hydroxy
Bromacil
Bromobutide
Bromoxynil
Bronopol # fragment 167.9
Butamifos
Captan: cis-1.2.3.4-THPI-3-hydroxy
Carbaryl: 1-Naphthol
Carbendazim: 2-Aminobenzimidazole
Carbendazim-5-hydroxy # fragment 174



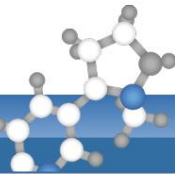
Carbofuranphenol-3-keto
Carboxin: Oxycarboxin
Carboxin-sulfoxide
Carpropamid
Chloramben
Chloramphenicol
Chlorantraniliprole
Chlorbenzuron
Chlorfluazuron
Chloridazon-methyl-desphenyl
Chlorothalonil-4-hydroxy
Chlorpropham: 4-HSA
Chlorpyrifos-desethyl # fragment 195.9
Chlorpyrifos-methyl-desmethyl # fragment 195.9
Chlorsulfuron
Chlorthiamid
Chromafenozide
Cinidon
Cinosulfuron
Clethodim-sulfone # Peak 1
Clethodim-sulfone # Peak 2
Clethodim-sulfoxide # Peak 1
Clethodim-sulfoxide # Peak 2
Climbazole
Clodinafop
Cloprop
Clopyralid
Clothianidin-desmethyl
Coumachlor
Coumafuryl
Coumaphos alcohol
Cyantraniliprole
Cyazofamid: CCIM
Cyclaniliprole
Cycloheximide
Cycloxydim # Peak 1
Cycloxydim # Peak 2
Cycloxydim: BH 517-TSO # Peak 1
Cycloxydim: BH 517-TSO # Peak 2
Cycloxydim: BH 517-TSO # Peak 3
Cycloxydim: BH 517-TSO2 # Peak 1
Cycloxydim: BH 517-TSO2 # Peak 2
Cyhalofop
Cyhalothric acid-lambda
Cyproconazole # Peak 1 small
Cyproconazole # Peak 2
Cyprosulfamide
Daimuron
Dalapon



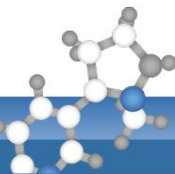
DEET omega-carboxylic acid
Deltamethrinic acid
Desmethyl-pyrazole-4-carboxylic acid # fragment 141
Diafenthiuron
Diafenthiuron: CGA 177960
Diazinon: 2-Isopropyl-6-methyl-4-pyrimidinol
Dicamba # fragment 174.9
Dicamba: 3,6-Dichloro-2-hydroxybenzoic acid # fragment 160
Dicamba-5-hydroxy
Dichlofluanid: DMSA
Dichlorprop # fragment 160
Dichlorprop glucosid
Diclofop
Diclomezine
Dicloran
Diclosulam
Difenacoum # Peak 1
Difenacoum # Peak 2
Difenoconazole alcohol # M+CH ₃ COOH
Difenoconazole ketone
Diflubenzuron: 4-Chlorophenylurea
Diflufenzopyr
Dikegulac
Dimethachlor: CGA 50266 # fragment 178
Dimethachlor: CGA 369873 # fragment 242 (M-Na)
Dimethachlor-sulfonic acid
Dimethenamid-P: M656PH023 # fragment 198
Dimethenamid-P: M656PH027
Dimethoate: O-desmethyl isodimethoate
Dimethoate-carboxylic acid # fragment 140.9
Dimethoate-O-desmethyl
Dimoxystrobin: 505M09
Dinocap # fragment 295
Dinotefuran-desmethyl
Dinoterb
Dithianon
DNOC
Drazoxolon
Endosulfan-sulfate
Ethaboxam # Fragment 292
Ethametsulfuron-methyl
Ethofumesate-carboxylic acid
Ethoxysulfuron
Ethyl-N-(3-hydroxyphenyl)-carbamate
Ethylparaben
Famoxadone
Fenamidone: 3-Anilino-5-methyl-5-phenyl-imidazolidine-2,4-dione
Fenarimol
Fenhexamid



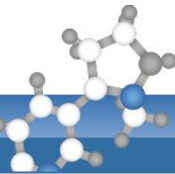
Fenoprop # fragment 195
Fenoxanil
Fenoxaprop: 6-Chloro-2-benzoxazolinone
Fenoxaprop-P
Fenpicoxamid: X12326349 # fragment 255
Fenpicoxamid: X642188 # fragment 237
Fenpropimorph-carboxylic acid
Fenpyroximate: M3
Fenvalerate: CPIA
Fipronil
Fipronil-amide
Fipronil-desulfinyl
Fipronil-sulfide
Fipronil-sulfone
Flonicamid: TFNA
Flonicamid: TFNG
Florasulam
Florpyrauxifen acid # -CO ₂
Florpyrauxifen-benzyl
Fluazifop
Fluazifop: CGA 142110
Fluazinam
Flucycloxuron
Fludioxonil: CGA 192155
Fludioxonil-carboxylic acid
Flufenacet-oxalate # fragment 152
Flufenacet-sulfonic acid
Flufenacet: Thiadone
Flufenacet-thioglycolate-sulfoxide # fragment 152
Flufiprole
Flumethrin acid
Flumiclorac
Fluometuron
Fluometuron-desmethyl
Fluometuron-N,N-desmethyl
Flupyradifurone
Flupyrimin
Fluridone # M+CH ₃ COOH-H
Fluroxypyr # fragment 195
Flurprimidol
Flurtamone
Flusulfamide
Flutolanil-desisopropyl
Flutolanil-hydroxy
Fluvalinate: 3-Phenoxybenzoic acid
Fluvalinate-enamine
Fluvalinate-tau: Anilino acid
Fluxapyroxad
Fluxapyroxad: M700F001



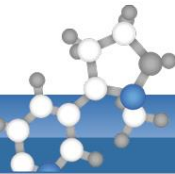
Fomesafen
Forchlorfenuron
Formetanate: 3-Acetamidophenol
Formetanate: 3-Hydroxyformanilide
Fuberidazole
Fumagillin
Gibberellic acid
Halauxifen
Halauxifen-methyl
Halofenozide
Halosulfuron-methyl
Haloxyfop
Haloxyfop glucoside
Heptylparaben
Hexachlorophene
Hexaconazole # fragment 166
Hexaflumuron
Imazalil: FK-284
Imazalil: FK-772
Imazamox
Imazamox-O-desmethyl
Imazapic
Imazapyr
Imazaquin
Imazethapyr
Imidacloprid-3-hydroxy
Imidacloprid-5-hydroxy
Imidacloprid-olefin
Imidacloprid: 6-Chloronicotinic acid
Inabenfide
Indole-3-acetate-ethyl
Indoxacarb-(S): IN-JT 333
Ioxynil
Iprodione: RP30228 # fragment 141
Iprodione-des-(N-isopropylcarboxamid)
Isofetamid
Isopyrazam
Isotianil
Isoxaben
Isoxaflutole
Isoxaflutole: RPA 202248
Isoxaflutole: RPA 203328 # fragment 223
Kinetin
Lenacil
Lincomycin
Lufenuron
MCPA # fragment 141
MCPA glucosid
MCPB # fragment 141



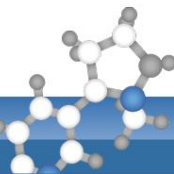
Mecoprop # fragment 141
Mefentrifluconazole # + CH ₃ COOH
Mefluidide
Mepronil
Meptyldinocap # fragment 295
Meptyldinocap-phenol
Mesosulfuron-methyl
Mesotrione # fragment 291
Mesotrione: AMBA
Mesotrione: MNBA
Metaflumizone-(E) # Peak 2
Metaflumizone-(Z) # Peak 1
Metaflumizone: 4-Cyanobenzoic acid
Metaflumizone ketone
Metalaxyl: CGA 62826
Metalaxyl: CGA 107955
Metamitron
Metamitron-desamino
Metazachlor: 479M04
Metazachlor: 479M08
Metconazole # +CH ₃ COOH
Methylparaben
Metobromuron: 4-Bromophenylurea
Metosulam
Metoxuron
Metribuzin-desamino
Metribuzin-desamino-diketo
Metribuzin-diketo
Metsulfuron-methyl
Myclobutanil: RH-9090 # +CH ₃ COOH
Naproanilide
Napropamide: 2-(2-Naphthyloxy)-propionic acid # fragment 143
Naptalam
Nicarbazin # (ISTD)
Niclosamide
Nitenpyram
Nitralin
Nitrofurazone
Norflurazon
Novaluron
Noviflumuron
Nuarimol
O,O-Diethyl thiophosphate
OPP 2-Phenylphenol
Oryzalin
Oxasulfuron
Pencycuron
Pendimethalin-4-hydroxymethyl
Pendimethalin: M455H001



Penflufen
Penfluron
Penoxsulam
Pentachlorophenol
Pentachlorophenol: 2.3.5.6-Tetrachlorophenol
Pentanochlor
Penthiopyrad
Penthiopyrad: DM-PCA
Penthiopyrad: PCA
Pentoxamid: MET-42
Perfluorobutanesulfonic acid
Perfluorobutanoic acid # fragment 168.9
Perfluorohexanoic acid # fragment 268.9
Perfluorooctanesulfonic acid
Perfluorooctanoic acid # fragment 368.9
Perfluoropentanoic acid # fragment 218.9
Permethrinic acid # (Racemat)
Phenamacril
Phenmedipham: MHPC
Phenothiazine-5-oxide
Phenothiazine-sulfone
Picolinafen
Pindon
Pinoxaden: M2
Pinoxaden: M4
Pinoxaden: M5
Pinoxaden: M6
Pirimicarb-desamido-desmethyl
Pirimiphos-methyl-desmethyl
Primisulfuron-methyl
Prochloraz: BTS 9608 # fragment 195
Profoxydim: BH 625-22
Profoxydim-sulfone # Peak 1
Profoxydim-sulfone # Peak 2
Profoxydim-sulfoxide # Peak 1
Profoxydim-sulfoxide # Peak 2
Prohexadione
Propanil
Propargite: Cyclohexanol-2-(4-tert-butyl-phenoxy) # M+HCOOH-H
Propiconazole: CGA 91304
Propiconazole: NOA436613
Propiconazole: SYN547889
Propoxycarbazone
Propoxycarbazone-2-hydroxy # fragment 172
Propylparaben
Propyzamide
Propyzamide D3 # (ISTD)
Propyzamide: 3.5-Dichlorobenzoic acid
Proquinazid: IN-MU210 # fragment 328.9



Prosulfuron
Prothioconazole
Pyracarbolid
Pyraclostrobin-desmethoxy # fragment 193
Pyraflufen
Pyrifluquinazon # fragment 421
Pyrifluquinazon-desacetyl
Pyrimethanil: 4.6-dimethyl-2-(phenylamino)pyrimidin-5-ol
Pyriminostrobin
Pyrimisulfan
Pyriproxyfen 4-hydroxy
Pyrithiobac # fragment 281
Pyroxasulfone M1
Pyroxasulfone M3
Quizalofop # Peak 1
Quizalofop # Peak 2
Quizalofop-pentanoic acid # fragment 271
Saflufenacil
Saflufenacil: M800H35
Saflufenacil-didesmethyl
Sedaxane # Peak 1
Sedaxane # Peak 2
Sethoxydim-sulfone
Sethoxydim-sulfoxide
Siduron
Sintofen
S-Metolachlor: CGA 357704 # Fragment 206
S-Metolachlor: CGA 368208
S-Metolachlor: CGA 37735
S-Metolachlor: CGA 50720 # fragment 134
S-Metolachlor: NOA 413173
S-Metolachlor-oxalamic acid # fragment 206
S-Metolachlor-sulfonic acid
Spiromesifen-enol
Spirotetramat-enol
Spirotetramat-enol-glucoside # fragment 300
Spirotetramat-keto-hydroxy
Spiroxamine-carboxylic acid
Sulcotrione # fragment 291
Sulcotrione: CMBA # fragment 189
Sulfachlorpyridazine
Sulfadiazine
Sulfadimethoxine
Sulfadimidine
Sulfamethoxazole
Sulfathiazole
Sulfentrazone
Sulfosulfuron
Sulfoxaflor



Sulfuramid
Sulfuron: AHMP
Swep
TCPy
Tebuconazole-hydroxy
Tecloftalam
Teflubenzuron
Tembotrione
Tembotrione-dihydroxy
Tepraloxym-dim-5-hydroxy # Peak 1
Tepraloxym-dim-5-hydroxy # Peak 2
Tepraloxym-dim-GP
Tepraloxym-dim-OH-GP
Terbacil
Thiacloprid-sulfonic acid # fragment 249
Thiamphenicol
Thidiazuron
Thiencarbazone-methyl
Thifensulfuron-methyl
Thifluzamide
Thiosultap
Tiadinil
Topramezone: M670H05
Tralopyril
Tri-allate: TCPSA
Triasulfuron
Tribenuron-methyl
Trichlamide
Triclopyr
Triclosan
Trifloxystrobin acid # fragment 317
Trifloxysulfuron
Triflomezopyrim # M+CH ₃ COOH-H
Triflumizole: FM-6-1 # (E-Isomer)
Triflumuron
Triflusulfuron-methyl
Triflusulfuron-methyl: IN-JK555 # fragment 214
Trinexapac
Trinexapac-methyl
Tritosulfuron # fragment 193
Tritosulfuron: AMTT
Tritosulfuron: TBSA
Uracil
Valifenalate # fragment 337
Valifenalate: beta-4-Chlorophenylalanine
Valifenalate acid
Warfarin