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Supplementary material

Automatic and predictive fractionation of organic micropollutants in contaminated water

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Table S1. Analytical characteristics of measured compounds (monitored ions and cone voltages)

Compounds families are highlighted in bold

Compound	CAS number	Ion 1 (*m*/*z*)	Ion 2 (*m*/*z*)	Cone voltage (V) Ion 1/Ion 2	Ion mode
Anilinopyrimidines					
Cyprodinil	121552-61-2	226.3	227.3	60/60	ESI+
Benzamides					
Tebutam	35256-85-0	192.3	234.4	50/15	ESI+
Isoxaben	82558-50-7	165.1	333.1	50/25	ESI+
Benzothiadiazinones					
Bentazone	25057-89-0	197.1	239.1	60/45	ESI–
Carbamates					
Carbofuran	1563-66-2	123.1	165.2	60/45	ESI+
Carboxamides					
Boscalid	188425-85-6	140	342.8	55/30	ESI+
Chloroacetamides					
Alachlor	15972-60-8	162.3	238.2	60/25	ESI+
Acetochlor	34256-82-1	148	224	45/25	ESI+
Dimethenamid	87674-68-8	168.2	276.1	60/25	ESI+
Metolachlor	51218-45-2	176.3	284.2	60/25	ESI+
Metazachlor	67129-08-2	210	278	25/25	ESI+
Propachlor	1918-16-7	105.9	212.2	62/25	ESI+
Dinitroanilines					
Pendimethaline	40487-42-1	212.2	282.2	25/25	ESI+
Hydroxybenzonitriles					
Bromoxynil	1689-84-5	273.9	276	60/60	ESI–
Ioxynil	1689-83-4	126.9	369.9	60/15	ESI–
Imidazoles					
Prochloraz	67747-09-5	375.8	377.8	15/15	ESI+
Imidazolinones					
Imazamethabenz-methyl	81405-85-8	257.2	289.2	45/25	ESI+
Isoxazoles					
Isoxaflutol	141112-29-0	250.9	357.9	50/25	ESI+
Oxadiazoles					
Oxadiazon	19666-30-9	220.1	303.2	60/45	ESI+
Oxyacetamides					
Fluthiamide	142459-58-3	152.2	364.1	45/25	ESI+
Phenylamides					
Oxadixyl	77732-09-3	219	279	30/15	ESI+
Phenoxycarboxylic acids					
2,4 D	94-75-7	160.9	219.1	47/25	ESI–
MCPA	94-74-6	141.2	199.2	45/25	ESI–
Dichlorprop	120-36-5	161	233.1	45/25	ESI–
Mecoprop	7085-19-0	141.1	143.1	45/60	ESI–
Pyridinecarboxamide					
Diflufenican	83164-33-4	266.2	395.2	60/25	ESI+
Pyridinecarboxylic acids					
Trichlopyr	55335-06-3	196	256	40/15	ESI–
Fluroxypyr	69377-81-7	180.9	208.8	50/40	ESI+
Triketones					
Mesotrione	104206-82-8	290.9	337.9	40/18	ESI–
Sulcotrione	99105-77-8	139	328.9	60/45	ESI+
Triazolopyrimidines					
Metosulam	139528-85-1	175.2	418.2	60/45	ESI+

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Compound	CAS number	Ion 1 (*m*/*z*)	Ion 2 (*m*/*z*)	Cone voltage (V) Ion 1/Ion 2	Ion mode
Strobilurins					
Azoxystrobin	131860-33-8	344.1	372.1	60/45	ESI+
Substituted ureas					
Chlortoluron	15545-48-9	213.2	215.1	25/25	ESI+
Diuron	330-54-1	231.1	233.1	25/25	ESI–
Isoproturon	34123-59-6	165.2	207.3	50/25	ESI+
Linuron	330-55-2	160.1	251.1	60/25	ESI+
Sulfonylureas					
Nicosulfuron	111991-09-4	182.3	411.2	60/25	ESI+
Triazines					
Simazine	122-34-9	104	202.2	60/45	ESI+
Terbutylazine	5915-41-3	230	232	25/25	ESI+
Terbumeton	33693-04-8	226.1	227.1	25/25	ESI+
Triazoles					
Epoxiconazole	133855-98-8	329.9	331.8	15/15	ESI+
Tetraconazole	112281-77-3	159.2	372.1	60/45	ESI+
Tebuconazole	107534-96-3	308.3	310.3	25/25	ESI+