

Chemicals of emerging concern (CECs) in river water

The chemical pollution cause huge damage to the aquatic environment. The simultaneous determination of pollutants with different physico-chemical properties, such as pesticides, metabolites, personal care products, plastic-related chemicals is always challenging. The application shows a sensitive LC/MS method for fast determination of diverse group of pollutants in river water.

Substance	Deisopropylatrazine, CAS number 1007-28-9
Substance	Hexazinon, CAS number 51235-04-2
Substance	Simazine, CAS number 122-34-9
Substance	Atrazine, CAS number 1912-24-9
Substance	Terbuthylazine, CAS number 5915-41-3
Substance	Terbutryn, CAS number 886-50-0
Substance	Prometryn, CAS number 7287-19-6
Substance	Metolachlor, CAS number 51218-45-2
Substance	Metazachlor, CAS number 67129-08-2
Substance	Diuron, CAS number 330-54-1
Substance	Isoproturon, CAS number 34123-59-6
Substance	Chlorotoluron, CAS number 15545-48-9
Substance	Desethylterbuthylazine, CAS number 30125-63-4
Substance	Acetochlor, CAS number 34256-82-1
Substance	Tebuconazole, CAS number 107534-96-3
Substance	Propiconazole, CAS number 60207-90-1
Substance	Ametryn, CAS number 834-12-8
Substance	Epoxiconazole, CAS number 135319-73-2
Substance	Cybutryne, CAS number 28159-98-0
Synonym	Irgarol
Substance	Alachlor, CAS number 15972-60-8
Substance	Chlorfenvinphos, CAS number 470-90-6
Substance	Ethofumesate, CAS number 26225-79-6
Substance	Linuron, CAS number 330-55-2
Substance	Pendimethalin, CAS number 40487-42-1
Substance	Fenthion, CAS number 55-38-9

Chemicals of emerging concern (CECs) in river water

Substance	Dichlorvos, CAS number 62-73-7
Substance	Quinoxifen, CAS number 124495-18-7
Substance	Thiamethoxam, CAS number 153719-23-4
Substance	Imidacloprid, CAS number 138261-41-3
Substance	Clothianidin, CAS number 210880-92-5
Substance	Fenpropimorph, CAS number 67564-91-4
Substance	Carbendazim, CAS number 10605-21-7
Substance	Thiacloprid, CAS number 111988-49-9
Substance	Spiroxamine, CAS number 118134-30-8
Substance	Metamitron, CAS number 41394-05-2
Substance	Propazine, CAS number 139-40-2
Substance	Thiophanate-methyl, CAS number 23564-05-8
Substance	(4-Chloro-2-methylphenoxy)acetic acid, CAS number 94-74-6
Synonym	MCPA
Substance	Mecoprop, CAS number 93-65-2
Synonym	MCPP+MCPP-p
Substance	2,4-Dichlorophenoxyacetic acid, CAS number 94-75-7
Synonym	2,4-D
Substance	4-(4-Chloro-2-methylphenoxy)butanoic acid, CAS number 94-81-5
Synonym	MCPB
Substance	Dichlorprop, CAS number 120-36-5
Synonym	2,4-DP
Substance	Bentazone, CAS number 25057-89-0
Substance	2,4,5-Trichlorophenoxyacetic acid, CAS number 93-76-5
Synonym	2,4,5-T
Substance	Perfluorooctanesulfonic acid, CAS number 1763-23-1
Synonym	PFOS
Substance	Desethylatrazine, CAS number 6190-65-4
Synonym	Desethyl-atrazine
Substance	Methiocarb, CAS number 2032-65-7

Chemicals of emerging concern (CECs) in river water

Column	CHROMSHELL® C18 Plus, 2.6 µm		
Dimensions	50 mm × 2.1 mm		
Part number	CSH-5722-GG21		
Mobile phase	A: 5mM ammonium formate in water B: 5mM ammonium formate in MeOH		
Gradient elution	Time (min)	%A	%B
	0	100	0
	2	100	0
	7	0	100
	8	0	100
	8.1	100	0
	11	100	0
Flow rate	0.350 mL/min		
Temperature	40 °C		
Detection	MS/MS Low Mass		
Injection volume	100 µL		
Analytes	See MS/MS method		

Validation parameters	LOD, µg/L	LOQ, µg/L
desethylatrazine	4.6	15.5
hexazinon	2.9	9.7
simazine	3.5	11.6
atrazine	2.1	7.1
terbuthylazin	3.8	12.6
terbutryn	3.5	11.7
prometryn	3.7	12.3
metolachlor	4.9	16.2
metazachlor	3	9.8
diuron	3.8	12.8
isoproturon	4	13.2
chlorotoluron	2.8	9.3
desethylterbuthylazine	6.3	21
acetochlor	4	13.4

Chemicals of emerging concern (CECs) in river water

Validation parameters	LOD, µg/L	LOQ, µg/L
tebuconazole	3.2	10.8
propiconazole	5	16.8
ametryn	3.4	11.4
epoxiconazole	2.7	8.9
cybutryne	3.9	12.8
alachlor	4.3	14.3
chlorfenvinphos	3	10
deisopropylatrazine	5.6	18.5
ethofumesat	2.7	8.9
linuron	4.7	15.6
pendimethalin	5.1	16.9
atrazin-desethyl desisopropyl	20	6
fenthion	2.3	7.6
dichlorvos	8.9	29.7
quinoxifen	3	10.1
thiamethoxam	3.3	11
imidacloprid	3.3	11
clothianidin	5.8	19.3
fenpropimorph	3	9.9
carbendazim	4.5	15.1
thiacloprid	4.4	14.6
spiroxamine	3.6	12.1
metamitron	2.9	9.5
propazin	3.5	11.8
thiophanate-methyl	5.2	17.4
(4-chloro-2-methylphenoxy)acetic acid	5.1	16.8
mecoprop	6	20.1
2,4-dichlorophenoxyacetic acid	3.8	12.7
4-(4-chloro-2-methylphenoxy)butanoic acid	6	20.1
dichlorprop	6	20
bentazon	3	9.9
2,4,5-trichlorophenoxyacetic acid	3.4	11.2
methiocarb	4.9	16.4
perfluorooctanesulfonic acid	5.4	18.1

* The LOD and LOQ were calculated from real surface river water samples, not pure standards.

Chemicals of emerging concern (CECs) in river water

Internal standard are used:

Bentazone D6 RT: 4.22

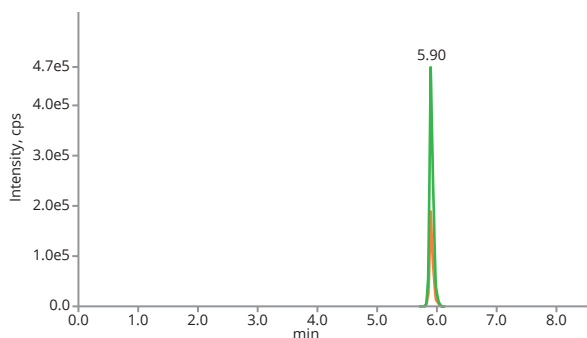
(-) Qualifier 244.9 > 132.0 [-38.0 V],
Quantifier 244.9 > 181.0 [-30.0 V]

Isoproturon D6 RT: 6.35

(+) Qualifier 213.3 > 78.2 [27.0 V],
Quantifier 213.3 > 52.2 [31.0 V]

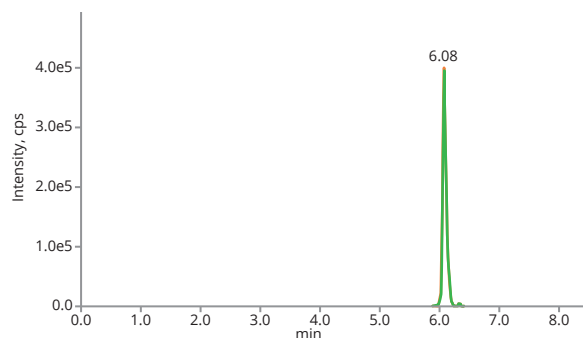
Simazine D10 RT: 5.84

(+) Qualifier 212.1 > 137.1 [25.0 V],
Quantifier 212.1 > 134.2 [25.0 V]



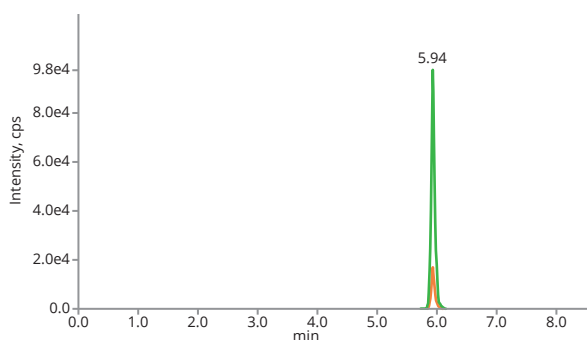
Mecoprop RT: 5.91

(-) Qualifier 213.0 > 141.0 [-18.0 V],
Quantifier 215.0 > 143.0 [-18.0 V]



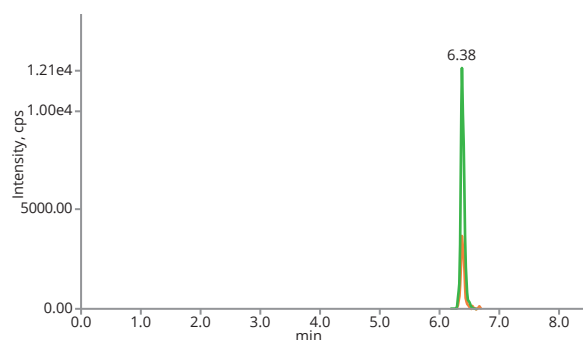
2,4,5-Trichlorophenoxyacetic acid RT: 6.07

(-) Qualifier 252.7 > 194.9 [-16.0 V],
Quantifier 254.7 > 196.8 [-16.0 V]



Dichlorprop RT: 5.92

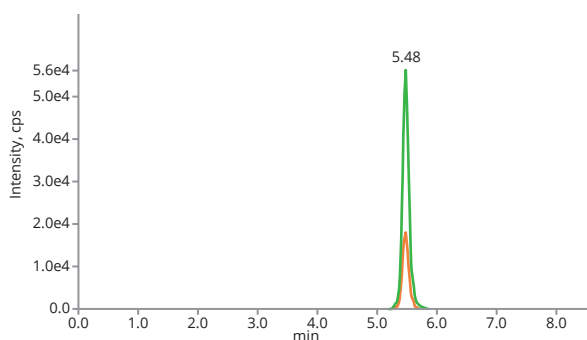
(-) Qualifier 233.0 > 161.0 [-18.0 V],
Quantifier 233.0 > 125.0 [-32.0 V]



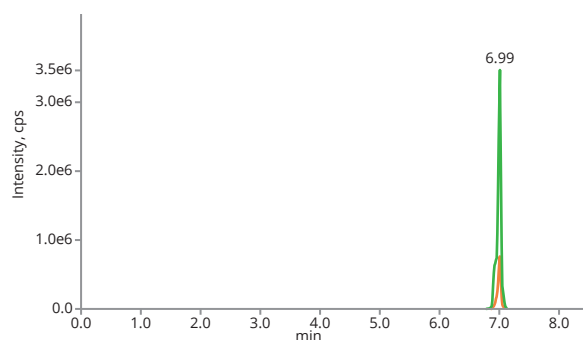
4-(4-Chloro-2-methylphenoxy)butanoic acid RT: 6.5

(-) Qualifier 227.0 > 141.0 [-12.0 V],
Quantifier 229.0 > 143.0 [-12.0 V]

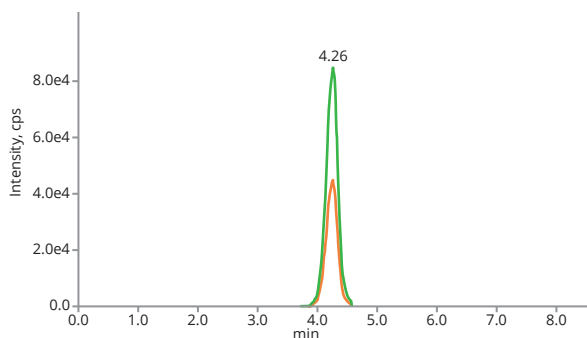
Chemicals of emerging concern (CECs) in river water



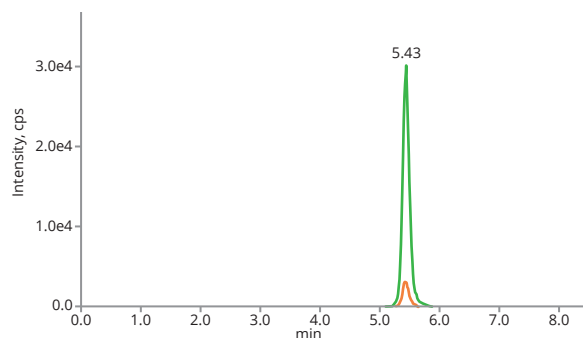
(4-Chloro-2-methylphenoxy)acetic acid RT: 5.48
 (-) Qualifier 199.0 > 141.0 [-20.0 V],
 Quantifier 201.0 > 143.0 [-20.0 V]



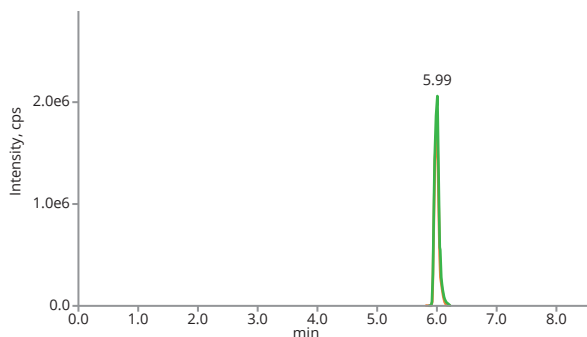
Perfluorooctanesulfonic acid RT: 7.0
 (-) Qualifier 498.8 > 79.8 [-118.0 V],
 Quantifier 498.8 > 98.8 [-98.0 V]



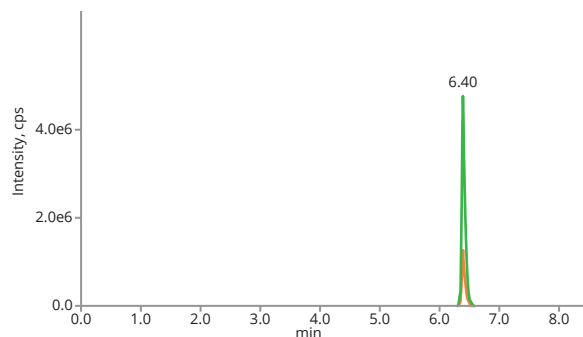
Bentazone RT: 4.22
 (-) Qualifier 239.0 > 132.0 [-36.0 V],
 Quantifier 239.0 > 197.0 [-30.0 V]



2,4-Dichlorophenoxyacetic acid RT: 5.44
 (-) Qualifier 219.0 > 161.0 [-18.0 V],
 Quantifier 219.0 > 125.0 [-36.0 V]

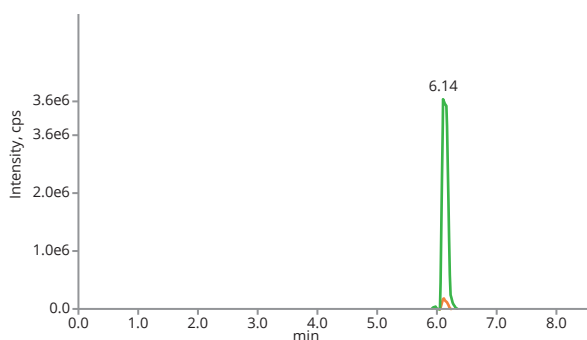


Simazine RT: 5.9
 (+) Qualifier 202.1 > 132.1 [25.0 V],
 Quantifier 202.1 > 124.3 [25.0 V]

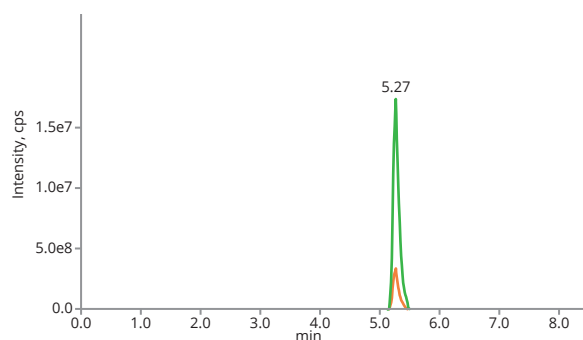


Isoproturon RT: 6.35
 (+) Qualifier 207.2 > 72.1 [29.0 V],
 Quantifier 207.2 > 46.1 [31.0 V]

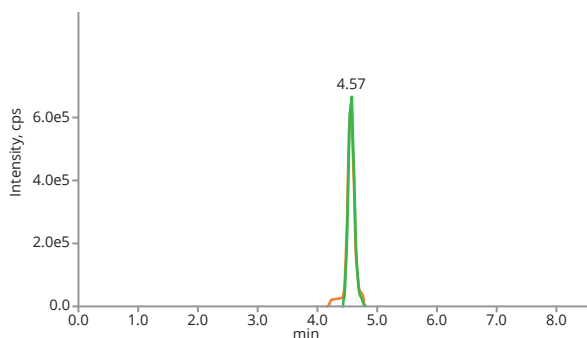
Chemicals of emerging concern (CECs) in river water



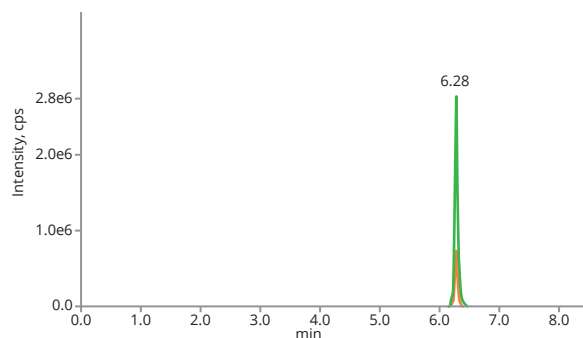
Desethylterbutylazine RT: 6.1
(+) Qualifier 202.1 > 146.0 [23.0 V],
Quantifier 202.1 > 79.0 [50.0 V]



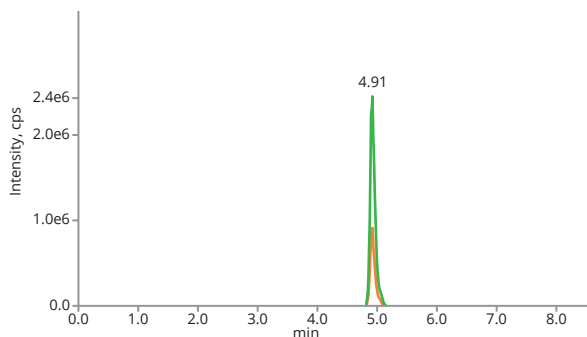
Carbendazim RT: 5.14
(+) Qualifier 192.2 > 160.2 [27.0 V],
Quantifier 192.2 > 132.1 [41.0 V]



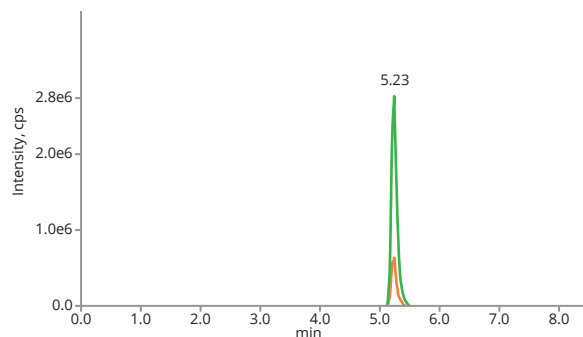
Deisopropylatrazine RT: 4.38
(+) Qualifier 174.1 > 104.1 [31.0 V],
Quantifier 174.1 > 96.1 [27.0 V]



Chlorotoluron RT: 6.21
(+) Qualifier 213.1 > 72.2 [31.0 V],
Quantifier 213.1 > 46.2 [27.0 V]

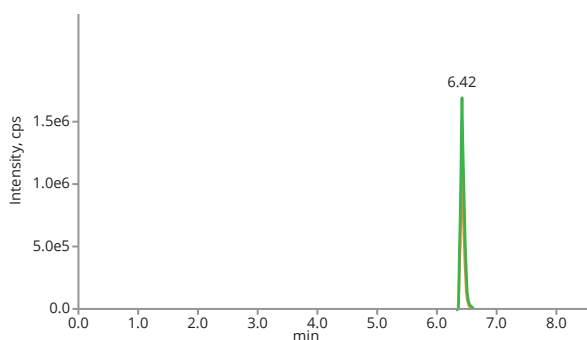


Metamitron RT: 4.8
(+) Qualifier 203.2 > 175.1 [23.0 V],
Quantifier 203.2 > 104.1 [33.0 V]

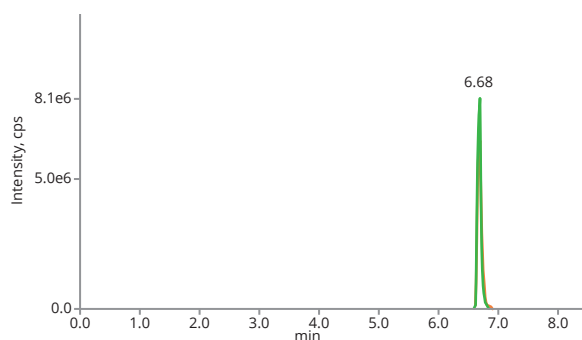


Desethylatrazine RT: 5.1
(+) Qualifier 188.1 > 146.2 [21.0 V],
Quantifier 188.1 > 104.1 [33.0 V]

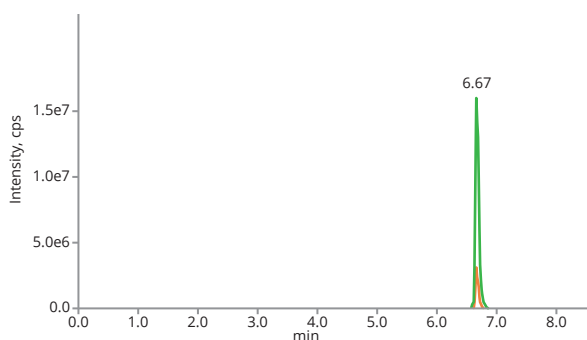
Chemicals of emerging concern (CECs) in river water



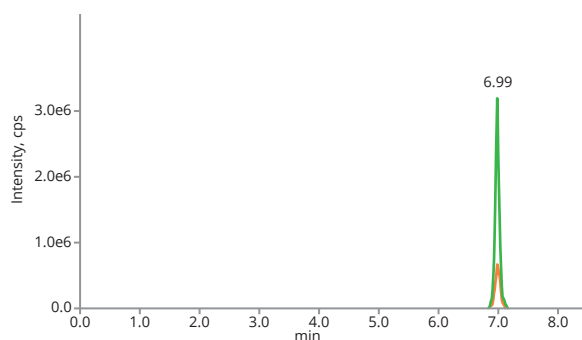
Diuron RT: 6.35
(+) Qualifier 233.1 > 72.0 [33.0 V],
Quantifier 235.1 > 72.1 [37.0 V]



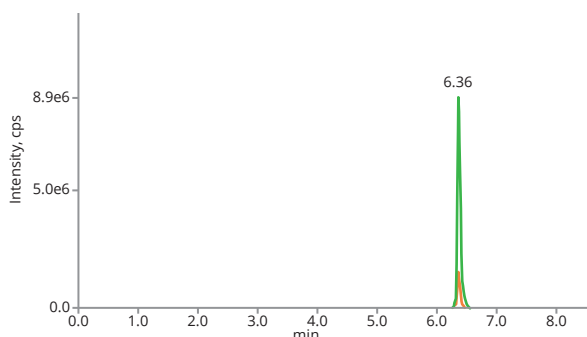
Propazin RT: 6.33
(+) Qualifier 230.1 > 188.0 [25.0 V],
Quantifier 230.1 > 146.0 [33.0 V]



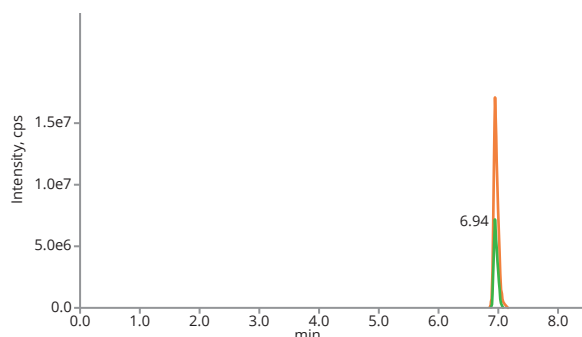
Amertyn RT: 6.63
(+) Qualifier 228.2 > 186.2 [23.0 V],
Quantifier 228.2 > 96.1 [33.0 V]



Acetochlor RT: 6.59
(+) Qualifier 224.1 > 148.1 [27.0 V],
Quantifier 270.0 > 224.0 [27.0 V]

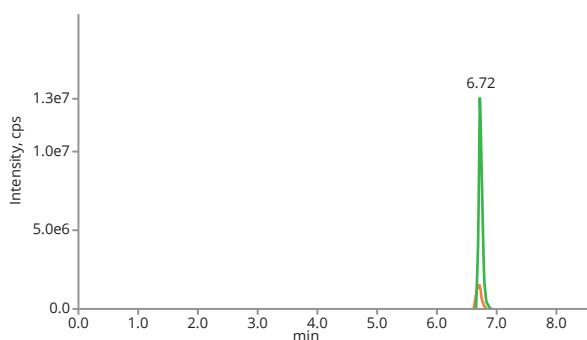


Atrazine RT: 6.31
(+) Qualifier 216.1 > 174.0 [23.0 V],
Quantifier 216.1 > 104.1 [39.0 V]

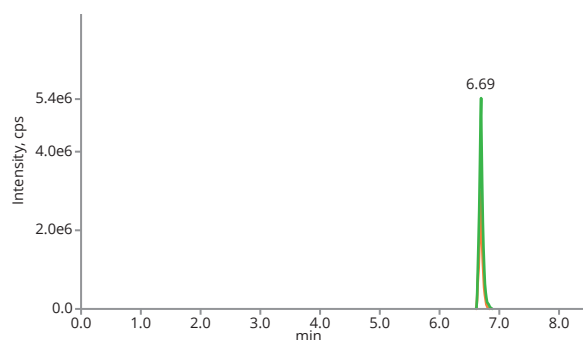


Prometryn RT: 6.9
(+) Qualifier 242.2 > 200.1 [19.0 V],
Quantifier 242.2 > 158.1 [35.0 V]

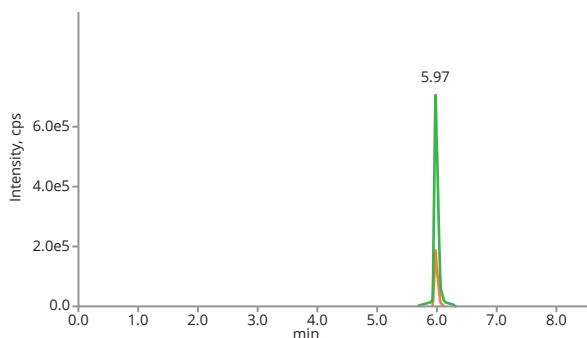
Chemicals of emerging concern (CECs) in river water



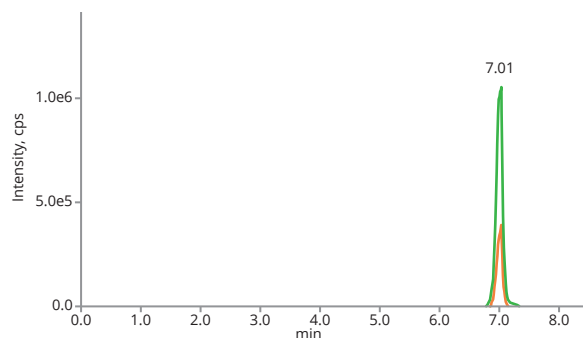
Terbutylazine RT: 6.7
(+) Qualifier 230.1 > 174.1 [23.0 V],
Quantifier 230.1 > 104.1 [41.0 V]



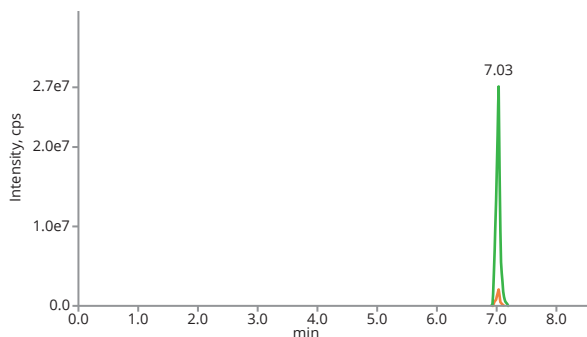
Methiocarb RT: 6.63
(+) Qualifier 226.1 > 169.2 [13.0 V],
Quantifier 226.1 > 121.1 [23.0 V]



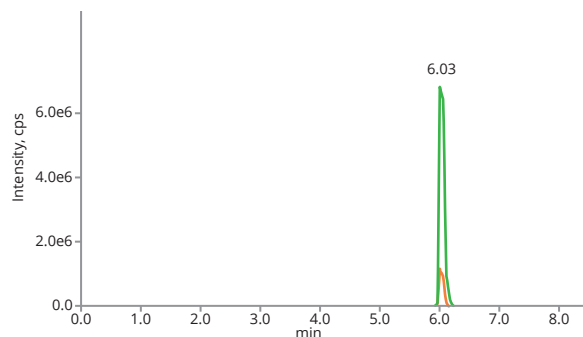
Dichlorvos RT: 5.88
(+) Qualifier 220.9 > 109.1 [25.0 V],
Quantifier 220.9 > 127.2 [23.0 V]



Alachlor RT: 7.0
(+) Qualifier 270.1 > 238.2 [17.0 V],
Quantifier 270.1 > 162.2 [28.0 V]

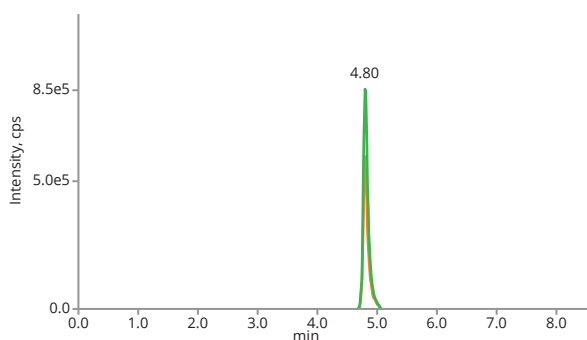


Cybutryne RT: 6.98
(+) Qualifier 254.2 > 198.2 [23.0 V],
Quantifier 254.2 > 83.2 [39.0 V]

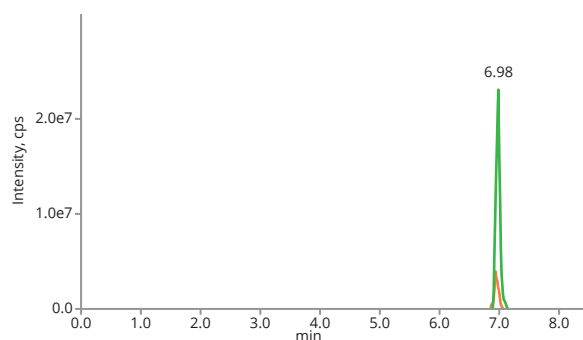


Hexazinon RT: 5.94
(+) Qualifier 253.2 > 171.2 [27.0 V],
Quantifier 253.2 > 85.1 [44.0 V]

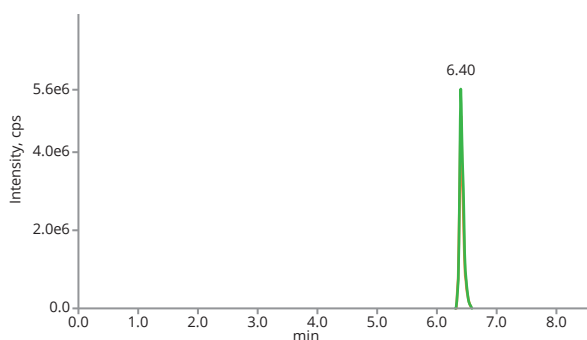
Chemicals of emerging concern (CECs) in river water



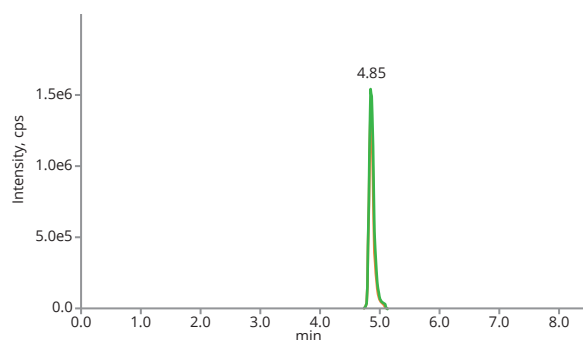
Clothianidin RT: 4.7
(+) Qualifier 250.0 > 169.1 [17.0 V],
Quantifier 250.0 > 132.0 [21.0 V]



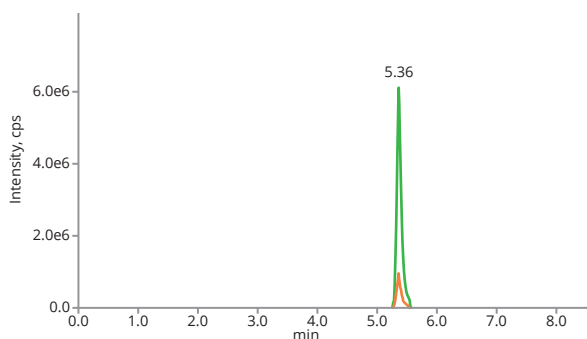
Terbutryn RT: 6.91
(+) Qualifier 242.2 > 186.1 [23.0 V],
Quantifier 242.2 > 68.1 [57.0 V]



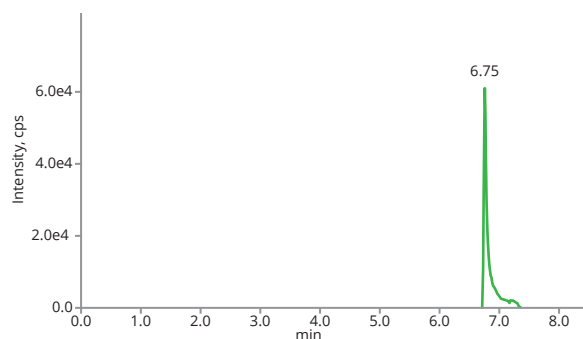
Metazachlor RT: 6.35
(+) Qualifier 278.2 > 134.2 [27.0 V],
Quantifier 278.2 > 210.2 [17.0 V]



Imidacloprid RT: 4.62
(+) Qualifier 256.2 > 209.0 [23.0 V],
Quantifier 256.2 > 175.2 [23.0 V]

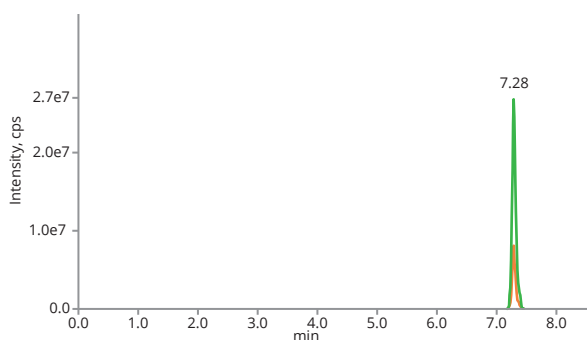


Thiachloprid RT: 5.22
(+) Qualifier 253.1 > 126.1 [29.0 V],
Quantifier 253.1 > 99.1 [57.0 V]

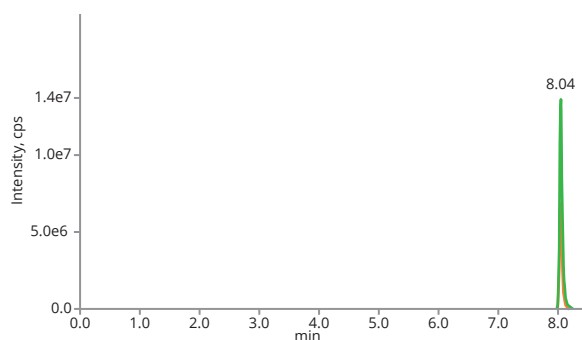


Linuron RT: 6.6
(+) Qualifier 249.1 > 160.0 [23.0 V],
Quantifier 249.1 > 182.1 [21.0 V]

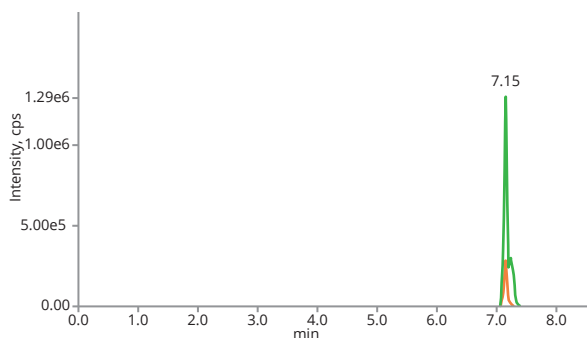
Chemicals of emerging concern (CECs) in river water



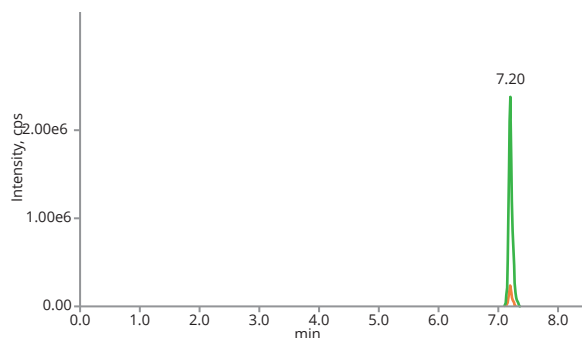
Spiroxamine RT: 7.1
(+) Qualifier 298.4 > 144.2 [27.0 V],
Quantifier 298.4 > 100.2 [43.0 V]



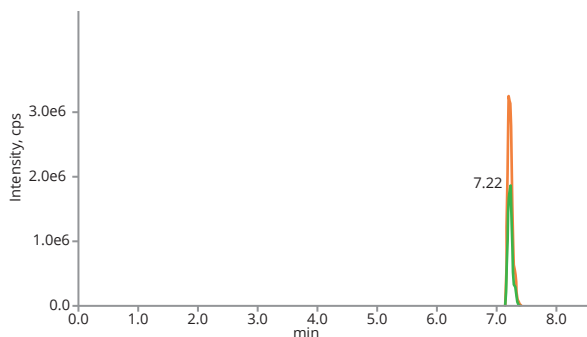
Fenpropimorph RT: 7.97
(+) Qualifier 304.0 > 147.0 [39.0 V],
Quantifier 304.0 > 117.0 [71.0 V]



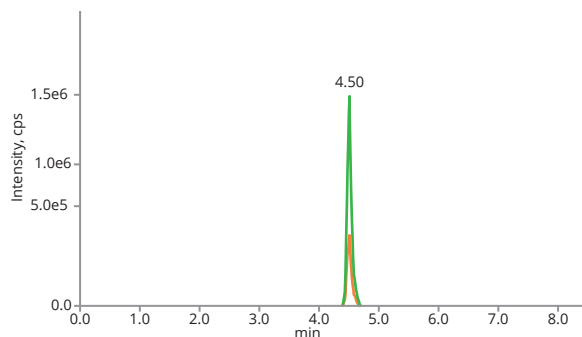
Tebuconazole RT: 7.1
(+) Qualifier 308.0 > 70.0 [39.0 V],
Quantifier 308.0 > 125.0 [47.0 V]



Propiconazole RT: 7.15
(+) Qualifier 342.1 > 159.1 [43.0 V],
Quantifier 342.1 > 69.1 [33.0 V]

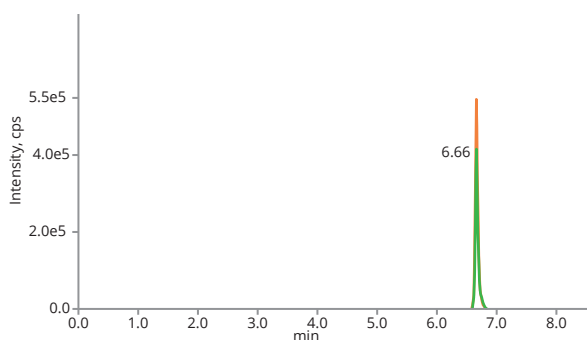


Chlorfenvinphos RT: 7.18
(+) Qualifier 358.9 > 99.0 [39.0 V],
Quantifier 358.9 > 155.1 [17.0 V]

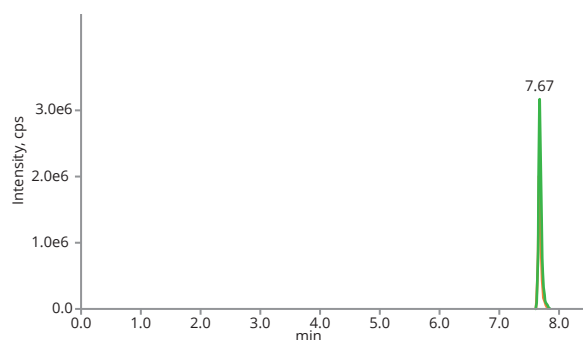


Thiamethoxam RT: 4.34
(+) Qualifier 292.0 > 211.0 [17.0 V],
Quantifier 292.0 > 181.0 [31.0 V]

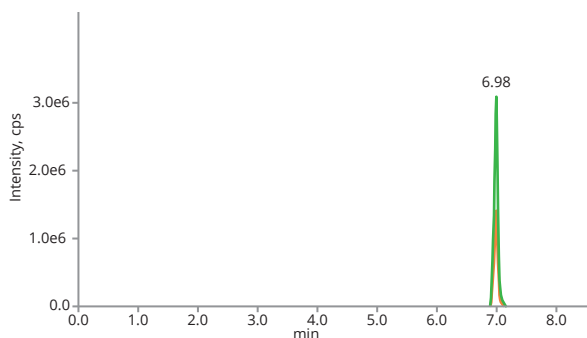
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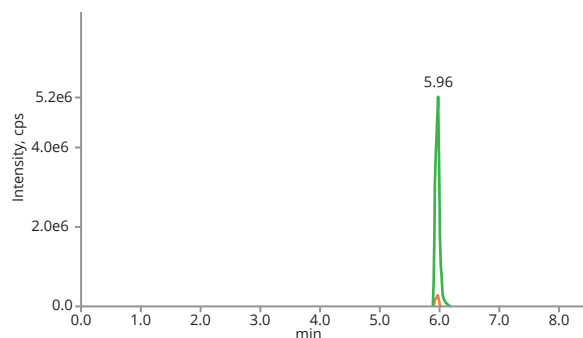
Ethofumesate RT: 6.62
(+) Qualifier 304.0 > 121.0 [27.0 V],
Quantifier 304.0 > 161.0 [31.0 V]



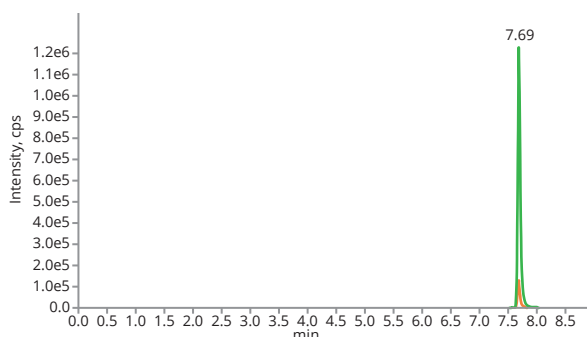
Quinoxifen RT: 7.61
(+) Qualifier 308.0 > 197.0 [43.0 V],
Quantifier 308.0 > 162.0 [57.0 V]



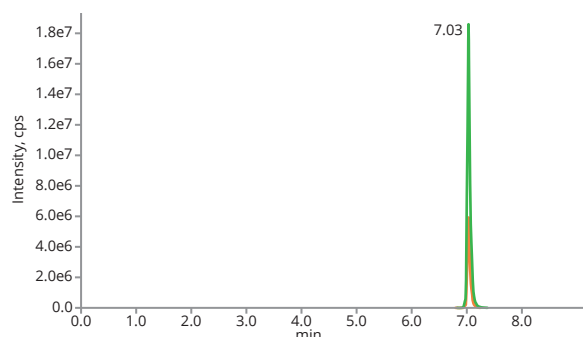
Epoxiconazole RT: 6.9
(+) Qualifier 330.0 > 121.0 [27.0 V],
Quantifier 330.0 > 101.0 [63.0 V]



Thiophanate-methyl RT: 5.84
(+) Qualifier 343.0 > 151.0 [25.0 V],
Quantifier 343.0 > 192.0 [21.0 V]

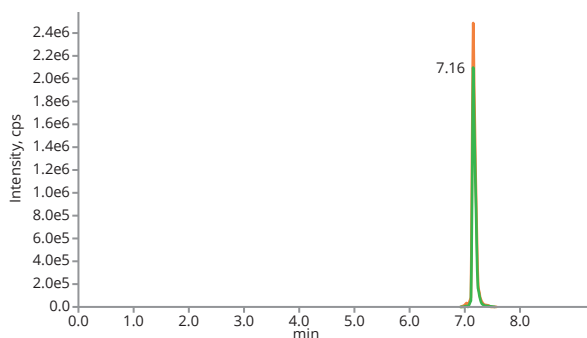


Pendimethalin RT: 7.65
(+) Qualifier 282.2 > 212.1 [15.0 V],
Quantifier 282.2 > 194.2 [21.0 V]

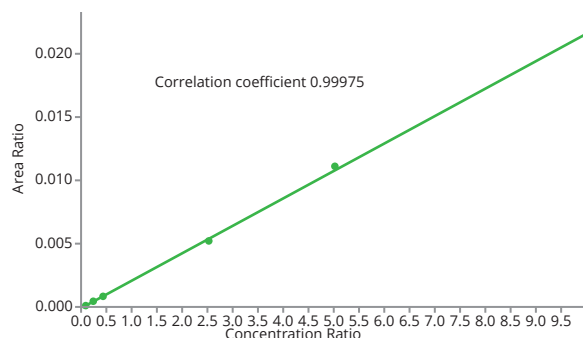


Metolachlor RT: 7.0
(+) Qualifier 284.2 > 252.2 [21.0 V],
Quantifier 284.2 > 176.2 [33.0 V]

Chemicals of emerging concern (CECs) in river water



Fenthion RT: 7.1
 (+) Qualifier 278.9 > 169.0 [25.0 V],
 Quantifier 278.9 > 246.9 [19.0 V]



*Example of calibration curve for
 4-(4-Chloro-2-methylphenoxy)butanoic acid
 (MCPB)*

Author of this application: Ohře river basin, state enterprise.

