Supporting Information for:

A LC-HRMS data processing strategy for reliable sample comparison exemplified by the assessment of water treatment processes

Tobias Bader[1,2*], Wolfgang Schulz[1], Klaus Kümmerer[2], Rudi Winzenbacher[1]

[1]*Laboratory for Operation Control and Research, Zweckverband Landeswasserversorgung, Am Spitzigen Berg 1, 89129 Langenau, Germany*
[2]*Sustainable Chemistry and Material Resources, Institute of Sustainable and Environmental Chemistry, Leuphana University of Lüneburg, Scharnhorststraße 1/C13, 21335 Lüneburg, Germany*

*Corresponding author
Email: Bader.T@lw-online.de
Phone: +49 7345 9638 2279
Fax: +49 7345 9638 2290

TABLE OF CONTENTS (clickable links)

Table S-1. List of 411 target compounds

#	Name	Formula	CAS Number
1	1-(2-Chlorophenyl)-3-phenylurea	$C_{13}H_{11}ClN_2O$	2989-99-3
2	1-(3,4-Dichlorophenyl)-3-methylurea	$C_8H_8Cl_2N_2O$	3567-62-2
3	1-(3,4-Dichlorophenyl)urea	$C_7H_6Cl_2N_2O$	2327-02-8
4	1,1-Dimethyl-3-phenylurea	$C_9H_{12}N_2O$	101-42-8
5	1,2,3-Benzotriazole	$C_6H_5N_3$	95-14-7
6	1-Hydroxyisoquinoline	C_9H_7NO	491-30-5
7	1-Methylisoquinoline	$C_{10}H_9N$	1721-93-3
8	2-(Methylthio)benzothiazole	$C_8H_7NS_2$	615-22-5
9	2,4-Dimethylquinoline	$C_{11}H_{11}N$	1198-37-4
10	2,5-Dichloroaniline	$C_6H_5Cl_2N$	95-82-9
11	2,6-Dichlorbenzamid	$C_7H_5Cl_2NO$	2008-58-4
12	2-Aminobenzothiazole	$C_7H_6N_2S$	136-95-8
13	2-Hydroxybenzothiazole	C_7H_5NOS	934-34-9
14	2-Methoxyphenyl isocyanate	$C_8H_7NO_2$	700-87-8
15	2-Methyl-8-quinolinol	$C_{10}H_9NO$	826-81-3
16	2-Methylphenyl isocyanate	C_8H_7NO	614-68-6
17	3-(2-Chloro-6-methylphenyl)-1,1-dimethylurea	$C_{10}H_{13}ClN_2O$	15441-90-4
18	3-(Trifluoromethyl)aniline	$C_7H_6F_3N$	98-16-8
19	3-Hydroxycarbofuran	$C_{12}H_{15}NO_4$	16655-82-6
20	4-Acetamidoantipyrine	$C_{13}H_{15}N_3O_2$	83-15-8
21	4-Chloro-o-toluidine	C_7H_8ClN	95-69-2
22	4'-Hydroxydiclofenac	$C_{14}H_{11}Cl_2NO_3$	64118-84-9
23	4-Isopropylaniline	$C_9H_{13}N$	99-88-7
24	5,6-Dimethyl-1H-benzotriazole	$C_8H_9N_3$	4184-79-6
25	5'-Chloro-2'-methylacetanilide	$C_9H_{10}ClNO$	5900-55-0
26	5-Methyl-1H-benzotriazole	$C_7H_7N_3$	136-85-6
27	8-Hydroxyquinoline	C_9H_7NO	148-24-3
28	Acebutolol	$C_{18}H_{28}N_2O_4$	37517-30-9
29	Acephate	$C_4H_{10}NO_3PS$	30560-19-1
30	Acetaminophen	$C_8H_9NO_2$	103-90-2
31	Acetamiprid	$C_{10}H_{11}ClN_4$	135410-20-7
32	Acetylsulfamethoxazole	$C_{12}H_{13}N_3O_4S$	21312-10-7
33	Aclonifen	$C_{12}H_9ClN_2O_3$	74070-46-5
34	Acridine	$C_{13}H_9N$	260-94-6
35	Alachlor	$C_{14}H_{20}ClNO_2$	15972-60-8
36	Aldicarb-sulfoxide	$C_7H_{14}N_2O_3S$	1646-87-3
37	Alprenolol	$C_{15}H_{23}NO_2$	13655-52-2
38	Amantadine	$C_{10}H_{17}N$	768-94-5
39	Ametryn	$C_9H_{17}N_5S$	834-12-8
40	Amidosulfuron	$C_9H_{15}N_5O_7S_2$	120923-37-7
41	Aminocarb	$C_{11}H_{16}N_2O_2$	2032-59-9
42	Amisulprid	$C_{17}H_{27}N_3O_4S$	71675-85-9
43	Amisulpride N-Oxide	$C_{17}H_{27}N_3O_5S$	71676-01-2
44	Aspartame	$C_{14}H_{18}N_2O_5$	22839-47-0
45	Asulam	$C_8H_{10}N_2O_4S$	3337-71-1
46	Atenolol	$C_{14}H_{22}N_2O_3$	29122-68-7
47	Atraton	$C_9H_{17}N_5O$	1610-17-9
48	Atrazine	$C_8H_{14}ClN_5$	1912-24-9
49	Atrazine-2-hydroxy	$C_8H_{15}N_5O$	2163-68-0
50	Azamethiphos	$C_9H_{10}ClN_2O_5PS$	35575-96-3
51	Azinphos-ethyl	$C_{12}H_{16}N_3O_3PS_2$	2642-71-9
52	Azoxystrobin	$C_{22}H_{17}N_3O_5$	131860-33-8
53	Benalaxyl-M	$C_{20}H_{23}NO_3$	98243-83-5
54	Benazolin	$C_9H_6ClNO_3S$	3813-05-6
55	Bensulfuron-methyl	$C_{16}H_{18}N_4O_7S$	83055-99-6
56	Bentazon	$C_{10}H_{12}N_2O_3S$	25057-89-0
57	Benzocaine	$C_9H_{11}NO_2$	94-09-7
58	Benzothiazole-6-carboxylic acid	$C_8H_5NO_2S$	3622-35-3
59	Betaxolol	$C_{18}H_{29}NO_3$	63659-18-7
60	Bezafibrate	$C_{19}H_{20}ClNO_4$	41859-67-0
61	Bisoprolol	$C_{18}H_{31}NO_4$	66722-44-9
62	Bisoprolol_M1	$C_{15}H_{23}NO_5$	109791-19-7
63	Bisoprolol_M3	$C_{13}H_{19}NO_4$	72570-70-8
64	Bisoprolol_M4	$C_{15}H_{25}NO_4$	109791-18-6
65	Bitertanol	$C_{20}H_{23}N_3O_2$	55179-31-2
66	Boscalid	$C_{18}H_{12}Cl_2N_2O$	188425-85-6
67	Bromacil	$C_9H_{13}BrN_2O_2$	314-40-9
68	Bromophos-ethyl	$C_{10}H_{12}BrCl_2O_3PS$	4824-78-6
69	Bromuconazole	$C_{13}H_{12}BrCl_2N_3O$	116255-48-2
70	Bupirimate	$C_{13}H_{24}N_4O_3S$	41483-43-6
71	Caffeine	$C_8H_{10}N_4O_2$	58-08-2
72	Candesartan	$C_{24}H_{20}N_6O_3$	139481-59-7
73	Carbamazepine	$C_{15}H_{12}N_2O$	298-46-4
74	Carbamazepine 10,11-epoxide	$C_{15}H_{12}N_2O_2$	36507-30-9
75	Carbanilide	$C_{13}H_{12}N_2O$	102-07-8
76	Carbaryl	$C_{12}H_{11}NO_2$	63-25-2
77	Carbendazim	$C_9H_9N_3O_2$	10605-21-7
78	Carbetamide	$C_{12}H_{16}N_2O_3$	16118-49-3
79	Carbofuran	$C_{12}H_{15}NO_3$	1563-66-2
80	Chloramben	$C_7H_5Cl_2NO_2$	133-90-4

#	Name	Formula	CAS Number
81	Chlorbromuron	$C_9H_{10}BrClN_2O_2$	13360-45-7
82	Chlordimeform	$C_{10}H_{13}ClN_2$	6164-98-3
83	Chlorfenvinphos	$C_{12}H_{14}Cl_3O_4P$	470-90-6
84	Chloridazon	$C_{10}H_8ClN_3O$	1698-60-8
85	Chloridazon-methyl-desphenyl	$C_5H_6ClN_3O$	17254-80-7
86	Chloroxuron	$C_{15}H_{15}ClN_2O_2$	1982-47-4
87	Chlorpyrifos	$C_9H_{11}Cl_3NO_3PS$	2921-88-2
88	Chlorthalonil R611965	$C_8H_4Cl_3NO_3$	142733-37-7
89	Chlortoluron	$C_{10}H_{13}ClN_2O$	15545-48-9
90	Chlortoluron benzoic acid (CGA 15140)	$C_{10}H_{11}ClN_2O_3$	59587-01-8
91	Clarithromycin	$C_{38}H_{69}NO_{13}$	81103-11-9
92	Clenbuterol	$C_{12}H_{18}Cl_2N_2O$	37148-27-9
93	Clindamycin	$C_{18}H_{33}ClN_2O_5S$	18323-44-9
94	Clodinafop-propargyl	$C_{17}H_{13}ClFNO_4$	105512-06-9
95	Clomazone	$C_{12}H_{14}ClNO_2$	81777-89-1
96	Clothianidin	$C_6H_8ClN_5O_2S$	210880-92-5
97	Codeine	$C_{18}H_{21}NO_3$	76-57-3
98	Crotamiton	$C_{13}H_{17}NO$	483-63-6
99	Cyanazine	$C_9H_{13}ClN_6$	21725-46-2
100	Cybutryne	$C_{11}H_{19}N_5S$	28159-98-0
101	Cyproconazole	$C_{15}H_{18}ClN_3O$	94361-06-5
102	Cyprodinil	$C_{14}H_{15}N_3$	121552-61-2
103	Dapsone	$C_{12}H_{12}N_2O_2S$	80-08-0
104	Deisopropylatrazine	$C_5H_8ClN_5$	1007-28-9
105	Desethylatrazine	$C_6H_{10}ClN_5$	6190-65-4
106	Desethylterbutylazine	$C_7H_{12}ClN_5$	30125-63-4
107	Diatrizoate	$C_{11}H_9I_3N_2O_4$	737-31-5
108	Diazepam	$C_{16}H_{13}ClN_2O$	439-14-5
109	Diazinon	$C_{12}H_{21}N_2O_3PS$	333-41-5
110	Dichlofenthion	$C_{10}H_{13}Cl_2O_3PS$	97-17-6
111	Dichlorvos	$C_4H_7Cl_2O_4P$	62-73-7
112	Diclofenac	$C_{14}H_{11}Cl_2NO_2$	15307-86-5
113	Dicrotophos	$C_8H_{16}NO_5P$	141-66-2
114	Didesmethylisoproturon	$C_{10}H_{14}N_2O$	56046-17-4
115	Diethofencarb	$C_{14}H_{21}NO_4$	87130-20-9
116	Difenoconazole	$C_{19}H_{17}Cl_2N_3O_3$	119446-68-3
117	Difenoxuron	$C_{16}H_{18}N_2O_3$	14214-32-5
118	Diflubenzuron	$C_{14}H_9ClF_2N_2O_2$	35367-38-5
119	Diflufenican	$C_{19}H_{11}F_5N_2O_2$	83164-33-4
120	Dihydrocodeine	$C_{18}H_{23}NO_3$	125-28-0
121	Dimefuron	$C_{15}H_{19}ClN_4O_3$	34205-21-5
122	Dimethachlor	$C_{13}H_{18}ClNO_2$	50563-36-5
123	Dimethachlor CGA 102935	$C_{12}H_{13}NO_5$	[1]
124	Dimethachlor CGA 354742	$C_{13}H_{19}NO_5S$	[1]
125	Dimethachlor CGA 369873	$C_{10}H_{13}NO_4S$	[1]
126	Dimethachlor CGA 373464	$C_{12}H_{15}NO_6S$	1196157-87-5
127	Dimethachlor CGA 50266	$C_{13}H_{17}NO_4$	1086384-49-7
128	Dimethachlor SYN 528702	$C_{15}H_{21}NO_5S$	1228182-52-2
129	Dimethachlor SYN 530561	$C_{13}H_{17}NO_5$	1138220-18-4
130	Dimethenamid	$C_{12}H_{18}ClNO_2S$	87674-68-8
131	Dimethenamid M23	$C_{12}H_{17}NO_4S$	380412-59-9
132	Dimethenamid M27	$C_{12}H_{19}NO_5S_2$	205939-58-8
133	Dimethenamid-P M31	$C_{14}H_{21}NO_5S_2$	[1]
134	Dimethoate	$C_5H_{12}NO_3PS_2$	60-51-5
135	Dimethomorph	$C_{21}H_{22}ClNO_4$	113210-97-2
136	Dimoxystrobin	$C_{19}H_{22}N_2O_3$	149961-52-4
137	Dimoxystrobin 505M08 (BF 505-7)	$C_{19}H_{20}N_2O_5$	[1]
138	Dimoxystrobin 505M09 (BF 505-8)	$C_{19}H_{20}N_2O_5$	[1]
139	Diniconazole	$C_{15}H_{17}Cl_2N_3O$	83657-24-3
140	Diphenylamine	$C_{12}H_{11}N$	122-39-4
141	Disulfoton-sulfone	$C_8H_{19}O_4PS_3$	2497-06-5
142	Disulfoton-sulfoxide	$C_8H_{19}O_3PS_3$	2497-07-6
143	Ditalimfos	$C_{12}H_{14}NO_4PS$	5131-24-8
144	Diuron	$C_9H_{10}Cl_2N_2O$	330-54-1
145	Doxycycline	$C_{22}H_{24}N_2O_8$	564-25-0
146	Epoxiconazole	$C_{17}H_{13}ClFN_3O$	135319-73-2
147	Eprosartan	$C_{23}H_{24}N_2O_4S$	133040-01-4
148	Erythromycin	$C_{37}H_{67}NO_{13}$	114-07-8
149	Estrone	$C_{18}H_{22}O_2$	53-16-7
150	Ethenzamide	$C_9H_{11}NO_2$	938-73-8
151	Ethidimuron	$C_7H_{12}N_4O_3S_2$	30043-49-3
152	Ethion	$C_9H_{22}O_4P_2S_4$	563-12-2
153	Ethirimol	$C_{11}H_{19}N_3O$	23947-60-6
154	Ethofumesate	$C_{13}H_{18}O_5S$	26225-79-6
155	Ethoprophos	$C_8H_{19}O_2PS_2$	13194-48-4
156	Etofibrate	$C_{18}H_{18}ClNO_5$	31637-97-5
157	Fenamiphos sulfone	$C_{13}H_{22}NO_5PS$	31972-44-8
158	Fenarimol	$C_{17}H_{12}Cl_2N_2O$	60168-88-9
159	Fenazaquin	$C_{20}H_{22}N_2O$	120928-09-8
160	Fenbuconazole	$C_{19}H_{17}ClN_4$	114369-43-6
161	Fenhexamid	$C_{14}H_{17}Cl_2NO_2$	126833-17-8
162	Fenitrothion	$C_9H_{12}NO_5PS$	122-14-5
163	Fenobucarb	$C_{12}H_{17}NO_2$	3766-81-2
164	Fenofibrate	$C_{20}H_{21}ClO_4$	49562-28-9

#	Name	Formula	CAS Number
165	Fenoxaprop	$C_{16}H_{12}ClNO_5$	95617-09-7
166	Fenoxycarb	$C_{17}H_{19}NO_4$	72490-01-8
167	Fenpropidin	$C_{19}H_{31}N$	67306-00-7
168	Fenpropimorph	$C_{20}H_{33}NO$	67564-91-4
169	Fenpyroximate	$C_{24}H_{27}N_3O_4$	111812-58-9
170	Fenthion	$C_{10}H_{15}O_3PS_2$	55-38-9
171	Fipronil	$C_{12}H_4Cl_2F_6N_4OS$	120068-37-3
172	Flamprop	$C_{16}H_{13}ClFNO_3$	58667-63-3
173	Flazasulfuron	$C_{13}H_{12}F_3N_5O_5S$	104040-78-0
174	Flecainide	$C_{17}H_{20}F_6N_2O_3$	54143-55-4
175	Florasulam	$C_{12}H_8F_3N_5O_3S$	145701-23-1
176	Fluazifop	$C_{15}H_{12}F_3NO_4$	69335-91-7
177	Fluazinam	$C_{13}H_4Cl_2F_6N_4O_4$	79622-59-6
178	Flufenacet	$C_{14}H_{13}F_4N_3O_2S$	142459-58-3
179	Flufenacet ESA	$C_{11}H_{14}FNO_4S$	201668-32-8
180	Flufenoxuron	$C_{21}H_{11}ClF_6N_2O_3$	101463-69-8
181	Fluometuron	$C_{10}H_{11}F_3N_2O$	2164-17-2
182	Fluopicolide	$C_{14}H_8Cl_3F_3N_2O$	239110-15-7
183	Fluquinconazole	$C_{16}H_8Cl_2FN_5O$	136426-54-5
184	Fluroxypyr	$C_7H_5Cl_2FN_2O_3$	69377-81-7
185	Flurtamone	$C_{18}H_{14}F_3NO_2$	96525-23-4
186	Flusilazole	$C_{16}H_{15}F_2N_3Si$	85509-19-9
187	Foramsulfuron	$C_{17}H_{20}N_6O_7S$	173159-57-4
188	Gabapentin	$C_9H_{17}NO_2$	60142-96-3
189	Gabapentin-Lactam	$C_9H_{15}NO$	64744-50-9
190	Haloxyfop	$C_{15}H_{11}ClF_3NO_4$	69806-34-4
191	Heptenophos	$C_9H_{12}ClO_4P$	23560-59-0
192	Hexa(methoxymethyl)melamine	$C_{15}H_{30}N_6O_6$	3089-11-0
193	Hexaconazole	$C_{14}H_{17}Cl_2N_3O$	79983-71-4
194	Hexazinone	$C_{12}H_{20}N_4O_2$	51235-04-2
195	Hexythiazox	$C_{17}H_{21}ClN_2O_2S$	78587-05-0
196	Ifosfamide	$C_7H_{15}Cl_2N_2O_2P$	3778-73-2
197	Imazalil	$C_{14}H_{14}Cl_2N_2O$	35554-44-0
198	Imazapyr	$C_{13}H_{15}N_3O_3$	81334-34-1
199	Imazaquin	$C_{17}H_{17}N_3O_3$	81335-37-7
200	Imidaclopride	$C_9H_{10}ClN_5O_2$	138261-41-3
201	Indomethacin	$C_{19}H_{16}ClNO_4$	53-86-1
202	Indoxacarb	$C_{22}H_{17}ClF_3N_3O_7$	173584-44-6
203	Iodofenphos	$C_8H_8Cl_2IO_3PS$	18181-70-9
204	Iodosulfuron-methyl	$C_{14}H_{14}IN_5O_6S$	185119-76-0
205	Iohexol	$C_{19}H_{26}I_3N_3O_9$	66108-95-0
206	Iomeprol	$C_{17}H_{22}I_3N_3O_8$	78649-41-9
207	Iopromide	$C_{18}H_{24}I_3N_3O_8$	73334-07-3
208	Iprodione	$C_{13}H_{13}Cl_2N_3O_3$	36734-19-7
209	Iprovalicarb	$C_{18}H_{28}N_2O_3$	140923-17-7
210	Irbesartan	$C_{25}H_{28}N_6O$	138402-11-6
211	Irbesartan_446	$C_{25}H_{30}N_6O_2$	[1]
212	Isoprocarb	$C_{11}H_{15}NO_2$	2631-40-5
213	Isoproturon	$C_{12}H_{18}N_2O$	34123-59-6
214	Ketoprofen	$C_{16}H_{14}O_3$	22071-15-4
215	Ketotifen	$C_{19}H_{19}NOS$	34580-14-8
216	Kresoxim (BF 490-1)	$C_{17}H_{17}NO_4$	137169-29-0
217	Kresoxim-methyl	$C_{18}H_{19}NO_4$	143390-89-0
218	Lamotrigine N2-Oxide	$C_9H_7Cl_2N_5O$	136565-76-9
219	Linuron	$C_9H_{10}Cl_2N_2O_2$	330-55-2
220	Losartan	$C_{22}H_{23}ClN_6O$	114798-26-4
221	Malaoxon	$C_{10}H_{19}O_7PS$	1634-78-2
222	Malathion	$C_{10}H_{19}O_6PS_2$	121-75-5
223	Mecarbam	$C_{10}H_{20}NO_5PS_2$	2595-54-2
224	Mefenpyr-diethyl	$C_{16}H_{18}Cl_2N_2O_4$	135590-91-9
225	Mepanipyrim	$C_{14}H_{13}N_3$	110235-47-7
226	Mephosfolan	$C_8H_{16}NO_3PS_2$	950-10-7
227	Mepronil	$C_{17}H_{19}NO_2$	55814-41-0
228	Mesosulfuron-methyl	$C_{17}H_{21}N_5O_9S_2$	208465-21-8
229	Mestranol	$C_{21}H_{26}O_2$	72-33-3
230	Metalaxyl	$C_{15}H_{21}NO_4$	57837-19-1
231	Metalaxyl-M CGA 108906	$C_{14}H_{17}NO_6$	104390-56-9
232	Metalaxyl-M CGA 62826	$C_{14}H_{19}NO_4$	75596-99-5
233	Metamitron	$C_{10}H_{10}N_4O$	41394-05-2
234	Metamitron-desamino	$C_{10}H_9N_3O$	36993-94-9
235	Metazachlor	$C_{14}H_{16}ClN_3O$	67129-08-2
236	Metazachlor BH 479-11	$C_{15}H_{19}N_3O_2S$	[1]
237	Metazachlor BH 479-12	$C_{14}H_{13}N_3O_5$	[1]
238	Metazachlor BH 479-4	$C_{14}H_{15}N_3O_3$	1231244-60-2
239	Metazachlor BH 479-8	$C_{14}H_{17}N_3O_4S$	172960-62-2
240	Metazachlor BH 479-9	$C_{16}H_{19}N_3O_4S$	[1]
241	Metconazole	$C_{17}H_{22}ClN_3O$	125116-23-6
242	Methabenzthiazuron	$C_{10}H_{11}N_3O_S$	18691-97-9
243	Methidathion	$C_6H_{11}N_2O_4PS_3$	950-37-8
244	Methiocarb	$C_{11}H_{15}NO_2S$	2032-65-7
245	Methiocarb sulfoxide	$C_{11}H_{15}NO_3S$	2635-10-1
246	Methiocarb-sulfone	$C_{11}H_{15}NO_4S$	2179-25-1
247	Methoxyfenozide	$C_{22}H_{28}N_2O_3$	161050-58-4
248	Methylphenidate	$C_{14}H_{19}NO_2$	113-45-1

#	Name	Formula	CAS Number
249	Metobromuron	$C_9H_{11}BrN_2O_2$	3060-89-7
250	Metolachlor	$C_{15}H_{22}ClNO_2$	51218-45-2
251	Metolachlor CGA 354743	$C_{15}H_{23}NO_5S$	171118-09-5
252	Metolachlor CGA 357704	$C_{14}H_{17}NO_5$	1217465-10-5
253	Metolachlor CGA 37735	$C_{11}H_{15}NO_2$	97055-05-5
254	Metolachlor CGA 50267	$C_{12}H_{17}NO_2$	82508-03-0
255	Metolachlor CGA 50720	$C_{11}H_{13}NO_3$	152019-74-4
256	Metolachlor CGA 51202	$C_{15}H_{21}NO_4$	152019-73-3
257	Metolachlor NOA 413173	$C_{14}H_{19}NO_6S$	[1]
258	Metolcarb	$C_9H_{11}NO_2$	1129-41-5
259	Metoprolol	$C_{15}H_{25}NO_3$	51384-51-1
260	Metoprolol acid	$C_{14}H_{21}NO_4$	56392-14-4
261	Metosulam	$C_{14}H_{13}Cl_2N_5O_4S$	139528-85-1
262	Metoxuron	$C_{10}H_{13}ClN_2O_2$	19937-59-8
263	Metribuzin	$C_8H_{14}N_4OS$	21087-64-9
264	Metronidazole	$C_6H_9N_3O_3$	443-48-1
265	Metsulfuron-methyl	$C_{14}H_{15}N_5O_6S$	74223-64-6
266	Metyrapone	$C_{14}H_{14}N_2O$	54-36-4
267	Monalide	$C_{13}H_{18}ClNO$	7287-36-7
268	Monocrotophos	$C_7H_{14}NO_5P$	6923-22-4
269	Monodemethylisoproturon	$C_{11}H_{16}N_2O$	34123-57-4
270	Monolinuron	$C_9H_{11}ClN_2O_2$	1746-81-2
271	Monuron	$C_9H_{11}ClN_2O$	150-68-5
272	Myclobutanil	$C_{15}H_{17}ClN_4$	88671-89-0
273	N,N-Diethyltoluamide	$C_{12}H_{17}NO$	134-62-3
274	N,N-Dimethylaniline	$C_8H_{11}N$	121-69-7
275	Naphazoline	$C_{14}H_{14}N_2$	835-31-4
276	Napropamide	$C_{17}H_{21}NO_2$	15299-99-7
277	Naproxen	$C_{14}H_{14}O_3$	22204-53-1
278	N-Ethylaniline	$C_8H_{11}N$	103-69-5
279	N-Formyl-4-aminoantipyrin	$C_{12}H_{13}N_3O_2$	1672-58-8
280	Nicosulfuron	$C_{15}H_{18}N_6O_6S$	111991-09-4
281	N-Methyl-2-pyrrolidone	C_5H_9NO	872-50-4
282	N-Methylbenzene-sulfonamide	$C_7H_9NO_2S$	5183-78-8
283	Norethisterone acetate	$C_{22}H_{28}O_3$	51-98-9
284	Norflurazon	$C_{12}H_9ClF_3N_3O$	27314-13-2
285	Nuarimol	$C_{17}H_{12}ClFN_2O$	63284-71-9
286	Olmesartan	$C_{24}H_{26}N_6O_3$	144689-24-7
287	Omethoate	$C_5H_{12}NO_4PS$	1113-02-6
288	Oseltamivir	$C_{16}H_{28}N_2O_4$	196618-13-0
289	Oxadixyl	$C_{14}H_{18}N_2O_4$	77732-09-3
290	Oxasulfuron	$C_{17}H_{18}N_4O_6S$	144651-06-9
291	Oxazepam	$C_{15}H_{11}ClN_2O_2$	604-75-1
292	Oxydemeton-methyl	$C_6H_{15}O_5PS_2$	301-12-2
293	Oxytetracycline	$C_{22}H_{24}N_2O_9$	2058-46-0
294	Paraoxon	$C_{10}H_{14}NO_6P$	311-45-5
295	Paraoxon-methyl	$C_8H_{10}NO_6P$	950-35-6
296	Parathion	$C_{10}H_{14}NO_5PS$	56-38-2
297	Parathion-methyl	$C_8H_{10}NO_5PS$	298-00-0
298	Penconazole	$C_{13}H_{15}Cl_2N_3$	66246-88-6
299	Pencycuron	$C_{19}H_{21}ClN_2O$	66063-05-6
300	Pendimethalin	$C_{13}H_{19}N_3O_4$	40487-42-1
301	Pentoxifylline	$C_{13}H_{18}N_4O_3$	6493-05-6
302	Pethoxamid	$C_{16}H_{22}ClNO_2$	106700-29-2
303	Pethoxamid sulphonic acid (MET-42)	$C_{16}H_{23}NO_5S$	1329805-71-1
304	Phenacetin	$C_{10}H_{13}NO_2$	62-44-2
305	Phenanthridinon	$C_{13}H_9NO$	1015-89-0
306	Phenazone	$C_{11}H_{12}N_2O$	60-80-0
307	Phenmedipham	$C_{16}H_{16}N_2O_4$	13684-63-4
308	Phenthoate	$C_{12}H_{17}O_4PS_2$	2597-03-7
309	Phenylalanine	$C_9H_{11}NO_2$	150-30-1
310	Phenylethylmalonamide	$C_{11}H_{14}N_2O_2$	7206-76-0
311	Phosalone	$C_{12}H_{15}ClNO_4PS_2$	2310-17-0
312	Phosphamidon	$C_{10}H_{19}ClNO_5P$	13171-21-6
313	Phoxim	$C_{12}H_{15}N_2O_3PS$	14816-18-3
314	Picloram	$C_6H_3Cl_3N_2O_2$	1918-02-1
315	Picolinafen	$C_{19}H_{12}F_4N_2O_2$	137641-05-5
316	Picoxystrobin	$C_{18}H_{16}F_3NO_4$	117428-22-5
317	Pilocarpine	$C_{11}H_{16}N_2O_2$	92-13-7
318	Pindolol	$C_{14}H_{20}N_2O_2$	13523-86-9
319	Piperophos	$C_{14}H_{28}NO_3PS_2$	24151-93-7
320	Pirimicarb	$C_{11}H_{18}N_4O_2$	23103-98-2
321	Pirimiphos-ethyl	$C_{13}H_{24}N_3O_3PS$	23505-41-1
322	Pirimiphos-methyl	$C_{11}H_{20}N_3O_3PS$	29232-93-7
323	Pregabalin	$C_8H_{17}NO_2$	148553-50-8
324	Prilocaine	$C_{13}H_{20}N_2O$	721-50-6
325	Primidone	$C_{12}H_{14}N_2O_2$	125-33-7
326	Primisulfuron-methyl	$C_{15}H_{12}F_4N_4O_7S$	86209-51-0
327	Prochloraz	$C_{15}H_{16}Cl_3N_3O_2$	67747-09-5
328	Procymidone	$C_{13}H_{11}Cl_2NO_2$	32809-16-8
329	Profenofos	$C_{11}H_{15}BrClO_3PS$	41198-08-7
330	Promecarb	$C_{12}H_{17}NO_2$	2631-37-0
331	Prometon	$C_{10}H_{19}N_5O$	1610-18-0
332	Propamocarb	$C_9H_{20}N_2O_2$	24579-73-5

#	Name	Formula	CAS Number
333	Propaquizafop	$C_{22}H_{22}ClN_3O_5$	111479-05-1
334	Propazine	$C_9H_{16}ClN_5$	139-40-2
335	Propazine-2-hydroxy	$C_9H_{17}N_5O$	7374-53-0
336	Propetamphos	$C_{10}H_{20}NO_4PS$	31218-83-4
337	Propiconazole	$C_{15}H_{17}Cl_2N_3O_2$	60207-90-1
338	Propoxur	$C_{11}H_{15}NO_3$	114-26-1
339	Propranolol	$C_{16}H_{21}NO_2$	13013-17-7
340	Propyphenazone	$C_{14}H_{18}N_2O$	479-92-5
341	Prosulfocarb	$C_{14}H_{21}NOS$	52888-80-9
342	Prosulfuron	$C_{15}H_{16}F_3N_5O_4S$	94125-34-5
343	Pyridaben	$C_{19}H_{25}ClN_2OS$	96489-71-3
344	Pyridate	$C_{19}H_{23}ClN_2O_2S$	55512-33-9
345	Pyrifenox	$C_{14}H_{12}Cl_2N_2O$	88283-41-4
346	Pyriproxyfen	$C_{20}H_{19}NO_3$	95737-68-1
347	Pyroquilon	$C_{11}H_{11}NO$	57369-32-1
348	Quinmerac	$C_{11}H_8ClNO_2$	90717-03-6
349	Quinmerac BH 518-2	$C_{11}H_6ClNO_4$	90717-07-0
350	Quinoline	C_9H_7N	91-22-5
351	Quinoxyfen	$C_{15}H_8Cl_2FNO$	124495-18-7
352	Rimsulfuron	$C_{14}H_{17}N_5O_7S_2$	122931-48-0
353	Ritalinic acid	$C_{13}H_{17}NO_2$	19395-41-6
354	Ronidazol	$C_6H_8N_4O_4$	7681-76-7
355	Roxithromycin	$C_{41}H_{76}N_2O_{15}$	80214-83-1
356	Schradan	$C_8H_{24}N_4O_3P_2$	152-16-9
357	Sebuthylazine	$C_9H_{16}ClN_5$	7286-69-3
358	Sebuthylazine-desethyl	$C_7H_{12}ClN_5$	37019-18-4
359	Simazine	$C_7H_{12}ClN_5$	122-34-9
360	Simazine-2-hydroxy	$C_7H_{13}N_5O$	2599-11-3
361	Simeton	$C_8H_{15}N_5O_1$	673-04-1
362	Simetryn	$C_8H_{15}N_5S$	1014-70-6
363	Sitagliptin	$C_{16}H_{15}F_6N_5O$	486460-32-6
364	S-Metolachlor Metabolite CGA 368208	$C_{11}H_{15}NO_4S$	1173021-76-5
365	Sotalol	$C_{12}H_{20}N_2O_3S$	3930-20-9
366	Spiroxamine	$C_{18}H_{35}NO_2$	118134-30-8
367	Sulfadiazine	$C_{10}H_{10}N_4O_2S$	68-35-9
368	Sulfadimidine	$C_{12}H_{14}N_4O_2S$	57-68-1
369	Sulfamerazine	$C_{11}H_{12}N_4O_2S$	127-79-7
370	Sulfamethoxazole	$C_{10}H_{11}N_3O_3S$	723-46-6
371	Sulfathiazole	$C_9H_9N_3O_2S_2$	72-14-0
372	Sulpirid	$C_{15}H_{23}N_3O_4S$	15676-16-1
373	Sulpiride N-Oxide	$C_{15}H_{23}N_3O_5S$	[1]
374	Swep	$C_8H_7Cl_2NO_2$	1918-18-9

#	Name	Formula	CAS Number
375	TCMTB	$C_9H_6N_2S_3$	21564-17-0
376	Tebuconazol	$C_{16}H_{22}ClN_3O$	107534-96-3
377	Tebufenpyrad	$C_{18}H_{24}ClN_3O$	119168-77-3
378	Tebutam	$C_{15}H_{23}NO$	35256-85-0
379	Telmisartan	$C_{33}H_{30}N_4O_2$	144701-48-4
380	Terbuthylazin-desethyl-2-hydroxy	$C_7H_{13}N_5O$	66753-06-8
381	Terbuthylazine	$C_9H_{16}ClN_5$	5915-41-3
382	Terbutryn	$C_{10}H_{19}N_5S$	886-50-0
383	Terbutylazin 1 SYN 545666	$C_8H_{14}N_4O_2$	[1]
384	Terbutylazin 2 CGA 324007	$C_7H_{12}N_4O_2$	309923-18-0
385	Tetraconazole	$C_{13}H_{11}Cl_2F_4N_3O$	112281-77-3
386	Tetramethylurea	$C_5H_{12}N_2O$	632-22-4
387	Thiacloprid	$C_{10}H_9ClN_4S$	111988-49-9
388	Thiamethoxam	$C_8H_{10}ClN_5O_3S$	153719-23-4
389	Thifensulfuron-methyl	$C_{12}H_{13}N_5O_6S_2$	79277-27-3
390	Tolfenamic acid	$C_{14}H_{12}ClNO_2$	13710-19-5
391	Topramezone	$C_{16}H_{17}N_3O_5S$	210631-68-8
392	Tramadol	$C_{16}H_{25}NO_2$	27203-92-5
393	Tramadol N-Oxide	$C_{16}H_{25}NO_3$	147441-56-3
394	trans-10,11-Dihydro-10,11-dihydroxy Carbamazepine	$C_{15}H_{14}N_2O_3$	58955-93-4
395	Triadimenol	$C_{14}H_{18}ClN_3O_2$	89482-17-7
396	Triallate	$C_{10}H_{16}Cl_3NOS$	2303-17-5
397	Triasulfuron	$C_{14}H_{16}ClN_5O_5S$	82097-50-5
398	Triazophos	$C_{12}H_{16}N_3O_3PS$	24017-47-8
399	Triethyl phosphate	$C_6H_{15}O_4P$	78-40-0
400	Trifloxistrobin CGA 321113	$C_{19}H_{17}F_3N_2O_4$	252913-85-2
401	Trifloxistrobin NOA 413161	$C_{19}H_{15}F_3N_2O_6$	[1]
402	Trifloxystrobin	$C_{20}H_{19}F_3N_2O_4$	141517-21-7
403	Triflusulfuron-methyl	$C_{17}H_{19}F_3N_6O_6S$	126535-15-7
404	Trimethoprim	$C_{14}H_{18}N_4O_3$	738-70-5
405	Tritosulfuron	$C_{13}H_9F_6N_5O_4S$	142469-14-5
406	Tritosulfuron BH 635-4	$C_{10}H_{10}F_3N_5O_4S$	[1]
407	Tritosulfuron BH 635-5	$C_5H_5F_3N_4O$	5311-05-7
408	Valsartan	$C_{24}H_{29}N_5O_3$	137862-53-4
409	Valsartan acid	$C_{14}H_{10}N_4O_2$	164265-78-5
410	Warfarin	$C_{19}H_{16}O_4$	81-81-2
411	Xanthone	$C_{13}H_8O_2$	90-47-1

[1]: For substances with missing CAS number, the smiles code is given in **Table S-2**

Table of contents

Table S-2. Smiles code for target compounds with missing CAS numbers

#[1)]	Name	Formula	Smiles code
123	Dimethachlor CGA 102935	$C_{12}H_{13}NO_5$	Cc1cccc(c1N(CC(=O)O)C(=O)C(=O)O)C
124	Dimethachlor CGA 354742	$C_{13}H_{19}NO_5S$	Cc1cccc(c1N(CCOC)C(=O)CS(=O)(=O)O)C
125	Dimethachlor CGA 369873	$C_{10}H_{13}NO_4S$	Cc1cccc(c1NC(=O)CS(=O)(=O)O)C
133	Dimethenamid-P M31	$C_{14}H_{21}NO_5S_2$	Cc1csc(c1N(C(C)COC)C(=O)CS(=O)CC(=O)O)C
137	Dimoxystrobin 505M08 (BF 505-7)	$C_{19}H_{20}N_2O_5$	Cc1ccc(c(c1)OCc2ccccc2/C(=N\OC)/C(=O)NC) C(=O)O
138	Dimoxystrobin 505M09 (BF 505-8)	$C_{19}H_{20}N_2O_5$	CNC(=O)C(=N\OC)\c1ccccc1COc1cc(ccc1C)C(O)=O
211	Irbesartan_446	$C_{25}H_{30}N_6O_2$	CCCCC(=O)NC1(CCCC1)C(=O) NCc2ccc(cc2)c3ccccc3c4[nH]nnn4
236	Metazachlor BH 479-11	$C_{15}H_{19}N_3O_2S$	Cc1cccc(C)c1N(Cn1cccn1)C(=O)CS(C)=O
237	Metazachlor BH 479-12	$C_{14}H_{13}N_3O_5$	Cc1cccc(C(O)=O)c1N(Cn1cccn1)C(=O)C(O)=O
240	Metazachlor BH 479-9	$C_{16}H_{19}N_3O_4S$	Cc1cccc(C)c1N(Cn1cccn1)C(=O)CS(=O)CC(O)=O
257	Metolachlor NOA 413173	$C_{14}H_{19}NO_6S$	CCc1cccc(c1N(C(C)C(=O)O)C(=O)CS(=O)(=O)O)C
373	Sulpiride N-Oxide	$C_{15}H_{23}N_3O_5S$	CC[N+]1(CCCC1CNC(=O)C2=C (C=CC(=C2)S(=O)(=O)N)OC)[O-]
383	Terbutylazin 1 SYN 545666	$C_8H_{14}N_4O_2$	CC(C)(C)Nc1[nH]c(=O)n(c(=O)n1)C
401	Trifloxystrobin NOA 413161	$C_{19}H_{15}F_3N_2O_6$	CO\N=C(\C(O)=O)c1ccccc1CO\N=C (/C(O)=O)c1cccc(c1)C(F)(F)F
406	Tritosulfuron BH 635-4	$C_{10}H_{10}F_3N_5O_4S$	NC(=O)NC(=N)NC(=O)NS(=O)(=O)c1ccccc1C(F)(F)F

[1)]: Numbers taken from **Table S-1**

Table of contents

Table S-3. LC-MS acquisition method

Name	
LC System	LC20 series Shimadzu
LC column	Zorbax Eclipse Plus C18 (2.1 x 150 mm, 3.5 µm) Agilent
Mobile phase A	Ultrapure water + 0.1 % v/v formic acid
Mobile phase B	Acetonitrile + 0.1 % v/v formic acid
Gradient (%B)	0 min (2%), 1 min (2%), 2 min (20%), 16.5 min (100%), 27 min (100%), 27.1 min (2%), 37 min (2%)
Flow rate	0.3 mL/min
Temperature	40 °C
Sample injection volume	95 µL
Internal standard injection volume	5 µL
MS System	TripleTOF™ 5600 (Sciex)
Ion source	DuoSpray Ion Source
Mass range	m/z 100 - 1200
Survey scan accumulation time	250 ms
Cycle time	ca. 1.1 sec[1)]
Ion Source Gas 1	35 psi
Ion Source Gas 2	45 psi
Curtain Gas	40 psi
Source Temperature	550 °C
IonSpray Voltage Floating	5500 V
Declustering Potential	60 V
Collision Energy	10 eV (for MS mode)

[1)]: In addition to MS, also MS^2 experiments have been performed (data dependent acquisition as well as data independent acquisition - SWATH™). The results of the study, however, are only based on the LC-MS data (survey scan). MS^2 acquisition was conducted to receive realistic cycle times comparable to approaches used in reality (where MS^2 is of great interest)

Table of contents

Table S-4. List of isotope-labeled standards (IS)

Name	Formula	Retention time [min]	Concentration[1)] [µg L^{-1}]
Benzotriazole D4	C_6 H N_3 $^2H_4$	5.5	10.0
Chloridazon D5	C_{10} H_3 Cl N_3 O $^2H_5$	6.4	0.20
Propazine D6	C_9 H_{10} Cl N_5 $^2H_6$	10.7	0.20
Diuron D6	C_9 H_4 Cl_2 N_2 O $^2H_6$	9.6	0.60
Lidocaine D10	C_{14} H_{12} N_2 O $^2H_{10}$	5.3	0.10
Sotalol D6	C_{12} H_{14} N_2 O_3 S $^2H_6$	4.5	0.40
Hydrochlorothiazide 13C, D2	C_6 H_6 Cl N_3 O_4 S_2 ^{13}C $^2H_2$	5.1	40.0
Diazinon D10	C_{12} H_{11} N_2 O_3 P S $^2H_{10}$	13.7	0.10
Sulfadimethoxine D6	C_{12} H_8 N_4 O_4 S $^2H_6$	7.5	0.40
Azoxystrobin D4	C_{22} H_{13} N_3 O_5 $^2H_4$	11.5	0.10
Irbesartan D4	C_{25} H_{24} N_6 O $^2H_4$	8.7	0.40
Bicalutamide D4	C_{18} H_{10} F_4 N_2 O_4 S $^2H_4$	10.7	0.50
Darunavir D9	C_{27} H_{28} N_3 O_7 S $^2H_9$	10.2	20.0

[1)]: Due to varying ionization efficiency, different concentrations were used to receive similar signal abundances

Table of contents

Table S-5. Parameters for data processing (*workflow LW_V2.0*)

Software package	Parameter	Value
MarkerView™ (1.2.1)	**Peak finding**	
	Minimum retention time	3.5 min
	Maximum retention time	19.0 min
	Subtraction offset	6 scans
	Subtraction multiple factor	1.3
	Noise threshold	25 cps
	Minimum spectral peak width	20 ppm
	Minimum RT peak width	3 scans
	Assign charge states	Enabled
	Peak alignment	
	Retention time tolerance	0.15 min
	Mass tolerance	20 ppm
	Intensity threshold	100 cps
MultiQuant™ 2.1.2 + Research Feature Software (Jan 2017)	**Peak integration by MQ4 algorithm**	
	Gaussian Smooth Width	1.0 points
	RT Half Window	9 sec
	Update Expected RT	No
	Report Largest Peak	No
	Min. Peak Width	6 points
	Min. Peak Height	100
	Noise Percentage	90.0%
	Baseline Sub. Window	0.3 min
	Peak Splitting	2
	Peak integration by Summation (SUM) algorithm	
	Gaussian Smooth Width	1.0 points
	Summation Window	15 sec
	Noise% for Baseline	-1[1)]
	Recentering	3.0
	Adjust Endpoints to Local Minima	Yes

Parameters for peak finding and peak alignment were optimized in a former study (data not shown).

[1)]: Option which is exclusively available in the research version of MultiQuant™, the data point with the smallest intensity within the summation window is used to fit the horizontal baseline of the peak

Table of contents

Table S-6. Optimized parameters for EIC filtering (*workflow LW_V2.0*)

Software package	Parameter	Value			
		min	max	RSD[1)]	SD[1)]
Matlab R2016b	**MQ4 algorithm**				
	(1) Expected RT[2)] [min]	**3.5**	**19**	-	-
	(2) Peak Area [cts]	**700**	**Inf**	0.50	-
	(3) Peak Height [cps]	**200**	**Inf**	0.45	-
	(4) Centroid RT[3)] [min]	**3.5**	**19**	-	0.07
	(5) Peak Width (FWHM) [min]	0.045	0.250	-	0.06
	(6) Baseline Delta[4)] [ ]	0	0.35	-	0.25
	(7) Apex RT[5)] [min]	**3.5**	**19**	-	0.08
	(8) Δ (Expected RT, Centroid RT) [min]	**-0.15**	**0.15**	-	0.08
	(9) Δ (Expected RT, Apex RT) [min]	**-0.15**	**0.15**	-	0.08
	(10) Δ (Centroid RT, Apex RT) [min]	-0.04	0.04	-	0.05
	Summation (SUM) algorithm				
	(11) Expected RT[2)] [min]	**3.5**	**19**	-	-
	(12) Peak Area [cts]	**700**	**Inf**	0.60	-
	(13) Peak Height [cps]	**200**	**Inf**	0.50	-
	(14) Centroid RT[3)] [min]	**3.5**	**19**	-	0.07
	(15) Peak Width (FWHM) [min]	0.050	0.250	-	0.06
	(16) Apex RT[5)] [min]	**3.5**	**19**	-	0.07
	(17) Δ(Expected RT, Centroid RT) [min]	**-0.15**	**0.15**	-	0.07
	(18) Δ(Expected RT, Apex RT) [min]	**-0.15**	**0.15**	-	0.07
	(19) Δ(Centroid RT, Apex RT) [min]	-0.04	0.04		0.06
	Between both algorithms				
	(20) Δ(Centroid RT MQ4, SUM) [min]	-0.06	0.06	-	0.05
	(21) Δ(Apex RT MQ4, SUM) [min]	-0.10	0.10	-	0.07
	(22) Δ(Peak Width MQ4, SUM) [min]	-0.09	0.09	-	0.07
	(23) Δ_{rel}(Peak Height MQ4, SUM)[6)] [ ]	-0.30	0.55	-	0.40

[1)]: Both the RSD and the SD are calculated across the triplicates; *note: RSD is dimensionless*

[2)]: Expected RT: initially set retention time value for a feature prior to integration (taken from peak alignment)

[3)]: Centroid RT: intensity weighted average retention time across a chromatographic peak (analogous to centroid mass)

[4)]: Baseline Delta: height difference of the baseline (at start and end of the peak) to the actual peak height

[5)]: Apex RT: retention time value reported for the most abundant data point across a chromatographic peak

[6)]: Δ_{rel} = (Peak Height (MQ4) - Peak Height (SUM)) / mean(Peak Height (MQ4), Peak Height (SUM))

bold printed: parameters were defined and not derived from the training data set; either empiric (e.g. peak height) or already determined by other settings (e.g. +/- 0.15 min taken from peak alignment)

Note: due to inadequate noise estimation in the MultiQuant software, the signal-to-noise ratio was not considered as a useful filter.

Componentization was conducted within 0.15 min and 20 ppm tolerances for the following species: 1st and 2nd isotope, $[M+Na]^+$, $[M+K]^+$, $[M+NH_4]^+$, $[M+CH_3CN+H]^+$, $[2M+H]^+$, $[2M+Na]^+$, $[2M+K]^+$, $[2M+NH_4]^+$.

Table of contents

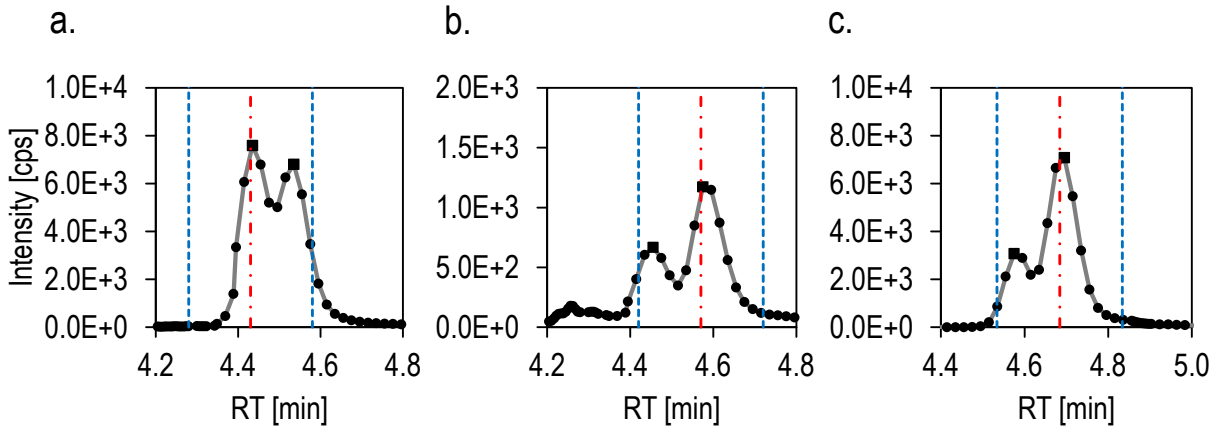

Figure S-1. Problem cases occurring during peak alignment. The smaller peak was not listed in the final peak list as the retention time tolerance during peak alignment (indicated by blue lines +/- of detected apex) includes the apex of the smaller peak. a. **Aminocarb** (2nd) and Pilocarpine (both $C_{11}H_{16}N_2O_2$), b. **N,N-Dimethylaniline** (1st) and N-Ethylaniline (both $C_8H_{11}N$), c. Simazine-2-hydroxy (2nd) and **Terbuthylazine-desethyl-2-hydroxy** (both $C_7H_{13}N_5O$), bold printed compounds were missed due to peak alignment.

Table of contents

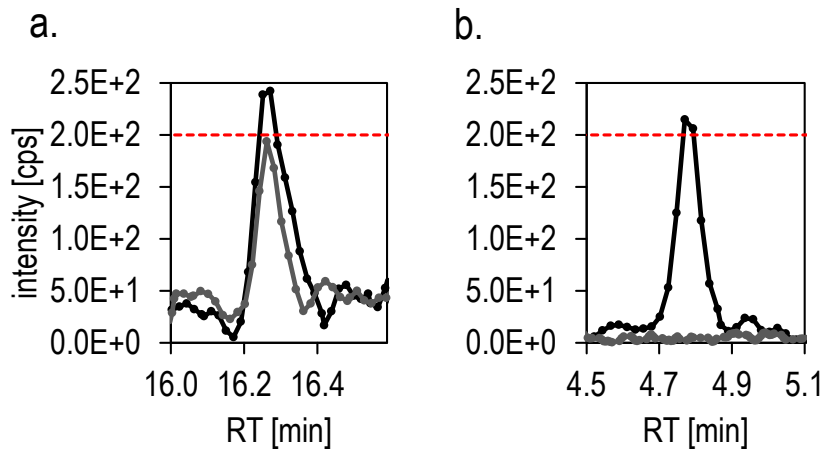

Figure S-2. Examples which emphasize possible misinterpretations that would occur if the fc calculations were conducted using a. the optimistic or b. the pessimistic view. Extracted ion chromatograms (EIC) of the influent (black) and effluent (grey) sample of a treatment process. The intensity threshold is indicated by the dashed lines.

Table of contents

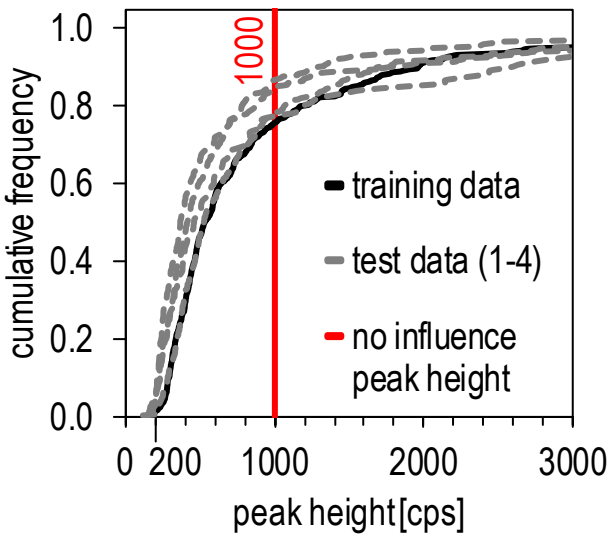

Figure S-3. Cumulative intensity distribution of the training data and the test data (sample 1-4). The "no influence peak height" of 1000 cps is depicted by the red line.

Table of contents

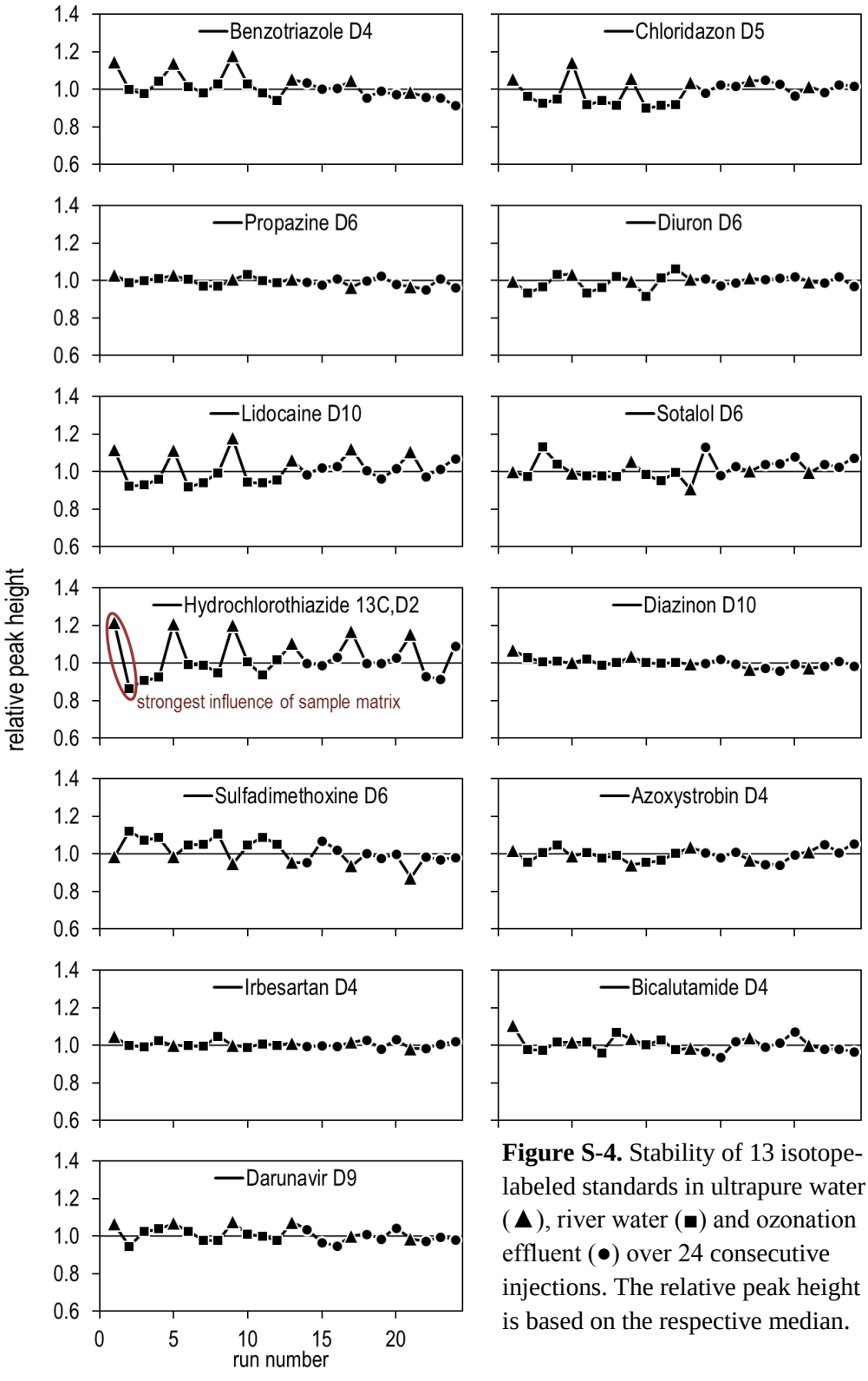

Figure S-4. Stability of 13 isotope-labeled standards in ultrapure water (▲), river water (■) and ozonation effluent (●) over 24 consecutive injections. The relative peak height is based on the respective median.

Table of contents

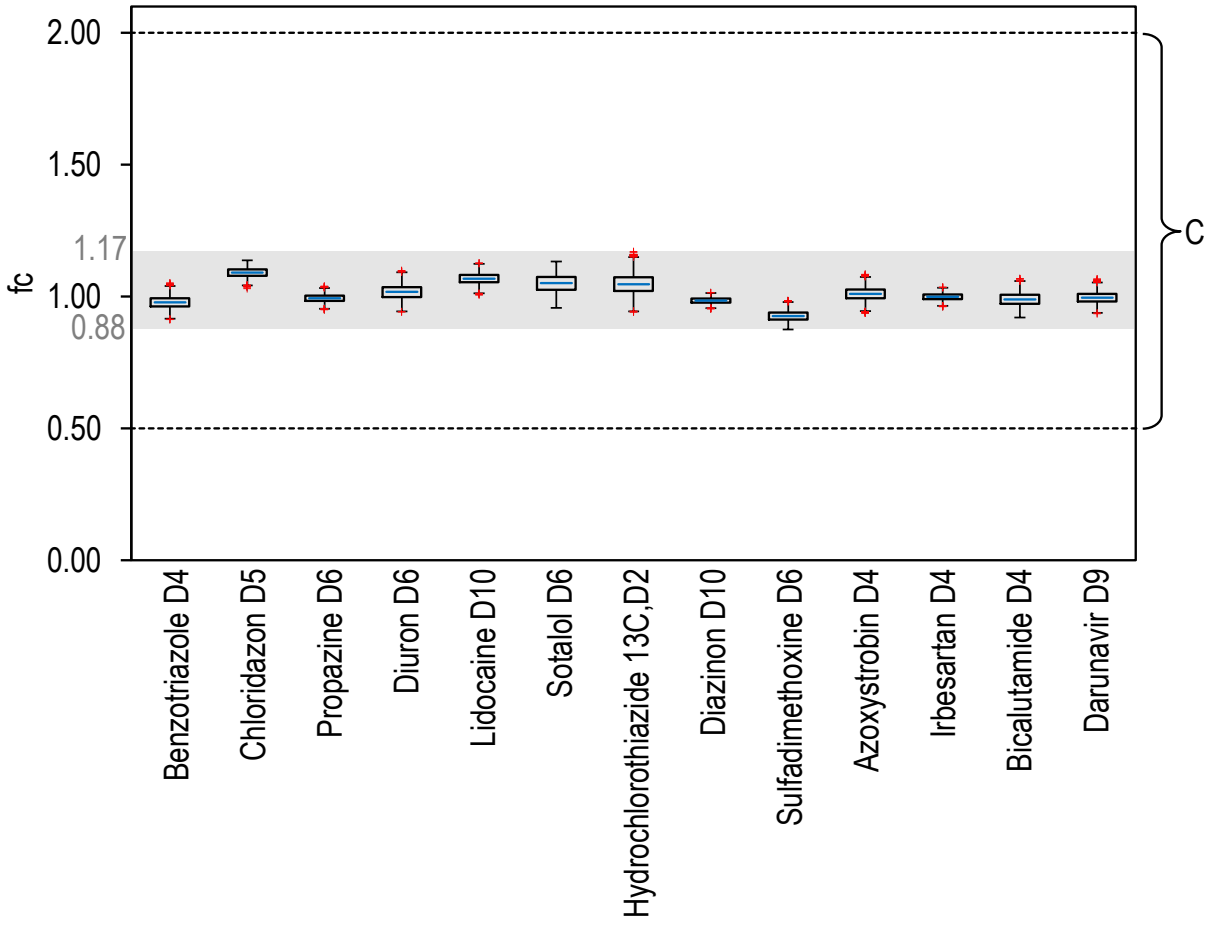

Figure S-5. Boxplots of the fold changes (fc) for the spiked isotope-labeled standards (IS) determined for all pairwise comparisons of triplicates (here: 7056 comparisons for each standard) between the influent (river water) and effluent sample (ozonation effluent) of the process. The intervals for the group *consistency* (C) are indicated by the dashed lines, the minimum (fc_{min} = 0.88) and maximum (fc_{max} = 1.17) value of the fold changes across all IS are emphasized by the grey rectangle. Boxes: 25th and 75th percentiles (q_1 and q_3), max whisker length: 1.5 (q_3-q_1), blue line: median value, red plus: outlier.
Note that the blank correction was omitted (IS also spiked to blanks) in order to illustrate the system stability and the low impact of matrix effects on the classification.

Table of contents

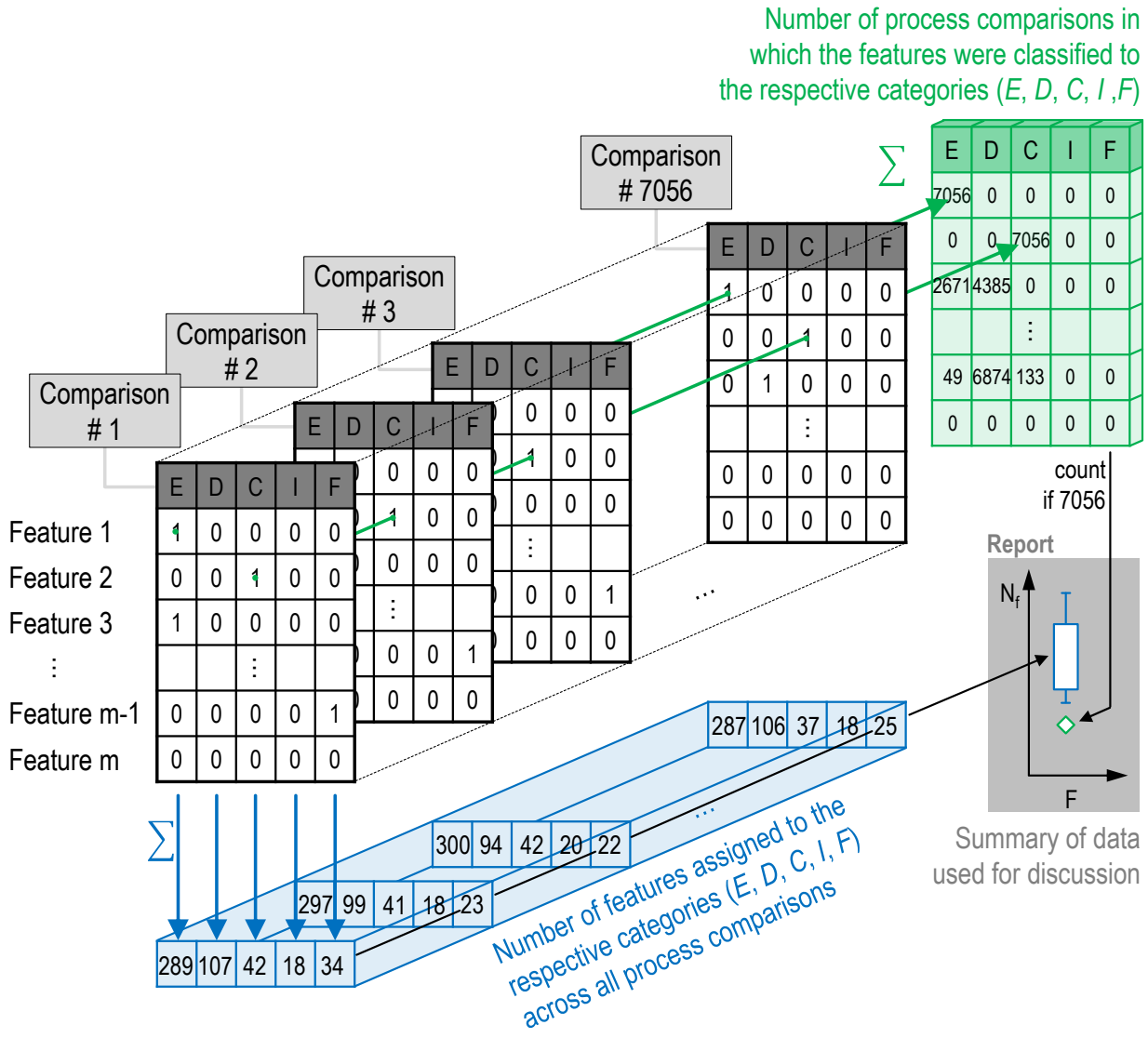

Figure S-6. Data processing strategy for assessing the repeatability of the process comparisons. For each process comparison, each feature was assigned to one respective class (*elimination E*, *decrease D*, *consistency C*, *increase I*, *formation F*) which is indicated by the binary numbers. Blue: sum of all features assigned to the respective category across all comparisons. The distributions of the feature numbers assigned to one certain class (here shown for *F*) were depicted by the boxplots (**Figure 5** in main article). Green: For each single feature, the number of process comparisons (here 7056) were tracked during data processing. Features which were always (across all possible comparison) assigned to one category were counted and additionally considered for the evaluation (green diamond).

Table of contents

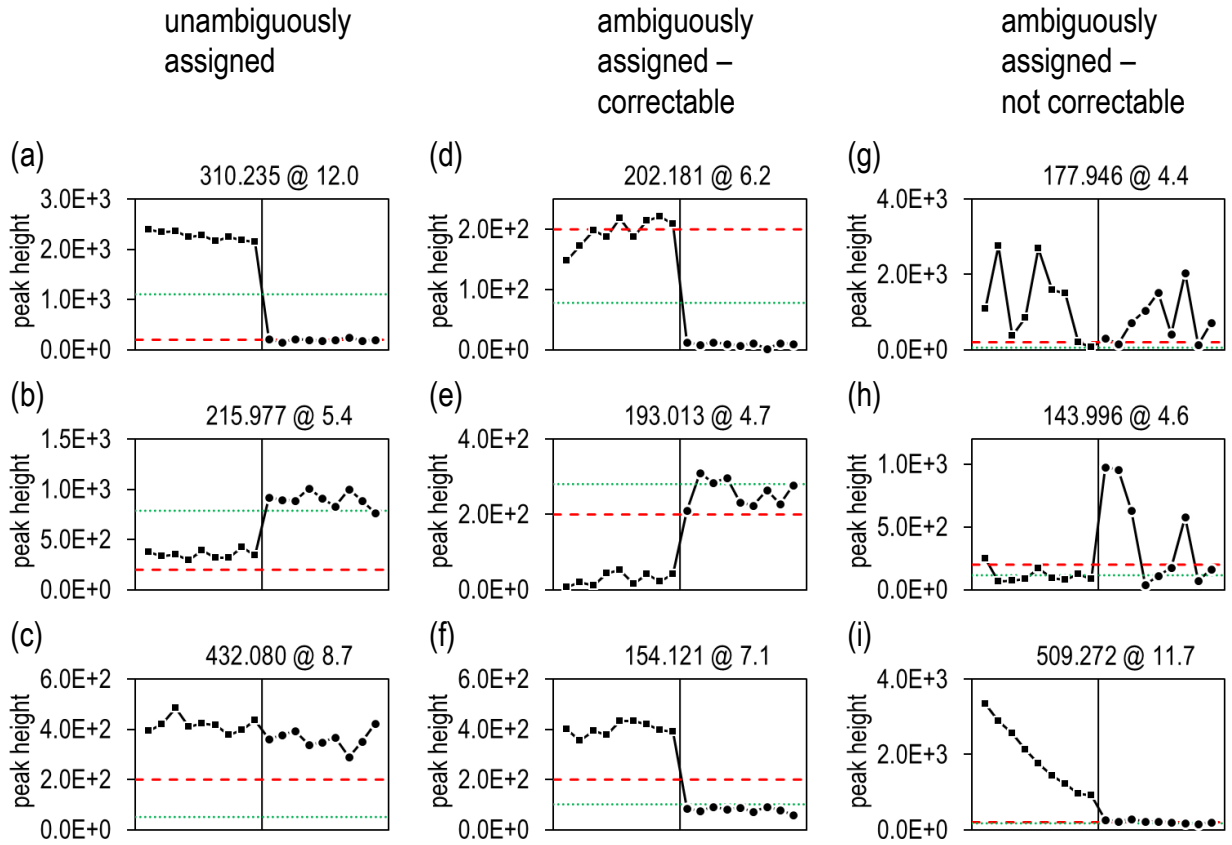

Figure S-7. Selected peak profiles from the ninefold injections of river water (■) and ozonation effluent (●) to illustrate the classification problems using the combinatorial approach. Red dashed line: intensity threshold (200 cps), green dotted line: threshold for blank correction (5 times the blank height).

- Signals unambiguously assigned (in all 7056 comparisons) to:

(a) *elimination*

(b) *increase*

(c) *consistency*

- Signals ambiguously (but correctable) assigned to multiple categories due to:

(d) some influent replicates below / above intensity threshold → feature assigned to *elimination* / *rejection*

(e) some effluent replicates below / above the blank threshold → feature assigned to *formation* / *rejection*

(f) fold change (fc) between sample triplicates of influent and effluent slightly below / above the 0.2 fc limit → feature assigned to *elimination* / *decrease*

- Signals ambiguously (and not correctable) assigned to multiple categories due to:

(g, h) implausible intensity profiles of real peaks; some triplicates fulfill all filter criteria and are thus not always rejected → feature assigned to multiple categories

(i) trend of peak height during analysis, some triplicates (e.g. Influent #1 #2 #3) fulfill the filtering criteria whereas others (e.g. #1 #2 #9) do not → feature assigned to multiple categories.

Table of contents

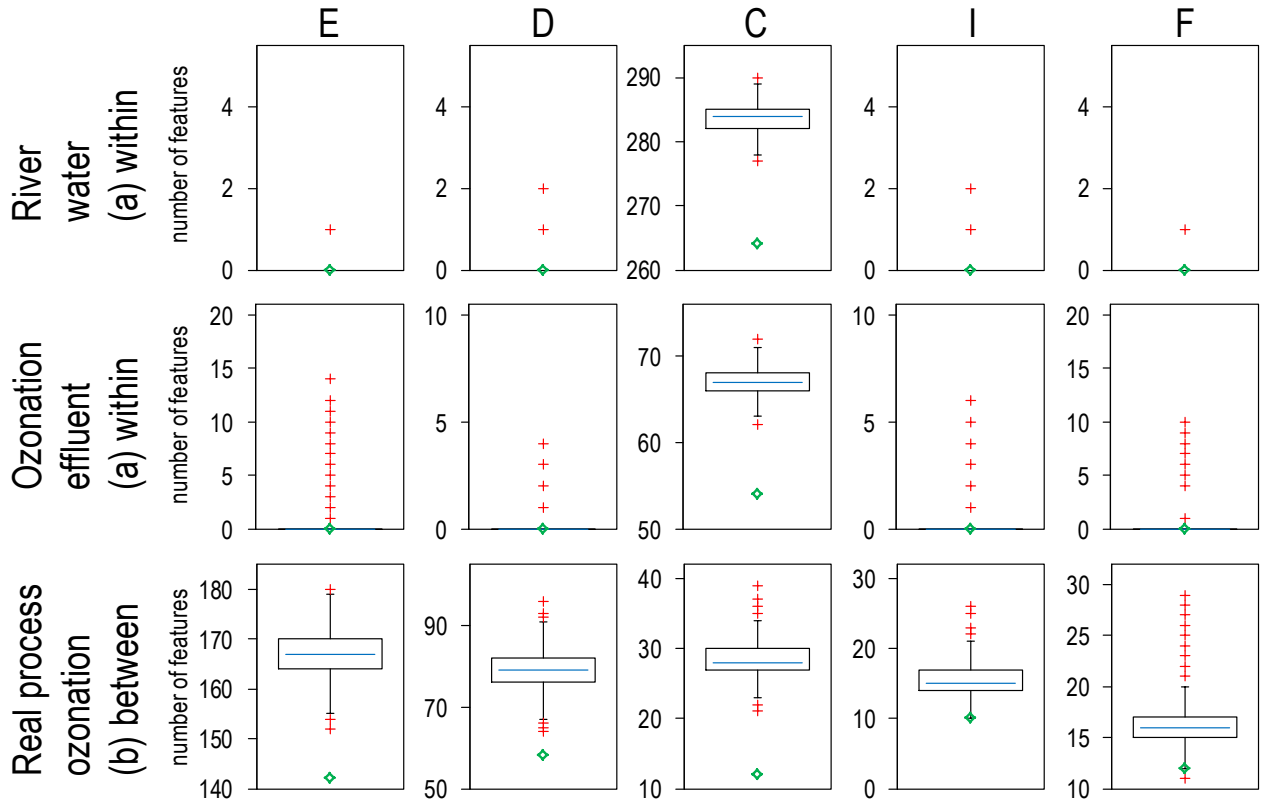

Figure S-8. Boxplots of feature numbers assigned to: *E elimination*, *D decrease*, *C consistency*, *I: increase* or *F formation*. The first and second line shows the within sample comparisons (840 comparisons). The third line shows the between sample comparisons of the real process of ozonation (7056 comparisons). Boxes: 25th and 75th percentiles (q_1 and q_3), max whisker length: 1.5 (q_3-q_1), blue line: median value, red plus: outlier, green diamond: features unambiguously assigned to this group.

Table of contents

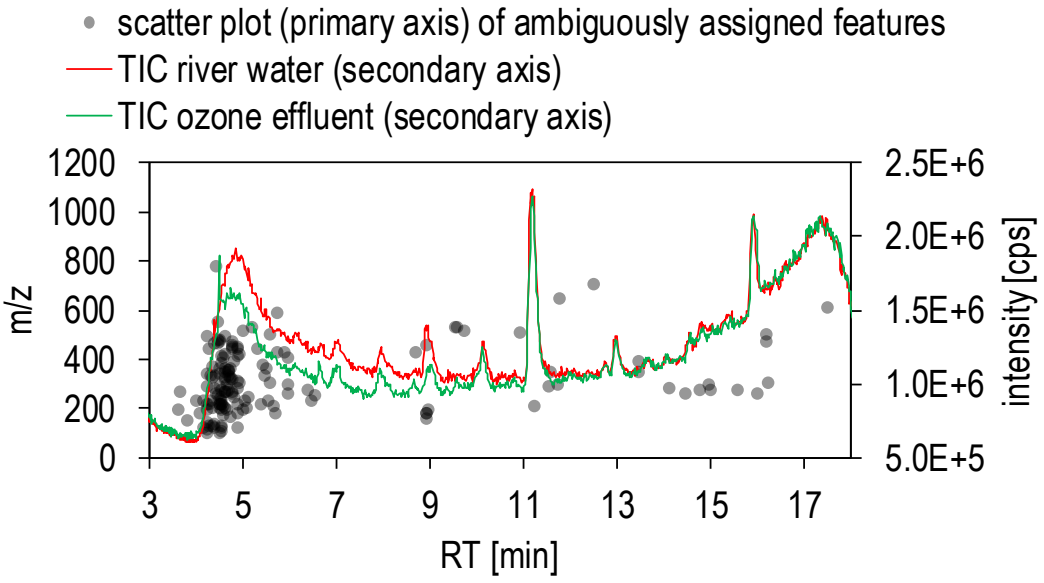

Figure S-9. m/z-RT-scatterplot (primary axis) of all features which are ambiguously assigned to multiple categories and superimposed line plots (secondary axis) of the total ion chromatograms (TIC) of river water and effluent of ozonation.

Table of contents