

図 1-4. ホルムアルデヒド-DNPH 誘導体の検量線

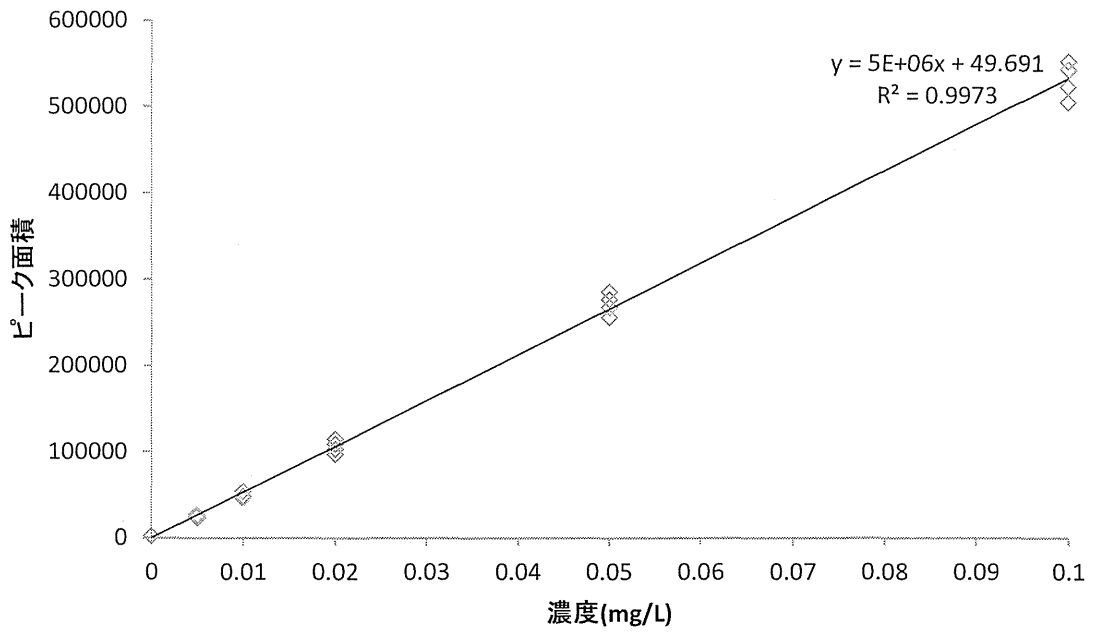


図 1-5. アセトアルデヒド-DNPH 誘導体の検量線

表 1-2. 添加回収試験の結果

測定対象物質	添加濃度 (mg/L)	回収率 (%)						併行精度 (RSD%)
		試料 1	試料 2	試料 3	試料 4	試料 5	平均値	
ホルムアルデヒド	0.08	108	109	112	112	111	110	2
	0.008	92	86	95	94	91	91	3
アセトアルデヒド	0.08	103	107	107	109	108	107	2
	0.008	110	106	107	106	109	108	2

表 2-1. 非イオン界面活性剤のFIA/MSスペクトル

ポリマー部 (n数)	マススペクトル* (m/z)					
	AE1-20	NPE	OPE	PEG	PPG	専用水道
	[M+23] ⁺	[M+23] ⁺	[M+23] ⁺	[M+23] ⁺	[M+23] ⁺	原水・浄水
0	165	243	229	85	99	-
1	209	310	273	129	157	-
2	253	331	317	173	215	-
3	297	375	361	217	273	-
4	341	419	405	261	331	331
5	385	463	449	305	389	389
6	429	507	538	349	447	447
7	473	552	582	393	505	505
8	518	596	626	437	564	564
9	562	640	670	481	622	622
10	606	684	714	525	680	680
11	650	728	-	570	738	738
12	694	772	-	614	796	796
13	738	816	-	658	854	854
14	782	860	-	702	912	912
15	826	904	-	746	970	-
16	870	-	-	790	1028	-
17	914	-	-	834	1086	-
18	958	-	-	878	1144	-
19	1002	-	-	922	1202	-
20	1046	-	-	966	1260	-
21	1090	-	-	1010	1318	-
22	-	-	-	1054	1376	-
23	-	-	-	1098	1434	-
24	-	-	-	1142	1492	-

*: Na⁺負荷体として検出

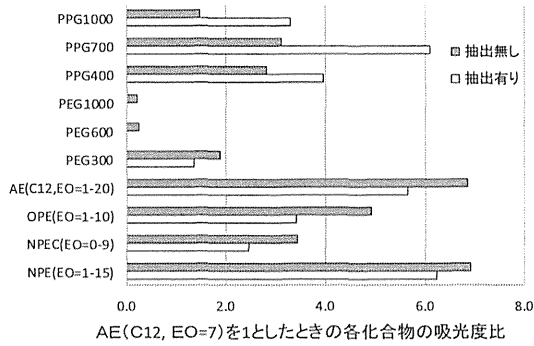
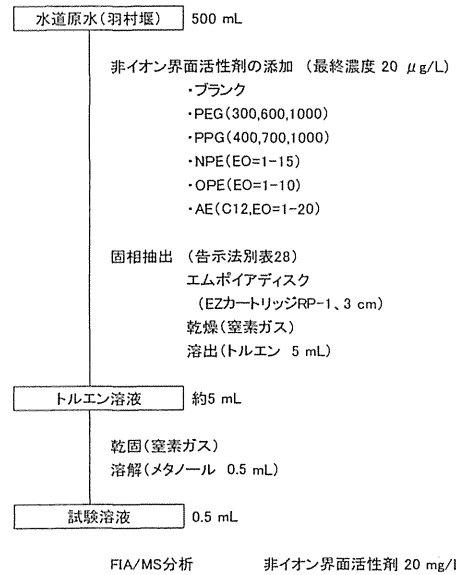


図2-1. PAR法における各種非イオン界面活性剤の発色



FIA/MS分析 非イオン界面活性剤 20 mg/L

図2-3. FIA/MS用の試験溶液の調製方法

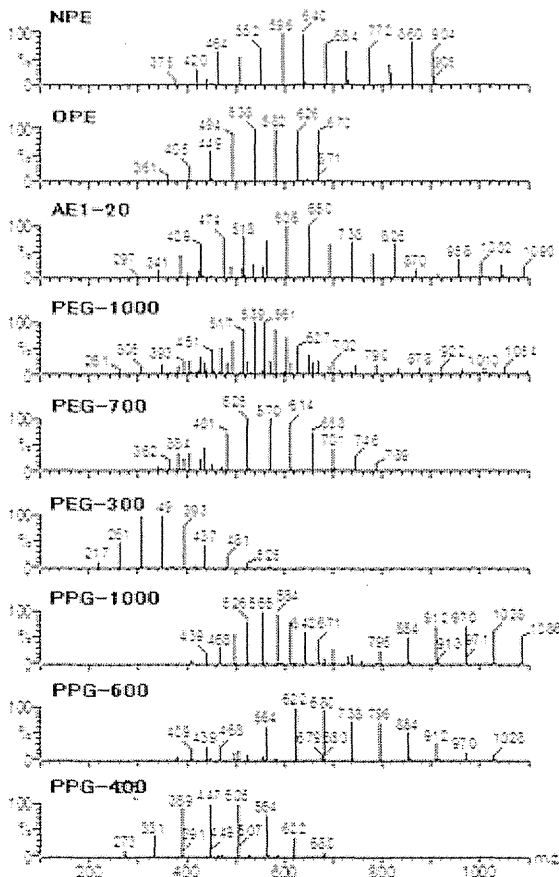


図2-2. FIA/MS法における非イオン界面活性剤および水溶性ポリマーのマススペクトル

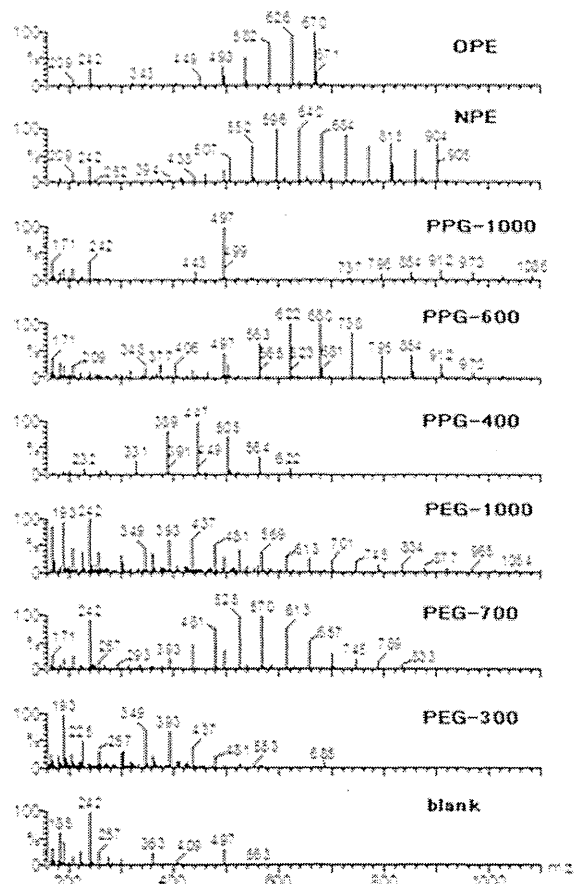


図2-4. 告示法(別表第28)により調製した試験溶液のFIA/MS法における非イオン界面活性剤および水溶性ポリマーのFIA/MSスペクトル(水試料:河川水)

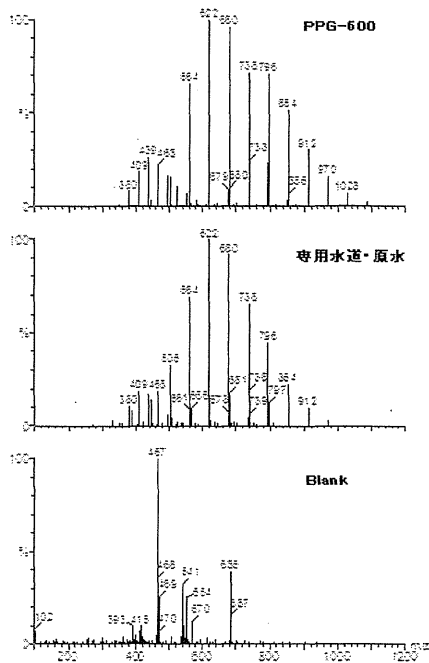


図 2-5. PAR 法により非イオン界面活性剤が基準値を超過した専用水道の FIA/MS スペクトル

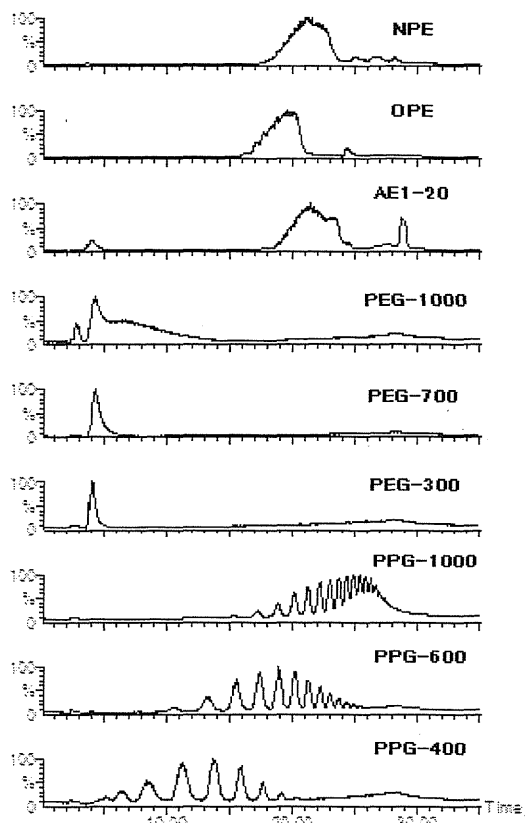


図 2-7. 非イオン界面活性剤および水溶性ポリマーの LC/MS クロマトグラム

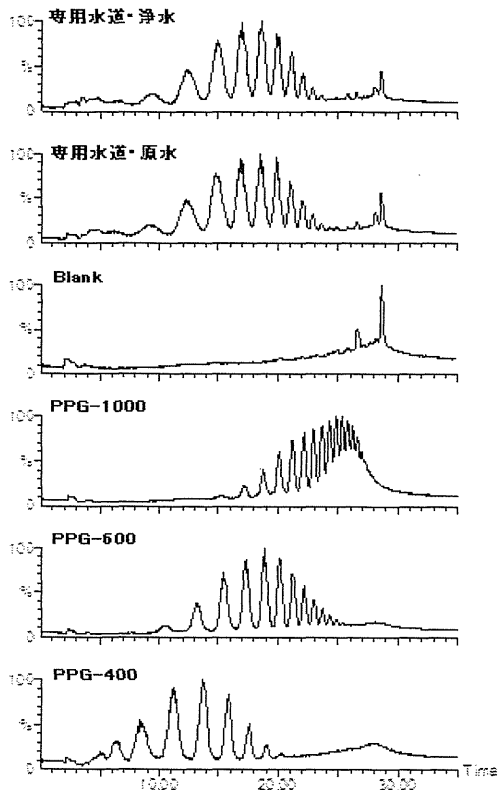


図 2-6. PAR 法により非イオン界面活性剤が基準値を超過した専用水道の LC/MS クロマトグラム

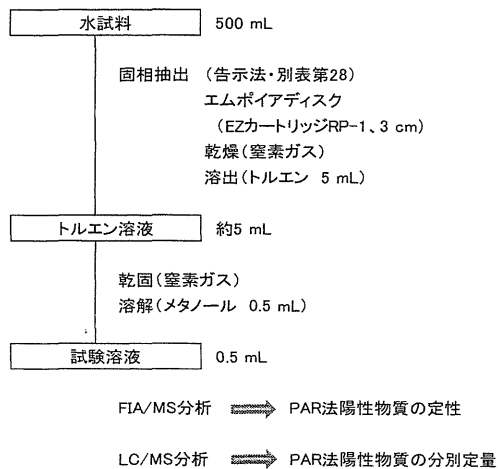


図 2-8. PAR 法により陽性となった水試料の混入物質の定性・分別定量方法

表 3-1. 対象金属と水道水規制値

金属	基準値(μg/L)	目標値等(μg/L)
Li	-	-
B	1000	-
Al	200	100
Cr	50	-
Mn	50	10
Fe	300	-
Ni	-	20
Co	-	-
Cu	1000	-
Zn	1000	-
As	10	-
Se	10	-
Sr	-	-
Y	-	-
Mo	-	70
Ag	-	(10)*
Cd	3	-
Sb	-	20
Ba	-	700
Pb	10	-
Bi	-	-
U	-	2

* USEPA飲料水基準

表 3-2. ICP-MS の測定条件

装置	パーキンエルマー社製 DRC-e
RF 出力	1500W
プラズマガス流量	17.0 L/min
補助ガス流量	1.20 L/min
ネブライザーガス流量	1.09 L/min
多原子イオン低減化用ガス	メタン (各金属のガス流量は表3を参照)
サンプル導入量	1.0 mL/min

表 3-3. 各金属に対する多原子イオン低減化用ガス流量と内部標準物質

金属	m/z	多原子イオン低減化用 ガス流量 (mL/min)	内部標準 物質
Li	7	0	⁹ Be
B	11	0	
Al	27	0	⁷¹ Ga
Cr	52	0.6	
Mn	55	0.6	
Fe	56	0.6	
Ni	58	0.6	
Co	59	0.6	
Cu	63	0.6	
Zn	64	0.6	
As	75	0.3	
Se	78	0.6	
Sr	88	0	¹¹⁵ In
Y	89	0	
Mo	98	0	
Ag	107	0	
Cd	111	0	
Sb	121	0	
Ba	135	0	
Pb	208	0	²⁰⁵ Tl
Bi	209	0	
U	238	0	

表 3-4. 各金属の検量線濃度 (単位: $\mu\text{g/L}$)

金属	BL	STD 1	STD 2	STD 3	STD 4	STD 5	STD 6	STD 7	STD 8	告示法 下限値	告示法 上限値	検量線点数 (BLを除く)	
Fe	0		3	6	15	30	60	120		1	300	6	
Al			1	2	5	10	20	40		0.4	40	6	
B				2	5	10	20	40	100	2	200	6	
Cu		0.5	1	2	5	10	20			0.2	20	6	
Zn		0.5	1	2	5	10	20			0.2	20	6	
Mo		0.35	0.7	1.4	3.5	7	14			-	-	6	
Cr		0.25	0.5	1	2.5	5	10	20		0.2	20	7	
Mn		0.25	0.5	1	2.5	5	10			0.08	8	6	
As			0.1	0.2	0.5	1	2	4		0.06	6	6	
Ni		0.05	0.1	0.2	0.5	1	2	4	10	[0.4]*	[40]*	8	
Pb				0.2	0.5	1	2	4	10	0.2	20	8	
Se					0.5	1	2	4	10	0.4	40	5	
Cd					0.15	0.3	0.6	1.2	3	0.07	7	5	
Sb		0.01	0.02	0.04	0.1	0.2	0.4	0.8	2	[0.3]*	[30]*	8	
U		0.01	0.02	0.04	0.1	0.2	0.4	0.8	2	[0.1]*	[10]*	8	
Sr			1	2	5	10	20	40	100	-	-	7	
Ba			1	2	5	10	20	40	100	-	-	7	
Li			0.2	0.4	1	2	4	8	20	-	-	7	
Bi				0.02	0.04	0.1	0.2	0.4	0.8	2	-	-	7
Ag				0.02	0.04	0.1	0.2	0.4	0.8	2	-	-	7
Y			0.1	0.2	0.5	1	2	4	10	-	-	7	
Co			0.1	0.2	0.5	1	2	4	10	-	-	7	

*: 水質管理目標設定項目の検査方法 別添4より引用

表 3-5. 真度、併行精度、室内精度の結果及び定量下限値

金属	サンプルBLの10σから求めた定量下限値 (μg/L)	添加濃度 (μg/L)	添加濃度の基準値等に対する割合	真度 (%) ¹⁾	併行精度 ²⁾ (RSD%)	室内精度 ³⁾ (RSD%)
Li	0.015	2	-	99.4	4.3	4.3
B	0.61	10	1/100	100.1	6.1	7.2
Al	0.28	10	1/20 (1/10)	101.9	2.2	7.2
Cr	0.039	5	1/10	100.6	1.1	4.3
Mn	0.036	5	1/10 (1/2)	99.6	1.3	3.9
Fe	0.50	30	1/10	100.2	1.4	4.1
Ni	0.033	1	1/20	98.8	1.4	5.5
Co	0.003	1	-	97.1	1.0	5.8
Cu	0.035	10	1/100	97.7	1.4	5.0
Zn	0.083	10	1/100	96.8	1.5	5.4
As	0.050	1	1/10	100.1	2.8	6.5
Se	0.11	1	1/10	98.3	2.3	3.0
Sr	0.041	10	-	102.5	5.2	11.7
Y	0.002	1	-	97.4	0.9	5.4
Mo	0.017	7	-	103.4	0.6	3.3
Ag	0.003	0.2	- [1/50] ⁴⁾	97.8	1.2	7.0
Cd	0.010	0.3	1/10	99.7	1.5	3.3
Sb	0.006	0.2	1/100	100.1	2.1	2.7
Ba	0.044	10	1/70	98.0	1.2	4.4
Pb	0.015	1	1/10	100.3	0.4	1.5
Bi	0.002	0.2	-	97.0	0.8	4.9
U	0.002	0.2	1/10	101.0	0.8	3.0

1) 5個以上の添加試料で実施

2,3) 自由度4以上で実施

室内精度の目標は、添加濃度の基準値等に対する割合が、1/100以下で<35 RSD%、1/100超1/10以下で<30 RSD%、1/10超 1倍以下で<20 RSD%、1倍超で<15 RSD%

4) USEPA飲料水基準を基に算出

表 4-1. LC-TOF-MS conditions

LC : Agilent 1200	
Column	GL Sciences Inertsil ODS-4 (2.1×150mm, 3μm)
Mobile phase	A : 5mmol CH ₃ COONH ₄ in H ₂ O B : 5mmol CH ₃ COONH ₄ in CH ₃ OH
Gradient profile	A 95:B 5 (0min) – A 5:B 95 (30min-50min)
Column temp	40°C
Injection volume	2μL
Flow rate	0.3 mL/min
MS : Agilent 6220 MSD	
Ionization	ESI-Positive
Measurement mode	Scan
Fragmentor Voltage	100, 150, 200, 250V
VCap voltage	3500V
Scan range (m/z)	50-1000

表 4-2. Columns used for prediction of retention times

Column	Size, mm	Particle size, μm
InertSustain C18	2.1×150	3
InertSustainSwift C18	2.1×150	3
Inertsil ODS-2	2.1×150	5
Inertsil ODS-3	2.1×150	3
Inertsil ODS-4	2.1×150	3
Inertsil ODS-SP	2.1×150	3
Inertsil ODS-80A	2.1×150	5

表 4-3. Columns used for evaluating applicability of the retention time prediction method

Column	Size, mm	Particle size, μm
ZORBAX Eclipse Plus C18	2.1×150	3.5
ZORBAX Eclipse XDB-C18	2.1×100	1.8
ZORBAX Eclipse XDB-C18	4.6×50	1.8
ZORBAX SB-C18	2.1×50	1.8
Xbridge C18	2.1×150	3.5
XSELECT CSH C18	4.6×150	3.5
Ascentis Express C18	2.1×150	2.7
Develosil C30-UG-3	2.0×150	3

表 4-4. Target compounds and their molecular-related ions and in-source fragment ions

Compound	Molecular formula	Molecular-related ion		Isotopic ion	Frag. ion 1	Frag. ion 2	Frag. ion 3	Frag. ion 4	Frag. ion 5
		Calculated exact mass	Type of ion						
2,3,5-Trimethacarb	C11H15NO2	194.1176	[M+H] ⁺						
Acephate	C4H10NO3PS	184.0192	[M+H] ⁺	186.0150	110.9670	94.9894	124.9826		
Acetaminophen	C8H9NO2	152.0706	[M+H] ⁺		110.0600	93.0476	134.0600		
Acetamiprid	C10H11ClN4	223.0745	[M+H] ⁺	225.0716	126.0111	72.9845			
Acetazolamide	C4H6N4O3S2	222.9954	[M+H] ⁺	224.9912	180.9842	163.9583			
Acetohexamide	C15H20N2O4S	325.1217	[M+H] ⁺	327.1175	138.0552	188.0863			
Aldicarb	C7H14N2O2S	208.1114	[M+NH4] ⁺	210.1072	116.0534	100.0221	89.0425		
Aldicarb sulfone	C7H14N2O4S	223.0747	[M+H] ⁺	225.0705	86.0606	148.0432	166.0538	76.0399	
Ametryn	C9H17N5S	228.1277	[M+H] ⁺	230.1235	186.0813	116.0282	144.0595		
Amitriptyline	C20H23N	278.1903	[M+H] ⁺		233.1330	191.0855	117.0699		
Ampicillin	C16H19N3O4S	350.1169	[M+H] ⁺	352.1127	160.0427				
Anilofos	C13H19NO3PS2Cl	368.0305	[M+H] ⁺	370.0276	124.9826	198.9652	170.9703		
Antipyrine	C11H12N2O	189.1022	[M+H] ⁺		147.0919	106.0649	104.0499	130.0650	
Aramite	C15H23O4SCl	352.1344	[M+NH4] ⁺	354.1314	191.1436	135.0810	91.0548	107.0497	
Asulam	C8H10N2O4S	248.0700	[M+NH4] ⁺	250.0657	156.0119	92.05	80.05		
Atenolol	C14H22N2O3	267.1703	[M+H] ⁺		190.0863	225.1234	145.0648		
Atrazine	C8H14ClN5	216.1011	[M+H] ⁺	218.0981	174.0546	104.0015			
Avermectin B1a	C48H72O14	895.4814	[M+Na] ⁺		528.2443	570.4583	746.5623	305.2117	
Azamethiphos	C9H10N2O5PSCl	324.9809	[M+H] ⁺	326.9780	182.9961	111.9951	139.0063		
Azimsulfuron	C13H16N10O5S	425.1099	[M+H] ⁺	427.1057	182.0566	244.0617			
Azinphos-methyl	C10H12N3O3PS2	318.0131	[M+H] ⁺	320.0088	132.0449	105.0453	160.0511	124.9826	
Azithromycin	C38H72N2O12	749.5158	[M+H] ⁺		591.4215	375.2615	158.1176		
Azoxystrobin	C22H17N3O5	404.1241	[M+H] ⁺		372.0984	344.1035			
Bendiocarb	C11H13NO4	224.0917	[M+H] ⁺		167.0708	109.0290	81.0340		
Benfuracarb	C20H30N2O5S	411.1948	[M+H] ⁺	413.1906	195.044	252.0694	190.0902		
Bensulfuron-methyl	C16H18N4O7S	411.0969	[M+H] ⁺	413.0927	149.0603	182.0566	91.0548	181.1054	
Bensulide	C14H24NO4PS3	398.0678	[M+H] ⁺	400.0636	313.9744	356.0214	158.0276	218.0309	
Benzobicyclon	C22H19ClO4S2	447.0486	[M+H] ⁺	449.0457	257.0636	411.0725			
Benzobicyclon metabolite	C16H15ClO5S	372.0667	[M+NH4] ⁺	374.0637	165.0585	319.064			
Benzofenap	C22H20N2O3Cl2	431.0924	[M+H] ⁺	433.0894	105.0704	320.0119			
Betaxolol	C18H29NO3	308.2220	[M+H] ⁺		290.2097	266.1736	98.0944		
Bezafibrate	C19H20NO4Cl	362.1154	[M+H] ⁺	364.1124	316.1109	276.0789	138.9974		
Bisoprolol	C18H31NO4	326.2326	[M+H] ⁺		116.1067	107.0488	74.0600		
Boscalid	C18H12N2OCl2	343.0399	[M+H] ⁺	345.0370	307.0638	139.9903	111.9954		
Bromacil	C9H13BrN2O2	261.0233	[M+H] ⁺	263.0213	204.9613	187.9347	161.9555		

Butafenacil	C20H18N2O6ClF3	492.1144	[M+NH4] ⁺	494.1114	331.0097	349.0203	179.9852	
Butocarboxim	C7H14N2O2S	208.1114	[M+NH4] ⁺	210.1072	100.0221	118.0492		
Butocarboxim sulfoxide	C7H14N2O3S	207.0798	[M+H] ⁺	209.0756	132.0477	75.0268	90.0377	
Candesartan	C24H20N6O3	441.1670	[M+H] ⁺		263.1295	423.1572	235.1114	
Carazolol	C18H22N2O2	299.1754	[M+H] ⁺		222.0914	184.0755		
Carbadox	C11H10N4O4	263.0775	[M+H] ⁺					
Carbamazepin	C15H12N2O	237.1022	[M+H] ⁺		194.0967	179.0736		
Carbaryl	C12H11O2N	219.1128	[M+NH4] ⁺		145.0653	117.0704	155.0602	
Carbendazim	C9H9N3O2	192.0768	[M+H] ⁺		160.0511	132.0562	105.0453	
Carbofuran	C12H15NO3	222.1125	[M+H] ⁺		165.0916	123.0446	109.0290	
Carbosulfan	C20H32N2O3S	381.2206	[M+H] ⁺	383.2164	118.069	160.116	165.0916	
Carpropamid	C15H18NOC13	334.0527	[M+H] ⁺	336.0497	139.0315			
Chloramphenicol	C11H12Cl2N2O5	323.0196	[M+H] ⁺	325.0167	305.0088	274.9979		
Chlorfluazuron	C20H9Cl3F5N3O3	539.9702	[M+H] ⁺	541.9673	158.0417	382.9369	141.0152	
Chloridazon	C10H8N3OC1	222.0429	[M+H] ⁺	224.0399	104.0500	92.0500	146.0121	
Chlorimuron-ethyl	C15H15N4O6SC1	415.0474	[M+H] ⁺	417.0444	186.0070	369.0060		
Chloroxuron	C15H15N2O2Cl	291.0895	[M+H] ⁺	293.0865	72.0449	218.0373	164.0950	
Chlorpheniramine maleate	C20H23N2O4Cl	275.1310	[C16H19CIN 2+H] ⁺	277.1280	230.0731	167.0729		
Chlorpromazine	C17H19CIN2S	319.1030	[M+H] ⁺	321.1001	86.1031	246.0192	248.0060	239.0723
Chlorsulfuron	C12H12N5O4SC1	358.0371	[M+H] ⁺	360.0342	141.0776			
Chromafenozide	C24H30N2O3	395.2329	[M+H] ⁺		175.0759	339.1709	147.0558	
Cimetidine	C10H16N6S	253.1230	[M+H] ⁺	255.1188	159.0699	117.0481	95.0604	
Cinosulfuron	C15H19N5O7S	414.1078	[M+H] ⁺	416.1036	183.0518	157.0726		
Clarithromycin	C38H69NO13	748.4842	[M+H] ⁺		718.4735	590.3899	558.3652	
Clenbuterol	C12H18Cl2N2O	277.0869	[M+H] ⁺	279.0839	203.0142	205.0111	132.0682	259.0768 168.0448
Clodinafop	C14H11NO4ClF	312.0433	[M+H] ⁺	314.0404	266.0384	239.0149		
Clofencet	C13H11N2O3Cl	279.0531	[M+H] ⁺	281.0501	261.0431	166.0424		
Clofentezine	C14H8N4Cl2	303.0199	[M+H] ⁺	305.0169	138.0111			
Clomeprop	C16H15NO2Cl2	324.0553	[M+H] ⁺	326.0523	120.0813	105.0578		
Cloquintocet-mexyl	C18H22NO3Cl	336.1361	[M+H] ⁺	338.1331	238.0271	179.0138	192.0216	
Clothianidin	C6H8N5O2SC1	250.0160	[M+H] ⁺	252.0130	169.0548	131.9675	113.0173	
Cotinine	C10H12N2O	177.1022	[M+H] ⁺		146.0600	98.0600	80.0495	
Cumyluron	C17H19N2OC1	303.1259	[M+H] ⁺	305.1229	185.0482			
Cyanazine	C9H13CIN6	241.0963	[M+H] ⁺	243.0933	214.0859	174.0546		
Cyazofamid	C13H13CIN4O2S	325.0521	[M+H] ⁺	327.0491	108.0119	217.0407	261.0907	
Cyclophosphamide	C7H15Cl2N2O2P	261.0321	[M+H] ⁺	263.0291	140.0028	120.0209	142.0185	
Cycloprothrin	C26H21Cl2NO4	499.1186	[M+NH4] ⁺	501.1156	208.0762	181.0653		
Cyclosulfamuron	C17H19N5O6S	422.1129	[M+H] ⁺	424.1087	261.0294	182.0566		
Cyflufenamid	C20H17N2O2F5	413.1283	[M+H] ⁺		295.0870	241.0400	203.0232	

Cyprodinil	C14H15N3	226.1339	[M+H] ⁺	108.0813	93.0578	210.1031		
Dexamethasone	C22H29O5F	393.2072	[M+H] ⁺	373.1999	147.0791	171.0803		
Dextromethorphan	C18H25NO	272.2009	[M+H] ⁺	213.1274	171.0804	147.0804		
Diazepam	C16H13N2OCl	285.0789	[M+H] ⁺	287.0760	257.0843	154.0418	193.0897	
Diclosulam	C13H10Cl2FN5O3S	405.9938	[M+H] ⁺	407.9909	160.9799	377.9632	314.0034	
Dicyclohexylamine	C12H23N	182.1903	[M+H] ⁺	83.0856	100.1122			
Difenoconazole	C19H17Cl2N3O3	406.0720	[M+H] ⁺	408.0690	251.003	337.0398		
Diflubenzuron	C14H9N2O2ClF2	311.0393	[M+H] ⁺	313.0364	158.0417	141.0152		
Diltiazem	C22H26N2O4S	415.1686	[M+H] ⁺	417.1644	178.0321	370.1108	150.0372	
Dimethirimol	C11H19N3O	210.1601	[M+H] ⁺	140.1075	167.1059	152.0824		
Dimethoate	C5H12NO3PS2	230.0069	[M+H] ⁺	232.0027	124.9826	170.9703	156.9547	
Dimethomorph(E)	C21H22NO4Cl	388.1310	[M+H] ⁺	390.1281	301.0631			
Dimethomorph(Z)	C21H22NO4Cl	388.1310	[M+H] ⁺	390.1281	301.0631			
Dinotefuran	C7H14N4O3	203.1139	[M+H] ⁺	129.0902	114.1031	112.0875		
Dioxacarb	C11H13NO4	224.0917	[M+H] ⁺	123.0446	95.04987			
Diphenidol	C21H27NO	310.2165	[M+H] ⁺	292.2060	129.0700	91.0543		
Dipyridamole	C24H40N8O4	505.3245	[M+H] ⁺	504.3176	429.2741	425.2511	473.2988	460.2911
Disopyramide	C21H29N3O	340.2383	[M+H] ⁺	239.1179	195.1042	221.1177		
Diuron	C9H10Cl2N2O	233.0243	[M+H] ⁺	235.0213	72.0449			
Dymron	C17H20N2O	269.1648	[M+H] ⁺	151.0871				
Epinastine	C16H15N3	250.1339	[M+H] ⁺	131.0609	91.0533	165.0690		
Epoxiconazole	C17H13N3OClF	330.0804	[M+H] ⁺	332.0774	123.033	129.0482	75.0264	141.0144 101.0415
Erythromycin	C37H67NO13	734.4685	[M+H] ⁺	576.3742	558.3637			
Ethametsulfuron-methyl	C15H18N6O6S	411.1081	[M+H] ⁺	413.1039	196.0834	168.0521	142.0729	
Ethenzamide	C9H11NO2	166.0863	[M+H] ⁺	149.0599	131.0499	138.0547		
Ethiofencarb	C11H15NO2S	226.0896	[M+H] ⁺	228.0854	107.0497	164.0712		
Ethoxyquin	C14H19NO	218.1539	[M+H] ⁺	202.1232	174.0919	188.1075		
Ethoxysulfuron	C15H18N4O7S	416.1235	[M+NH4] ⁺	401.0992				
Etobenzanid	C16H15Cl2NO3	340.0502	[M+H] ⁺	342.0472				
Etodolac	C17H21NO3	288.1594	[M+H] ⁺	172.1128	143.0731	270.1498		
Fenamidone	C17H17N3OS	312.1165	[M+H] ⁺	314.1123	236.1188			
Fenarimol	C17H12Cl2N2O	331.0399	[M+H] ⁺	333.0370				
Fenhexamid	C14H17NO2Cl2	302.0709	[M+H] ⁺	304.0680	97.1017	177.9826		
Fenobucarb	C12H17NO2	208.1332	[M+H] ⁺	95.0497	152.0712	77.0391		
Fenoxaprop-ethyl	C18H16NO5Cl	362.0790	[M+H] ⁺	364.0760	288.0427			
Fenoxycarb	C17H19NO4	302.1387	[M+H] ⁺	88.0399	256.0974	116.0712		
Fenpyroximate	C24H27N3O4	422.2074	[M+H] ⁺	366.1454				
Fenthion oxon sulfone	C10H15O6PS	312.0665	[M+NH4] ⁺	314.0623	217.0452			
Fenthion oxon sulfoxide	C10H15O5PS	279.0451	[M+H] ⁺	281.0409	264.0221	216.0551	247.0194	
Fenthion sulfone	C10H15O5PS2	328.0437	[M+NH4] ⁺	330.0395	124.9826			

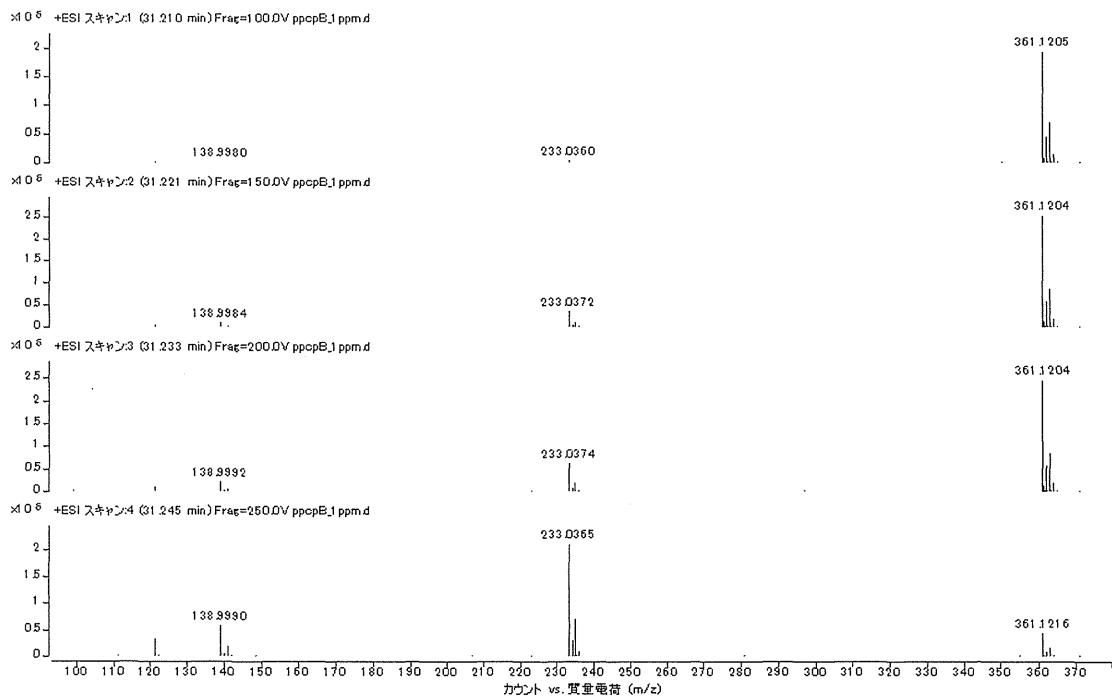
Fenthion sulfoxide	C10H15O4PS2	295.0222	[M+H] ⁺	297.0180	279.9993	109.0055	232.0323	
Fentrazamide	C16H20CIN5O2	350.1378	[M+H] ⁺	352.1349	197.129	154.1232	115.0508	83.0861
Fenvalerate	C25H22CINO3	437.1627	[M+NH4] ⁺	439.1597	129.0704	259.1698		
Ferimzone(E)	C15H18N4	255.1604	[M+H] ⁺		132.0813	163.0984	238.1344	
Ferimzone(Z)	C15H18N4	255.1604	[M+H] ⁺		132.0813	163.0984	238.1344	
Fipronil	C12H4Cl2F6N4OS	453.9725	[M+NH4] ⁺	455.9696				
Flazasulfuron	C13H12N5O5SF3	408.0584	[M+H] ⁺	410.0542	182.0563	301.0912	182.0558	
Florasulam	C12H8N5O3SF3	360.0373	[M+H] ⁺	362.0331	129.0390	296.0759		
Fluazifop	C15H12NO4F3	328.0791	[M+H] ⁺		282.0742	255.0499		
Flufenacet	C14H13N3O2SF4	364.0737	[M+H] ⁺	366.0695	152.0512			
Flumequine	C14H12FNO3	262.0874	[M+H] ⁺		244.0838	202.0299	174.0350	
Flumetsulam	C12H9F2N5O2S	326.0518	[M+H] ⁺	328.0476	262.0904			
Fluoxetine	C17H18NOF3	310.1413	[M+H] ⁺		148.1121			
Fluridone	C19H14NOF3	330.1100	[M+H] ⁺		310.1043	290.0981		
Fluvoxamine	C15H21N2O2F3	319.1628	[M+H] ⁺		258.1100	200.0682	71.0491	
Fomesafen	C15H10ClF3N2O6S	456.0238	[M+NH4] ⁺	458.0209	343.9937	379.0308		
Foramsulfuron	C17H20N6O7S	453.1187	[M+H] ⁺	455.1145	182.0566	272.0705	255.0440	
Forchlorfenuron	C12H10ClN3O	248.0585	[M+H] ⁺	250.0556	129.0220	155.0012	111.0558	
Furametpyr	C17H20N3O2Cl	334.1317	[M+H] ⁺	336.1287	316.1217			
Furathiocarb	C18H26N2O5S	383.1635	[M+H] ⁺	385.1593	195.0440	167.0490	252.0694	
Griseofulvin	C17H17O6Cl	353.0786	[M+H] ⁺	355.0757	285.0493	215.0074	165.0512	
Haloperidol	C21H23NO2ClF	376.1474	[M+H] ⁺	378.1445	165.0709	123.0276	358.1379	
Halosulfuron-methyl	C13H15N6O7SCl	435.0484	[M+H] ⁺	437.0455	182.0566	139.0508	83.0245	
Hexamethylenetetramine	C6H12N4	141.1135	[M+H] ⁺		112.0871			
Hexythiazox	C17H21N2O2SCl	353.1085	[M+H] ⁺	355.1056	228.0250	168.0580	271.0308	
Ifenprodil	C21H27NO2	326.2115	[M+H] ⁺		308.2018	176.1435	151.0757	
Ifosfamide	C7H15N2O2PCl2	261.0321	[M+H] ⁺	263.0291	92.0262	182.0132	78.0246	153.9821
Imazalil	C14H14N2OCl2	297.0556	[M+H] ⁺	299.0526	158.9768	109.0766	255.0092	
Imazaquin	C17H17N3O3	312.1343	[M+H] ⁺		284.1399	267.1134	199.0508	266.1293
Imazosulfuron	C14H13ClN6O5S	413.0429	[M+H] ⁺	415.0400	156.0773	257.974	231.9947	
Imibenconazole	C17H13Cl3N4S	410.9999	[M+H] ⁺	412.9970	125.0158	341.9678	194.0485	
Imidacloprid	C9H10N5O2Cl	256.0596	[M+H] ⁺	258.0566	175.0984	209.0594	84.0562	
Imipramine	C19H24N2	281.2012	[M+H] ⁺		86.0967	208.1122	236.1437	
Inabenfide	C19H15ClN2O2	339.0895	[M+H] ⁺	341.0865	321.0795			
Indanofan	C20H17O3Cl	341.0939	[M+H] ⁺	343.0909	175.0759	131.0861		
Indoxacarb	C22H17N3O7ClF3	528.0780	[M+H] ⁺	530.0750	293.0329	249.0431	263.0223	203.0195
Iodosulfuron-methyl-sodium	C14H13N5O6SINa	529.9602	[M+H] ⁺	531.9560	167.0569			
Iprodione	C13H13Cl2N3O3	330.0407	[M+H] ⁺	332.0377				
Iprovalicarb	C18H28N2O3	321.2173	[M+H] ⁺		119.0861	203.1396	98.0606	144.0661

Isoprocarb	C11H15NO2	194.1176	[M+H] ⁺	95.0497	137.0966			
Isouron	C10H17N3O2	212.1394	[M+H] ⁺	167.0821	194.1293			
Isoxaflutole	C15H12NO4SF3	360.0512	[M+H] ⁺	362.0470	250.9990	377.0777		
Ketoprofen	C16H14O3	272.1281	[M+NH4] ⁺	105.0335	209.0961	77.0386		
Lactofen	C19H15NO7CIF3	479.0827	[M+NH4] ⁺	481.0798	343.9937			
Lidocaine	C14H22N2O	235.1805	[M+H] ⁺	86.0966				
Lincomycin	C18H34N2O6S	407.2210	[M+H] ⁺	409.2168	359.2196	317.2071	126.1277	
Linuron	C9H10N2O2Cl2	249.0192	[M+H] ⁺	251.0163	182.0247			
Losartan	C22H23ClN6O	423.1695	[M+H] ⁺	425.1665	207.0919	192.0798	180.0828	
Mefenacet	C16H14N2O2S	299.0849	[M+H] ⁺	301.0807	148.0762	120.0813		
Mepanipyrim	C14H13N3	224.1182	[M+H] ⁺	131.0609	106.0646			
Mepanipyrim metabolite	C14H17N3O	244.1444	[M+H] ⁺	226.1344	200.1188	82.0657		
Mepirizole	C11H14N4O2	235.1190	[M+H] ⁺	220.0952	192.1004	156.0533		
Mesosulfuron-methyl	C17H21N5O9S2	504.0854	[M+H] ⁺	506.0811	306.0106			
Metformin	C4H11N5	130.1087	[M+H] ⁺	113.0822	88.0869	71.0604		
Methabenzthiazuron	C10H11N3OS	222.0696	[M+H] ⁺	224.0654	165.0486	150.0252	124.0221	80.0500
Methamidophos	C2H8NO2PS	142.0086	[M+H] ⁺	144.0044	94.0058	124.9826	78.9949	
Methiocarb	C11H15NO2S	226.0896	[M+H] ⁺	228.0854	169.0561	105.0340	154.0327	
Methomyl	C5H10N2O2S	163.0536	[M+H] ⁺	165.0494	88.0221	106.0327	72.9986	
Methoxyfenozide	C22H28N2O3	369.2173	[M+H] ⁺	313.1552	149.0603	91.0548		
Metoclopramide	C14H22N3O2Cl	300.1473	[M+H] ⁺	302.1444	227.0588	184.0166	140.9979	
Metolcarb	C9H11NO2	166.0863	[M+H] ⁺	109.0653	94.0419	91.0548		
Metominostrobin(E)	C16H16N2O3	285.1234	[M+H] ⁺	194.0606	196.0762	238.0868		
Metoprolol	C15H25NO3	268.1907	[M+H] ⁺	116.1070	133.0648	159.0804	56.0495	
Metosulam	C14H13N5O4SCl2	418.0138	[M+H] ⁺	420.0109	174.9944	354.0525	140.0262	
Metribuzin	C8H14N4OS	215.0961	[M+H] ⁺	217.0919	187.1017	84.0813		
Metsulfuron-methyl	C14H15N5O6S	382.0816	[M+H] ⁺	384.0774	167.0569	199.0065		
Monolinuron	C9H11N2O2Cl	215.0582	[M+H] ⁺	217.0552	126.0111	148.0637		
Naproanilide	C19H17NO2	292.1332	[M+H] ⁺	171.0810	120.0813			
Naproxen	C14H14O3	248.1281	[M+NH4] ⁺	185.0961	170.0737			
Naptalam	C18H13NO3	292.0968	[M+H] ⁺	144.0813	274.0868			
Nitenpyram	C11H15ClN4O2	271.0956	[M+H] ⁺	273.0927	225.1033	237.0907	126.0111	196.0642
Norgestimate	C23H31NO3	370.2377	[M+H] ⁺	149.0240	301.1417	310.2177		
Ormetoprim	C14H18N4O2	275.1503	[M+H] ⁺	259.1189	123.0661	81.0446		
Oryzalin	C12H18N4O6S	347.1020	[M+H] ⁺	349.0978				
Oxadiargyl	C15H14Cl2N2O3	358.0720	[M+NH4] ⁺	360.0690	257.9725	151.0144	183.9801	
Oxamyl	C7H13N3O3S	237.1016	[M+NH4] ⁺	239.0974	90.0555	72.0449		
Oxaziclomefone	C20H19NO2Cl2	376.0866	[M+H] ⁺	378.0836	190.0868	161.0607		
Oxycarboxin	C12H13NO4S	268.0638	[M+H] ⁺	270.0596	175.0065	146.9752		
Paroxetine	C19H20NO3F	330.1500	[M+H] ⁺	192.1183	123.0605	151.0390		

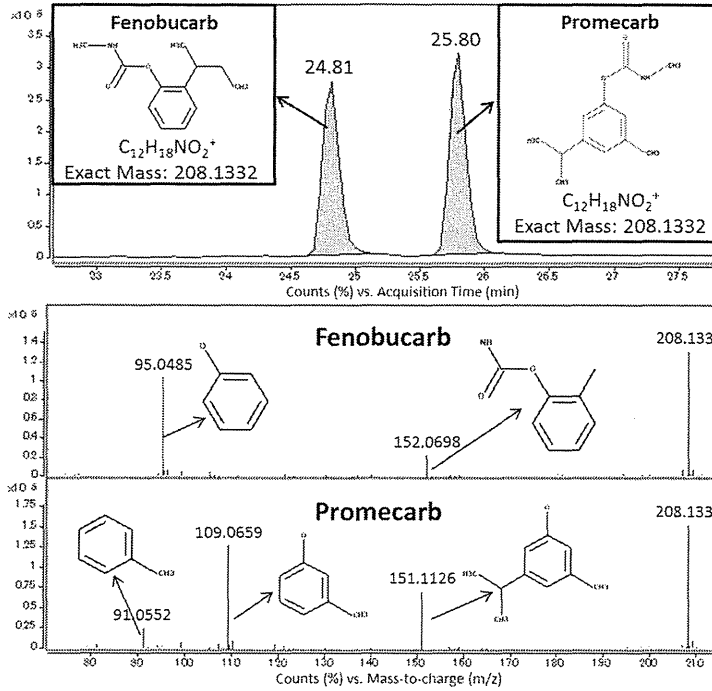
Pencycuron	C19H21N2OC1	329.1415	[M+H] ⁺	331.1386	125.0158	261.0795	89.0391	218.0737
Penicillin G	C16H18N2O4S	335.1060	[M+H] ⁺	337.1018	160.0427	217.0649	114.0372	
Penoxsulam	C16H14N5O5SF5	484.0709	[M+H] ⁺	486.0667	228.1494	195.0751		
Pentoxifylline	C13H18N4O3	279.1452	[M+H] ⁺		181.0720	138.0659	163.0608	
Phenacetin	C10H13NO2	180.1019	[M+H] ⁺		110.0610	138.0921	152.0713	93.0558 109.0531
Phenytoin	C15H12N2O2	253.0972	[M+H] ⁺		182.0964	104.0495		
Phoxim	C12H15N2O3PS	299.0614	[M+H] ⁺	301.0572	96.9513	129.0453	153.0139	
Pirenzepine	C19H21N5O2	352.1768	[M+H] ⁺		113.1077	252.0775	70.0657	
Pirimicarb	C11H18N4O2	239.1503	[M+H] ⁺		182.1293	72.0444	85.0766	137.0715
Pirimiphos-methyl	C11H20N3O3PS	306.1036	[M+H] ⁺	308.0994				
Prednisolone	C21H28O5	361.2010	[M+H] ⁺		343.1870	325.1872	147.0766	
Primidone	C12H14N2O2	219.1128	[M+H] ⁺		91.0542	162.0913	119.0855	
Prochloraz	C15H16Cl3N3O2	376.0381	[M+H] ⁺	378.0351	308.0012	265.9542	70.0293	
Promecarb	C12H17NO2	208.1332	[M+H] ⁺		109.0653	151.1123	91.0548	
Promethazine	C17H20N2S	285.1420	[M+H] ⁺		86.0967	198.0376	240.0848	
Prometryn	C10H19N5S	242.1434	[M+H] ⁺	244.1392	200.097	158.05	116.0282	
Propamocarb	C9H20N2O2	189.1598	[M+H] ⁺		102.0555	144.1025	74.0242	
Propanil	C9H9Cl2NO	218.0134	[M+H] ⁺	220.0104	127.0189	161.9877		
Propaquizafop	C22H22N3O5Cl	444.1321	[M+H] ⁺	446.1291	299.0587	371.0799		
Propoxur	C11H15NO3	210.1125	[M+H] ⁺		111.0446	168.0661	93.034	
Propoxycarbazone-sodium	C15H17N4O7SNa	421.0788	[M+H] ⁺	423.0746	180.0751	399.0967		
Propranolol	C16H21NO2	260.1645	[M+H] ⁺		183.0804	155.0809		
Propyphenazone	C14H18N2O	231.1492	[M+H] ⁺		189.1022	201.1022	112.1118	
Pymetrozin	C10H11N5O	218.1036	[M+H] ⁺		105.0453	78.0344	79.0422	
Pyraclostrobin	C19H18N3O4Cl	388.1059	[M+H] ⁺	390.1029	163.0633	194.0817	164.0712	296.0591
Pyrazolynate/Pyrazolate	C19H16N2O4SCl2	439.0281	[M+H] ⁺	441.0251	172.9561	249.0431		
Pyrazosulfuron-ethyl	C14H18N6O7S	415.1030	[M+H] ⁺	417.0988	182.0566	369.0617	139.0508	
Pyrifthalid	C15H14N2O4S	319.0747	[M+H] ⁺	321.0705	301.0647	139.0508	220.0432	
Pyriminobac-methyl(Z)	C17H19N3O6	362.1347	[M+H] ⁺		330.109	284.0671		
Quizalofop-ethyl	C19H17N2O4Cl	373.0950	[M+H] ⁺	375.0920	299.0587	255.0325	345.0642	
Ranitidine	C13H22N4O3S	315.1485	[M+H] ⁺	317.1443	270.0907	224.0978	176.0488	130.0559
Roxithromycin	C41H76N2O15	837.5319	[M+H] ⁺		679.4376	158.1176	419.2715	
Salbutamol	C13H21NO3	240.1594	[M+H] ⁺		222.1489	166.0863	148.0757	
Salinomycin	C42H70O11	768.5256	[M+NH4] ⁺		733.4901			
Scopolamine	C17H21NO4	304.1543	[M+H] ⁺		138.0812	156.0917	79.0471	
Sethoxydim	C17H29NO3S	328.1941	[M+H] ⁺	330.1899	282.1528	178.0868	180.1025	
Siduron	C14H20N2O	233.1648	[M+H] ⁺		94.0657	137.0715	120.0449	
Simazine	C7H12ClN5	202.0854	[M+H] ⁺	204.0825	104.0015	132.0328	96.0562	
Simeconazole	C14H20N3OFSi	294.1432	[M+H] ⁺		135.0610	70.0405	115.0548	

Sotalol	C12H20N2O3S	273.1267	[M+H] ⁺	275.1225	255.1162	213.0695	133.0759		
Spinosyn A	C41H65NO10	732.4681	[M+H] ⁺		142.1232	558.3795			
Spinosyn D	C42H67NO10	746.4838	[M+H] ⁺		142.1232	558.3795			
Spiramycin	C43H74N2O14	843.5213	[M+H] ⁺		174.1126	83.0493	342.7035	142.1225	438.2785
Sulfadiazine	C10H10N4O2S	251.0597	[M+H] ⁺	253.0555	156.0114	108.0444	92.0495		
Sulfadimethoxine	C12H14N4O4S	311.0809	[M+H] ⁺	313.0766	156.0768	108.0444	245.1031		
Sulfamerazine	C11H12N4O2S	265.0754	[M+H] ⁺	267.0712	156.0114	110.0713	108.0444	92.0495	
Sulfamethizole	C9H10N4O2S2	271.0318	[M+H] ⁺	273.0276	156.0114	108.0444	293.0145		
Sulfamethoxazole	C10H11N3O3S	254.0594	[M+H] ⁺	256.0552	156.0114	108.0444	92.0495		
Sulfamonomethoxine	C11H12N4O3S	281.0703	[M+H] ⁺	283.0661					
Sulfanilamide	C6H8N2O2S	190.0645	[M+NH4] ⁺	192.0603	156.0114	108.0444	92.0495		
Sulfapyridine	C11H11N3O2S	250.0645	[M+H] ⁺	252.0603	95.0599	108.0438	156.0114		
Sulfathiazole	C9H9N3O2S2	256.0209	[M+H] ⁺	258.0167	156.0117	108.0446	92.0497		
Sulfentrazone	C11H10N4O3SCl2F2	404.0157	[M+NH4] ⁺	406.0127	306.9965				
Sulfosulfuron	C16H18N6O7S2	471.0751	[M+H] ⁺	473.0709	211.0541	156.0773	165.0123		
Sulpiride	C15H23N3O4S	342.1482	[M+H] ⁺	344.1440	112.1122	214.0169	84.0810		
Tebuconazole	C16H22ClN3O	308.1524	[M+H] ⁺	310.1495	70.0405	125.0158	151.0315		
Tebufenozide	C22H28N2O2	353.2224	[M+H] ⁺		297.1603	133.0653			
Tebufenpyrad	C18H24ClN3O	334.1681	[M+H] ⁺	336.1651					
Tebuthiuron	C9H16N4OS	229.1118	[M+H] ⁺	231.1076	172.0908	116.0282			
Tepraloxymid	C17H24ClNO4	342.1467	[M+H] ⁺	344.1437	166.0761				
Terbucarb	C17H27NO2	295.2380	[M+NH4] ⁺		222.1494	109.0653	166.0868		
Terbutaline	C12H19NO3	226.1438	[M+H] ⁺		152.0706	107.0494	125.0595		
Testosterone	C19H28O2	289.2162	[M+H] ⁺		97.0647	109.0647	271.2054	253.1949	
Tetrachlorvinphos	C10H9O4PCl4	381.9331	[M+NH4] ⁺	383.9301	127.0160	109.0055	203.9300		
Tetraconazole	C13H11Cl2F4N3O	372.0288	[M+H] ⁺	374.0259	158.9768				
Theophylline	C7H8N4O2	203.0540	(M+Na) ⁺		124.0506	181.0721			
Thiabendazole	C10H7N3S	202.0433	[M+H] ⁺	204.0391	175.0330	131.0609	92.0500		
Thiabendazole metabolite	C10H7N3OS	218.0383	[M+H] ⁺	220.0341	191.0279				
Thiacloprid	C10H9N4SCl	253.0309	[M+H] ⁺	255.0280	126.0111	90.0344	72.9860		
Thiamethoxam	C8H10N5O3SCl	292.0266	[M+H] ⁺	294.0236	211.0654	152.0282	181.0548		
Thiamphenicol	C12H15NO5Cl2S	373.0386	[M+NH4] ⁺	375.0357	307.9913	338.0021			
Thidiazuron	C9H8N4OS	221.0492	[M+H] ⁺		102.0126	127.9919			
Thifensulfuron-methyl	C12H13N5O6S2	388.0380	[M+H] ⁺	390.0338	269.9493	167.0563			
Thifluzamide	C13H6Br2F6N2O2S	526.8494	[M+H] ⁺	528.8473	168.0095				
Thiodicarb	C10H18N4O4S3	355.0563	[M+H] ⁺	357.0521	88.0221		107.9908	78.9676	
Thiofanox sulfone	C9H18N2O4S	268.1326	[M+NH4] ⁺	270.1283	76.0399	194.0851			
Thiofanox sulfoxide	C9H18N2O3S	252.1376	[M+NH4] ⁺	254.1334	104.017	178.0902	76.0399		
Tiadinil	C11H10ClN3OS	268.0306	[M+H] ⁺	270.0276					

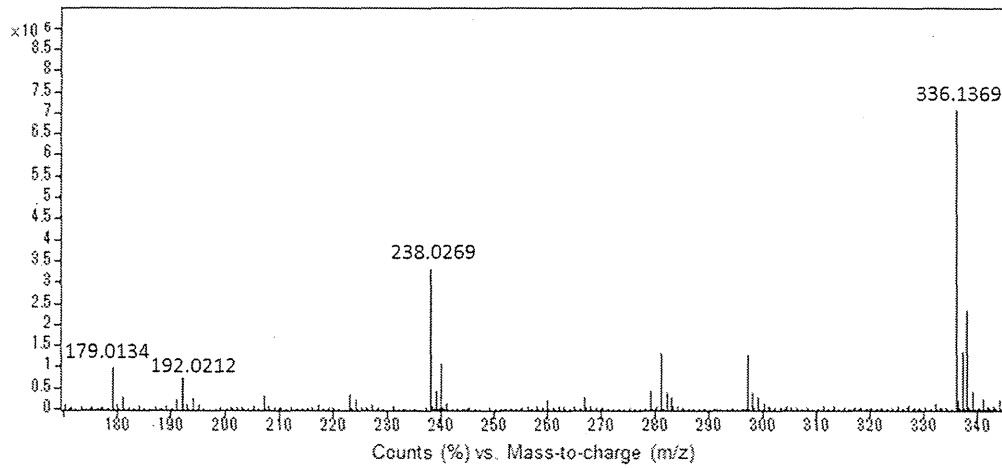
Tolbutamide	C12H18N2O3S	271.1111	[M+H] ⁺	273.1069	91.0540	172.0428	155.0162
Tolperisone	C16H23NO	246.1852	[M+H] ⁺		98.0964		
Tralkoxydim-1	C20H27NO3	330.2064	[M+H] ⁺		284.1651	138.0555	
Tralkoxydim-2	C20H27NO3	330.2064	[M+H] ⁺		284.1651	138.0555	
Triasulfuron	C14H16N5O5SCl	402.0634	[M+H] ⁺	404.0604	141.0776	167.0569	
Tribenuron-methyl	C15H17N5O6S	396.0972	[M+H] ⁺	398.0930	155.0933	181.0726	364.0716
Tricyclazole	C9H7N3S	190.0433	[M+H] ⁺	192.0391	163.033	136.0221	
Trifloxysulfuron-sodium	C14H13N5O6SF3Na	460.0509	[M+H] ⁺	462.0467			
Triflumizole	C15H15ClF3N3O	346.0929	[M+H] ⁺	348.0899	278.056	205.9984	248.0528
Triflumizole metabolite	C12H14ClF3N2O	295.0820	[M+H] ⁺	297.0790	253.0356		
Triflururon	C15H10N2O3ClF3	359.0405	[M+H] ⁺	361.0375	156.0216		
Trimethoprim	C14H18N4O3	291.1452	[M+H] ⁺	261.0992	275.1134	230.1158	123.0662
Trinexapac-ethyl	C13H16O5	253.1071	[M+H] ⁺		207.0657	179.0708	165.0188
Triticonazole	C17H20N3OC1	318.1368	[M+H] ⁺	320.1338	70.0405		
Vamidotion	C8H18NO4PS2	288.0488	[M+H] ⁺	290.0446	146.064	118.037	86.0606
Verapamil	C27H38N2O4	455.2904	[M+H] ⁺		165.0898	303.2061	
Virginiamycin M1	C28H35N3O7	526.2548	[M+H] ⁺		508.2452	355.1305	395.1975
Warfarin	C19H16O4	309.1121	[M+H] ⁺		251.0699	163.0392	
XMC	C10H13NO2	180.1019	[M+H] ⁺		123.0810	108.0575	
Xylylcarb	C10H13NO2	180.1019	[M+H] ⁺		123.081	108.0575	



☒ 4-1. Mass spectra of Fenofibrate at 100, 150, 200 and 250V



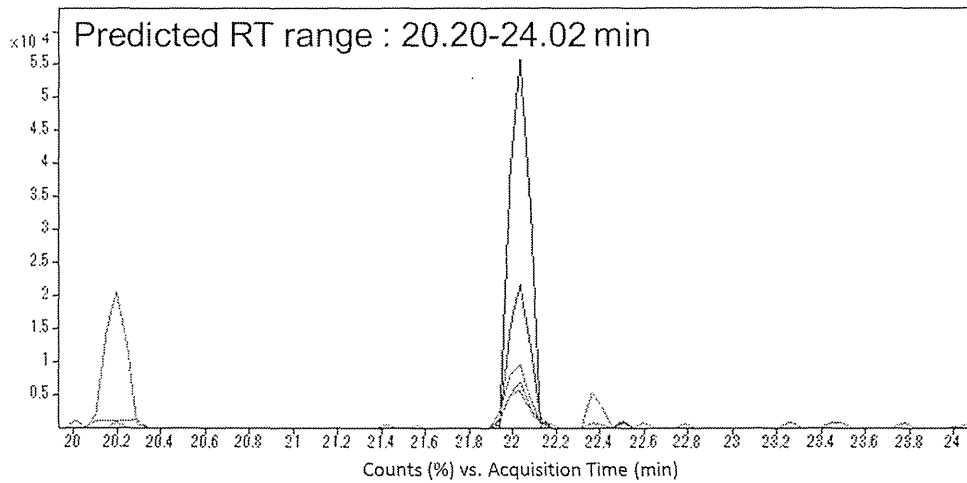
☒ 4-2. Distinction of two insecticides (isomers) by in-source fragment ions



☒ 4-3. Mass spectrum of Cloquintocet-mexyl at 250V

表 4-5. Result of RT prediction

Columns	5分以内の予測範囲かつ、 RT 予測が成功した物質数 (%)
InertSustain C18	261 (89)
InertSustainSwift C18	258 (88)
Inertsil ODS-2	261 (89)
Inertsil ODS-3	255 (87)
Inertsil ODS-4	254 (87)
Inertsil ODS-SP	262 (89)
Inertsil ODS-80A	253 (86)
ZORBAX Eclipse Plus C18	255 (87)
ZORBAX Eclipse XDB-C18 (50mm)	239 (82)
ZORBAX Eclipse XDB-C18 (100mm)	141 (48)
ZORBAX SB-C18	113 (39)
Xbridge C18	262 (89)
XSELECT CSH C18	100 (34)
Ascentis Express C18	168 (57)
Develosil C30-UG-3	246 (84)



☒ 4-4. Extracted ion chromatograms of molecular-related ions and 3 fragment ions of Bezaifibrate

表 4-6. Compounds found in an influent and an effluent of a municipal sewage treatment plant

Compound	Formula	Use
Azithromycin	C ₃₈ H ₇₂ N ₂ O ₁₂	Antibiotic
Clarithromycin	C ₃₈ H ₆₉ N ₃ O ₁₃	Antibiotic
Trimethoprim	C ₁₄ H ₁₈ N ₄ O ₃	Antibiotic
Atenolol	C ₁₄ H ₂₂ N ₂ O ₃	Antihypertensive drugs
Diltiazem	C ₂₂ H ₂₆ N ₂ O ₄ S	Antihypertensive drugs
Losartan	C ₂₂ H ₂₃ ClN ₆ O	Antihypertensive drugs
Disopyramide	C ₂₁ H ₂₉ N ₃ O	Antiarrhythmic
Lidocaine	C ₁₄ H ₂₂ N ₂ O	Antiarrhythmic drugs
Sulpiride	C ₁₅ H ₂₃ N ₃ O ₄ S	Antidepressants
Chlorpheniramine maleate	C ₂₀ H ₂₃ N ₂ O ₄ Cl	Antihistamine
Sulfamethoxazole	C ₁₀ H ₁₁ N ₃ O ₃ S	Anti-infective agent
Ketoprofen	C ₁₆ H ₁₄ O ₃	Anti-inflammatory agents
Etodolac	C ₁₇ H ₂₁ N ₃ O	Antipyretic analgesics
Acetaminophen	C ₈ H ₉ N ₂ O	Analgesic
Theophylline	C ₇ H ₈ N ₄ O ₂	Bronchodilators, vasodilators
Dicyclohexylamine	C ₁₂ H ₂₃ N	Enzyme Inhibitors
Metformin	C ₄ H ₁₁ N ₅	Hypoglycemic agent
Bezafibrate	C ₁₉ H ₂₀ NO ₄ Cl	Hypolipidemic agent
Fenofibrate	C ₂₀ H ₂₁ O ₄ Cl	Hypolipidemic agent
Carbamazepine	C ₁₅ H ₁₂ N ₂ O	Psychotropic drug
Sulfapyridine	C ₁₁ H ₁₁ N ₃ O ₂ S	Sulfonamide antibacterial
Carbendazim	C ₉ H ₉ N ₃ O ₂	Fungicide
Ferimzone(E)	C ₁₅ H ₁₈ N ₄	Fungicide
Ferimzone(Z)	C ₁₅ H ₁₈ N ₄	Fungicide
Thiabendazole	C ₁₀ H ₇ N ₃ S	Fungicide
Diuron	C ₉ H ₁₀ Cl ₂ N ₂ O	Herbicide