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Article

Application of Headspace-SIFT-MS to Direct Analysis of Hazardous Volatiles in Drinking Water

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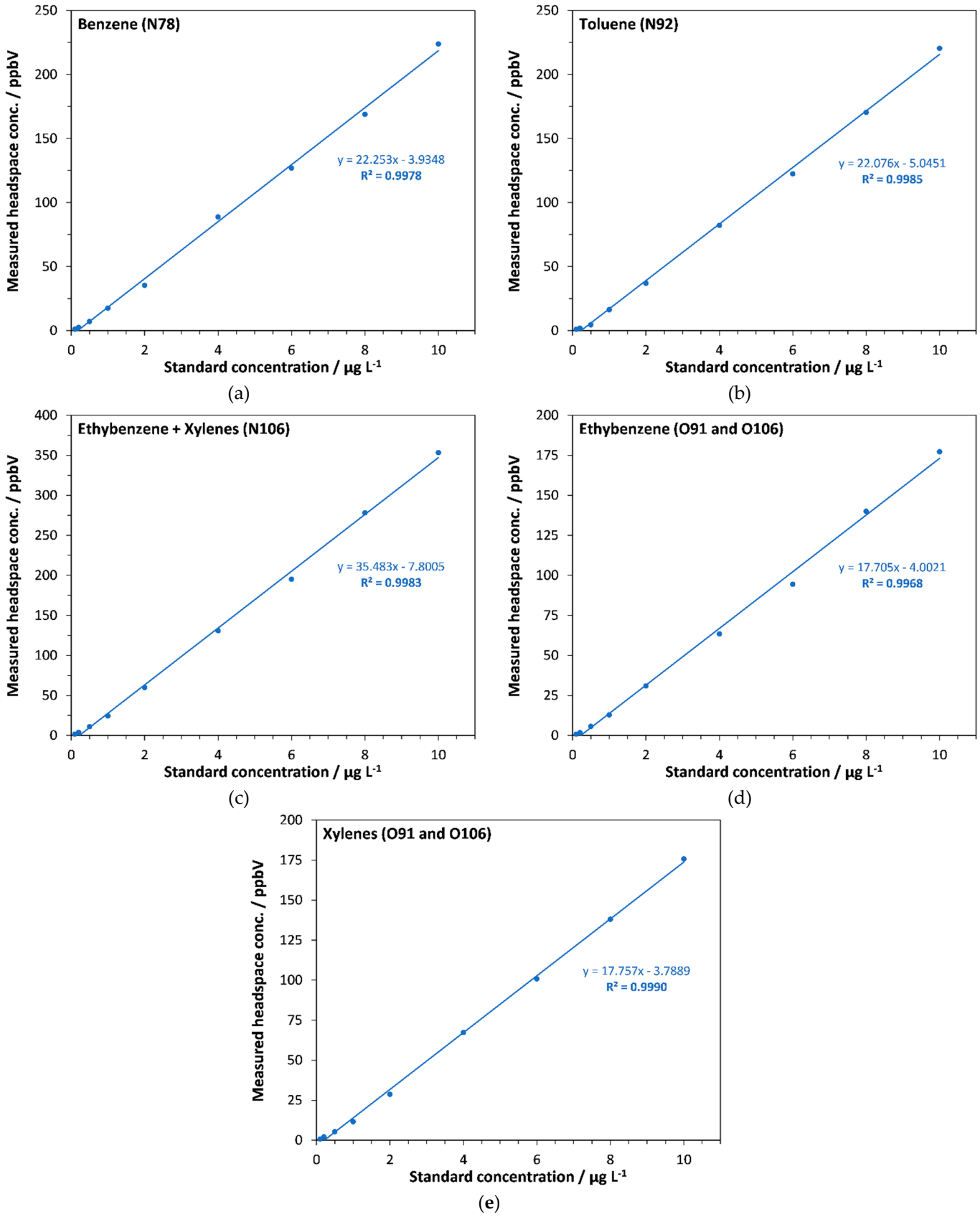

Figure S1. Linearity of headspace measurements of BTEX compounds: (**a**) benzene; (**b**) toluene; (**c**) total ethylbenzene and xylenes; (**d**) ethylbenzene; (**e**) xylenes. The linear fit and its regression coefficient, R^2, are shown.

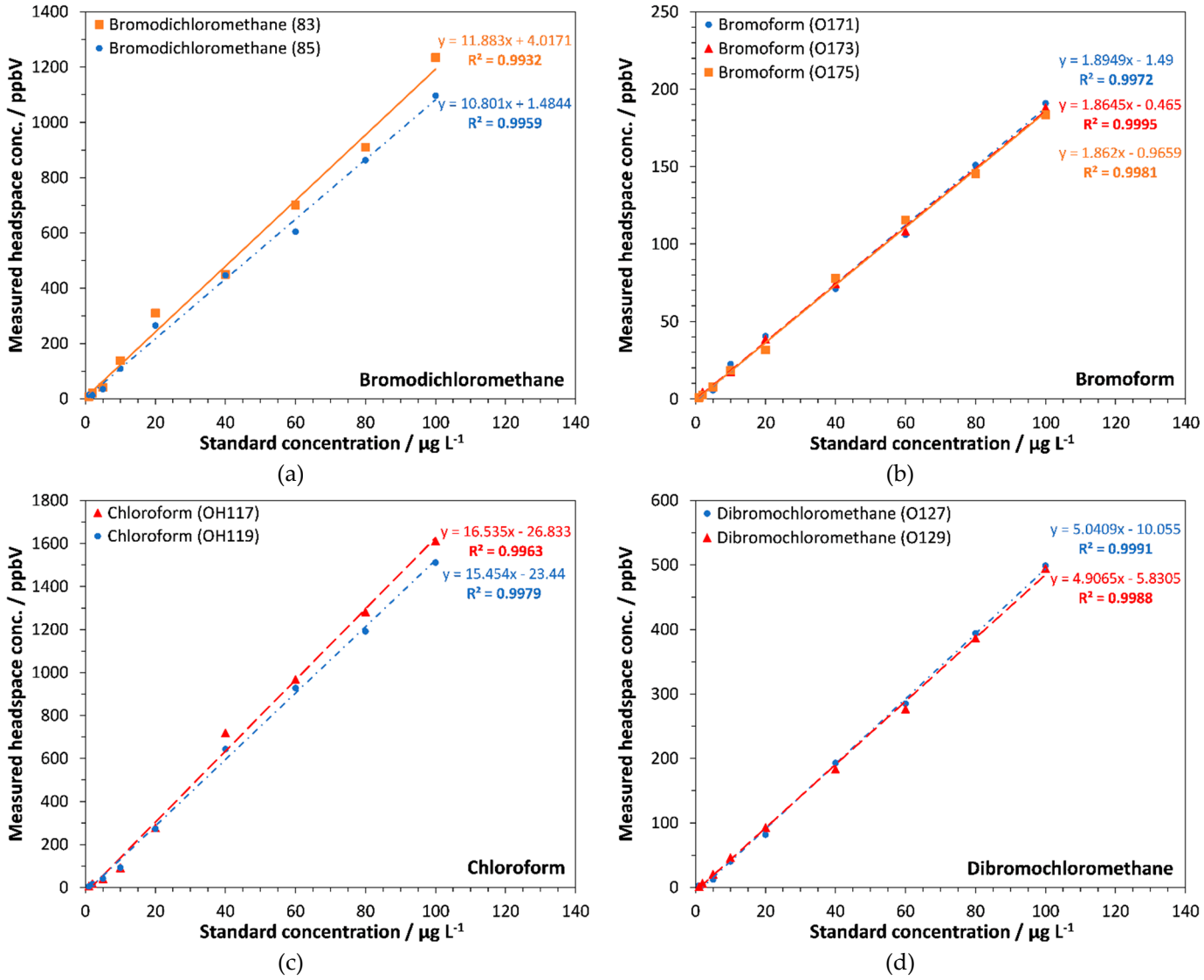

Figure S2. Linearity of headspace measurements of individual quantitation ions of the THMs: (**a**) bromodichloromethane; (**b**) bromoform; (**c**) chloroform; (**d**) dibromochloromethane. The linear fit and its regression coefficient, R^2, are shown.

2. Supplementary Tables

Table S1. Linearity data for BTEX. The linear regression coefficient, R^2, is also shown. Headspace concentrations are in parts per billion by volume (ppbV).

Solution Conc. / μg L^{-1}	Benzene (NO^+ 78)	Toluene (NO^+ 92)	Ethylbenzene + Xylenes (NO^+ 106)	Ethylbenzene (O_2^+ 91 and 106)*	Xylenes (O_2^+ 91 and 106)*
0.1	1.21	1.12	1.51	0.772	0.737
0.2	2.54	1.96	3.84	1.75	2.10
0.5	7.12	4.56	11.0	5.61	5.37
1	17.5	16.3	24.4	12.8	11.6
2	35.3	37.0	59.7	30.9	28.7
4	88.8	82.2	131	63.4	67.4
6	127	122	195	94.5	101
8	169	170	278	140	138
10	224	220	353	177	176
R^2	*0.9978*	*0.9985*	*0.9983*	*0.9968*	*0.9990*

* See the article for details of deconvolution of ethylbenzene and the xylenes using the O_2^+ product ions.

Table S2. Linearity data for the individual quantitation ions of the THM compounds. The linear regression coefficient, R^2, is also shown. Headspace concentrations are in ppbV.

Solution Conc. / μg L^{-1}	Bromodichloromethane (O_2^+ 83)*	Bromodichloromethane (O_2^+ 85)*	Bromoform (O_2^+ 171)	Bromoform (O_2^+ 173)	Bromoform (O_2^+ 175)	Chloroform (OH^- 117)	Chloroform (OH^- 119)	Dibromochloromethane (O_2^+ 127)	Dibromochloromethane (O_2^+ 129)
1	7.46	14.3	-1.26	1.82	0.802	6.78	5.42	3.07	1.27
2	20.3	12.4	2.76	4.30	2.49	18.1	16.2	3.68	6.34
5	41.5	35.1	5.54	7.92	7.70	41.0	41.5	12.4	20.4
10	139	109	22.4	17.6	18.4	91.4	92.7	40.4	46.0
20	310	265	40.4	38.4	31.6	277	273	81.9	93.0
40	450	447	71.1	74.4	77.8	719	644	193	183
60	701	605	106	108	116	968	928	285	276
80	910	863	151	148	146	1282	1192	394	386
100	1235	1096	191	188	184	1612	1512	499	494
R^2	*0.9932*	*0.9959*	*0.9972*	*0.9995*	*0.9981*	*0.9963*	*0.9979*	*0.9991*	*0.9988*

* See the article for details of subtraction of chloroform interference.

Table S3. Data obtained for determination of the lower limit of quantitation (LLOQ) of BTEX compounds at sub-μg L^{-1} concentrations (0.1, 0.2, 0.5 μg L^{-1}) in solution. Mean, standard deviation (SD), and relative standard deviation (RSD, in %) are shown in for the triplicate measurements made at each level. Headspace concentrations are in ppbV.

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Benzene (NO^+ 78)	Toluene (NO^+ 92)	Ethylbenzene + Xylenes (NO^+ 106)	Ethylbenzene (O_2^+ 91 and 106)*	Xylenes (O_2^+ 91 and 106)*
0.1	1	0.810	0.990	1.45	0.720	0.730
	2	0.880	0.530	1.33	0.727	0.595
	3	1.08	0.820	1.10	0.570	0.530
	Mean	0.923	0.780	1.29	0.672	0.619
	SD	0.114	0.190	0.145	0.073	0.083
	%RSD	12.4	24.3	11.2	10.8	13.5
0.2	1	3.31	2.26	3.51	2.04	1.46

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Benzene (NO^+ 78)	Toluene (NO^+ 92)	Ethylbenzene + Xylenes (NO^+ 106)	Ethylbenzene (O_2^+ 91 and 106)*	Xylenes (O_2^+ 91 and 106)*
	2	3.40	1.98	3.87	2.39	1.45
	3	2.79	2.08	3.85	2.24	1.59
	Mean	3.17	2.11	3.74	2.22	1.50
	SD	0.269	0.116	0.165	0.146	0.062
	%RSD	8.5	5.5	4.4	6.6	4.2
0.5	1	4.53	4.63	6.02	2.71	3.32
	2	3.94	3.89	6.79	3.34	3.45
	3	4.29	4.07	5.81	2.81	3.01
	Mean	*4.25*	*4.20*	6.21	*2.95*	*3.26*
	SD	*0.242*	*0.315*	0.422	*0.277*	*0.186*
	%RSD	*5.7*	*7.5*	6.8	*9.4*	*5.7*

* See the article for details of deconvolution of ethylbenzene and the xylenes using the O_2^+ product ions.

Table S4. Data obtained for determination of the LLOQ of THM compounds by individual quantitation ions at low μg L^{-1} concentrations (1, 2, 5 μg L^{-1}) in solution. Mean, standard deviation (SD), and RSD (in %) are shown in for the triplicate measurements made at each level. Headspace concentrations are in ppbV.

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Bromodichloromethane (O_2^+ 83)*	Bromodichloromethane (O_2^+ 85)*	Bromoform (O_2^+ 171)	Bromoform (O_2^+ 173)	Bromoform (O_2^+ 175)	Chloroform (OH^- 117)	Chloroform (OH^- 119)	Dibromochloromethane (O_2^+ 127)	Dibromochloromethane (O_2^+ 129)
1	1	23.9	24.7	-2.35	2.01	0.963	7.92	6.31	2.97	1.72
	2	33.2	33.7	2.76	1.52	1.77	8.02	5.51	2.51	1.88
	3	31.9	31.2	0.340	0.977	1.31	8.62	5.91	1.00	1.76
	Mean	*29.7*	*29.9*	*0.250*	*1.50*	*1.35*	*8.19*	*5.91*	*2.16*	*1.79*
	SD	*4.10*	*3.80*	*2.09*	*0.421*	*0.332*	*0.309*	*0.327*	*0.841*	*0.068*
	%RSD	*13.8*	*12.7*	*834.8*	*28.0*	*24.6*	*3.8*	*5.5*	*39.0*	*3.8*
2	1	21.2	22.8	3.08	3.43	3.00	16.3	14.8	4.55	4.58
	2	18.3	25.2	2.27	3.88	3.25	18.8	14.6	5.71	5.18
	3	16.0	20.9	2.72	2.88	2.69	17.5	12.7	5.11	5.17
	Mean	*18.51*	*22.94*	*2.69*	*3.39*	*2.98*	*17.55*	*14.0*	*5.12*	*4.98*
	SD	*2.12*	*1.76*	*0.331*	*0.409*	*0.229*	*1.02*	*0.946*	*0.474*	*0.281*
	%RSD	*11.4*	*7.7*	*12.3*	*12.0*	*7.7*	*5.8*	*6.7*	*9.2*	*5.6*
5	1	34.8	38.9	5.57	6.80	7.70	36.4	31.2	16.6	14.0
	2	42.7	45.7	6.57	6.99	6.80	35.8	29.4	18.1	15.9
	3	32.0	36.2	5.97	8.22	6.71	38.2	31.7	16.0	15.2
	Mean	*36.5*	*40.2*	*6.04*	*7.33*	*7.07*	*36.8*	*30.8*	*16.9*	*15.1*
	SD	*4.55*	*3.99*	*0.411*	*0.629*	*0.447*	*1.02*	*0.988*	*0.883*	*0.785*
	%RSD	*12.5*	*9.9*	*6.8*	*8.6*	*6.3*	*2.8*	*3.2*	*5.2*	*5.2*

* See the article for details of subtraction of chloroform interference.

Table S5. Precision data for BTEX, with the mean and standard deviation (SD) shown in ppbV measured in the headspace, RSD as a percentage.

Solution Conc. / μg L^{-1}	**Replicate No. / *Statistical Parameter***	**Benzene (NO^+ 78)**	**Toluene (NO^+ 92)**	**Ethylbenzene + Xylenes (NO^+ 106)**	**Ethylbenzene (O_2^+ 91 and 106)***	**Xylenes (O_2^+ 91 and 106)***
1	1	17.2	16.4	25.1	13.3	11.7
	2	15.8	15.3	25.8	13.3	12.5
	3	13.2	13.2	22.5	10.9	11.7
	4	14.9	15.1	24.9	13.1	11.8
	5	16.4	14.8	25.4	12.1	13.3
	6	15.4	15.5	23.7	11.2	12.4
	Mean	*15.5*	*15.0*	24.6	*12.3*	*12.2*
	SD	*1.25*	*0.964*	1.128	*0.980*	*0.579*
	%RSD	*8.1*	*6.4*	4.6	*8.0*	*4.7*
5	1	95.9	94.8	154	74.4	79.9
	2	98.8	100	158	80.7	77.3
	3	109	106	181	94.7	85.9
	4	97.8	104	159	77.0	82.3
	5	110	104	159	78.0	80.7
	6	102	108	159	81.3	77.8
	Mean	*102*	*103*	161.7	*81.0*	*80.6*
	SD	*5.36*	*4.48*	8.67	*6.56*	*2.91*
	%RSD	*5.2*	*4.3*	5.4	*8.1*	*3.6*
9	1	196	197	314	158	156
	2	196	192	318	160	158
	3	171	178	279	143	135
	4	201	199	315	157	157
	5	187	188	307	153	154
	6	209	205	328	162	165
	Mean	*193*	*194*	310	*155*	*154*
	SD	*12.0*	*8.63*	15.27	*6.25*	*9.20*
	%RSD	*6.2*	*4.5*	4.9	*4.0*	*6.0*

* See the article for details of deconvolution of ethylbenzene and the xylenes using the O_2^+ product ions.

Table S6. Precision data for the individual quantitation ions of the THM compounds, with the mean and standard deviation (SD) shown in ppbV measured in the headspace, and RSD as a percentage.

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Bromodichloromethane (O_2^+ 83)*	Bromodichloromethane (O_2^+ 85)*	Bromoform (O_2^+ 171)	Bromoform (O_2^+ 173)	Bromoform (O_2^+ 175)	Chloroform (OH^- 117)	Chloroform (OH^- 119)	Dibromochloromethane (O_2^+ 127)	Dibromochloromethane (O_2^+ 129)
10	1	136	126	13.0	13.9	14.4	91.6	91.2	38.5	38.1
	2	92.4	100	14.0	15.5	13.9	96.5	93.2	39.3	36.2
	3	118	98.1	10.3	14.5	12.7	81.5	89.3	33.7	35.9
	4	99.7	111	12.3	13.6	15.2	92.5	93.0	33.8	35.5
	5	112	103	13.9	14.5	12.1	87.1	91.5	36.5	38.8
	6	98.4	92.9	12.9	14.3	15.9	96.5	94.0	40.3	40.1
	Mean	*109*	*105*	*12.7*	*14.4*	*14.1*	*91.0*	*92.0*	*37.0*	*37.4*
	SD	*14.7*	*10.9*	*1.24*	*0.60*	*1.32*	*5.30*	*1.56*	*2.58*	*1.68*
	%RSD	*13.4*	*10.4*	*9.7*	*4.1*	*9.4*	*5.8*	*1.7*	*7.0*	*4.5*
50	1	605	546	81.5	96.3	93.5	729	687	232	227
	2	589	529	80.3	92.0	83.4	746	718	223	234
	3	806	527	97.3	106	111	690	785	286	274
	4	521	547	89.4	80.5	87.1	757	686	236	241
	5	736	706	90.9	86.8	87.6	767	713	264	243
	6	661	664	94.3	97.7	89.9	789	754	262	264
	Mean	*653*	*586*	*88.9*	*93.3*	*92.0*	*746*	*724*	*251*	*247*
	SD	*95.0*	*71.2*	*6.2*	*8.2*	*8.8*	*31.2*	*35.6*	*21.9*	*16.5*
	%RSD	*14.5*	*12.1*	*7.0*	*8.8*	*9.6*	*4.2*	*4.9*	*8.7*	*6.7*
90	1	845	890	156	173	156	1523	1394	427	429
	2	1034	1052	153	158	149	1453	1294	445	422
	3	944	812	136	165	152	1133	1084	376	387
	4	1047	1012	158	150	155	1413	1294	442	443
	5	813	826	154	157	155	1473	1344	401	426
	6	1145	1119	158	156	176	1523	1434	477	476
	Mean	*971*	*952*	*153*	*160*	*157*	*1419*	*1307*	*428*	*431*
	SD	*117*	*116*	*7.61*	*7.34*	*8.74*	*134*	*112*	*32.5*	*26.5*
	%RSD	*12.0*	*12.2*	*5.0*	*4.6*	*5.6*	*9.4*	*8.6*	*7.6*	*6.2*

* See the article for details of subtraction of chloroform interference.

Table S7. Measured concentrations (in μg L^{-1}) in a drinking water sample (Cambridge, UK)for BTEX using the individual quantitation ions. The mean, standard deviation (SD), and RSD are also shown.

Amount / μg L^{-1}	Benzene (NO^+ 78)	Toluene (NO^+ 92)	Ethylbenzene + Xylenes (NO^+ 106)	Ethylbenzene (O_2^+ 91 and 106)*	Xylenes (O_2^+ 91 and 106)*
Repl. 1	0.05	−0.25	0.00	0.01	−0.03
Repl. 2	0.20	−0.30	0.01	0.01	0.01
Repl. 3	−0.11	−0.38	−0.02	−0.01	−0.04
Repl. 4	0.06	−0.27	0.00	0.01	−0.02
Repl. 5	0.12	−0.22	−0.02	0.01	−0.04
Repl. 6	0.08	−0.32	0.00	0.00	0.00
Mean	*0.07*	*−0.29*	*−0.01*	*0.01*	*−0.02*
SD	*0.09*	*0.05*	*0.01*	*0.01*	*0.02*
%RSD	*135.9*	*−17.5*	*−160.3*	*162.2*	*−95.3*

* See the article for details on deconvolution of ethylbenzene and the xylenes using the O_2^+ product ions.

Table S8. Measured concentrations (in μg L^{-1}) in a drinking water sample (Cambridge, UK) for the THMs using the individual quantitation ions. The mean, standard deviation (SD), and RSD are also shown.

Amount / μg L^{-1}	Bromodichloromethane (O_2^+ 83)*	Bromodichloromethane (O_2^+ 85)*	Bromoform (O_2^+ 171)	Bromoform (O_2^+ 173)	Bromoform (O_2^+ 175)	Chloroform (OH^- 117)	Chloroform (OH^- 119)	Dibromochloromethane (O_2^+ 127)	Dibromochloromethane (O_2^+ 129)
Repl. 1	3.34	1.48	8.62	6.58	9.53	0.30	0.22	3.71	4.16
Repl. 2	2.97	1.81	10.6	8.92	8.85	0.34	0.26	5.56	4.01
Repl. 3	7.62	5.40	8.46	6.74	7.65	0.26	0.48	4.74	4.24
Repl. 4	2.47	2.39	9.92	8.56	8.93	0.33	0.22	4.43	4.08
Repl. 5	1.98	2.09	10.7	6.42	9.46	0.51	0.33	4.17	3.83
Repl. 6	2.51	1.11	10.2	7.35	8.70	0.31	0.19	4.10	3.47
Mean	*3.48*	*2.38*	*9.73*	*7.43*	*8.85*	*0.34*	*0.29*	*4.45*	*3.97*
SD	*1.90*	*1.41*	*0.88*	*0.98*	*0.62*	*0.079*	*0.10*	*0.58*	*0.25*
%RSD	*54.5*	*59.4*	*9.0*	*13.1*	*7.0*	*23.1*	*34.2*	*13.1*	*6.4*

* See the article for details of subtraction of chloroform interference.

Table S9. Accuracy data (μg L^{-1} in solution) for BTEX spiked in triplicate at three levels in drinking water (Cambridge, UK). The mean, standard deviation (SD), and RSD (in %) are also shown.

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Benzene (NO^+ 78)	Toluene (NO^+ 92)	Ethylbenzene + Xylenes (NO^+ 106)	Ethylbenzene (O_2^+ 91 and 106)*	Xylenes (O_2^+ 91 and 106)*
2.5	1	2.29	2.09	2.17	2.30	2.05
	2	2.15	1.92	2.02	2.02	2.03
	3	2.26	2.02	2.13	2.12	2.14
	Mean	*2.24*	*2.01*	*2.11*	*2.15*	*2.07*
	SD	*0.060*	*0.067*	*0.061*	*0.12*	*0.047*
	%RSD	*2.66*	*3.34*	*2.90*	*5.41*	*2.29*
5.0	1	4.81	4.83	4.76	5.18	4.37
	2	4.66	4.18	4.78	4.97	4.61
	3	4.20	3.72	3.98	3.95	4.01
	Mean	*4.56*	*4.24*	*4.51*	*4.70*	*4.33*
	SD	*0.26*	*0.45*	*0.37*	*0.54*	*0.25*
	%RSD	*5.67*	*10.72*	*8.24*	*11.48*	*5.72*

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Benzene (NO^+ 78)	Toluene (NO^+ 92)	Ethylbenzene + Xylenes (NO^+ 106)	Ethylbenzene (O_2^+ 91 and 106)*	Xylenes (O_2^+ 91 and 106)*
7.5	1	7.18	6.68	7.35	7.31	7.39
	2	6.83	6.48	6.78	7.10	6.49
	3	7.24	6.68	7.19	7.88	6.57
	Mean	*7.08*	*6.62*	*7.11*	*7.43*	*6.82*
	SD	*0.18*	*0.094*	*0.24*	*0.33*	*0.41*
	%RSD	*2.55*	*1.42*	*3.37*	*4.40*	*5.94*

* See the article for details of deconvolution of ethylbenzene and the xylenes using the O_2^+ product ions.

Table S10. Accuracy data (μg L^{-1} in solution) for the individual quantitation ions of the THMs spiked in triplicate at three levels in drinking water (Cambridge, UK). The mean, standard deviation (SD), and RSD (in %) are also shown.

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Bromodichloromethane* (O_2^+ 83)*	Bromodichloromethane (O_2^+ 85)*	Bromoform (O_2^+ 171)	Bromoform (O_2^+ 173)	Bromoform (O_2^+ 175)	Chloroform (OH^- 117)	Chloroform (OH^- 119)	Dibromochloromethane (O_2^+ 127)	Dibromochloromethane (O_2^+ 129)
25	1	31.6	27.1	37.9	35.9	38.6	23.1	23.9	33.5	31.0
	2	33.3	36.8	52.9	45.4	39.6	18.9	20.2	34.0	33.8
	3	32.9	27.9	37.7	31.0	33.0	20.6	21.7	31.0	28.9
	Mean	*32.6*	*30.6*	*42.8*	*37.4*	*37.1*	*20.9*	*21.9*	*32.8*	*31.2*
	SD	*0.74*	*4.4*	*7.1*	*6.0*	*2.9*	*1.7*	*1.5*	*1.3*	*2.0*
	%RSD	*2.3*	*14.3*	*16.6*	*16.1*	*7.8*	*8.2*	*6.9*	*4.1*	*6.4*
50	1	107.3	117.0	68.5	61.2	63.4	29.9	29.7	57.6	59.5
	2	61.2	57.3	69.0	58.5	58.6	44.5	46.6	55.8	51.4
	3	40.3	38.6	55.6	48.9	49.9	42.3	43.1	48.9	46.5
	Mean	*69.6*	*71.0*	*64.4*	*56.2*	*57.3*	*38.9*	*39.8*	*54.1*	*52.5*
	SD	*28.0*	*33.5*	*6.2*	*5.3*	*5.6*	*6.4*	*7.3*	*3.8*	*5.4*
	%RSD	*40.2*	*47.2*	*9.6*	*9.4*	*9.8*	*16.6*	*18.3*	*6.9*	*10.2*
75	1	93.2	86.6	90.8	81.1	90.5	68.5	71.3	78.6	80.9
	2	88.7	78.6	82.6	74.0	76.9	64.7	67.2	72.7	72.5
	3	83.9	88.9	77.9	76.1	76.9	71.4	69.4	86.5	73.0
	Mean	*88.6*	*84.7*	*83.8*	*77.1*	*81.5*	*68.2*	*69.3*	*79.3*	*75.5*
	SD	*3.8*	*4.4*	*5.3*	*3.0*	*6.4*	*2.8*	*1.7*	*5.7*	*3.9*
	%RSD	*4.3*	*5.2*	*6.3*	*3.9*	*7.9*	*4.1*	*2.5*	*7.1*	*5.1*

* See the article for details of subtraction of chloroform interference.

Table S11. Recovery data (%) for BTEX spiked in triplicate at three levels in drinking water (Cambridge, UK). The mean, standard deviation (SD), and RSD are also shown.

Solution Conc. / μg L^{-1}	**Replicate No. / *Statistical Parameter***	**Benzene (NO^+ 78)**	**Toluene (NO^+ 92)**	**Ethylbenzene + Xylenes (NO^+ 106)**	**Ethylbenzene (O_2^+ 91 and 106)***	**Xylenes (O_2^+ 91 and 106)***
2.5	1	91.8	83.5	86.6	92.0	81.8
	2	86.2	77.0	80.9	80.7	81.2
	3	90.4	80.9	85.2	84.9	85.5
	Mean	*89.5*	*80.5*	*84.2*	*85.9*	*82.8*
	SD	*2.4*	*2.7*	*2.4*	*4.6*	*1.9*
	%RSD	*2.7*	*3.3*	*2.9*	*5.4*	*2.3*
5.0	1	96.2	96.6	95.1	103.7	87.4
	2	93.3	83.5	95.6	99.4	92.2
	3	84.1	74.4	79.6	79.0	80.2
	Mean	*91.2*	*84.8*	*90.1*	*94.0*	*86.6*
	SD	*5.2*	*9.1*	*7.4*	*10.8*	*5.0*
	%RSD	*5.7*	*10.7*	*8.2*	*11.5*	*5.7*
7.5	1	95.7	89.1	98.0	97.4	98.5
	2	91.0	86.5	90.4	94.7	86.6
	3	96.5	89.1	95.8	105.0	87.6
	Mean	*94.4*	*88.2*	*94.8*	*99.1*	*90.9*
	SD	*2.4*	*1.3*	*3.2*	*4.4*	*5.4*
	%RSD	*2.5*	*1.4*	*3.4*	*4.4*	*5.9*

* See the article for details of deconvolution of ethylbenzene and the xylenes using the O_2^+ product ions.

Table S12. Recovery data (%) for the individual quantitation ions of the THMs spiked in triplicate at three levels in drinking water (Cambridge, UK). The mean, standard deviation (SD), and RSD are also shown.

Solution Conc. / μg L^{-1}	Replicate No. / *Statistical Parameter*	Bromodichloromethane (O_2^+ 83)*	Bromodichloromethane (O_2^+ 85)*	Bromoform (O_2^+ 171)	Bromoform (O_2^+ 173)	Bromoform (O_2^+ 175)	Chloroform (OH^- 117)	Chloroform (OH^- 119)	Dibromochloromethane (O_2^+ 127)	Dibromochloromethane (O_2^+ 129)
25	1	112.4	99.0	112.7	113.8	119.1	94.4	91.1	116.3	108.0
	2	119.2	137.5	172.6	152.0	123.0	79.7	74.4	118.3	119.2
	3	117.8	102.0	112.0	94.1	96.7	85.5	81.1	106.0	99.8
	Mean	*116.5*	*112.8*	*132.4*	*120.0*	*112.9*	*86.5*	*82.2*	*113.6*	*109.0*
	SD	*2.9*	*17.5*	*28.4*	*24.0*	*11.6*	*6.1*	*6.9*	*5.4*	*7.9*
	%RSD	*2.5*	*15.5*	*21.4*	*20.0*	*10.3*	*7.0*	*8.3*	*4.7*	*7.3*
50	1	207.6	229.3	117.5	107.5	109.1	58.9	59.0	106.3	111.1
	2	115.4	109.8	118.5	102.1	99.4	92.7	88.3	102.7	94.8
	3	73.6	72.4	91.8	82.9	82.0	85.6	83.9	88.9	85.1
	Mean	*132.2*	*137.2*	*109.3*	*97.5*	*96.8*	*79.1*	*77.1*	*99.3*	*97.0*
	SD	*56.0*	*66.9*	*12.4*	*10.6*	*11.2*	*14.5*	*12.9*	*7.5*	*10.7*
	%RSD	*42.3*	*48.8*	*11.3*	*10.9*	*11.6*	*18.4*	*16.7*	*7.6*	*11.1*
75	1	119.7	112.3	108.1	98.2	108.9	94.7	90.9	98.9	102.6
	2	113.6	101.6	97.2	88.7	90.8	89.2	85.8	91.0	91.4
	3	107.3	115.4	90.9	91.6	90.8	92.2	94.8	109.5	92.1
	Mean	*113.5*	*109.8*	*98.7*	*92.8*	*96.8*	*92.0*	*90.5*	*99.8*	*95.4*
	SD	*5.1*	*5.9*	*7.1*	*4.0*	*8.5*	*2.3*	*3.7*	*7.6*	*5.1*
	%RSD	*4.5*	*5.4*	*7.2*	*4.3*	*8.8*	*2.5*	*4.1*	*7.6*	*5.4*

* See the article for details of subtraction of chloroform interference.