Supplementary Information

Penetration of polar brominated DBPs through the activated carbon columns during total organic bromine analysis

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This supplementary information includes 5 pages, 2 tables, and 3 figures.

Table S1 Ion intensities in the ESI-tqMS PIS spectra of *m/z* 79 of the chlorinated SRHA sample.

Table S2 Ion intensities in the ESI-tqMS PIS spectra of *m/z* 79 of the chlorinated wastewater effluent sample.

Fig. S1 Relationship of molecular ion intensity to molecular weight of polar brominated DBPs formed in chlorinated SRFA.

Fig. S2 Minimization of the penetration of polar brominated DBPs formed in chlorinated SRFA when OAC was used in the TOBr method.

Fig. S3 ESI-tqMS PIS spectra of the chlorinated SRHA sample: (a) ORI PIS m/z 81, (b) ORI PIS m/z 79, (c) FAC PIS m/z 79, (d) FOAC PIS m/z 79, (e) FAC PIS m/z 79 enlarged, and (f) FOAC PIS m/z 79 enlarged. (a), (b), (c), and (d) are on the same y-axis scale (6.52×10^6); (e) and (f) are on the same y-axis scale (1.14×10^6).

Table S1 Ion intensities in the ESI-tqMS PIS spectra of *m/z* 79 of the chlorinated SRHA sample.

m/z	ORI	FAC	Change by AC vs. ORI	FOAC	Change by OAC vs. ORI	Change by OAC vs. AC
127/129	492227	54888	*–88.9%*	57698	*–88.3%*	*–5.1%*
137	96821	8623	*–91.1%*	25002	*–74.2%*	*189.9%*
142	146652	33983	*–76.8%*	5945	*–95.9%*	*–82.5%*
161/163/165	2557733	82574	*–96.8%*	43717	*–98.3%*	*–47.1%*
171/173	7897162	1550978	*–80.4%*	1183545	*–85.0%*	*–23.7%*
193	648107	4913	*–99.2%*	2439	*–99.6%*	*–50.4%*
205/207/209	2830034	76959	*–97.3%*	37354	*–98.7%*	*-51.5%*
215/217	1967954	129046	*–93.4%*	146514	*–92.6%*	*13.5%*
234	657497	106221	*–83.8%*	44447	*–93.2%*	*–58.2%*
251	214931	8979	*–95.8%*	2541	*–98.8%*	*–71.7%*
259	524823	3504	*–99.3%*	3168	*–99.4%*	*–9.6%*
268/270	907897	17942	*–98.0%*	6364	*–99.3%*	*–64.5%*
275/277	1027897	5510	*–99.5%*	21051	*–98.0%*	*282.1%*
293	330985	3484	*–98.9%*	2792	*–99.2%*	*–19.9%*
339	214325	10418	*–95.1%*	1333	*–99.4%*	*–87.2%*
353	107437	3047	*–97.2%*	1770	*–98.4%*	*–41.9%*
367	116739	3526	*–97.0%*	3210	*–97.3%*	*–9.0%*
373	107589	3504	*–96.7%*	1956	*–98.2%*	*–44.2%*
381/383	161553	8996	*–94.4%*	5872	*–96.4%*	*–34.7%*
389	81745	1251	*–98.5%*	5968	*–92.7%*	*377.1%*
TII	21784739	2263799	*–89.6%*	1734285	*–92.0%*	*–23.4%*

Table S2 Ion intensities in the ESI-tqMS PIS spectra of *m/z* 79 of the chlorinated wastewater effluent sample.

m/z	ORI	FAC	Change by AC vs. ORI	FOAC	Change by OAC vs. ORI	Change by OAC vs. AC
142	417314	142042	*–66.0%*	111400	*–73.3%*	*–21.6%*
164	276735	173562	*–37.3%*	68840	*–75.1%*	*–60.3%*
167	122176	50461	*–58.7%*	17621	*–85.6%*	*–65.1%*
171/173	496519	234875	*–52.7%*	122676	*–75.3%*	*–47.8%*
183/185	138899	82127	*–40.9%*	53743	*–61.3%*	*–34.6%*
189	101189	44315	*–56.2%*	84059	*–16.9%*	*89.7%*
193	525711	75490	*–85.6%*	40590	*–92.3%*	*–46.2%*
201/203/205	588177	136031	*–76.9%*	93615	*–84.1%*	*–31.2%*
215/217	1472538	368267	*–75.0%*	343748	*–76.7%*	*–6.7%*
220	72565	21301	*–70.6%*	10451	*–85.6%*	*–50.9%*
223	66691	18917	*–71.6%*	17599	*–73.6%*	*–7.0%*
230	199209	52495	*–73.6%*	14736	*–92.6%*	*–71.9%*
243	234446	33051	*–85.9%*	16327	*–93.0%*	*–50.6%*
249/251	308827	124826	*–59.6%*	80615	*–73.9%*	*–35.4%*
259/261	561810	110282	*–80.4%*	121486	*–78.4%*	*10.2%*
271/273	373653	51054	*–86.3%*	21761	*–94.2%*	*–57.4%*
274	158305	12458	*–92.1%*	21446	*–86.5%*	*72.1%*
280	125937	36572	*–71.0%*	16198	*–87.1%*	*–55.7%*
287	172562	8949	*–94.8%*	4432	*–97.4%*	*–50.5%*
288	107631	8949	*–91.7%*	10995	*–89.8%*	*22.9%*
294/296	1635975	74666	*–95.4%*	89964	*–94.5%*	*20.5%*
301	211592	37798	*–82.1%*	14130	*–93.3%*	*–62.6%*
313	209620	56756	*–72.9%*	21718	*–89.6%*	*–61.7%*
324	129097	30231	*–76.6%*	28909	*–77.6%*	*–4.4%*
328	424073	24546	*–94.2%*	19023	*–95.5%*	*–22.5%*
329	254974	24546	*–90.4%*	17245	*–93.2%*	*–29.7%*
356	297632	29995	*–89.9%*	8361	*–97.2%*	*–72.1%*
357	237465	15909	*–93.3%*	6705	*–97.2%*	*–57.9%*
387	168469	21011	*–87.5%*	36827	*–78.1%*	*75.3%*
401	340602	11101	*–96.7%*	31371	*–90.8%*	*182.6%*
409	134933	19670	*–85.4%*	12330	*–90.9%*	*–37.3%*
414	143995	20590	*–85.7%*	4956	*–96.6%*	*–75.9%*
44	127193	4433	*–96.5%*	672	*–99.5%*	*–84.8%*
453	111732	27907	*–75.0%*	4934	*–95.6%*	*–82.3%*
456	96434	17663	*–81.7%*	13231	*–86.3%*	*–25.1%*
464	107818	25044	*–76.8%*	4494	*–95.8%*	*–82.1%*
471	74737	5856	*–92.2%*	6729	*–91.0%*	*14.9%*
477	88380	3011	*–96.6%*	3554	*–96.0%*	*18.0%*
490	112213	12775	*–88.6%*	3636	*–96.8%*	*–71.5%*
494	91770	4224	*–95.4%*	4471	*–95.1%*	*5.8%*
TII	11519598	2253756	*–80.4%*	1605598	*–86.1%*	*–28.8%*

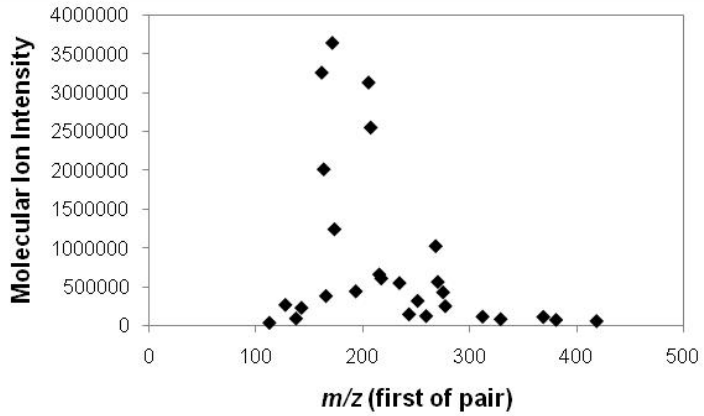

Fig. S1 Relationship of molecular ion intensity to molecular weight of polar brominated DBPs formed in chlorinated SRFA.

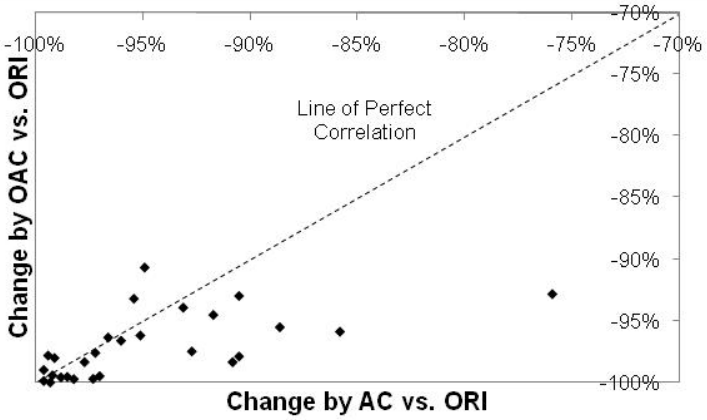

Fig. S2 Minimization of the penetration of polar brominated DBPs formed in chlorinated SRFA when OAC was used in the TOBr method.

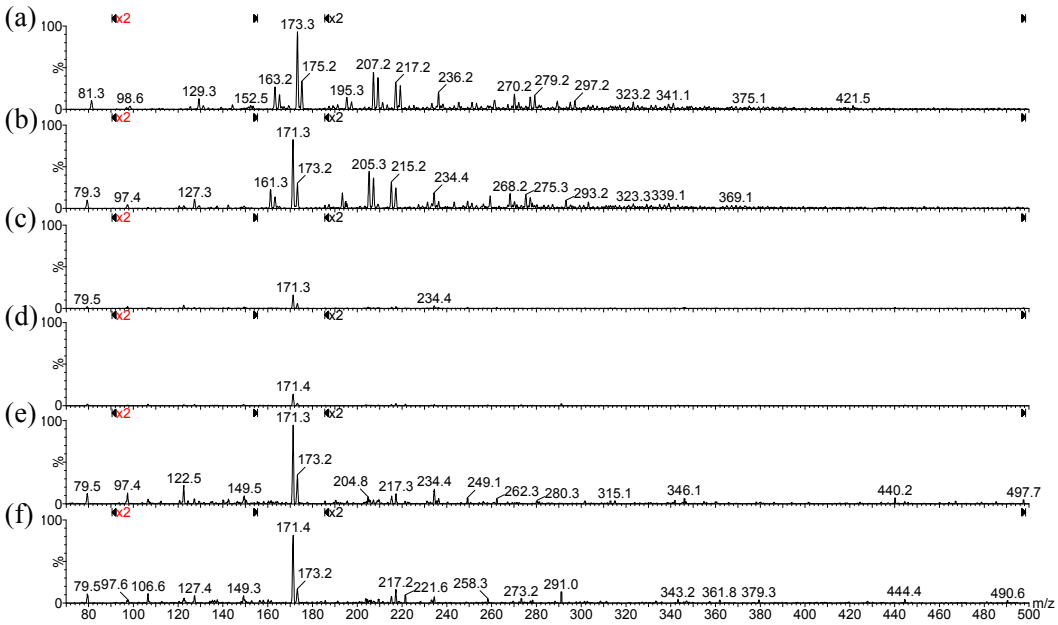

Fig. S3 ESI-tqMS PIS spectra of the chlorinated SRHA sample: (a) ORI PIS *m/z* 81, (b) ORI PIS *m/z* 79, (c) FAC PIS *m/z* 79, (d) FOAC PIS *m/z* 79, (e) FAC PIS *m/z* 79 enlarged, and (f) FOAC PIS *m/z* 79 enlarged. (a), (b), (c), and (d) are on the same y-axis scale (6.52×10^6); (e) and (f) are on the same y-axis scale (1.14×10^6).