

Table S1 Characteristic ion fragments (m/z) of the contaminants detected in wastewaters from the chemical production site and reference compounds used for quantification

Compound	m/z	Reference compound used for quantification (if different)
Bromoform	173, 175	
1,2,3,4-Tetrachlorobutane	123, 125	1,1,2,2-Tetrachlorethane
Chlorobicyclo[3.2.1]oct-2-ene	113, 142	
Dichlorobenzene	146, 148	
Chlorophenol	128, 130	
Dichlorophenol	162, 164	
Dichloroveratrol	191, 206	2,3-Dichloroanisole
Trichlorobenzoic acid ^a	207, 209	2,3,5-Trichlorobenzoic acid, methyl ester
Dichloroaniline	161, 163	
Trichloroaniline	195, 197	
Chlorofluoroaniline	145, 147	
Bromofluoroaniline	189, 191	
4-Bromo-2,6-dichloroaniline	239, 241	
2-Bromo-6-chloro-4-fluoroaniline	223, 225	
Chloroquinolinol	179, 181	
Chloroindole	151, 153	
5-Fluoroindole	108, 135	
Chlorothieno[2,3-c]pyridine	169, 171	2-Chlorobenzothiazole
2,3,5,6-Tetrafluorophenol ^b	137, 180	2,3,5,6-Tetrafluoroanisole
3'-(Trifluoromethyl)acetophenone	173, 188	
3,4-Dichloromethylthiobenzene	192, 194	
Dichlorothiophenol ^c	192, 194	3,4-Dichloromethylthiobenzene (derivatized from 3,4-dichlorothiophenol)
Tetramethylbutanedinitrile	69	3'-(Trifluoromethyl)acetophenone
3,3-Diphenyl-2-propenenitrile	165, 205	3'-(Trifluoromethyl)acetophenone
N-Formylmorpholine	110, 115	
Dimercaptomethane ^d	61, 108	2,5-Dithiohexane (derivatized from 1,2-dimercaptoethane)
1,2-Dimercaptoethane ^e	61, 122	2,5-Dithiohexane (derivatized from 1,2-dimercaptoethane)
2-(Methylthio)acetic acid ^a	74, 120	
TCPP (Tris(chloropropyl)phosphate)	277	
TEP (Triethylphosphate)	127, 155	
Tributylphosphate (TBP)	99, 211	
DBMP (Dibutylmethylphosphonate)	97	TEP
BEHP (Bis(2-ethylhexyl)hydrogen phosphate)	99, 211	
Bisphenol A	213, 228	
TXIB (Trimethylpentanedioldiisobutyrate)	111	
Benzoic acid ^a	105, 136	
Phenylacetic acid ^a	91, 150	
4- <i>tert</i> -Butylbenzoic acid ^a	177, 192	
DIPN (Diisopropyl-naphthalene)	197, 212	

^a Derivatized, detected and quantified as corresponding methylester

^b Methylation product 2,3,5,6-tetrafluoroanisole was detected and quantified.

^c Methylation product dichloromethylthiobenzene was detected and quantified.

^d Methylation product 2,4-dithiopentane was detected and quantified.

^e Methylation product 2,5-dithiohexane was detected and quantified.