Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Information

Reactivity-directed analysis – A novel approach for the identification of toxic organic electrophiles in drinking water

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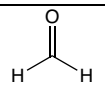
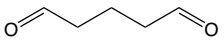
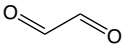
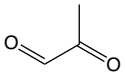
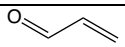
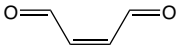
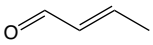
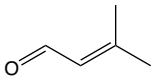
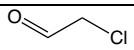
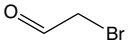
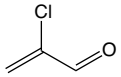
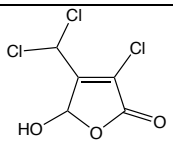
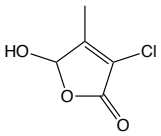
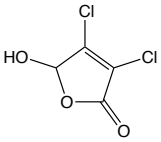
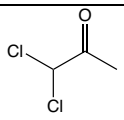
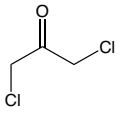
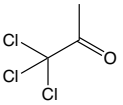
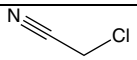
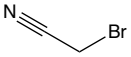
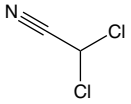
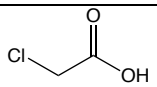
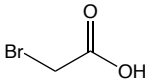
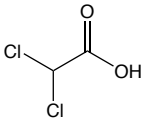
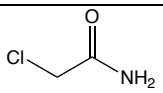
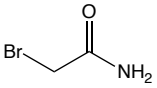
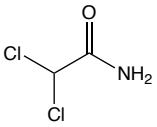
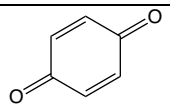
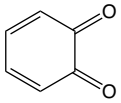
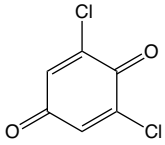
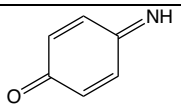
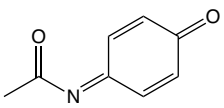
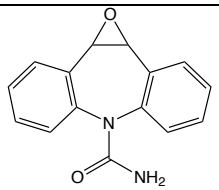
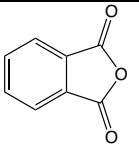
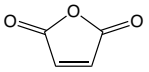
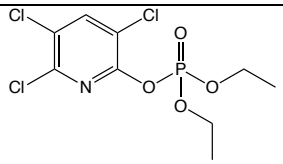
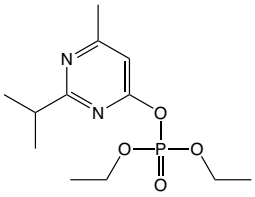
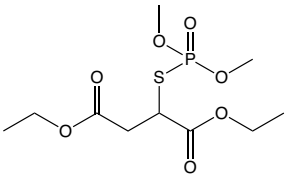
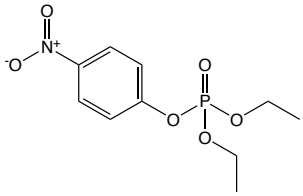
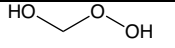
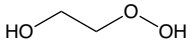
Content

Table S1. Electrophiles classes, chemical structures of electrophiles previously identified in drinking water and relevant precursors (pro-electrophiles).

Electrophile class	Examples		Relevant pro-electrophiles
Aldehydes	formaldehyde		aliphatic and aromatic compounds containing double bonds, amino acids
	acetaldehyde		
	glutaraldehyde		
	glyoxal		
	methylglyoxal		
α,β-Unsaturated aldehydes	acrolein		phenols, aromatics, unsaturated fatty acids
	2-butene-1,4-dial		
	crotonaldehyde		
	3-methyl-crotonaldehyde		
Haloaldehydes	chloroacetaldehyde		amino acids, low molecular weight NOM, phenolics
	bromoacetaldehyde		
	2-chloropropenal		
Chlorinated hydroxyfuranones	MX		fulvic acids, humic acids
	MCF		
	MCA		
Haloketones	1,1-dichloropropanone		amino acids, humic acids
	1,3-dichloropropanone		
	1,1,1-trichloropropanone		

Haloacetonitriles	chloroacetonitrile		phenols, DON, haloaldehydes
	bromoacetonitrile		
	dichloroacetonitrile		
Haloacetic acids	chloroacetic acid		hydrophilic, neutral NOM, hydrophobic NOM
	bromoacetic acid		
	dichloroacetic acid		
Haloacetamides	chloroacetamide		organic acids, phenols
	bromoacetamide		
	dichloroacetamide		
Quinones	benzoquinone		aromatic compounds, phenols, aromatic amines
	ortho-quinone		
	2,6-dichlorobenzoquinone		
Quinone imines	benzoquinone imine		aromatic amines
	N-acetyl-p-benzoquinone imine		

Epoxides	carbamazepine epoxide		unsaturated aliphatic and aromatic compounds
	oxirane		
	methyloxirane		
Cyclic anhydrides	phthalic anhydride		azo dyes, hydroxylated aromatics
	maleic anhydride		
Organo-phosphorus esters	chlorpyrifos oxon		thiophosphates such as chlorpyrifos, malathion, parathion
	diazinon oxon		
	malaoxon		
	parathion oxon		
Cyanogen halides	cyanogen chloride		aliphatic amino acids, formaldehyde
	cyanogen bromide		
Hydro-peroxides	Hydroxymethyl hydroperoxide		Unsaturated alkyl compounds, thymidine, vinyl chloride
	2-hydroxyethyl hydroperoxide		

Abbreviations: AOP – advanced oxidation process; ClO_2 – chlorine dioxide; DON – dissolved organic nitrogen; NOM – natural organic matter; MCA – 3,4-dichloro-5-hydroxy- 2(5H)-furanone; MCF – 3-chloro-4-methyl-5-hydroxy-2(5H)-furanone; MX – 3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone; S_N2 – Nucleophilic substitution; UV - ultraviolet.