

Supplementary Materials for

Occurrence of the persistent antimicrobial triclosan in microwave pretreated and anaerobically digested municipal sludges under various process conditions

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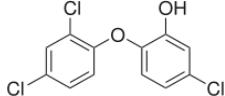
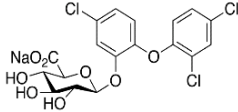
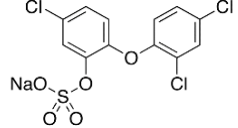
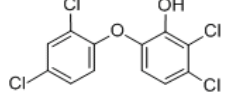
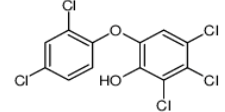
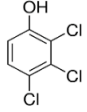
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Table S1. Further information about triclosan and five of its transformation products.

Analyte	IUPAC Name	Molecular Weight (g/mol)	Chemical structure
Parent compound			
Triclosan (TCS)	5-chloro-2-(2,4-dichlorophenoxy)phenol	289.54	
Transformation products			
Triclosan O-β-D-glucuronide	5-chloro-2-(2,4-dichlorophenoxy)phenyl β-D-glucopyranosiduronic acid	487.65 ^a	
Triclosan-O-Sulfate	Sodium 5-chloro-2-(2,4-dichlorophenoxy)phenyl sulfate	391.59 ^a	
Tetra-III	5,6-dichloro-2-(2,4-dichlorophenoxy)phenol	323.978	
Penta	4,5,6-trichloro-2-(2,4-dichlorophenoxy)phenol	358.432	
2,3,4-TCP	2,3,4-trichlorophenol	197.45	
Internal standard			
Triclocarban (TCC-d ₄)	1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea-d ₄	319.61	-

^aas sodium salt.

Table S2. Optimized MS/MS conditions used for each analyte quantification.

Compound	Ion Source	Parent ion (m/z)	Cone potential (V)	Fragment ion (m/z)	Collision Energy (V)	Capillary voltage (kV)	
						^a ESI-	^b ESI+
<i>Parent compound:</i>							
Triclosan (TCS)	ESI-	286.9	20	34.9	10	0.6	0.6
<i>Transformation products:</i>							
Triclosan O- β -D-glucuronide	ESI-	465.0	34	113.0	18	0.6	0.6
Triclosan-O-Sulfate	ESI-	368.9	34	288.9	18	0.6	0.6
Tetra-III	ESI-	322.8	24	34.9	12	0.6	0.6
Penta	ESI-	356.8	26	34.8	14	0.6	0.6
2,3,4-trichlorophenol	ESI-	194.8	38	158.8	18	0.6	0.6
Triclocarban-d ₄ (TCC-d ₄)	ESI-	317.0	44	129.9834 159.9541	24, 14	varies	varies

^anegative ionization mode, ^bpositive ionization mode.

Table S3. Validation of developed method for each analyte.

Compound	LOD^a (ppb)	LOQ^b (ppb)	RL^c (ppb)	Recovery (%)
<i>Parent compound:</i>				
Triclosan (TCS)	0.33	0.50	1.10	112.50
<i>Transformation products:</i>				
Triclosan O- β -D-glucuronide	1.44	5.22	5.46	107.24
Triclosan-O-Sulfate	0.12	0.31	0.50	317.64
Tetra-III	0.58	0.95	4.92	110.3
Penta	0.09	0.25	0.46	105.18
2,3,4-trichlorophenol	0.26	0.57	0.69	114.2

^aLOD: limit of detection, ^bLOQ: limit of quantification, ^cRL: reporting limit.