

Supplementary Data

Doxycycline transformation and emergence of antibacterially active products during
water disinfection with chlorine

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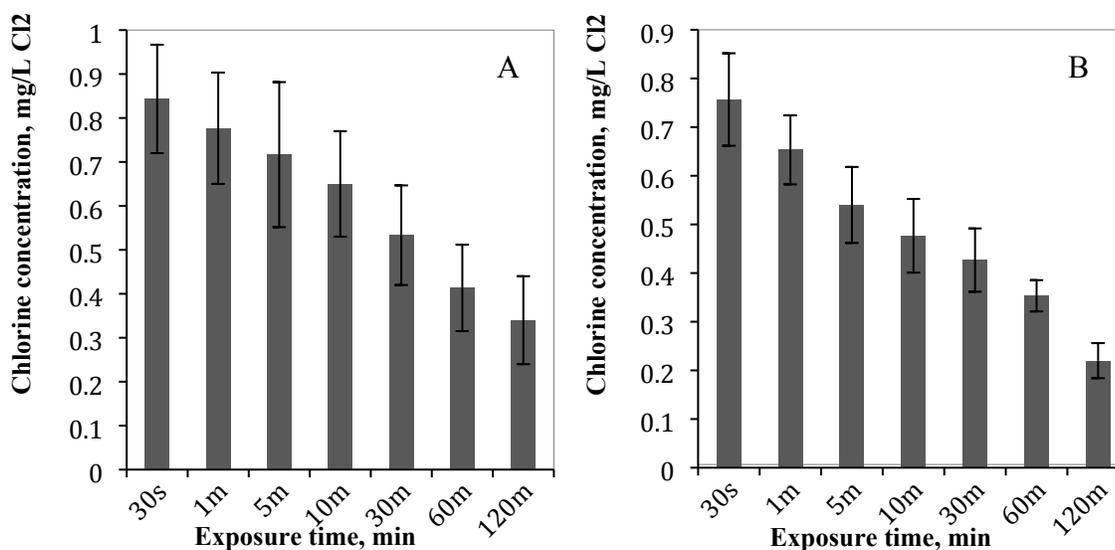


Figure S1. Chlorine concentration over time in ultrapure water (A) and wastewater (B). Results are based on three sets of replicated data. Error bars represent the standard deviation from three repeated experiments.

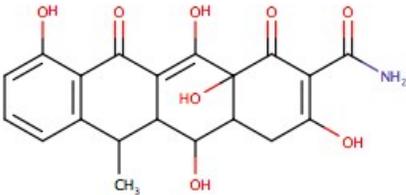
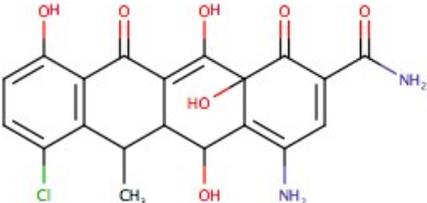
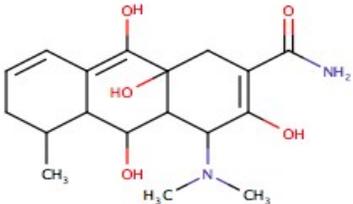
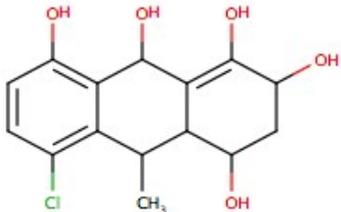
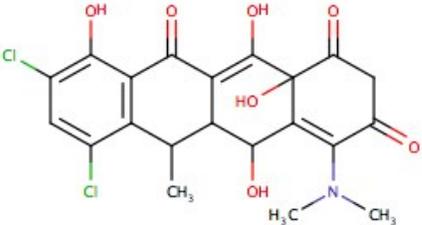
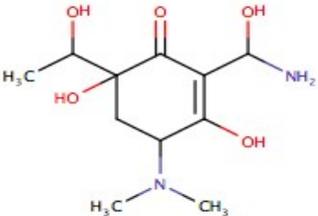
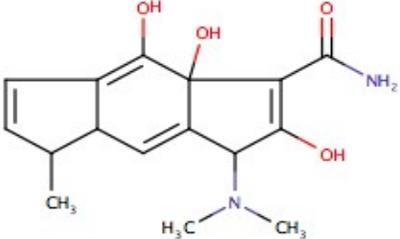
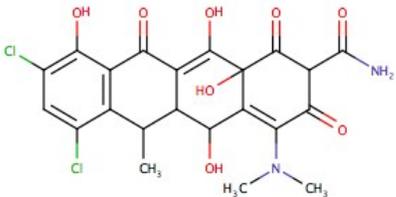
Transformation Product	Major Fragment	Proposed Structure of Fragment	Minor Fragment	Proposed Structure of Fragment
417	400 ¹		-	-
451	433 ²		-	-
479	349 ¹		312 ^{1,3}	
513	468 ⁴		260	
547	303 ²		511 ⁴	

Figure S2. Proposed transformation products with corresponding MS/MS fragments and proposed major/minor structures.

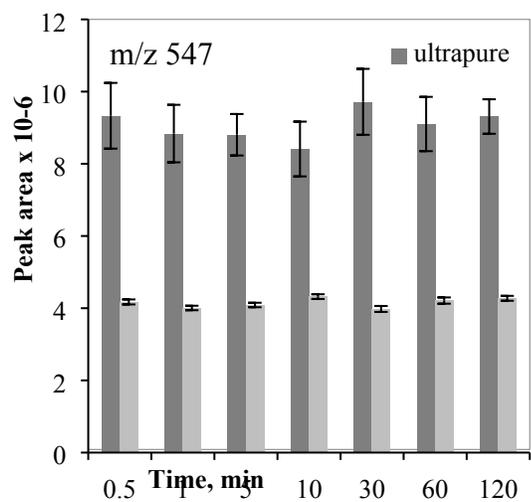
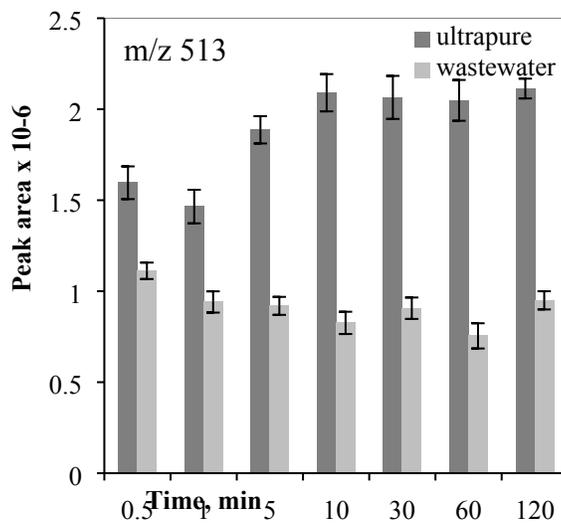
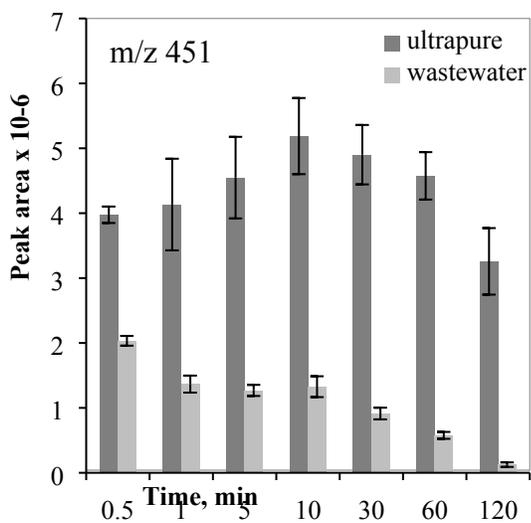
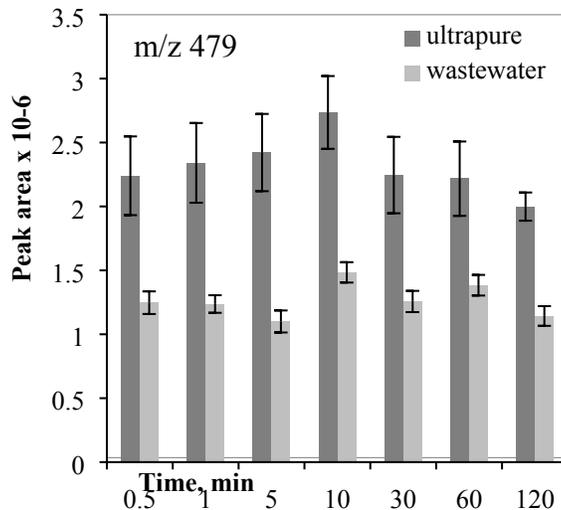
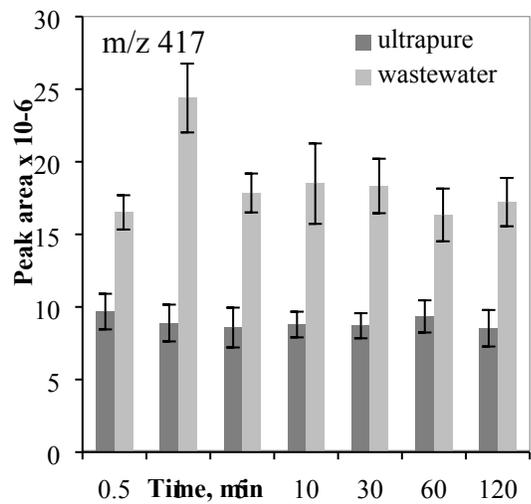


Figure S3. Transformation product mass spectrum peak area over time. Results are based on three sets of replicated data. Error bars represent the standard deviation from three repeated experiments.

References:

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