**Supplementary Data**

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

Nicole Kennedy Neth\(^a\), Clifford M. Carlin\(^b\) and Olya S. Keen\(^a,\#\)

\(^a\) University of North Carolina at Charlotte, Department of Civil and Environmental Engineering

\(^b\) University of North Carolina at Charlotte, Department of Chemistry

\(^\#\) corresponding author: okeen@uncc.edu, 704-687-5048

9201 University City Blvd, EPIC 3355

Charlotte, NC 28223

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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.
<table>
<thead>
<tr>
<th>Transformation Product</th>
<th>Major Fragment</th>
<th>Proposed Structure of Fragment</th>
<th>Minor Fragment</th>
<th>Proposed Structure of Fragment</th>
</tr>
</thead>
<tbody>
<tr>
<td>417</td>
<td>400&lt;sup&gt;1&lt;/sup&gt;</td>
<td><img src="image1" alt="Proposed Structure of Fragment" /></td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>451</td>
<td>433&lt;sup&gt;2&lt;/sup&gt;</td>
<td><img src="image2" alt="Proposed Structure of Fragment" /></td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>479</td>
<td>349&lt;sup&gt;3&lt;/sup&gt;</td>
<td><img src="image3" alt="Proposed Structure of Fragment" /></td>
<td>312&lt;sup&gt;1,3&lt;/sup&gt;</td>
<td><img src="image4" alt="Proposed Structure of Fragment" /></td>
</tr>
<tr>
<td>513</td>
<td>468&lt;sup&gt;4&lt;/sup&gt;</td>
<td><img src="image5" alt="Proposed Structure of Fragment" /></td>
<td>260</td>
<td><img src="image6" alt="Proposed Structure of Fragment" /></td>
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<tr>
<td>547</td>
<td>303&lt;sup&gt;2&lt;/sup&gt;</td>
<td><img src="image7" alt="Proposed Structure of Fragment" /></td>
<td>511&lt;sup&gt;4&lt;/sup&gt;</td>
<td><img src="image8" alt="Proposed Structure of Fragment" /></td>
</tr>
</tbody>
</table>

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: