

### Supplemental Information

Transformation of common antibiotics during water disinfection with chlorine and formation of antibacterially active products.

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Table S1. CT values for selected antibiotics

Antibiotic	CT Value			
	Ultrapure water (mg-min/L)		Wastewater (mg-min/L)	
	10 min	120 min	10 min	120 min
Ciprofloxacin	14.8	140	17.9	71.3
Levofloxacin	6.7	36.8	20.6	72.4
Ofloxacin	12.5	75.2	20.0	96.9
Trimethoprim	11.7	67.0	31.0	106.4
Sulfamethoxazole	16.9	192	17.8	81.0
Sulfamethoxazole/Trimethoprim	17.3	188	17.8	70.8

Table S2. Summary of antibiotics used, including initial concentration, initial chlorine concentration, and residual chlorine for both ultrapure water and wastewater. Error represents standard deviation from three repeated experiments.

Antibiotic	Antibiotic Initial concentration (mg/L)	Initial chlorine concentration (mg/L)		Residual Chlorine (mg/L as Cl <sub>2</sub> )			
		Ultrapure water	Wastewater	Ultrapure water	error	Wastewater	error
CIP	2.33	2.0	6.5	0.99	0.02	0.23	0.02
LVF	2.0	3.0	7.0	0.22	0.05	0.25	0.01
OFL	2.0	3.0	7.0	0.46	0.03	0.33	0.01
TMP	20	5.0	10	0.33	0.02	0.21	0.01
SMX	2.0	2.0	5.0	1.55	0.03	0.34	0.09
SMX/TMP	2.0/0.4	2.0	5.0	1.44	0.03	0.23	0.02

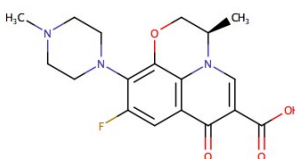
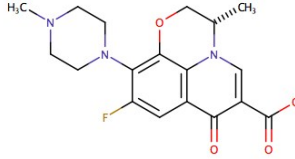
Ciprofloxacin (CIP), Levofloxacin (LVF), Ofloxacin (OFL), Trimethoprim (TMP), Sulfamethoxazole (SMX), Sulfamethoxazole/Trimethoprim (SMX/TMP)

Table S3. Antibiotics and their respective pK<sub>a</sub> values

Antibiotic	pK <sub>a1</sub>	pK <sub>a2</sub>	Reference
ciprofloxacin	4.34	10.03	1
sulfamethoxazole	1.6	5.7	2
trimethoprim	7.12	-	3
levofloxacin	5.59	7.94	1
ofloxacin*	5.56	7.94	1

\*Reflects pK<sub>a</sub> values of ofloxacin components: levofloxacin and dextroflaxacin

Table S4. The parent compounds of levofloxacin or dextroflaxacin (component of ofloxacin), both *m/z* 362.

<i>m/z</i>	RT	Chlorine	Levofloxacin	Dextroflaxacin
362	3.27	0		

### References:

1. Singh, B. K.; Parwate, D. V.; Shukla, S. K., Rapid Color Test Identification System for Screening of Counterfeit Fluoroquinolone. *E-Journal of Chemistry* **2009**, *6* (2), 377-384.
2. Boreen, A. L.; Arnold, W. A.; McNeill, K., Photochemical fate of sulfa drugs in the aquatic environment: sulfa drugs containing five-membered heterocyclic groups. *Environmental science & technology* **2004**, *38* (14), 3933-3940.
3. Perrin, D. D., *Dissociation constants of organic bases in aqueous solution: supplement 1972*. Butterworths: 1972.