SUPPLEMENTAL DATA

ASCE *Journal of Environmental Engineering*

Identification of Transformation Products for Benzotriazole, Triclosan, and Trimethoprim by Aerobic and Anoxic-Activated Sludge

Rebecca A. Trenholm, Brett J. Vanderford, Narasimman Lakshminarasimman, Drew C. McAvoy, and Eric R. V. Dickenson

DOI: 10.1061/(ASCE)EE.1943-7870.0001691

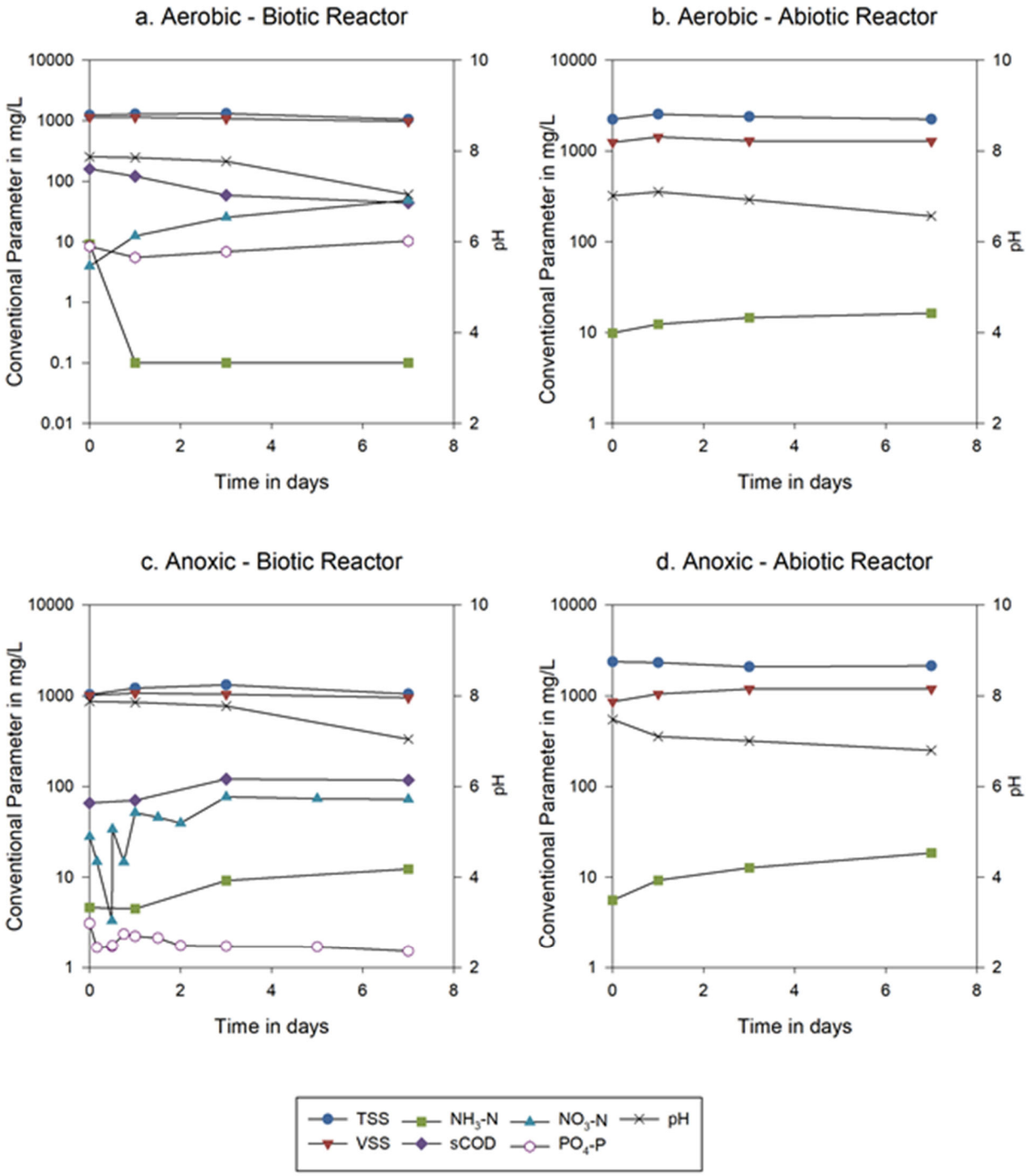


Fig. S1. Results from conventional parameters analysis in samples from biotic and abiotic reactors containing BNR activated sludge from aerobic and anoxic redox conditions.

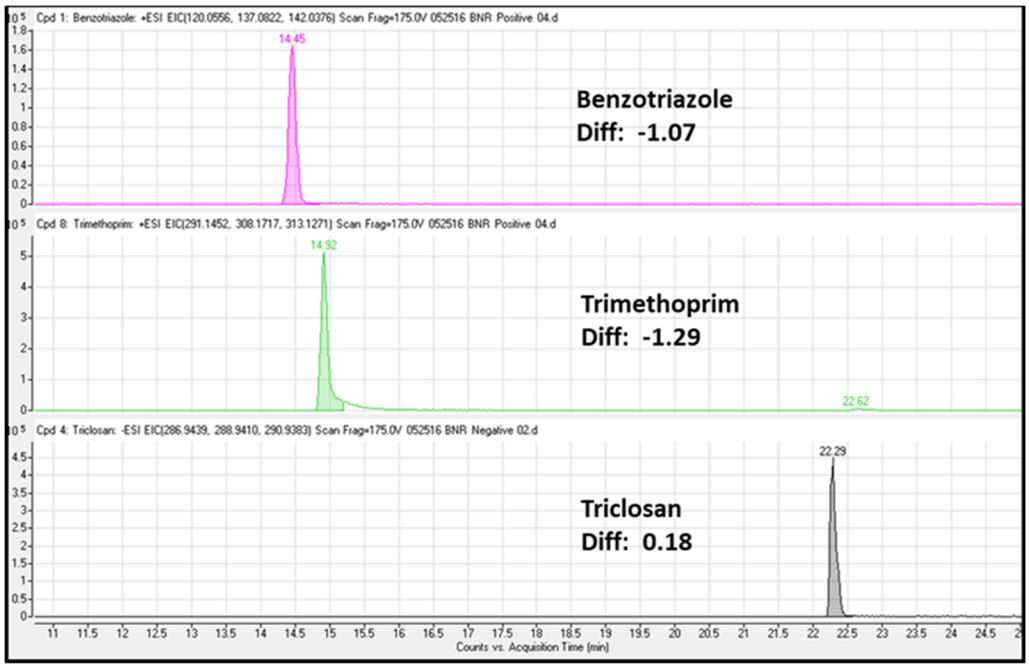


Fig. S2. Example chromatogram of parent compounds and Q-TOF results (includes the mass difference between the exact mass (calculated) and observed mass (accurate mass) of each standard)

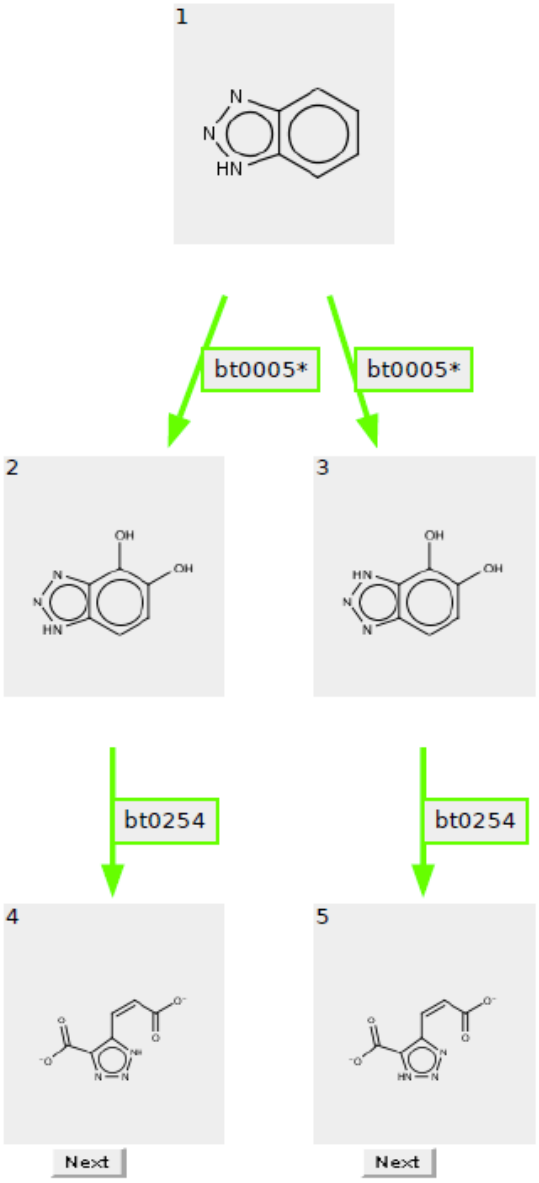


Fig. S3. EAWAG-PPS pathway for benzotriazole.

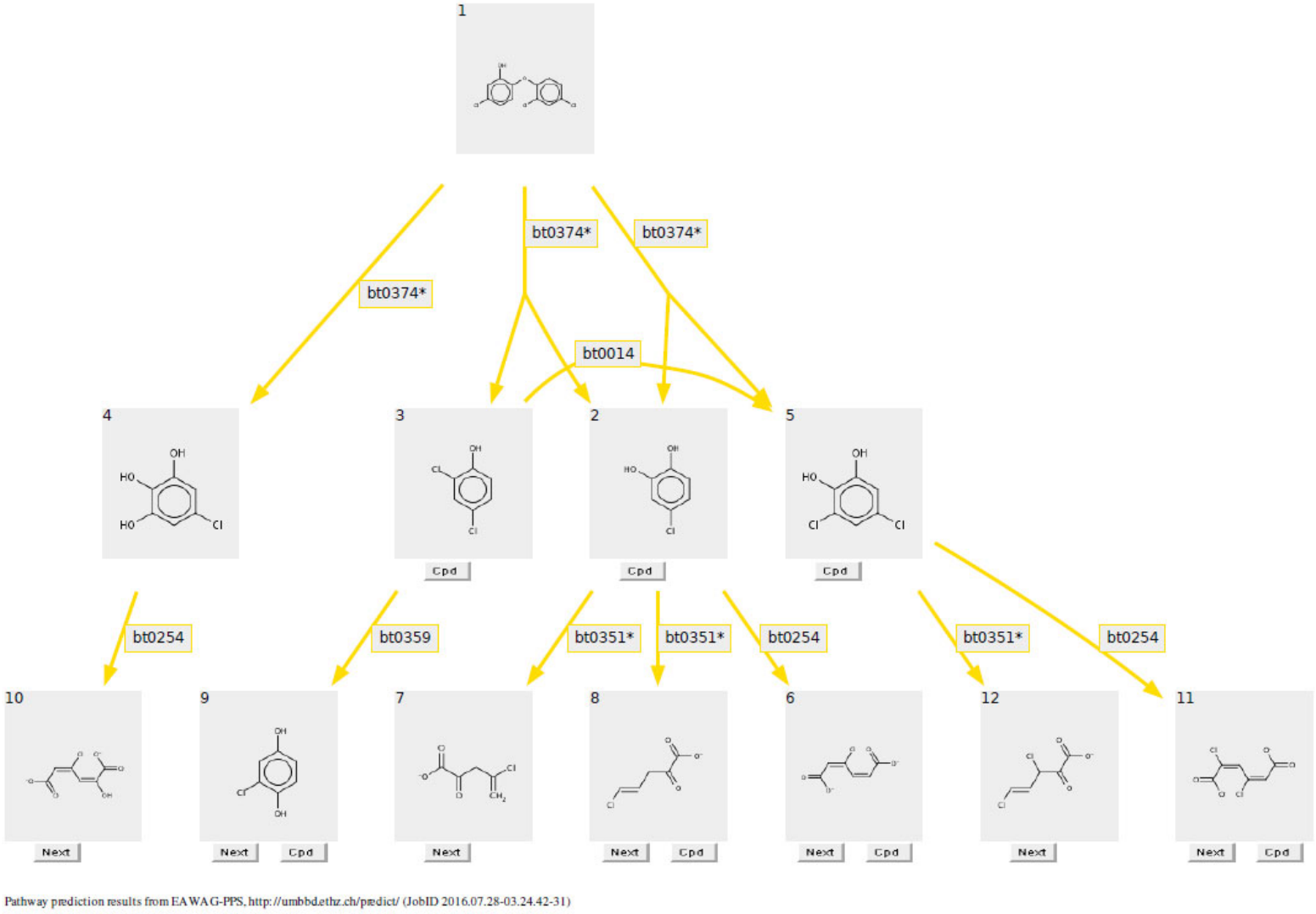


Fig. S4. EAWAG-PPS pathway for triclosan.

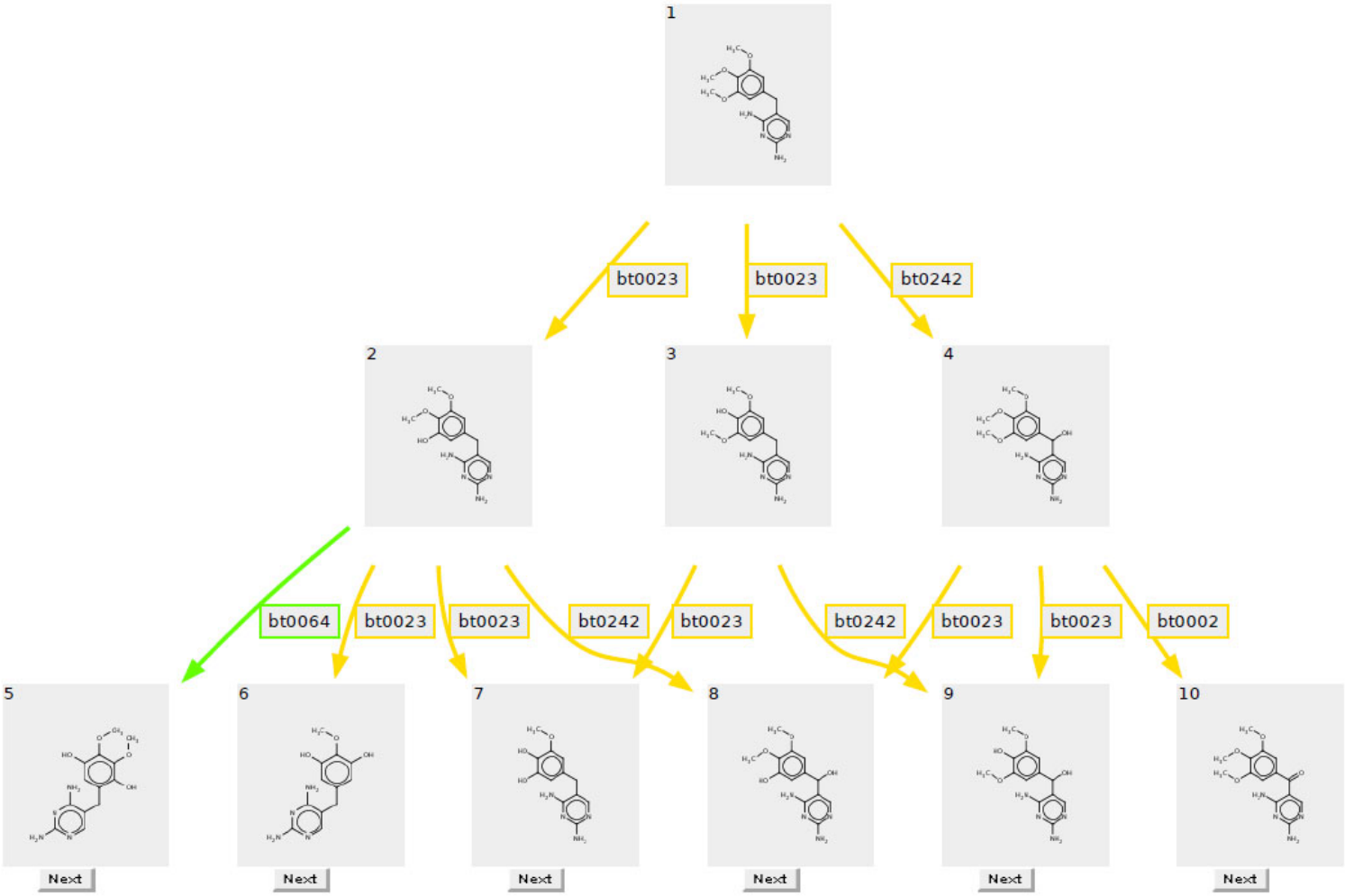
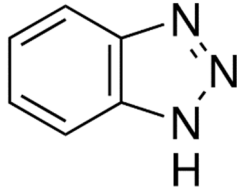
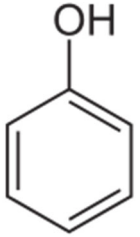
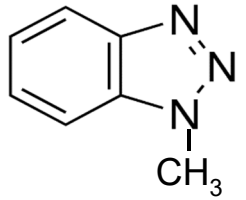
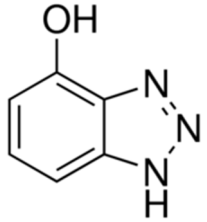
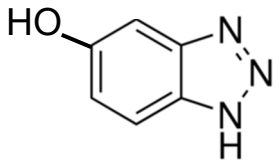
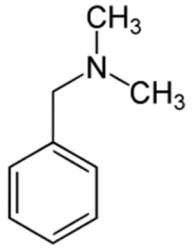
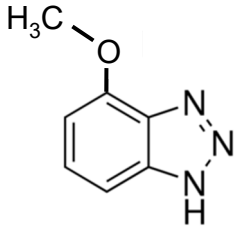
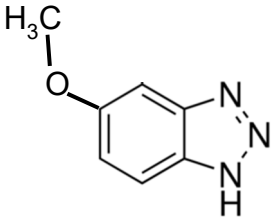
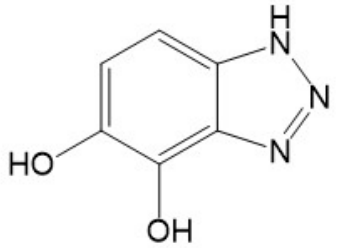
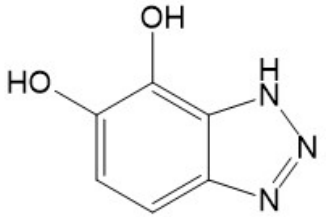
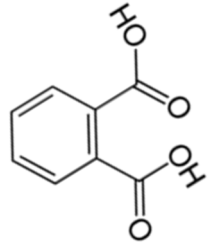
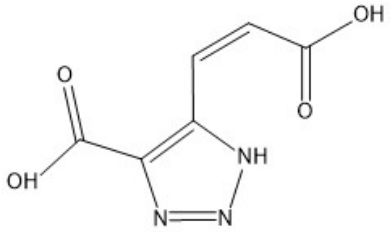
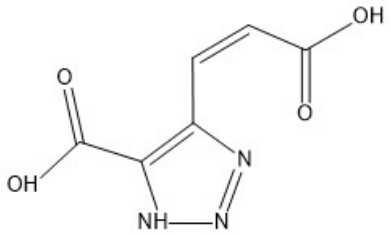
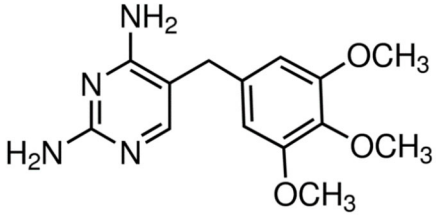
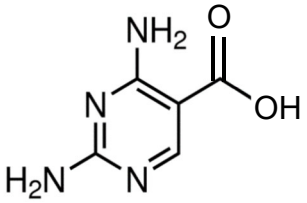
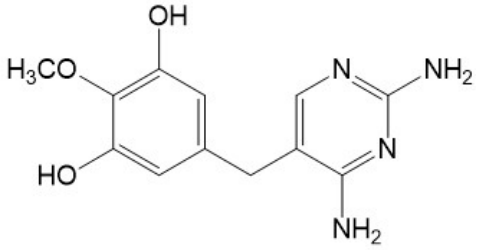


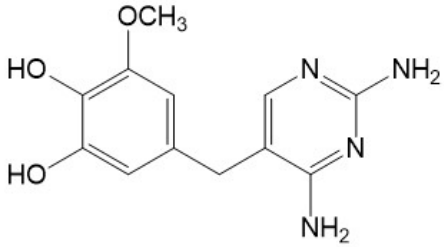
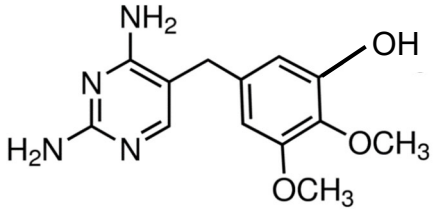
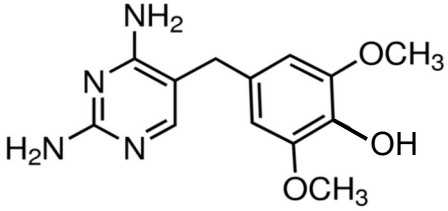
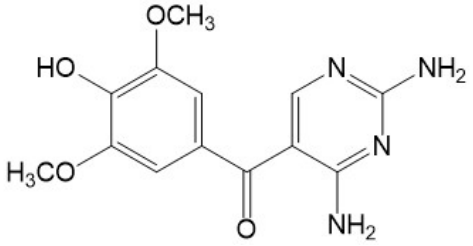
Fig. S5. EAWAG-PPS pathway for trimethoprim.

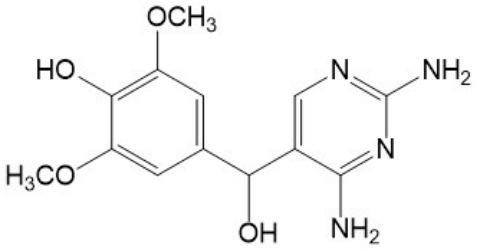
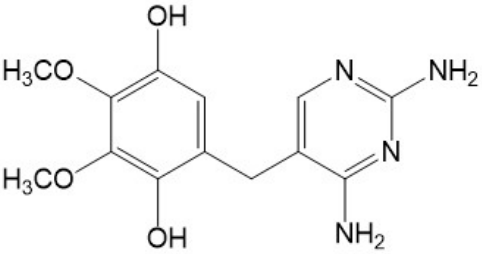
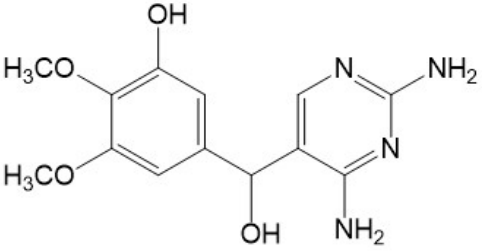
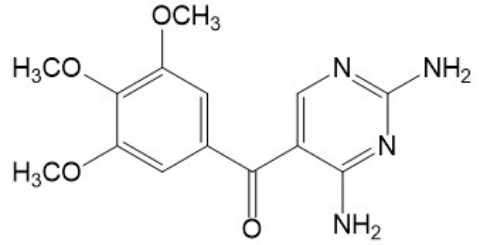
Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
Benzotriazole	$C_6H_5N_3$	119.04835	1H-benzo[d][1,2,3]triazole	
Phenol	C_6H_6O	94.04186	Phenol	
1-methylbenzotriazole	$C_7H_7N_3$	133.064	1-methyl-1H-benzo[d][1,2,3]triazole	
4-hydroxybenzotriazole	$C_6H_5N_3O$	135.04326	1H-benzo[d][1,2,3]triazol-4-ol	

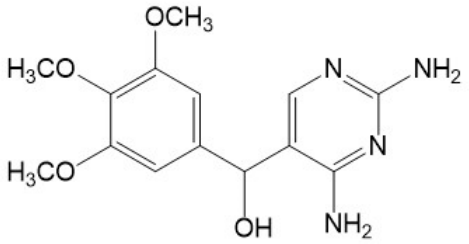
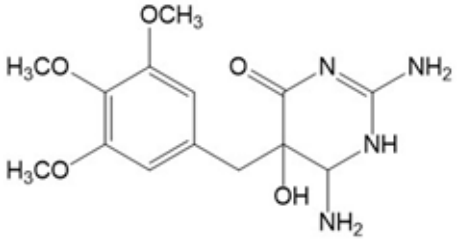
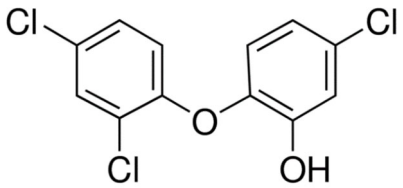
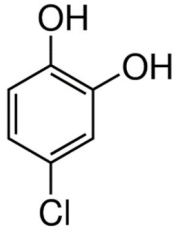
Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
5-hydroxybenzotriazole	$C_6H_5N_3O$	135.04326	1H-benzo[d][1,2,3]triazol-5-ol	
dimethylbenzylamine	$C_9H_{13}N$	135.1048	N,N-dimethyl-1-phenylmethanamine	
4-methoxybenzotriazole	$C_7H_7N_3O$	149.05891	4-methoxy-1H-benzo[d][1,2,3]triazole	
5-methoxybenzotriazole	$C_7H_7N_3O$	149.05891	5-methoxy-1H-benzo[d][1,2,3]triazole	

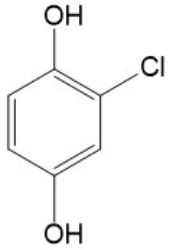
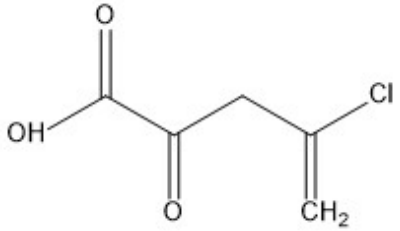
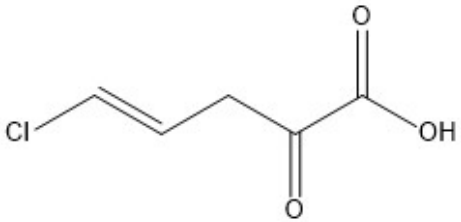
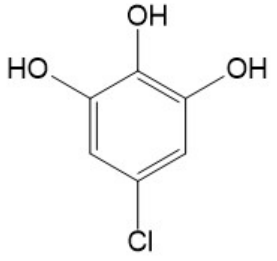
Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
benzotriazole -2	$C_6H_5N_3O_2$	151.03818	1H-benzo[d][1,2,3]triazole-4,5-diol	
benzotriazole -3	$C_6H_5N_3O_2$	151.03818	1H-benzo[d][1,2,3]triazole-6,7-diol	
phthalic acid	$C_8H_6O_4$	166.02661	phthalic acid	
benzotriazole -4	$C_6H_3N_3O_4$	181.01236	(Z)-5-(2-carboxyvinyl)-1H-1,2,3-triazole-4-carboxylic acid	

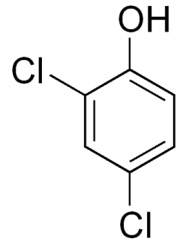
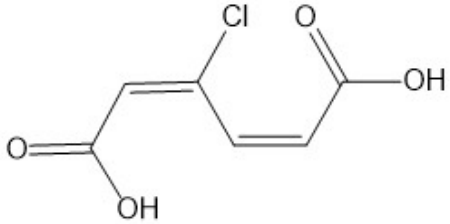
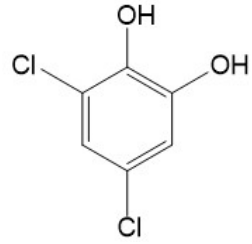
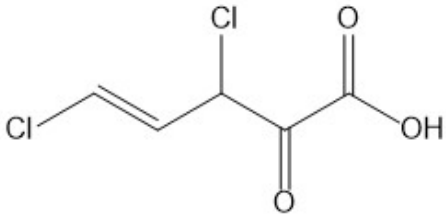
Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
benzotriazole -5	$C_6H_3N_3O_4$	181.01236	(Z)-4-(2-carboxyvinyl)-1H-1,2,3-triazole-5-carboxylic acid	
Trimethoprim	$C_{14}H_{18}N_4O_3$	290.13789	5-(3,4,5-trimethoxybenzyl)pyrimidine-2,4-diamine	
2,4-diaminopyrimidine-5-carboxylic acid (DAPC)	$C_5H_6N_4O_2$	154.04908	2,4-diaminopyrimidine-5-carboxylic acid	
trimethoprim -6	$C_{12}H_{14}N_4O_3$	262.10659	5-((2,4-diaminopyrimidin-5-yl)methyl)-2-methoxybenzene-1,3-diol	

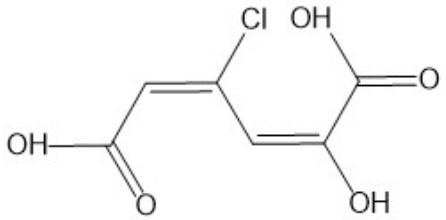
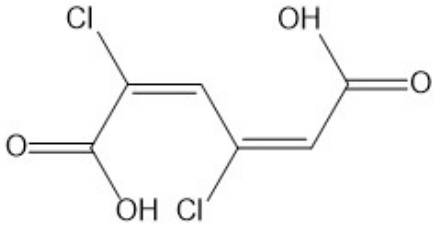
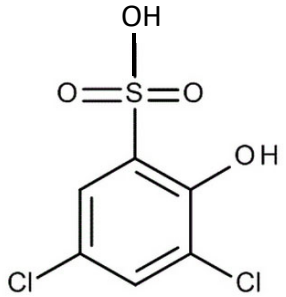
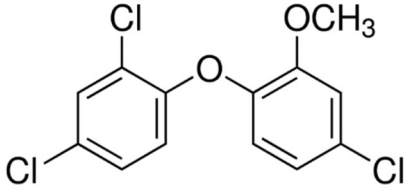
Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
trimethoprim -7	$C_{12}H_{14}N_4O_3$	262.10659	5-((2,4-diaminopyrimidin-5-yl)methyl)-3-methoxybenzene-1,2-diol	
3-desmethyl-trimethoprim	$C_{13}H_{16}N_4O_3$	276.12224	5-((2,4-diaminopyrimidin-5-yl)methyl)-2,3-dimethoxyphenol	
4-desmethyl-trimethoprim	$C_{13}H_{16}N_4O_3$	276.12224	4-((2,4-diaminopyrimidin-5-yl)methyl)-2,6-dimethoxyphenol	
TMP 290	$C_{13}H_{14}N_4O_4$	290.1015	(2,4-diaminopyrimidin-5-yl)(4-hydroxy-3,5-dimethoxyphenyl)methanone	

Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
TMP 292	$C_{13}H_{16}N_4O_4$	292.11716	4-((2,4-diaminopyrimidin-5-yl)(hydroxy)methyl)-2,6-dimethoxyphenol	
trimethoprim -5	$C_{13}H_{16}N_4O_4$	292.11716	5-((2,4-diaminopyrimidin-5-yl)methyl)-2,3-dimethoxybenzene-1,4-diol	
trimethoprim -8	$C_{13}H_{16}N_4O_4$	292.11716	5-((2,4-diaminopyrimidin-5-yl)(hydroxy)methyl)-2,3-dimethoxyphenol	
trimethoprim -10	$C_{14}H_{16}N_4O_4$	304.11716	(2,4-diaminopyrimidin-5-yl)(3,4,5-trimethoxyphenyl)methanone	

Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
TMP 306	$C_{14}H_{18}N_4O_4$	306.13281	(2,4-diaminopyrimidin-5-yl)(3,4,5-trimethoxyphenyl)methanol	
TMP 324	$C_{14}H_{20}N_4O_5$	324.14337	2,6-diamino-5-hydroxy-5-(3,4,5-trimethoxybenzyl)-5,6-dihydropyrimidin-4(1H)-one	
triclosan	$C_{12}H_7Cl_3O_2$	287.95116	5-chloro-2-(2,4-dichlorophenoxy)phenol	
4-chlorocatechol	$C_6H_5ClO_2$	143.99781	4-chlorobenzene-1,2-diol	

Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
triclosan -9	$C_6H_5ClO_2$	143.99781	2-chlorobenzene-1,4-diol	
triclosan -7	$C_5H_4ClO_3$	146.9849	4-chloro-2-oxopent-4-enoic acid	
triclosan -8	$C_5H_4ClO_3$	146.9849	(E)-5-chloro-2-oxopent-4-enoic acid	
triclosan -4	$C_6H_5ClO_3$	159.99272	5-chlorobenzene-1,2,3-triol	

Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
2,4-dichlorophenol	$C_6H_4Cl_2O$	161.96392	2,4-dichlorophenol	
triclosan -6	$C_6H_3ClO_4$	173.97199	(2E,4Z)-3-chlorohexa-2,4-dienedioic acid	
triclosan -5	$C_6H_4Cl_2O_2$	177.95883	3,5-dichlorobenzene-1,2-diol	
triclosan -12	$C_5H_3Cl_2O_3$	180.94592	(E)-3,5-dichloro-2-oxopent-4-enoic acid	

Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
triclosan -10	$C_6H_3ClO_5$	189.9669	(2E,4E)-4-chloro-2-hydroxyhexa-2,4-dienedioic acid	
triclosan -11	$C_6H_2Cl_2O_4$	207.93301	(2E,4E)-2,4-dichlorohexa-2,4-dienedioic acid	
3,5-dichloro-2-hydroxybenzene sulfonate	$C_6H_4Cl_2O_4S$	241.92073	3,5-dichloro-2-hydroxybenzenesulfonic acid	
methyl-triclosan	$C_{13}H_9Cl_3O_2$	301.96681	2,4-dichloro-1-(4-chloro-2-methoxyphenoxy)benzene	

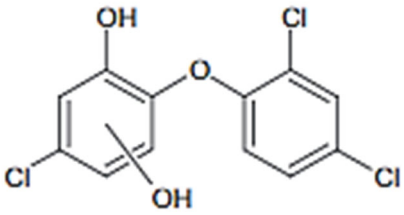
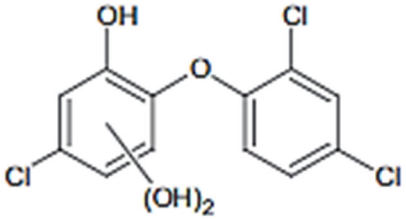
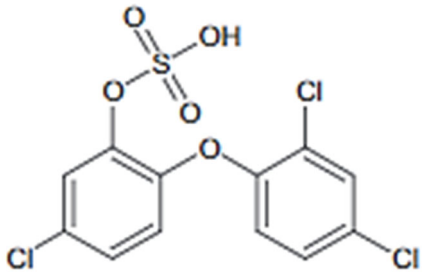
Compound	Molecular Formula	Molecular Weight	IUPAC Name	Structure
monohydroxytriclosan	$C_{12}H_7Cl_3O_3$	303.94608		
dihydroxytriclosan	$C_{12}H_7Cl_3O_4$	319.94099		
triclosan-o-sulfate	$C_{12}H_7Cl_3O_5S$	367.90798	5-chloro-2-(2,4-dichlorophenoxy)phenyl hydrogen sulfate	

Figure S6. Full list of possible transformation product intermediates for three parent compounds (in bold) used in the qualitative screening personal compounds database and their molecular formula, molecular weight, IUPAC name where no common name is given, and corresponding structure.

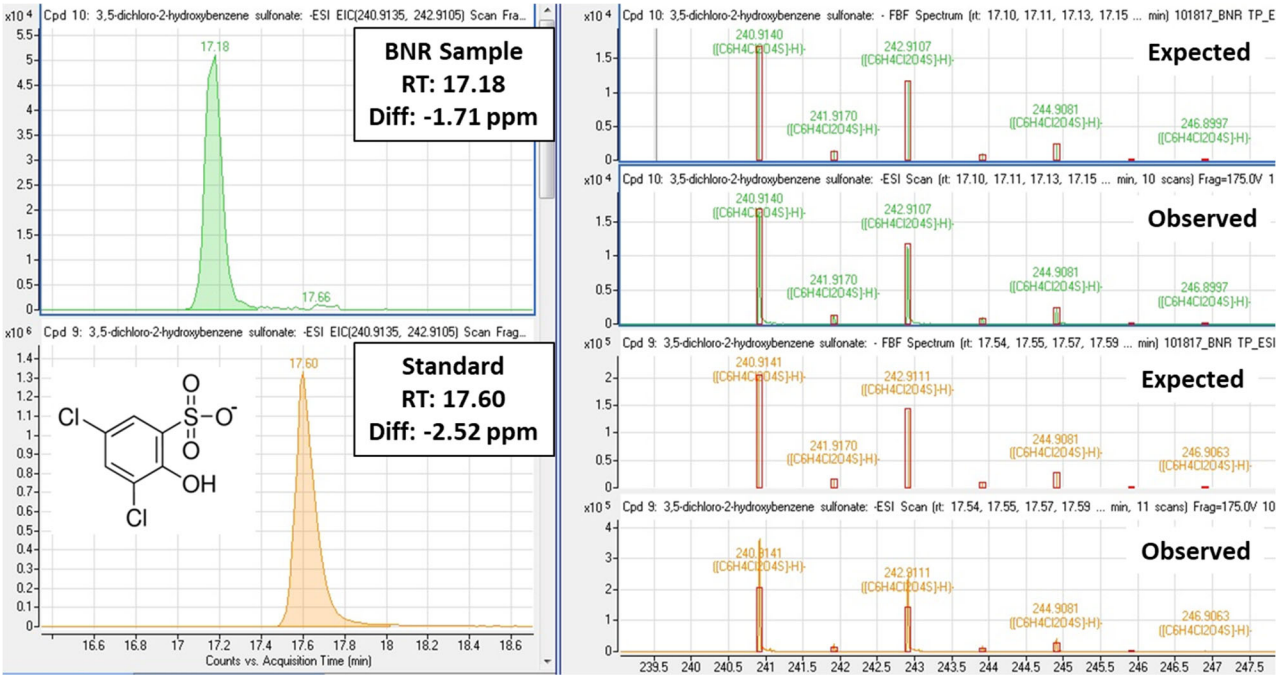


Fig. S7. Comparison of retention times for 3,5-dichloro-2-hydroxybenzene sulfonate standard to potential transformation product observed in sample, including expected and observed mass spectrum for each peak and mass error

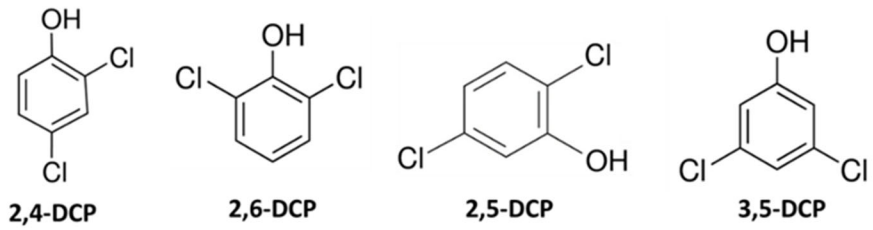


Fig. S8. Dichlorophenol (DCP) isomers tested