Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Electronic Supplementary Information for:

TITLE: Clustering micropollutants based on initial biotransformations for improved prediction of micropollutant removal during conventional activated sludge treatment

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Table S1. List of publications used for secondary treatment data extraction (alphabetical order)

Reference	**Citation**
Batt et al., 2007	Batt, A, S Kim, and D Aga. 2007. "Comparison of the Occurrence of Antibiotics in Four Full-Scale Wastewater Treatment Plants with Varying Designs and Operations." *Chemosphere* 68 (3): 428–35
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Bernhard et al., 2006	Bernhard, M, J Müller, and T Knepper. 2006. "Biodegradation of Persistent Polar Pollutants in Wastewater: Comparison of an Optimised Lab-Scale Membrane Bioreactor and Activated Sludge Treatment." *Water Research* 40 (18): 3419–28
Carballa et al., 2004	Carballa, M, F Omil, J Lema, M Llompart, C Gracía-Jares, I Rodríguez, M Gómez, and T Ternes. 2004. "Behavior of Pharmaceuticals, Cosmetics And Hormones in a Sewage Treatment Plant." *Water Research* 38 (12): 2918–26
Clara et al., 2005	Clara, M, B Strenn, O Gans, E Martinez, N Kreuzinger, and H Kroiss. 2005. "Removal of Selected Pharmaceuticals , Fragrances and Endocrine Disrupting Compounds in a Membrane Bioreactor and Conventional Wastewater Treatment Plants." *Water Research* 39 (19): 4797–4807
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	Pharmaceuticals and Corresponding Metabolites in Wastewater of a Sewage Treatment Plant." *Science of the Total Environment* 532: 762–70
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Meyer et al. 2004	Meyer, J, and K Bester. 2004. "Organophosphate Flame Retardants and Plasticisers in Wastewater Treatment Plants." *Journal of Environmental Monitoring* 6 (7): 559–605
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Salgado et al. 2012	Salgado, R, R Marques, J Noronha, G Carvalho, A Oehmen, and M Reis. 2012. “Assessing the Removal of Pharmaceuticals and Personal Care Products in a Full-Scale Activated Sludge Plant.” *Environ Sci Pollut Res Int* 19 (5): 1818–27
Sim et al. 2010	Sim, W-J, J-W Lee, and J-E Oh. 2010. “Occurrence and Fate of Pharmaceuticals in Wastewater Treatment Plants and Rivers in Korea.” *Environmental Pollution* 158 (5): 1938–47
Simonich et al. 2000	Simonich, S, W Begley, G Bedaere, and W Eckhoff. 2000. “Trace Analysis of Fragrance Materials in Wastewater and Treated Wastewater.” *Environ. Sci. Technol.* 34 (6): 959–65
Simonich et al. 2002	Simonich, S, T Federle, W Eckhoff, A Rottiers, S Webb, D Saballiuans, and W Wolf. 2002. “Removal of Fragrance Materials during U.S. and European Wastewater Treatment.” *Environ. Sci. Technol.* 36 (13): 2839–47
Smyth et al. 2007	Smyth, S, L Lishman, E McBean, S Kleywegt, J-J Yang, ML Svoboda, S Ormonde, V Pileggi, H-B Lee, and P Seto. 2007. “Polycyclic and Nitro Musks in Canadian MunicipalWastewater: Occurrence and Removal InWastewater Treatment.” *Water Quality Research Journal of Canada* 42 (3): 138–52
Spongberg et al. 2008	Spongberg, A, and J Witter. 2008. “Pharmaceutical Compounds in the Wastewater Process Stream in Northwest Ohio.” *Science of the Total Environment* 397 (1–3): 148–57
Ternes 1998	Ternes, T. 1998. “Occurrence of Drugs in German Sewage Treatment Plants and Rivers.” *Water Research* 32 (11): 3245–60
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Zotita et al. 2009	Zotita, S, L Martensson, and L Mathiasson. 2009. “Occurrence and Removal of Pharmaceuticals in a Municipal Sewage Treatment System in the South of Sweden.” *Science of the Total Environment* 407 (8): 2760–70

Table S2. Summary of process parameters included in the final database.

Process parameter[a]	Abbreviation	Units
Plant location	*Location*	NA
Population served	P	$person\ equivalents$
Design capacity	DC	$m^3 \cdot day^{-1}$
Flow rate	Q	$m^3 \cdot day^{-1}$
Composition of raw influent	*Composition*	*domestic, industrial, or mixed*
Sample month	*Season*	NA
Sample type	*Type*	*grab or composite*
Hydraulic retention time[b]	HRT	$hours$
Hydraulic retention time offset	HRT_{offset}	*yes or no*
Volume of primary settler	V_{ps}	m^3
Volume of activated sludge basin	V_a	m^3
Volume of secondary settler	V_{ss}	m^3
BOD_5 in influent	$BOD_{5,in}$	$mg \cdot L^{-1}$
BOD_5 in effluent	$BOD_{5,out}$	$mg \cdot L^{-1}$
COD in influent	COD_{in}	$mg \cdot L^{-1}$
COD in effluent	COD_{out}	$mg \cdot L^{-1}$
Micropollutant concentration in influent	C_{inf}	$mg \cdot L^{-1}$
Micropollutant concentration in effluent	C_{eff}	$mg \cdot L^{-1}$
Mixed liquor suspended solids	$MLSS$	$mg \cdot L^{-1}$
Total suspended solids in influent	TSS_{in}	$g \cdot L^{-1}$
Total suspended solids in effluent	TSS_{out}	$g \cdot L^{-1}$
Volatile suspended solids in influent	VSS_{in}	$g \cdot L^{-1}$
Volatile suspended solids in effluent	VSS_{out}	$g \cdot L^{-1}$
Total organic carbon in influent	TOC_{in}	$g \cdot L^{-1}$
Total organic carbon in effluent	TOC_{out}	$g \cdot L^{-1}$
Food to microorganism ratio	$F/M\ ratio$	NA
Biomass concentration	*Biomass*	$g \cdot L^{-1}$
Solids retention time	SRT	$hours$
Nitrification/Denitrification[c]	NDN	mgO_2/L
pH influent	pH_{in}	NA
pH effluent	pH_{out}	NA
Temperature	T	$°C$
Total nitrogen concentration	N_{total}	$mg \cdot L^{-1}$
Total phosphate concentration	P_{total}	$mg \cdot L^{-1}$

[a]when a process parameter was reported as a range of values (e.g., flow rate), the average value was used for our study; [b]some studies did not specify if reported *HRT* was for the whole plant or for the activated sludge process; [c]nitrification and denitrification (*NDN*) conditions were translated into equivalent dissolved oxygen levels. Conventional activated sludge was assigned a value of 2.5 mg/L, nitrification was assigned a value of 2 mg/L[1,2], and denitrification was assigned a value of 0.55 mg/L[3].

Table S3. Matched literature reported initial transformation pathways with predicted initial transformation pathways in Eawag-PPS for micropollutants.

	Literature reported initial reaction	eawag-PPS corresponding bt rules	Citations
Atenolol	Primary amide to carboxylate	bt0027	4–6
Bezafibrate	Secondary amide to carboxylate	bt0067	5
Citalopram	Amine to aldehyde or ketone	bt0063	7
Codeine	Alcohol to ketone or ester	bt0002	8,9
DEET	N-substituted amide to aldehyde or ketone	bt0243	10
Diuron	N-substituted amide to aldehyde or ketone	bt0243	11
Ibuprofen	Hydroxylation	bt0241	12
Iopromide	Primary alcohol to aldehyde	bt0001	13
Isoproturon	N-substituted amide to aldehyde or ketone	bt0243	4,6
Levetiracetam	Primary amide to carboxylate	bt0027	5
Ranitidine	Disubstituted sulfide to disubstituted sulfoxide	bt0162	6
N4-Acetylsulfamethoxazole	Secondary amide to carboxylate	bt0067	14
Sulfamethazine	Sulfamate to amine	bt0144	15
Sulfamethoxazole	Sulfamate to amine	bt0144	15
Trimethoprim	Hydroxylation	bt0242	13,16

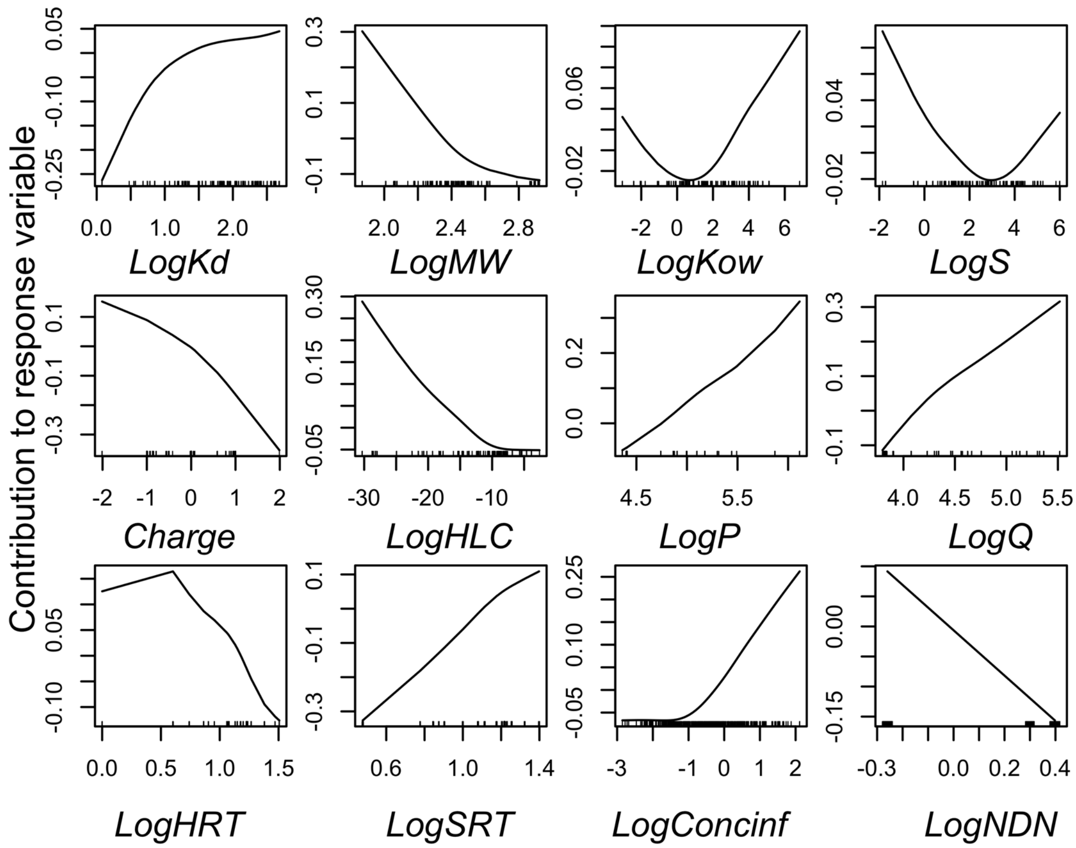

Figure S1. Shape functions describing the relationships between micropollutant removal efficiency (*R%*) and each of the predictor variables included in GAM model for 84 micropollutants.

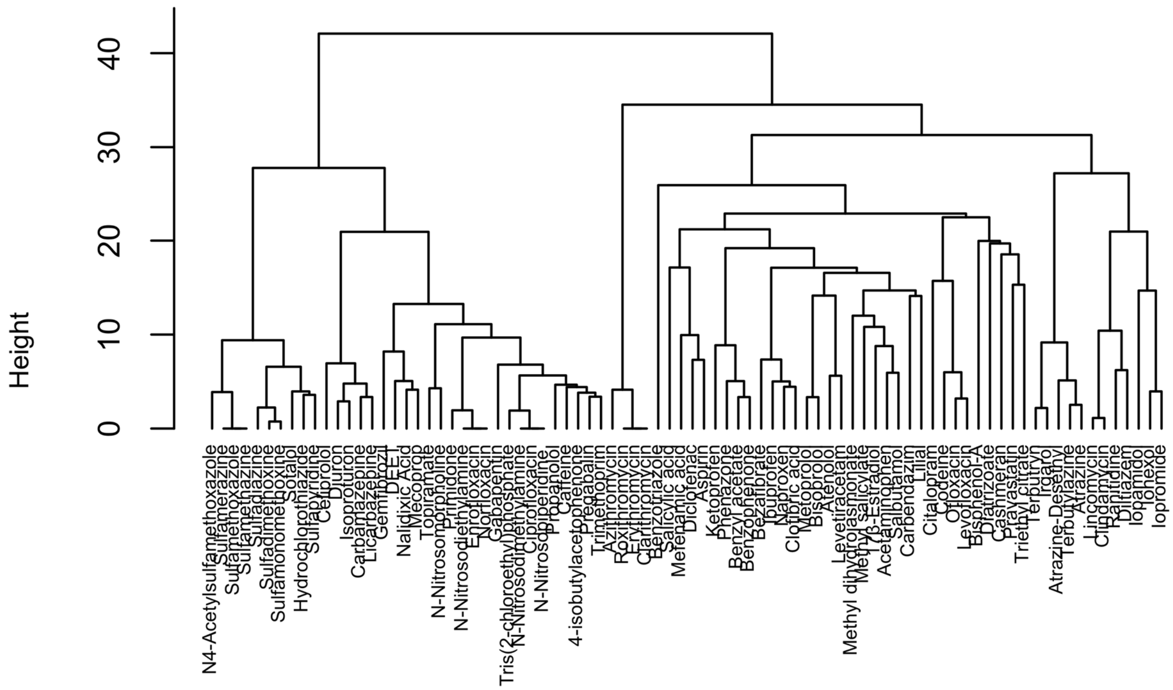

Figure S2. Hierarchical clustering of micropollutants based on their predicted initial biotransformation reactions using prediction method (2) use relative reasoning, neutral likelihood cutoff in eawag-PPS.

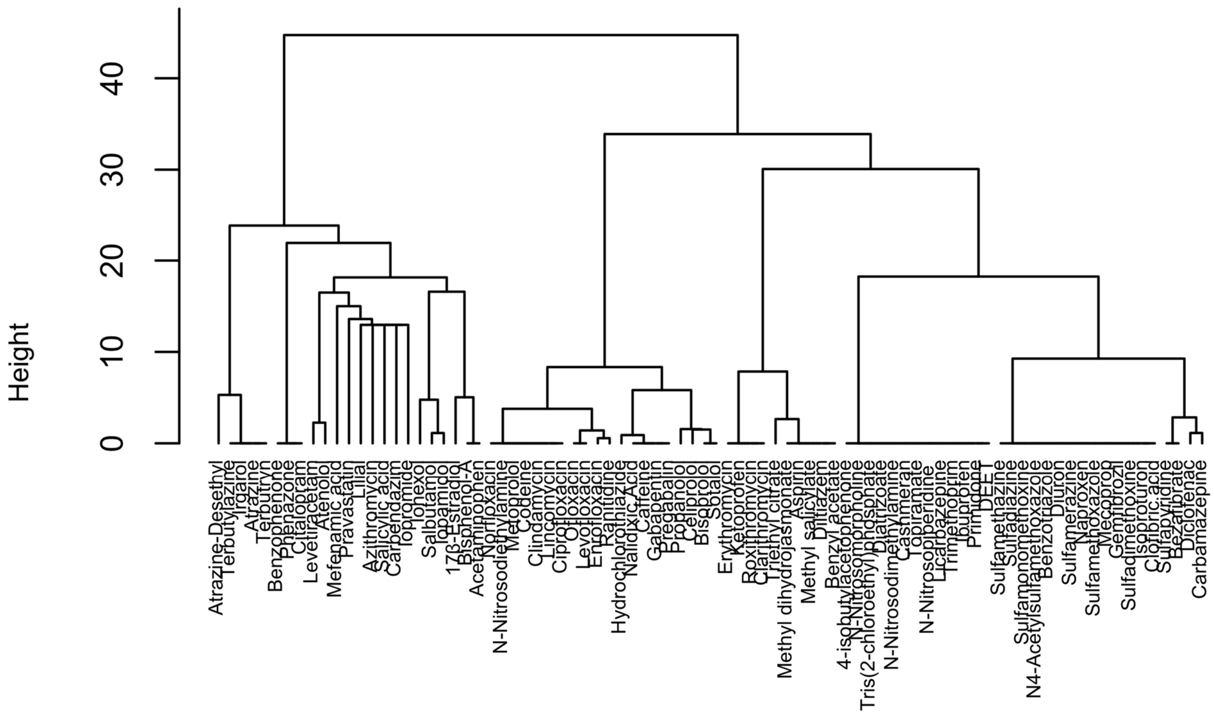

Figure S3. Hierarchical clustering of micropollutants based on their predicted initial biotransformation reactions using prediction method (3) use relative reasoning, likely likelihood cutoff in eawag-PPS.

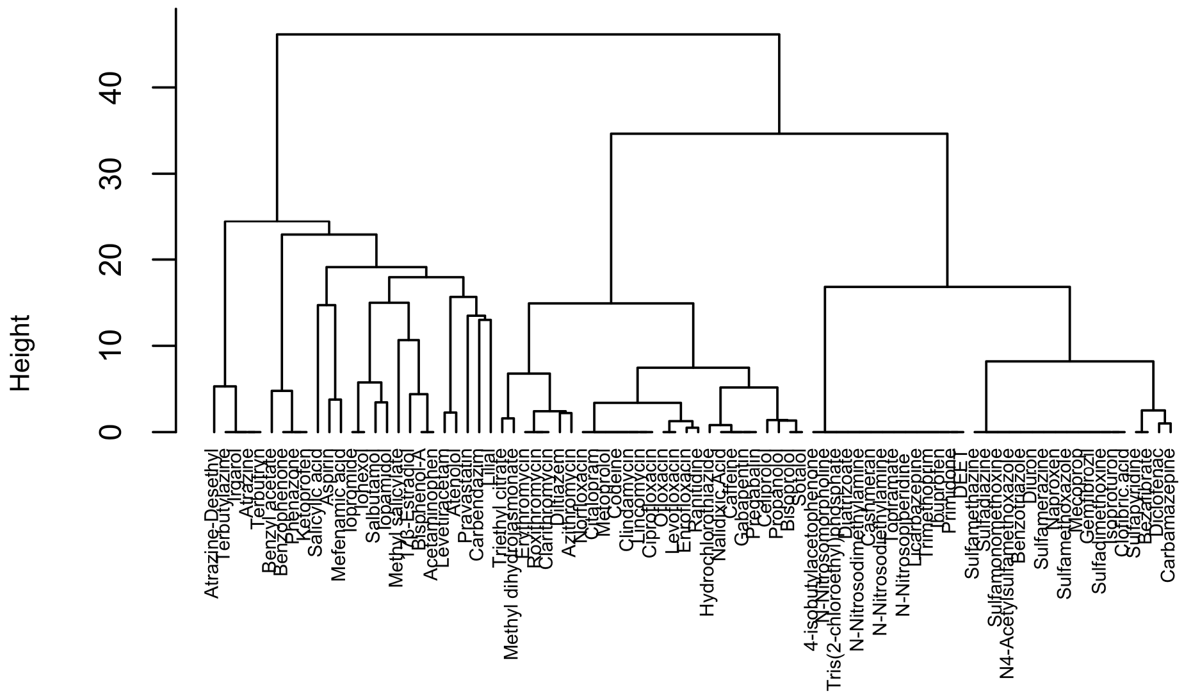

Figure S4. Hierarchical clustering of micropollutants based on their predicted initial biotransformation reactions using prediction method (4) no relative reasoning, likely likelihood cutoff in eawag-PPS.

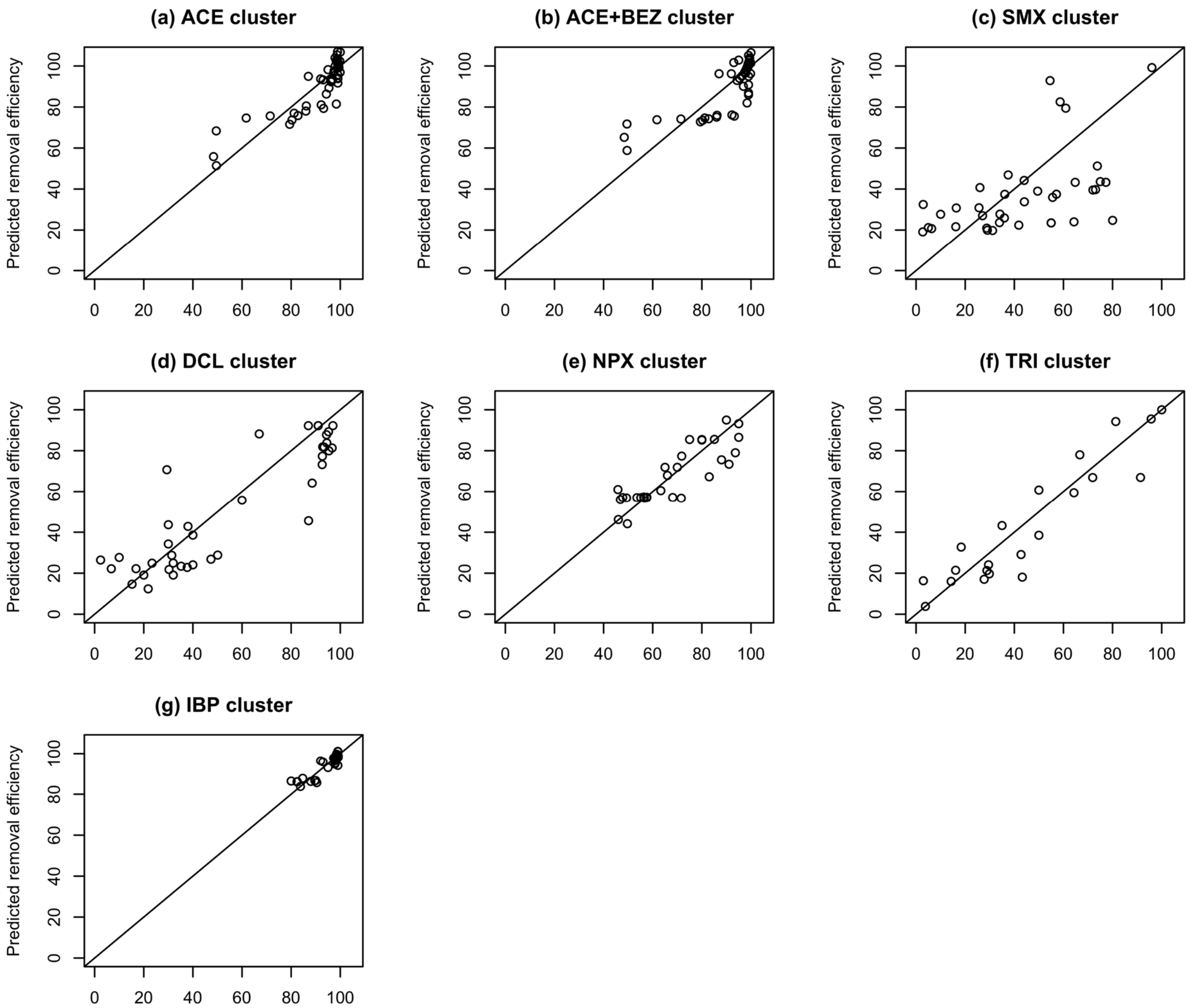

Figure S5. Comparison of experimental removal efficiency and predicted removal efficiency of the clusters using GAM and stepwise modeling. ACE cluster includes acetaminophen and SMX-acetate. ACE+BEZ cluster includes acetaminophen, SMX-acetate, and bezafibrate. SMX cluster includes sulfamethazine, sulfadiazine, sulfamethoxazole, and sulfamerazine. DCL cluster includes diclofenac and mefenamic. NPX cluster includes naproxen and sulfamonomethoxine. TRI cluster contains trimethoprim, tris(2-chloroethyl)phosphate and 4-isobutylacetophenone. IBP cluster includes ibuprofen and lilial.

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