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




**SUPPORTING INFORMATION**

to

# Removal of 293 organic compounds in 15 WWTPs studied with non-targeted suspect screening

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Table S1: Internal standards

| **Chemical** |
|---|
| 2,4-D ($^{13}C_6$) |
| Acesulfame ($D_4$) |
| Atenolol ($D_7$) |
| Atrazine ($D_5$) |
| Caffeine ($^{13}C_3$) |
| Carbamazepine ($D_{10}$) |
| Codeine ($D_3$) |
| Cotinine ($D_3$) |
| DEET ($D_7$) |
| Deisopropylatrazine ($D_5$) |
| Desethyl atrazine ($D_6$) |
| Diuron ($D_6$) |
| Fluoxetine ($D_6$) |
| Gabapentin ($D_{10}$) |
| Hexazinone ($D_6$) |
| Hydrochlorothiazide ($^{13}C_1$,$D_2$) |
| Ibuprofen ($D_3$) |
| Imidacloprid ($D_4$) |
| MCPA ($D_6$) |
| Metolachlor ($D_6$) |
| Paracetamol ($D_4$) |
| Simazine ($D_{10}$) |
| Temazepam ($D_5$) |
| Venlafaxine ($D_6$) |

Table S2: Liquid chromatography program

| **Time (min)** | **Flow (mL min$^{-1}$)** | **%A** | **%B** |
|---|---|---|---|
| 0 | 0.4 | 95 | 5 |
| 10 | 0.4 | 5 | 95 |
| 12 | 0.4 | 5 | 95 |
| 12.1 | 0.4 | 95 | 5 |
| 14 | 0.4 | 95 | 5 |

Sampler compartment temperature = 10 °C.
Column temperature = 40 °C.

Table S3: Comparison of mean removal efficiency (= 1-*B*) in WWTPs with modern conventional treatment measured in this study with values reported in the literature. Green shading = WWTPs with nitrification/denitrification (N/DN); blue shading = activated sludge without N/DN.

| | This study[a] | Gaffney et al. (2017)[b] | Angeles et al. (2020)[c] | Sun et al. (2014)[b] | Collado et al. (2014)[b] | Bijllsma et al. (2021) | Luo et al. (2014) | Gros et al. (2010) | Bourgin et al. (2018) |
|---|---|---|---|---|---|---|---|---|---|
| Treatment technology | AS-N/DN[d] | AS-N/DN[d] (Bardenpho) | Sequential batch reactor | Orbal oxidation ditch | AS-N/DN[d] | AS (A20 type) with N/DN[d] | Mean from review of many WWTPs | Mean of 7 WWTPs, 6 with AS | AS[e] |
| Caffeine | 100 | 100 | 100 | 100 | | | 89 | | >99 |
| Acetaminophen | 99 | 100 | 100 | 100 | 85 | 100 | 100 | 99 | 100 |
| Metformin | 98 | 100 | | | | | | | 92 |
| DEET | 97 | | | | | | 74 | | 76 |
| Codeine | 95 | | | 80 | | | | | 21 |
| Valsartan | 93 | | | | 93 | 90 | | | 77 |
| Atenolol | 88 | 70 | | | 80 | | 63 | 59 | 58 |
| Ranitidine | 84 | | | | 73 | | | 66 | 58 |
| Trimethoprim | 82 | | 83 | | 56 | 89 | 47 | | 8 |
| Sulfapyridine | 58 | 47 | | | | | | | 52 |
| Gabapentin | 36 | | | | | 68 | | | 24 |
| Metoprolol | 19 | 14 | | | 52 | | 38 | | 29 |
| Tramadol | 1 | | | | | 18 | | | |
| Citalopram | -1[f] | | 23 | | 71 | | | | 5 |
| Irbesartan | -4 | | | | 15 | 25 | | | 9 |
| Venlafaxine | -6 | | 28 | | 26 | 13 | | | -3[f] |
| Carbamazepine | -40 | 55 | -10[e] | | | | 33 | | -29[f] |

[a] mean of S2, S5, S11, S24, and S40

[b] values read off of figures in the publication and hence approximate

[c] mean of WWTPs 4 & 6

[d] activated sludge with nitrification/denitrification

[e] removal in the biological treatment portion of the plant

[f] negative values indicate that concentrations in the effluent were greater than in the influent

Table S4: Linear regressions for chemicals whose log *B* was highly correlated (r > 0.9) with log *B* for 4-pyridoxic acid. These chemicals are characterized by very good abatement in WWTPs with activated sludge and N/DN (*B* < 2%), satisfactory removal in trickling filter plants (*B* ≈ 10%) and negligible removal in WWTPs with primary treatment only.

| **Chemical** | **Slope** | **Intercept** | **r** |
|---|---|---|---|
| Docosahexaenoic acid ethyl ester | 1.988 | -1.402 | 0.99 |
| Dodecyl sulfate | 1.309 | -0.438 | 0.99 |
| (-)-Camphanic acid | 1.169 | -0.150 | 0.98 |
| Cyclo(leucylprolyl) | 0.937 | 0.208 | 0.98 |
| Paraxanthine | 1.511 | -0.724 | 0.97 |
| Cholic acid | 2.010 | -1.555 | 0.97 |
| Theobromine | 1.097 | -0.116 | 0.97 |
| Caffeine | 1.494 | -0.583 | 0.96 |
| Deoxycholic acid | 2.452 | -1.776 | 0.96 |
| 4-Picoline | 1.550 | -0.620 | 0.96 |
| (S)-Nicotine | 1.116 | -0.288 | 0.95 |
| Theophylline | 1.218 | -0.254 | 0.95 |
| 7-Methylxanthine | 1.472 | -0.742 | 0.95 |
| Methylimidazoleacetic acid | 1.172 | -0.295 | 0.94 |
| 5-Sulfosalicylic acid | 1.140 | 0.200 | 0.94 |
| Kynurenic acid | 1.126 | -0.078 | 0.94 |
| 2-Hydroxyhippuric acid | 1.352 | -0.567 | 0.94 |
| 3-Indoxyl sulphate | 2.000 | -0.495 | 0.94 |
| 5-Nitro-o-toluidine | 1.461 | -0.700 | 0.94 |
| PEG n16 | 0.939 | 0.373 | 0.93 |
| Paracetamol | 1.402 | -0.521 | 0.93 |
| 3-(4-Hydroxyphenyl)propionic acid | 0.967 | -0.001 | 0.93 |
| 2,6-Bis[(2-hydroxyethyl)amino]-3-nitrobenzonitrile | 1.131 | -0.134 | 0.93 |
| 3-Methylxanthine | 1.522 | -0.798 | 0.93 |
| Inosine | 1.673 | -0.302 | 0.93 |
| Acetyl-β-methylcholine | 1.547 | -0.487 | 0.93 |
| 6-(3,4,5-Trimethoxystyryl)-2,3,4,5-tetrahydropyridazin-3-one | 1.419 | -0.431 | 0.92 |
| 4-Dodecylbenzenesulfonic acid | 0.913 | -0.105 | 0.92 |
| N-Methyl-2-pyrrolidone | 0.906 | 0.262 | 0.92 |
| N-Acetylornithine | 1.359 | -0.301 | 0.92 |
| Cotinine | 1.072 | 0.039 | 0.92 |
| PEG n5 | 1.221 | 0.004 | 0.92 |
| Panthenol | 1.326 | -0.328 | 0.92 |
| 3,3-Dimethylglutaric acid | 0.854 | 0.449 | 0.92 |
| L-threo-3-Phenylserine | 0.884 | 0.735 | 0.92 |
| Mesalamine | 1.010 | -0.124 | 0.92 |
| PEG n6 | 1.274 | -0.152 | 0.92 |
| 7-Methylguanine | 1.033 | 0.071 | 0.91 |
| PEG n15 | 0.880 | 0.471 | 0.91 |
| Myricetin | 1.053 | 0.103 | 0.91 |
| PEG n7 | 1.250 | -0.105 | 0.91 |
| PEG n14 | 0.921 | 0.434 | 0.91 |
| PEG n11 | 1.025 | 0.289 | 0.91 |
| Butylparaben | 0.855 | 0.262 | 0.91 |
| PEG n13 | 0.914 | 0.399 | 0.91 |
| Acetylcholine | 1.470 | -0.332 | 0.90 |
| Indole-3-acetic acid | 0.838 | -0.460 | 0.90 |
| PEG n8 | 1.188 | 0.020 | 0.90 |

Table S5: Chemicals showing a strong reduction in *B* due to activated sludge treatment with N/DN compared to trickling filter treatment. The difference between mean log *B* (S39 and S53) and mean log *B* (S2, S5, S11, S24, S40) is shown together with a p-value from a one-sided t-test, unequal variance.

| **Chemical** | **Log *B* difference** | **p** |
|---|---|---|
| Deoxycholic acid | 2.32 | 0.048 |
| L-Norleucine | 2.27 | 0.063 |
| L-Phenylalanine | 1.96 | 0.074 |
| Leucylproline | 1.85 | 0.067 |
| Indole-3-acrylic acid | 1.78 | 0.138 |
| Guanosine | 1.72 | 0.145 |
| Valylproline | 1.71 | 0.002 |
| tert-Butyl N-[1-(aminocarbonyl)-3-methylbutyl]carbamate | 1.70 | 0.001 |
| Glycyl-L-leucine | 1.67 | 0.052 |
| Cholic acid | 1.67 | |
| Valine | 1.67 | 0.090 |
| 2-Hydroxycinnamic acid | 1.66 | 0.083 |
| Prolylleucine | 1.62 | 0.064 |
| L-Tyrosine | 1.60 | 0.087 |
| (15Z)-9,12,13-Trihydroxy-15-octadecenoic acid | 1.58 | 0.095 |
| Acesulfame | 1.57 | 0.001 |
| Uridine | 1.56 | 0.071 |
| Pantothenic acid | 1.55 | 0.071 |
| Docosahexaenoic acid ethyl ester | 1.55 | |
| Inosine | 1.47 | 0.005 |
| Acetylcholine | 1.47 | 0.104 |
| 2,6-Diaminotoluene | 1.45 | 0.002 |
| L-Tryptophan | 1.44 | 0.159 |
| Cytidine | 1.43 | 0.172 |
| Isophthalic acid | 1.43 | 0.003 |
| Acetyl-β-methylcholine | 1.43 | 0.114 |
| N-Acetylornithine | 1.39 | 0.003 |
| Choline | 1.37 | 0.146 |
| Uracil | 1.36 | 0.033 |
| Ibuprofen metabolite B | 1.34 | 0.181 |
| 2'-Deoxyinosine | 1.34 | 0.000 |
| Nicotinic acid | 1.32 | 0.161 |
| Hypoxanthine | 1.31 | 0.134 |
| 4-Picoline | 1.29 | 0.091 |
| Guanine | 1.28 | 0.010 |
| Isoamylamine | 1.28 | 0.003 |
| Acetophenone | 1.28 | 0.001 |
| 2'-Deoxyguanosine | 1.23 | 0.010 |
| δ-Valerolactam | 1.23 | 0.073 |
| Methionine | 1.23 | 0.217 |
| Caffeine | 1.21 | 0.000 |
| Thymine | 1.19 | 0.001 |
| 2-Hydroxyhippuric acid | 1.18 | 0.110 |
| 3-Methylxanthine | 1.17 | 0.001 |
| D-Panthenol | 1.15 | 0.000 |
| 3-Phenyllactic acid | 1.15 | 0.230 |
| Phthalic acid | 1.15 | |
| Panthenol | 1.14 | 0.000 |
| 9-Oxo-10(E),12(E)-octadecadienoic acid | 1.14 | 0.088 |

Table S5 (continued)

| **Chemical** | **Log *B* difference** | **p** |
|---|---|---|
| 3-Morpholino-4-tetrahydro-1H-pyrrol-1-ylcyclobut-3-ene-1,2-dione | 1.14 | 0.144 |
| Meprylcaine | 1.12 | 0.000 |
| α-Aspartylphenylalanine | 1.11 | 0.001 |
| Tyramine | 1.10 | 0.001 |
| Metformin | 1.08 | 0.002 |
| Paraxanthine | 1.05 | 0.072 |
| Phenethylamine | 1.05 | 0.091 |
| α-Linolenic acid | 1.05 | 0.183 |
| 5-Nitro-o-toluidine | 1.03 | 0.119 |
| 4-Guanidinobutyric acid | 1.03 | 0.001 |
| L-Pyroglutamic acid | 1.03 | 0.167 |
| 5-Methoxyindole | 1.03 | 0.122 |
| 2-Naphthalenesulfonic acid | 1.02 | |
| Levetiracetam | 1.01 | 0.000 |
| Porphobilinogen | 1.00 | 0.113 |
| Cytosine | 0.99 | 0.189 |
| Tetraglyme | 0.99 | 0.008 |
| Coumarin | 0.98 | 0.097 |
| DL-Arginine | 0.98 | 0.201 |
| DL-Stachydrine | 0.98 | 0.177 |
| Pipecolic acid | 0.97 | 0.093 |
| Sulcatol | 0.96 | 0.103 |
| Pregabalin | 0.94 | 0.005 |
| PEG n5 | 0.93 | 0.001 |
| PEG n6 | 0.92 | 0.065 |
| Creatinine | 0.92 | 0.221 |
| Thymidine | 0.92 | 0.001 |
| Paracetamol | 0.90 | 0.002 |
| PEG n7 | 0.90 | 0.001 |
| Pseudoephedrine | 0.88 | 0.006 |
| Desisopropylatrazine | 0.87 | |
| 3-Hydroxypyridine | 0.86 | 0.002 |
| 2,3,5,6-Tetramethylpyrazine | 0.86 | 0.013 |
| 6-(3,4,5-Trimethoxystyryl)-2,3,4,5-tetrahydropyridazin-3-one | 0.86 | 0.001 |
| Theophylline | 0.85 | 0.000 |
| PEG n8 | 0.84 | 0.001 |
| 5-Sulfosalicylic acid | 0.84 | |
| 3-Hydroxydecanoic acid | 0.84 | 0.048 |
| D-Carnitine | 0.84 | 0.039 |
| N,N-Diethylethanolamine | 0.84 | |
| Uric acid | 0.84 | 0.239 |
| 7-Methylxanthine | 0.83 | 0.115 |
| 4-[(6E)-3-Hydroxy-8,10-dimethyl-2-(methylamino)-6-dodecen-1-yl]phenol | 0.83 | 0.304 |
| 3-(2,1,3-Benzothiadiazol-4-ylamino)-2-(2,2-dimethylpropanoyl)acrylonitrile | 0.83 | |
| D-(+)-Proline | 0.81 | 0.230 |
| 2,6-Dimethylpyrazine | 0.81 | 0.007 |
| trans-Zeatin | 0.80 | 0.003 |
| 6-Methylquinoline | 0.80 | 0.132 |
| DEET | 0.79 | 0.030 |

Table S5 (continued)

| **Chemical** | **Log *B* difference** | **p** |
|---|---|---|
| Cotinine | 0.79 | 0.062 |
| 6-Aminocaproic acid | 0.78 | 0.165 |
| PEG n10 | 0.77 | 0.001 |
| N-Methyl-2-AI | 0.76 | 0.002 |
| Dodecyl sulfate | 0.76 | 0.021 |
| Kynurenic acid | 0.74 | |
| PEG n11 | 0.74 | 0.001 |
| N-Methylhydantoin | 0.74 | 0.122 |
| Creatine | 0.73 | 0.160 |
| 4-Dodecylbenzenesulfonic acid | 0.72 | 0.096 |
| 7-Methylguanine | 0.71 | 0.079 |
| Xylenesulfonate | 0.71 | 0.237 |
| (-)-Camphanic acid | 0.70 | |
| (S)-Nicotine | 0.70 | 0.010 |
| Diethanolamine | 0.69 | 0.183 |
| Glycylproline | 0.69 | 0.148 |
| PEG n12 | 0.69 | 0.001 |
| N-Acetyl-D-galactosamine | 0.67 | 0.235 |
| Ethyl palmitoleate | 0.67 | 0.143 |
| Chrysin | 0.66 | 0.160 |
| PEG n16 | 0.66 | 0.000 |
| Codeine | 0.66 | 0.044 |
| PEG n14 | 0.65 | 0.000 |
| Tryptamine | 0.65 | 0.186 |
| 2,6-Bis[(2-hydroxyethyl)amino]-3-nitrobenzonitrile | 0.65 | 0.111 |
| Urocanic acid | 0.64 | 0.255 |
| PEG n13 | 0.64 | 0.001 |
| Methylimidazoleacetic acid | 0.64 | 0.078 |
| 4-Pyridoxic acid | 0.64 | 0.001 |
| Desthiobiotin | 0.64 | 0.155 |
| PPG n11 | 0.63 | 0.062 |
| PEG n15 | 0.61 | 0.001 |
| Myricetin | 0.60 | 0.033 |
| PPG n8 | 0.57 | 0.010 |
| 1-(4-Chlorobenzyl)-4,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile | 0.57 | 0.202 |
| Theobromine | 0.56 | 0.039 |
| 3-Indoxyl sulphate | 0.56 | |
| Acetanilide | 0.56 | 0.205 |
| Palmitoyl ethanolamide | 0.55 | 0.003 |
| PPG n9 | 0.54 | 0.016 |
| N-(tert-Butyl)-N'-(2-hydroxyethyl)urea | 0.54 | 0.272 |
| N-Acetyl-DL-glutamic acid | 0.53 | 0.171 |
| Piperine | 0.53 | 0.213 |
| 1-(Carboxymethyl)cyclohexanecarboxylic acid | 0.52 | 0.239 |
| Azelaic acid | 0.51 | 0.254 |
| 9-Methyluric acid | 0.51 | 0.339 |
| Tropinone | 0.50 | 0.226 |
| 3,3-Dimethylglutaric acid | 0.50 | 0.205 |

Table S6: Chemicals whose log B was highly correlated (r > 0.85, WWTPs S2, S5, S11, S24, S39, S40, S53) with log B for meprylcaine and with mean log B in S39 and S53 >1.5. These chemicals are characterized by poor removal in trickling filter plants and good abatement in WWTPs with activated sludge and N/DN.

| **Chemical** | **r** |
|---|---|
| trans-Zeatin | 0.97 |
| tert-Butyl N-[1-(aminocarbonyl)-3-methylbutyl]carbamate | 0.94 |
| Uridine | 0.93 |
| 9-Oxo-10(E),12(E)-octadecadienoic acid | 0.91 |
| α-Aspartylphenylalanine | 0.91 |
| 2,6-Diaminotoluene | 0.91 |
| Acesulfame | 0.87 |
| (15Z)-9,12,13-Trihydroxy-15-octadecenoic acid | 0.86 |

Table S7: Chemicals showing a strong reduction in *B* due to filtration compared to activated sludge treatment with N/DN. The difference between mean log *B* (S2, S5, S11, S24, S40) and mean log *B* (S9, S29, S51) is shown together with the p-value from a one-sided t-test, unequal variance.

| **Chemical** | **Log B difference** | **p** |
|---|---|---|
| O-Desmethylvenlafaxine* | 2.03 | 0.036 |
| Tapentadol* | 1.90 | 0.000 |
| O-Desmethyl-cis-tramadol* | 1.83 | 0.002 |
| Sulfapyridine* | 1.50 | 0.000 |
| Sotalol* | 1.44 | 0.076 |
| Desacetyl diltiazem* | 1.44 | 0.000 |
| Tramadol* | 1.44 | 0.079 |
| Gabapentin* | 1.38 | 0.074 |
| Citalopram* | 1.36 | 0.013 |
| Venlafaxine* | 1.25 | 0.083 |
| Trimethoprim* | 1.21 | 0.001 |
| Moclobemide* | 1.19 | 0.065 |
| Lidocaine* | 1.15 | 0.054 |
| L-Phenylalanine* | 1.12 | 0.004 |
| Guanine* | 1.11 | 0.011 |
| Ranitidine* | 1.04 | 0.001 |
| 3-Morpholino-4-tetrahydro-1H-pyrrol-1-ylcyclobut-3-ene-1,2-dione | 1.01 | 0.012 |
| 2'-Deoxyguanosine* | 0.99 | 0.009 |
| Codeine | 0.97 | 0.009 |
| Fexofenadine* | 0.89 | 0.166 |
| L-Tryptophan* | 0.79 | 0.014 |
| 5-Methylbenzotriazole* | 0.77 | 0.077 |
| Amisulpride* | 0.76 | |
| 2,6-Dimethylpyrazine* | 0.76 | 0.015 |
| Guanosine | 0.75 | 0.001 |
| N-Desmethyltramadol* | 0.75 | 0.082 |
| Phenibut* | 0.71 | 0.034 |
| Pregabalin* | 0.69 | 0.149 |
| Irbesartan* | 0.69 | 0.143 |
| Metoprolol* | 0.68 | 0.099 |
| 2,3,5,6-Tetramethylpyrazine* | 0.67 | 0.031 |
| L-Norleucine* | 0.66 | 0.010 |
| Climbazole* | 0.63 | 0.093 |
| Cytosine | 0.63 | 0.082 |
| Pseudoephedrine* | 0.63 | 0.129 |
| Choline* | 0.60 | 0.043 |
| 2-Pyridylacetic acid | 0.60 | 0.083 |
| Pyridostigmine* | 0.59 | 0.002 |
| N-Methyl-2-AI | 0.59 | 0.092 |
| Metformin | 0.58 | 0.122 |
| Methamphetamine* | 0.57 | 0.021 |
| 6-(3,4,5-Trimethoxystyryl)-2,3,4,5-tetrahydropyridazin-3-one | 0.56 | 0.019 |
| Triisopropanolamine* | 0.52 | 0.037 |
| Indole-3-acrylic acid* | 0.52 | 0.060 |
| Atenolol acid* | 0.51 | 0.017 |
| Cytidine | 0.51 | 0.032 |
| 2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile* | 0.51 | 0.062 |

*For these compounds, log B for the WWTP with ozonation (S1) was also >0.5 log units lower than mean log B for activated sludge WWTPs with N/DN (S2, S5, S11, S24, S40)

Table S8: Chemicals showing a strong reduction in *B* due to ozonation compared to activated sludge treatment with N/DN. The difference between mean log *B* (S2, S5, S11, S24, S40) and log *B* (S1) is shown.

| **Chemical** | **Log B difference** |
|---|---|
| O-Desmethylvenlafaxine | 2.99 |
| 5-Methylbenzotriazole | 2.36 |
| Fexofenadine | 2.33 |
| Tramadol | 2.31 |
| Irbesartan | 2.30 |
| Atenolol acid | 2.27 |
| Venlafaxine | 2.08 |
| Telmisartan | 2.05 |
| Sotalol | 2.05 |
| Tapentadol | 2.04 |
| Metoprolol | 2.04 |
| Lidocaine | 1.97 |
| Benzotriazole | 1.95 |
| Gabapentin | 1.89 |
| Carbamazepine | 1.80 |
| Flecainide | 1.77 |
| O-Desmethyl-cis-tramadol | 1.73 |
| Citalopram | 1.69 |
| Amisulpride | 1.67 |
| Moclobemide | 1.66 |
| 2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile | 1.59 |
| 8-(4-Sulfophenyl) octanoic acid | 1.58 |
| Sitagliptin | 1.54 |
| Sulfapyridine | 1.49 |
| Desacetyl diltiazem | 1.40 |
| Norfenefrine | 1.33 |
| Triisopropanolamine | 1.33 |
| Xylenesulfonate | 1.32 |
| Valsartan | 1.28 |
| Pyridostigmine | 1.18 |
| 10,11-Dihydro-10,11-dihydroxycarbamazepine | 1.18 |
| L-Tryptophan | 1.17 |
| Pregabalin | 1.16 |
| 2,6-Dimethylpyrazine | 1.15 |
| Desnitro-imidacloprid | 1.09 |
| Trimethoprim | 1.08 |
| Hypoxanthine | 1.04 |
| L-Phenylalanine | 1.04 |
| 2,3,5,6-Tetramethylpyrazine | 1.02 |
| Methionine | 0.96 |
| Urocanic acid | 0.93 |
| Creatinine | 0.92 |
| Methamphetamine | 0.90 |
| 2'-Deoxyguanosine | 0.90 |

Table S8 (continued)

| Chemical | Log B difference |
|---|---|
| Icaridin | 0.89 |
| 2-Amino-4-cresol | 0.89 |
| Indole-3-acrylic acid | 0.89 |
| L-Tyrosine | 0.84 |
| 1-(4-Chlorobenzyl)-4,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile | 0.82 |
| Climbazole | 0.81 |
| 4-Hydroxybenzaldehyde | 0.81 |
| N-Acetyl-L-phenylalanine | 0.80 |
| Ranitidine | 0.79 |
| Atenolol | 0.79 |
| Pseudoephedrine | 0.79 |
| Guanine | 0.78 |
| Threonine | 0.77 |
| D-(+)-Proline | 0.74 |
| Triisopropanolamine cyclic borate | 0.72 |
| Desthiobiotin | 0.71 |
| L-Norleucine | 0.70 |
| Phenethylamine | 0.69 |
| Ibuprofen metabolite B | 0.68 |
| Isoamylamine | 0.68 |
| Choline | 0.67 |
| Phenibut | 0.66 |
| N-Acetyl-D-alloisoleucine | 0.65 |
| D-(+)-Galactose | 0.65 |
| Meprylcaine | 0.65 |
| Thymidine | 0.64 |
| Pyridoxamine | 0.63 |
| L-Pyroglutamic acid | 0.63 |
| 2-Hydroxycinnamic acid | 0.61 |
| Eprosartan | 0.60 |
| Nicotinic acid | 0.60 |
| L-(+)-Citrulline | 0.59 |
| L-(+)-Lactic acid | 0.58 |
| 3-Aminophenol | 0.58 |
| N-Acetyl-L-tyrosine | 0.58 |
| trans-Zeatin | 0.57 |
| 2'-O-Methylguanosine | 0.57 |
| N-Desmethyltramadol | 0.55 |
| Tryptamine | 0.55 |
| 6-Methylquinoline | 0.54 |
| L-Glutamic acid | 0.53 |
| N-Acetyl-D-galactosamine | 0.52 |
| 2-(Acetylamino)hexanoic acid | 0.51 |
| Tris(2-butoxyethyl) phosphate | 0.51 |

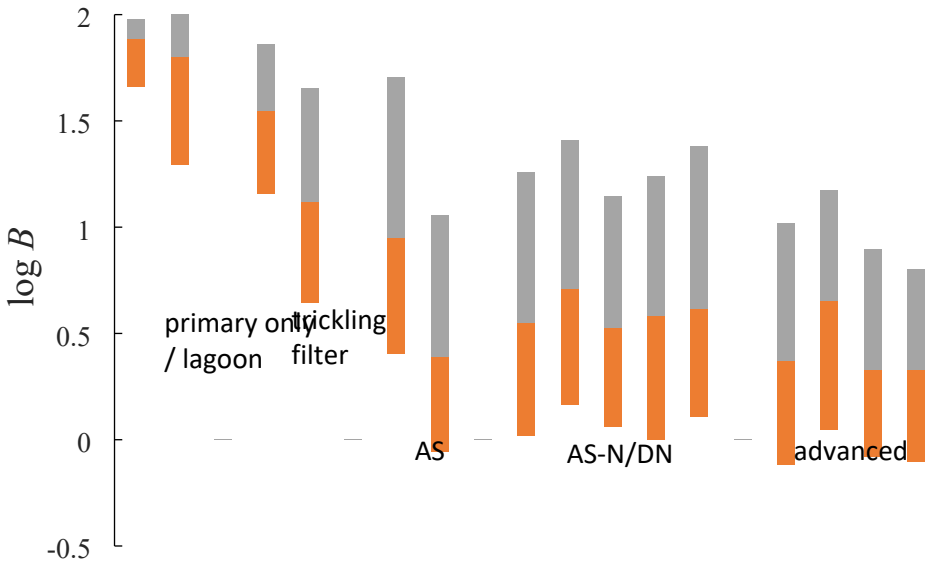



Figure S1: Plot of the second (orange bar) and third (grey bar) quartiles of log *B* (*n* = 293 chemicals) for the 15 WWTPs, ordered according to the most advanced treatment step. The meeting point of the two bars is the median, while the upper and lower ends are the 25$^{th}$ and 75$^{th}$ percentiles, respectively.

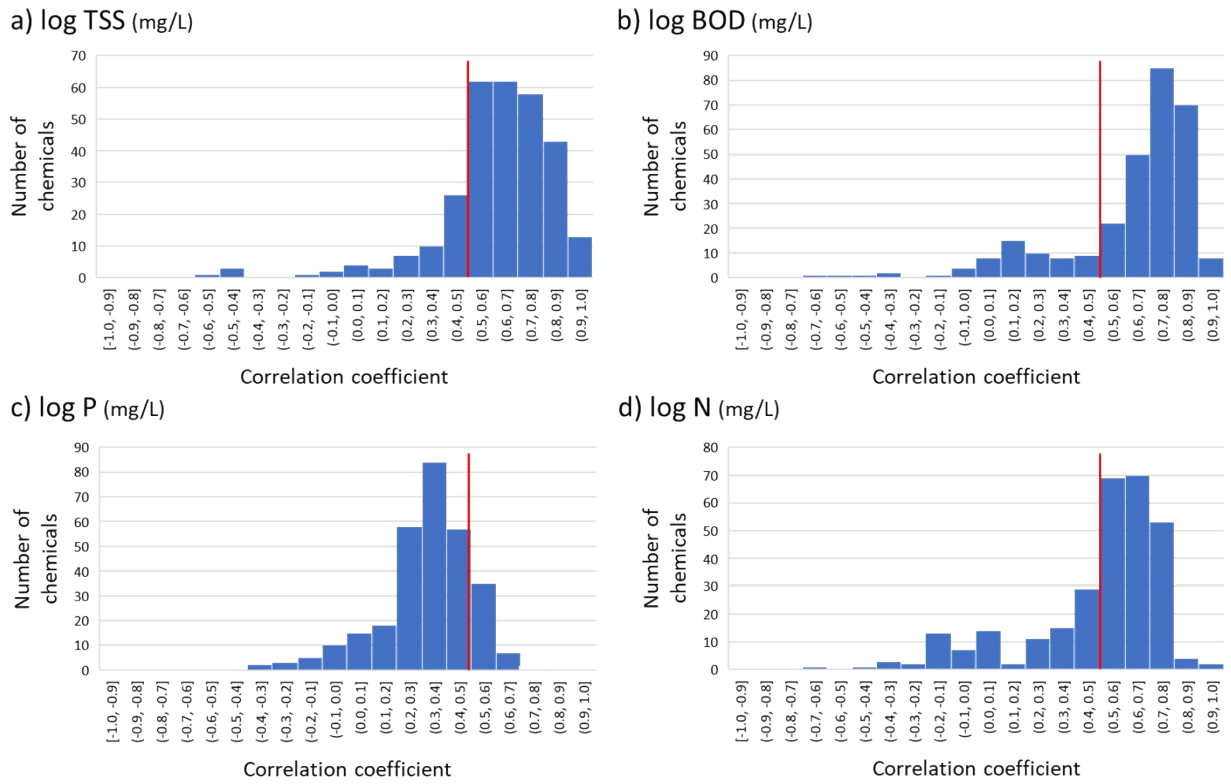
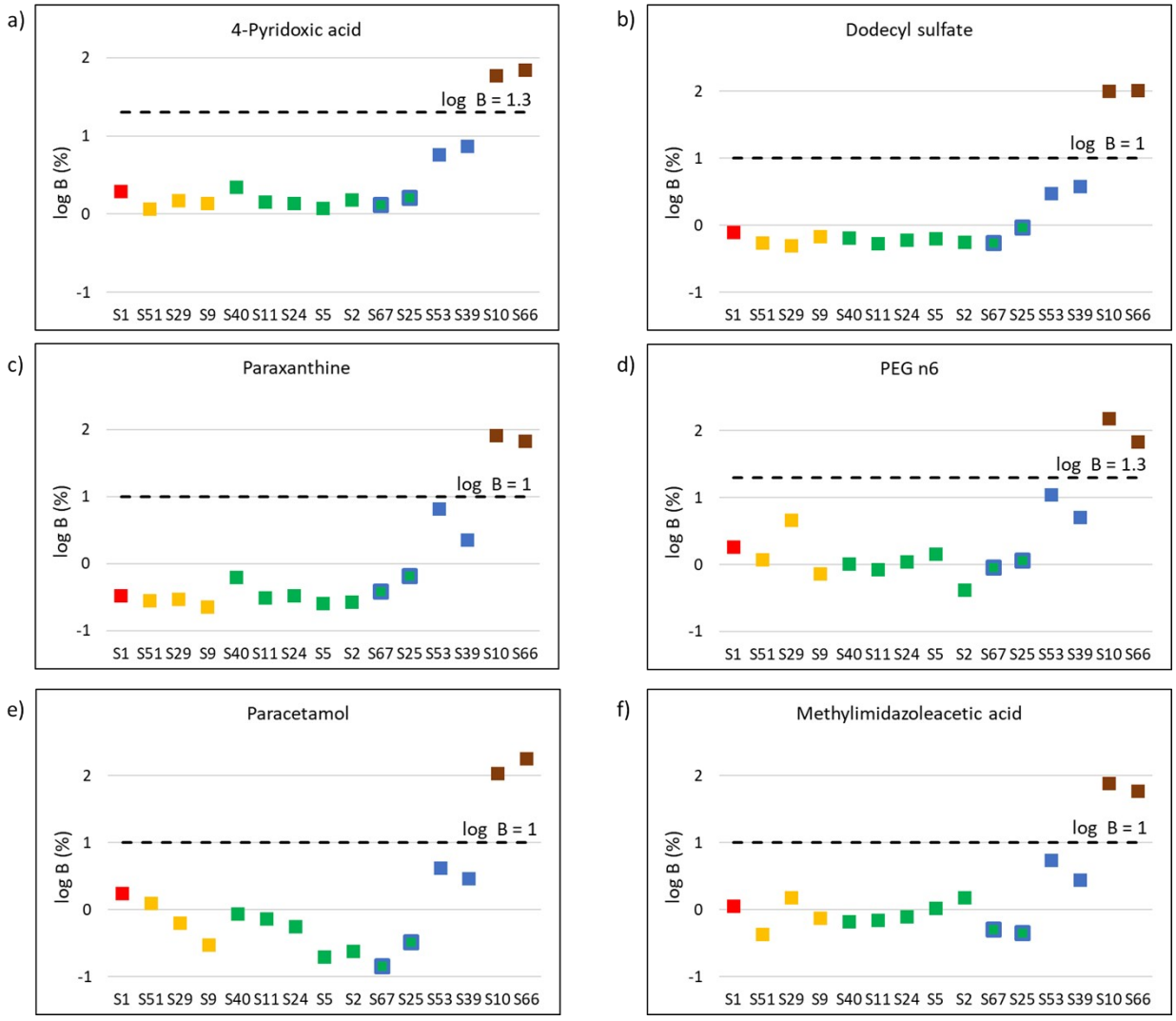



Figure S2: Histograms of the correlation coefficient for 293 chemicals for the correlation of log *Signal in effluent* vs: a) log *TSS*; b) log *BOD*; c) log *P*; d) log *N* in the effluent of 13 WWTPs. Bars to the right of the red line have a correlation coefficient >0.5.




Figures S3: Example chemicals illustrating the influence of trickling filter treatment on breakthrough (*B*). The dotted line shows the selected *B* threshold indicating trickling filter quality treatment compared to primary treatment only. The colors indicate the treatment standard (see Table 1): red = ozonation; yellow = filtration; green = AS-N/DN; blue around green = AS; blue = trickling filter; brown = primary treatment (S10) or anaerobic lagoon (S66).

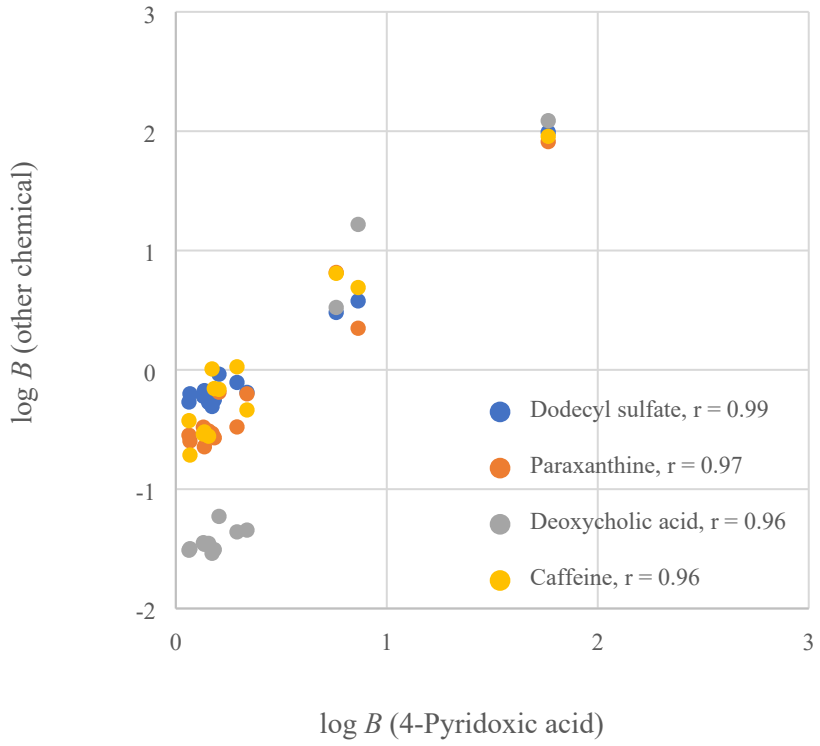
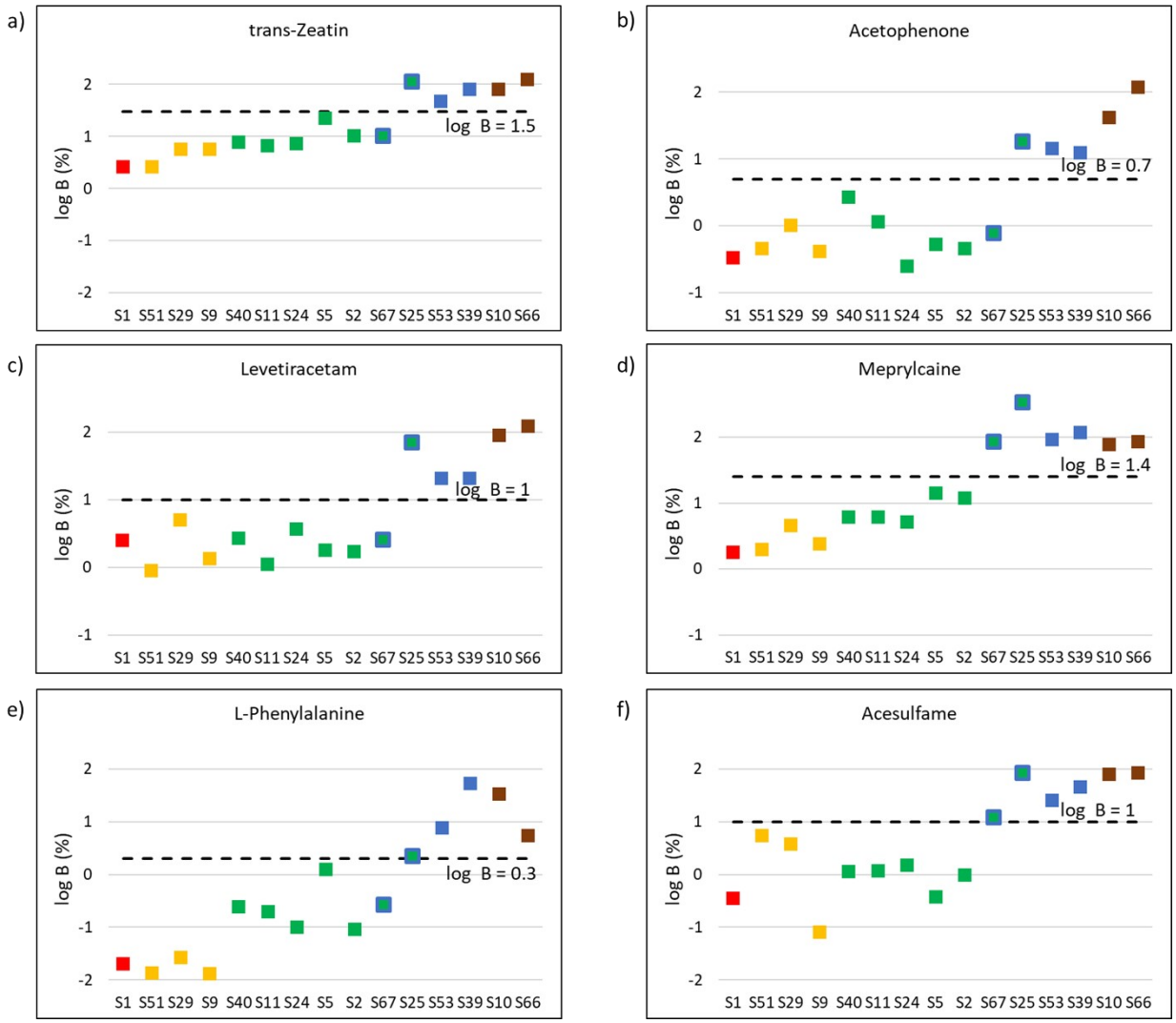
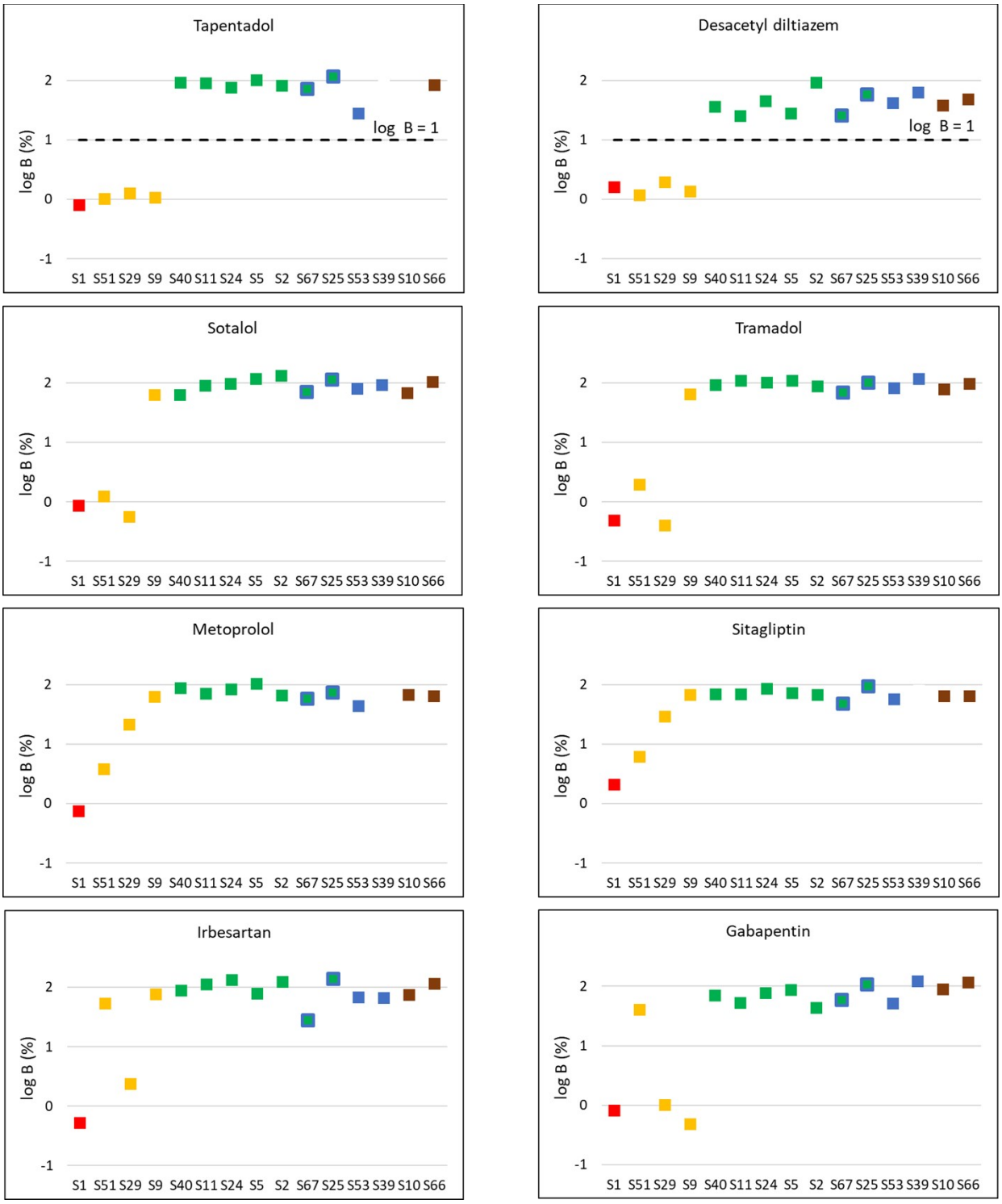


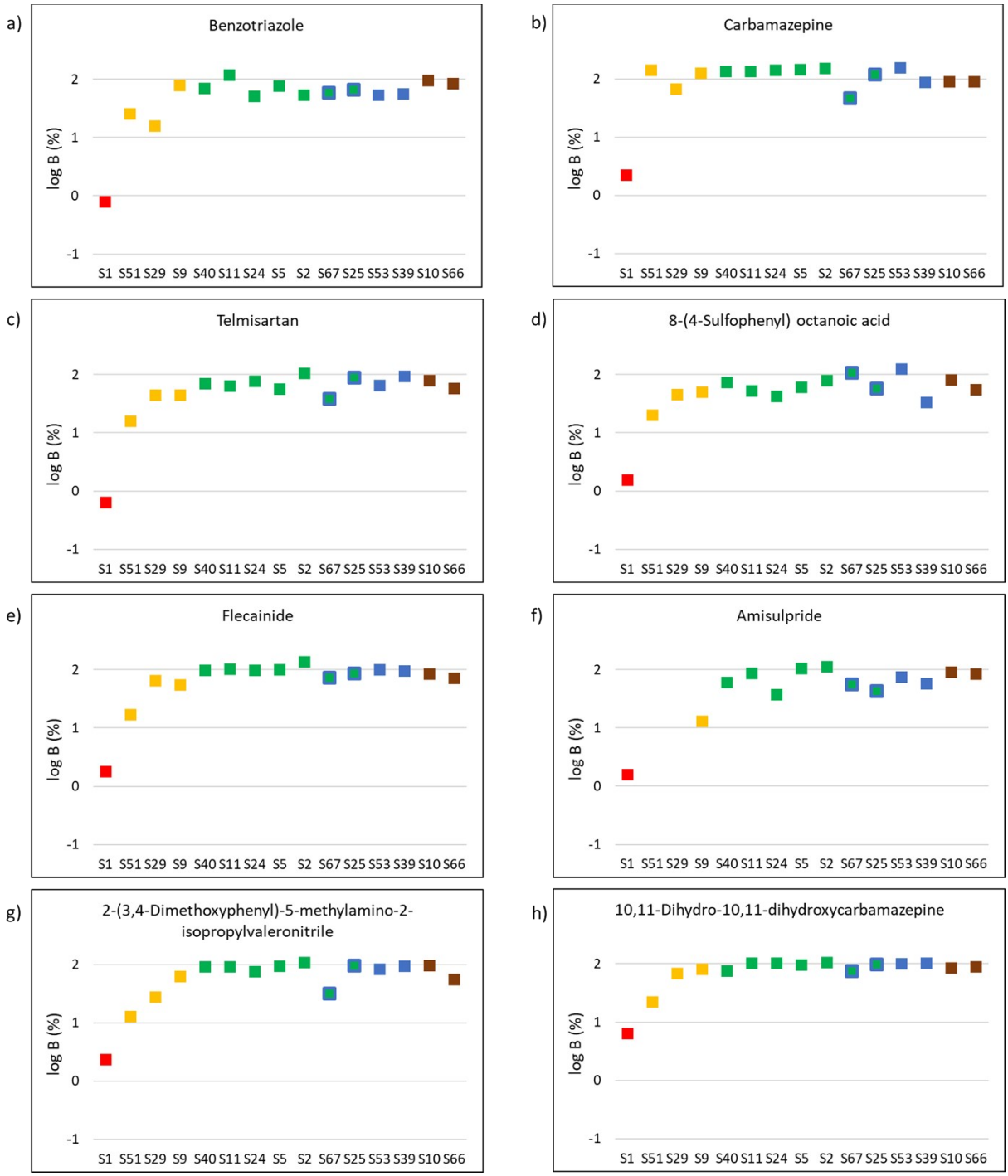

Figure S4: Correlation between log *B* for 4-pyridoxic acid and log *B* for several other chemicals. The data for the 13 WWTPs that satisfied the inclusion criteria are shown.




Figures S5: Example chemicals illustrating the influence of activated sludge with N/DN on breakthrough (*B*). The dotted line shows the selected *B* threshold indicating AS-N/DN quality treatment compared to trickling filter treatment. The colors indicate the treatment standard (see Table 1): red = ozonation; yellow = filtration; green = AS; blue around green = biofilter/activated sludge; blue = trickling filter; brown = primary treatment (S10) or anaerobic lagoon (S66).




Figures S6: Example chemicals illustrating the influence of advanced treatment on breakthrough (*B*). The colors indicate the treatment standard (see Table 1): red = ozonation; yellow = filtration; green = AS-N/DN; blue around green = AS; blue = trickling filter; brown = primary treatment (S10) or anaerobic lagoon (S66).




Figures S7: Chemicals for which log *B* was at least 0.5 units lower for the WWTP with ozonation (S1) than the WWTP with the next lowest breakthrough, and for which log *B* was > 1 for the WWTP with the next lowest breakthrough. The colors indicate the treatment standard (see Table 1): red = ozonation; yellow = filtration; green = AS-N/DN; blue around green = AS; blue = trickling filter; brown = primary treatment (S10) or anaerobic lagoon (S66).