

## Supplementary Information

### ***Multimodal 3D-printed passive samplers to monitor, model and prioritise in situ chemical pollution risks to an aquatic freshwater invertebrate, Gammarus pulex***

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## S1. List of analytical standards

Reference standards for 2-(thiocyanomethylthio)benzothiazole, 4-fluoromethacationone, 4-methylethcathinone, acetamiprid, aclonifen, alprazolam, ametryn, amiodarone, amitriptyline, amlodipine, amphetamine, antipyrine, atorvastatin, atrazine, azelnidipine, azithromycin, azoxystrobin, benoxacor, bensulide, benzatropine, benzoylecgonine, betaxolol, bezafibrate, bisoprolol, bupropion, buspirone, carazolol, carbamazepine, carbamazepine-10, 11-epoxide, carboxine, carfentrazone-ethyl, celecoxib, chloramphenicol, cilazapril, citalopram, clarithromycin, clodinafop-propargyl, clofibric acid, clopidogrel, clothianidin, clozapine, cocaine, cyclouron, cycloxydim, cymoxanil, cyphenothrin, cyromazine, diazepam, diclofenac, diflubenzuron, dimethametryn, dimethomorph, diphenhydramine, disulfoton sulfone, diuron, enalapril, ethofumesate, famoxadone, fenoxaprop-ethyl, fenuron, flufenoxuron, fluocinonide, fluoxetine, flurbiprofen, flurochloridone, flutamide, flutolanil, fuberidazole, gemfibrozil, haloperidol, hydrochlorothiazide, ibuprofen, imidacloprid, indomethacin, isocarbamid, isradipine, josamycin, ketamine, ketoconazole, ketoprofen, ketotifen, levamisole, levocabastine, lidocaine, lincomycin, lorazepam, MDMA, meclizine, meclofenamic acid, medroxyprogesterone, mefenamic acid, memantine, mephedrone, mephosfolan, metformin, methamphetamine, methcathinone, methedrone, methylphenidate, metoprolol, morphine, nadolol, naproxen, nicotine, nifedipine, nitenpyram, nordiazepam, norethisterone, nortriptyline, orphenadrine, oxamyl, oxazepam, oxycarboxin, oxycodone, picoxystrobin, piperophos, pirenzepine, pretilachlor, prodiamine, prometon, prometryn, propamocarb, propranolol, propazine, pymetrozine, pyracarbolid, pyraclostrobin, pyraflufen-ethyl, pyridaben, risperidone, rizatriptan, ronidazole, roxithromycin, salbutamol, salicylic acid, sertraline, simazine, spinosyn A, spinosyn B, spiramycin, sulfadimethoxine, sulfamerazine, sulfamethazine, sulfamethoxazole, sulfamonomethoxine, sulfapyridine, sulfathiazole, sulfisoxazole, tacrine, tamsulosin, temazepam, terbutryn, terfenadine, thiacloprid, thiamethoxam, thiazopyr, timolol, tramadol, trimethoprim, valsartan, venlafaxine, verapamil, warfarin and ziprasidone were sourced from QMX (Essex, UK).

Deuterated internal standards for amitriptyline-d3, amphetamine-d6, benzoylecgonine-d3, betaxolol-d7, celecoxib-d7, cetirizine-d4, clarithromycin-d3, clothianidin-d3, cocaine-d3, cotinine-d3, diazepam-d6, fluoxetine-d6, gemfibrozil-d6, haloperidol-d4, ketamine-d4, lidocaine-d10, lorazepam-d4, MDMA-d5, methylone-d3, methylphenidate-d9, metoprolol-d7, morphine-d3, nicotine-d4, nifedipine-d4, nordiazepam-d5, nortriptyline-d3, oxazepam-d5, risperidone-d4, sertraline-d3, sulfamethazine-d4, temazepam-d5, thiamethoxam-d3, tramadol-d3, trimethoprim-d3, venlafaxine-d6 and verapamil-d3 were purchased from Sigma Aldrich (Gillingham, Dorset, UK) and QMX (Essex, UK).

Table S1. Collection events per month across the course of the study for all sample types

| Month & collection event |                               | Water | 3D-PSD | <i>Gammarus pulex</i> |
|--------------------------|-------------------------------|-------|--------|-----------------------|
| July                     | Deployment – 20 <sup>th</sup> | 🔗     |        | 🔗                     |
|                          | Midpoint – 24 <sup>th</sup>   | 🔗     |        | 🔗                     |
|                          | Retrieval – 27 <sup>th</sup>  | 🔗     | 🔗      | 🔗                     |
| August                   | Deployment – 10 <sup>th</sup> | 🔗     |        | 🔗                     |
|                          | Midpoint – 15 <sup>th</sup>   | 🔗     |        | 🔗                     |
|                          | Retrieval – 17 <sup>th</sup>  | 🔗     | 🔗      | 🔗                     |
|                          | Extra – 27 <sup>th</sup>      | 🔗     |        | 🔗                     |
| September                | Deployment – 7 <sup>th</sup>  | 🔗     |        | 🔗                     |
|                          | Midpoint – 10 <sup>th</sup>   | 🔗     |        | 🔗                     |
|                          | Retrieval – 14 <sup>th</sup>  | 🔗     | 🔗      | 🔗                     |
|                          | Extra – 27 <sup>th</sup>      | 🔗     |        | 🔗                     |
| October                  | Deployment – 13 <sup>th</sup> | 🔗     |        | 🔗                     |
|                          | Retrieval – 20 <sup>th</sup>  | 🔗     | 🔗      | 🔗                     |
|                          | Extra – 29 <sup>th</sup>      | 🔗     |        | 🔗                     |
| November                 | Deployment – 9 <sup>th</sup>  | 🔗     |        | 🔗                     |
|                          | Midpoint – 12 <sup>th</sup>   | 🔗     |        | 🔗                     |
|                          | Retrieval – 16 <sup>th</sup>  | 🔗     | 🔗      | 🔗                     |
|                          | Extra – 26 <sup>th</sup>      | 🔗     |        | 🔗                     |
| December                 | Deployment – 7 <sup>th</sup>  | 🔗     |        | 🔗                     |
|                          | Midpoint – 12 <sup>th</sup>   | 🔗     |        | 🔗                     |
|                          | Retrieval – 14 <sup>th</sup>  | 🔗     | 🔗      | 🔗                     |

## **S2. Site selection and sample collection - additional details**

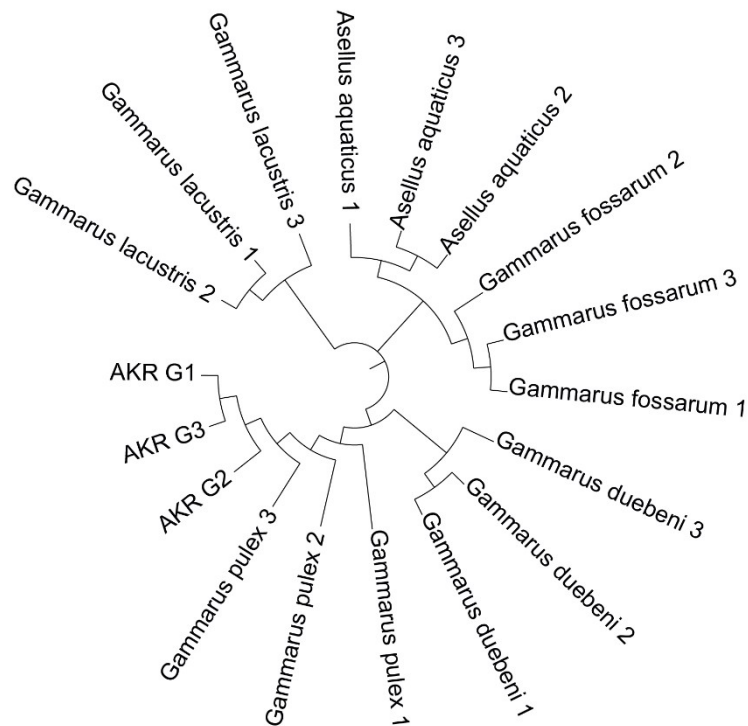
Of the ten 3D-PSDs deployed each month, three devices contained the same chemistry for all sorbent disks contained within the same device (i.e., one 3D-PSD contained five HLB sorbent disks) for the HLB, MM-anion, and MM-cation phases, respectively. In addition, a single device was multiplexed with all three sorbent chemistries and deployed alongside the other 3D-PSDs. The 3D-PSDs were securely anchored to the riverbed as described in Richardson *et al.* (2022) using U-shaped galvanised pegs (15 x 0.29 cm, G&B, UK) which were pushed into the sediment so that the 3D-PSD was sitting approximately 3-5 cm from the bottom of the river with the water flowing over the top of the device (Richardson *et al.*, 2022). During retrieval, the 3D-PSDs were removed from the riverbed and rinsed in river water before the transport cap was fitted, the device was then wrapped in methanol-washed aluminium foil and stored in a food-grade plastic container for transport to the laboratory in a cool box as standard practice in passive sampling (Taylor *et al.*, 2021). A separate 3D-PSD was used as the field blank during deployment and retrieval to account for contamination occurring from handling the 3D-PSDs in the field and laboratory. Upon return to the laboratory, all 3D-PSDs were rinsed with ultra-pure water, disassembled, the PES membrane removed, and the sorbent disks were allowed to air dry overnight on MeOH rinsed foil alongside the field blanks. Once dry, the sorbent disks were wrapped in fresh MeOH-washed foil and stored at -20 °C until extraction and analysis.

*G. pulex* samples were collected by kick-sampling multiple organisms using a D-frame net (NHBS, Totnes, UK). The net composed of a stainless-steel frame with a wooden handle fitted with a woven polyester net (diameter 30 cm, depth 50 cm, 500 µm mesh size). Kick sampling is a sample collection technique where a net is placed downstream of the operator, and then the riverbed is disturbed by kicking the upper layers of sediment in a perpendicular fashion to the direction of flow to collect benthic organisms (Storey *et al.*, 1991). An area of approximately 2-3 m<sup>2</sup> was covered to collect organisms and water depth at this site was relatively shallow (0.5 m at a maximum). All collected macroinvertebrates were returned to the laboratory and sorted using 1,000 and 500 µm sieves, where all *G. pulex* individuals larger than 0.5 mm were collected using forceps ( $n > 15$  specimens). Pure *G. pulex* samples were stored at -20 °C in preparation for sample analysis and the other invertebrates (including polychaetes and larvae) and isopods (including *Asellus aquaticus*) were disposed of.

### S3. Sample preparation - additional details

Extractions were performed using pre-fritted, empty SPE cartridges (Agilent Technologies UK Ltd., Cheshire, UK) configured to an SPE manifold with the taps closed. Before extraction, all sorbent disks were directly spiked with 0.5 ng of SIL-IS in MeOH and left to dry. Initially, 1 mL of elution solvent was added on top of the 9 mm disks and allowed to soak for 15 min. After which, the taps were opened and the elution solvent was allowed to percolate into 2 mL microcentrifuge tubes. An additional 0.6 mL of elution solvent was added to the SPE cartridges and gently pulled through under vacuum. The eluent was then filtered through 0.2  $\mu\text{m}$  polytetrafluoroethylene (PTFE) membrane using a BD Plastipak™ syringe (FisherScientific UK Ltd., Loughborough, UK) directly into pointed glass tubes (Merck Life Science UK, Ltd., Dorset, UK) for the subsequent evaporation step. Extracts were dried at 35 °C under N<sub>2</sub> before reconstitution in 200  $\mu\text{L}$  of starting mobile phase conditions. Per month,  $n = 3$  separate disks from one 3D-PSD device were extracted as measurement replicates. To perform quantification, the spare 9 mm disks from the same deployment were directly spiked with analytical standards to form an 11-point calibration series (0.005 to 10 ng disk<sup>-1</sup>) per sorbent phase and extracted as above.

All frozen *G. pulex* samples at each timepoint (typically 15 to 50 individuals) were lyophilised at -40 °C under vacuum for at least 24 h. These were pooled and homogenised to a fine powder in a 2 mL microcentrifuge tube with a 3 mm tungsten carbide bead using a TissueLyser LT benchtop system (50 Hz, Qiagen, Hilden, Germany). Homogenised material was weighed into a new 2 mL microcentrifuge tube ( $20 \pm 0.1$  mg,  $n = 3$  per collection timepoint), all analytical standards and SIL-IS (50 ng g<sup>-1</sup>) were spiked directly onto the dried material in a total volume of 100  $\mu\text{L}$  of MeOH. Samples were extracted in 2 mL of 0.1 % (v/v) glacial acetic acid in 3:1 MeCN:H<sub>2</sub>O using an ultrasonic bath for 15 min. Insoluble material was pelleted out by centrifugation at 18,407 rcf for 5 min, 1.9 mL of the supernatant was removed and diluted in 100 mL of 10 mM ammonium acetate<sub>(aq)</sub>. Sample clean-up and preconcentration was performed using tandem solid-phase extraction with an upper matrix removal cartridge (Strata Alumina-N cartridge, 6 mL, 1 g, Phenomenex Ltd., Cheshire, UK) and a lower Oasis HLB cartridge (6 mL, 200 mg, Waters Corp., Hertfordshire, UK) for analyte preconcentration (Miller et al., 2019). Cartridges were conditioned with 6 mL each of MeOH and 10 mM ammonium acetate<sub>(aq)</sub> prior to sample loading. The SPE system was subsequently washed with 1 mL of ultra-pure water, the upper cartridge removed, and the lower cartridge dried under vacuum. Analytes were eluted with a total of 5 mL of MeOH split into two 2.5 mL aliquots and dried under N<sub>2</sub> at 35 °C before reconstitution in 100  $\mu\text{L}$  of initial mobile phase conditions, briefly centrifuged twice for 5 min at 254 rcf to pellet any particulates that formed during the reconstitution step before transfer to silanised HPLC vial inserts for analysis. Quantification was performed by comparing to an 11-point calibration series (0.05 to 150 ng g<sup>-1</sup>) using homogenised *G. pulex* material collected from a relatively contaminant-free site in the south of London (51.385972; 0.109000, Miller et al., 2017, 2015) and prepared as above.



**Figure S1.** Maximum likelihood estimation phylogenetic tree generated from Cytochrome C Oxidase (COI) DNA barcode sequencing comparing three individuals (AKR G1-3) collected from the Gammarid population at the Ravensbury study site to published known COI sequences from four freshwater gammarid species (*G. pulex*, *G. duebeni*, *G. lacustris*, and *G. fossarum*) and an evolutionary distant water louse (*Asellus aquaticus*). Forward (5'-ACGTCATAGTCACCGCTCAC-3') and reverse (5'-CGTTCACCCTGTTCTACCC-3') primers were designed using the Primer3Plus platform (Untergasser et al., 2012). Reference COI sequences (S4) were retrieved from the National Center for Biotechnology Information (NCBI) GenBank (Benson et al., 2013). Results indicate that the sampled individuals share a common ancestor with *G. pulex*. Created using MegaX software and maximumhood likelihood estimation was used.

#### **S4. Aligned COI haplotype sequences with NCBI GenBank reference codes**

G1

TATAATAATTGGTGGTTTCGGGAATTGACTGGTGCCATTAATGCTAGGTAGACC  
TGATATAGCTTTTCCGCGTATAAACAATATAAGATTTTGACTTTTACCTCCTTCTC  
TCACCCTTCTGCTTATAAGTAGTATAGTAGAAAGAGGGGTAGGAACAGGGTGAA  
CG

G2

TTATAATTGGGTGGGTTTCGGGGAATTGACTGGTGCCACTAATGCTAGGTAGACC  
TGATATAGCTTTTCCGCGTATAAACAATATAAGATTTTGACTTTTACCTCCTTCTC  
TCACCCTTCTGCTTATAAGTAGTATAGTAGAAAGAGGGGTAGGAACAGGGTGAA  
GGA

G3

TATNATAATTGGTGGTTTCGGGAATTGACTGGTGCCATTAATGCTAGGTAGACC  
TGATATAGCTTTTCCGCGTATAAACAATATAAGATTTTGACTTTTACCTCCTTCTC  
TCACCCTTCTGCTTATAAGTAGTATAGTAGAAAGAGGGGTAGGAACAGGGTGAA  
CG

*Gammarus pulex*1 (MW459741.1)

GATTATAATCGGGGGTTTCGGAAATTGACTAGTACCTTTAATATTAGGTAGACCT  
GATATAGCTTTCCCGCGAATAAACAATATAAGATTTTGACTTTTACCCCCTTCCC  
TAACACTTCTGCTTATAAGTAGTATAGTAGAAAGAGGGGTAGGAACAGGGTGAA  
CG

*Gammarus pulex*2 (MG986849.1)

TATTATAATTGGCGGTTTCGGAAATTGATTGGTTCCATTAATATTAGGTAGACCT  
GATATAGCTTTCCCGCGTATAAATAATATAAGGTTTTGACTTTTACCTCCTTCTCT  
AACCCTTCTACTTATAAGTAGTATAGTAGAAADAGGCGTAGGAACGGGTTGGAC  
G

*Gammarus pulex*3 (KY464959.1)

TATTATAATTGGTGGTTTCGGGAATTGACTGGTGCCATTAATGCTAGGTAGACC  
TGATATAGCTTTTCCGCGTATAAACAATATAAGATTTTGACTTTTACCTCCTTCTC  
TCACCCTTCTGCTTATAAGTAGTATAGTAGAAAGAGGTGTAGGAACGGGTTGAA  
CG

*Gammarus duebeni*1 (HF930488.1)

TATTATAATCGGTGGATTTCGGTAACTGACTAGTGCCGCTTATGCTAGGTAGCCC  
AGACATAGCCTTCCCGCGTATAAATAATATAAGATTTTGACTTTTACCCCCTTCT  
CTAACTTTACTACTTATAAGGGGGCTTGTAGAAAGAGGGGTGTTGGTACAGGTTGA  
ACC

*Gammarus duebeni*2 (KT209188.1)

TATTATAATCGGTGGATTTCGGTAACTGACTAGTACCGCTTATGCTAGGTAGCCC  
AGACATAGCCTTCCCCCGTATAAATAATATAAGATTTTGACTTTTACCCCCTTCT  
CTAACTTTACTACTTATAAGGGGGCTTGTAGAAAGAGGGGTGTTGGTACAGGTTGA  
ACC

*Gammarus duebeni*3 (HF930481.1)

TATTATAATCGGGGGGATTTCGGTAATTGACTAGTGCCGCTTATGCTAGGTAGCCC  
AGACATAGCCTTCCCCCGTATAAACAAACATAAGATTTTACTTTTACCACCTTCT  
CTAACTTTACTACTTATAAGGGGGGCTTGTAGAAAGAGGGGTGGCACAGGTTGA  
ACC

*Gammarus lacustris*1 (KU376166.1)

TATCATAATTGGGGGGTTCGGCAACTGACTAGTGCCCTTTAATACTAGGTAGACC  
TGATATAGCTTTCCCTCGTATAAACAAACATGAGATTCTGGCTTTTACCCCCCTCC  
TTAACTCTTCTTCTTATAAGAGGTCTAGTGGANAGCGNAGTGNGTACTGGGTGA  
ACT

*Gammarus lacustris*2 (FJ756329.1)

TATCATAATTGGGGGGTTCGGCAACTGACTAGTGCCCTTTAATACTAGGTAGACC  
TGATATAGCTTTCCCTCGTATAAACAAACATGAGATTCTGGCTTTTACCCCCCTCC  
TTAACTCTTCTTCTTATAAGAGGTCTAGTGGAGAGCGGAGTGGGTACTGGGTGA  
ACT

*Gammarus lacustris*3 (DQ889100.1)

TATCATAATTGGAGGGTTCGGCAACTGACTAGTGCCCTTTAATACTAGGTAGACC  
TGATATAGCTTTCCCTCGTATGAATAACATGAGATTCTGGCTTTTACCCCCCTCC  
TTAACTCTTCTTCTTATAAGAGGTCTAGTGGAGAGCGGAGTGGGTACTGGATGA  
ACT

*Gammarus fossarum*1 (KY464960.1)

CATTATAATCGGCGGATTTGGAAACTGATTAGTTCCTTTAATGCTAGGTAGCCCT  
GATATAGCCTTTCCACGTATAAATAACATAAGATTTTATTACCCCCCTCATT  
AACCCTGCTTCTAATAAGAAGTTTAGTAGAAAGGGGAGTGGGCACGGGTTGAA  
CT

*Gammarus fossarum*2 (KX065397.1)

CATTATAATCGGCGGATTTGGAAACTGATTAGTTCCTTTAATGCTAGGTAGCCCT  
GATATAGCCTTTCCACGTATAAATAACATAAGATTCTGATTATTACCCCCCTCAT  
TAACCCTACTTCTAACAAGAAGTTTAGTAGAAAGGGGAGTGGGCACGGGTTGAA  
CT

*Gammarus fossarum*3 (KY464962.1)

CATTATAATCGGCGGATTTGGAAACTGATTAGTTCCTTTAATGCTAGGTAGCCCT  
GATATAGCCTTTCCACGTATAAATAACATAAGATTTTATTACCCCCCTCAT  
TAACCCTGCTTCTAATAAGAAGTTTAGTAGAAAGGGGAGTGGGCACGGGTTGAA  
CT

*Asellus aquaticus*1 (AY531819.1)

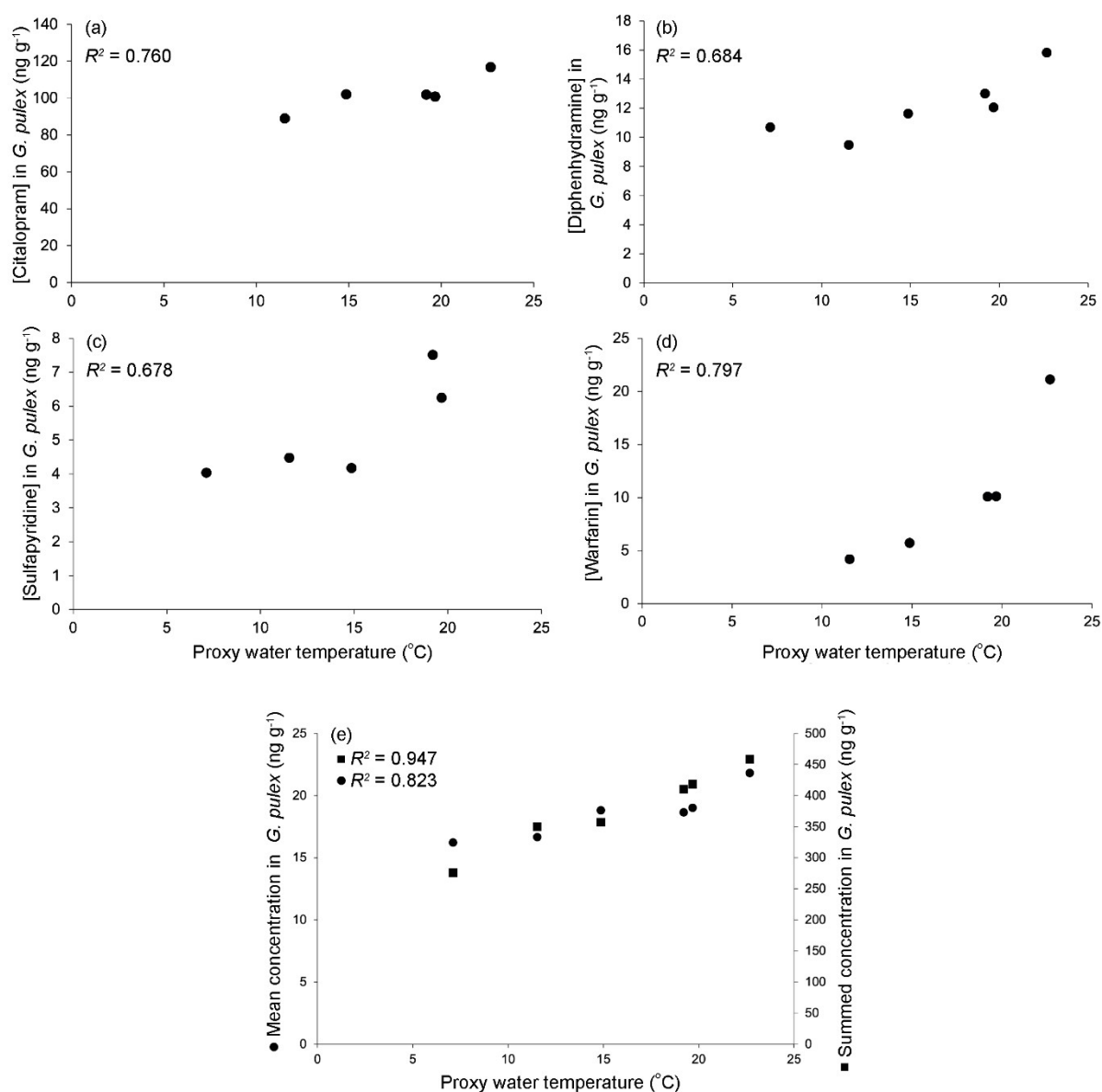
AGTAATAATTGGAGGGTTTGGAAATTGATTAATTCCTTTAATACTAGGCGCCCCC  
GATATAGCATTCCCTCGTATAAATAATATAAGATTCTGATTATTACCTCCCTCTCT  
TACTCTACTCCTATCAAGAGGGTTAATTGAAAGAGGGGTAGGGACCGGTTGAAC  
A

Asellus aquaticus2 (DQ144891.1)

AGTGATAATCGGAGGGTTTGGAAATTGATTAATTCCCCTAATGCTAGGTGCCCC  
AGATATAGCATTTCCTCGCATAAATAATATAAGATTCTGACTATTACCTCCTTCTC  
TAACCCTGCTCCTGTCTAGGGGGTTAATTGAAAGAGGAGTAGGAACTGGCTGA  
ACA

Asellus aquaticus3 (MG986872.1)

AGTGATAATCCGACGGTTTGGAAATTGATTAATTCCCCTAATGCTAGGTGCTCC  
AGATATAGCATTTCCTCGTATAAATAATATAAGATTCTGACTATTACCTCCTTCTC  
TAACCCTGCTCCTGTCTAGGGGGCTAATTGAAAGAGGAGTAGGAACTGGCTGA  
ACA



**Figure S2.** Linear relationships between the water temperature and the concentration of citalopram (a), diphenhydramine (b), sulfapyridine (c), and warfarin (d).  $R^2$  values are indicated on the graphs. (e) Correlation between the mean concentration in *G. pulex* (left axis), cumulative concentration in the *G. pulex* (right axis) and proxy water temperatures.

Table S2. Average concentration  $\pm$  standard deviation of 89 compounds quantified over the entire 6-month study for each compound. Please refer to Tables S9 to S13 in the separate

supplementary data file for monthly data for all matrices.

| <b>Compounds</b>            | <b>HLB<br/>(ng disk<sup>-1</sup>)</b> | <b>MM-anion<br/>(ng disk<sup>-1</sup>)</b> | <b>MM-cation<br/>(ng disk<sup>-1</sup>)</b> | <b>G. pulex<br/>(ng g<sup>-1</sup>)</b> | <b>H<sub>2</sub>O<br/>(ng L<sup>-1</sup>)</b> |
|-----------------------------|---------------------------------------|--------------------------------------------|---------------------------------------------|-----------------------------------------|-----------------------------------------------|
| 4-Methylethcathinone        | 0.05 ± 0.01                           | < LLOQ                                     | 0.13 ± 0.03                                 | -                                       | -                                             |
| Acetamidiprid               | 1.15 ± 0.40                           | 2.24 ± 1.80                                | 3.39 ± 1.00                                 | < LLOQ                                  | 86 ± 20                                       |
| Amitriptyline               | 1.85 ± 0.30                           | 0.47 ± 0.20                                | 1.08 ± 0.30                                 | D                                       | 32 ± 8                                        |
| Amlodipine                  | < LLOQ                                | 0.22 ± 0.10                                | 0.92 ± 0.30                                 | 14 ± 5                                  | -                                             |
| Amphetamine                 | 0.61 ± 0.1                            | < LLOQ                                     | -                                           | D                                       | -                                             |
| Antipyrine                  | 0.1 ± 0.1                             | 0.05 ± 0.02                                | 0.08 ± 0.03                                 | 9.1 ± 5.0                               | -                                             |
| Atorvastatin                | 0.27 ± 0.05                           | D                                          | 2.98 ± 1.00                                 | -                                       | 35 ± 20                                       |
| Atrazine                    | 0.85 ± 0.40                           | 0.56 ± 0.30                                | 0.78 ± 0.30                                 | -                                       | 12 ± 2                                        |
| Azithromycin                | -                                     | 0.21 ± 0.05                                | D                                           | D                                       | 160 ± 40                                      |
| Azoxystrobin                | 0.1 ± 0.07                            | 0.15 ± 0.20                                | 0.11 ± 0.07                                 | < LLOQ                                  | -                                             |
| Benzatropine                | -                                     | -                                          | -                                           | 7.3 ± 1.0                               | -                                             |
| Benzoylecgonine             | 0.4 ± 0.2                             | 0.08 ± 0.04                                | 0.34 ± 0.20                                 | -                                       | 20 ± 7                                        |
| Bezafibrate                 | 0.82 ± 0.20                           | 0.63 ± 0.20                                | 0.84 ± 0.40                                 | -                                       | -                                             |
| Bisoprolol                  | 1 ± 0.5                               | 0.44 ± 0.20                                | 1.11 ± 1.00                                 | -                                       | 19 ± 5                                        |
| Bupropion                   | 0.05 ± 0.02                           | < LLOQ                                     | < LLOQ                                      | -                                       | -                                             |
| Buspirone                   | < LLOQ                                | 0.07 ± 0.01                                | 0.1 ± 0.02                                  | -                                       | -                                             |
| Carbamazepine               | -                                     | D                                          | D                                           | 12.2 ± 7.0                              | 333 ± 100                                     |
| Carbamazepine-10,11-epoxide | 4.23 ± 2.00                           | 2.06 ± 0.50                                | 4.2 ± 2.0                                   | < LLOQ                                  | 47 ± 9                                        |
| Celecoxib                   | < LLOQ                                | 0.06 ± 0.03                                | 0.24 ± 0.09                                 | -                                       | -                                             |
| Citalopram                  | D                                     | 2.75 ± 2.00                                | D                                           | 100.2 ± 14.0                            | 259 ± 60                                      |
| Clarithromycin              | D                                     | 0.96 ± 1.00                                | D                                           | 9.2 ± 3.0                               | 121 ± 50                                      |
| Clopidogrel                 | 1.51 ± 0.40                           | 1.31 ± 1.00                                | 1.9 ± 1.4                                   | 7.2 ± 2.0                               | 29 ± 7                                        |
| Clothianidin                | < LLOQ                                | -                                          | -                                           | 49.5 ± 40.0                             | -                                             |
| Clozapine                   | D                                     | 1.21 ± 0.40                                | D                                           | 11.9 ± 6.0                              | 21 ± 5                                        |
| Cocaine                     | 0.22 ± 0.08                           | 0.41 ± 0.60                                | 0.29 ± 0.20                                 | < LLOQ                                  | 22 ± 20                                       |
| Cyromazine                  | -                                     | -                                          | 1.62 ± 0.20                                 | -                                       | 30 ± 6                                        |
| Diazepam                    | 0.10 ± 0.03                           | -                                          | 0.10 ± 0.02                                 | -                                       | -                                             |
| Diclofenac                  | D                                     | D                                          | D                                           | 10.5 ± 5.0                              | 266 ± 40                                      |
| Diphenhydramine             | 2.25 ± 0.60                           | 0.65 ± 0.40                                | D                                           | 11.8 ± 3.0                              | 53 ± 100                                      |
| Fluoxetine                  | 0.78 ± 0.30                           | 0.27 ± 0.10                                | D                                           | 33.3 ± 14.0                             | 15 ± 2                                        |
| Flurbiprofen                | 2.34 ± 0.50                           | -                                          | 2.41 ± 0.40                                 | -                                       | -                                             |
| Hydrochlorothiazide         | 1.58 ± 0.40                           | 0.85 ± 0.20                                | 2.05 ± 0.80                                 | -                                       | -                                             |
| Imidacloprid                | 4.54 ± 2.00                           | 4.71 ± 0.20                                | 3.73 ± 2.00                                 | 64 ± 13                                 | 66 ± 20                                       |
| Isocarbamid                 | -                                     | 0.2 ± 0.09                                 | -                                           | D                                       | -                                             |
| Ketamine                    | D                                     | 1.97 ± 1.00                                | D                                           | < LLOQ                                  | 46 ± 10                                       |
| Ketoconazole                | D                                     | < LLOQ                                     | D                                           | 17.8 ± 4.0                              | -                                             |
| Levamisole                  | 1.47 ± 0.80                           | 0.93 ± 0.50                                | 3.32 ± 1.00                                 | -                                       | 53 ± 30                                       |
| Levocabastine               | -                                     | -                                          | 0.09 ± 0.01                                 | -                                       | -                                             |
| Lidocaine                   | D                                     | 2.09 ± 0.80                                | D                                           | 21.2 ± 17.0                             | 100 ± 30                                      |

Table S2. Continued

| Compounds           | HLB<br>(ng disk <sup>-1</sup> ) | MM-anion<br>(ng disk <sup>-1</sup> ) | MM-cation<br>(ng disk <sup>-1</sup> ) | G. pulex<br>(ng g <sup>-1</sup> ) | H <sub>2</sub> O<br>(ng L <sup>-1</sup> ) |
|---------------------|---------------------------------|--------------------------------------|---------------------------------------|-----------------------------------|-------------------------------------------|
| Lincomycin          | 0.15 ± 0.03                     | 0.04 ± 0.01                          | 0.10 ± 0.07                           | 6.8 ± 2.0                         | -                                         |
| Lorazepam           | < LLOQ                          | -                                    | 1.54 ± 0.40                           | -                                 | -                                         |
| MDMA                | 1.02 ± 0.60                     | 0.21 ± 0.09                          | D                                     | -                                 | 26 ± 20                                   |
| Medroxyprogesterone | 1.75 ± 0.80                     | 0.75 ± 0.30                          | 0.7 ± 0.14                            | -                                 | -                                         |
| Mefenamic acid      | D                               | D                                    | D                                     | D                                 | 32 ± 10                                   |
| Memantine           | 0.96 ± 0.30                     | 0.27 ± 0.10                          | 2.5 ± 0.90                            | -                                 | 19 ± 3                                    |
| Mephedrone          | 0.02 ± 0.02                     | < LLOQ                               | 0.3 ± 0.30                            | -                                 | < LLOQ                                    |
| Methamphetamine     | 0.75 ± 0.60                     | 0.12 ± 0.05                          | D                                     | < LLOQ                            | 20 ± 6                                    |
| Methylphenidate     | 0.1 ± 0.06                      | 0.04 ± 0.01                          | 0.13 ± 0.04                           | -                                 | -                                         |
| Metoprolol          | 0.2 ± 0.07                      | 0.08 ± 0.04                          | 0.33 ± 0.20                           | -                                 | 12 ± 1                                    |
| Nadolol             | < LLOQ                          | -                                    | 0.04 ± 0.01                           | -                                 | -                                         |
| Nicotine            | 2.74 ± 0.50                     | 1.92 ± 0.70                          | D                                     | D                                 | 240 ± 400                                 |
| Nordiazepam         | 0.34 ± 0.10                     | 0.36 ± 0.20                          | 0.43 ± 0.20                           | -                                 | -                                         |
| Nortriptyline       | 0.42 ± 0.10                     | 0.14 ± 0.10                          | 0.58 ± 0.30                           | 7.5 ± 3.0                         | < LLOQ                                    |
| Orphenadrine        | 0.16 ± 0.04                     | 0.05 ± 0.02                          | 0.11 ± 0.05                           | < LLOQ                            | -                                         |
| Oxamyl              | -                               | -                                    | -                                     | 17.9 ± 13.0                       | -                                         |
| Oxazepam            | 0.8 ± 0.30                      | 0.77 ± 0.40                          | 4.48 ± 0.40                           | < LLOQ                            | < LLOQ                                    |
| Oxycodone           | 0.28 ± 0.10                     | 0.12 ± 0.04                          | 0.3 ± 0.1                             | -                                 | -                                         |
| Pirenzepine         | 0.44 ± 0.20                     | 0.09 ± 0.10                          | 0.74 ± 0.40                           | -                                 | 14 ± 2                                    |
| Prometryn           | 0.2 ± 0.1                       | -                                    | < LLOQ                                | -                                 | -                                         |
| Propamocarb         | 0.06 ± 0.01                     | -                                    | < LLOQ                                | -                                 | < LLOQ                                    |
| Propranolol         | 4.65 ± 0.60                     | 2.27 ± 0.40                          | 0.98 ± 0.70                           | 8.2 ± 2.0                         | 50 ± 9                                    |
| Propazine           | 0.19 ± 0.05                     | < LLOQ                               | 0.18 ± 0.02                           | -                                 | -                                         |
| Risperidone         | < LLOQ                          | -                                    | 0.09 ± 0.03                           | 6.6 ± 0.1                         | 21 ± 8                                    |
| Rizatriptan         | -                               | -                                    | 0.03 ± 0.01                           | -                                 | -                                         |
| Roxithromycin       | 0.10 ± 0.06                     | 0.05 ± 0.02                          | 0.10 ± 0.05                           | -                                 | -                                         |
| Salbutamol          | 0.34 ± 0.10                     | 0.06 ± 0.04                          | 0.82 ± 0.50                           | -                                 | 12 ± 1                                    |
| Salicylic acid      | D                               | D                                    | D                                     | D                                 | 294 ± 200                                 |
| Sertraline          | 2.77 ± 0.40                     | 1.14 ± 0.50                          | D                                     | D                                 | D                                         |
| Simazine            | 0.64 ± 0.05                     | 0.22 ± 0.10                          | 0.34 ± 0.10                           | -                                 | -                                         |
| Spiramycin          | D                               | 0.22 ± 0.20                          | < LLOQ                                | D                                 | -                                         |
| Sulfadimethoxine    | 0.05 ± 0.01                     | 0.13 ± 0.04                          | -                                     | < LLOQ                            | -                                         |
| Sulfamethazine      | < LLOQ                          | 0.05 ± 0.01                          | 0.05 ± 0.03                           | -                                 | -                                         |
| Sulfamethoxazole    | 2.88 ± 0.80                     | 1.51 ± 0.50                          | 1.86 ± 0.40                           | 17 ± 14.0                         | 34 ± 20                                   |
| Sulfamonomethoxine  | 0.59 ± 0.10                     | 0.49 ± 0.20                          | 0.36 ± 0.1                            | -                                 | < LLOQ                                    |
| Sulfapyridine       | D                               | 1.97 ± 1.00                          | D                                     | 5.5 ± 2.0                         | 104 ± 50                                  |
| Sulfathiazole       | -                               | -                                    | -                                     | 20.8 ± 17.0                       | -                                         |
| Tamsulosin          | 0.13 ± 0.09                     | 0.12 ± 0.10                          | 0.16 ± 0.09                           | -                                 | -                                         |
| Temazepam           | 1.46 ± 0.60                     | 1.18 ± 0.70                          | 5.03 ± 0.60                           | < LLOQ                            | 22 ± 5                                    |
| Terbutryn           | 0.28 ± 0.06                     | 0.52 ± 0.50                          | 1.48 ± 0.80                           | -                                 | 14 ± 4                                    |
| Table S2. Continued |                                 |                                      |                                       |                                   |                                           |

| Compounds    | HLB<br>(ng disk <sup>-1</sup> ) | MM-anion<br>(ng disk <sup>-1</sup> ) | MM-cation<br>(ng disk <sup>-1</sup> ) | <i>G. pulex</i><br>(ng g <sup>-1</sup> ) | H <sub>2</sub> O<br>(ng L <sup>-1</sup> ) |
|--------------|---------------------------------|--------------------------------------|---------------------------------------|------------------------------------------|-------------------------------------------|
| Terfenadine  | -                               | 0.22 ± 0.04                          | -                                     | -                                        | -                                         |
| Thiacloprid  | 0.03 ± 0.01                     | 2.24 ± 2.00                          | 0.02 ± 0.001                          | < LLOQ                                   | -                                         |
| Thiamethoxam | 0.09 ± 0.01                     | < LLOQ                               | -                                     | -                                        | -                                         |
| Timolol      | 0.13 ± 0.10                     | 0.15 ± 0.20                          | 0.13 ± 0.07                           | -                                        | -                                         |
| Tramadol     | D                               | 0.47 ± 0.05                          | D                                     | < LLOQ                                   | 246 ± 50                                  |
| Trimethoprim | D                               | 3.36 ± 0.20                          | D                                     | 6.1 ± 2.0                                | 95 ± 20                                   |
| Valsartan    | 0.55 ± 0.09                     | 1.05 ± 1.00                          | 0.35 ± 0.10                           | -                                        | -                                         |
| Venlafaxine  | D                               | 2.31 ± 2.00                          | D                                     | 6.9 ± 2.0                                | 178 ± 30                                  |
| Verapamil    | 0.29 ± 0.30                     | 0.23 ± 0.10                          | 0.44 ± 0.40                           | < LLOQ                                   | 17 ± 2                                    |
| Warfarin     | 0.14 ± 0.07                     | 0.17 ± 0.03                          | 0.11 ± 0.05                           | 11.6 ± 7.0                               | < LLOQ                                    |

< LLOQ: concentrations below LLOQ; D: compound detected but not quantifiable; - not detected.

Refer to Table S3 for method performance data for the MM-anion, MM-cation, and *G. pulex*. For HLB method performance, refer to (Richardson et al., 2022).

Refer to Table S4 for MM-anion and MM-cation recovery data.

Table S3. Selected method performance data of the analysis of passive sampler extracts from the *G. pulex*, MM-anion, and MM-cation sorbent phases. Weekly LOD and LLOQs were calculated using the determined  $R_s$  value over an exposure period of seven days for the 3D-PSD sorbents, refer to (Richardson et al., 2022) for additional details.

| Compound                             | MM-anion         |                       |                           |                       |                           | MM-cation        |                       |                           |                       |                           | <i>G. pulex</i>  |                              |                               |
|--------------------------------------|------------------|-----------------------|---------------------------|-----------------------|---------------------------|------------------|-----------------------|---------------------------|-----------------------|---------------------------|------------------|------------------------------|-------------------------------|
|                                      | LIN<br>( $R^2$ ) | LOD                   |                           | LLOQ                  |                           | LIN<br>( $R^2$ ) | LOD                   |                           | LLOQ                  |                           | LIN<br>( $R^2$ ) | LOD<br>(ng g <sup>-1</sup> ) | LLOQ<br>(ng g <sup>-1</sup> ) |
|                                      |                  | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> |                  | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> |                  |                              |                               |
| 2-(Thiocyanomethylthio)benzothiazole | 0.995            | 95                    | -                         | 285                   | -                         | 0.985            | 174                   | -                         | 523                   | -                         | -                | -                            | -                             |
| 4-Fluoromethacationone               | 0.994            | 87                    | -                         | 261                   | -                         | -                | -                     | -                         | -                     | -                         | 0.600            | 5.2                          | 15.6                          |
| 4-Methylethcathinone                 | 0.993            | 18                    | 0.8                       | 55                    | 2.3                       | 0.991            | 55                    | 0.2                       | 165                   | 0.5                       | 0.982            | 1.2                          | 3.7                           |
| Acetamiprid                          | 0.998            | 11                    | 0.2                       | 34                    | 0.5                       | 0.999            | 6                     | 0.1                       | 17                    | 0.2                       | 0.985            | 1.3                          | 3.8                           |
| Alprazolam                           | 0.997            | 32                    | 0.4                       | 97                    | 1.1                       | 0.974            | 45                    | 0.4                       | 136                   | 1.3                       | 0.935            | 1.7                          | 5.1                           |
| Ametryn                              | 0.981            | 30                    | 0.7                       | 89                    | 2.1                       | 0.982            | 80                    | 0.5                       | 239                   | 1.5                       | 0.979            | 1.3                          | 4                             |
| Amiodarone                           | -                | -                     | -                         | -                     | -                         | 0.250            | 259                   | -                         | 777                   | -                         | -                | -                            | -                             |
| Amitriptyline                        | 0.993            | 12                    | 0.7                       | 36                    | 2.2                       | 0.995            | 11                    | 0.1                       | 32                    | 0.2                       | -                | -                            | -                             |
| Amlodipine                           | 0.996            | 78                    | -                         | 233                   | -                         | 0.983            | 36                    | -                         | 109                   | -                         | 0.970            | 1.4                          | 4.3                           |
| Amphetamine                          | 0.993            | 100                   | 12.5                      | 299                   | 37.4                      | 0.988            | 74                    | -                         | 221                   | -                         | -                | -                            | -                             |
| Antipyrine                           | 0.995            | 11                    | 0.3                       | 32                    | 0.9                       | 0.986            | 18                    | 0.2                       | 54                    | 0.6                       | 0.996            | 1.1                          | 3.4                           |
| Atorvastatin                         | 0.989            | 144                   | 3.1                       | 433                   | 9.3                       | 0.982            | 191                   | -                         | 573                   | -                         | 0.915            | 1.9                          | 5.6                           |
| Atrazine                             | 0.985            | 145                   | -                         | 436                   | -                         | 0.998            | 62                    | 0.3                       | 187                   | 0.9                       | 0.993            | 1.2                          | 3.6                           |
| Azithromycin                         | 0.999            | 33                    | -                         | 100                   | -                         | 0.990            | 27                    | 0.2                       | 82                    | 0.5                       | 0.660            | 4.2                          | 12.7                          |
| Azoxystrobin                         | 0.998            | 11                    | 0.2                       | 32                    | 0.5                       | 0.995            | 11                    | 0.2                       | 33                    | 0.5                       | 0.981            | 1.3                          | 4                             |
| Benoxacor                            | 0.803            | 707                   | -                         | 2121                  | -                         | -                | 211                   | -                         | 632                   | -                         | 0.340            | 0.1                          | 0.2                           |
| Bensulide                            | 0.996            | 76                    | -                         | 229                   | -                         | 0.996            | 72                    | -                         | 215                   | -                         | -                | -                            | -                             |
| Benzatropine                         | 0.980            | 22                    | 0.6                       | 65                    | 1.8                       | 0.989            | 16                    | 0.1                       | 48                    | 0.2                       | 0.933            | 1.5                          | 4.5                           |
| Benzoylcegonine                      | 0.991            | 14                    | 1.1                       | 42                    | 3.2                       | 0.996            | 13                    | 0.6                       | 40                    | 1.9                       | 0.994            | 1.2                          | 3.5                           |
| Betaxolol                            | 0.994            | 11                    | 0.3                       | 34                    | 1                         | 0.997            | 15                    | 0.1                       | 46                    | 0.3                       | 0.917            | 1.7                          | 5.1                           |
| Bezafibrate                          | 0.983            | 20                    | 0.2                       | 60                    | 0.6                       | 0.998            | 6                     | 0.1                       | 18                    | 0.4                       | 0.907            | 1.5                          | 4.5                           |
| Bisoprolol                           | 0.993            | 13                    | 0.3                       | 38                    | 0.9                       | 0.999            | 5                     | 0.03                      | 16                    | 0.1                       | 0.986            | 1.3                          | 3.8                           |
| Bupropion                            | 0.996            | 76                    | 1.8                       | 229                   | 5.3                       | 0.997            | 69                    | 0.3                       | 208                   | 0.9                       | 0.981            | 1.3                          | 4                             |
| Buspirone                            | 0.998            | 6                     | 0.1                       | 19                    | 0.3                       | 0.982            | 20                    | 0.1                       | 60                    | 0.3                       | 0.991            | 1.2                          | 3.6                           |
| Carazolol                            | 0.999            | 6                     | -                         | 17                    | -                         | 0.997            | 15                    | 0.1                       | 45                    | 0.2                       | 0.971            | 1.4                          | 4.3                           |
| Carbamazepine                        | 0.996            | 75                    | 0.9                       | 224                   | 2.8                       | 0.996            | 9                     | 0.1                       | 28                    | 0.3                       | 0.878            | 2.1                          | 6.4                           |
| Carbamazepine-10,11-epoxide          | 0.986            | 26                    | -                         | 78                    | -                         | 0.992            | 103                   | 0.6                       | 310                   | 1.9                       | 0.996            | 1.1                          | 3.4                           |
| Carboxine                            | 0.983            | 77                    | -                         | 231                   | -                         | 0.997            | 85                    | -                         | 255                   | -                         | 0.957            | 1.3                          | 3.8                           |
| Carfentrazone-ethyl                  | 0.990            | 21                    | -                         | 63                    | -                         | 0.996            | 76                    | -                         | 229                   | -                         | 0.796            | 2.2                          | 6.6                           |
| Celecoxib                            | 0.995            | 11                    | -                         | 33                    | -                         | 0.985            | 26                    | 0.3                       | 78                    | 1                         | 0.965            | 1.5                          | 4.4                           |
| Chloramphenicol                      | 0.981            | 83                    | -                         | 248                   | -                         | 0.979            | 22                    | -                         | 66                    | -                         | -                | -                            | -                             |
| Cilazapril                           | 0.999            | 6                     | 0.1                       | 19                    | 0.4                       | 0.997            | 16                    | 0.7                       | 48                    | 2.1                       | 0.989            | 1.2                          | 3.7                           |
| Citalopram                           | 0.999            | 7                     | -                         | 20                    | -                         | 0.995            | 11                    | -                         | 32                    | -                         | 0.736            | 3.3                          | 10                            |
| Clarithromycin                       | 0.994            | 16                    | -                         | 49                    | -                         | 0.979            | 22                    | 0.1                       | 65                    | 0.2                       | 0.952            | 1.6                          | 4.7                           |
| Clodinafop-propargyl                 | 0.996            | 38                    | -                         | 113                   | -                         | 0.977            | 219                   | -                         | 657                   | -                         | 0.890            | 2                            | 6.1                           |
| Clofibrilic acid                     | 0.983            | 154                   | -                         | 461                   | -                         | 0.887            | 54                    | -                         | 161                   | -                         | 0.837            | 2.4                          | 7.3                           |
| Clopidogrel                          | 0.992            | 20                    | 0.4                       | 59                    | 1.2                       | 0.989            | 63                    | 0.8                       | 189                   | 2.5                       | 0.984            | 1.3                          | 3.9                           |
| Clothianidin                         | 0.993            | 13                    | 0.2                       | 39                    | 0.6                       | 0.999            | 10                    | 0.1                       | 30                    | 0.3                       | 0.688            | 2.5                          | 7.6                           |
| Clozapine                            | 0.995            | 88                    | 3.8                       | 264                   | 11.5                      | -                | -                     | -                         | -                     | -                         | 0.880            | 2.1                          | 6.3                           |
| Cocaine                              | 0.999            | 9                     | 0.1                       | 27                    | 0.3                       | 0.994            | 11                    | 0.1                       | 34                    | 0.2                       | 0.978            | 1.4                          | 4.1                           |
| Cyclouron                            | 0.989            | 132                   | -                         | 397                   | -                         | 0.992            | 146                   | -                         | 437                   | -                         | 0.937            | 1.7                          | 5.1                           |
| Cycloxydim                           | -                | -                     | -                         | -                     | -                         | -                | 492                   | -                         | 1477                  | -                         | -                | -                            | -                             |
| Cymoxanil                            | 0.991            | 132                   | -                         | 395                   | -                         | -                | -                     | -                         | -                     | -                         | -                | -                            | -                             |
| Cyromazine                           | 0.992            | 119                   | -                         | 357                   | -                         | 0.976            | 210                   | -                         | 630                   | -                         | -                | -                            | -                             |
| Diazepam                             | 0.991            | 111                   | 1.3                       | 332                   | 3.8                       | 0.981            | 163                   | 1.8                       | 489                   | 5.5                       | 0.988            | 1.2                          | 3.7                           |
| Diclofenac                           | 0.991            | 111                   | 1.5                       | 333                   | 4.4                       | 0.985            | 18                    | 0.5                       | 55                    | 1.5                       | 0.910            | 1.9                          | 5.7                           |
| Diffubenzuron                        | 0.994            | 12                    | -                         | 36                    | -                         | 0.987            | 17                    | -                         | 52                    | -                         | 0.860            | 2.3                          | 6.8                           |
| Dimethametryn                        | 0.984            | 19                    | -                         | 58                    | -                         | 0.977            | 42                    | -                         | 127                   | -                         | 0.880            | 2.1                          | 6.3                           |
| Dimethomorph                         | 0.992            | 108                   | -                         | 323                   | -                         | 0.988            | 24                    | -                         | 72                    | -                         | 0.963            | 1.5                          | 4.5                           |
| Diphenhydramine                      | 0.997            | 8                     | 1.3                       | 25                    | 4                         | 0.992            | 14                    | 0.1                       | 41                    | 0.2                       | 0.930            | 1.7                          | 5.2                           |

Table S3. Continued

| Compound            | MM-anion                 |                       |                           |                       |                           | MM-cation                |                       |                           |                       |                           | <i>G. pulex</i>          |                              |                               |
|---------------------|--------------------------|-----------------------|---------------------------|-----------------------|---------------------------|--------------------------|-----------------------|---------------------------|-----------------------|---------------------------|--------------------------|------------------------------|-------------------------------|
|                     | LIN<br>(R <sup>2</sup> ) | LOD                   |                           | LLOQ                  |                           | LIN<br>(R <sup>2</sup> ) | LOD                   |                           | LLOQ                  |                           | LIN<br>(R <sup>2</sup> ) | LOD<br>(ng g <sup>-1</sup> ) | LLOQ<br>(ng g <sup>-1</sup> ) |
|                     |                          | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> |                          | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> |                          |                              |                               |
| Enalapril           | 0.997                    | 59                    | -                         | 176                   | -                         | 0.984                    | 27                    | -                         | 81                    | -                         | 0.881                    | 2.1                          | 6.3                           |
| Famoxadone          | 0.984                    | 19                    | -                         | 57                    | -                         | 0.995                    | 88                    | -                         | 264                   | -                         | 0.849                    | 2.3                          | 7                             |
| Fenoxaprop-ethyl    | 0.012                    | 12757                 | -                         | 38270                 | -                         | -                        | -                     | -                         | -                     | -                         | 0.370                    | 6.1                          | 18.3                          |
| Fenuron             | 0.980                    | 31                    | -                         | 92                    | -                         | 0.993                    | 95                    | -                         | 284                   | -                         | 0.994                    | 1.1                          | 3.4                           |
| Fluocinonide        | -                        | 82                    | -                         | 245                   | -                         | 0.967                    | 262                   | -                         | 786                   | -                         | 0.948                    | 1.3                          | 4                             |
| Fluoxetine          | 0.993                    | 17                    | 2.1                       | 52                    | 6.2                       | 0.986                    | 18                    | -                         | 54                    | -                         | 0.976                    | 1.4                          | 4.1                           |
| Flurbiprofen        | -                        | -                     | -                         | -                     | -                         | -                        | -                     | -                         | -                     | -                         | -                        | -                            | -                             |
| Flurochloridone     | 0.997                    | 70                    | -                         | 211                   | -                         | 0.980                    | 167                   | -                         | 500                   | -                         | 0.836                    | 2.2                          | 6.6                           |
| Flutamide           | 0.998                    | 10                    | 0.1                       | 29                    | 0.4                       | 0.998                    | 12                    | 0.2                       | 35                    | 0.5                       | 0.982                    | 1.3                          | 3.8                           |
| Flutolanil          | 0.997                    | 8                     | -                         | 23                    | -                         | 0.995                    | 16                    | -                         | 47                    | -                         | 0.860                    | 2.1                          | 6.2                           |
| Fuberidazole        | 0.999                    | 6                     | -                         | 18                    | -                         | 0.998                    | 10                    | -                         | 31                    | -                         | 0.871                    | 2.2                          | 6.5                           |
| Gemfibrozil         | -                        | -                     | -                         | -                     | -                         | 0.869                    | 450                   | -                         | 1350                  | -                         | -                        | -                            | -                             |
| Hydrochlorothiazide | 0.985                    | 72                    | -                         | 217                   | -                         | 0.989                    | 29                    | -                         | 86                    | -                         | 0.813                    | 2.6                          | 7.9                           |
| Imidacloprid        | 0.986                    | 33                    | 0.3                       | 98                    | 1                         | 0.984                    | 19                    | 0.2                       | 58                    | 0.7                       | 0.847                    | 2.4                          | 7.1                           |
| Isocarbamid         | 0.988                    | 25                    | -                         | 74                    | -                         | 0.996                    | 70                    | -                         | 210                   | -                         | 0.604                    | 4.2                          | 12.7                          |
| Isradipine          | 0.901                    | 76                    | -                         | 227                   | -                         | 0.852                    | 116                   | -                         | 348                   | -                         | 0.942                    | 1.4                          | 4.2                           |
| Josamycin           | 0.997                    | 12                    | -                         | 36                    | -                         | 0.989                    | 155                   | -                         | 466                   | -                         | 0.983                    | 1.3                          | 3.9                           |
| Ketamine            | 0.983                    | 28                    | 0.4                       | 84                    | 1.1                       | 0.987                    | 67                    | 0.2                       | 200                   | 0.5                       | 0.992                    | 1.2                          | 3.6                           |
| Ketoconazole        | 0.991                    | 112                   | -                         | 337                   | -                         | -                        | -                     | -                         | -                     | -                         | 0.695                    | 3.8                          | 11.4                          |
| Ketoprofen          | 0.940                    | 335                   | -                         | 1005                  | -                         | 0.007                    | -                     | -                         | -                     | -                         | -                        | -                            | -                             |
| Ketotifen           | 0.994                    | 11                    | 0.4                       | 33                    | 1.2                       | 0.997                    | 9                     | 0.1                       | 27                    | 0.2                       | 0.887                    | 2.1                          | 6.2                           |
| Levamisole          | 0.995                    | 14                    | 0.5                       | 43                    | 1.5                       | 0.996                    | 10                    | 0.1                       | 29                    | 0.2                       | -                        | -                            | -                             |
| Levocabastine       | 0.995                    | 16                    | 0.1                       | 49                    | 0.4                       | 0.993                    | 23                    | 0.2                       | 68                    | 0.6                       | 0.981                    | 1.3                          | 4                             |
| Lidocaine           | 0.997                    | 12                    | 0.2                       | 35                    | 0.7                       | 0.991                    | 14                    | 0.1                       | 42                    | 0.2                       | 0.997                    | 1.1                          | 3.3                           |
| Lincomycin          | 0.999                    | 24                    | -                         | 72                    | -                         | 0.999                    | 7                     | 0.2                       | 22                    | 0.7                       | 0.996                    | 1.1                          | 3.4                           |
| Lorazepam           | 0.994                    | 95                    | -                         | 285                   | -                         | -                        | 205                   | -                         | 616                   | -                         | 0.986                    | 1.3                          | 3.8                           |
| MDMA                | 0.999                    | 8                     | 1.2                       | 25                    | 3.6                       | 0.985                    | 27                    | -                         | 80                    | -                         | 0.993                    | 1.2                          | 3.5                           |
| Meclizine           | 0.987                    | 137                   | -                         | 411                   | -                         | 0.068                    | 5301                  | -                         | 15904                 | -                         | 0.507                    | 7.3                          | 21.9                          |
| Medroxyprogesterone | 0.991                    | 26                    | -                         | 79                    | -                         | 0.997                    | 11                    | -                         | 33                    | -                         | 0.976                    | 1.4                          | 4.1                           |
| Mefenamic acid      | 0.990                    | 128                   | -                         | 383                   | -                         | 0.957                    | 59                    | 1.9                       | 178                   | 5.7                       | -                        | -                            | -                             |
| Memantine           | 0.997                    | 13                    | 0.8                       | 38                    | 2.5                       | 0.989                    | 62                    | 0.1                       | 187                   | 0.4                       | 0.961                    | 1.5                          | 4.5                           |
| Mephedrone          | 0.995                    | 15                    | 3.6                       | 46                    | 10.7                      | 0.993                    | 48                    | 0.2                       | 145                   | 0.6                       | 0.997                    | 1.1                          | 3.4                           |
| Mephosfolan         | 0.999                    | 11                    | -                         | 32                    | -                         | 0.997                    | 8                     | -                         | 23                    | -                         | 0.859                    | 2.3                          | 6.8                           |
| Metformin           | 0.987                    | 135                   | -                         | 405                   | -                         | 0.701                    | 858                   | -                         | 2574                  | -                         | -                        | -                            | -                             |
| Methamphetamine     | 0.993                    | 18                    | 4.9                       | 55                    | 14.8                      | 0.986                    | 71                    | -                         | 213                   | -                         | 0.984                    | 1.3                          | 3.9                           |
| Methcathinone       | 0.993                    | 18                    | 6.8                       | 55                    | 20.4                      | 0.995                    | 16                    | 0.03                      | 48                    | 0.1                       | 0.973                    | 1.4                          | 4.2                           |
| Methedrone          | 0.990                    | 15                    | 3.1                       | 44                    | 9.2                       | 0.978                    | 42                    | 0.2                       | 127                   | 0.7                       | 0.909                    | 1.6                          | 4.9                           |
| Methylphenidate     | 0.999                    | 10                    | -                         | 31                    | -                         | 0.982                    | 20                    | 0.1                       | 60                    | 0.2                       | 0.993                    | 1.2                          | 3.6                           |
| Metoprolol          | 0.998                    | 12                    | 0.4                       | 36                    | 1.2                       | 0.997                    | 12                    | 0.1                       | 35                    | 0.2                       | 0.981                    | 1.3                          | 4                             |
| Morphine            | 0.985                    | 34                    | -                         | 102                   | -                         | 0.977                    | 90                    | -                         | 269                   | -                         | 0.951                    | 1.4                          | 4.3                           |
| Nadolol             | 0.997                    | 12                    | 0.7                       | 37                    | 2.1                       | 0.999                    | 9                     | 0.1                       | 26                    | 0.2                       | 0.991                    | 1.2                          | 3.7                           |
| Nicotine            | 0.991                    | 115                   | -                         | 346                   | -                         | -                        | -                     | -                         | -                     | -                         | -                        | -                            | -                             |
| Nifedipine          | 0.979                    | 95                    | -                         | 285                   | -                         | 0.991                    | 114                   | -                         | 341                   | -                         | 0.851                    | 1.6                          | 4.8                           |
| Nitenpyram          | 0.999                    | 10                    | 1                         | 29                    | 3                         | 0.991                    | 75                    | -                         | 225                   | -                         | 0.967                    | 1.5                          | 4.4                           |
| Nordiazepam         | 0.995                    | 20                    | 0.4                       | 59                    | 1.3                       | 0.990                    | 15                    | 0.3                       | 44                    | 0.9                       | 0.983                    | 1.3                          | 3.9                           |
| Norethisterone      | 0.999                    | 45                    | -                         | 136                   | -                         | -                        | 54                    | -                         | 162                   | -                         | -                        | -                            | -                             |
| Nortriptyline       | 0.994                    | 17                    | 2.3                       | 50                    | 7                         | 0.977                    | 23                    | 0.1                       | 69                    | 0.3                       | 0.983                    | 1.2                          | 3.5                           |
| Orphenadrine        | 0.999                    | 5                     | 0.5                       | 16                    | 1.6                       | 0.995                    | 11                    | 0.1                       | 33                    | 0.2                       | 0.825                    | 1.8                          | 5.4                           |
| Oxamyl              | 0.998                    | 25                    | 8.2                       | 76                    | 24.6                      | 0.997                    | 15                    | -                         | 44                    | -                         | 0.992                    | 1.2                          | 3.6                           |
| Oxazepam            | 0.996                    | 14                    | 0.2                       | 43                    | 0.7                       | 0.995                    | 20                    | 0.8                       | 59                    | 2.5                       | 0.986                    | 1.3                          | 3.8                           |
| Oxycarboxin         | 0.999                    | 10                    | -                         | 31                    | -                         | 0.986                    | 32                    | -                         | 96                    | -                         | 0.836                    | 2.4                          | 7.3                           |

Table S3. Continued

| Compound           | MM-anion                         |                       |                           |                       |                           | MM-cation                        |                       |                           |                       |                           | <i>G. pulex</i>                  |                              |                               |
|--------------------|----------------------------------|-----------------------|---------------------------|-----------------------|---------------------------|----------------------------------|-----------------------|---------------------------|-----------------------|---------------------------|----------------------------------|------------------------------|-------------------------------|
|                    | LIN<br>( <i>R</i> <sup>2</sup> ) | LOD                   |                           | LLOQ                  |                           | LIN<br>( <i>R</i> <sup>2</sup> ) | LOD                   |                           | LLOQ                  |                           | LIN<br>( <i>R</i> <sup>2</sup> ) | LOD<br>(ng g <sup>-1</sup> ) | LLOQ<br>(ng g <sup>-1</sup> ) |
|                    |                                  | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> |                                  | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> | pg disk <sup>-1</sup> | Weekly ng L <sup>-1</sup> |                                  |                              |                               |
| Oxycodone          | 0.999                            | 5                     | 0.2                       | 14                    | 0.6                       | 0.999                            | 5                     | 0                         | 14                    | 0.1                       | 0.937                            | 1.7                          | 5.1                           |
| Picoxystrobin      | 0.998                            | 59                    | 1.1                       | 177                   | 3.4                       | 0.989                            | 30                    | -                         | 90                    | -                         | 0.969                            | 1.4                          | 4.3                           |
| Piperophos         | 0.996                            | 9                     | -                         | 27                    | -                         | 0.993                            | 13                    | -                         | 39                    | -                         | 0.893                            | 2                            | 6                             |
| Pirenzepine        | 0.999                            | 4                     | 0.4                       | 11                    | 1.3                       | 0.996                            | 18                    | 0.3                       | 54                    | 1                         | 0.995                            | 1.2                          | 3.5                           |
| Pretilachlor       | 0.993                            | 100                   | -                         | 301                   | -                         | 0.989                            | 124                   | -                         | 372                   | -                         | 0.764                            | 2.2                          | 6.5                           |
| Prodiamine         | -                                | -                     | -                         | -                     | -                         | 0.886                            | 487                   | -                         | 1462                  | -                         | -                                | -                            | -                             |
| Prometon           | 0.982                            | 29                    | 0.5                       | 86                    | 1.5                       | 0.997                            | 37                    | 0.2                       | 110                   | 0.7                       | 0.996                            | 1.1                          | 3.4                           |
| Prometryn          | 0.996                            | 77                    | 1.3                       | 232                   | 4                         | 0.987                            | 74                    | 0.4                       | 222                   | 1.1                       | 0.988                            | 1.2                          | 3.7                           |
| Propamocarb        | 0.998                            | 9                     | -                         | 28                    | -                         | 0.986                            | 18                    | 0.1                       | 53                    | 0.3                       | 0.912                            | 1.9                          | 5.6                           |
| Propranolol        | 0.999                            | 5                     | 0.2                       | 16                    | 0.5                       | 0.976                            | 24                    | 0.1                       | 71                    | 0.3                       | 0.981                            | 1.3                          | 4                             |
| Propazine          | 0.984                            | 153                   | -                         | 459                   | -                         | 0.998                            | 57                    | 0.3                       | 171                   | 0.8                       | 0.989                            | 1.2                          | 3.6                           |
| Pymetrozine        | 0.999                            | 5                     | 0.8                       | 14                    | 2.3                       | 0.999                            | 6                     | 0.2                       | 17                    | 0.7                       | 0.951                            | 1.6                          | 4.7                           |
| Pyracarbolid       | 0.991                            | 21                    | -                         | 62                    | -                         | 0.984                            | 35                    | -                         | 106                   | -                         | 0.980                            | 1.3                          | 3.9                           |
| Pyraclostrobin     | 0.993                            | 110                   | -                         | 331                   | -                         | 0.999                            | 36                    | -                         | 109                   | -                         | 0.934                            | 1.4                          | 4.3                           |
| Pyraflufen-ethyl   | 0.984                            | 36                    | -                         | 108                   | -                         | 0.997                            | 73                    | -                         | 219                   | -                         | 0.585                            | 3.2                          | 9.6                           |
| Pyridaben          | -                                | -                     | -                         | -                     | -                         | 0.986                            | 79                    | -                         | 237                   | -                         | -                                | -                            | -                             |
| Risperidone        | 0.994                            | 99                    | 2.9                       | 296                   | 8.6                       | -                                | -                     | -                         | -                     | -                         | 0.967                            | 1.3                          | 4                             |
| Rizatriptan        | 0.993                            | 13                    | -                         | 39                    | -                         | 0.986                            | 71                    | 1.1                       | 214                   | 3.2                       | 0.984                            | 1.3                          | 3.9                           |
| Ronidazole         | 0.999                            | 7                     | 1.2                       | 22                    | 3.5                       | 0.999                            | 6                     | 0.2                       | 19                    | 0.7                       | 0.975                            | 1.4                          | 4.1                           |
| Roxithromycin      | 0.998                            | 7                     | -                         | 21                    | -                         | 0.995                            | 11                    | -                         | 32                    | -                         | 0.967                            | 1.3                          | 4                             |
| Salbutamol         | 0.999                            | 7                     | 3.2                       | 20                    | 9.5                       | 0.999                            | 10                    | 0.1                       | 30                    | 0.3                       | 0.971                            | 1.4                          | 4.2                           |
| Salicylic acid     | 0.552                            | 1046                  | -                         | 3138                  | -                         | 0.469                            | 159                   | -                         | 478                   | -                         | -                                | -                            | -                             |
| Sertraline         | 0.981                            | 30                    | -                         | 90                    | -                         | 0.878                            | 56                    | -                         | 167                   | -                         | -                                | -                            | -                             |
| Simazine           | 0.987                            | 155                   | -                         | 465                   | -                         | 0.990                            | 119                   | 0.6                       | 357                   | 1.9                       | 0.985                            | 1.3                          | 3.9                           |
| Spinosyn A         | 0.995                            | 83                    | -                         | 250                   | -                         | 0.917                            | 45                    | -                         | 135                   | -                         | 0.961                            | 1.4                          | 4.3                           |
| Spinosyn D         | 0.809                            | 73                    | -                         | 218                   | -                         | 0.984                            | 19                    | -                         | 57                    | -                         | 0.936                            | 1.4                          | 4.3                           |
| Spiramycin         | 0.981                            | 21                    | -                         | 62                    | -                         | -                                | -                     | -                         | -                     | -                         | 0.773                            | 3                            | 9                             |
| Sulfadimethoxine   | 0.996                            | 9                     | 0.1                       | 27                    | 0.2                       | 0.997                            | 16                    | 0.6                       | 48                    | 1.7                       | 0.982                            | 1.3                          | 3.9                           |
| Sulfamerazine      | 0.997                            | 85                    | -                         | 255                   | -                         | -                                | -                     | -                         | -                     | -                         | -                                | -                            | -                             |
| Sulfamethazine     | 0.993                            | 13                    | 0.3                       | 38                    | 0.8                       | 0.999                            | 5                     | 0.4                       | 15                    | 1.3                       | 0.989                            | 1.2                          | 3.7                           |
| Sulfamethoxazole   | 0.993                            | 60                    | 0.8                       | 180                   | 2.5                       | 0.989                            | 30                    | 2.2                       | 90                    | 6.7                       | 0.994                            | 1.1                          | 3.3                           |
| Sulfamonomethoxine | 0.985                            | 73                    | -                         | 218                   | -                         | 0.995                            | 81                    | 4.6                       | 244                   | 13.9                      | 0.992                            | 1.2                          | 3.6                           |
| Sulfapyridine      | 0.995                            | 11                    | 3.6                       | 32                    | 10.8                      | 0.996                            | 9                     | 0.4                       | 27                    | 1.2                       | 0.987                            | 1.3                          | 3.8                           |
| Sulfathiazole      | 0.988                            | 31                    | 3.3                       | 92                    | 9.9                       | 0.999                            | 3                     | 0.2                       | 10                    | 0.6                       | 0.966                            | 1.5                          | 4.4                           |
| Sulfisoxazole      | 0.989                            | 23                    | 0.4                       | 68                    | 1.3                       | 0.996                            | 10                    | -                         | 30                    | -                         | 0.990                            | 1.2                          | 3.7                           |
| Tacrine            | 0.996                            | 10                    | 0.4                       | 30                    | 1.3                       | 0.978                            | 41                    | -                         | 122                   | -                         | 0.988                            | 1.3                          | 3.8                           |
| Tamsulosin         | 0.998                            | 11                    | 0.2                       | 34                    | 0.7                       | 0.990                            | 15                    | 0.1                       | 44                    | 0.3                       | 0.988                            | 1.2                          | 3.7                           |
| Temazepam          | 0.995                            | 11                    | 0.2                       | 33                    | 0.6                       | -                                | 6                     | 0.1                       | 19                    | 0.4                       | 0.99                             | 1.2                          | 3.7                           |
| Terbutryn          | 0.996                            | 75                    | 1                         | 226                   | 3.1                       | 0.987                            | 73                    | 0.3                       | 220                   | 1                         | -                                | -                            | -                             |
| Terfenadine        | 0.959                            | 31                    | -                         | 92                    | -                         | 0.991                            | 14                    | -                         | 43                    | -                         | 0.950                            | 1.6                          | 4.8                           |
| Thiacloprid        | 0.997                            | 15                    | 0.1                       | 44                    | 0.3                       | 0.997                            | 8                     | 0.1                       | 23                    | 0.2                       | 0.974                            | 1.4                          | 4.2                           |
| Thiamethoxam       | 0.997                            | 15                    | 0.3                       | 45                    | 0.8                       | 0.976                            | 35                    | 0.7                       | 105                   | 2.2                       | 0.947                            | 1.6                          | 4.8                           |
| Thiazopyr          | 0.986                            | 143                   | -                         | 430                   | -                         | 0.985                            | 143                   | -                         | 429                   | -                         | 0.851                            | 2.3                          | 7                             |
| Timolol            | 0.999                            | 8                     | 0.2                       | 23                    | 0.6                       | 0.999                            | 5                     | 0.03                      | 16                    | 0.1                       | 0.991                            | 1.2                          | 3.6                           |
| Tramadol           | 0.998                            | 11                    | 0.3                       | 32                    | 0.9                       | 0.996                            | 10                    | 0.04                      | 29                    | 0.1                       | 0.922                            | 1.8                          | 5.4                           |
| Trimethoprim       | 0.996                            | 18                    | 0.6                       | 53                    | 1.9                       | 0.998                            | 6                     | 0.1                       | 19                    | 0.2                       | 0.978                            | 1.4                          | 4.1                           |
| Valsartan          | 0.988                            | 141                   | 3                         | 423                   | 8.9                       | 0.994                            | 92                    | 7.3                       | 275                   | 21.8                      | 0.976                            | 1.2                          | 3.7                           |
| Venlafaxine        | 0.990                            | 15                    | 0.8                       | 45                    | 2.3                       | 0.999                            | 5                     | 0                         | 16                    | 0.1                       | 0.973                            | 1.4                          | 4.2                           |
| Verapamil          | 0.998                            | 7                     | 0.1                       | 22                    | 0.3                       | 0.993                            | 13                    | 0.1                       | 38                    | 0.2                       | 0.983                            | 1.3                          | 3.9                           |
| Warfarin           | 0.997                            | 66                    | 1.2                       | 199                   | 3.6                       | 0.998                            | 13                    | 0.4                       | 38                    | 1.2                       | 0.986                            | 1.3                          | 3.8                           |
| Ziprasidone        | 0.996                            | 74                    | -                         | 221                   | -                         | 0.976                            | 35                    | -                         | 106                   | -                         | 0.935                            | 1.7                          | 5.1                           |

Table S4. Comparison of the mean (standard deviation,  $n = 9$ ) percentage recovery of each compound using the MM-anion and MM-cation sorbents. Refer to Richardson *et al.*, 2022 for HLB recovery data.

| Compound                             | MM-anion | MM-cation | Compound             | MM-anion | MM-cation | Compound            | MM-anion | MM-cation |
|--------------------------------------|----------|-----------|----------------------|----------|-----------|---------------------|----------|-----------|
| 2-(Thiocyanomethylthio)benzothiazole | 48 (21)  | 2 (1)     | Carazolol            | 62 (13)  | 40 (7)    | Fenoxaprop-ethyl    | 27 (16)  | 2 (0)     |
| 4-Fluoromethacationone               | 43 (13)  | 24 (8)    | Carbamazepine        | 75 (9)   | 76 (10)   | Fenuron             | 50 (14)  | 50 (17)   |
| 4-Methylethcathinone                 | 60 (11)  | 25 (14)   | Carboxine            | 3 (4)    | 12 (8)    | Flufenoxuron        | 10 (5)   | 44 (22)   |
| Acetamiprid                          | 72 (9)   | 70 (8)    | Carfentrazone-ethyl  | 61 (11)  | 2 (1)     | Fluocinonide        | 83 (11)  | 40 (17)   |
| Aclonifen                            | 93 (8)   | 98 (9)    | CBZ epoxide          | 49 (29)  | 15 (1)    | Fluoxetine          | 83 (29)  | 29 (9)    |
| Alprazolam                           | 54 (14)  | 55 (13)   | Celecoxib            | 55 (10)  | 61 (10)   | Flurochloridone     | 61 (11)  | 45 (13)   |
| Ametryn                              | 50 (10)  | 42 (13)   | Chloramphenicol      | 65 (16)  | 76 (15)   | Flutamide           | 70 (9)   | 80 (11)   |
| Amiodarone                           | 44 (7)   | 27 (14)   | Cilazapril           | 70 (8)   | 76 (8)    | Flutolanil          | 68 (8)   | 73 (7)    |
| Amitriptyline                        | 87 (26)  | 32 (10)   | Citalopram           | 79 (13)  | 52 (10)   | Fuberidazole        | 67 (7)   | 62 (6)    |
| Amlodipine                           | 39 (11)  | 16 (5)    | Clarithromycin       | 59 (33)  | 15 (7)    | Hydrochlorothiazide | 39 (5)   | 72 (10)   |
| Amphetamine                          | 57 (8)   | 28 (15)   | Clodinafop-propargyl | 60 (9)   | 16 (2)    | Imidacloprid        | 74 (9)   | 77 (13)   |
| Antipyrine                           | 60 (8)   | 68 (12)   | Clopidogrel          | 64 (8)   | 56 (10)   | Isocarbamid         | 63 (11)  | 53 (9)    |
| Atorvastatin                         | 12 (6)   | 15 (6)    | Clothianidin         | 63 (11)  | 61 (15)   | Isradipine          | 39 (11)  | 52 (13)   |
| Atrazine                             | 35 (10)  | 44 (18)   | Clothianidin-d3      | 45 (33)  | 80 (51)   | Josamycin           | 23 (10)  | 9 (3)     |
| Azelnidipine                         | 3 (2)    | 31 (24)   | Clozapine            | 45 (18)  | 43 (35)   | Ketamine            | 56 (9)   | 38 (19)   |
| Azithromycin                         | 48 (27)  | 15 (8)    | Cocaine              | 74 (9)   | 54 (10)   | Ketoconazole        | 38 (17)  | 39 (25)   |
| Azoxystrobin                         | 70 (9)   | 73 (7)    | Cyclouron            | 45 (14)  | 42 (21)   | Ketotifen           | 73 (11)  | 45 (11)   |
| Benoxacor                            | 33 (21)  | 29 (24)   | Cymoxanil            | 162 (8)  | 36 (12)   | Levamisole          | 75 (13)  | 49 (14)   |
| Bensulide                            | 39 (20)  | 53 (14)   | Diazepam             | 65 (10)  | 73 (8)    | Levocabastine       | 75 (10)  | 71 (8)    |
| Benzatropine                         | 85 (27)  | 45 (11)   | Diclofenac           | 55 (13)  | 72 (8)    | Lidocaine           | 59 (8)   | 42 (18)   |
| Benzoylcegonine                      | 66 (8)   | 72 (13)   | Diffubenzuron        | 63 (12)  | 68 (8)    | Lincomycin          | 25 (15)  | 42 (9)    |
| Betaxolol                            | 66 (9)   | 56 (9)    | Dimethametryn        | 61 (8)   | 47 (9)    | Lorazepam           | 78 (10)  | 71 (14)   |
| Bezafibrate                          | 73 (10)  | 83 (11)   | Dimethomorph         | 77 (8)   | 73 (11)   | MDMA                | 60 (6)   | 45 (51)   |
| Bisoprolol                           | 71 (9)   | 59 (11)   | Diphenhydramine      | 78 (12)  | 33 (11)   | Meclizine           | 37 (21)  | 42 (24)   |
| Bupropion                            | 47 (16)  | 19 (14)   | Enalapril            | 73 (11)  | 77 (10)   | Medroxyprogesterone | 77 (9)   | 77 (9)    |
| Buspirone                            | 49 (7)   | 44 (12)   | Famoxadone           | 51 (17)  | 59 (6)    | Mefenamic acid      | 32 (9)   | 59 (10)   |

Table S4. Continued

| Compound        | MM-anion | MM-cation | Compound         | MM-anion | MM-cation | Compound           | MM-anion | MM-cation |
|-----------------|----------|-----------|------------------|----------|-----------|--------------------|----------|-----------|
| Memantine       | 63 (8)   | 28 (12)   | Pirenzepine      | 27 (4)   | 44 (18)   | Sulfadimethoxine   | 17 (9)   | 72 (8)    |
| Mephedrone      | 50 (12)  | 18 (12)   | Pretilachlor     | 44 (6)   | 44 (16)   | Sulfamerazine      | 85 (20)  | 44 (12)   |
| Mephosfolan     | 68 (12)  | 72 (7)    | Prodiamine       | 20 (11)  | 25 (13)   | Sulfamethazine     | 14 (9)   | 69 (8)    |
| Metformin       | 25 (16)  | 8 (2)     | Prometon         | 51 (13)  | 45 (19)   | Sulfamethoxazole   | 15 (9)   | 69 (9)    |
| Methamphetamine | 55 (7)   | 26 (12)   | Prometryn        | 49 (10)  | 38 (14)   | Sulfamonomethoxine | 48 (12)  | 89 (18)   |
| Methcathinone   | 53 (18)  | 18 (9)    | Propamocarb      | 106 (16) | 44 (14)   | Sulfapyridine      | 9 (6)    | 58 (15)   |
| Methedrone      | 51 (8)   | 29 (14)   | Propanolol       | 67 (8)   | 47 (8)    | Sulfathiazole      | 8 (4)    | 52 (11)   |
| Methylphenidate | 69 (7)   | 35 (13)   | Propazine        | 35 (10)  | 39 (18)   | Sulfisoxazole      | 16 (9)   | 62 (10)   |
| Metoprolol      | 69 (8)   | 55 (14)   | Pymetrozine      | 73 (14)  | 75 (6)    | Tacrine            | 73 (8)   | 30 (11)   |
| Morphine        | 109 (27) | 62 (15)   | Pyracarbolid     | 28 (17)  | 11 (2)    | Tamsulosin         | 67 (8)   | 63 (8)    |
| Nadolol         | 51 (8)   | 58 (6)    | Pyraclostrobin   | 51 (10)  | 68 (12)   | Temazepam          | 66 (10)  | 71 (8)    |
| Nicotine        | 33 (19)  | 30 (30)   | Pyraflufen-ethyl | 58 (11)  | 3 (1)     | Terbutryn          | 51 (10)  | 37 (12)   |
| Nifedipine      | 25 (14)  | 32 (12)   | Pyridaben        | 28 (3)   | 48 (11)   | Terfenadine        | 72 (29)  | 37 (9)    |
| Nitenpyram      | 29 (9)   | 58 (7)    | Risperidone      | 42 (15)  | 36 (27)   | Thiacloprid        | 70 (8)   | 71 (8)    |
| Nordiazepam     | 69 (10)  | 71 (13)   | Rizatriptan      | 20 (3)   | 34 (13)   | Thiamethoxam       | 54 (6)   | 57 (6)    |
| Norethisterone  | 71 (9)   | 79 (20)   | Ronidazole       | 64 (8)   | 73 (8)    | Thiazopyr          | 33 (14)  | 32 (16)   |
| Nortriptyline   | 72 (20)  | 23 (10)   | Roxithromycin    | 52 (31)  | 14 (5)    | Timolol            | 49 (10)  | 50 (10)   |
| Orphenadrine    | 84 (16)  | 33 (11)   | Salbutamol       | 102 (40) | 67 (8)    | Tramadol           | 74 (8)   | 44 (16)   |
| Oxamyl          | 54 (8)   | 19 (11)   | Salicylic acid   | 57 (16)  | 103 (18)  | Trimethoprim       | 59 (9)   | 55 (6)    |
| Oxazepam        | 62 (8)   | 65 (7)    | Sertraline       | 85 (27)  | 40 (11)   | Valsartan          | 37 (13)  | 73 (10)   |
| Oxycarboxin     | 66 (9)   | 2 (2)     | Simazine         | 36 (7)   | 46 (16)   | Venlafaxine        | 72 (9)   | 49 (14)   |
| Oxycodone       | 44 (7)   | 41 (15)   | Spinosyn A       | 58 (39)  | 24 (12)   | Verapamil          | 66 (9)   | 44 (12)   |
| Picoxystrobin   | 55 (8)   | 56 (10)   | Spinosyn D       | 58 (47)  | 27 (15)   | Warfarin           | 65 (6)   | 73 (9)    |
| Piperophos      | 46 (16)  | 60 (7)    | Spiramycin       | 12 (8)   | 1 (1)     | Ziprasidone        | 59 (17)  | 20 (16)   |

## S5. Calibration of the 3D-PSD for the anion and cation phases

The sampling rates ( $R_s$ ) for the 9 mm MM-anion and MM-cation phases were determined as described previously (Richardson et al., 2022). In summary, 5 L of artificial freshwater (AFW, (OECD, 2019)) was fortified to 100 ng L<sup>-1</sup> with a mix of 164 analytical standards and agitated using a magnetic stirrer. Twelve fully assembled 3D-PSDs per sorbent phase were exposed within the beaker and a single device was removed at the following timepoints: 8, 24, 48, 72, 96, 120, 144, and 168 hours. A sample of water was taken from the beaker coinciding with the 3D-PSD collection and the fortified AFW was replaced after sampling. An unused, fully assembled 3D-PSD was exposed to the air and underwent the same handling to act as a negative control. The 9 mm sorbent disks were prepared for analysis as described in the methods. Water samples were prepared for LC-MS analysis as described previously (Ng et al., 2020; Richardson et al., 2022). Briefly, 900 µL of river water sample was spiked with 100 µL of SIL-IS in MeOH (500 ng L<sup>-1</sup>). After vortexing, water samples were filtered (0.2 µm PTFE) directly into deactivated HPLC vials. Sample quantification was done with a 14-point external AFW calibration series. Calibrants were prepared as above with the 900 µL of AFW water spiked with 100 µL of MeOH containing analytical standards to a final concentration over the range of 5 to 2,000 ng L<sup>-1</sup> with the SIL-IS concentration remaining to 500 ng L<sup>-1</sup> for all samples.

The  $R_s$  values were determined as the ratio between the slope of the regression line representing the contaminant mass on the sorbent disk per unit of time and the mean concentration in the fortified AFW over the same time period (Eqn. S1) (Castle et al., 2018; Vrana et al., 2005). Refer to Table S1 for  $R_s$  values determined on the MM-anion and MM-cation phases.

$$R_s = \frac{C_s}{C_w \cdot t} \quad \text{Eqn. S1}$$

Table S5. Experimentally determined  $R_s$  values ( $\pm$  standard deviation (SD)) for 93 compounds on the 9 mm HLB, anion, and cation 9 mm phases,

| Compound                    | $R_s \pm SD$ (mL/d) |                |                 | LogP  | LogD<br>(pH 7.4) |
|-----------------------------|---------------------|----------------|-----------------|-------|------------------|
|                             | HLB*                | MM-anion       | MM-cation       |       |                  |
| 4-Methylethcathinone        | -                   | $3.4 \pm 0.5$  | $47.9 \pm 1.9$  | 2.18  | 1.87             |
| Acetamiprid                 | -                   | $9.4 \pm 0.5$  | $10 \pm 0.8$    | 1.06  | 1.06             |
| Alprazolam                  | -                   | $12.7 \pm 2.6$ | $16 \pm 0.8$    | 2.63  | 2.63             |
| Ametryn                     | -                   | $6 \pm 2.1$    | $27.5 \pm 1.4$  | 3.04  | 3.04             |
| Amitriptyline               | -                   | $3.2 \pm 0.3$  | $22.6 \pm 4.7$  | 4.72  | 2.95             |
| Amphetamine                 | $1.6 \pm 0.1$       | -              | -               | 1.82  | -0.62            |
| Antipyrine                  | -                   | $4.8 \pm 0.3$  | $13.7 \pm 0.8$  | 0.72  | 0.72             |
| Atorvastatin                | -                   | $4.6 \pm 0.3$  | -               | 4.36  | 1.26             |
| Atrazine                    | -                   | -              | $31.8 \pm 9.6$  | 2.66  | 2.66             |
| Azithromycin                | -                   | -              | $25.8 \pm 3.3$  | 3.29  | 1.36             |
| Azoxystrobin                | $10.2 \pm 0.8$      | $7.8 \pm 2.8$  | $9.5 \pm 1.9$   | 3.54  | 3.54             |
| Benzatropine                | $3.2 \pm 0.1$       | $6.1 \pm 0.1$  | $33.8 \pm 9$    | 4.71  | 1.89             |
| Benzoylecgonine             | $8.5 \pm 0.7$       | $1.9 \pm 0.1$  | $3.1 \pm 0.3$   | 2.29  | -0.21            |
| Betaxolol                   | -                   | $5 \pm 1.2$    | $23.4 \pm 3.4$  | 2.87  | 0.77             |
| Bezafibrate                 | -                   | $13.7 \pm 3.4$ | $6.4 \pm 1.2$   | 3.48  | -0.11            |
| Bisoprolol                  | $3.7 \pm 0.3$       | $5.8 \pm 0.8$  | $27.4 \pm 2.7$  | 2.21  | 0.12             |
| Bupropion                   | -                   | $6.2 \pm 1.1$  | $28.1 \pm 2.1$  | 3.08  | 2.88             |
| Buspirone                   | $2.4 \pm 0.4$       | $10.1 \pm 3.9$ | $33.6 \pm 3.7$  | 2.95  | 2.59             |
| Carazolol                   | $4.9 \pm 0.5$       | -              | $30.3 \pm 6.3$  | 3.33  | 1.15             |
| Carbamazepine               | $12.3 \pm 1$        | $11.1 \pm 0.9$ | $13 \pm 1.4$    | 2.28  | 2.28             |
| Carbamazepine-10,11-epoxide | $4.2 \pm 0.4$       | -              | $23.3 \pm 2$    | 6.09  | 6.09             |
| Celecoxib                   | -                   | -              | $10.7 \pm 3$    | 3.24  | 3.24             |
| Cilazapril                  | -                   | $6.2 \pm 1.9$  | $3.2 \pm 0.5$   | 1     | -2.5             |
| Citalopram                  | $1.6 \pm 0.2$       | -              | -               | 3.39  | 1.27             |
| Clarithromycin              | -                   | -              | $60.8 \pm 10.6$ | 3.12  | 2.37             |
| Clopidogrel                 | -                   | $7.3 \pm 2.7$  | $11.4 \pm 1.7$  | 4.21  | 4.21             |
| Clothianidin                | -                   | $9.7 \pm 1$    | $13 \pm 1.4$    | -0.03 | -0.03            |
| Cocaine                     | -                   | $12.5 \pm 2.2$ | $22 \pm 3.9$    | 2.78  | 1.21             |
| Diazepam                    | -                   | $12.5 \pm 2.5$ | $12.8 \pm 1.7$  | 2.92  | 2.92             |
| Diclofenac                  | -                   | $10.9 \pm 4.3$ | $5.4 \pm 1.5$   | 4.48  | 1.37             |
| Dimethametryn               | $3.4 \pm 0.9$       | -              | -               | 3.73  | 3.73             |
| Diphenhydramine             | -                   | $0.9 \pm 0.3$  | $25.4 \pm 3.2$  | 3.71  | 2.34             |
| Flutamide                   | -                   | $11.2 \pm 2.9$ | $10.9 \pm 2.5$  | 3.14  | 3.14             |
| Flutolanil                  | $6 \pm 0.6$         | -              | -               | 4.06  | 4.06             |
| Fuberidazole                | $8.3 \pm 0.6$       | -              | -               | 2.54  | 2.54             |
| Imidacloprid                | -                   | $14.2 \pm 1.1$ | $11.1 \pm 1.2$  | 0.81  | -0.52            |
| Isocarbamid                 | $6.3 \pm 0.5$       | -              | -               | 0.65  | 0.65             |
| Ketamine                    | $2.7 \pm 0$         | $11.5 \pm 0.8$ | $53.6 \pm 8.3$  | 2.12  | 2.07             |
| Ketotifen                   | $1.3 \pm 0.2$       | $4 \pm 1.3$    | $15.7 \pm 2.7$  | 4.06  | 2.61             |

Table S5. Continued

| Compound           | $R_s \pm SD$ (mL/d) |                |                | LogP  | LogD<br>(pH 7.4) |
|--------------------|---------------------|----------------|----------------|-------|------------------|
|                    | HLB*                | MM-anion       | MM-cation      |       |                  |
| Levamisole         | -                   | 4.4 $\pm$ 0.2  | 21.6 $\pm$ 2.3 | 2.15  | 0.25             |
| Levocabastine      | -                   | 17.4 $\pm$ 7   | 15.1 $\pm$ 4.4 | 4.48  | 1.98             |
| Lidocaine          | 0.8 $\pm$ 0.1       | 7.6 $\pm$ 0.9  | 31.8 $\pm$ 2.4 | 2.33  | 1.81             |
| Lincomycin         | -                   | -              | 4.1 $\pm$ 0.2  | 0.63  | -0.44            |
| MDMA               | 3.3 $\pm$ 0.4       | 1 $\pm$ 0.1    | -              | 1.93  | -0.77            |
| Mefenamic acid     | -                   | -              | 3.9 $\pm$ 1.1  | 5     | 2.04             |
| Memantine          | 5.9 $\pm$ 0.3       | -              | 67.4 $\pm$ 3.7 | 3.48  | 0.56             |
| Mephedrone         | -                   | 0.6 $\pm$ 0.1  | 37.9 $\pm$ 2   | 1.9   | 1.59             |
| Mephosfolan        | 6.7 $\pm$ 0.5       | -              | -              | 1.57  | 1.57             |
| Methamphetamine    | 1.4 $\pm$ 0.1       | 0.5 $\pm$ 0    | -              | 2.17  | -0.57            |
| Methcathinone      | -                   | 0.4 $\pm$ 0    | 74.6 $\pm$ 6.1 | 1.51  | 1.32             |
| Methedrone         | -                   | -              | 27.9 $\pm$ 2.9 | 1.33  | 0.99             |
| Methylphenidate    | -                   | -              | 43.1 $\pm$ 3.2 | 2.33  | 0.26             |
| Metoprolol         | 4.1 $\pm$ 0.4       | 4.2 $\pm$ 0.5  | 27.3 $\pm$ 1.8 | 1.85  | -0.25            |
| Nadolol            | -                   | 2.4 $\pm$ 0.2  | 18.5 $\pm$ 2.2 | 1.24  | -0.86            |
| Nitenpyram         | -                   | 1.4 $\pm$ 0.3  | -              | 0.4   | 0.4              |
| Nordiazepam        | -                   | 6.6 $\pm$ 1.4  | 6.7 $\pm$ 0.7  | 2.94  | 2.94             |
| Nortriptyline      | -                   | -              | 37.9 $\pm$ 4   | 4.76  | 2.28             |
| Orphenadrine       | -                   | 1.4 $\pm$ 0.4  | 24.6 $\pm$ 3.9 | 4.05  | 2.71             |
| Oxazepam           | -                   | 9.2 $\pm$ 1.5  | 3.6 $\pm$ 0.7  | 2.06  | 2.06             |
| Oxycodone          | 2.8 $\pm$ 0.3       | 3.4 $\pm$ 0.4  | 16.3 $\pm$ 2.1 | 0.91  | 0.45             |
| Picoxystrobin      | -                   | 7.3 $\pm$ 2.7  | -              | 3.84  | 3.84             |
| Pirenzepine        | 1 $\pm$ 0.1         | 1.2 $\pm$ 0.2  | 8.1 $\pm$ 0.8  | 0.31  | 0.03             |
| Prometon           | -                   | 8.1 $\pm$ 2.2  | 26.2 $\pm$ 3.7 | 2.79  | 2.79             |
| Prometryn          | -                   | 9.8 $\pm$ 1.1  | 25 $\pm$ 0.5   | 3.4   | 3.4              |
| Propamocarb        | 0.3 $\pm$ 0.2       | -              | 26.5 $\pm$ 1.6 | 1.15  | -0.67            |
| Propranolol        | -                   | 4.1 $\pm$ 1.4  | 37.4 $\pm$ 6.5 | 3.26  | 1.15             |
| Propazine          | -                   | -              | 26.7 $\pm$ 7.2 | 2.98  | 2.98             |
| Pymetrozine        | 3.5 $\pm$ 0.4       | -              | 4.3 $\pm$ 0.1  | 0.3   | 0.3              |
| Pyracarbolid       | 5.4 $\pm$ 0.4       | -              | -              | 2.03  | 2.03             |
| Rizatriptan        | -                   | -              | 9.6 $\pm$ 0.9  | 1.97  | 0.04             |
| Ronidazole         | 2.1 $\pm$ 0.2       | 0.9 $\pm$ 0    | 4 $\pm$ 0.3    | -0.42 | -0.42            |
| Salbutamol         | 4.8 $\pm$ 0.6       | 0.3 $\pm$ 0    | 15.2 $\pm$ 1.8 | 0.61  | -1.52            |
| Simazine           | -                   | -              | 26.7 $\pm$ 4.5 | 2.29  | 2.29             |
| Sulfadimethoxine   | -                   | 15.3 $\pm$ 3.1 | 4.2 $\pm$ 0.3  | 1.46  | -0.49            |
| Sulfamethazine     | 6 $\pm$ 0.6         | 7 $\pm$ 0.5    | 1.6 $\pm$ 0.1  | 0.44  | 0.3              |
| Sulfamethoxazole   | -                   | 10 $\pm$ 1.2   | 1.9 $\pm$ 0    | 0.65  | -0.55            |
| Sulfamonomethoxine | -                   | -              | 2.5 $\pm$ 0.2  | 0.56  | -1.31            |
| Sulfapyridine      | 6 $\pm$ 0.7         | 0.4 $\pm$ 0.1  | 3.1 $\pm$ 0.3  | 0.47  | 0.41             |
| Sulfathiazole      | -                   | 1.3 $\pm$ 0.3  | 2.6 $\pm$ 0.1  | 0.42  | 0.04             |
| Sulfisoxazole      | -                   | 7.4 $\pm$ 1.1  | -              | 0.85  | -0.77            |

Table S5. Continued

| Compound     | $R_s \pm SD$ (mL/d) |                |                | LogP  | LogD<br>(pH 7.4) |
|--------------|---------------------|----------------|----------------|-------|------------------|
|              | HLB*                | MM-anion       | MM-cation      |       |                  |
| Tacrine      | 11.9 $\pm$ 1.1      | 3.9 $\pm$ 0.2  | -              | 2.87  | 0.81             |
| Tamsulosin   | 8.1 $\pm$ 0.5       | 6.6 $\pm$ 2.3  | 20.4 $\pm$ 2.9 | 2.14  | 0.77             |
| Temazepam    | 8.2 $\pm$ 0.6       | 8 $\pm$ 2      | 6.4 $\pm$ 0.9  | 2.11  | 2.11             |
| Terbutryn    | 6.1 $\pm$ 1         | 10.4 $\pm$ 4   | 27.6 $\pm$ 1.3 | 3.35  | 3.35             |
| Thiacloprid  | -                   | 18.8 $\pm$ 2.1 | 17.6 $\pm$ 2.2 | 1.22  | 1.22             |
| Thiamethoxam | -                   | 8.4 $\pm$ 0.5  | 6.8 $\pm$ 0.6  | -0.33 | -0.33            |
| Timolol      | -                   | 5.5 $\pm$ 0.6  | 21.5 $\pm$ 2.1 | 1.53  | -0.35            |
| Tramadol     | 1.9 $\pm$ 0.3       | 5.4 $\pm$ 0.2  | 30.7 $\pm$ 3   | 2.54  | 0.52             |
| Trimethoprim | 6.3 $\pm$ 0.5       | 3.9 $\pm$ 0.8  | 17.3 $\pm$ 1.9 | 1.12  | 1                |
| Valsartan    | -                   | 6.7 $\pm$ 2.5  | 2.2 $\pm$ 0.2  | 3.87  | -0.86            |
| Venlafaxine  | 1.6 $\pm$ 0.3       | 2.8 $\pm$ 0.4  | 23.5 $\pm$ 2.2 | 3.15  | 1.43             |
| Verapamil    | 3.7 $\pm$ 0.5       | 10 $\pm$ 2.9   | 22.5 $\pm$ 5.1 | 3.95  | 2.38             |
| Warfarin     | -                   | 11.7 $\pm$ 3.2 | 4.5 $\pm$ 0.7  | 3.1   | 0.31             |

\* Adapted from Richardson *et al.* (2022) with permission from Elsevier.

Table S6. Mean concentration of contaminants detected across the 6-month study on the three 3D-PSD phases represented as time-weighted average water concentration calculated using the indicated  $R_s$  value and in water samples. Data is reported  $\pm$  standard deviation and all water concentrations are in  $\text{ng L}^{-1}$  and  $R_s$  is in  $\text{mL day}^{-1}$ .

| Compound                    | [CEC]<br>water | HLB   |              | MM-anion |              | MM-cation |               |
|-----------------------------|----------------|-------|--------------|----------|--------------|-----------|---------------|
|                             |                | $R_s$ | TWA [CEC]    | $R_s$    | TWA [CEC]    | $R_s$     | TWA [CEC]     |
| 4-Methylethcathinone        | -              | -     | -            | -        | -            | 47.9      | $0.4 \pm 0.1$ |
| Acetamidiprid               | $86 \pm 22$    | -     | -            | 9.4      | $34 \pm 28$  | 10        | $48 \pm 18$   |
| Amitriptyline               | $32 \pm 8$     | -     | -            | 2.3      | $29 \pm 13$  | 22.6      | $7 \pm 2$     |
| Amphetamine                 | -              | 1.6   | $54 \pm 9$   | -        | -            | -         | -             |
| Antipyrine                  | -              | -     | -            | 4.8      | $2 \pm 1$    | 13.7      | $1 \pm 0.3$   |
| Atrazine                    | $12 \pm 2$     | -     | -            | -        | -            | 31.8      | $4 \pm 1$     |
| Azithromycin                | $160 \pm 37$   | -     | -            | -        | -            | -         | -             |
| Azoxystrobin                | -              | 10.2  | $1 \pm 1$    | 9.3      | $2 \pm 2$    | 9.5       | $2 \pm 1$     |
| Benzoylcegonine             | $20 \pm 7$     | 8.5   | $7 \pm 3$    | 1.9      | $6 \pm 3$    | 3.1       | $16 \pm 7$    |
| Bezafibrate                 | -              | -     | -            | 13.8     | $7 \pm 2$    | 6.4       | $19 \pm 9$    |
| Bisoprolol                  | $19 \pm 5$     | 3.7   | $39 \pm 20$  | 5.9      | $11 \pm 6$   | 27.4      | $6 \pm 6$     |
| Buspirone                   | -              | -     | -            | 10.1     | $1 \pm 0.1$  | 33.6      | $0.4 \pm 0.1$ |
| Carbamazepine-10,11-epoxide | $47 \pm 9$     | 4.2   | $144 \pm 62$ | -        | -            | 23.3      | $26 \pm 11$   |
| Celecoxib                   | -              | -     | -            | -        | -            | 10.7      | $3 \pm 1$     |
| Clopidogrel                 | $29 \pm 7$     | -     | -            | 7.3      | $26 \pm 19$  | 11.4      | $24 \pm 18$   |
| Cocaine                     | $22 \pm 19$    | -     | -            | 12.7     | $5 \pm 6$    | 22        | $2 \pm 1$     |
| Diazepam                    | -              | -     | -            | -        | -            | 12.8      | $1 \pm 0.3$   |
| Diphenhydramine             | $53 \pm 12$    | -     | -            | 0.9      | $107 \pm 57$ | -         | -             |
| Imidacloprid                | $66 \pm 21$    | 7.8   | $83 \pm 33$  | 14.3     | $47 \pm 2$   | 11.1      | $48 \pm 20$   |
| Ketamine                    | $46 \pm 10$    | -     | -            | 11       | $26 \pm 18$  | -         | -             |
| Levamisole                  | $53 \pm 27$    | -     | -            | 4.2      | $32 \pm 17$  | 21.6      | $22 \pm 7$    |
| Levocabastine               | -              | -     | -            | -        | -            | 15.1      | $1 \pm 0.1$   |
| Lidocaine                   | $100 \pm 30$   | -     | -            | 7.7      | $39 \pm 14$  | -         | -             |
| Lincomycin                  | -              | -     | -            | -        | -            | 4.1       | $3 \pm 2$     |
| MDMA                        | $26 \pm 17$    | 3.3   | $44 \pm 28$  | 1        | $30 \pm 13$  | -         | -             |
| Memantine                   | $19 \pm 3$     | 5.9   | $23 \pm 8$   | -        | -            | 67.4      | $5 \pm 2$     |
| Mephedrone                  | -              | -     | -            | -        | -            | 37.9      | $1 \pm 1$     |
| Methamphetamine             | $20 \pm 6$     | 1.4   | $77 \pm 57$  | 0.5      | $33 \pm 12$  | -         | -             |
| Methylphenidate             | -              | -     | -            | -        | -            | 43.1      | $0.4 \pm 0.1$ |
| Metoprolol                  | $12 \pm 0.4$   | 4.1   | $7 \pm 2$    | 4.2      | $3 \pm 1$    | 27.3      | $2 \pm 1$     |
| Nadolol                     | -              | -     | -            | -        | -            | 18.5      | $0.3 \pm 0.1$ |
| Nordiazepam                 | -              | -     | -            | -        | -            | 6.7       | $9 \pm 4$     |
| Nortriptyline               | -              | -     | -            | -        | -            | 37.9      | $2 \pm 1$     |
| Orphenadrine                | -              | -     | -            | 1.4      | $5 \pm 2$    | 24.6      | $1 \pm 0.3$   |
| Oxazepam                    | -              | -     | -            | 9.2      | $12 \pm 6$   | 3.6       | $178 \pm 14$  |
| Oxycodone                   | -              | 2.8   | $15 \pm 5$   | 3.4      | $5 \pm 2$    | 16.3      | $3 \pm 1$     |
| Pirenzepine                 | $14 \pm 2$     | 1     | $63 \pm 24$  | 1.2      | $11 \pm 12$  | 8.1       | $13 \pm 6$    |
| Propamocarb                 | -              | 0.3   | $26 \pm 1$   | -        | -            | -         | -             |

Table S6. Continued

| Compound           | [CEC]<br>water | HLB   |           | MM-anion |           | MM-cation |           |
|--------------------|----------------|-------|-----------|----------|-----------|-----------|-----------|
|                    |                | $R_s$ | TWA [CEC] | $R_s$    | TWA [CEC] | $R_s$     | TWA [CEC] |
| Propranolol        | 50 ± 9         | -     | -         | 4.2      | 78 ± 15   | 37.4      | 4 ± 2     |
| Propazine          | -              | -     | -         | -        | -         | 26.7      | 1 ± 0.1   |
| Rizatriptan        | -              | -     | -         | -        | -         | 9.6       | 0.5 ± 0.1 |
| Salbutamol         | 12 ± 1         | 4.8   | 10 ± 3    | 0.3      | 30 ± 20   | 15.2      | 8 ± 5     |
| Simazine           | -              | -     | -         | -        | -         | 26.7      | 2 ± 1     |
| Sulfadimethoxine   | -              | -     | -         | 15.4     | 1 ± 0.4   | -         | -         |
| Sulfamethazine     | -              | -     | -         | 7        | 1 ± 0.3   | 1.6       | 5 ± 2     |
| Sulfamethoxazole   | 34 ± 15        | -     | -         | 10.1     | 21 ± 7    | 1.9       | 140 ± 28  |
| Sulfamonomethoxine | -              | -     | -         | -        | -         | 2.5       | 21 ± 6    |
| Sulfapyridine      | 104 ± 47       | -     | -         | 0.4      | 630 ± 423 | -         | -         |
| Tamsulosin         | -              | 8.1   | 2 ± 2     | -        | -         | 20.4      | 1 ± 1     |
| Temazepam          | 22 ± 5         | 8.2   | 25 ± 10   | 8.6      | 20 ± 11   | 6.4       | 112 ± 13  |
| Terbutryn          | 14 ± 4         | 6.1   | 6 ± 1     | 10.4     | 7 ± 6     | 27.6      | 8 ± 4     |
| Thiacloprid        | -              | -     | -         | 18.8     | 17 ± 16   | 17.6      | 0.2 ± 0   |
| Timolol            | -              | -     | -         | 5.5      | 4 ± 6     | 21.5      | 1 ± 0.5   |
| Tramadol           | 246 ± 45       | -     | -         | 5.2      | 13 ± 1    | -         | -         |
| Trimethoprim       | 95 ± 20        | -     | -         | 3.9      | 122 ± 7   | -         | -         |
| Valsartan          | -              | -     | -         | 6.8      | 22 ± 29   | 2.2       | 22 ± 7    |
| Venlafaxine        | 178 ± 33       | -     | -         | 2.8      | 117 ± 76  | -         | -         |
| Verapamil          | 16 ± 2         | 3.7   | 11 ± 10   | 9        | 4 ± 2     | 22.5      | 3 ± 2     |
| Warfarin           | -              | -     | -         | 7.9      | 3 ± 1     | 4.5       | 4 ± 2     |

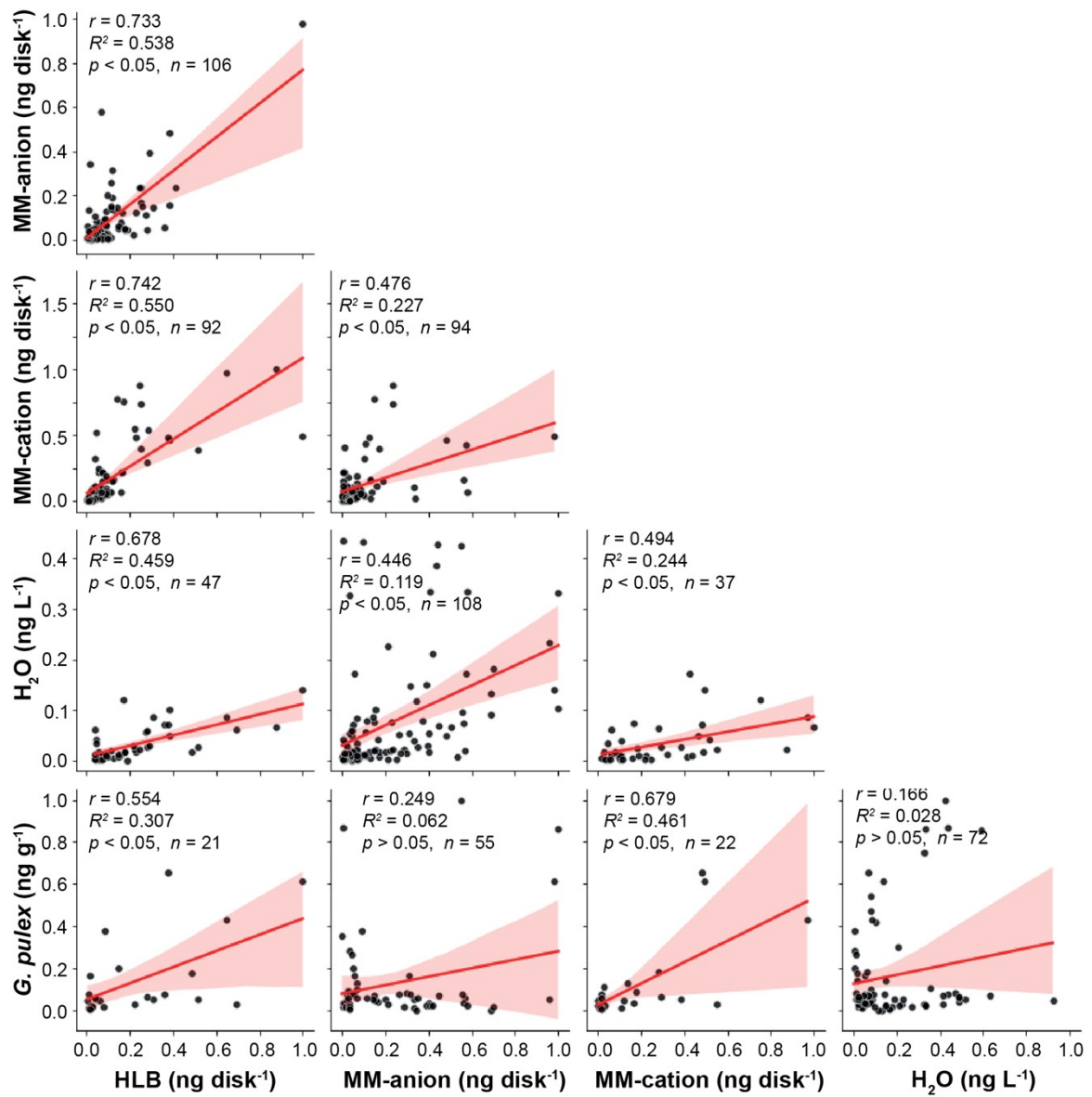


**Figure S3.** Heatmap of the risk quotients (RQs) calculated for the HLB, MM-anion, and MM-cation passive sampler sorbents (for compounds with  $R_s$  values), and from the water CEC data for all compounds. Light grey tiles indicates compounds not quantified, compounds with a RQ of 0 are < 0.1.

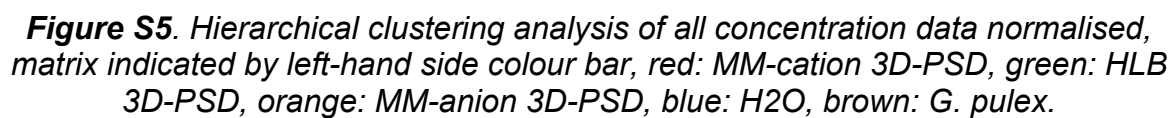
Table S7. Values used to calculate the toxic and effect units in *G. pulex* as per Eqn. 2 and 4. References for values are indicated.

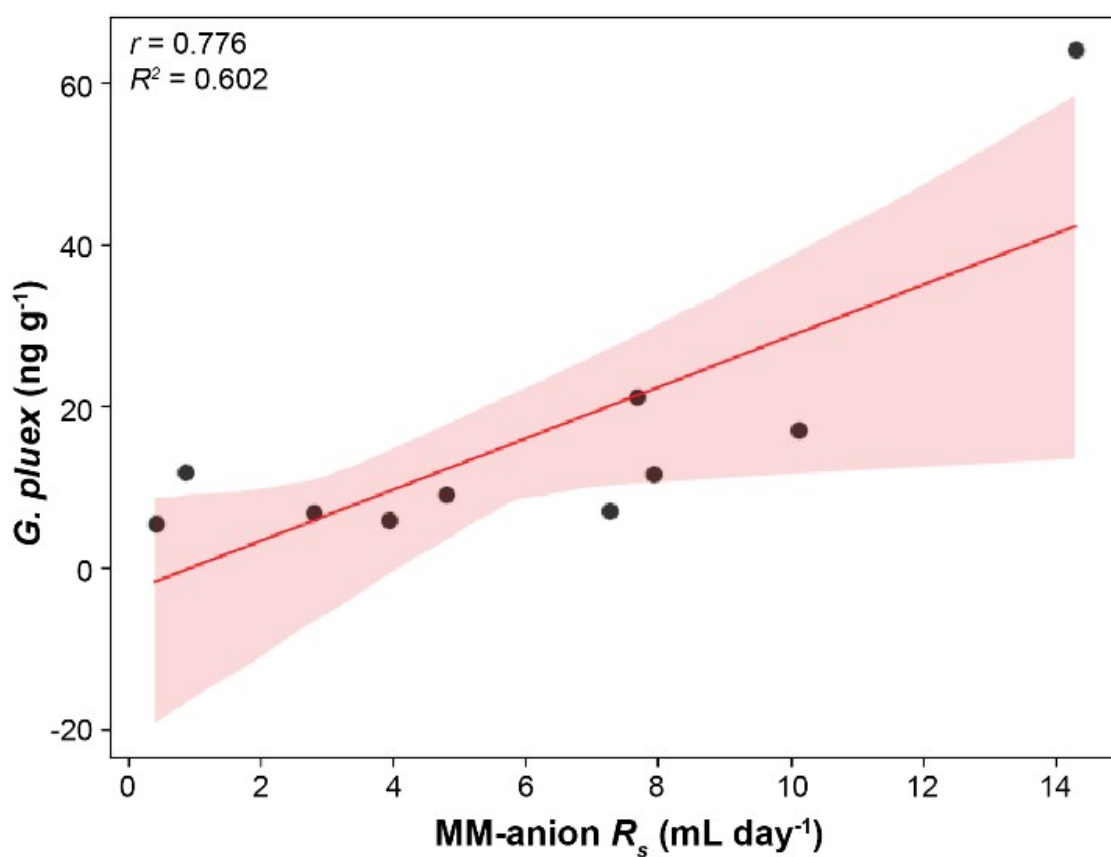
| Pesticide        | Toxic units                                   |                                   |                                                 | Refs                                      |
|------------------|-----------------------------------------------|-----------------------------------|-------------------------------------------------|-------------------------------------------|
|                  | <i>EC</i> <sub>50</sub> (mg L <sup>-1</sup> ) | <i>BCF</i>                        | <i>EC</i> <sub>50</sub> <sub>int</sub>          |                                           |
| Clothianidin     | 11.43                                         | 3                                 | 34,290                                          | (Olker et al., 2022, EPA, 2015)           |
| Imidacloprid     | 0.021                                         | 9                                 | 185                                             | (Agatz et al., 2014, Miller et al., 2019) |
| Oxamyl           | 0.42                                          | 6                                 | 2,520                                           | (Olker et al., 2022, Miller et al., 2019) |
| PPCPs            | Effect units                                  |                                   |                                                 |                                           |
|                  | <i>logD</i> <sub>pH 7.4</sub> <sup>a</sup>    | <i>HtPC</i> (mg L <sup>-1</sup> ) | <i>PC</i> <sub>crit</sub> (mg L <sup>-1</sup> ) |                                           |
| Amlodipine       | 1.91                                          | -                                 | 7.0x10 <sup>-3</sup>                            | (Fick et al., 2010)                       |
| Antipyrine       | 0.72                                          | -                                 | 14                                              | (Fick et al., 2010)                       |
| Benzatropine*    | 1.89                                          | 0.01                              | 3.2x10 <sup>-3</sup>                            | (Schulz et al., 2012)                     |
| Carbamazepine    | 2.28                                          | -                                 | 0.35                                            | (Fick et al., 2010)                       |
| Citalopram       | 1.27                                          | -                                 | 1.4x10 <sup>-4</sup>                            | (Fick et al., 2010)                       |
| Clarithromycin   | 2.37                                          | -                                 | 7.3x10 <sup>-3</sup>                            | (Fick et al., 2010)                       |
| Clopidogrel*     | 4.21                                          | 0.001                             | 6.4x10 <sup>-6</sup>                            | (Schulz et al., 2012)                     |
| Clozapine        | 2.71                                          | -                                 | 0.32                                            | (Fick et al., 2010)                       |
| Diclofenac       | 1.37                                          | -                                 | 4.6x10 <sup>-3</sup>                            | (Fick et al., 2010)                       |
| Diphenhydramine  | 2.34                                          | -                                 | 2.0x10 <sup>-3</sup>                            | (Fick et al., 2010)                       |
| Fluoxetine       | 1.75                                          | -                                 | 4.9x10 <sup>-4</sup>                            | (Fick et al., 2010)                       |
| Ketoconazole     | 3.49                                          | -                                 | 4.3x10 <sup>-3</sup>                            | (Fick et al., 2010)                       |
| Lidocaine        | 1.81                                          | -                                 | 0.47                                            | (Fick et al., 2010)                       |
| Lincomycin*      | -0.44                                         | 1.5                               | 24                                              | (Nielsen and Gyrd-Hansen, 1998)           |
| Nortriptyline    | 2.28                                          | -                                 | 5.6e <sup>-5</sup>                              | (Fick et al., 2010)                       |
| Propranolol      | 1.15                                          | -                                 | 2.0e <sup>-3</sup>                              | (Fick et al., 2010)                       |
| Risperidone      | 1.18                                          | -                                 | 1.3e <sup>-4</sup>                              | (Fick et al., 2010)                       |
| Sulfamethoxazole | -0.55                                         | -                                 | 98                                              | (Fick et al., 2010)                       |
| Sulfathiazole*   | 0.04                                          | 37.1                              | 263                                             | (Strum et al., 1978)                      |
| Trimethoprim     | 1.00                                          | -                                 | 3.3                                             | (Fick et al., 2010)                       |
| Venlafaxine      | 1.43                                          | -                                 | 6.1x10 <sup>-3</sup>                            | (Fick et al., 2010)                       |
| Warfarin         | 0.31                                          | -                                 | 0.19                                            | (Fick et al., 2010)                       |

<sup>a</sup> Predicted from SMILES using Percepta PhysChem Profiler; \* Compounds for which the *PC*<sub>crit</sub> was calculated from *logD* and *H<sub>T</sub>PC* values.



**Figure S4.** Linear regressions of CEC concentrations between the different matrices with all data normalised between 1 and 0. The red trendline represents the line of best fit with a 95 % confidence interval (shaded).





**Figure S6.** Correlation between the MM-anion  $R_s$  values and the average contaminant concentration in the *G. pulex* across the whole study. The red trendline represents the line of best fit with a 95 % confidence interval (shaded).

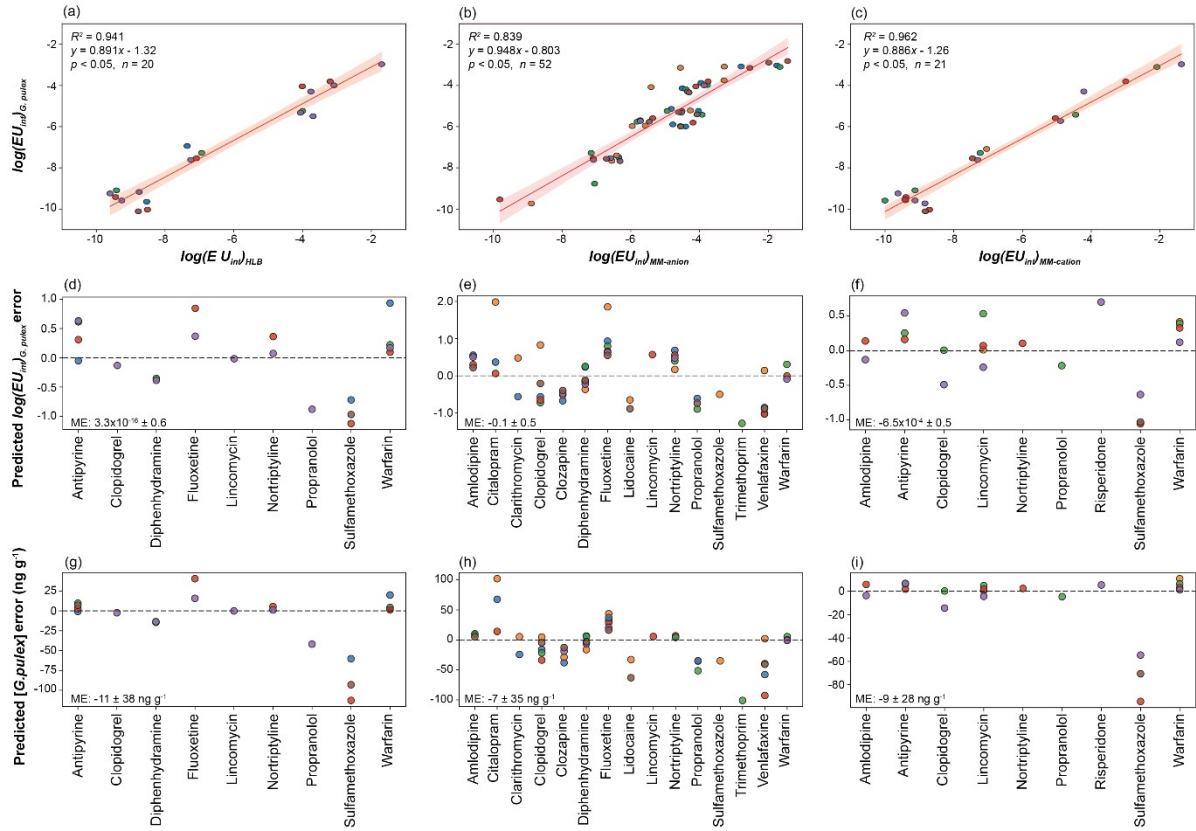
Table S8. Toxic units calculated from literature-derived data, values in bold exceed the -3 effect threshold.

| Compounds                 | Calculated toxic units |                  |             |             |             |
|---------------------------|------------------------|------------------|-------------|-------------|-------------|
|                           | <i>Gammarid</i>        | H <sub>2</sub> O | HLB         | MM-anion    | MM-cation   |
| Azoxystrobin <sup>1</sup> | -4.2                   | -5.1             | <b>-2.5</b> | <b>-2.5</b> | <b>-2.5</b> |
| Azoxystrobin <sup>1</sup> | -4.2                   | -4.7             | <b>-2.1</b> | <b>-2.2</b> | <b>-2.2</b> |
| Azoxystrobin <sup>1</sup> | -3.9                   | -5.1             | <b>-2.5</b> | <b>-2.5</b> | <b>-2.5</b> |
| Azoxystrobin <sup>1</sup> | -3.8                   | -4.4             | <b>-1.9</b> | <b>-1.9</b> | <b>-1.9</b> |
| Imidacloprid <sup>1</sup> | <b>-2.2</b>            | -3.4             | -           | <b>-0.4</b> | <b>-0.6</b> |
| Imidacloprid <sup>1</sup> | <b>-1.9</b>            | -3.6             | -           | <b>-0.7</b> | <b>-0.8</b> |
| Imidacloprid <sup>1</sup> | <b>-1.7</b>            | -3.7             | -           | <b>-0.8</b> | <b>-0.9</b> |
| Imidacloprid <sup>2</sup> | <b>-1.4</b>            | -2.2             | -           | <b>0.7</b>  | <b>0.6</b>  |
| Propamocarb <sup>3</sup>  | -6.6                   | -8.9             | -7.4        | -           | -5.5        |
| Propamocarb <sup>3</sup>  | -6.5                   | -9.0             | -7.5        | -           | -5.6        |
| Thiacloprid <sup>1</sup>  | -4.0                   | -6.8             | -           | -3.9        | -4.0        |
| Thiacloprid <sup>1</sup>  | -3.9                   | -6.6             | -           | -3.8        | -3.8        |

<sup>1</sup>(Munz et al., 2018, 2017)

<sup>2</sup>(Miller et al., 2019)

<sup>3</sup>(Miller et al., 2021)



**Figure S7.** (a) to (c), linear regression models for each passive sampler sorbent. (d) to (f), residual root of the predicted effect units in *G. pulex* using the corresponding model. (g) to (i), residual error of the predicted contaminant concentration using each of the models. Coloured dots indicate the month of sample collection, blue = July, orange = August, green = September, red = October, purple = November, and brown = December. The red trendline represents the line of best fit with a 95 % confidence interval (shaded).

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