Application of a predicative model to the seasonal changes in contaminant occurrence of a London urban river system measured using passive sampling

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1. Introduction

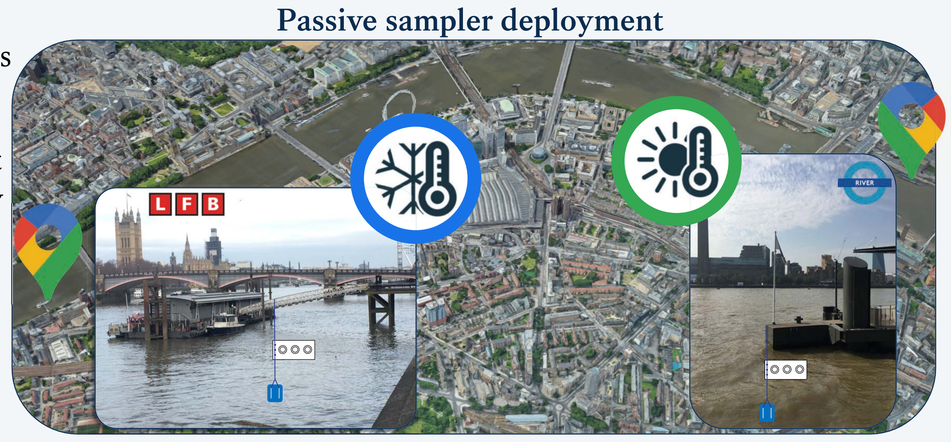
- Pharmaceuticals and personal care products, pesticides and controlled drugs have now been identified as emerging contaminants of concern over the past 20 years.
- The abundance and distribution of contaminants in the water system is a cause for concern as they potentially pose a significant threat to the ecosystem and organisms.

Aim: To determine the seasonal difference in emerging contaminants in the River Thames, UK and use machine learning to predict bioconcentration factor in an invertebrate.

2. Methods

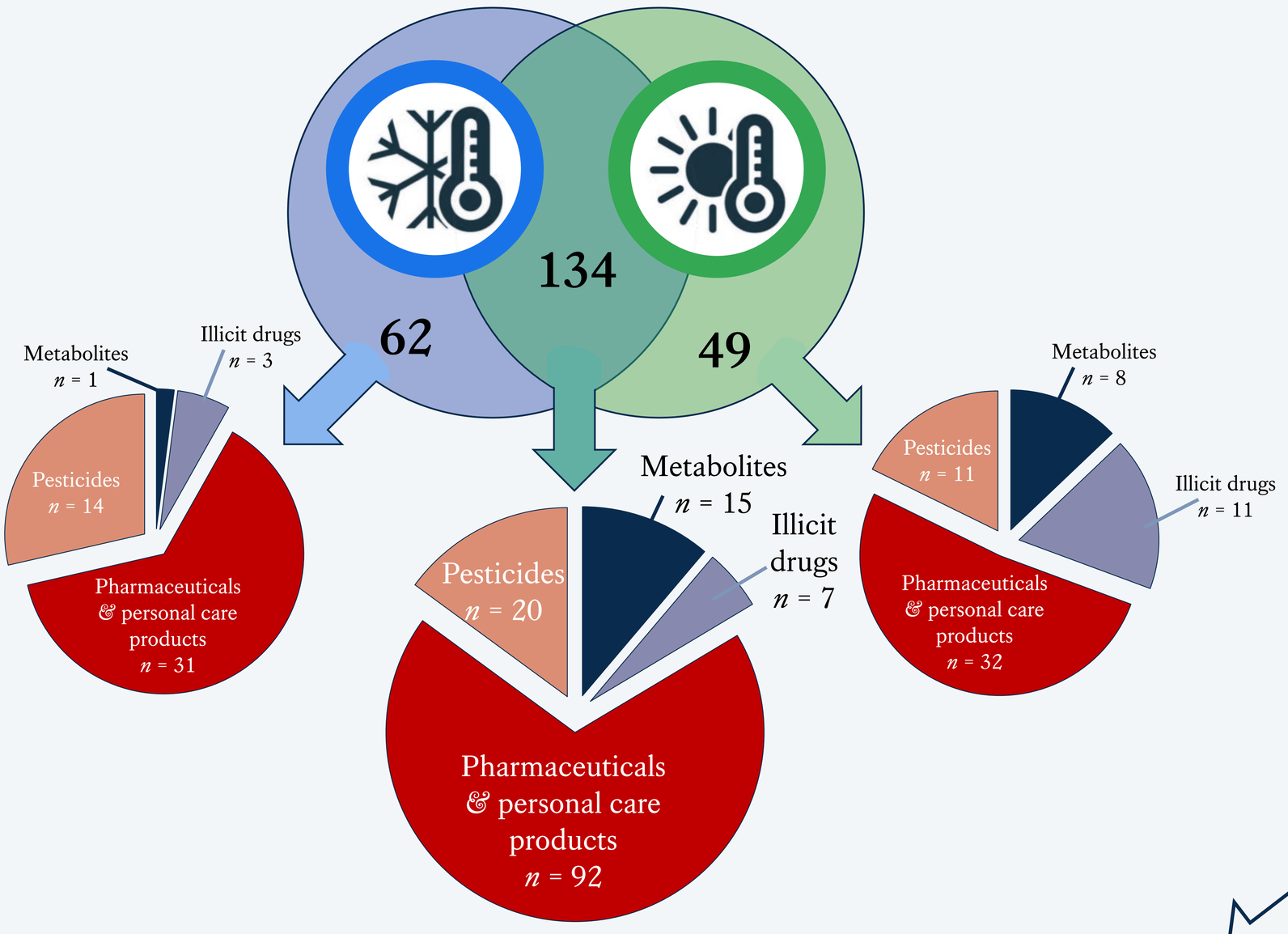
- HLB configured Chemcatcher® passive samplers were deployed for at least 14 days during winter and summer.
- Extracts were analysed using two different liquid chromatography-mass spectrometry (LC-MS) methods.[1,2]
- A machine learning model for the prediction of bioconcentration factor (BCF)[3] in the invertebrate *G. pulex* was applied to the compounds common to both seasons.

Passive sampler deployment

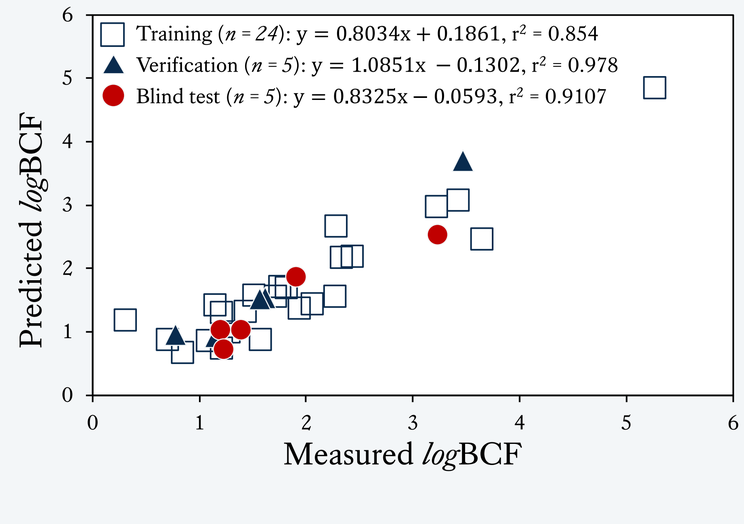


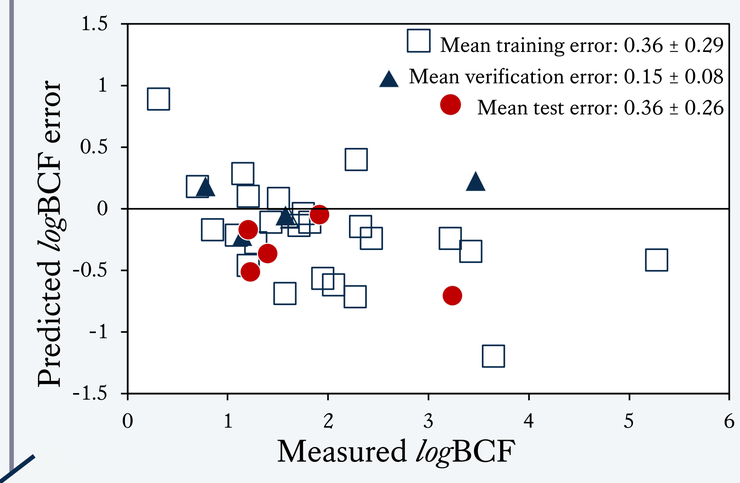
3. Results

3.1. Contaminants detected on passive sampler using LC-MS/MS and LC-QTOF



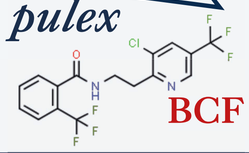
3.2. Predicting BCF using machine learning





3.3. BCF prediction in *G. pulex*

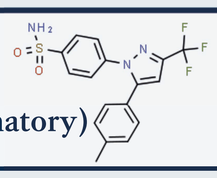
fluopyram (fungicide)



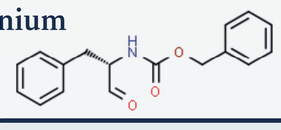
BCF > 5000 L/kg – very bioaccumulative (*n* = 1)

BCF < 2000 L/kg
n = 115, unable to predict for *n* = 16 contaminants

celecoxib (anti-inflammatory)



benzododecinium (antiseptic)



BCF > 2000 L/kg – bioaccumulative (*n* = 2)

4. Conclusions

134 contaminants were common to the passive samplers deployed in the River Thames over winter and summer.

62 contaminants were unique to the winter deployment.

49 contaminants were unique to the summer deployment.

One contaminant was predicted to be very bioaccumulative (fluopyram) and two were predicted to be bioaccumulative (benzododecinium & celecoxib).

Next steps:

- Shortlist of compounds for further *G. pulex* BCF experiments.
- Attempt to model invertebrate BCF from *in situ* data collected using passive samplers

Acknowledgements

Thanks are extended to James Fielding and Adam Taylor for training and advice in the use of Chemcatchers. Thanks are also extended to the London Fire Brigade, TFL and Helen Czerski for their assistance in access to sampler deployment locations.

References

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