Implementing Rules for Improved Quantification of Transformation Products and Metabolites

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— 1. Introduction —

Environmental water samples are complex mixtures of anthropogenic chemicals and their **transformation products (TPs)**, formed via processes like hydrolysis, photolysis, and metabolism. (1) As TP formation is largely unknown and difficult to assess, **non-target screening (NTS)** is needed to detect and evaluate novel TPs. However, **the lack of analytical standards** makes identification, quantification, and risk assessment challenging.
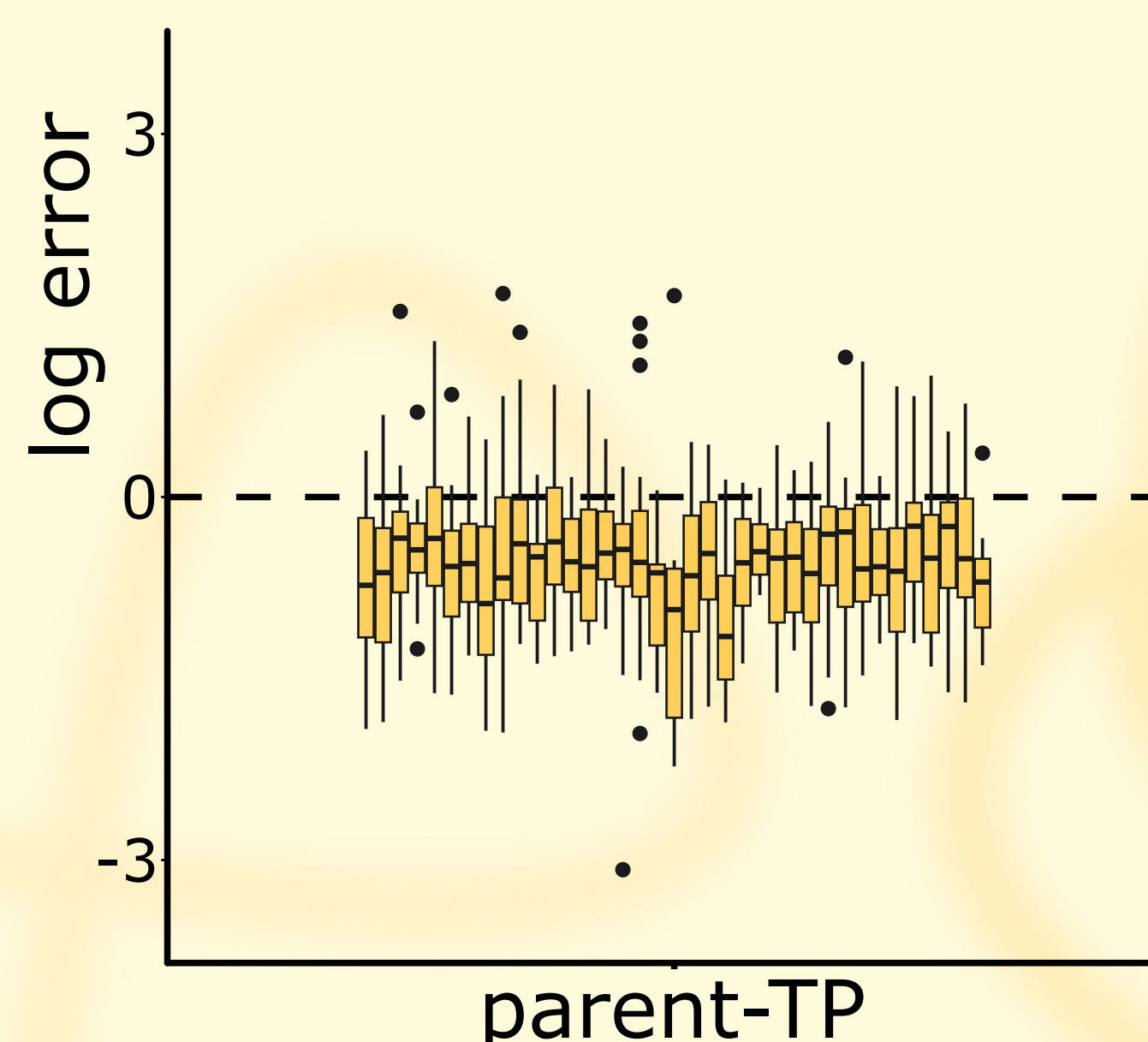
A common workaround is to **estimate TP concentrations** using the **parent compound's calibration curve**, assuming similar ionization efficiency (*IE*). However, our previous work shows this often **leads to underestimation**, with errors depending on parent–TP structural similarity. (2)

2. Preliminary results
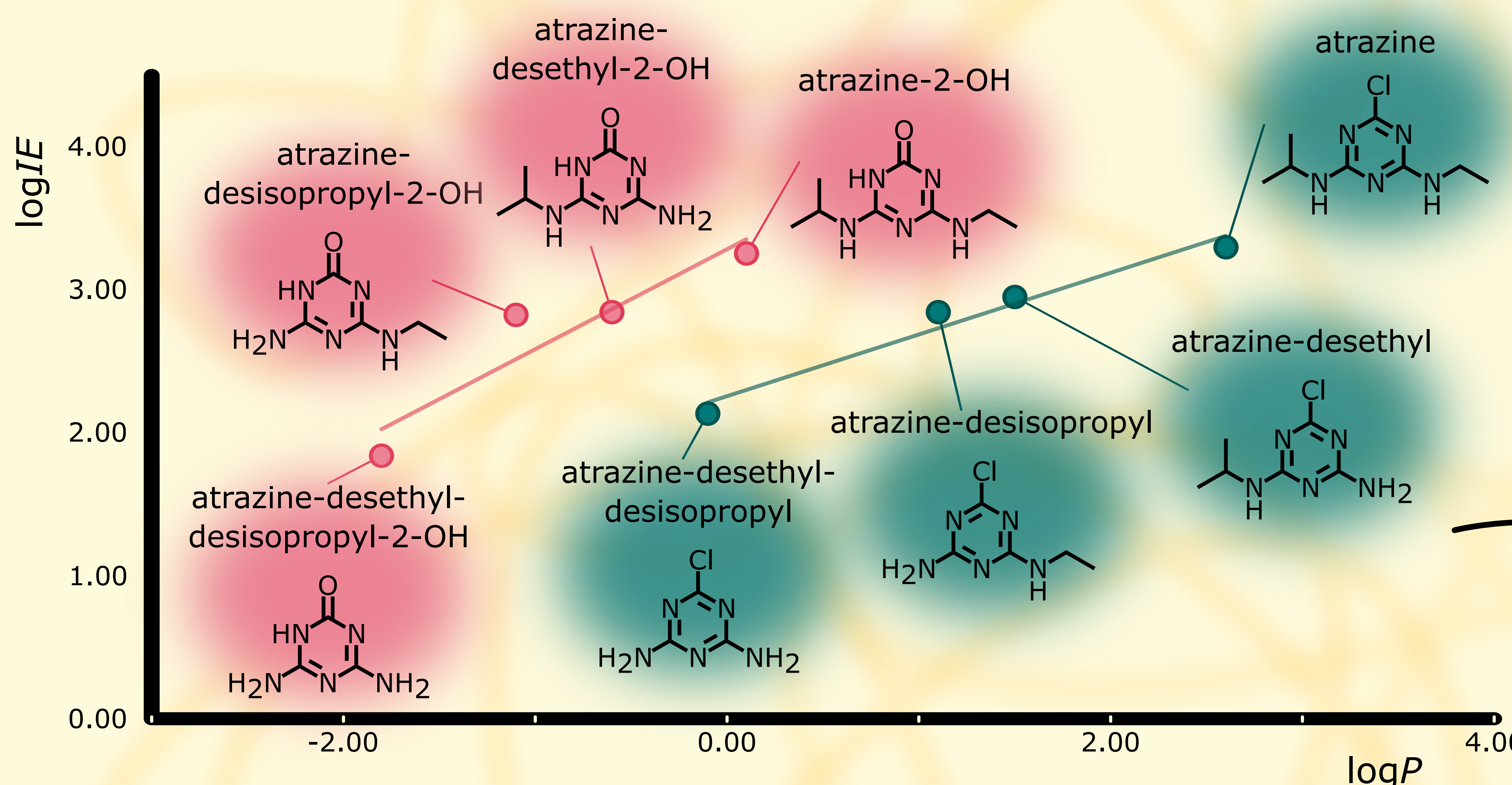
In a pre-study, we observed a **linear relationship** between **logIE and log$P$** (or pKa) within several parent–TP series.
As shown for **atrazine** and its TPs, a **linear trend** was observed, however separate for hydroxylated and non-hydroxylated TPs.
The accompanying graph highlights how the **quantification error increased with decreasing structural similarity** between the TP and its parent.
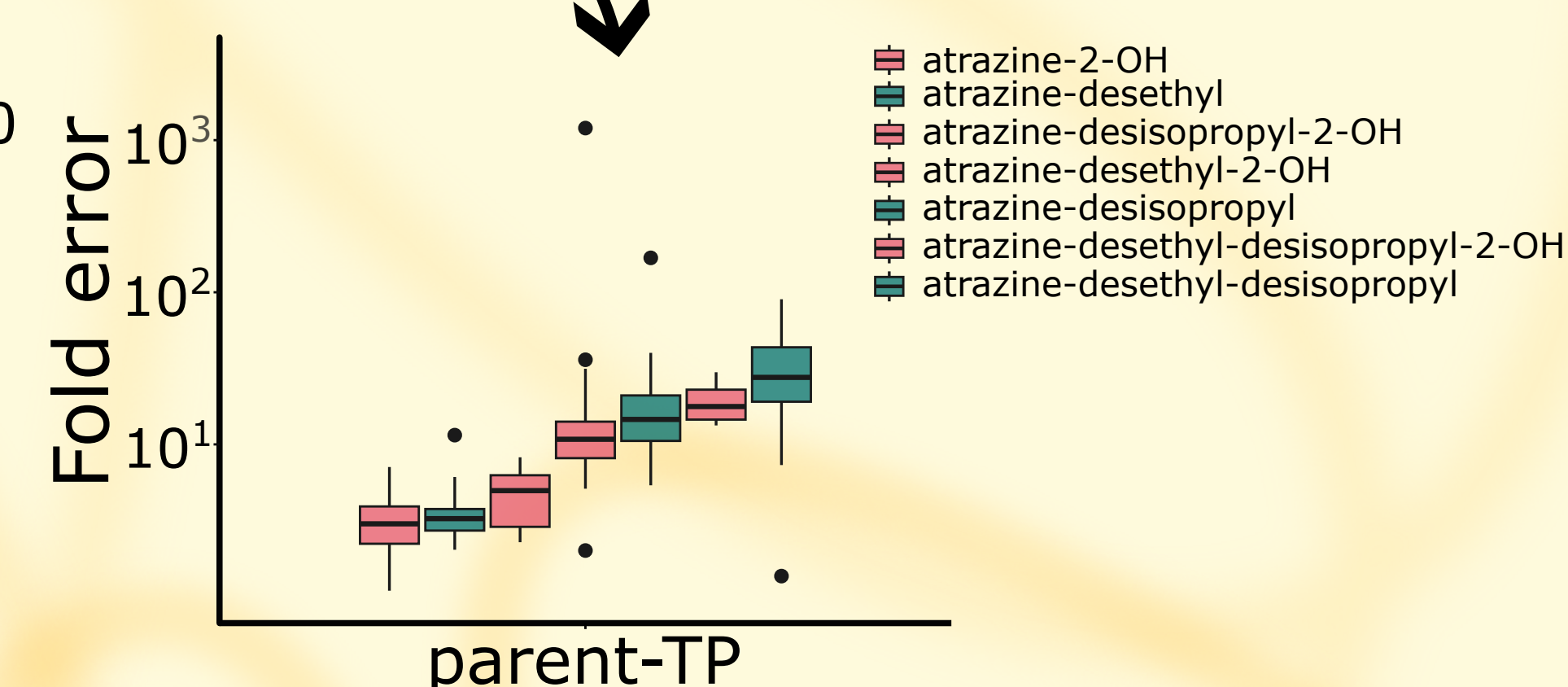

3. Workflow / future plan
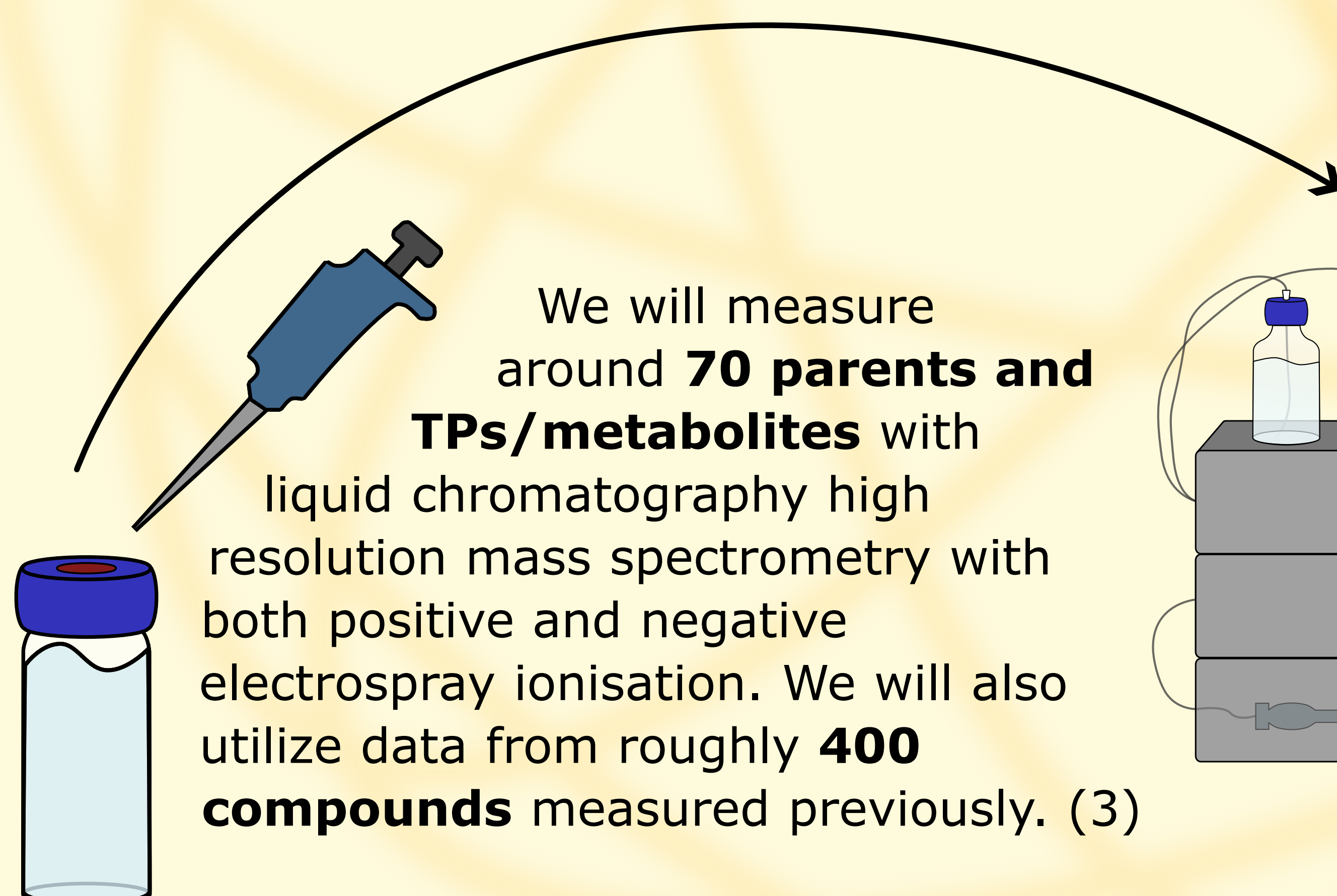
We will measure around **70 parents and TPs/metabolites** with liquid chromatography high resolution mass spectrometry with both positive and negative electrospray ionisation. We will also utilize data from roughly **400 compounds** measured previously. (3)
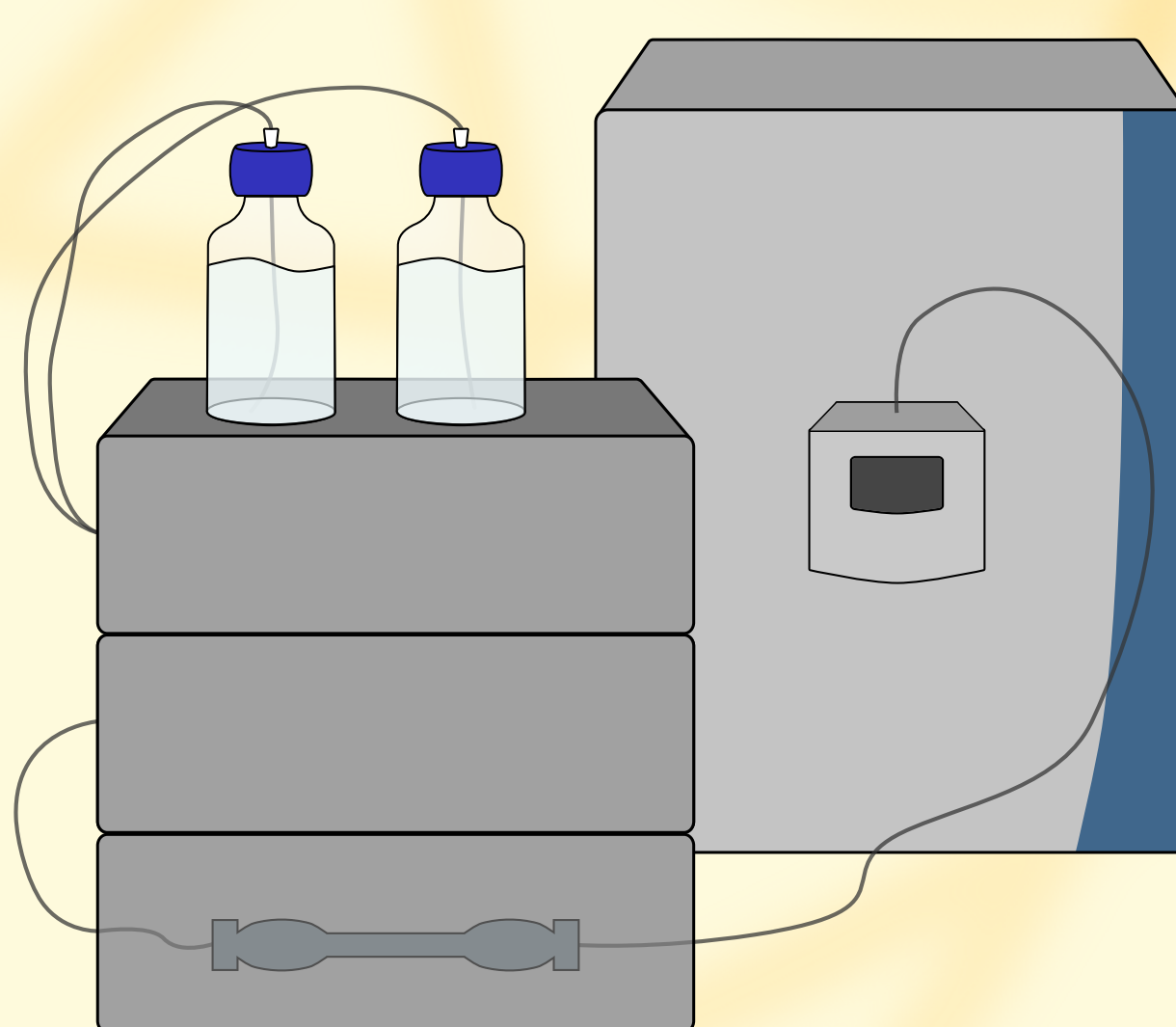
From the measurements, the *IE* will be determined and different similarity measures such as **cosine, Tanimoto, and maximum common edge subgraph similarity** will be determined.
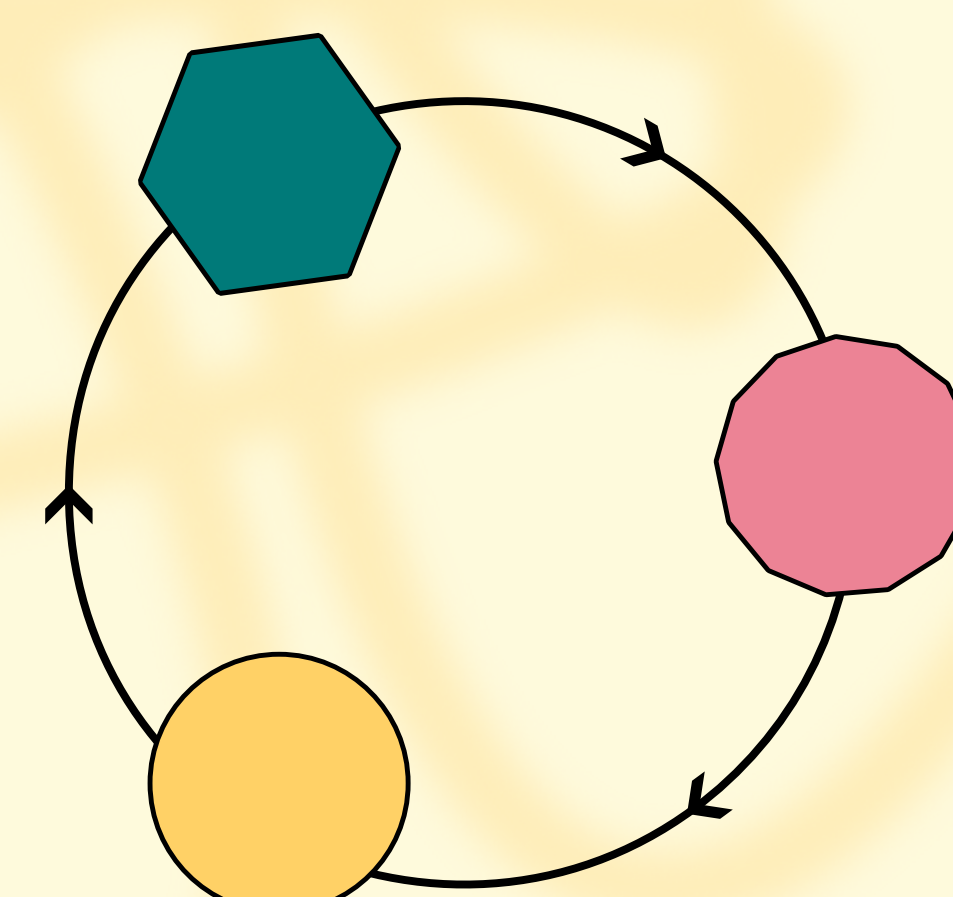
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(1) J. Wilkinson, et al. Environ. Pollut. 231 (2017) 954–70.
(2) L. Malm, et al. Anal. Chem. 96 (2024) 16215–26.
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