RapToxMix – predicting toxicity from LC/HRMS data

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Research problem

Understanding the toxicity of real-world **complex mixtures** is an essential starting point for intelligent design of water treatment solutions. However from hundreds of different **chemicals** present in **water samples**, only small fraction is usually **identififed** and their **toxity** evaluated.

Non-target LC/HRMS analysis. →

Proposal for solution

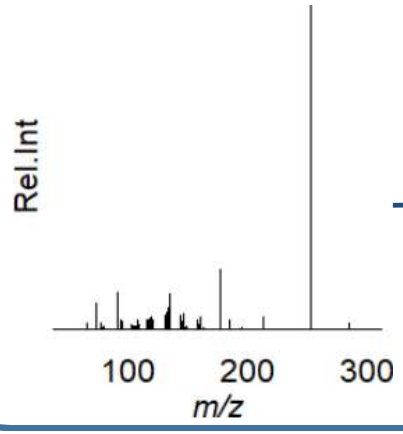
High-resolution mass spectromety (**HRMS**) with **fragmentation** spectra give **information** about the structure of the compound which can be **correlated** to its **toxicity** through **structural alerts**.

Machine learning →

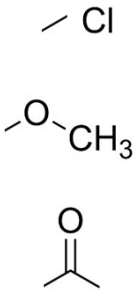
Results

In this work we developed method which uses fragmentation information from HRMS spectra to **predict** compounds **toxicity**. For fish LC_{50} values root mean square error (**RMSE**) less than **10x** was achieved.

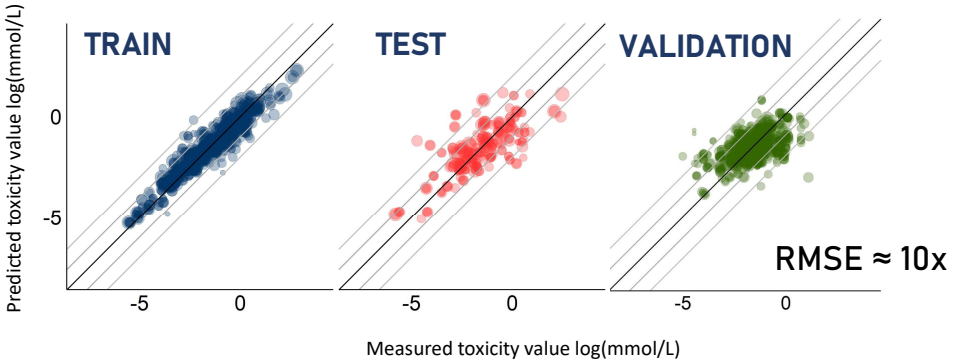
HRMS data



Fragments/ Structural alerts



Predicted toxicity



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