Ionization efficiency (*IE*) prediction for atmospheric pressure chemical ionization (APCI) coupling with gas chromatography (GC) and high-resolution mass spectrometry (HRMS) for environmental analysis

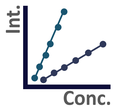
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1 Introduction



GC/APCI has been increasingly used in NTA of environmental samples.



The different ionization efficiency (*IE*) across chemicals affect the accuracy of quantification.



The *IE* in APGC is less understood, and no *in silico* prediction tools have been developed.

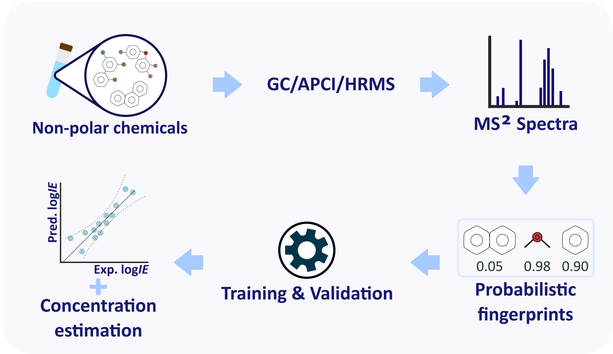
2 Objectives

A Evaluate the effect of water content on the ionization process in GC/APCI.

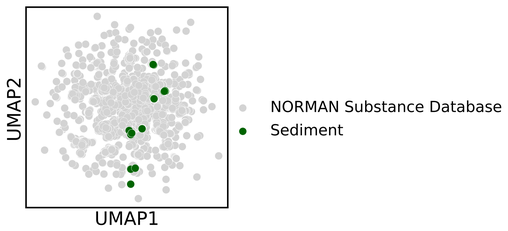
B Design a workflow to predict log*IE* and estimate the concentrations of detected chemicals from MS² spectra.

C Expand the application domain of *IE* predictions to GC-APCI-HRMS

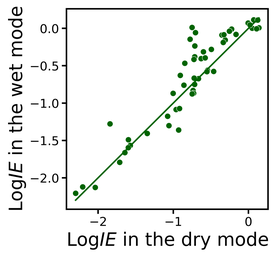
3 Workflow



4 Results

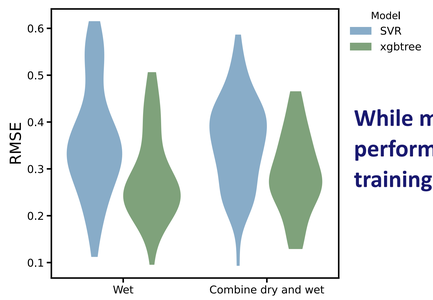


The chemical space for the pilot test



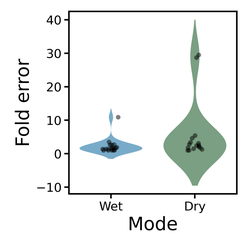
The high correlation indicates the potential for developing a universal model to predict log*IE*.

Correlation of logIE with different environments in GC/APCI



While models trained using *xgbtree* performed better, the effect of the training sets remained unclear.

Model's performance with different training sets and algorithms



The models provided more accurate predictions for chemicals ionized in wet mode.

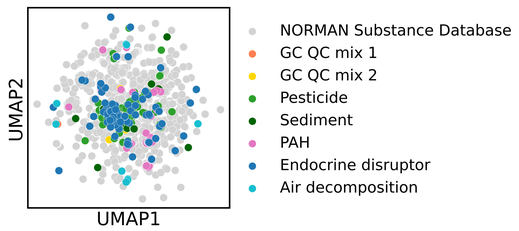
Validation of model performance using sediment samples

5 Conclusions

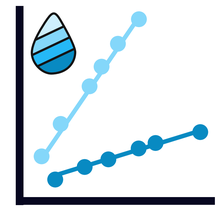
Chemicals detected with GC/APCI in NTA can be quantified from MS2 spectra based on predicted logIE values.

Water content did not largely affect *IE* values but the model's preformance in the GC/APCI pilot test.

6 Future perspectives



Chemical space expansion



Water content evaluation

[1] González-Gaya, B. et al. Anal. Methods 2021, 13 (16), 1876–1904.

[2] Dührkop, K. *et al.* Nat Methods 2019, 16 (4), 299–302.

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