

Comparison of semi-quantification methods for non-targeted screening of emerging contaminants with LC/ESI/HRMS

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Introduction

- Increased pollution of water worldwide
- Need for robust non-targeted screening semi-quantification approaches

Methods

- Water samples spiked with 68 representative compounds (30 stds, 37 suspects, 3 isotope labelled IS) analysed on LC/ESI(+)/HRMS
- Peak areas obtained using vendor software
- Concentration of 37 of the compounds estimated with four semi-quantitative approaches: (1a) structurally similar compounds; (1b) parent-TP pairs; (2) close eluting compounds; (3) ionisation efficiency prediction model
- Estimated concentrations compared to real concentrations to evaluate semi-quantification methods

Instrumentation

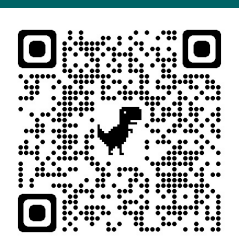
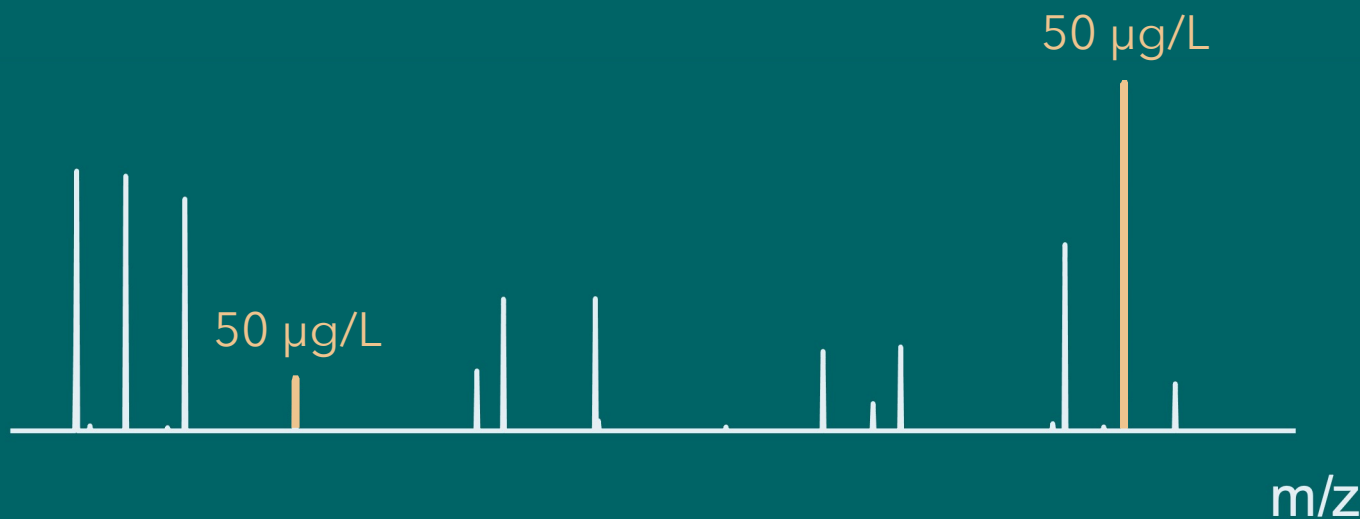
- Dionex UltiMate™ 3000 UHPLC
- Kinetex 2.6 μm, EVO C18, 100 Å, 150×3.0 mm column
- Positive electrospray ionisation
- Q Exactive Orbitrap HRMS
- Xcalibur Qual Browser
- R studios

Prediction error calculations

$$\text{pred error} = \begin{cases} \frac{c_{\text{pred}}}{c_{\text{real}}}, & \text{if } c_{\text{pred}} > c_{\text{real}} \\ \frac{c_{\text{real}}}{c_{\text{pred}}}, & \text{otherwise} \end{cases}$$

Standardised methods to quantify compounds before identification are expected to aid in decision making

Intensity



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The funding for this project has been generously provided by NORMAN network, JPA 2020

Semi-quantification approaches

$$RF = \frac{\text{peak area}}{\text{concentration}}$$

$$(1a) \quad c_{\text{suspect}} = \frac{\text{peak area}_{\text{suspect}}}{RF_{\text{structurally similar std}}}$$

$$(1b) \quad c_{TP} = \frac{\text{peak area}_{TP}}{RF_{\text{parent}}}$$

$$(2) \quad c_{\text{suspect}} = \frac{\text{peak area}_{\text{suspect}}}{RF_{\text{close eluting std}}}$$

(3) IE predicted using random forest regression based on 2D PaDEL descriptors and eluent descriptors

Results

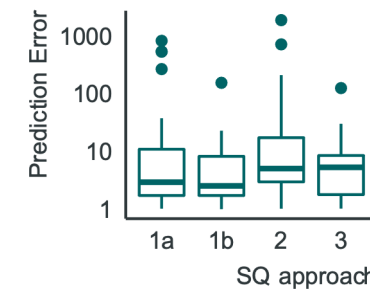


Fig 1. The prediction errors related to each semi-quantification approach

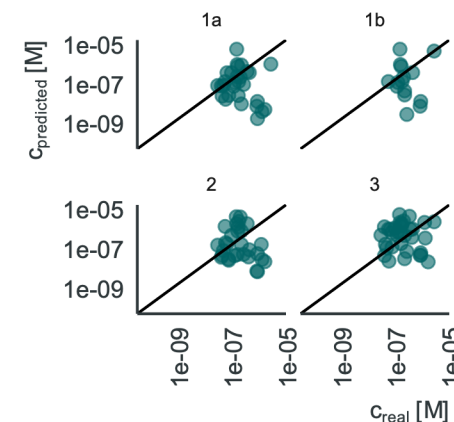


Fig 2. Predicted vs real concentration for each semi-quantification approach