Evaluation of Semi-Quantification Methods in Suspect Screening of Water Samples Using LC/ESI/HRMS

A NORMAN Collaborative Trial

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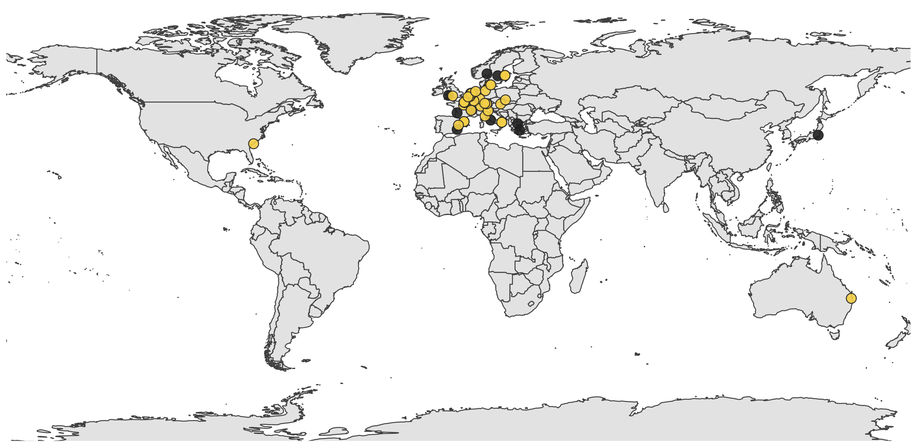
Introduction

Non-targeted LC/ESI/HRMS analysis of environmental samples have expanded the known universe of contaminants,[1] however, the ionisation efficiency (*IE*) in ESI varies tremendously between compounds.[2] Therefore, to determine the relevance of environmental contaminants, semi-quantitative methods can be used.[3] In this work we evaluate the performance of five semi-quantification methods in the largest collaborative trial organised by NORMAN network.

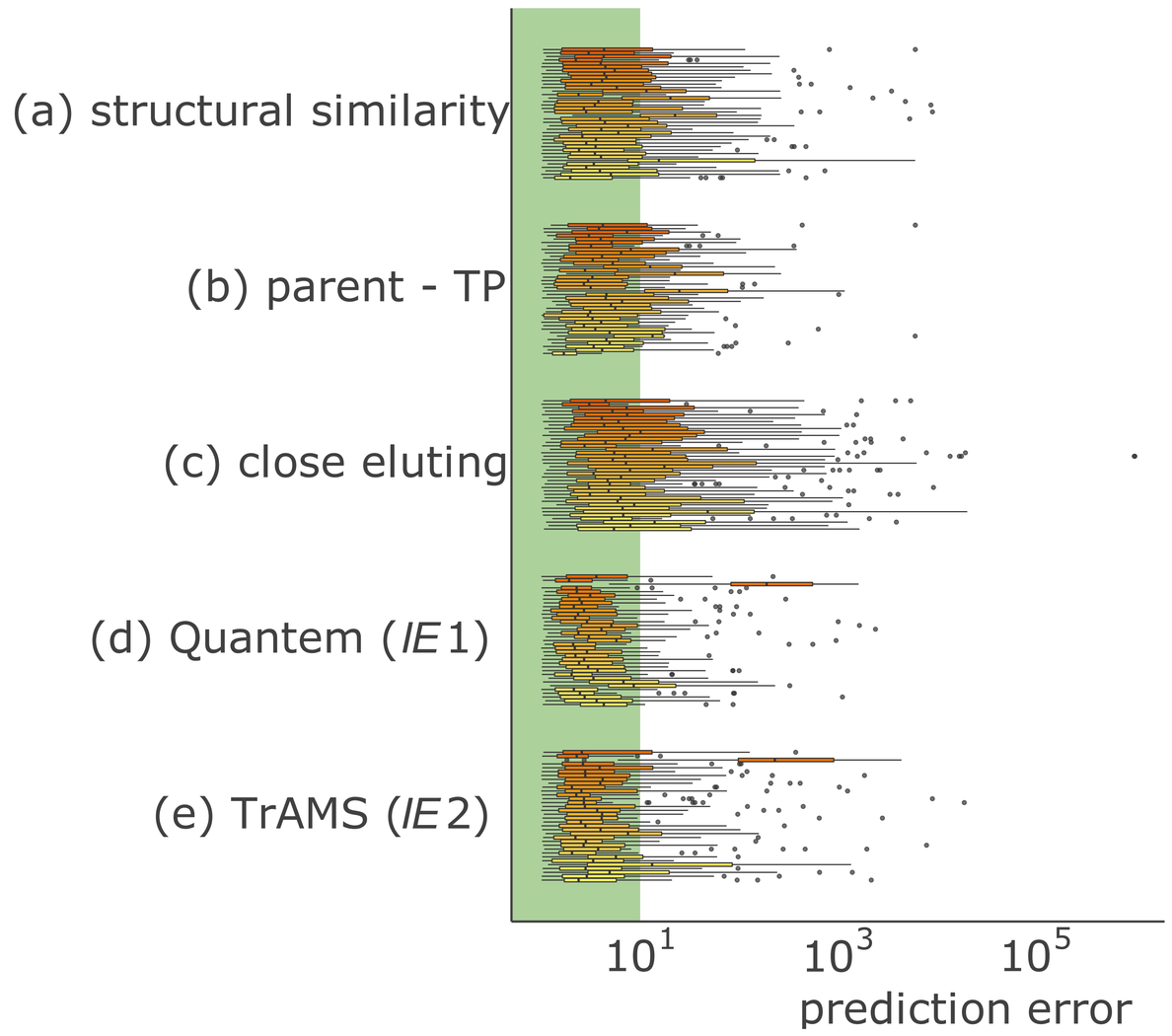
Fig. 1. Participating laboratories



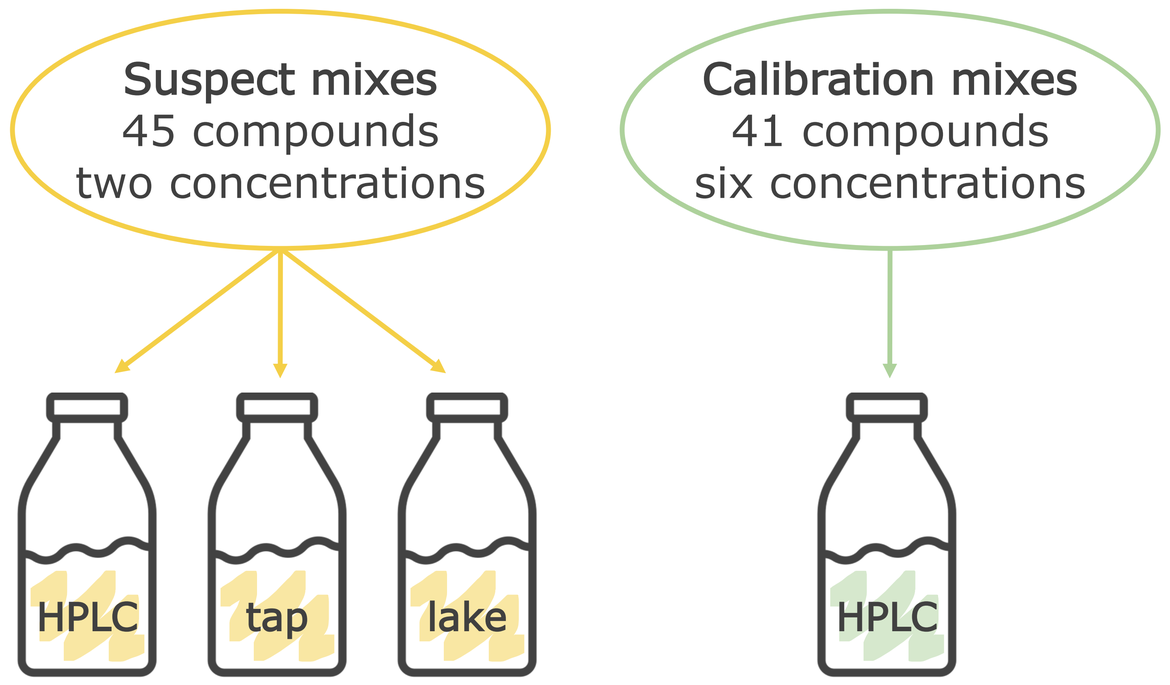
Results

- Better performance of IE prediction based methods
- Median error for all methods < 10× for most laboratories
- Generally, methods performance agrees well across laboratories

Fig. 3. Prediction errors for all laboratories

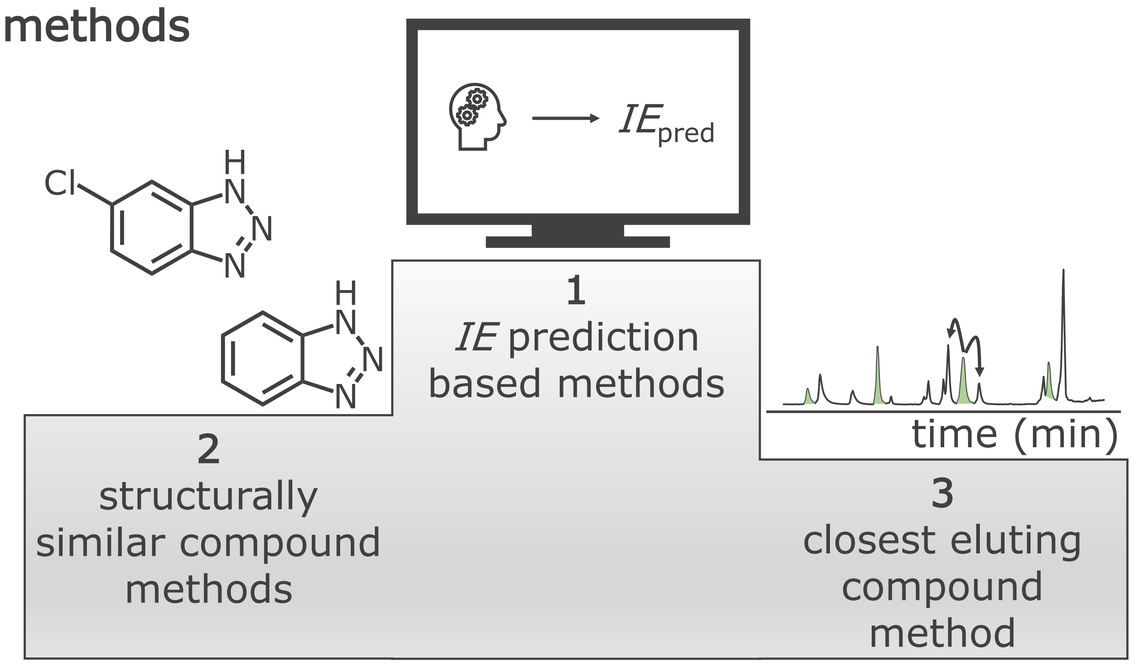


Methods



- Spiked water samples sent to 45 laboratories (Fig.1)
- Analysed with LC/ESI(+)/HRMS by 34 laboratories (Fig. 1, yellow dots)
- Concentrations estimated using either response factor of (a) structurally similar compound[4]; (b) parent compound; (c) close eluting compound[5]; or (d) & (e) *IE* prediction models[6,7]
- Semi-quantification methods evaluated based on fold prediction error

Fig. 2. Overall performance of semi-quantification methods



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References

[1] Pérez-Fernández, V.; et al. *Anal. Chim. Acta* **2017**, *983*, 9–41. [2] Kruve, A. *Anal. Chem.* **2020**, *92*, 4691–4699. [3] McCord, J. P.; et al. *Environ. Int.* **2022**, *158*, 107011. [4] Kalogiouri, N. P.; et al. *Anal. Bioanal. Chem.* **2017**, *409*, 5413–5426. [5] Pieke, E. N.; et al. *Anal. Chim. Acta* **2017**, *975*, 30–41. [6] Liigand, J.; et al. *Sci. Rep.* **2020**, 53. [7] Aalizadeh, R.; et al. *Anal. Bioanal. Chem.* **2022**, *414*, 7435-7450.