

# Standard substance free quantification of LC/ESI/MS on example of pesticides in cereals



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## Overview

**Purpose:** Enabling standard substance free semi-quantitation in LC/ESI/MS and interlaboratory comparison of suspect screening analyses via ionization efficiency (IE) predictions.

**Methods:** Cereal matrices spiked with pesticides were analysed with two different mass spectrometric setups in two different laboratories.

**Results:** Quantem approach resulted in standard substance free concentration estimation with error on average **3.8-times**. The result of suspect screening from different laboratories have average difference of 3.2-times.

## Chemicals

- 139 pesticides and mycotoxins
  - 6 concentration levels
  - 10 nM – 35 µM

## Matrices

- 6 cereals (proficiency test materials EU-PTs):
  - Barley C6
  - Wheat CF8
  - Rye CF10
  - Oat C3
  - Maize CF9
  - Rice SRM6
- QuEChERS sample preparation

## Instrumentation

### University of Tartu - UT

- Agilent 1290 UPLC with Agilent 6495 Triple Quadrupole
  - Agilent Zorbax RRHD SB-C18 (1.8 µm, 2.1 × 50 mm)
  - A 0.1% formic acid
  - B Acetonitrile

### Technical University of Denmark - DTU

- Agilent 1200 HPLC with Bruker Daltonics micro-TOFq
  - Nucleoshell C18 (2.7 µm, 2 × 100 mm)
  - A 2.5 mM ammonium formate pH = 3.0
  - B Acetonitrile

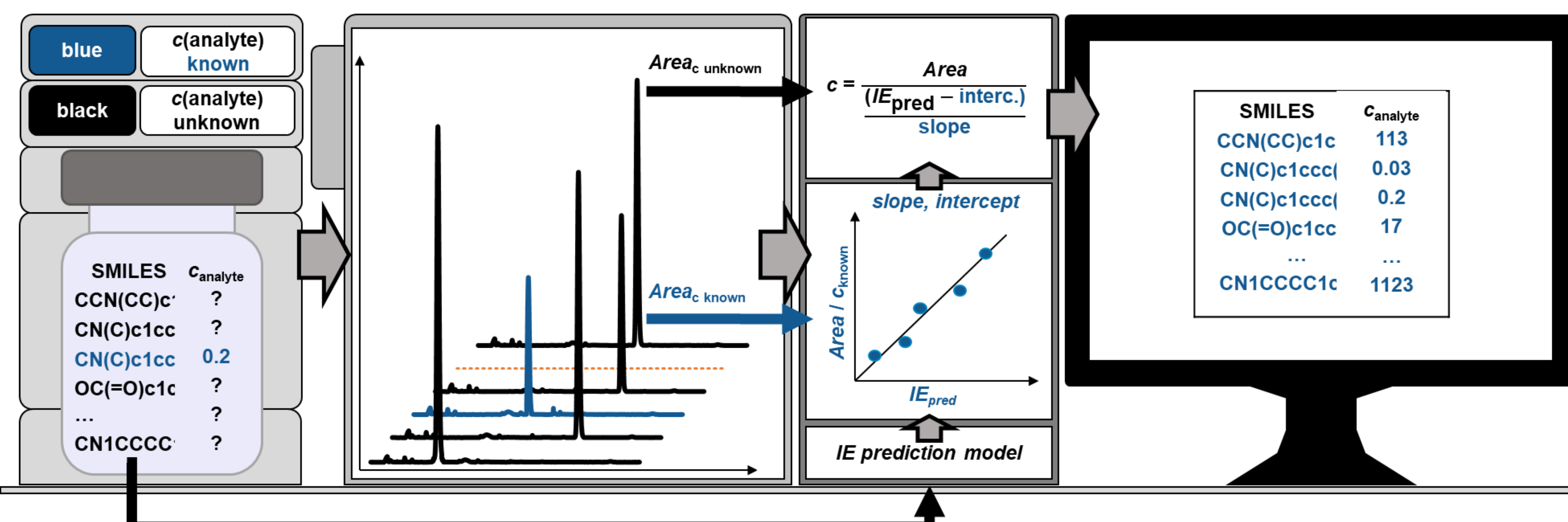
## Quantification

ESI ionization efficiency predictions

- Quantem approach
  - PaDEL descriptors for compound
  - Viscosity, surface tension, polarity, pH for eluent
  - Random Forest Regression

Transformation with 6 compounds

## Workflow



UT

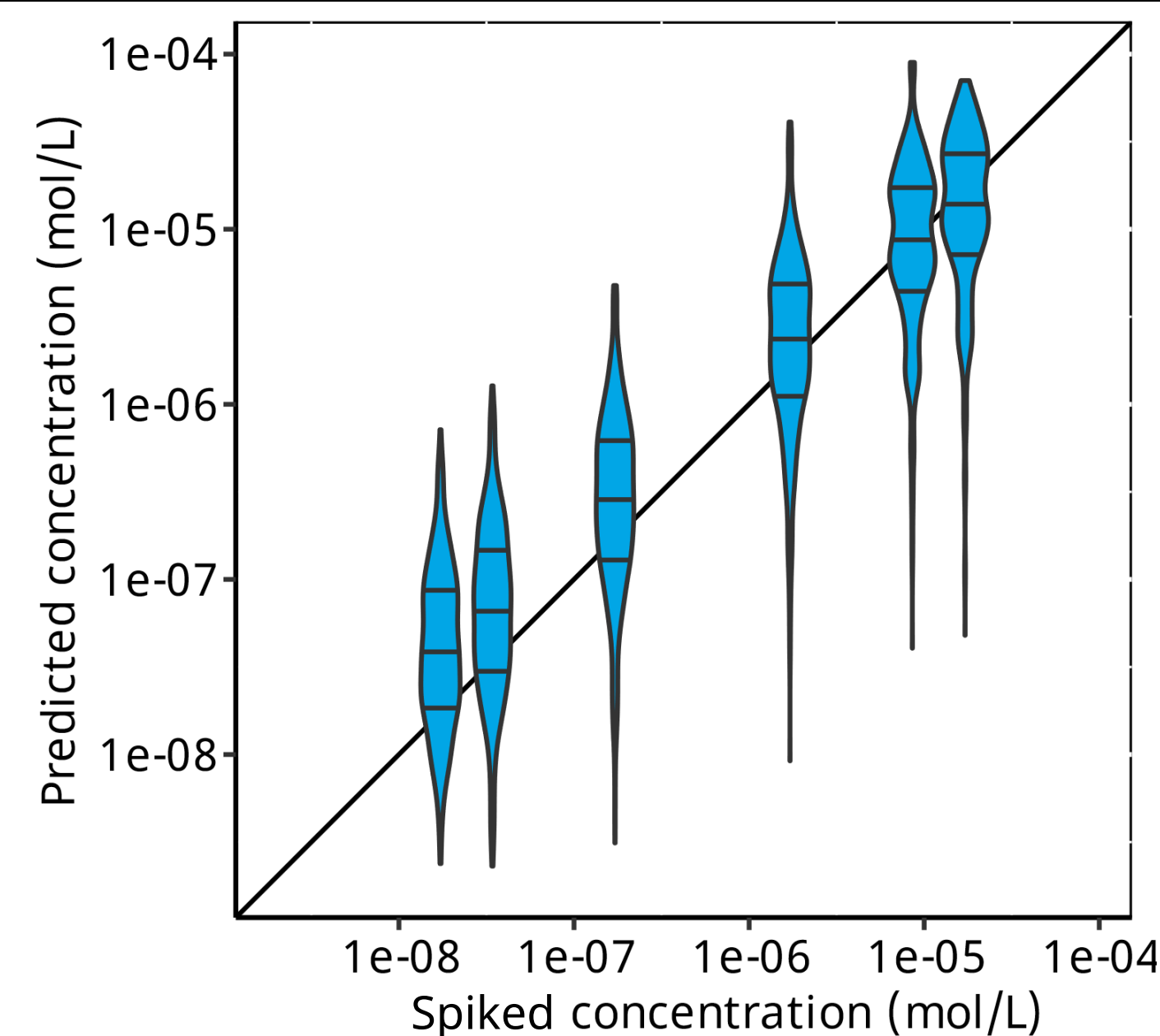


Figure 1 Predicted vs spiked concentrations on triple quadrupole in University of Tartu presented as violin plot. Horizontal lines denote 25%, 50% and 75% quantiles. Black line denotes ideal fit.

DTU

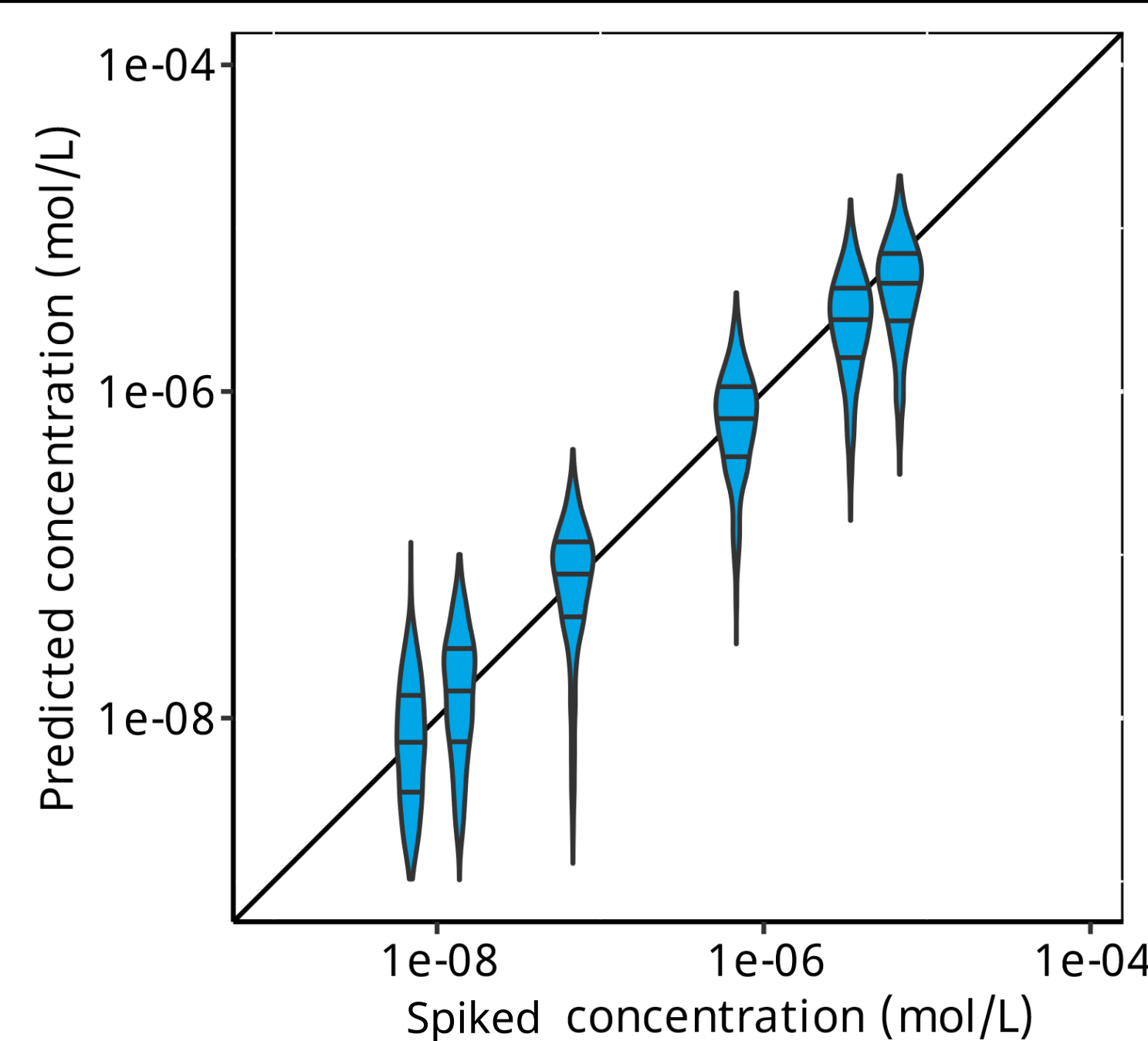


Figure 2 Predicted vs spiked concentrations on micro TOFq in Technical University of Denmark presented as violin plot. Horizontal lines denote 25%, 50% and 75% quantiles. Black line denotes ideal fit.

UT vs DTU

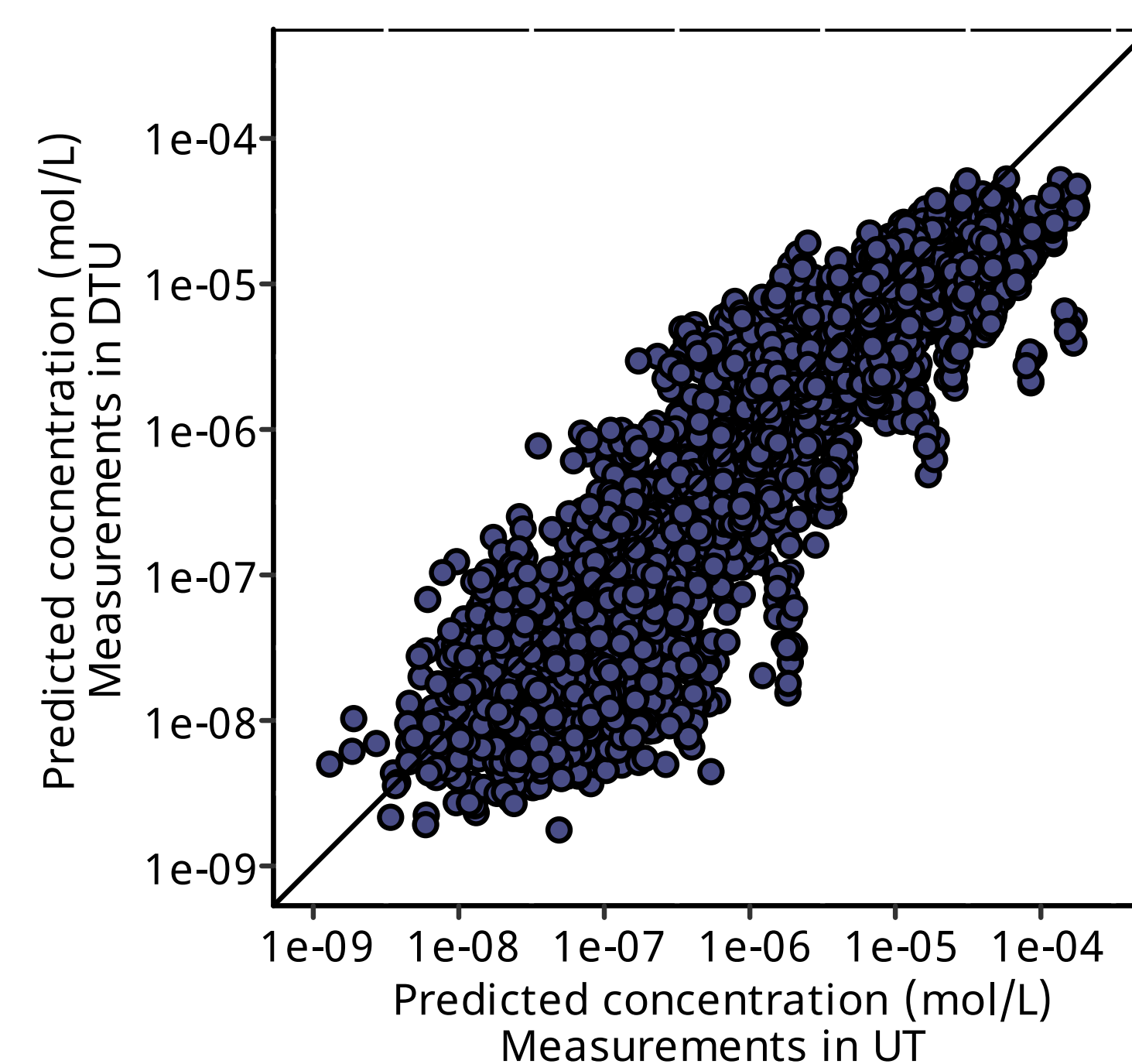


Figure 3 Comparison of predicted concentrations on micro TOFq vs triple quadrupole. Black line denotes ideal fit.

Conclusions

Standard substance free quantification in LC/ESI/MS analysis using Quantem approach is feasible

Average concentration prediction error **3.8-times**

Average difference on two instruments **3.2-times**



## References

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