

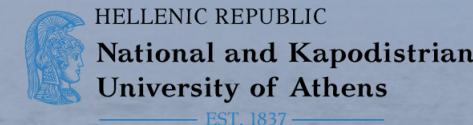
Evaluation of Quantification Approaches Without Analytical Standards in Non-Targeted Screening Using LC/ESI/HRMS

L. Malm, J. Liigand, R. Aalizadeh, N.
Alygizakis, N. Thomaidis, A. Kruve, et al.

Oct 19, 2023

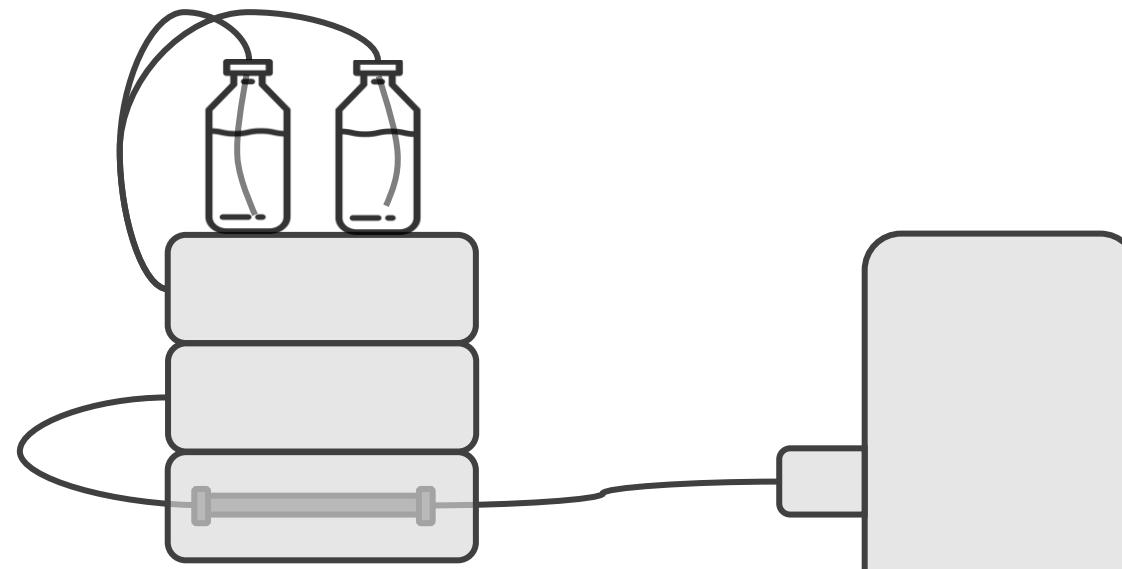
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Kruvelab.com



Stockholm
University

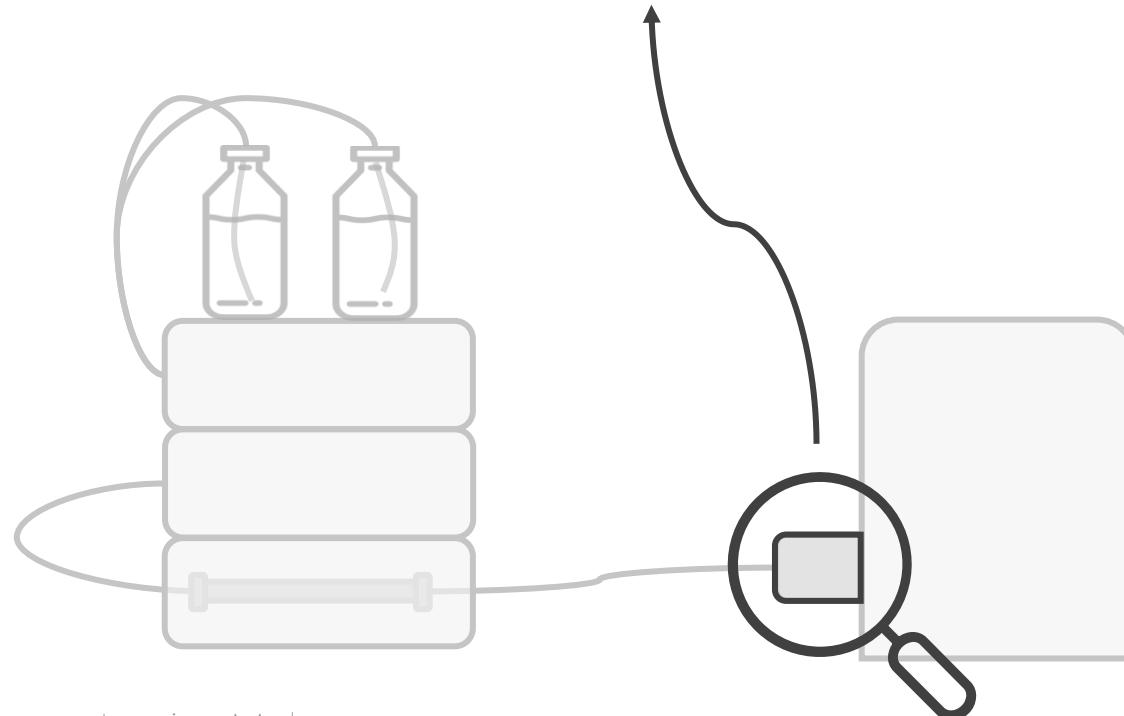
Brief background



Louise Malm

Brief background

Polarity, acid-base properties, eluent properties, ion source geometry, etc.



Quantification in NTS

A photograph showing a humpback whale breaching the surface of the ocean. The whale's body is arched upwards, with its white pectoral fin visible on the left side. The background consists of a cloudy sky and the blue ocean.

Several quantification methods developed

Quantification in NTS

Several quantification methods developed

Thorough evaluation lacking

Quantification in NTS

A photograph of a humpback whale breaching the surface of the ocean. The whale is captured mid-air, its body arched as it comes out of the water. The background is a bright, slightly overexposed sky and sea.

Several quantification methods developed

Thorough evaluation lacking

5 approaches compared and evaluated

Quantification approaches: similarity

$$\text{concentration} = \frac{\text{peak area}_{\text{suspect}}}{R F_{\text{calibrant}}}$$



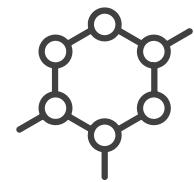
Parent – transformation
product (TP)

Quantification approaches: similarity

$$\text{concentration} = \frac{\text{peak area}_{\text{suspect}}}{R F_{\text{calibrant}}}$$



Parent – transformation
product (TP)



Tanimoto similarity

Quantification approaches: similarity

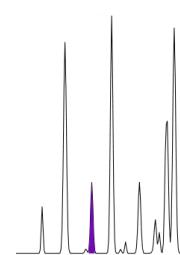
$$\text{concentration} = \frac{\text{peak area}_{\text{suspect}}}{R F_{\text{calibrant}}}$$



Parent – transformation
product (TP)

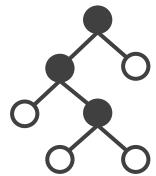
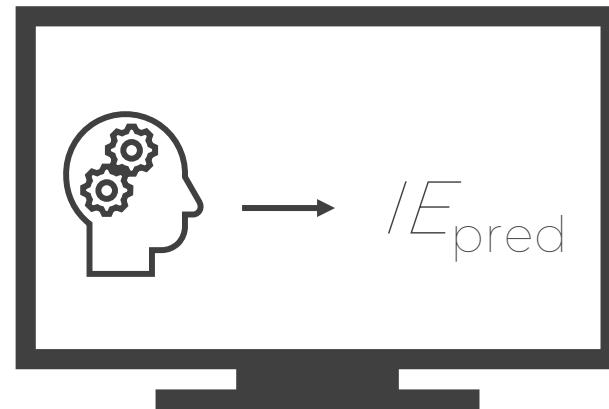
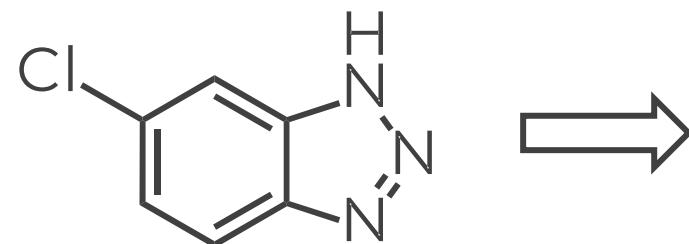


Tanimoto similarity



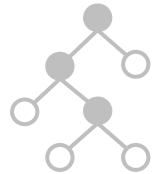
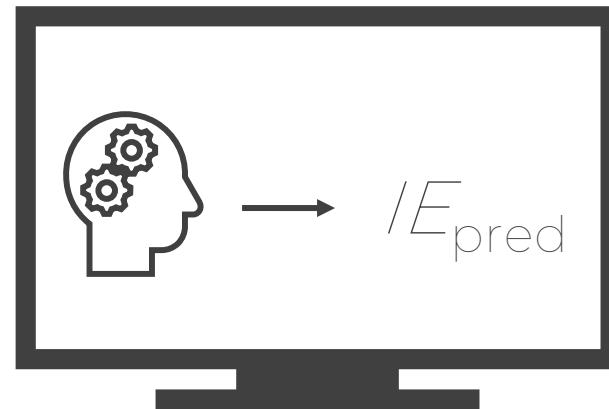
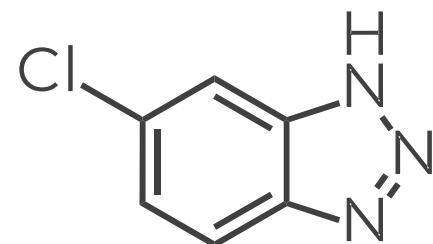
Close eluting compound

Quantification approaches: ionisation efficiency ($/E$)

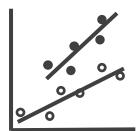


RF- $/E$: molecular & eluent
descriptors

Quantification approaches: ionisation efficiency ($/E$)

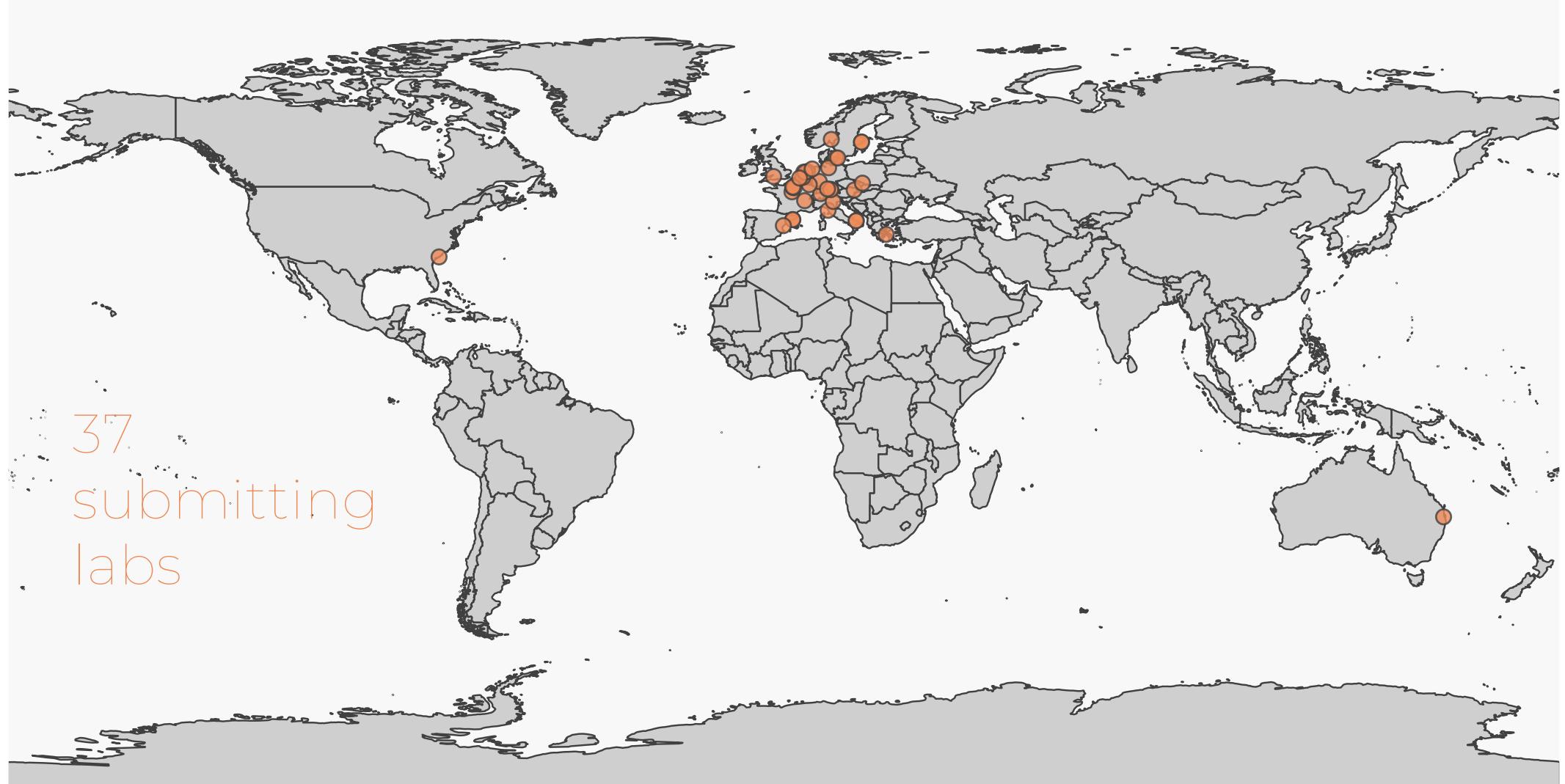


RF- $/E$: molecular & eluent
descriptors



MLR- $/E$: molecular
descriptors

Participants



Samples

Suspect samples

45 compounds

Three matrices



HPLC



tap



lake

High and low spike level

Samples

Suspect samples

45 compounds

Three matrices



HPLC



tap



lake

High and low spike level

Calibration samples

41 compounds



HPLC

Six known concentrations



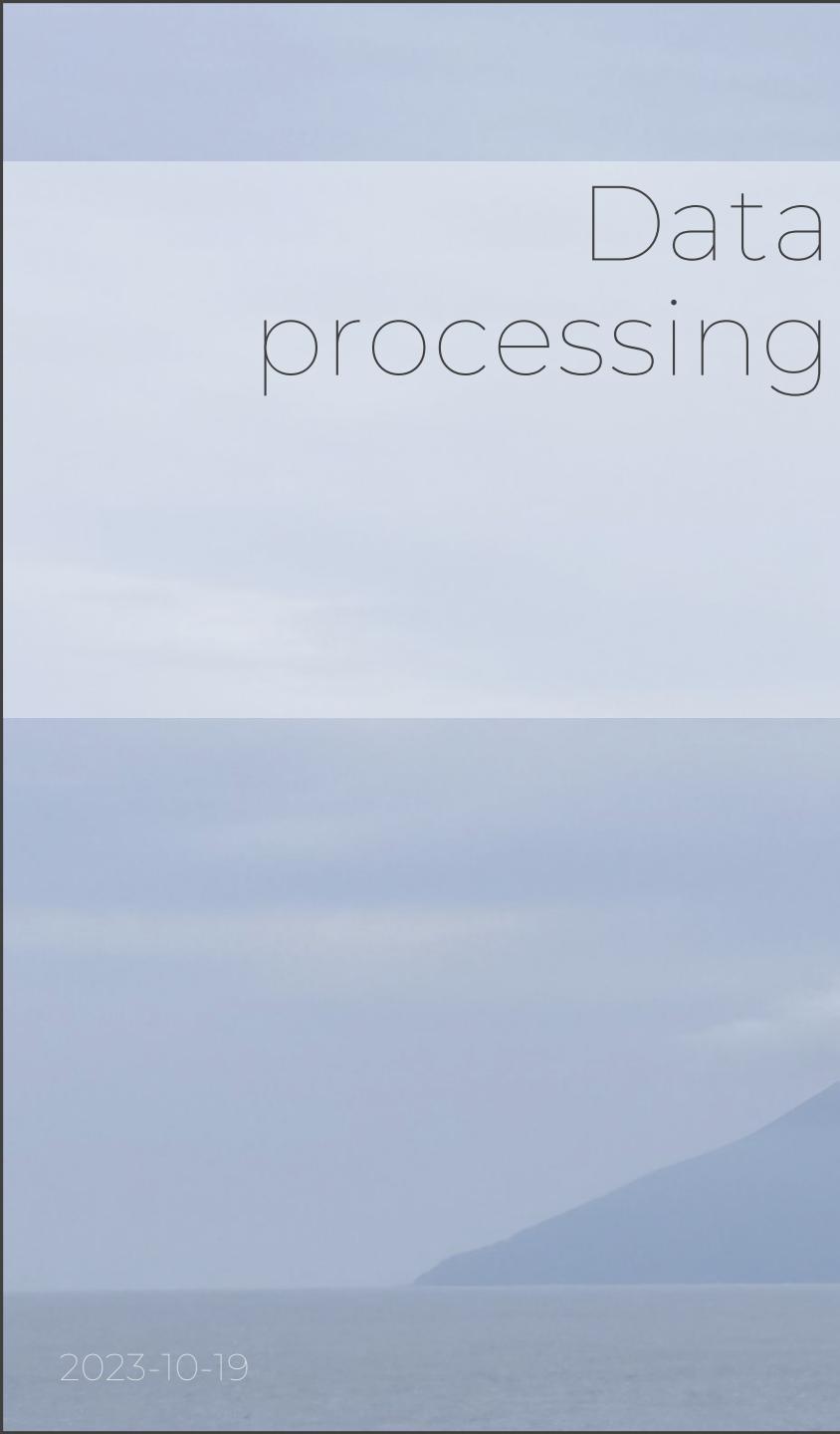
Data processing

Concentration estimates and raw data

Data processing

Concentration estimates and raw data

Reported and reprocessed



Data processing

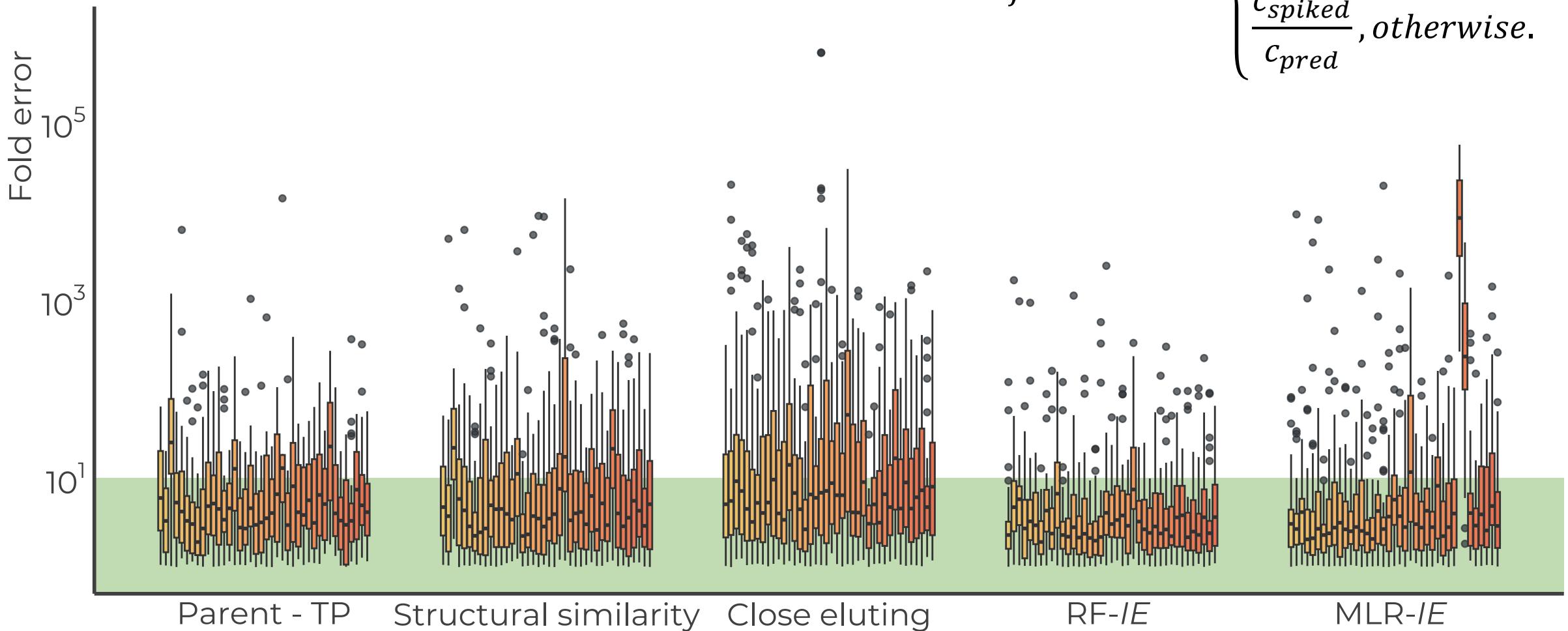
Concentration estimates and raw data

Reported and reprocessed

Quality assessment of reprocessed data

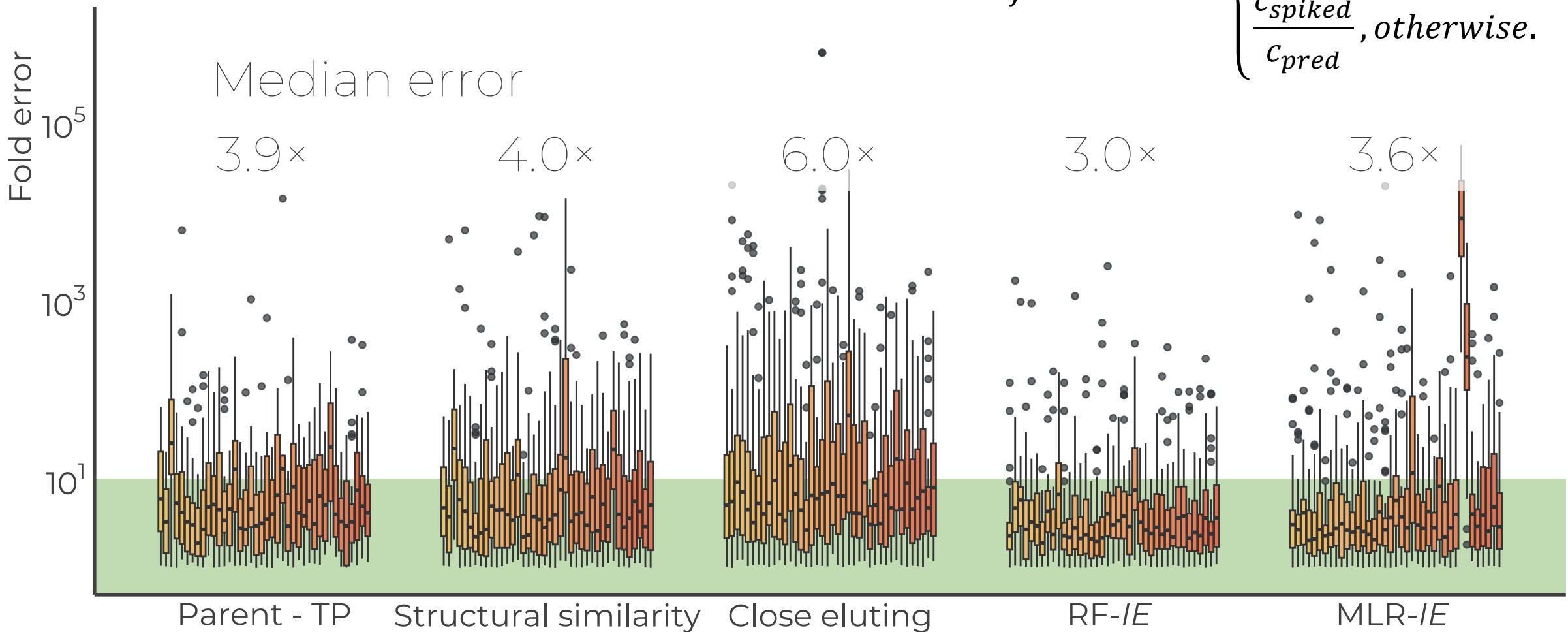
Fold error, reported data

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



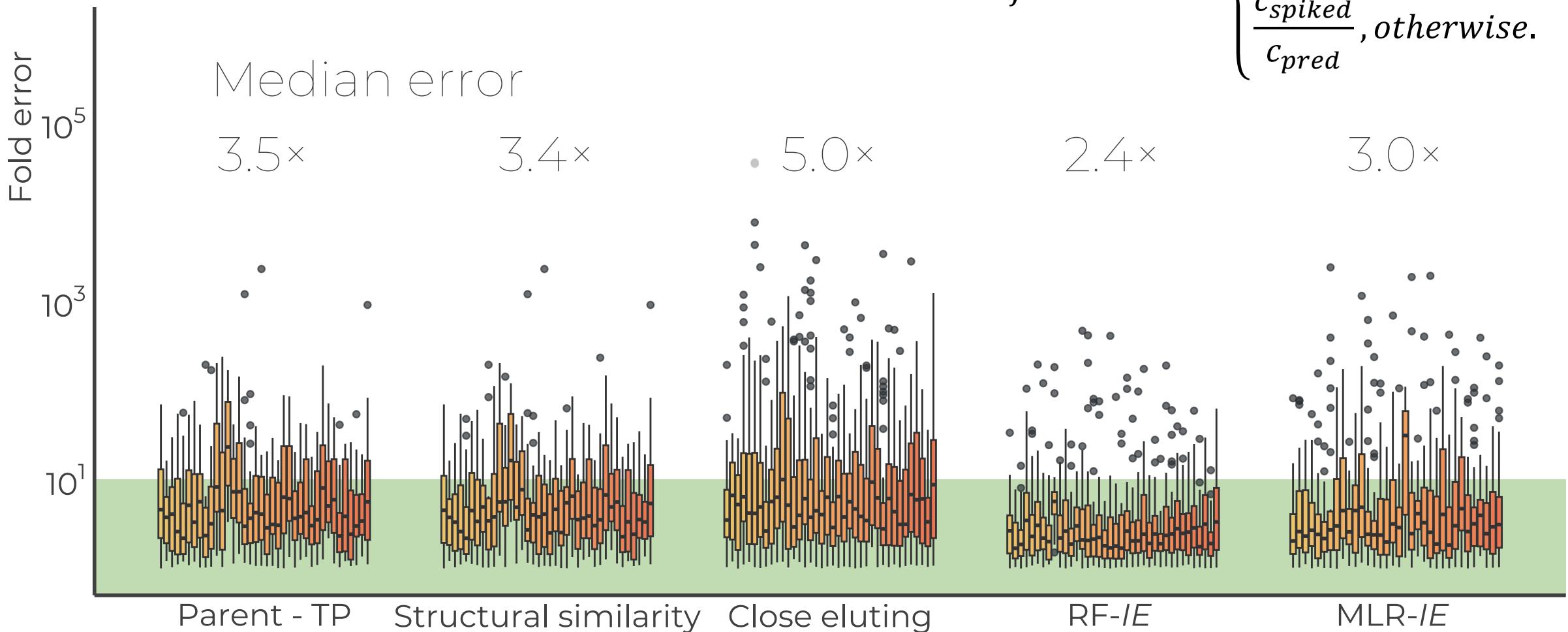
Fold error, reported data

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



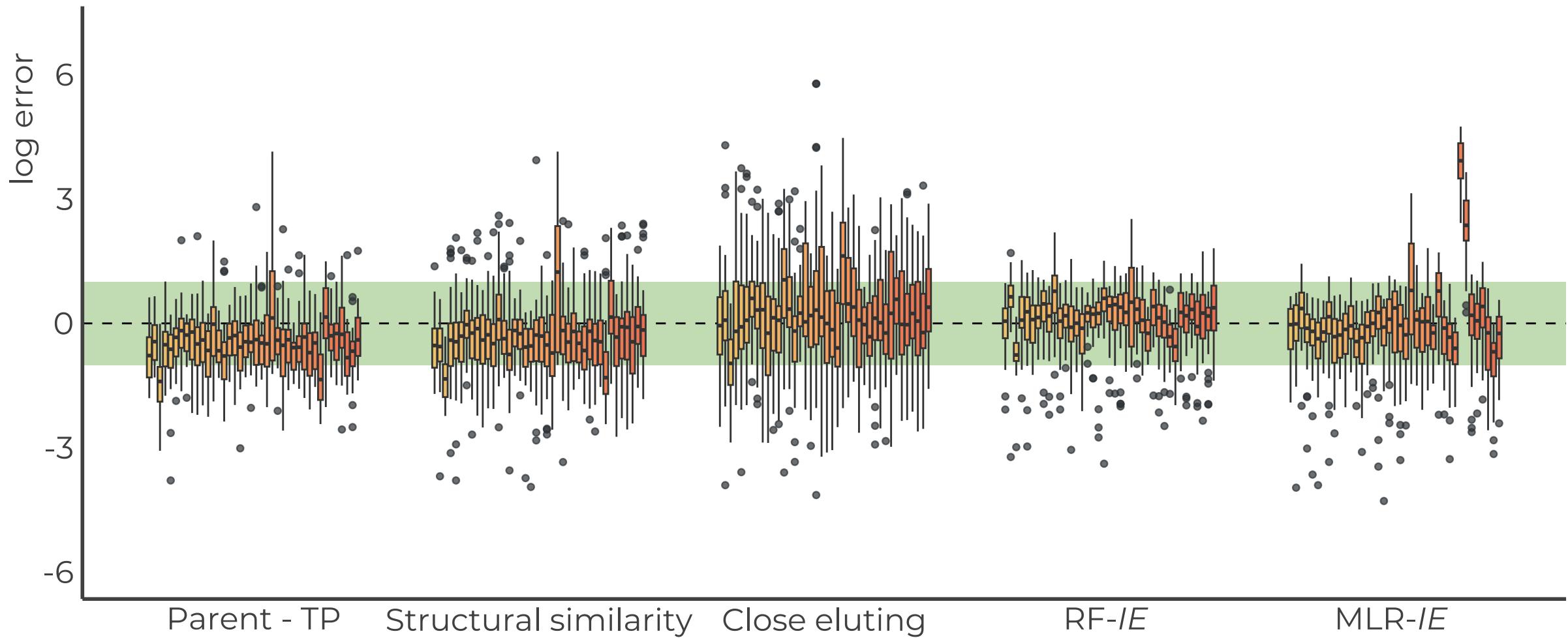
Fold error, reprocessed data

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



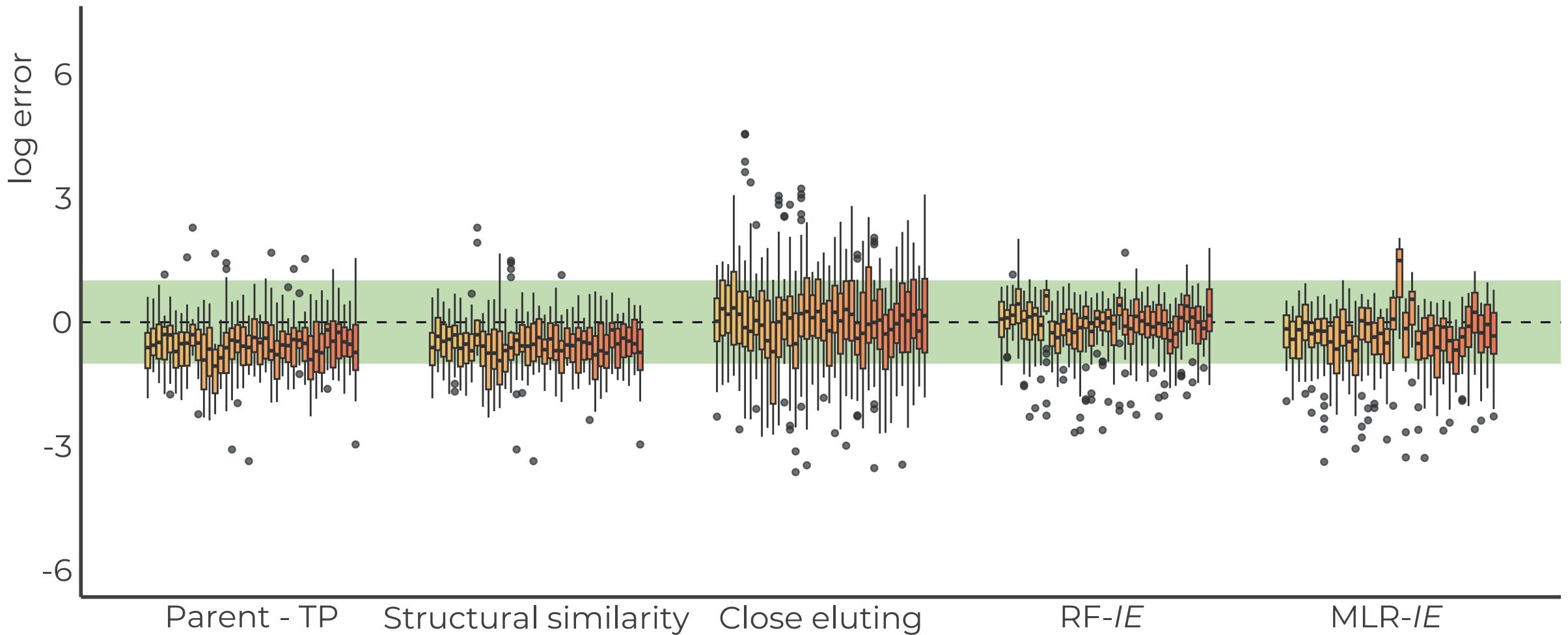
log error, reported data

$$\log \text{error} = \log_{10} \left(\frac{c_{\text{pred}}}{c_{\text{spiked}}} \right)$$



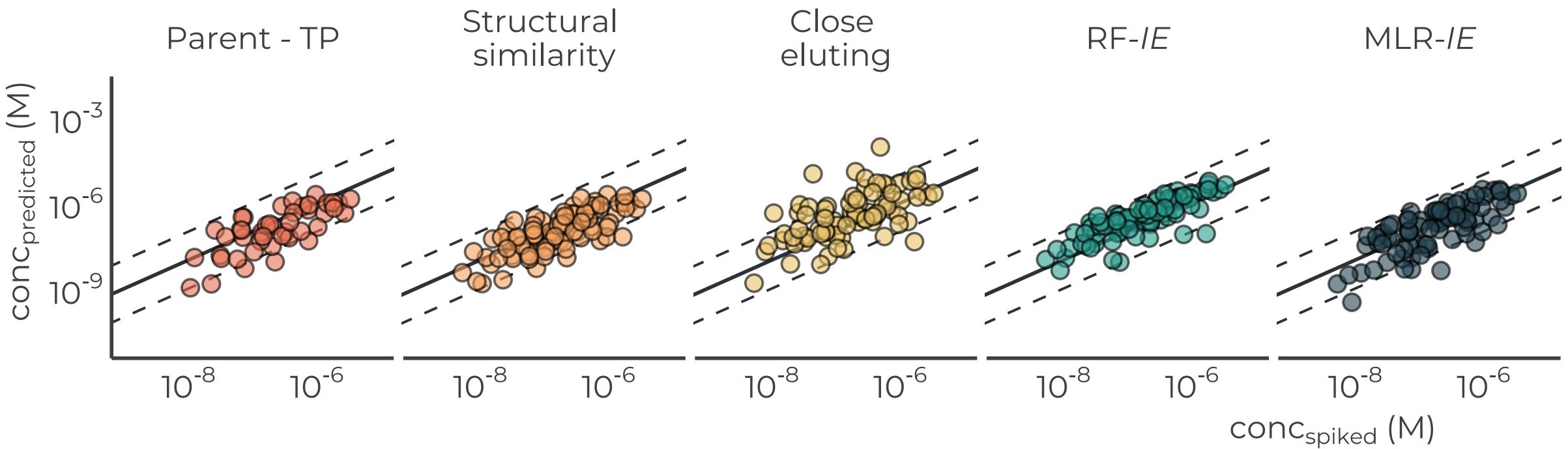
log error, reprocessed data

$$\log \text{error} = \log_{10} \left(\frac{c_{\text{pred}}}{c_{\text{spiked}}} \right)$$



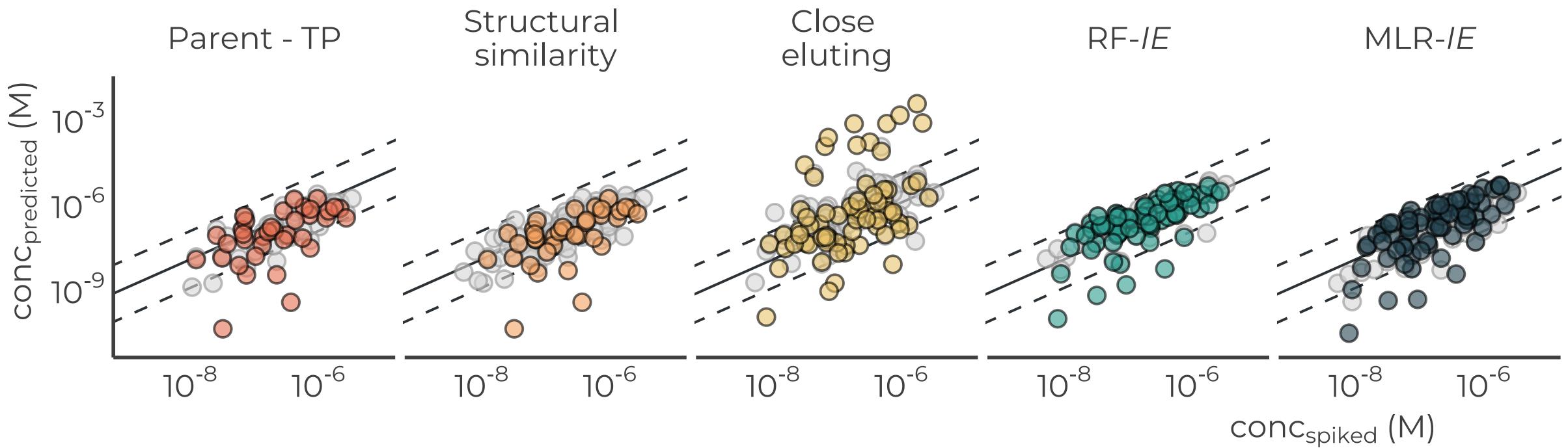
Correlation, reported

Lab 1



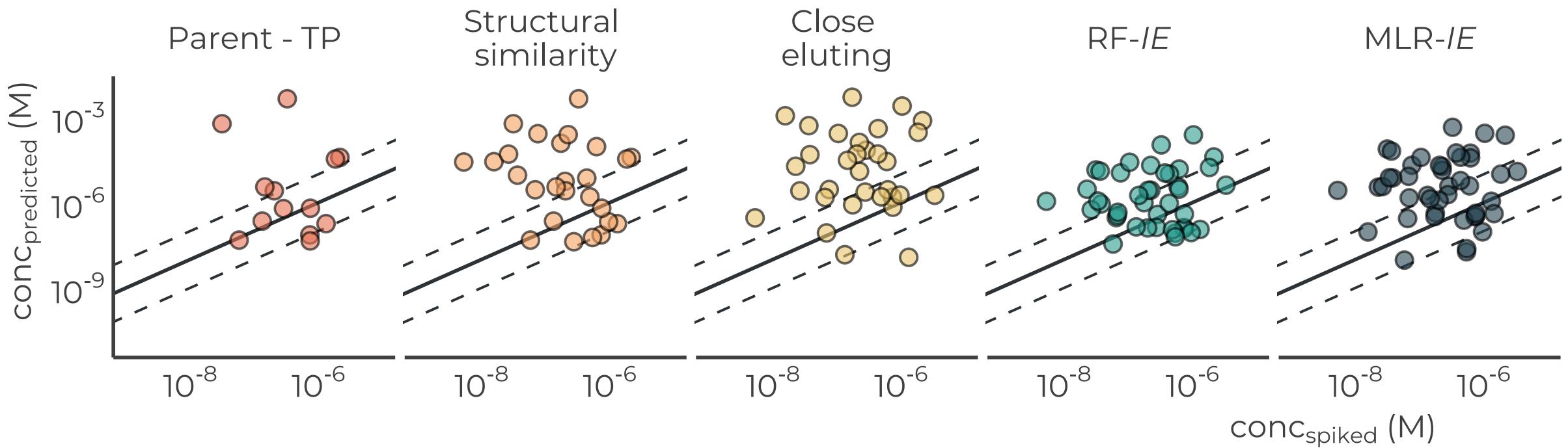
Correlation, reprocessed

Lab 1



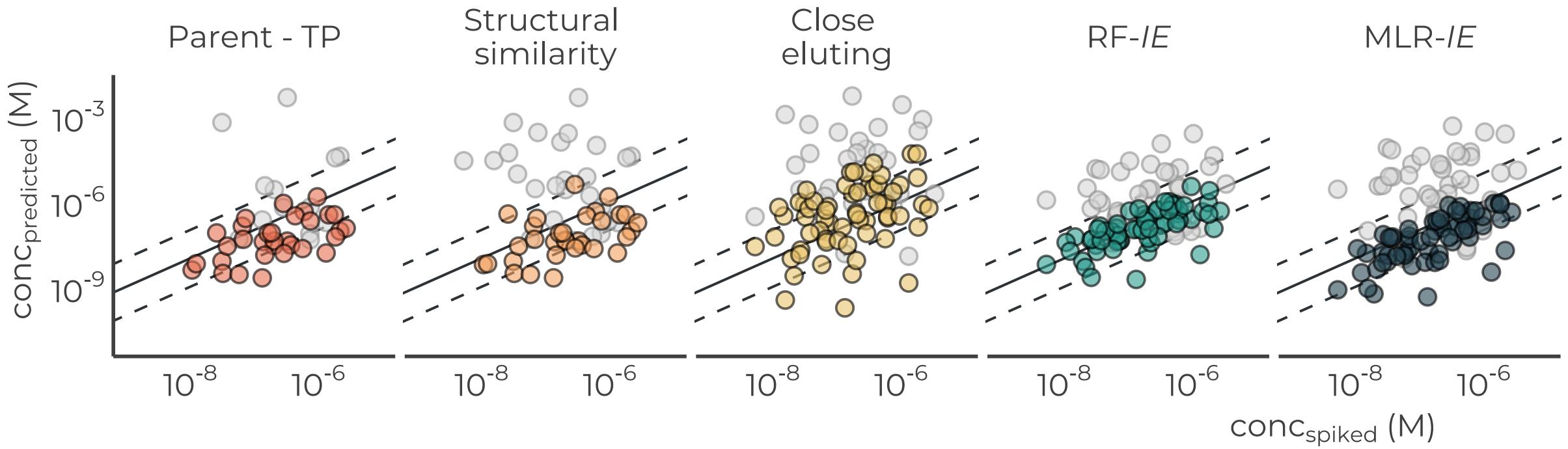
Correlation, reported

Lab 2



Correlation, reprocessed

Lab 2



Conclusions

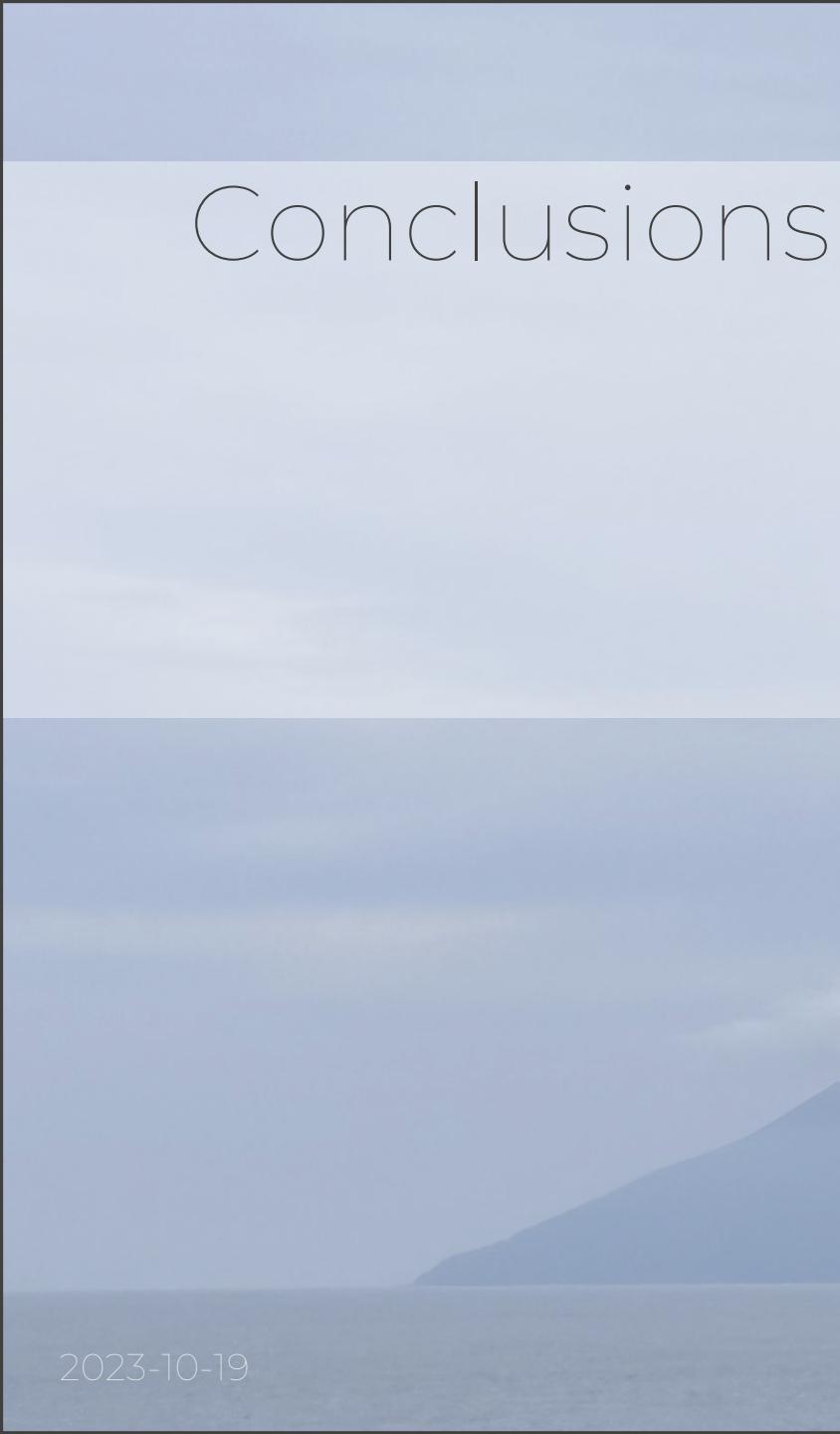
Lowest prediction error for /E-based approaches

Conclusions

Lowest prediction error for /E-based approaches

Underprediction issue for most approaches

Conclusions

A photograph showing a humpback whale breaching the surface of the ocean. The whale is positioned in the lower right quadrant of the frame, its dark body contrasting with the lighter blue of the water and sky. The background consists of a cloudy, overcast sky.

Lowest prediction error for /E-based approaches

Underprediction issue for most approaches

Importance of thorough quality assessment

Thank You!

All participants

NORMAN network

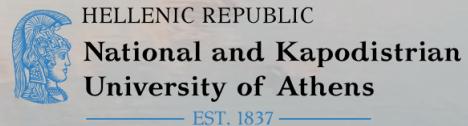
Jaanus Liigand, Reza Aalizadeh,
Nikiforos Alygizakis & Kelsey Ng

Nikolaos Thomaidis & Anneli Kruve

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