

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

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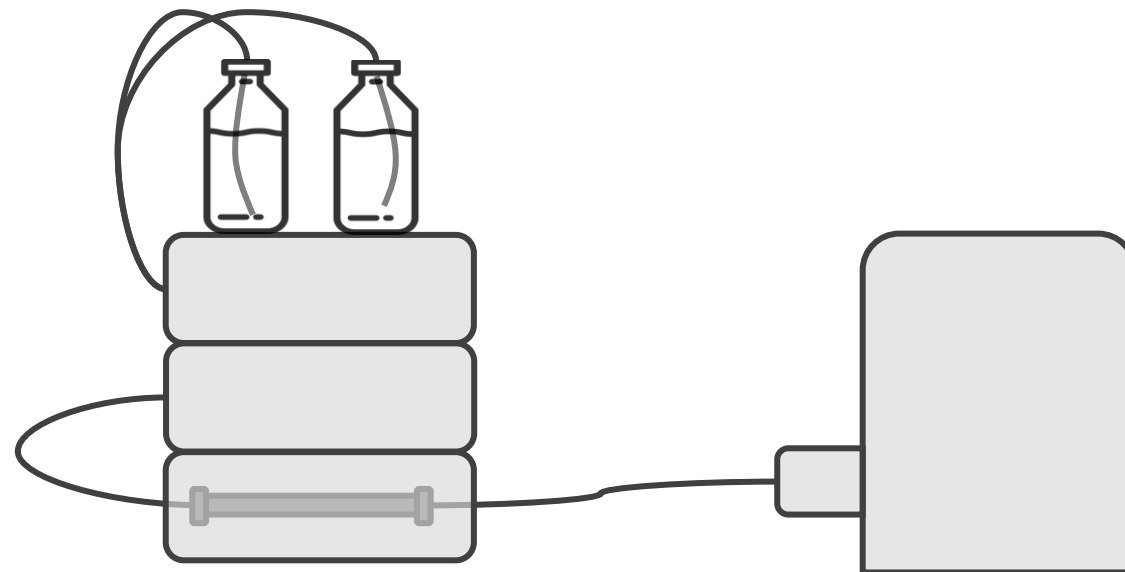
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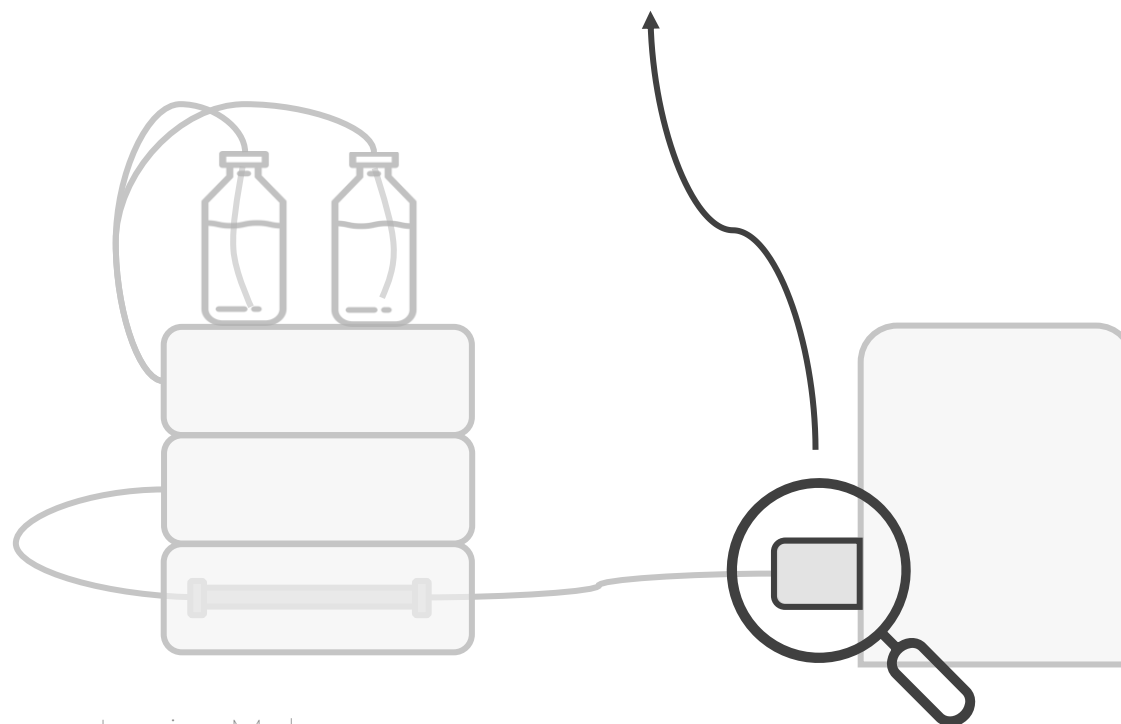
Stockholm
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Brief background



Brief background

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





Quantification in NTS

Several quantification methods
developed



Quantification in NTS

Several quantification methods
developed

Thorough evaluation lacking



Quantification in NTS

Several quantification methods
developed

Thorough evaluation lacking

5 approaches compared and
evaluated

Quantification approaches: similarity

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



Parent – transformation product (TP)

Quantification approaches: similarity

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



Parent – transformation product (TP)



Tanimoto similarity

Quantification approaches: similarity

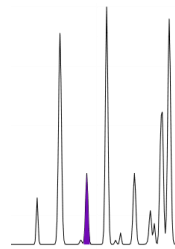
$$\text{concentration} = \frac{\text{peak area}_{\text{suspect}}}{RF_{\text{calibrant}}}$$



Parent – transformation product (TP)

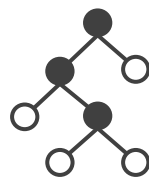
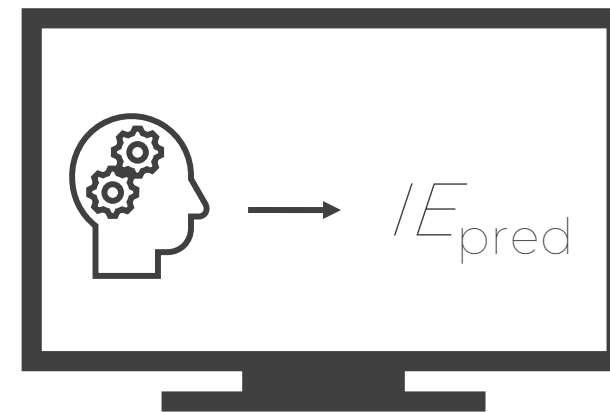
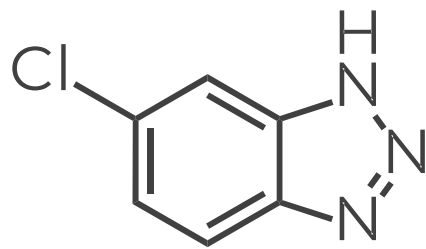


Tanimoto similarity



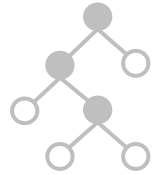
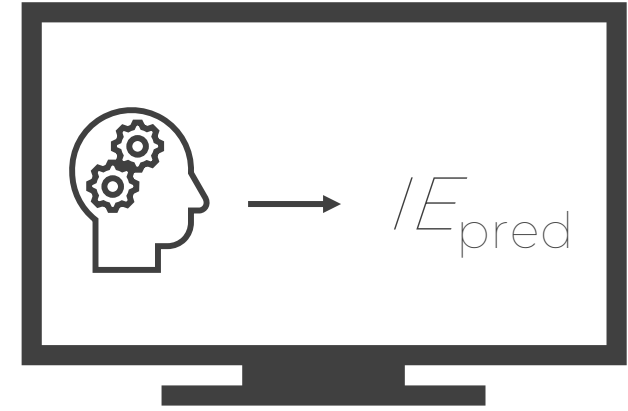
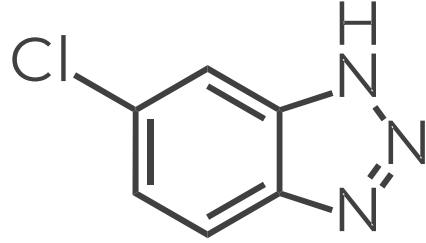
Close eluting compound

Quantification
approaches:
ionisation
efficiency (I/E)

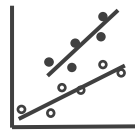


RF- I/E : molecular & eluent
descriptors

Quantification
approaches:
ionisation
efficiency (I/E)

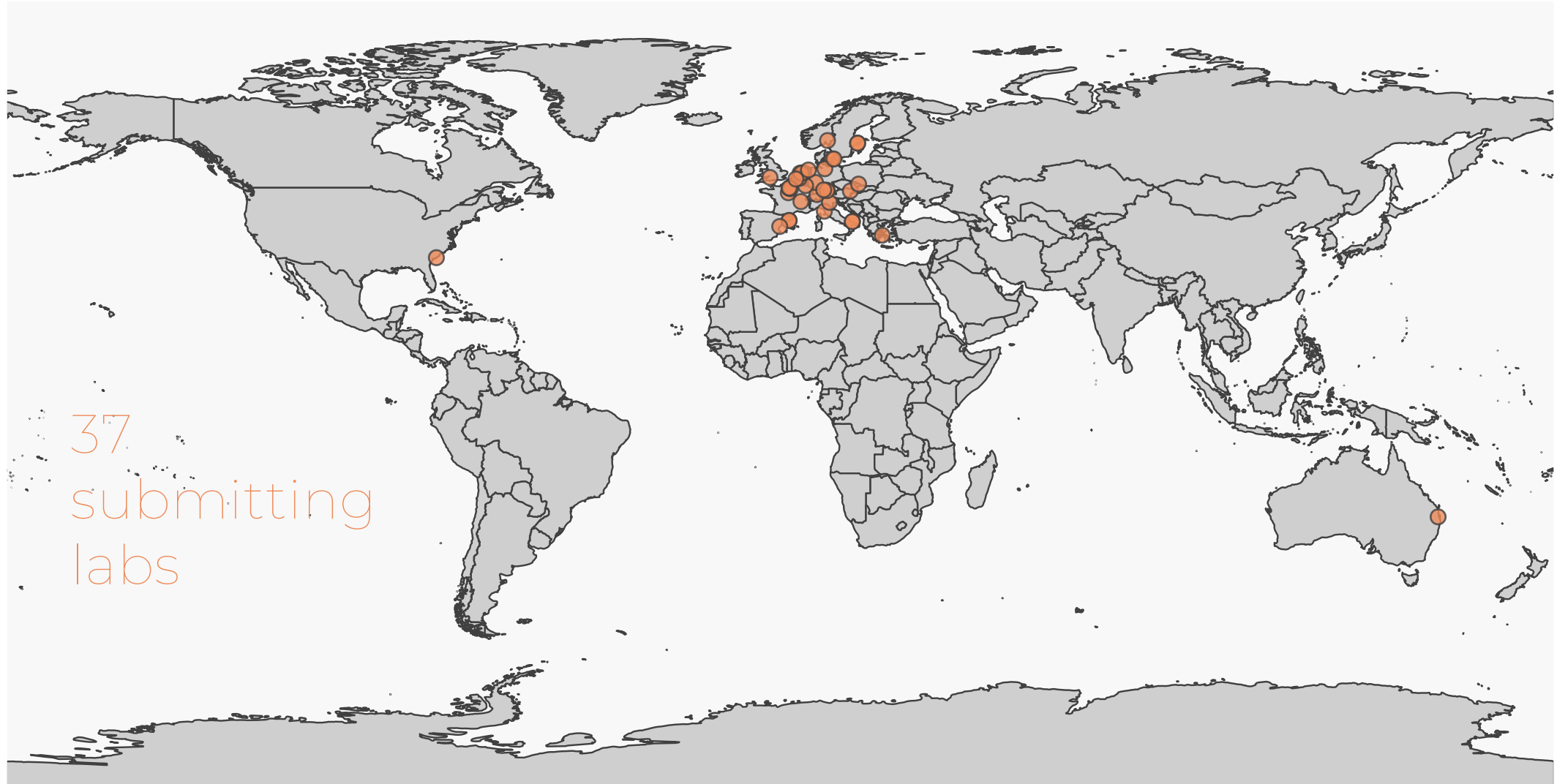


RF- I/E : molecular & eluent
descriptors



MLR- I/E : molecular
descriptors

Participants



37
submitting
labs

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



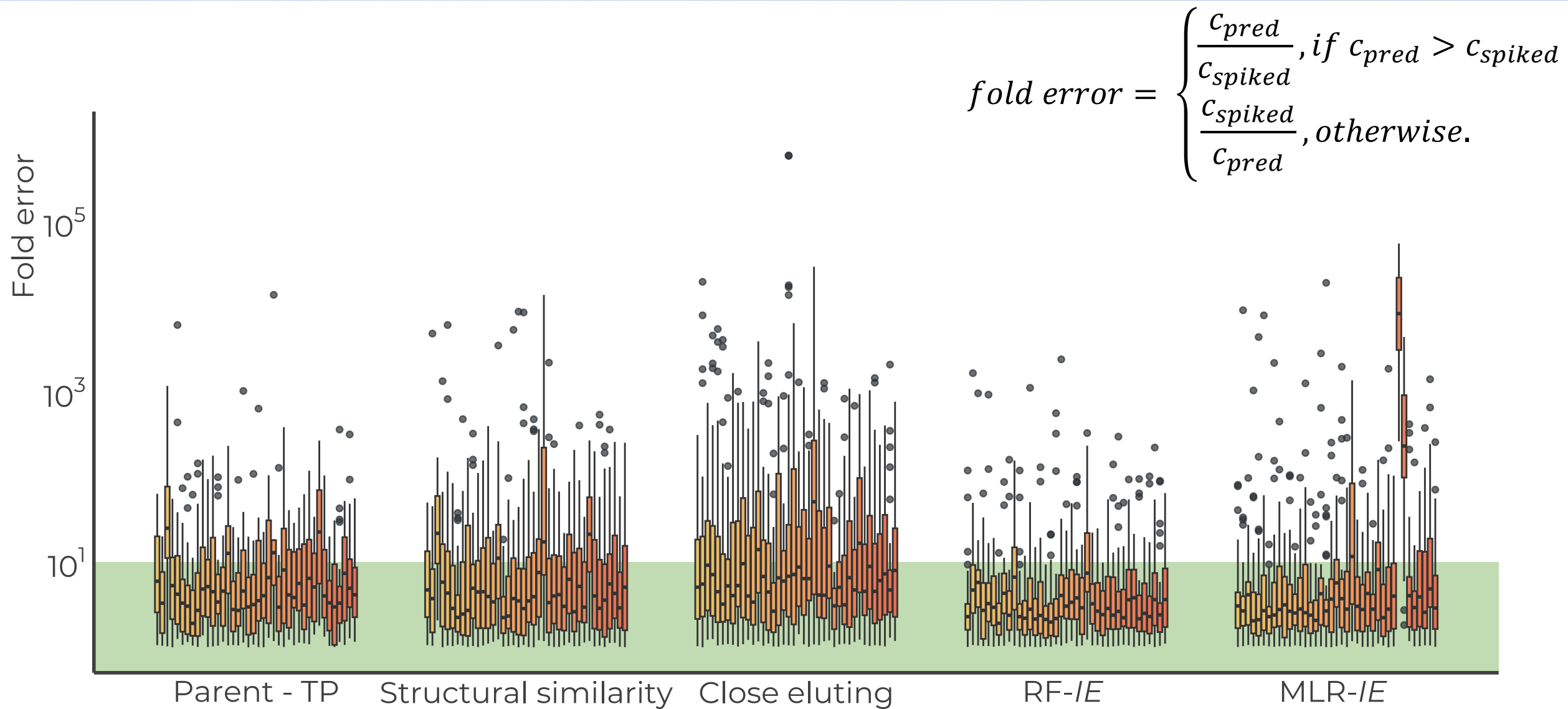
Data processing

Concentration estimates and raw
data

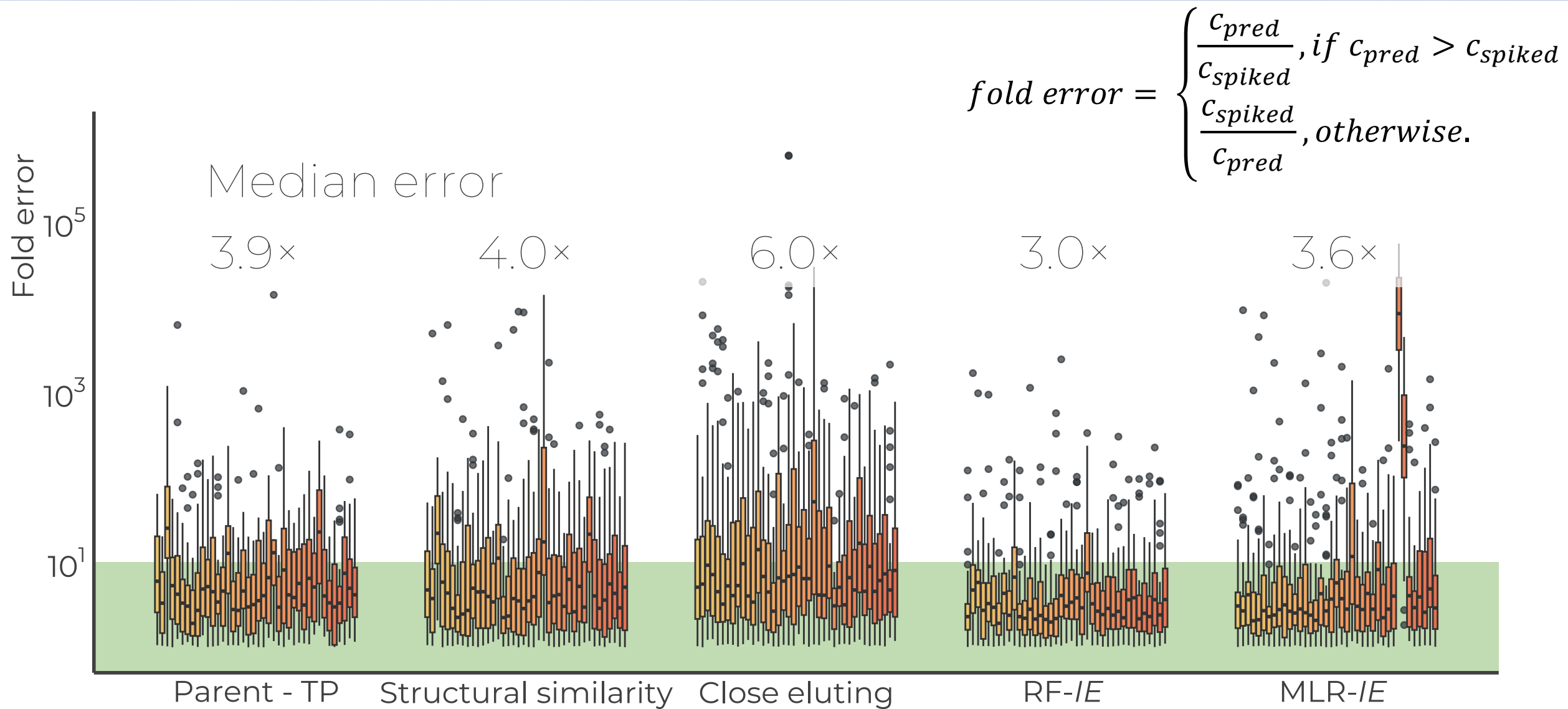
Reported and reprocessed

Quality assessment of reprocessed
data

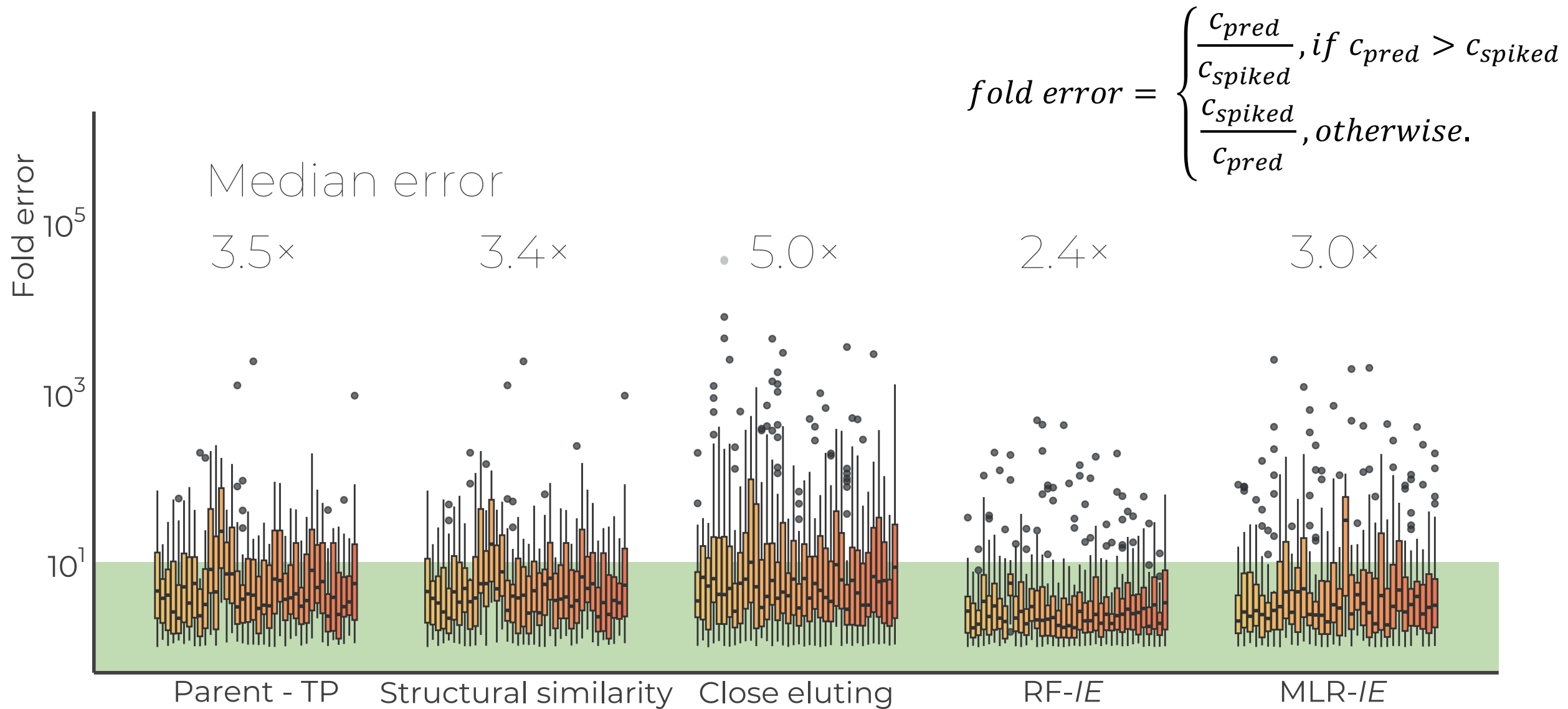
Fold error, reported data



Fold error, reported data

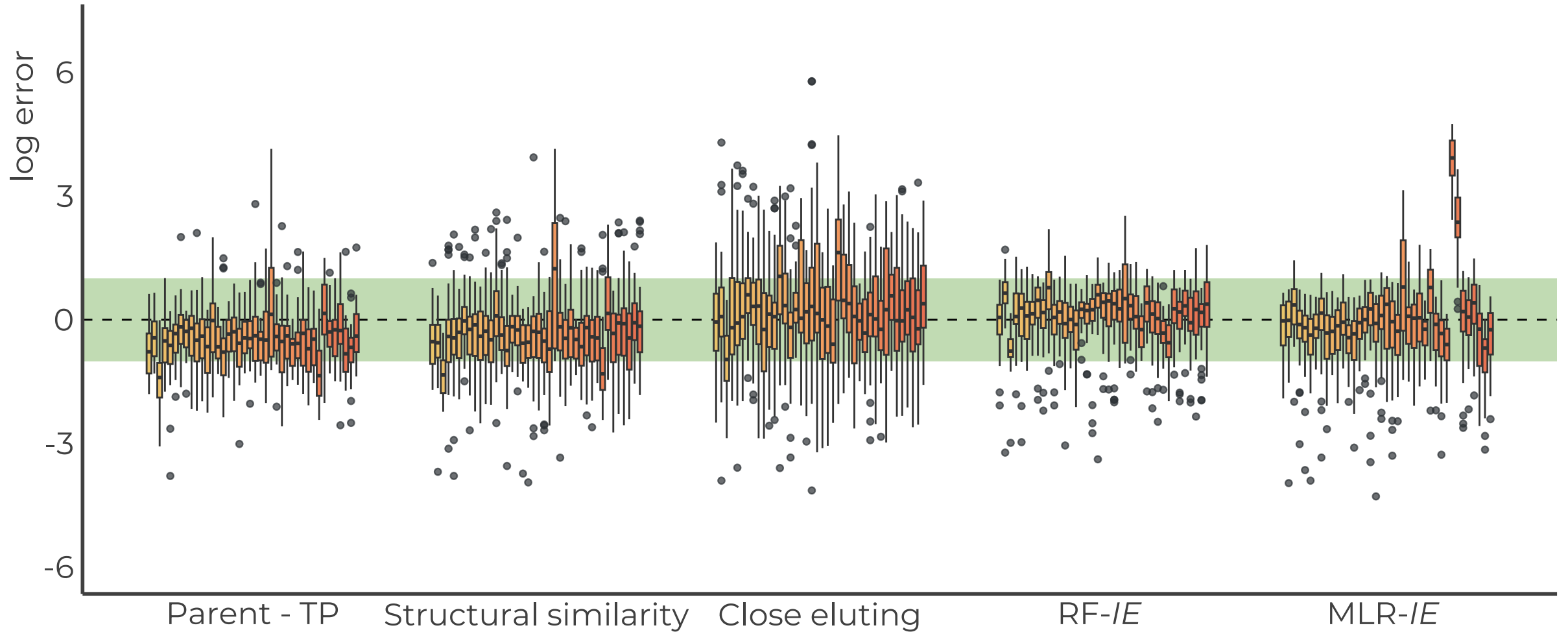


Fold error, reprocessed data



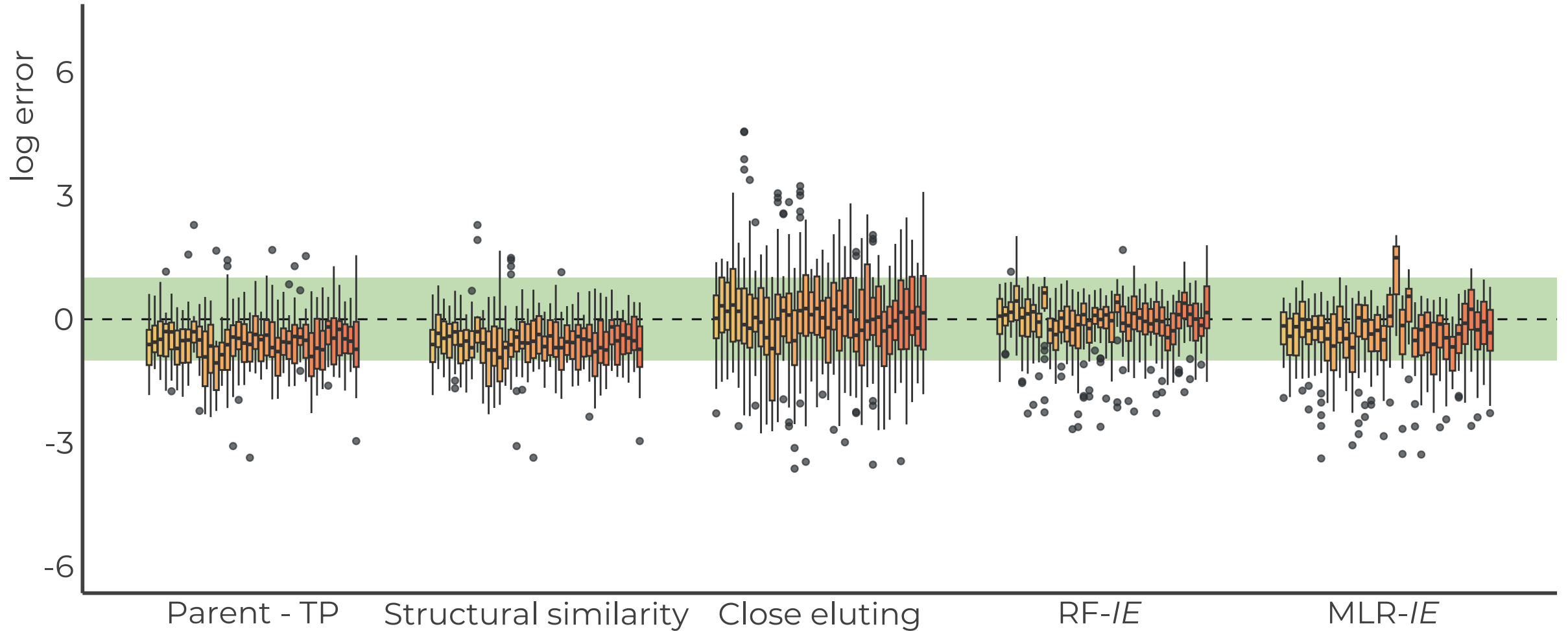
log error, reported data

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



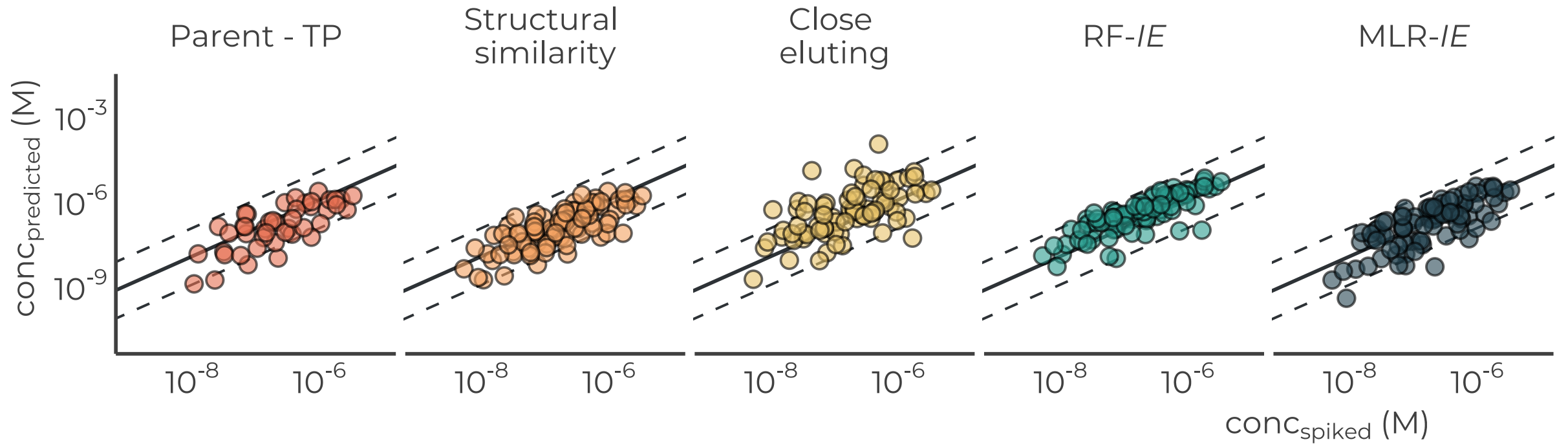
log error, reprocessed data

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



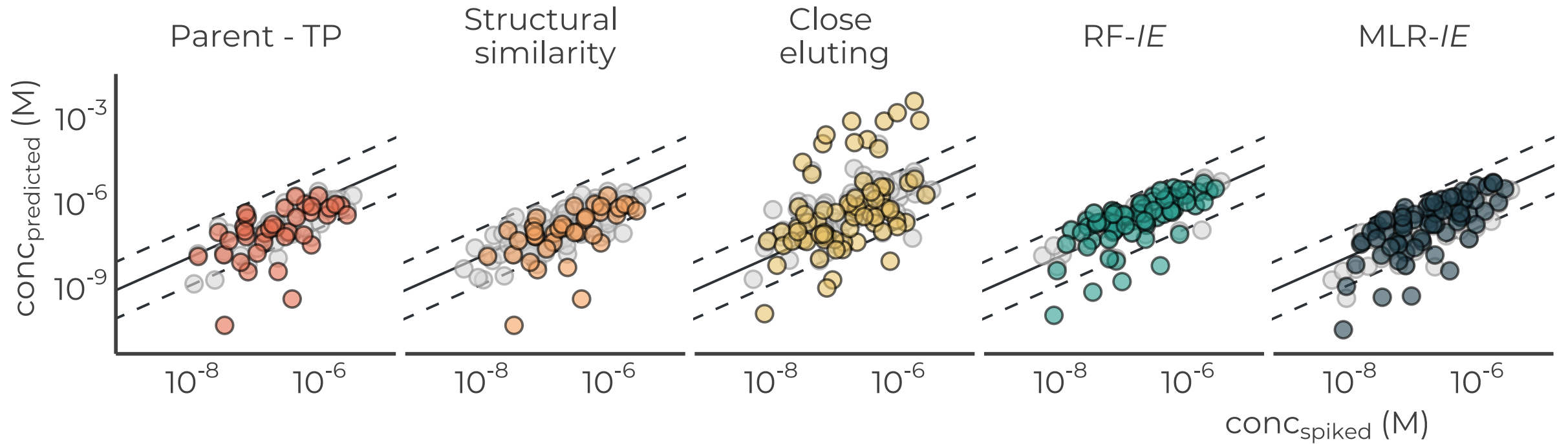
Correlation, reported

Lab 1



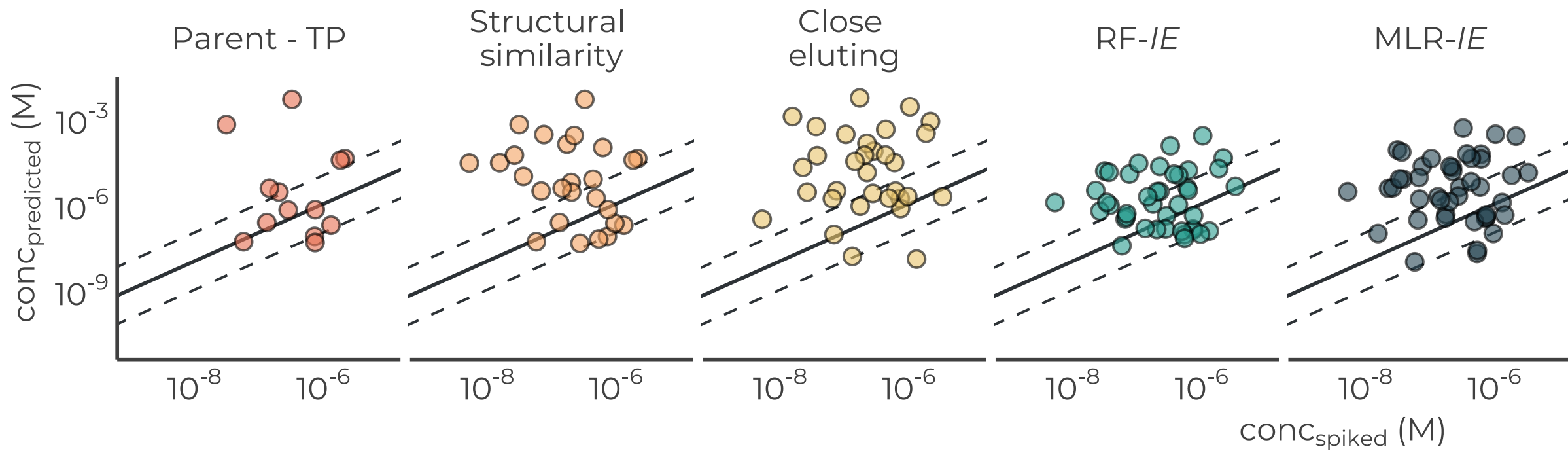
Correlation, reprocessed

Lab 1



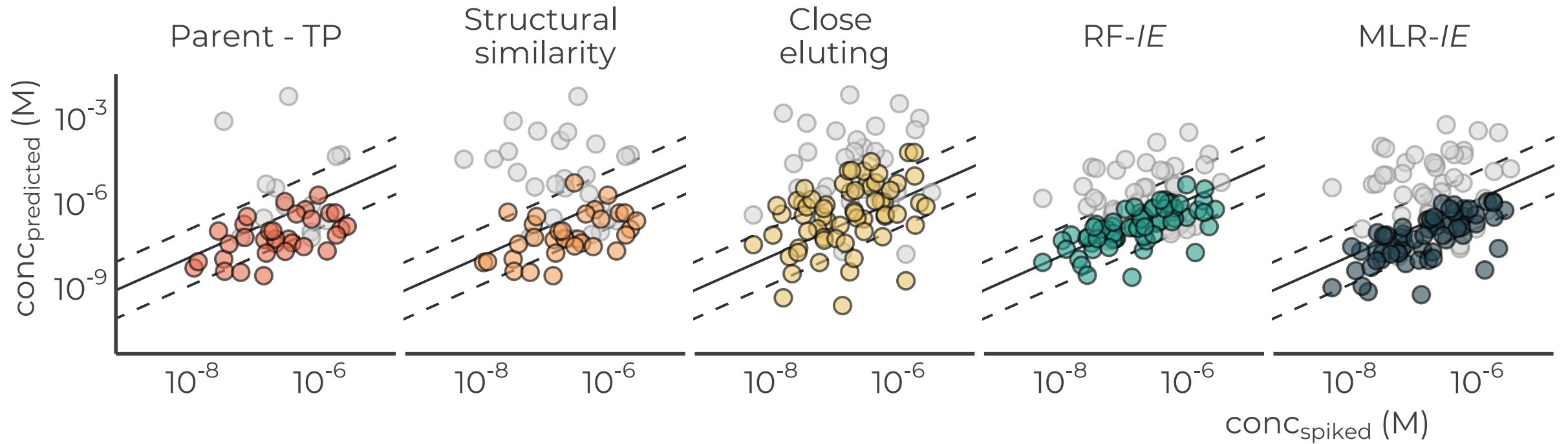
Correlation, reported

Lab 2



Correlation, reprocessed

Lab 2



Conclusions

Lowest prediction error for $1/E$ -based approaches

Conclusions

Lowest prediction error for $1/E$ -based approaches

Underprediction issue for most approaches

Conclusions

Lowest prediction error for $1/E$ -based approaches

Underprediction issue for most approaches

Importance of thorough quality assessment

Thank You!

All participants
NORMAN network

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Nikiforos Alygizakis & Kelsey Ng

Nikolaos Thomaidis & Anneli Kruve

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