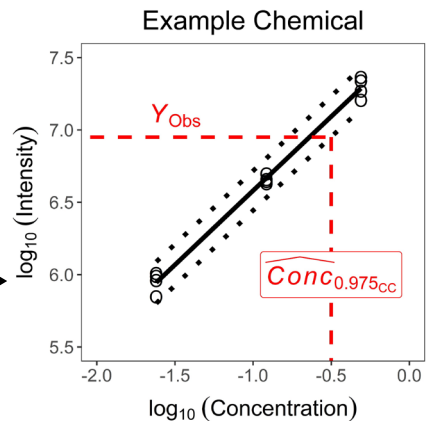


Substances Spiked in ENTACT Mixtures (n = 1269)

Correctly Identified Chemicals (n = 530 [+]; 237 [-])

Subset with Repeat Measures (n = 73 [+]; 10 [-])

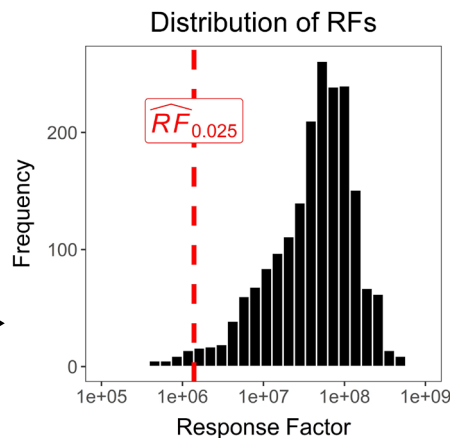
Inverse Prediction Using Calibration Curves (CC)



Given Y_{obs}

$$\widehat{\text{Conc}}_{0.975_{\text{CC}}}$$

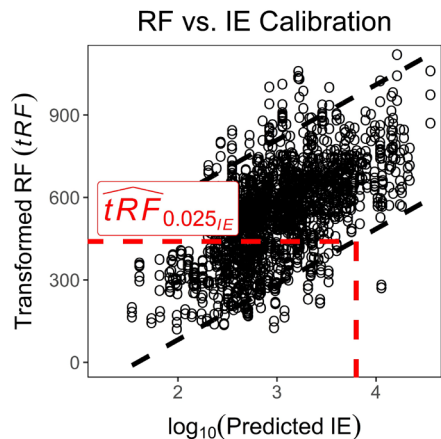
Inverse Prediction Using a Bounded Response Factor (RF)



Given Y_{obs}

$$Y_{\text{obs}} \div \widehat{\text{RF}}_{0.025} = \widehat{\text{Conc}}_{0.975_{\text{RF}}}$$

Inverse Prediction Using Ionization Efficiency (IE) Estimation



Given Y_{obs} and Predicted IE

$$Y_{\text{obs}} \div \widehat{\text{RF}}_{0.025_{\text{IE}}} = \widehat{\text{Conc}}_{0.975_{\text{IE}}}$$