Posterior predictive samples

- For model validation we can feed posterior samples into the ODE system
- Voilá : a set of posterior predictive samples
  - Given the set of modeling assumptions and data how would the pharmacokinetics evolve in time probabilistically
  - We can compare the predicted distribution to *validation* datasets!
- In addition, we can investigate the sensitivity of the model to the evolution of PFOS in time (e.g. using area-under-curve (AUC) performance metric and increasing the value of estimated parameters by 1%)

Predictive performance

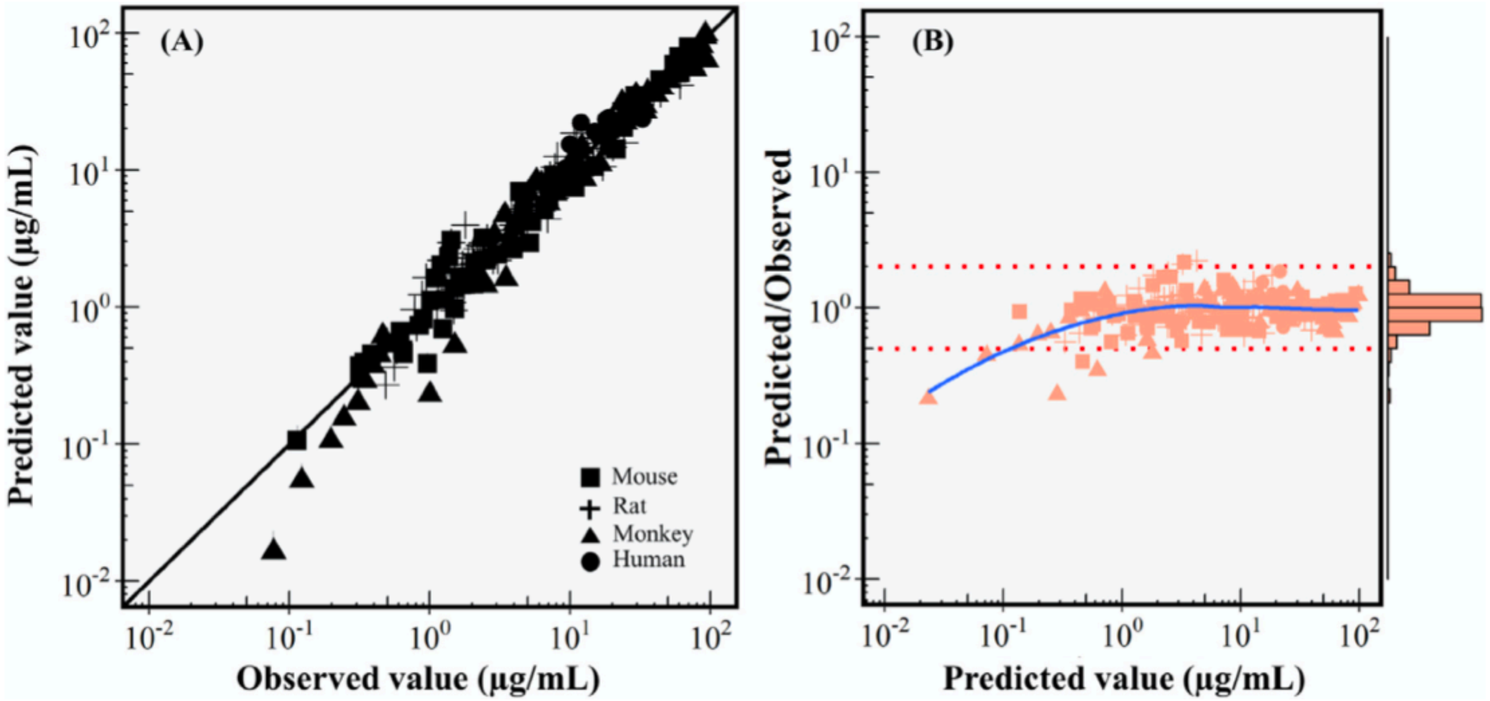

Fig. 4. Comparisons of model predictions (y-axis) with observed data (x-axis) with (A) global evaluation of goodness of model fit and (B) predicted-to-observed ratio versus model prediction plot. In plot (A), the different symbol shapes are used for different species, including the mouse (square), rat (cross), monkey (triangle) and human (round). The solid black diagonal line represents the unity line where the observed value and the predicted value are equal. In plot (B), the dashed line represents over a predicted-to-observed ratio of 2 or lower 0.5, and the blue line is the smoothed high order polynomial curve. The histogram of residuals is shown on the right of the panel. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)