



**Figure 1S: Normalised Predictive Distribution Error (NPDE)**

Top left: QQ-plot of the distribution of the NPDE vs. the theoretical  $N(0,1)$  distribution. Top right: Histogram of the distribution of the NPDE along with the density of the standard Gaussian distribution. Bottom left: NPDE vs. time. Bottom right: NPDE vs. population predicted concentrations. Dashed lines in the top graphs represent the 95% prediction intervals for the normal distribution. Dashed lines in the bottom graphs represent 10<sup>th</sup>; 50<sup>th</sup> and 90<sup>th</sup> percentiles of the NPDE corresponding to the observed data. Shaded areas represent the 95% prediction intervals for the 2.5, 50 and 97.5<sup>th</sup> percentiles. Red lines/shade depict the median, whereas blue lines/shade indicate the 2.5<sup>th</sup> and 97.5<sup>th</sup> quantiles of observed data. Blue dots represent the individual observed values.