

Supporting Information: Model diagnostics

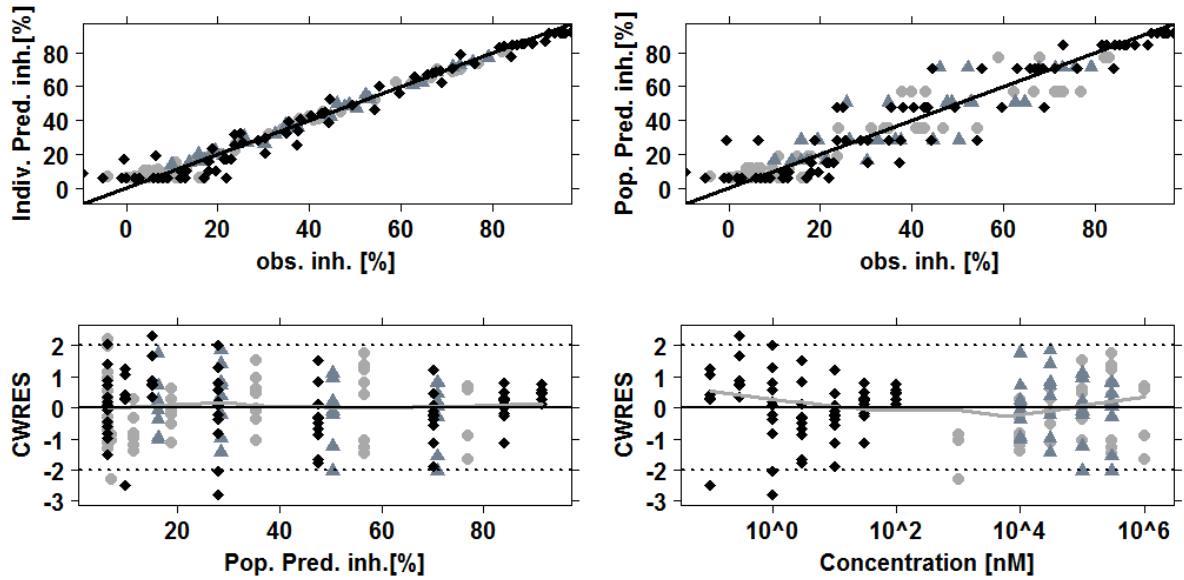


Figure S1: Goodness-of-fit plots. Upper panels show the individual (left) and population (right) predictions vs. observed inhibition in the whole cell patch clamp assay. Lower panels show the conditional weighted residuals vs. population predicted inhibition values (left) and drug concentration (right). Symbols indicate the different compounds, namely cisapride, sotalol and moxifloxacin.

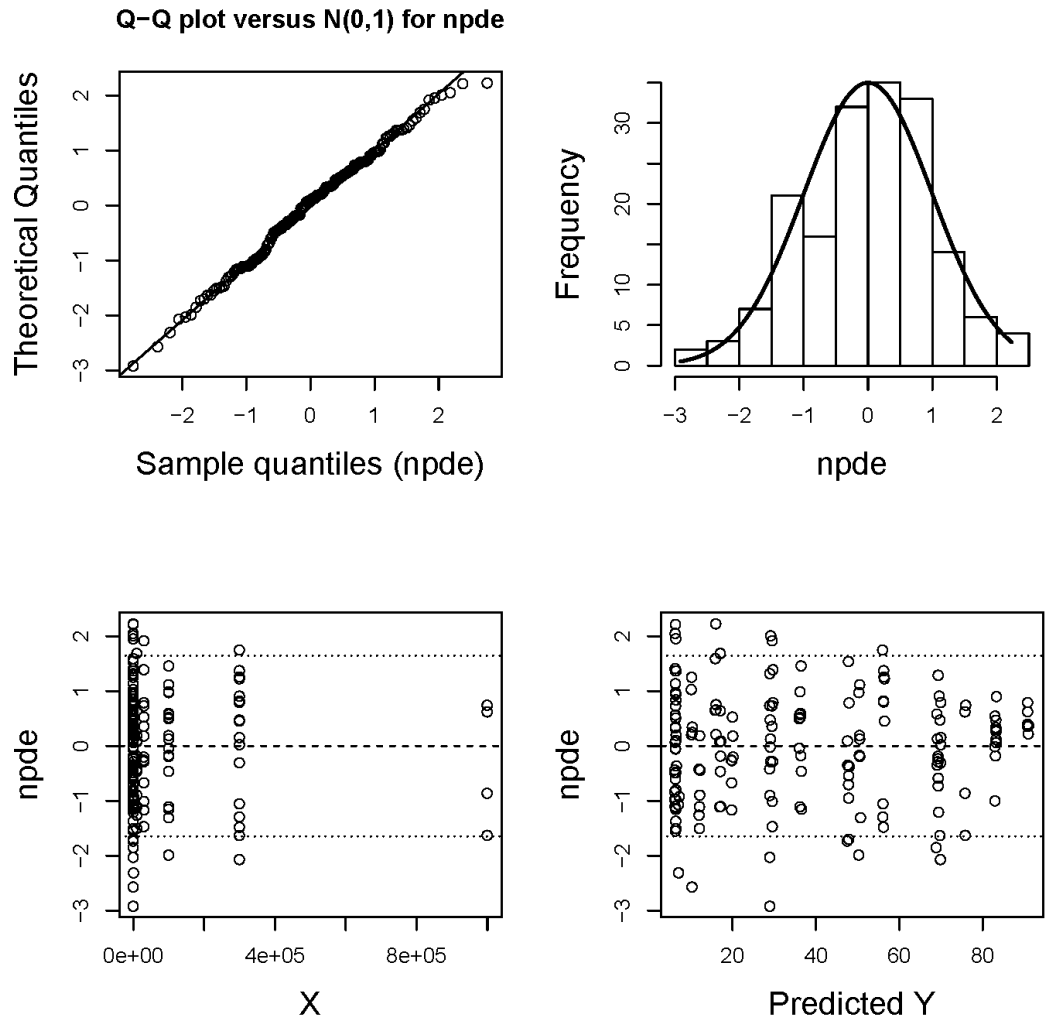


Figure 2S: NPDE summaries for the pharmacokinetic-pharmacodynamic model describing hERG inhibition in the whole cell patch clamp assay. Upper panels show the QQ-plot of the distribution of the NPDEs for a theoretical $N(0, 1)$ distribution (left) and the histogram of the distribution of the NPDE together with the density of the standard normal distribution (right). Lower panels show the NPDEs vs. concentrations (left) and NPDEs vs. individual predictions (right).