

Supplementary Figure S3

Supplement to:

Title: Machine learning and pharmacometrics for prediction of pharmacokinetic data: Differences, similarities and challenges illustrated with rifampicin

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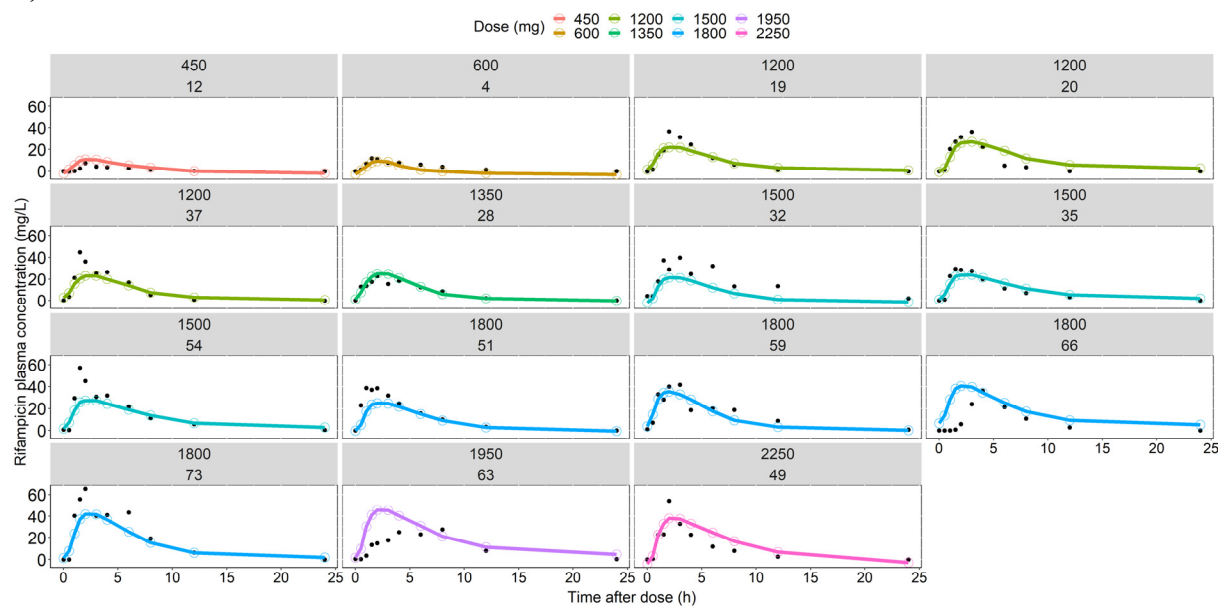
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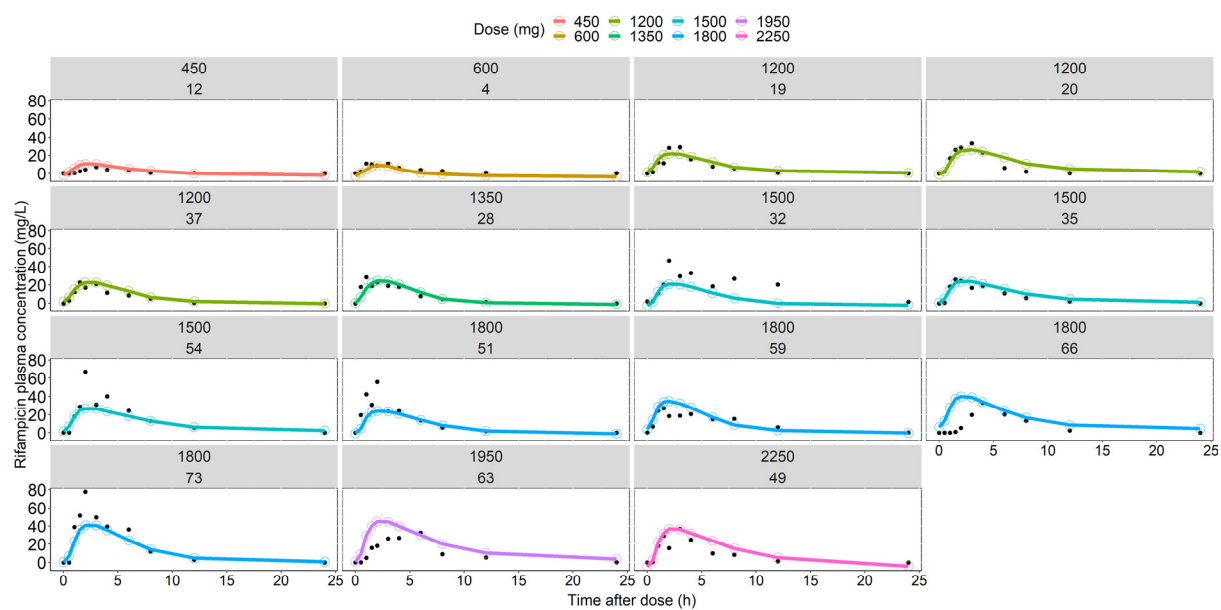
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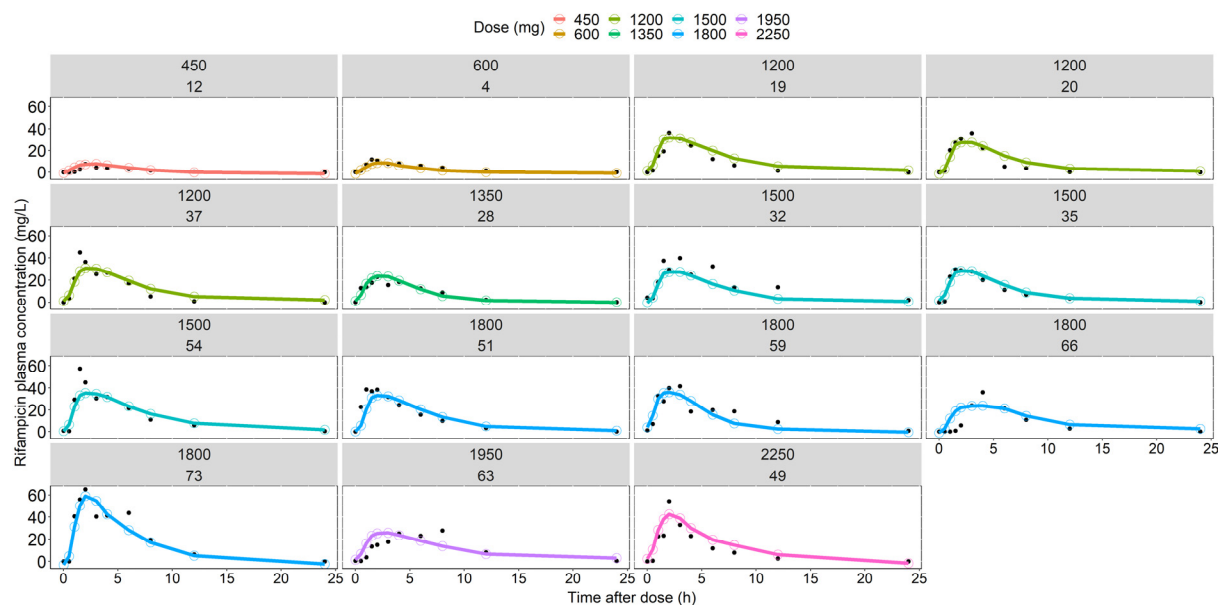
A)



B)



C)



D)

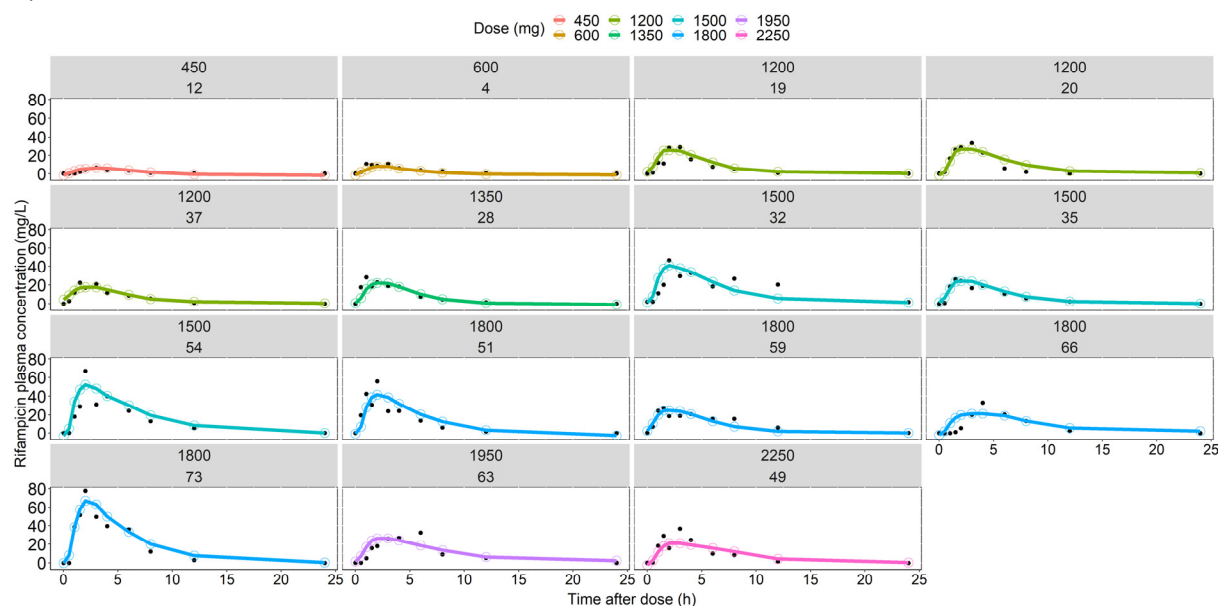


Figure S3. Individual rifampicin plasma concentrations predicted from the eXtreme Gradient Boosting (XGBoost) model (solid line and open circles) compared to the true concentrations (black closed circles). Panel A) represents the predictions for each individual in the test dataset at the first week of rifampicin treatment for scenario 1 (predictions based on features only). Panel B) represents the predictions for each individual in the test dataset at the second week of rifampicin treatment for scenario 1 (predictions based on features only). Panel C) represents the predictions for each individual in the test dataset at the first week of rifampicin treatment for scenario 2 (predictions based on features and 2 rifampicin plasma concentrations). Panel D) represents the predictions for each individual in the test dataset at the second week of rifampicin treatment for scenario 2 (predictions based on features and 2 rifampicin plasma concentrations). The different colors indicate the different daily rifampicin doses.