Supplementary Table S1

Supplement to:

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

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Table S1. Final model hyperparameters for the different machine learning models.

Algorithm	Hyperparameter	Hyperparameter interval	Hyperparameter values AUC models	Hyperparameter values longitudinal models
LASSO	Lambda	(5:20, steps = 1)	5	5
Random Forest	Mtry	(1:20, steps = 1)	6	9
Gradient Boosting Machine (GBM)	n.trees	(100, 150, 200, 250, 300, 350, 400)	350	200
	Interaction.depth	(1:18, steps = 1)	1	5
	Shrinkage	(0.01, 0.1, 0.9)	0.01	0.1
	n.minobsinnode	(0.005, 0.01, 0.1, 0.5, 1, 5, 10, 20)	0.01	5
Extreme Gradient Boosting (XGBoost)	Nrounds	(200:1000, steps = 50)	650	1000
	Eta	(0.005, 0.01, 0.015, 0.025, 0.05, 0.1)	0.005	0.01
	Max_depth	(1, 2, 3, 4, 5, 6, 10)	3	4
	Gamma	(0, 0.05, 0.1, 0.5, 0.7, 0.9, 1.0)	0.5	0.9
	Colsample_bytree	(0.4, 0.6, 0.8, 1)	1	0.8
	Min_child_weight	(1:20, steps = 1)	3	8
	Subsample	(0.1, 0.2, 0.5, 0.75, 1)	0. 2	0.5

Colsample_bytree, subsample ratio of columns when constructing each tree; *eta*, scales the contribution of each tree by a factor (between 0 an 1); *gamma*, minimum loss reduction required to make a further partition on a leaf node of the tree; *interaction.depth*, maximum depth of each tree; *max_depth*, maximum tree depth; *min_child_weight*, minimum number of instances needed in each node; *mtry*, number of variables randomly sampled as candidates at each split; *n-minobsinnode*, minimum number of observations in the terminal nodes of the trees; *nrounds*, maximum number of iterations; *n.trees*, total number of trees to fit; *shrinkage*, learning rate or step-size reduction; *subsample*, subsample ratio of the training data used priot to growing trees.