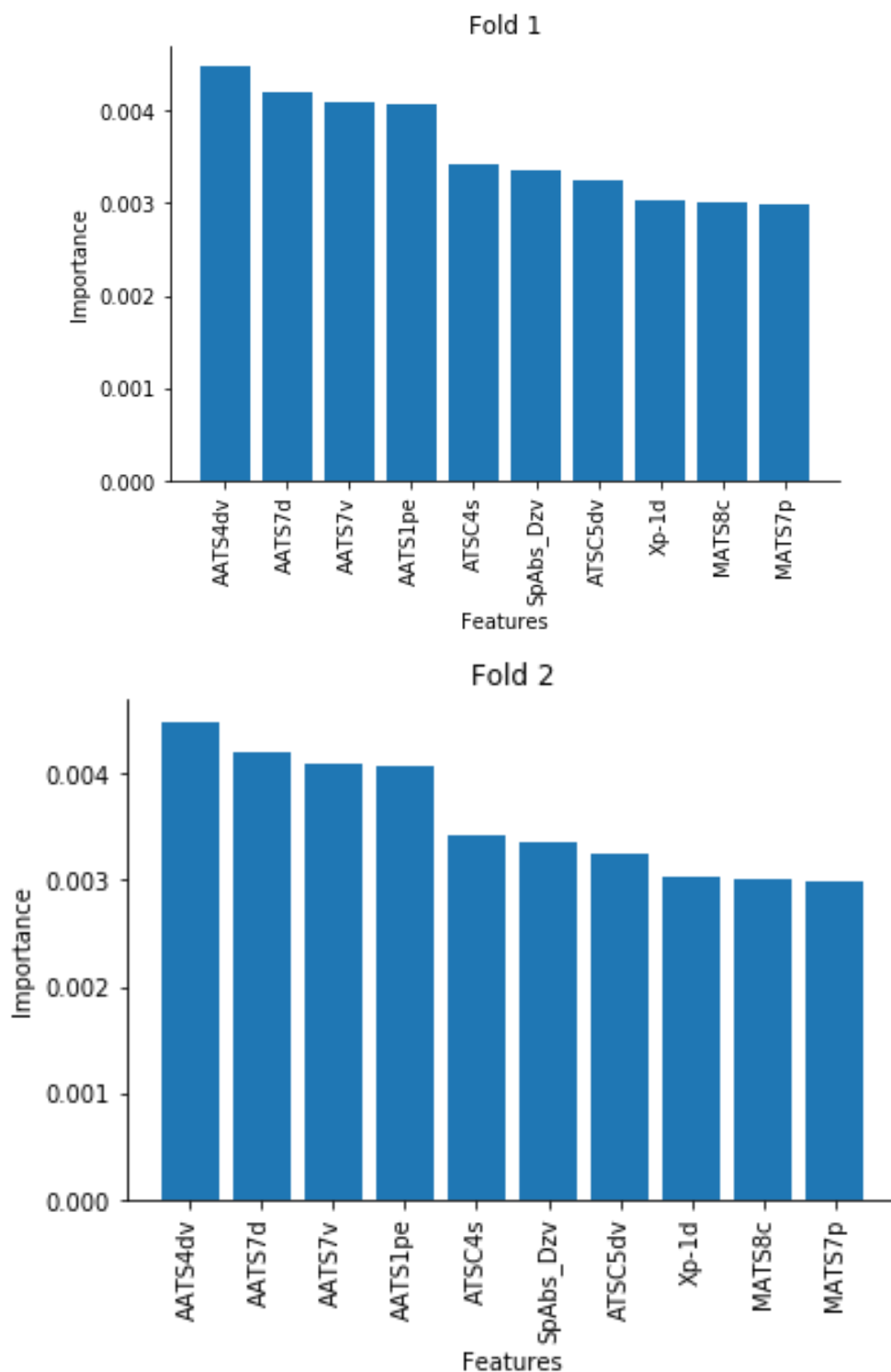
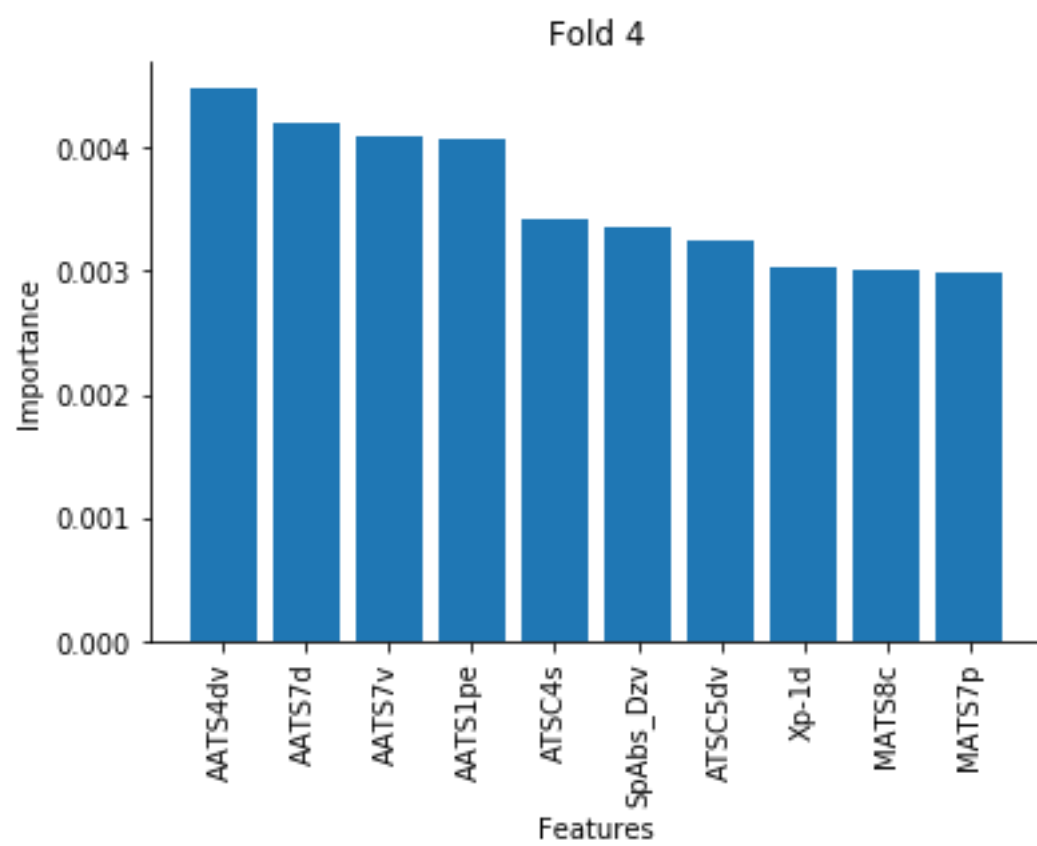
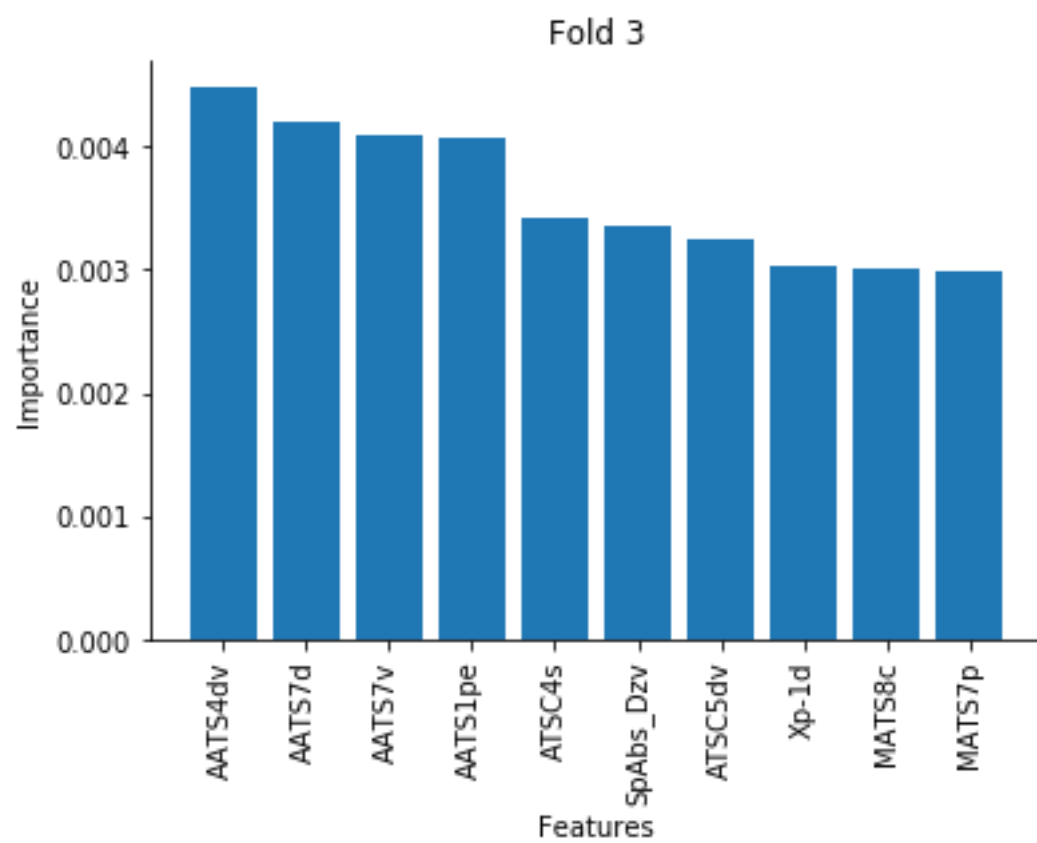


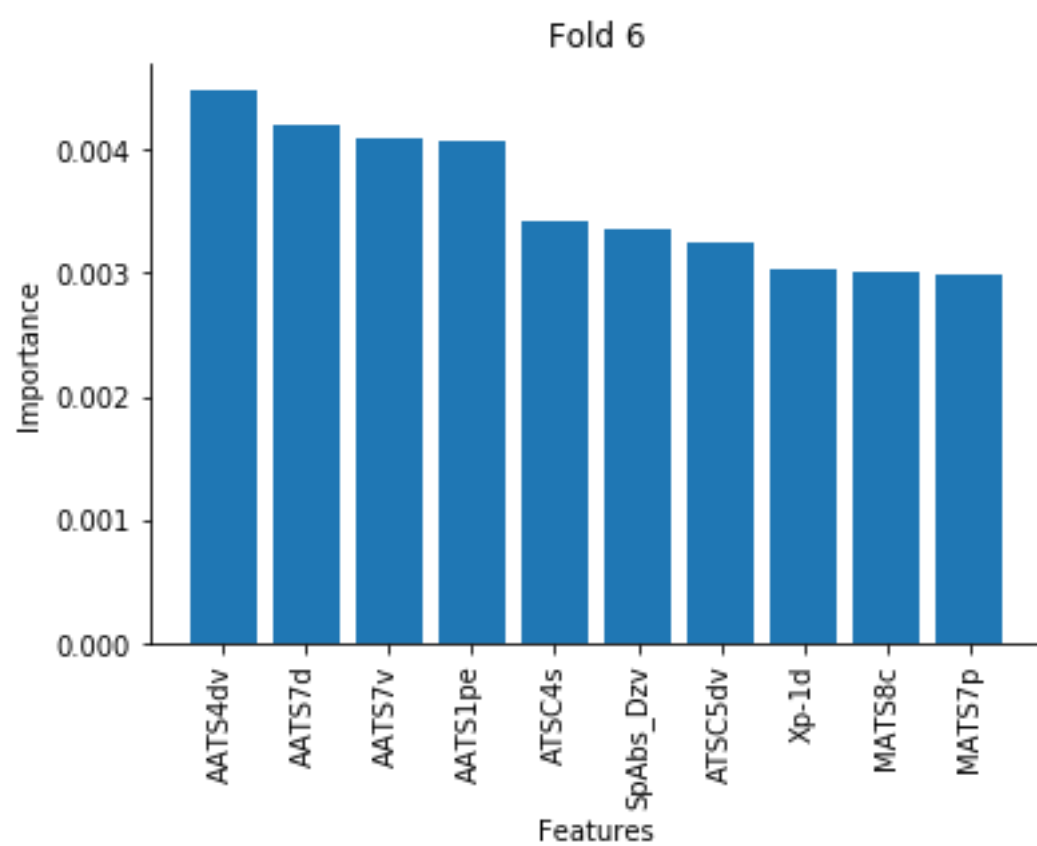
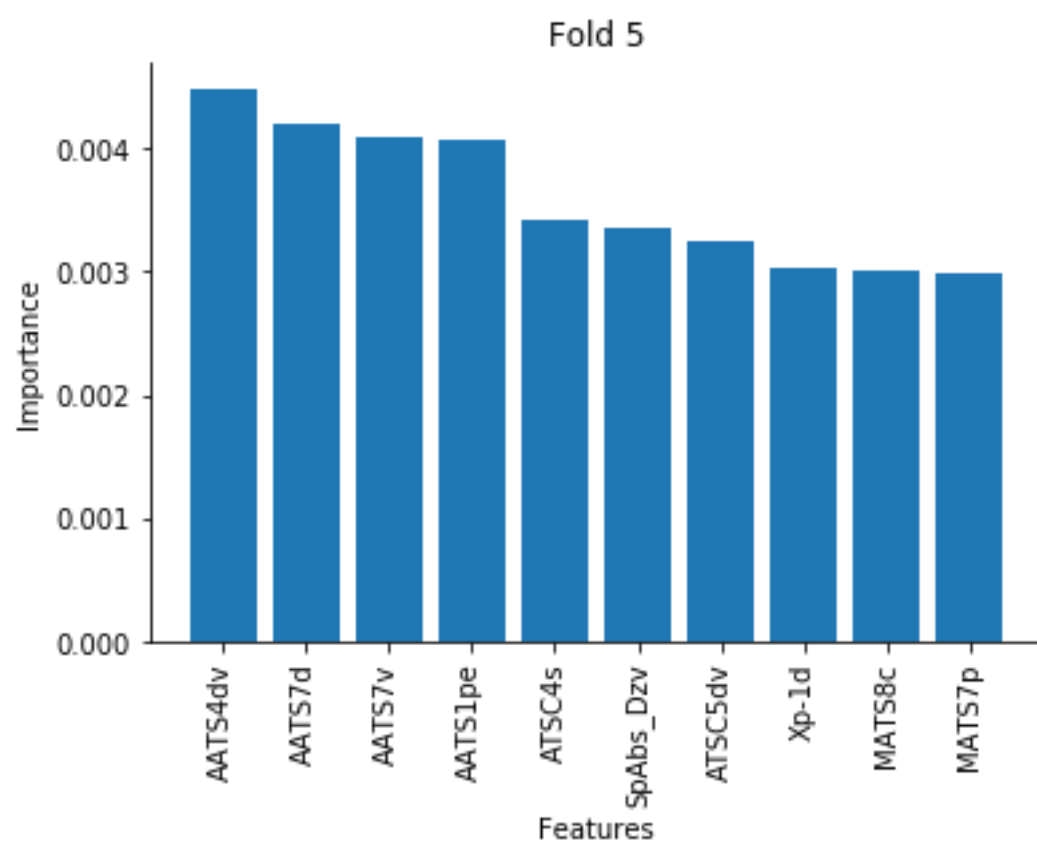
Supplementary Materials: Machine Learning Uncovers Adverse Drug Effects on Intestinal Bacteria

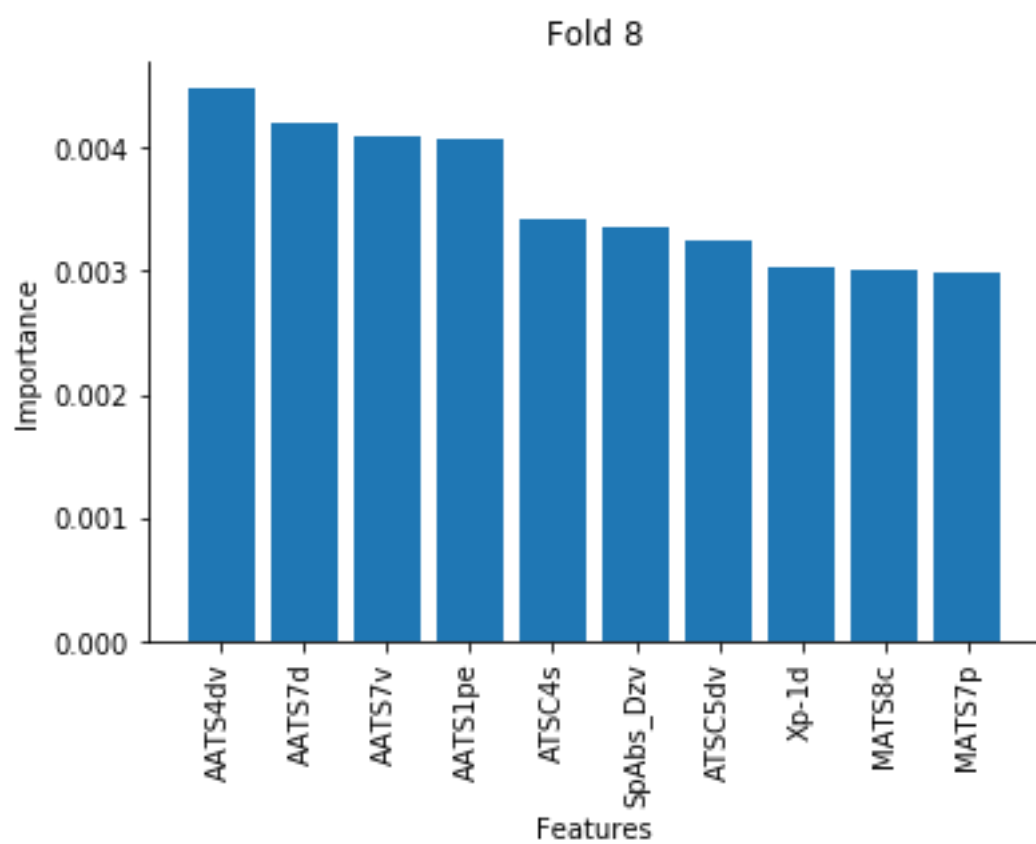
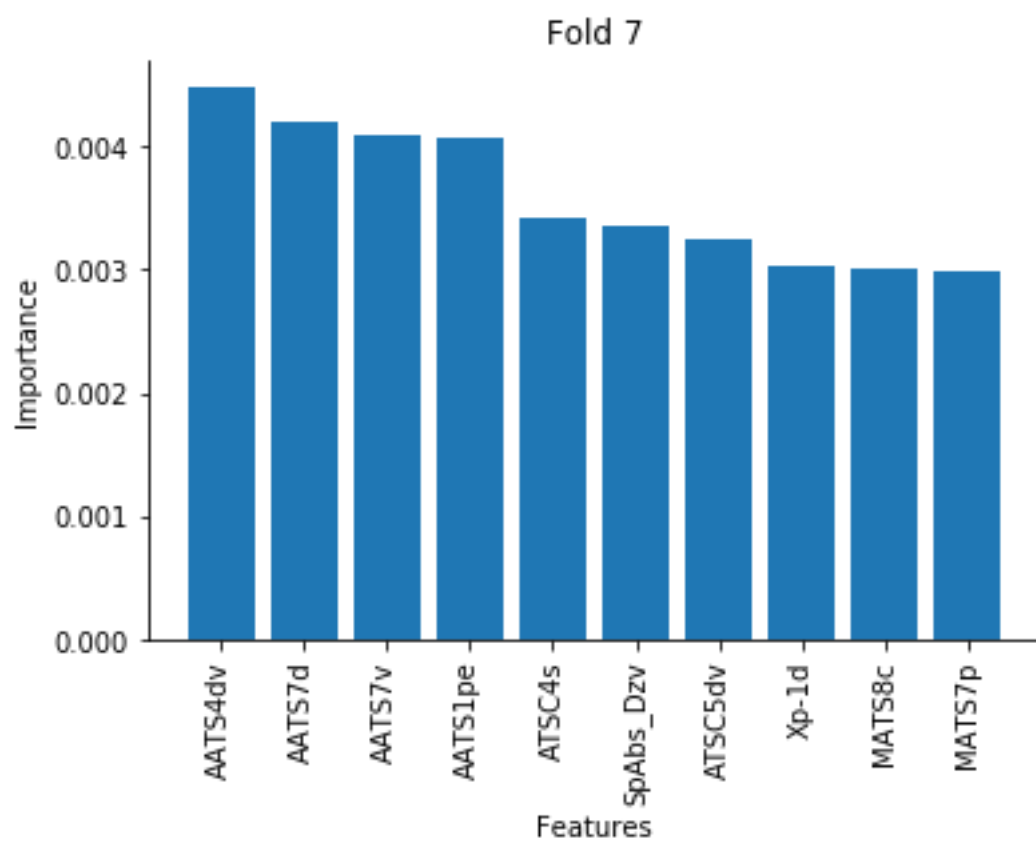
Laura E. McCoubrey, Moe Elbadawi, Mine Orlu, Simon Gaisford and Abdul W. Basit

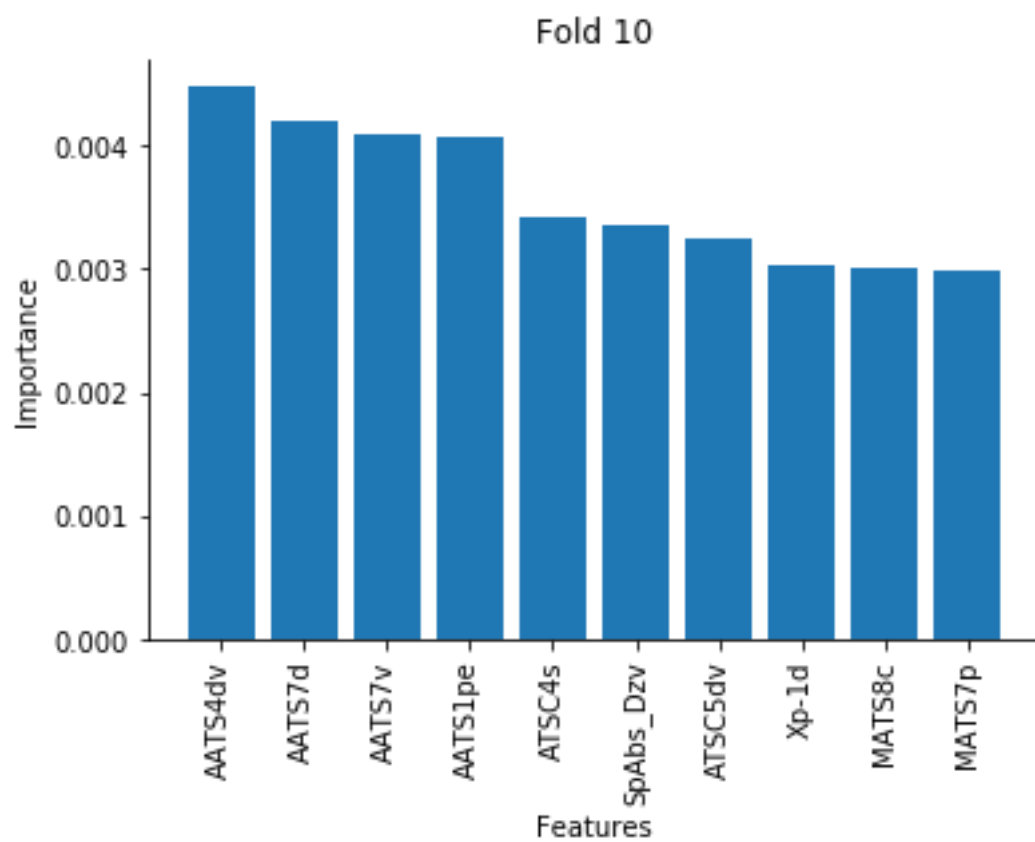
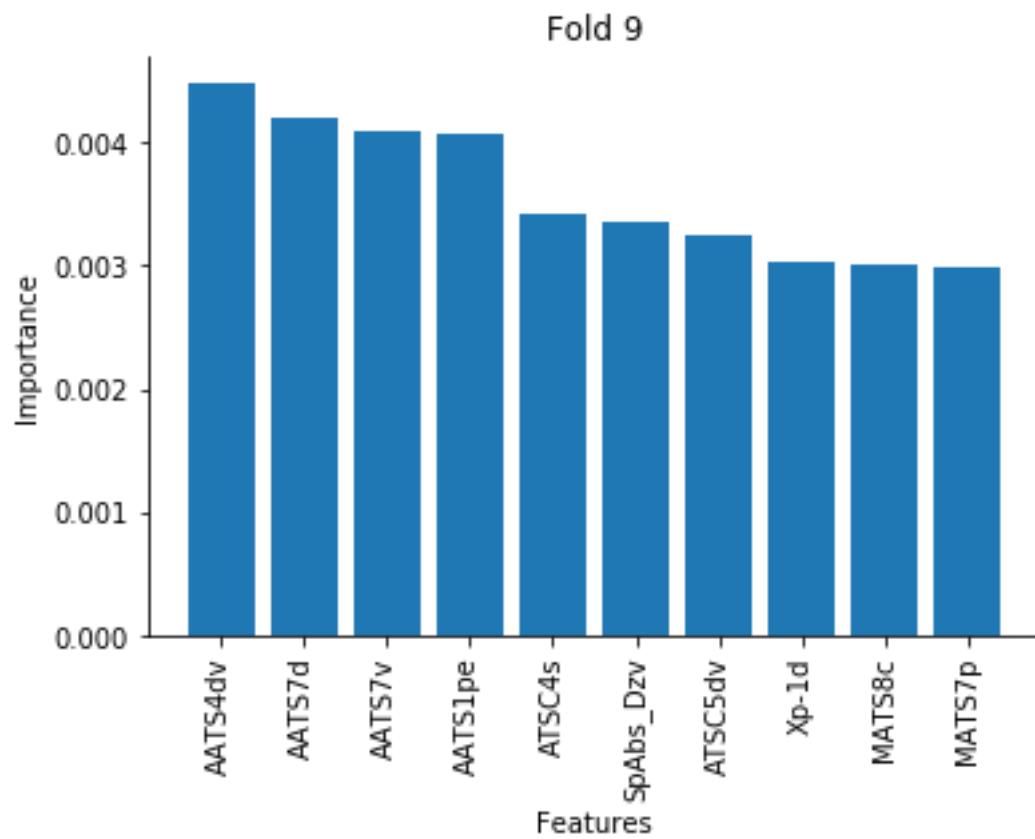
Feature Importance for Each Cross-Validation Fold of the Final Model











Performance Metrics at Labelling Threshold of $p < 0.01$

Table S1. All models are baseline models (random state = 0) without hyperparameter tuning.

Extra trees	0.866 AUROC with a standard deviation of 0.013
	0.584 recall_weighted with a standard deviation of 0.074
	0.793 precision_weighted with a standard deviation of 0.048
	0.663 f1_weighted with a standard deviation of 0.049
Random forest	0.859 AUROC with a standard deviation of 0.016
	0.541 recall_weighted with a standard deviation of 0.072
	0.790 precision_weighted with a standard deviation of 0.057
	0.630 f1_weighted with a standard deviation of 0.055
K-nearest neighbours	0.796 AUROC with a standard deviation of 0.014
	0.553 recall_weighted with a standard deviation of 0.043
	0.671 precision_weighted with a standard deviation of 0.053
	0.600 f1_weighted with a standard deviation of 0.030
MLP	0.838 AUROC with a standard deviation of 0.019
	0.654 recall_weighted with a standard deviation of 0.042
	0.686 precision_weighted with a standard deviation of 0.038
	0.665 f1_weighted with a standard deviation of 0.029
Decision trees	0.698 AUROC with a standard deviation of 0.029
	0.592 recall_weighted with a standard deviation of 0.039
	0.589 precision_weighted with a standard deviation of 0.066
	0.586 f1_weighted with a standard deviation of 0.045
Support vector machines	0.846 AUROC with a standard deviation of 0.012
	0.488 recall_weighted with a standard deviation of 0.077
	0.832 precision_weighted with a standard deviation of 0.049
	0.603 f1_weighted with a standard deviation of 0.058
Gradient boosting	0.847 AUROC with a standard deviation of 0.012
	0.596 recall_weighted with a standard deviation of 0.050
	0.738 precision_weighted with a standard deviation of 0.047
	0.652 f1_weighted with a standard deviation of 0.034
Logistic regression	0.809 AUROC with a standard deviation of 0.020
	0.650 recall_weighted with a standard deviation of 0.032
	0.646 precision_weighted with a standard deviation of 0.043
	0.643 f1_weighted with a standard deviation of 0.029
Logistic regression CV	0.824 AUROC with a standard deviation of 0.017
	0.577 recall_weighted with a standard deviation of 0.049
	0.699 precision_weighted with a standard deviation of 0.050
	0.623 f1_weighted with a standard deviation of 0.031
Gaussian process	0.703 AUROC with a standard deviation of 0.100
	0.575 recall_weighted with a standard deviation of 0.112
	0.656 precision_weighted with a standard deviation of 0.077
	0.602 f1_weighted with a standard deviation of 0.086
Stochastic gradient descent	0.793 AUROC with a standard deviation of 0.020
	0.571 recall_weighted with a standard deviation of 0.045
	0.644 precision_weighted with a standard deviation of 0.039
	0.600 f1_weighted with a standard deviation of 0.032
Perceptron	0.777 AUROC with a standard deviation of 0.017
	0.684 recall_weighted with a standard deviation of 0.030
	0.563 precision_weighted with a standard deviation of 0.033
	0.613 f1_weighted with a standard deviation of 0.024
Passive aggressive	0.794 AUROC with a standard deviation of 0.017
	0.695 recall_weighted with a standard deviation of 0.029
	0.590 precision_weighted with a standard deviation of 0.038
	0.634 f1_weighted with a standard deviation of 0.028

Performance Metrics at Labelling Threshold of $p < 0.005$

Table S2. All models are baseline models (random state = 0) without hyperparameter tuning.

Extra trees	0.870 AUROC with a standard deviation of 0.015
	0.571 recall_weighted with a standard deviation of 0.081
	0.790 precision_weighted with a standard deviation of 0.049
	0.654 f1_weighted with a standard deviation of 0.061
Random forest	0.864 AUROC with a standard deviation of 0.017
	0.533 recall_weighted with a standard deviation of 0.080
	0.786 precision_weighted with a standard deviation of 0.056
	0.623 f1_weighted with a standard deviation of 0.061
K-nearest neighbours	0.801 AUROC with a standard deviation of 0.017
	0.547 recall_weighted with a standard deviation of 0.041
	0.668 precision_weighted with a standard deviation of 0.057
	0.595 f1_weighted with a standard deviation of 0.031
MLP	0.839 AUROC with a standard deviation of 0.018
	0.646 recall_weighted with a standard deviation of 0.045
	0.680 precision_weighted with a standard deviation of 0.037
	0.658 f1_weighted with a standard deviation of 0.032
Decision trees	0.699 AUROC with a standard deviation of 0.029
	0.600 recall_weighted with a standard deviation of 0.055
	0.563 precision_weighted with a standard deviation of 0.052
	0.576 f1_weighted with a standard deviation of 0.039
Support vector machines	0.851 AUROC with a standard deviation of 0.013
	0.480 recall_weighted with a standard deviation of 0.079
	0.833 precision_weighted with a standard deviation of 0.047
	0.597 f1_weighted with a standard deviation of 0.062
Gradient boosting	0.849 AUROC with a standard deviation of 0.012
	0.587 recall_weighted with a standard deviation of 0.052
	0.731 precision_weighted with a standard deviation of 0.048
	0.644 f1_weighted with a standard deviation of 0.038
Logistic regression	0.812 AUROC with a standard deviation of 0.020
	0.643 recall_weighted with a standard deviation of 0.040
	0.636 precision_weighted with a standard deviation of 0.043
	0.635 f1_weighted with a standard deviation of 0.034
Logistic regression CV	0.829 AUROC with a standard deviation of 0.016
	0.568 recall_weighted with a standard deviation of 0.047
	0.693 precision_weighted with a standard deviation of 0.048
	0.615 f1_weighted with a standard deviation of 0.032
Gaussian process	0.711 AUROC with a standard deviation of 0.106
	0.567 recall_weighted with a standard deviation of 0.115
	0.645 precision_weighted with a standard deviation of 0.093
	0.594 f1_weighted with a standard deviation of 0.093
Stochastic gradient descent	0.799 AUROC with a standard deviation of 0.022
	0.567 recall_weighted with a standard deviation of 0.050
	0.635 precision_weighted with a standard deviation of 0.037
	0.593 f1_weighted with a standard deviation of 0.035
Perceptron	0.778 AUROC with a standard deviation of 0.016
	0.683 recall_weighted with a standard deviation of 0.030
	0.548 precision_weighted with a standard deviation of 0.036
	0.603 f1_weighted with a standard deviation of 0.027
Passive aggressive	0.795 AUROC with a standard deviation of 0.016
	0.695 recall_weighted with a standard deviation of 0.031
	0.575 precision_weighted with a standard deviation of 0.041
	0.625 f1_weighted with a standard deviation of 0.031