

Neural Network Similarity: A New Measure to Assist Decision Making in Chemical Toxicology

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Links to source code and models generated

Python 3 code for fingerprint generation, chemical clustering, model construction, and model recall and network similarity calculation, as well as data used for training and testing the models and model files for optimized models can be found in GitHub (https://github.com/teha2/chemical_toxicology) and in the University of Cambridge repository (<https://doi.org/10.17863/CAM.50429>).

DNN Model Details

The cost function used in DNN training was sparse categorical cross-entropy including class weights to allow for binary classification with an imbalanced data set. The Adam optimizer was used to provide efficient model training. L2 regularization was added to the cost function to prevent overfitting.

A multi-class multi-label predictor was considered for this task, incorporating several biological targets into a single network. This dataset would have contained many “unknown” labels (cases where a compound was tested against one target but not against others) leaving holes in the dataset that caused difficulty in training and evaluation. As a result of this, several binary classification networks were pursued, each predicting the activity at a single biological target without the requirement for any “unknown” data labels.

Hyperparameters.

The learning rate was adjusted on a case by case basis to give a smooth training curve and fast gradient descent. The regularization rate for L2 regularization was adjusted to prevent a large gap between the statistical performance values of the training and validation data. In addition, early stopping was used to prevent overfitting, by reducing the number of training iterations while maintaining a smooth training curve.

Performance Statistics.

Values provided in the output layer of each of the DNNs were interpreted using the Argmax and Softmax functions, yielding binary predictions of molecular activity and probability of positive activity respectively. The Argmax function yielded numbers of true positives (chemical predicted positive, experimentally positive, TP), false positives (chemical predicted positive, experimentally negative, FP), true negatives (chemical predicted negative, experimentally negative, TN) and false negatives (chemical predicted negative, experimentally positive FN). These values were used to calculate evaluation statistics on the training and test sets, including sensitivity (SE), specificity (SP), accuracy (ACC) and Matthews correlation coefficient.

$$SE = \frac{TP}{TP + FN}$$

$$SP = \frac{TN}{TN + FP}$$

$$ACC = \frac{TP + TN}{TP + TN + FP + FN}$$

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

The SE, SP and ACC give percentages based on the number of positives, negatives and molecules correctly assigned respectively. The MCC gives a value between -1 and +1 and removes bias in the available data. An MCC value of +1 is obtained if every prediction is correct, a value of -1 if every prediction is incorrect, and 0 if predictions are random.

The positive probability values generated using the Softmax function allow for the plotting of a receiver operating curve (ROC) and the calculation of the area under this curve (ROC-AUC). This value can be between 0 and 1 and represents the probability that an experimentally positive compound is given a higher positive probability than an experimentally negative one. Higher SE, SP, ACC, MCC and ROC-AUC values are associated with better predictive models.

For each network architecture, for each biological target five networks were produced, changing the chemical cluster used in the test set and randomizing the training/validation shuffle and split seeding values to provide five-fold clustered cross-validation. The performance on each of the training, validation and test sets were then averaged to prevent any single cluster affecting the overall results.

The highest performing networks provide optimized predictive models for use in safety evaluation. These models are provided via GitHub (https://github.com/teha2/chemical_toxicology) and in the University of Cambridge repository (<https://doi.org/10.17863/CAM.50429>).

Initial investigations into fingerprints and activation functions

[10]		Training				Test				
Fingerprint	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
MACCS	86.7	76.7	85.6	0.673	0.89	85.9	74.3	85.1	0.648	0.87
ECFP6 1000	88.0	82.4	88.7	0.743	0.92	87.5	81.3	87.9	0.728	0.90
ECFP6 5000	89.0	85.4	90.1	0.775	0.94	88.1	83.8	89.0	0.750	0.92
ECFP6 10000	89.4	81.8	89.0	0.754	0.93	87.7	79.0	87.1	0.708	0.90
ECFP4 1000	87.7	83.4	89.0	0.749	0.93	86.7	80.6	87.2	0.708	0.91
ECFP4 5000	87.9	88.0	90.7	0.788	0.94	85.9	84.6	88.2	0.732	0.91
ECFP4 10000	88.5	87.2	90.5	0.785	0.94	87.1	85.9	89.6	0.760	0.92
ECFP4 20000	89.3	87.0	90.8	0.791	0.94	86.3	82.6	87.9	0.726	0.91

[10,10]		Training				Test				
Fingerprint	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
MACCS	87.1	74.6	85.4	0.666	0.88	81.8	74.4	79.6	0.593	0.88
ECFP6 1000	88.0	84.7	89.3	0.756	0.93	86.2	83.4	87.7	0.722	0.92
ECFP6 5000	88.5	90.4	91.6	0.811	0.95	86.4	86.3	89.1	0.750	0.92
ECFP6 10000	88.4	88.3	91.3	0.800	0.95	85.8	84.6	88.7	0.739	0.92
ECFP4 1000	88.3	86.9	89.9	0.770	0.94	86.6	82.6	87.5	0.715	0.91
ECFP4 5000	88.5	90.8	92.2	0.820	0.96	85.9	85.0	88.6	0.740	0.92
ECFP4 10000	89.4	89.4	91.9	0.814	0.95	86.4	85.5	88.9	0.747	0.92
ECFP4 20000	89.2	86.4	90.7	0.789	0.94	87.7	82.2	88.0	0.735	0.91

[10,10,10]		Training				Test				
Fingerprint	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
MACCS	86.7	81.9	87.5	0.715	0.90	85.6	81.6	86.9	0.701	0.89
ECFP6 1000	92.3	96.3	95.4	0.897	0.98	84.8	86.0	87.6	0.722	0.91
ECFP6 5000	96.1	98.5	98.2	0.957	1.00	87.4	86.7	89.1	0.756	0.92
ECFP6 10000	98.9	99.4	99.3	0.985	1.00	88.4	86.2	89.2	0.757	0.93
ECFP4 1000	93.0	95.8	95.7	0.903	0.98	86.8	85.4	88.3	0.730	0.91
ECFP4 5000	98.9	99.5	99.4	0.987	1.00	86.8	84.9	87.7	0.723	0.92
ECFP4 10000	99.1	99.6	99.5	0.988	1.00	87.8	87.2	89.1	0.752	0.92
ECFP4 20000	98.4	99.7	99.3	0.984	1.00	86.4	89.4	89.8	0.771	0.93

Table S1. A summary of the results shown in Table S2 comparing the model performance of several chemical fingerprints across three network architectures and five biological targets. Highest accuracy (ACC) Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC) values are highlighted in red. ECFP4 at length 10000 was chosen as the best performing fingerprint across the single

layer [10] and two layer [10,10] networks of 10 neurons, and three-layer networks [10,10,10] were dropped from further investigation due to high levels of overfitting.

MACCS Keys**Training Data****Test Data**

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]	ADORA2A	98.2	85.9	93.9	0.865	0.97	97.8	85.7	93.6	0.858	0.97
	hERG	88.1	51.5	73.4	0.434	0.79	89.3	49.4	73.7	0.432	0.75
	AR	60.7	96.0	86.5	0.638	0.86	57.2	95.7	85.9	0.602	0.84
	AChE	87.8	68.4	79.4	0.579	0.86	86.4	67.4	78.6	0.552	0.85
	SERT	98.7	81.6	94.9	0.849	0.97	98.8	73.3	93.5	0.795	0.95
	avg	86.7	76.7	85.6	0.673	0.89	85.9	74.3	85.1	0.648	0.87
		Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC
[10,10]	ADORA2A	97.9	87.6	94.4	0.874	0.97	97.6	87.1	93.8	0.865	0.96
	hERG	94.9	35.4	71.2	0.394	0.75	64.2	37.8	42.6	0.016	0.75
	AR	57.3	96.5	86.1	0.621	0.85	61.3	96.6	87.1	0.655	0.86
	AChE	86.7	71.1	80.0	0.589	0.86	86.7	69.5	79.3	0.574	0.86
	SERT	98.7	82.6	95.2	0.854	0.97	99.2	81.0	95.1	0.856	0.97
	avg	87.1	74.6	85.4	0.666	0.88	81.8	74.4	79.6	0.593	0.88
		Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC
[10,10,10]	ADORA2A	97.9	89.5	95.0	0.889	0.98	97.9	89.6	95.0	0.889	0.98
	hERG	87.7	57.0	75.5	0.476	0.81	87.3	60.8	77.4	0.505	0.79
	AR	63.2	97.0	88.1	0.677	0.87	60.7	97.0	87.0	0.660	0.86

AChE	86.4	77.2	82.5	0.641	0.85	84.3	72.1	79.0	0.569	0.85
SERT	98.5	88.9	96.4	0.892	0.98	98.0	88.5	95.9	0.880	0.97
avg	86.7	81.9	87.5	0.715	0.90	85.6	81.6	86.9	0.701	0.89

ECFP6 1000

Training Data

Test Data

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]	ADORA2A	97.9	90.3	95.3	0.894	0.98	98.4	86.8	94.3	0.875	0.97
	hERG	92.9	50.7	76.2	0.498	0.84	91.1	48.9	74.0	0.453	0.81
	AR	62.4	98.5	88.9	0.705	0.88	61.3	98.4	88.5	0.694	0.87
	AChE	87.9	84.8	86.6	0.726	0.93	87.9	84.8	86.6	0.726	0.90
	SERT	98.8	87.7	96.3	0.892	0.99	98.8	87.7	96.3	0.892	0.97
	avg	88.0	82.4	88.7	0.743	0.92	87.5	81.3	87.9	0.728	0.90

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10]	ADORA2A	97.7	91.7	95.6	0.903	0.98	97.6	91.1	95.4	0.897	0.98
	hERG	89.7	64.6	79.9	0.570	0.88	87.8	61.1	76.6	0.514	0.88
	AR	65.4	98.0	89.4	0.716	0.88	62.5	97.5	88.0	0.683	0.86
	AChE	88.4	80.1	84.8	0.690	0.92	85.5	79.6	83.0	0.652	0.90
	SERT	98.8	89.3	96.7	0.902	0.99	97.6	87.6	95.5	0.865	0.99
	avg	88.0	84.7	89.3	0.756	0.93	86.2	83.4	87.7	0.722	0.92

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10,10]	ADORA2A	99.4	98.5	99.0	0.979	1.00	96.4	92.2	95.0	0.889	0.98

hERG	90.6	90.5	90.6	0.805	0.96	77.8	72.6	75.7	0.500	0.83
AR	76.6	98.8	93.0	0.815	0.93	66.7	95.2	87.5	0.669	0.85
AChE	94.9	94.3	94.7	0.892	0.99	84.9	85.3	85.1	0.697	0.90
SERT	99.9	99.4	99.8	0.993	1.00	98.1	84.6	95.0	0.855	0.97
avg	92.3	96.3	95.4	0.897	0.98	84.8	86.0	87.6	0.722	0.91

ECFP6 5000

Training Data

Test Data

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]	ADORA2A	97.9	95.9	97.2	0.938	0.99	97.4	91.0	95.2	0.894	0.99
	hERG	89.7	63.3	79.2	0.560	0.87	87.9	59.3	76.7	0.500	0.83
	AR	69.9	99.3	91.5	0.778	0.93	67.4	98.8	90.2	0.748	0.87
	AChE	88.2	85.5	87.0	0.736	0.94	88.8	83.9	86.7	0.729	0.92
	SERT	99.0	83.1	95.5	0.866	0.99	98.8	85.9	96.0	0.880	0.98
	avg	89.0	85.4	90.1	0.775	0.94	88.1	83.8	89.0	0.750	0.92

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10]	ADORA2A	97.5	91.3	95.4	0.897	0.99	97.6	92.1	95.7	0.904	0.98
	hERG	88.1	82.9	86.0	0.709	0.93	83.2	71.2	78.6	0.545	0.86
	AR	69.8	99.0	91.3	0.771	0.91	65.6	98.2	89.4	0.721	0.86
	AChE	87.9	89.5	88.6	0.770	0.95	87.3	85.9	86.7	0.730	0.93
	SERT	98.9	89.5	96.9	0.907	0.99	98.1	84.1	95.0	0.852	0.98
	avg	88.5	90.4	91.6	0.811	0.95	86.4	86.3	89.1	0.750	0.92

Model	SE	SP	ACC	MCC	ROC-	SE	SP	ACC	MCC	ROC-
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						AUC					AUC
[10,10,10]	ADORA2A	99.7	98.9	99.4	0.987	1.00	96.7	92.3	95.2	0.893	0.98
	hERG	98.5	96.6	97.8	0.953	1.00	83.4	70.4	78.1	0.542	0.85
	AR	83.1	99.8	95.4	0.881	0.98	69.9	96.6	89.4	0.721	0.87
	AChE	99.3	98.9	99.2	0.983	1.00	88.6	82.4	85.9	0.712	0.92
	SERT	99.7	98.4	99.4	0.982	1.00	98.5	91.7	96.9	0.913	0.99
	avg	96.1	98.5	98.2	0.957	1.00	87.4	86.7	89.1	0.756	0.92

ECFP 10000

Training Data

Test Data

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]	ADORA2A	97.6	91.7	95.5	0.901	0.99	96.4	91.9	94.8	0.885	0.98
	hERG	95.4	42.9	74.3	0.470	0.84	94.9	39.7	73.5	0.433	0.81
	AR	66.2	98.9	90.4	0.742	0.89	63.6	98.2	88.3	0.705	0.86
	AChE	89.1	86.5	88.0	0.755	0.94	85.4	83.0	84.4	0.684	0.90
	SERT	98.9	89.0	96.7	0.903	0.99	98.1	82.1	94.7	0.836	0.97
	avg	89.4	81.8	89.0	0.754	0.93	87.7	79.0	87.1	0.708	0.90

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10]	ADORA2A	97.9	93.7	96.4	0.921	0.99	96.3	93.3	95.3	0.895	0.98
	hERG	91.7	77.6	85.9	0.706	0.93	86.9	67.7	79.6	0.560	0.86
	AR	63.7	99.3	89.8	0.732	0.89	59.8	99.2	88.9	0.703	0.85
	AChE	89.8	87.6	88.9	0.773	0.95	87.0	82.5	85.1	0.694	0.92
	SERT	98.9	83.3	95.5	0.865	0.98	98.8	80.3	94.7	0.842	0.98
	avg	88.4	88.3	91.3	0.800	0.95	85.8	84.6	88.7	0.739	0.92

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10,10]	ADORA2A	99.9	99.4	99.8	0.995	1.00	96.9	92.6	95.4	0.898	0.99
	hERG	99.3	99.5	99.4	0.987	1.00	83.2	72.0	78.7	0.554	0.85
	AR	96.1	99.6	98.6	0.965	1.00	73.3	93.8	88.3	0.694	0.86
	AChE	99.5	98.7	99.2	0.983	1.00	89.1	82.6	86.4	0.720	0.93
	SERT	99.9	99.7	99.8	0.995	1.00	99.3	90.3	97.4	0.921	1.00
	avg	98.9	99.4	99.3	0.985	1.00	88.4	86.2	89.2	0.757	0.93

ECFP4 1000

Training Data

Test Data

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]	ADORA2A	98.1	89.7	95.2	0.893	0.98	96.6	88.5	93.8	0.863	0.97
	hERG	91.3	58.1	78.2	0.538	0.86	89.0	54.7	74.9	0.474	0.83
	AR	61.0	98.6	88.7	0.697	0.89	62.5	98.2	88.4	0.698	0.87
	AChE	88.9	83.4	86.6	0.725	0.93	87.4	80.2	84.2	0.679	0.90
	SERT	99.0	87.1	96.3	0.893	0.99	97.9	81.2	94.5	0.825	0.98
	avg	87.7	83.4	89.0	0.749	0.93	86.7	80.6	87.2	0.708	0.91

[10,10]

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10]	ADORA2A	98.2	90.1	95.4	0.898	0.99	97.4	90.0	94.8	0.885	0.98
	hERG	86.8	70.5	80.3	0.584	0.88	81.8	62.9	74.2	0.457	0.82
	AR	69.0	96.5	89.2	0.711	0.89	66.4	96.1	88.2	0.682	0.85
	AChE	88.9	85.8	87.6	0.747	0.94	89.3	79.6	85.0	0.695	0.91

SERT	98.5	91.4	96.9	0.911	0.99	98.2	84.7	95.4	0.855	0.98
avg	88.3	86.9	89.9	0.770	0.94	86.6	82.6	87.5	0.715	0.91

[10,10,10]

Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
ADORA2A	99.8	99.1	99.6	0.989	1.00	97.6	89.8	95.7	0.881	0.98
hERG	94.1	85.0	90.5	0.801	0.96	83.9	68.5	77.9	0.532	0.84
AR	76.1	99.4	93.2	0.824	0.95	69.7	94.3	87.7	0.675	0.86
AChE	95.2	95.7	95.4	0.907	0.98	86.1	83.6	85.1	0.696	0.91
SERT	99.8	99.9	99.8	0.995	1.00	96.5	90.7	95.1	0.868	0.98
avg	93.0	95.8	95.7	0.903	0.98	86.8	85.4	88.3	0.730	0.91

ECFP4 5000

Training Data

Test Data

[10]

Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
ADORA2A	97.9	93.3	96.3	0.917	0.99	96.1	90.7	94.2	0.872	0.98
hERG	89.0	70.4	81.5	0.612	0.90	85.4	66.5	78.2	0.531	0.85
AR	65.3	99.3	90.4	0.745	0.90	62.8	98.3	88.4	0.701	0.85
AChE	88.5	88.9	88.7	0.771	0.94	86.8	82.5	84.9	0.693	0.91
SERT	98.8	87.9	96.5	0.894	0.99	98.4	84.9	95.4	0.864	0.98
avg	87.9	88.0	90.7	0.788	0.94	85.9	84.6	88.2	0.732	0.91

[10,10]

Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
ADORA2A	98.1	93.3	96.5	0.922	0.99	98.0	90.6	95.5	0.899	0.98
hERG	91.7	81.4	87.6	0.740	0.95	86.3	65.1	77.8	0.531	0.86

AR	62.6	99.4	89.6	0.727	0.90	61.0	98.8	88.8	0.703	0.87
AChE	90.8	87.8	89.6	0.786	0.95	86.5	83.7	85.2	0.701	0.92
SERT	99.1	91.8	97.5	0.926	0.99	97.9	86.9	95.4	0.867	0.99
avg	88.5	90.8	92.2	0.820	0.96	85.9	85.0	88.6	0.740	0.92

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10,10]	ADORA2A	99.9	99.9	99.9	0.998	1.00	96.3	93.8	95.4	0.900	1.00
	hERG	99.5	99.3	99.4	0.987	1.00	81.6	69.0	76.7	0.508	0.83
	AR	95.3	99.8	98.6	0.965	1.00	72.3	92.2	86.8	0.659	0.85
	AChE	99.7	99.1	99.4	0.989	1.00	85.8	80.2	83.3	0.661	0.91
	SERT	99.9	99.7	99.8	0.996	1.00	98.2	89.1	96.3	0.888	0.99
	avg	98.9	99.5	99.4	0.987	1.00	86.8	84.9	87.7	0.723	0.92

ECFP4 10000

Training Data

Test Data

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]	ADORA2A	97.6	93.0	96.0	0.911	0.99	97.2	91.2	95.3	0.892	0.98
	hERG	91.5	65.2	81.2	0.600	0.89	91.5	65.2	81.2	0.600	0.83
	AR	66.7	98.8	90.4	0.744	0.89	62.1	97.7	87.9	0.685	0.88
	AChE	88.1	87.6	87.9	0.754	0.94	86.2	89.4	87.6	0.751	0.93
	SERT	98.7	91.3	97.0	0.915	0.99	98.6	85.7	96.1	0.871	0.98
	avg	88.5	87.2	90.5	0.785	0.94	87.1	85.9	89.6	0.760	0.92

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
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[10,10]	ADORA2A	97.7	94.1	96.4	0.922	0.99	97.4	93.2	96.0	0.908	0.99
	hERG	91.0	73.7	84.0	0.665	0.92	87.8	68.3	80.3	0.578	0.88
	AR	67.6	99.0	90.8	0.754	0.90	65.0	98.5	89.0	0.723	0.87
	AChE	91.7	91.0	91.4	0.825	0.97	83.5	84.3	83.8	0.674	0.90
	SERT	98.9	89.0	96.7	0.904	0.99	98.3	83.4	95.1	0.852	0.97
	avg	89.4	89.4	91.9	0.814	0.95	86.4	85.5	88.9	0.747	0.92

[10,10,10]	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
	ADORA2A	99.9	99.9	99.9	0.998	1.00	95.7	92.0	94.4	0.877	0.98
	hERG	99.3	99.1	99.3	0.985	1.00	82.7	74.6	79.5	0.571	0.86
	AR	97.0	99.6	98.9	0.972	1.00	74.4	92.7	88.1	0.680	0.87
	AChE	99.6	99.4	99.5	0.990	1.00	87.8	85.4	86.8	0.731	0.91
	SERT	99.9	99.9	99.9	0.997	1.00	98.2	91.3	96.7	0.903	0.99
	avg	99.1	99.6	99.5	0.988	1.00	87.8	87.2	89.1	0.752	0.92

ECFP4 20000

Training Data

Test Data

[10]	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
	ADORA2A	97.9	92.1	95.9	0.909	0.99	98.1	88.6	94.8	0.884	0.99
	hERG	91.5	66.7	81.6	0.612	0.89	89.7	60.7	78.0	0.536	0.85
	AR	66.8	98.9	90.2	0.746	0.89	61.7	98.9	89.6	0.712	0.86
	AChE	91.4	85.8	89.0	0.775	0.95	83.1	79.7	81.7	0.626	0.88
	SERT	98.7	91.5	97.2	0.915	0.99	98.7	84.9	95.5	0.871	0.98
	avg	89.3	87.0	90.8	0.791	0.94	86.3	82.6	87.9	0.726	0.91

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10]	ADORA2A	97.9	93.8	96.5	0.922	0.99	97.4	90.2	94.8	0.887	0.98
	hERG	93.2	55.4	78.3	0.542	0.88	92.7	49.4	74.7	0.480	0.84
	AR	66.1	99.0	90.3	0.745	0.89	65.8	98.6	89.7	0.732	0.86
	AChE	89.9	91.7	90.7	0.812	0.96	84.9	87.6	86.1	0.721	0.92
	SERT	99.0	92.2	97.5	0.926	0.99	97.8	85.1	94.8	0.853	0.97
	avg	89.2	86.4	90.7	0.789	0.94	87.7	82.2	88.0	0.735	0.91
	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10,10]	ADORA2A	99.7	99.9	99.8	0.995	1.00	97.3	93.0	95.8	0.907	0.99
	hERG	99.4	99.5	99.4	0.988	1.00	80.8	75.3	78.6	0.557	0.86
	AR	94.1	99.7	98.3	0.955	1.00	68.7	97.0	89.4	0.719	0.86
	AChE	98.9	99.6	99.2	0.983	1.00	86.7	91.1	88.5	0.768	0.93
	SERT	99.9	99.8	99.9	0.996	1.00	98.5	90.7	96.8	0.906	0.99
	avg	98.4	99.7	99.3	0.984	1.00	86.4	89.4	89.8	0.771	0.93

Table S2. Results comparing the model performance of several chemical fingerprints across three network architectures and five biological targets (adenosine A2a receptor = ADORA2A, human ether a go-go related gene channel = hERG, androgen receptor = AR, acetylcholinesterase AChE, serotonin transporter (SERT). Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC).

	Training					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10]										
Sigmoid	88.5	87.2	90.5	0.785	0.94	87.1	85.9	89.6	0.760	0.92
ReLU	92.6	94.7	95.0	0.887	0.98	87.2	88.2	89.9	0.773	0.93
[10,10]										
Sigmoid, Sigmoid	89.4	89.4	91.9	0.814	0.95	86.4	85.5	88.9	0.747	0.92
Sigmoid, ReLU	90.7	88.6	92.1	0.822	0.96	88.6	83.3	89.1	0.753	0.93
ReLU, Sigmoid	89.2	88.7	91.8	0.811	0.96	86.8	83.0	88.3	0.733	0.92
ReLU, ReLU	96.0	92.6	95.6	0.903	0.99	90.2	84.0	90.0	0.770	0.93

Table S3. A summary of the results shown in Table S4 comparing the model performance sigmoid and ReLU activation functions across two network architectures and five biological targets. Highest accuracy (ACC) Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC) values are highlighted in red. ReLU was chosen as the best performing activation function in both single and double-layer cases.

[10] ECFP4 10000

		Training Data					Test Data					
	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	
Sigmoid	ADORA2A	97.6	93.0	96.0	0.911	0.99	97.2	91.2	95.3	0.892	0.98	
	hERG	91.5	65.2	81.2	0.600	0.89	91.5	65.2	81.2	0.600	0.83	
	AR	66.7	98.8	90.4	0.744	0.89	62.1	97.7	87.9	0.685	0.88	
	AChE	88.1	87.6	87.9	0.754	0.94	86.2	89.4	87.6	0.751	0.93	
	SERT	98.7	91.3	97.0	0.915	0.99	98.6	85.7	96.1	0.871	0.98	
	avg	88.5	87.2	90.5	0.785	0.94	87.1	85.9	89.6	0.760	0.92	
		Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
ReLU	ADORA2A	98.5	96.9	98.0	0.955	1.00	97.1	92.9	95.6	0.904	0.98	
	hERG	95.0	84.9	91.0	0.811	0.97	84.9	71.0	79.3	0.567	0.87	
	AR	77.7	99.2	93.5	0.830	0.96	68.4	97.6	89.9	0.730	0.87	
	AChE	92.4	95.4	93.7	0.873	0.98	87.3	90.2	88.6	0.770	0.93	
	SERT	99.2	97.3	98.8	0.966	1.00	98.3	89.2	96.4	0.891	0.99	
	avg	92.6	94.7	95.0	0.887	0.98	87.2	88.2	89.9	0.773	0.93	

[10,10] ECFP4 10000

	Training Data					Test Data					
	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
Sigmoid,Sigmoid	ADORA2A	97.7	94.1	96.4	0.922	0.99	97.4	93.2	96.0	0.908	0.99
	hERG	91.0	73.7	84.0	0.665	0.92	87.8	68.3	80.3	0.578	0.88
	AR	67.6	99.0	90.8	0.754	0.90	65.0	98.5	89.0	0.723	0.87
	AChE	91.7	91.0	91.4	0.825	0.97	83.5	84.3	83.8	0.674	0.90
	SERT	98.9	89.0	96.7	0.904	0.99	98.3	83.4	95.1	0.852	0.97
	avg	89.4	89.4	91.9	0.814	0.95	86.4	85.5	88.9	0.747	0.92
	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
Sigmoid,ReLU	ADORA2A	98.0	92.7	96.1	0.915	0.99	97.1	92.0	95.4	0.896	0.98
	hERG	94.6	65.5	83.0	0.646	0.92	92.1	55.2	77.2	0.522	0.86
	AR	68.8	99.1	91.0	0.765	0.92	66.6	98.3	90.1	0.731	0.92
	AChE	93.2	92.3	92.8	0.854	0.98	88.5	84.3	86.7	0.727	0.92
	SERT	98.9	93.3	97.7	0.931	1.00	98.9	86.5	95.9	0.886	0.98
	avg	90.7	88.6	92.1	0.822	0.96	88.6	83.3	89.1	0.753	0.93

	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
ReLU,Sigmoid	ADORA2A	97.6	93.4	96.2	0.915	0.99	97.9	89.1	94.9	0.886	0.98
	hERG	93.3	76.3	86.5	0.717	0.94	87.5	61.9	77.2	0.518	0.86
	AR	65.2	99.2	90.1	0.741	0.90	64.0	98.3	89.3	0.713	0.88
	AChE	91.1	89.4	90.4	0.803	0.96	86.2	85.7	85.9	0.715	0.92
	SERT	98.9	85.3	96.0	0.879	0.99	98.5	80.1	94.4	0.834	0.97
	avg	89.2	88.7	91.8	0.811	0.96	86.8	83.0	88.3	0.733	0.92
	Model	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
ReLU, ReLU	ADORA2A	99.2	98.2	98.8	0.974	1.00	97.3	92.5	95.7	0.903	0.99
	hERG	96.1	70.2	85.7	0.706	0.94	90.5	58.4	77.9	0.528	0.86
	AR	87.3	99.7	96.4	0.907	0.99	72.8	97.5	90.9	0.759	0.87
	AChE	97.9	98.1	98.0	0.959	1.00	91.8	86.6	89.6	0.786	0.94
	SERT	99.5	97.1	99.0	0.970	1.00	98.7	85.0	95.8	0.872	0.98
	avg	96.0	92.6	95.6	0.903	0.99	90.2	84.0	90.0	0.770	0.93

Table S4. Results comparing the model performance of Sigmoid and ReLU activation function across two network architectures and five biological targets (adenosine A2a receptor = ADORA2A, human ether a go-go related gene channel = hERG, androgen receptor = AR, acetylcholinesterase AChE, serotonin transporter (SERT). Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC).

AChE

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[10]	1	Train 1	1442	178	947	179	89.0	84.1	87.0	0.731	0.93
	2	Train 2	1313	214	1062	156	86.0	87.2	86.5	0.729	0.93
	3	Train 3	1397	177	964	207	88.8	82.3	86.0	0.713	0.93
	4	Train 4	1394	159	973	219	89.8	81.6	86.2	0.719	0.92
	5	Train 5	1422	164	974	185	89.7	84.0	87.3	0.739	0.93
		Avg	1394	178	984	189	88.7	83.9	86.6	0.726	0.93
		SD	49	22	45	25	1.5	2.2	0.5	0.010	0.00
		Validation 1	416	80	325	94	83.9	77.6	81.0	0.616	0.90
		Validation 2	434	76	334	71	85.1	82.5	83.9	0.675	0.91
		Validation 3	456	76	323	60	85.7	84.3	85.1	0.697	0.91
		Validation 4	456	73	296	90	86.2	76.7	82.2	0.633	0.89
		Validation 5	434	87	326	68	83.3	82.7	83.1	0.657	0.89
		Avg	439.2	78.4	320.8	76.6	84.9	80.7	83.1	0.655	0.90
		SD	17	5	14	15	1.2	3.4	1.6	0.032	0.01
		Test 1	416	80	325	94	83.9	77.6	81.0	0.616	0.88
		Test 2	468	107	287	53	81.4	84.4	82.5	0.642	0.90
		Test 3	436	70	320	89	86.2	78.2	82.6	0.648	0.89
	Test 4	461	69	288	97	87.0	74.8	81.9	0.625	0.89	
	Test 5	419	86	328	82	83.0	80.0	81.6	0.629	0.89	

Avg	440.0	82.4	309.6	83.0	84.2	78.9	81.9	0.631	0.89
SD	24	15	20	18	2.3	3.6	0.7	0.013	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[100]	6	Train 1	1411	158	1064	112	89.9	90.5	90.2	0.801	0.96	
	7	Train 2	1396	142	1047	160	90.8	86.7	89.0	0.776	0.95	
	8	Train 3	1419	141	1054	131	91.0	88.9	90.1	0.798	0.96	
	9	Train 4	1429	125	1013	178	92.0	85.1	89.0	0.775	0.95	
	10	Train 5	1437	157	1047	104	90.2	91.0	90.5	0.807	0.96	
		Avg	1418	145	1045	137	90.7	88.4	89.7	0.791	0.96	
		SD	16	14	19	31	0.8	2.5	0.7	0.015	0.01	
			Validation 1	473	74	313	55	86.5	85.1	85.9	0.710	0.92
			Validation 2	436	63	340	76	87.4	81.7	84.8	0.693	0.91
			Validation 3	494	52	306	63	90.5	82.9	87.4	0.738	0.93
			Validation 4	464	64	310	77	87.9	80.1	84.6	0.683	0.91
			Validation 5	435	78	347	55	84.8	86.3	85.5	0.708	0.91
			Avg	460.4	66.2	323.2	65.2	87.4	83.2	85.6	0.706	0.92
			SD	25	10	19	11	2.1	2.5	1.1	0.021	0.01
			Test 1	413	83	347	72	83.3	82.8	83.1	0.660	0.89
			Test 2	501	74	277	63	87.1	81.5	85.0	0.682	0.91
			Test 3	442	64	329	80	87.4	80.4	84.3	0.681	0.91

Test 4	478	52	283	102	90.2	73.5	83.2	0.653	0.90
Test 5	418	87	348	62	82.8	84.9	83.7	0.674	0.91
Avg	450.4	72.0	316.8	75.8	86.2	80.7	83.8	0.670	0.90
SD	38	14	34	16	3.1	4.3	0.8	0.013	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000]	11	Train 1	1424	169	942	210	89.4	81.8	86.2	0.715	0.92
	12	Train 2	1292	216	1061	176	85.7	85.8	85.7	0.713	0.93
	13	Train 3	1388	203	979	175	87.2	84.8	86.2	0.719	0.93
	14	Train 4	1388	177	987	193	88.7	83.6	86.5	0.725	0.93
	15	Train 5	1405	172	961	207	89.1	82.3	86.2	0.717	0.93
		Avg	1379	187	986	192	88.0	83.7	86.2	0.718	0.93
		SD	51	21	45	17	1.5	1.7	0.3	0.004	0.00
		Validation 1	461	62	292	100	88.1	74.5	82.3	0.636	0.89
		Validation 2	434	95	316	70	82.0	81.9	82.0	0.635	0.89
		Validation 3	447	68	305	95	86.8	76.3	82.2	0.636	0.90
		Validation 4	439	78	319	79	84.9	80.2	82.8	0.651	0.89
		Validation 5	453	77	297	88	85.5	77.1	82.0	0.629	0.89
		Avg	446.8	76.0	305.8	86.4	85.5	78.0	82.3	0.637	0.89
		SD	11	13	12	12	2.3	3.0	0.4	0.008	0.00
		Test 1	418	78	319	100	84.3	76.1	80.5	0.607	0.87

Test 2	468	107	285	55	81.4	83.8	82.3	0.637	0.89
Test 3	434	72	323	86	85.8	79.0	82.7	0.650	0.89
Test 4	461	69	294	91	87.0	76.4	82.5	0.639	0.89
Test 5	424	81	325	85	84.0	79.3	81.9	0.633	0.88
Avg	441.0	81.4	309.2	83.4	84.4	78.8	82.0	0.632	0.88
SD	22	15	18	17	2.1	3.1	0.9	0.016	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[10,10]	16	Train 1	1424	140	1073	108	91.0	90.9	91.0	0.817	0.96
	17	Train 2	1364	169	1097	115	89.0	90.5	89.7	0.792	0.95
	18	Train 3	1463	148	996	138	90.8	87.8	89.6	0.785	0.96
	19	Train 4	1429	125	1066	125	92.0	89.5	90.9	0.815	0.96
	20	Train 5	1420	145	1058	122	90.7	89.7	90.3	0.802	0.96
		Avg	1420	145	1058	122	90.7	89.7	90.3	0.802	0.96
		SD	36	16	38	11	1.1	1.2	0.7	0.014	0.00
		Validation 1	472	80	310	53	85.5	85.4	85.5	0.701	0.92
		Validation 2	424	80	346	65	84.1	84.2	84.2	0.681	0.91
		Validation 3	430	65	338	82	86.9	80.5	83.9	0.676	0.91
		Validation 4	461	67	308	79	87.3	79.6	84.0	0.672	0.91
		Validation 5	469	73	318	55	86.5	85.3	86.0	0.713	0.93
	Avg	451.2	73.0	324.0	66.8	86.1	82.9	84.7	0.688	0.92	
	SD	23	7	17	13	1.3	2.8	1.0	0.018	0.01	

Test 1	416	80	353	66	83.9	84.2	84.0	0.680	0.90
Test 2	464	111	296	44	80.7	87.1	83.1	0.659	0.91
Test 3	434	72	328	81	85.8	80.2	83.3	0.661	0.90
Test 4	468	62	298	87	88.3	77.4	83.7	0.664	0.90
Test 5	419	86	343	67	83.0	83.7	83.3	0.664	0.91
Avg	440.2	82.2	323.6	69.0	84.3	82.4	83.5	0.664	0.90
SD	25	18	26	17	2.9	3.8	0.4	0.008	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[100,100]	21	Train 1	1487	113	1037	108	92.9	90.6	91.9	0.835	0.97	
	22	Train 2	1389	122	1110	124	91.9	90.0	91.0	0.819	0.97	
	23	Train 3	1444	126	1074	101	92.0	91.4	91.7	0.832	0.97	
	24	Train 4	1466	108	1060	111	93.1	90.5	92.0	0.837	0.97	
	25	Train 5	1377	194	1106	68	87.7	94.2	90.5	0.811	0.97	
		Avg	1433	133	1077	102	91.5	91.3	91.4	0.827	0.97	
		SD	48	35	31	21	2.2	1.7	0.7	0.011	0.00	
			Validation 1	466	50	331	68	90.3	83.0	87.1	0.737	0.92
			Validation 2	467	59	330	59	88.8	84.8	87.1	0.736	0.93
			Validation 3	454	82	325	54	84.7	85.8	85.1	0.698	0.92
		Validation 4	440	68	335	72	86.6	82.3	84.7	0.690	0.91	
		Validation 5	458	78	343	36	85.4	90.5	87.5	0.751	0.94	

Avg	457	67	333	58	87.2	85.3	86.3	0.722	0.92
SD	11	13	7	14	2.3	3.2	1.3	0.027	0.01
Test 1	425	71	343	76	85.7	81.9	83.9	0.676	0.90
Test 2	508	67	284	56	88.3	83.5	86.6	0.714	0.92
Test 3	430	76	351	58	85.0	85.8	85.4	0.706	0.91
Test 4	471	59	302	83	88.9	78.4	84.5	0.680	0.91
Test 5	386	119	373	37	76.4	91.0	83.0	0.672	0.91
Avg	444	78	331	62	84.9	84.1	84.7	0.690	0.91
SD	47	24	37	18	5.0	4.7	1.4	0.019	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000,1000]	26	Train 1	1452	139	1086	68	91.3	94.1	92.5	0.848	0.98
	27	Train 2	1444	61	1210	30	95.9	97.6	96.7	0.933	0.99
	28	Train 3	1528	30	1123	64	98.1	94.6	96.6	0.930	0.99
	29	Train 4	1475	75	1173	22	95.2	98.2	96.5	0.929	0.99
	30	Train 5	1526	66	1133	20	95.9	98.3	96.9	0.937	0.99
		Avg	1485	74	1145	41	95.3	96.5	95.8	0.915	0.99
		SD	40	40	48	23	2.5	2.0	1.9	0.038	0.00
		Validation 1	446	79	341	49	85.0	87.4	86.0	0.718	0.92
		Validation 2	480	52	339	44	90.2	88.5	89.5	0.785	0.94
		Validation 3	507	41	295	72	92.5	80.4	87.7	0.741	0.95

Validation 4	448	84	331	52	84.2	86.4	85.1	0.700	0.91
Validation 5	452	63	361	39	87.8	90.3	88.9	0.776	0.94
Avg	467	64	333	51	87.9	86.6	87.4	0.744	0.93
SD	26	18	24	13	3.5	3.8	1.8	0.037	0.02
Test 1	402	94	365	54	81.0	87.1	83.8	0.679	0.91
Test 2	499	76	293	47	86.8	86.2	86.6	0.719	0.93
Test 3	455	51	301	108	89.9	73.6	82.6	0.649	0.91
Test 4	445	85	324	61	84.0	84.2	84.0	0.676	0.91
Test 5	411	94	366	44	81.4	89.3	84.9	0.703	0.92
Avg	442	80	330	63	84.6	84.1	84.4	0.685	0.92
SD	39	18	35	26	3.8	6.1	1.5	0.027	0.01

Table S5. Results comparing model performance for various network architectures at the AChE. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC). Averages (Avg) and standard deviations (SD) are shown.

ADORA2A

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[10]	1	Train 1	2309	57	1141	108	97.6	91.4	95.4	0.899	0.99
	2	Train 2	2279	60	1156	120	97.4	90.6	95.0	0.890	0.98
	3	Train 3	2376	51	1047	141	97.9	88.1	94.7	0.879	0.98
	4	Train 4	2303	65	1113	134	97.3	89.3	94.5	0.877	0.98
	5	Train 5	2316	48	1124	127	98.0	89.8	95.2	0.893	0.98
		Avg	2317	56	1116	126	97.6	89.9	95.0	0.888	0.98
		SD	36	7	42	13	0.3	1.2	0.4	0.009	0.00
		Validation 1	742	18	399	46	97.6	89.7	94.7	0.886	0.98
		Validation 2	744	27	390	44	96.5	89.9	94.1	0.871	0.98
		Validation 3	795	26	350	34	96.8	91.1	95.0	0.885	0.98
		Validation 4	759	14	384	48	98.2	88.9	94.9	0.888	0.98
		Validation 5	758	25	387	35	96.8	91.7	95.0	0.890	0.98
		Avg	759.6	22.0	382.0	41.4	97.2	90.2	94.7	0.884	0.98
		SD	21	6	19	6	0.7	1.1	0.4	0.007	0.00
		Test 1	798	19	342	46	97.7	88.1	94.6	0.875	0.98
		Test 2	816	17	328	44	98.0	88.2	94.9	0.880	0.97
		Test 3	671	24	462	48	96.5	90.6	94.0	0.878	0.97
		Test 4	778	24	360	43	97.0	89.3	94.4	0.874	0.97
		Test 5	769	27	351	58	96.6	85.8	92.9	0.841	0.96

Avg	766.4	22.2	368.6	47.8	97.2	88.5	94.2	0.871	0.97
SD	56	4	54	6	0.6	1.8	0.8	0.016	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[100]	6	Train 1	2327	52	1150	86	97.8	93.0	96.2	0.915	0.99
	7	Train 2	2287	56	1185	87	97.6	93.2	96.0	0.913	0.99
	8	Train 3	2391	45	1070	109	98.2	90.8	95.7	0.902	0.99
	9	Train 4	2309	59	1175	72	97.5	94.2	96.4	0.920	0.99
	10	Train 5	2301	50	1177	87	97.9	93.1	96.2	0.916	0.99
		Avg	2323	52	1151	88	97.8	92.9	96.1	0.913	0.99
		SD	41	5	47	13	0.3	1.3	0.2	0.007	0.00
		Validation 1	721	26	425	33	96.5	92.8	95.1	0.896	0.98
		Validation 2	747	20	386	52	97.4	88.1	94.0	0.870	0.98
		Validation 3	788	24	360	33	97.0	91.6	95.3	0.892	0.99
		Validation 4	747	26	392	40	96.6	90.7	94.5	0.880	0.98
		Validation 5	773	23	337	32	97.1	91.3	95.3	0.890	0.98
		Avg	755.2	23.8	380.0	38.0	96.9	90.9	94.8	0.886	0.98
		SD	26	2	33	8	0.4	1.7	0.6	0.010	0.00
		Test 1	793	24	349	39	97.1	89.9	94.8	0.879	0.98
	Test 2	824	9	332	40	98.9	89.2	95.9	0.904	0.97	
	Test 3	675	20	465	45	97.1	91.2	94.6	0.890	0.98	

Test 4	773	29	372	31	96.4	92.3	95.0	0.888	0.98
Test 5	768	28	361	48	96.5	88.3	93.7	0.858	0.97
Avg	766.6	22.0	375.8	40.6	97.2	90.2	94.8	0.884	0.98
SD	56	8	52	7	1.0	1.6	0.8	0.017	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000]	11	Train 1	2284	55	1158	118	97.6	90.8	95.2	0.895	0.98
	12	Train 2	2274	69	1165	107	97.1	91.6	95.1	0.893	0.98
	13	Train 3	2389	52	1030	144	97.9	87.7	94.6	0.875	0.98
	14	Train 4	2295	54	1151	115	97.7	90.9	95.3	0.897	0.98
	15	Train 5	2282	64	1173	96	97.3	92.4	95.6	0.902	0.99
		Avg	2305	59	1135	116	97.5	90.7	95.2	0.893	0.98
		SD	48	7	59	18	0.3	1.8	0.4	0.010	0.00
		Validation 1	764	23	364	54	97.1	87.1	93.6	0.858	0.97
		Validation 2	743	24	397	41	96.9	90.6	94.6	0.883	0.98
		Validation 3	795	12	351	47	98.5	88.2	95.1	0.889	0.98
		Validation 4	766	26	372	41	96.7	90.1	94.4	0.876	0.97
		Validation 5	776	25	369	35	96.9	91.3	95.0	0.888	0.98
		Avg	768.8	22.0	370.6	43.6	97.2	89.5	94.6	0.879	0.98
	SD	19	6	17	7	0.7	1.8	0.6	0.013	0.01	
	Test 1	798	19	340	48	97.7	87.6	94.4	0.871	0.98	

Test 2	815	18	333	39	97.8	89.5	95.3	0.888	0.97
Test 3	673	22	453	57	96.8	88.8	93.4	0.866	0.97
Test 4	771	31	370	33	96.1	91.8	94.7	0.881	0.98
Test 5	766	30	360	49	96.2	88.0	93.4	0.853	0.96
Avg	764.6	24.0	371.2	45.2	97.0	89.1	94.3	0.872	0.97
SD	55	6	48	9	0.8	1.7	0.8	0.014	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[10,10]	16	Train 1	2270	59	1166	120	97.5	90.7	95.0	0.891	0.99	
	17	Train 2	2268	54	1217	76	97.7	94.1	96.4	0.922	0.99	
	18	Train 3	2376	49	1084	106	98.0	91.1	95.7	0.902	0.99	
	19	Train 4	2290	45	1194	86	98.1	93.3	96.4	0.920	0.99	
	20	Train 5	2314	57	1170	74	97.6	94.1	96.4	0.920	0.99	
		Avg	2304	53	1166	92	97.8	92.7	96.0	0.911	0.99	
		SD	45	6	50	20	0.3	1.6	0.6	0.014	0.00	
			Validation 1	784	13	373	35	98.4	91.4	96.0	0.911	0.98
			Validation 2	766	22	369	48	97.2	88.5	94.2	0.871	0.97
			Validation 3	808	15	341	41	98.2	89.3	95.4	0.892	0.98
			Validation 4	782	24	361	38	97.0	90.5	94.9	0.883	0.98
			Validation 5	755	21	400	29	97.3	93.2	95.9	0.909	0.98
		Avg	779.0	19.0	368.8	38.2	97.6	90.6	95.3	0.893	0.98	
		SD	20	5	21	7	0.6	1.9	0.7	0.017	0.00	

Test 1	797	20	343	45	97.6	88.4	94.6	0.875	0.98
Test 2	819	14	334	38	98.3	89.8	95.7	0.898	0.97
Test 3	672	23	466	44	96.7	91.4	94.4	0.886	0.98
Test 4	776	26	371	32	96.8	92.1	95.2	0.892	0.98
Test 5	762	34	360	49	95.7	88.0	93.1	0.845	0.97
Avg	765.2	23.4	374.8	41.6	97.0	90.0	94.6	0.880	0.98
SD	56	7	53	7	1.0	1.8	1.0	0.021	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[100,100]	21	Train 1	2296	39	1196	84	98.3	93.4	96.6	0.925	0.99
	22	Train 2	2295	29	1164	127	98.8	90.2	95.7	0.906	0.99
	23	Train 3	2388	58	1108	61	97.6	94.8	96.7	0.925	0.99
	24	Train 4	2307	45	1185	78	98.1	93.8	96.6	0.925	0.99
	25	Train 5	2290	56	1224	45	97.6	96.5	97.2	0.939	0.99
		Avg	2315	45	1175	79	98.1	93.7	96.6	0.924	0.99
		SD	41	12	43	31	0.5	2.3	0.5	0.012	0.00
		Validation 1	769	22	364	50	97.2	87.9	94.0	0.867	0.98
		Validation 2	767	19	378	41	97.6	90.2	95.0	0.890	0.98
		Validation 3	775	27	373	30	96.6	92.6	95.3	0.894	0.98
		Validation 4	761	28	379	37	96.5	91.1	94.6	0.880	0.98
		Validation 5	770	31	373	31	96.1	92.3	94.9	0.885	0.98

Avg	768	25	373	38	96.8	90.8	94.8	0.883	0.98
SD	5	5	6	8	0.6	1.9	0.5	0.010	0.00
Test 1	800	17	349	39	97.9	89.9	95.4	0.893	0.98
Test 2	823	10	318	54	98.8	85.5	94.7	0.875	0.98
Test 3	670	25	476	34	96.4	93.3	95.1	0.900	0.98
Test 4	774	28	373	30	96.5	92.6	95.2	0.892	0.98
Test 5	752	44	368	41	94.5	90.0	92.9	0.843	0.98
Avg	764	25	377	40	96.8	90.3	94.7	0.880	0.98
SD	59	13	60	9	1.7	3.1	1.0	0.023	0.00

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000,1000]	26	Train 1	2318	23	47	1227	99.0	3.7	65.4	0.094	1.00
	27	Train 2	2292	31	1256	36	98.7	97.2	98.1	0.960	1.00
	28	Train 3	2412	18	1120	65	99.3	94.5	97.7	0.948	1.00
	29	Train 4	2337	23	1223	32	99.0	97.5	98.5	0.966	1.00
	30	Train 5	2348	25	1215	27	98.9	97.8	98.6	0.968	1.00
		Avg	2341	24	972	277	99.0	78.1	91.7	0.787	1.00
		SD	45	5	520	531	0.2	41.6	14.7	0.388	0.00
		Validation 1	737	24	410	34	96.8	92.3	95.2	0.896	0.99
		Validation 2	765	22	393	25	97.2	94.0	96.1	0.914	0.99
		Validation 3	800	18	353	34	97.8	91.2	95.7	0.900	0.98

Validation 4	762	19	383	41	97.6	90.3	95.0	0.890	0.98
Validation 5	752	22	405	26	97.2	94.0	96.0	0.913	0.98
Avg	763	21	389	32	97.3	92.4	95.6	0.903	0.98
SD	23	2	23	7	0.4	1.6	0.5	0.010	0.01
Test 1	773	44	364	24	94.6	93.8	94.4	0.873	0.99
Test 2	817	16	337	35	98.1	90.6	95.8	0.900	0.98
Test 3	674	21	462	48	97.0	90.6	94.3	0.883	0.98
Test 4	780	22	373	30	97.3	92.6	95.7	0.903	0.98
Test 5	767	29	363	46	96.4	88.8	93.8	0.860	0.98
Avg	762	26	380	37	96.7	91.3	94.8	0.884	0.98
SD	53	11	48	10	1.3	2.0	0.9	0.018	0.00

Table S6. Results comparing model performance for various network architectures at the ADORA2A. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC). Averages (Avg) and standard deviations (SD) are shown.

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	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[10]	1	Train 1	908	654	4358	32	58.1	99.3	88.5	0.693	0.88	
	2	Train 2	884	664	4372	32	57.1	99.3	88.3	0.685	0.88	
	3	Train 3	932	699	4285	36	57.1	99.2	87.7	0.681	0.88	
	4	Train 4	931	634	4358	29	59.5	99.3	88.9	0.704	0.88	
	5	Train 5	938	669	4312	33	58.4	99.2	88.2	0.692	0.88	
		Avg	919	664	4337	32	58.0	99.3	88.3	0.691	0.88	
		SD	22	24	37	3	1.0	0.1	0.4	0.009	0.00	
			Validation 1	304	231	1436	13	56.8	99.1	87.7	0.677	0.86
			Validation 2	327	224	1418	15	59.3	99.0	88.0	0.691	0.87
			Validation 3	342	192	1433	17	64.0	98.8	89.5	0.724	0.87
			Validation 4	273	230	1466	15	54.3	99.0	87.7	0.658	0.88
			Validation 5	311	201	1454	18	60.7	98.8	89.0	0.700	0.87
			Avg	311.4	215.6	1441.4	15.6	59.1	98.9	88.3	0.691	0.87
			SD	26	18	19	2	3.7	0.1	0.8	0.025	0.01
			Test 1	297	243	1432	12	55.0	99.2	87.1	0.665	0.85
			Test 2	298	240	1432	14	55.4	99.0	87.2	0.665	0.85
			Test 3	272	200	1496	16	57.6	98.9	89.1	0.684	0.86
			Test 4	300	269	1399	16	52.7	98.9	85.6	0.638	0.84

Test 5	305	213	1449	17	58.9	98.8	88.4	0.688	0.88
Avg	294.4	233.0	1441.6	15.0	55.8	99.0	87.5	0.667	0.86
SD	13	27	35	2	2.4	0.1	1.3	0.020	0.02

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[100]	6	Train 1	1046	493	4365	48	68.0	98.9	90.9	0.756	0.91	
	7	Train 2	1172	421	4263	96	73.6	97.8	91.3	0.772	0.91	
	8	Train 3	1100	484	4321	47	69.4	98.9	91.1	0.766	0.90	
	9	Train 4	996	540	4386	30	64.8	99.3	90.4	0.743	0.91	
	10	Train 5	1094	480	4318	60	69.5	98.6	90.9	0.760	0.90	
		Avg	1082	484	4331	56	69.1	98.7	90.9	0.759	0.91	
		SD	66	42	48	25	3.1	0.6	0.3	0.011	0.01	
			Validation 1	344	214	1408	18	61.6	98.7	88.3	0.703	0.85
			Validation 2	344	162	1442	36	68.0	97.6	90.0	0.726	0.85
			Validation 3	393	188	1372	31	67.6	97.8	89.0	0.726	0.88
			Validation 4	248	184	1430	22	57.4	98.5	89.1	0.671	0.87
			Validation 5	360	185	1408	31	66.1	97.8	89.1	0.717	0.88
			Avg	337.8	186.6	1412.0	27.6	64.4	98.1	89.1	0.711	0.87
			SD	54	18	27	7	4.5	0.5	0.6	0.023	0.02
			Test 1	333	207	1427	17	61.7	98.8	88.7	0.706	0.85
		Test 2	376	162	1408	38	69.9	97.4	89.9	0.736	0.86	

Test 3	309	163	1486	26	65.5	98.3	90.5	0.725	0.87
Test 4	333	236	1397	18	58.5	98.7	87.2	0.679	0.85
Test 5	351	167	1438	28	67.8	98.1	90.2	0.736	0.88
Avg	340.4	187.0	1431.2	25.4	64.5	98.3	89.3	0.715	0.86
SD	25	33	35	9	4.6	0.6	1.3	0.024	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000]	11	Train 1	1027	531	4332	62	65.9	98.6	90.0	0.733	0.89
	12	Train 2	1038	555	4298	61	65.2	98.6	89.7	0.728	0.89
	13	Train 3	1032	578	4280	62	64.1	98.6	89.2	0.719	0.89
	14	Train 4	1063	502	4319	68	67.9	98.4	90.4	0.745	0.89
	15	Train 5	983	601	4322	46	62.1	98.9	89.1	0.713	0.89
		Avg	1029	553	4310	60	65.0	98.6	89.7	0.727	0.89
		SD	29	39	21	8	2.2	0.2	0.5	0.012	0.00
		Validation 1	336	203	1412	33	62.3	97.7	88.1	0.687	0.86
		Validation 2	323	183	1447	31	63.8	97.9	89.2	0.703	0.87
		Validation 3	334	221	1408	21	60.2	98.5	87.8	0.688	0.87
		Validation 4	317	186	1454	27	63.0	98.2	89.3	0.703	0.86
		Validation 5	316	219	1432	17	59.1	98.8	88.1	0.687	0.85
		Avg	325.2	202.4	1430.6	25.8	61.6	98.2	88.5	0.693	0.86
		SD	9	18	20	7	2.0	0.5	0.7	0.009	0.01

Test 1	329	211	1422	22	60.9	98.5	88.3	0.693	0.86
Test 2	342	196	1418	28	63.6	98.1	88.7	0.703	0.86
Test 3	284	188	1487	25	60.2	98.3	89.3	0.687	0.87
Test 4	347	222	1388	27	61.0	98.1	87.4	0.683	0.84
Test 5	321	197	1447	19	62.0	98.7	89.1	0.707	0.88
Avg	324.6	202.8	1432.4	24.2	61.5	98.3	88.6	0.695	0.86
SD	25	14	37	4	1.3	0.3	0.7	0.010	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[10,10]	16	Train 1	1103	479	4337	33	69.7	99.2	91.4	0.775	0.91	
	17	Train 2	1025	513	4377	37	66.6	99.2	90.8	0.752	0.91	
	18	Train 3	1129	498	4276	49	69.4	98.9	90.8	0.764	0.91	
	19	Train 4	1042	542	4316	52	65.8	98.8	90.0	0.737	0.89	
	20	Train 5	1017	574	4307	54	63.9	98.8	89.4	0.722	0.89	
		Avg	1063	521	4323	45	67.1	99.0	90.5	0.750	0.90	
		SD	50	37	38	9	2.5	0.2	0.8	0.021	0.01	
			Validation 1	347	168	1446	23	67.4	98.4	90.4	0.741	0.87
			Validation 2	349	212	1402	21	62.2	98.5	88.3	0.702	0.87
			Validation 3	335	203	1422	24	62.3	98.3	88.6	0.700	0.85
			Validation 4	307	177	1481	19	63.4	98.7	90.1	0.720	0.88
			Validation 5	309	219	1435	21	58.5	98.6	87.9	0.677	0.84
		Avg	329.4	195.8	1437.2	21.6	62.7	98.5	89.0	0.708	0.86	

SD	20	22	29	2	3.2	0.1	1.1	0.024	0.02
Test 1	343	197	1422	22	63.5	98.5	89.0	0.712	0.87
Test 2	307	231	1426	20	57.1	98.6	87.3	0.667	0.86
Test 3	312	160	1489	23	66.1	98.5	90.8	0.734	0.87
Test 4	342	227	1394	21	60.1	98.5	87.5	0.686	0.88
Test 5	320	198	1449	17	61.8	98.8	89.2	0.709	0.87
Avg	324.8	202.6	1436.0	20.6	61.6	98.6	88.8	0.701	0.87
SD	17	29	35	2	3.4	0.2	1.4	0.026	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[100,100]	21	Train 1	1229	340	4340	43	78.3	99.0	93.6	0.831	0.95
	22	Train 2	1231	356	4329	36	77.6	99.2	93.4	0.829	0.94
	23	Train 3	1195	420	4323	14	74.0	99.7	92.7	0.814	0.96
	24	Train 4	1206	354	4372	20	77.3	99.5	93.7	0.836	0.96
	25	Train 5	1162	421	4346	23	73.4	99.5	92.5	0.806	0.95
		Avg	1205	378	4342	27	76.1	99.4	93.2	0.823	0.95
		SD	28	39	19	12	2.3	0.3	0.5	0.012	0.01
		Validation 1	373	155	1409	47	70.6	96.8	89.8	0.729	0.87
		Validation 2	356	156	1443	29	69.5	98.0	90.7	0.748	0.86
		Validation 3	371	179	1398	36	67.5	97.5	89.2	0.720	0.88
	Validation 4	346	162	1451	25	68.1	98.3	90.6	0.743	0.88	

Validation 5	377	159	1424	24	70.3	98.3	90.8	0.759	0.88
Avg	365	162	1425	32	69.2	97.8	90.2	0.740	0.87
SD	13	10	22	10	1.4	0.7	0.7	0.016	0.01
Test 1	361	179	1407	37	66.9	97.4	89.1	0.715	0.86
Test 2	371	167	1412	34	69.0	97.6	89.9	0.735	0.87
Test 3	318	154	1489	23	67.4	98.5	91.1	0.743	0.88
Test 4	379	190	1385	30	66.6	97.9	88.9	0.721	0.85
Test 5	364	154	1450	16	70.3	98.9	91.4	0.772	0.89
Avg	359	169	1429	28	68.0	98.1	90.1	0.737	0.87
SD	24	16	41	9	1.6	0.6	1.1	0.023	0.02

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000,1000]	26	Train 1	937	610	4366	39	60.6	99.1	89.1	0.707	0.89
	27	Train 2	1318	290	4298	46	82.0	98.9	94.4	0.855	0.95
	28	Train 3	1180	438	4322	12	72.9	99.7	92.4	0.808	0.96
	29	Train 4	1108	427	4408	9	72.2	99.8	92.7	0.806	0.98
	30	Train 5	1234	336	4352	30	78.6	99.3	93.9	0.840	0.94
		Avg	1155	420	4349	27	73.2	99.4	92.5	0.803	0.94
		SD	144	123	42	16	8.2	0.4	2.1	0.058	0.03
		Validation 1	329	221	1418	16	59.8	98.9	88.1	0.693	0.85
		Validation 2	351	140	1425	68	71.5	95.4	89.5	0.708	0.87

Validation 3	361	186	1421	16	66.0	98.9	89.8	0.739	0.90
Validation 4	336	197	1438	13	63.0	99.1	89.4	0.723	0.87
Validation 5	381	168	1395	40	69.4	97.2	89.5	0.729	0.88
Avg	352	182	1419	31	65.9	97.9	89.3	0.718	0.87
SD	21	31	16	24	4.7	1.6	0.7	0.018	0.02
Test 1	313	227	1431	13	58.0	99.1	87.9	0.685	0.86
Test 2	384	154	1381	65	71.4	95.5	89.0	0.711	0.87
Test 3	305	167	1497	15	64.6	99.0	90.8	0.737	0.87
Test 4	328	241	1403	12	57.6	99.2	87.2	0.682	0.85
Test 5	368	150	1439	27	71.0	98.2	91.1	0.761	0.88
Avg	340	188	1430	26	64.5	98.2	89.2	0.715	0.87
SD	35	43	44	22	6.7	1.6	1.7	0.034	0.01

Table S7. Results comparing model performance for various network architectures at the AR. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC). Averages (Avg) and standard deviations (SD) are shown.

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	Model Number		TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	
[10]	1	Train 1	2707	194	1073	910	0.87	93.3	54.1	77.4	0.531	0.87	
	2	Train 2	2753	195	1064	872	0.87	93.4	55.0	78.2	0.541	0.87	
	3	Train 3	2748	169	922	1045	0.86	94.2	46.9	75.1	0.484	0.86	
	4	Train 4	2690	247	1227	720	0.88	91.6	63.0	80.2	0.582	0.88	
	5	Train 5	2823	148	925	991	0.86	95.0	48.3	76.7	0.511	0.86	
		Avg	2744	191	1042	908	0.87	93.5	53.5	77.5	0.529	0.87	
		SD	52	37	126	125	0.01	1.3	6.4	1.9	0.037	0.01	
			Validation 1	918	88	327	295	0.83	91.3	52.6	76.5	0.489	0.83
			Validation 2	913	73	296	346	0.82	92.6	46.1	74.3	0.452	0.82
			Validation 3	939	51	303	335	0.83	94.8	47.5	76.3	0.501	0.83
			Validation 4	836	136	340	316	0.80	86.0	51.8	72.2	0.408	0.80
			Validation 5	889	66	290	383	0.81	93.1	43.1	72.4	0.431	0.81
			Avg	899.0	82.8	311.2	335.0	0.82	91.6	48.2	74.3	0.454	0.82
			SD	39	33	21	33	0.01	3.4	4.0	2.0	0.039	0.01
			Test 1	890	98	290	350	0.78	90.1	45.3	72.5	0.406	0.78
			Test 2	875	86	314	353	0.82	91.1	47.1	73.0	0.436	0.82
			Test 3	929	59	273	367	0.81	94.0	42.7	73.8	0.445	0.81
			Test 4	886	100	351	291	0.83	89.9	54.7	76.0	0.486	0.83
			Test 5	921	51	268	388	0.81	94.8	40.9	73.0	0.440	0.81

Avg	900.2	78.8	299.2	349.8	0.81	92.0	46.1	73.7	0.441	0.81
SD	23	23	34	36	0.02	2.3	5.3	1.4	0.029	0.02

	Model Number		TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	
[100]	6	Train 1	2698	212	1053	921	0.87	92.7	53.3	76.8	0.516	0.87	
		Avg	2752	172	977	982	0.86	94.1	49.9	76.4	0.508	0.86	
	7	Train 2	2782	172	996	934	0.87	94.2	51.6	77.4	0.525	0.87	
		Avg	2752	172	977	982	0.86	94.1	49.9	76.4	0.508	0.86	
	8	Train 3	2718	201	1027	938	0.86	93.1	52.3	76.7	0.513	0.86	
		Avg	2752	172	977	982	0.86	94.1	49.9	76.4	0.508	0.86	
	9	Train 4	2764	157	942	1021	0.85	94.6	48.0	75.9	0.500	0.85	
		Avg	2752	172	977	982	0.86	94.1	49.9	76.4	0.508	0.86	
	10	Train 5	2800	117	869	1098	0.86	96.0	44.2	75.1	0.491	0.86	
		Avg	2752	172	977	982	0.86	94.1	49.9	76.4	0.508	0.86	
			SD	43	38	73	76	0.01	1.3	3.8	0.9	0.013	0.01
			Validation 1	902	95	317	314	0.82	90.5	50.2	74.9	0.456	0.82
			Validation 2	893	87	297	351	0.81	91.1	45.8	73.1	0.426	0.81
			Validation 3	920	68	308	332	0.81	93.1	48.1	75.4	0.478	0.81
			Validation 4	917	71	264	347	0.79	92.8	43.2	73.9	0.430	0.79
			Validation 5	939	67	258	364	0.81	93.3	41.5	73.5	0.423	0.81
			Avg	914.2	77.6	288.8	341.6	0.81	92.2	45.8	74.2	0.443	0.81
			SD	18	13	26	19	0.01	1.3	3.6	1.0	0.024	0.01
		Test 1	893	95	288	352	0.78	90.4	45.0	72.5	0.407	0.78	
		Test 2	895	66	298	369	0.81	93.1	44.7	73.3	0.446	0.81	
		Test 3	911	77	307	333	0.80	92.2	48.0	74.8	0.462	0.80	

Test 4	918	68	295	347	0.80	93.1	46.0	74.5	0.459	0.80
Test 5	930	42	242	414	0.80	95.7	36.9	72.0	0.421	0.80
Avg	909.4	69.6	286.0	363.0	0.80	92.9	44.1	73.4	0.438	0.80
SD	16	19	26	31	0.01	1.9	4.2	1.2	0.024	0.01

	Model Number		TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[1000]	11	Train 1	2447	483	1459	495	0.88	83.5	74.7	80.0	0.582	0.88
	12	Train 2	2718	238	1188	740	0.87	91.9	61.6	80.0	0.576	0.87
	13	Train 3	2686	248	1167	783	0.87	91.5	59.8	78.9	0.555	0.87
	14	Train 4	2703	265	1182	734	0.87	91.1	61.7	79.5	0.564	0.87
	15	Train 5	2667	279	1234	704	0.87	90.5	63.7	79.9	0.573	0.87
		Avg	2644	303	1246	691	0.87	89.7	64.3	79.7	0.568	0.87
		SD	112	102	122	113	0.00	3.5	6.0	0.5	0.011	0.00
		Validation 1	776	201	445	206	0.83	79.4	68.4	75.0	0.478	0.83
		Validation 2	877	101	371	279	0.81	89.7	57.1	76.7	0.505	0.81
		Validation 3	882	91	320	335	0.81	90.6	48.9	73.8	0.446	0.81
		Validation 4	833	265	1182	734	0.83	75.9	61.7	66.9	0.362	0.83
		Validation 5	863	114	374	277	0.82	88.3	57.5	76.0	0.490	0.82
		Avg	846.2	154.4	538.4	366.2	0.82	84.6	59.5	72.7	0.458	0.82
		SD	44	76	363	211	0.01	6.7	7.1	4.0	0.057	0.01
		Test 1	763	225	406	234	0.78	77.2	63.4	71.8	0.408	0.78

Test 2	859	102	346	321	0.81	89.4	51.9	74.0	0.454	0.81
Test 3	890	98	335	305	0.81	90.1	52.3	75.2	0.469	0.81
Test 4	884	102	344	298	0.82	89.7	53.6	75.4	0.474	0.82
Test 5	863	109	353	303	0.82	88.8	53.8	74.7	0.463	0.82
Avg	851.8	127.2	356.8	292.2	0.81	87.0	55.0	74.2	0.450	0.81
SD	51	55	28	34	0.02	5.5	4.8	1.5	0.027	0.02

	Model Number		TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[10,10]	16	Train 1	2771	150	1698	265	0.97	94.9	86.5	91.5	0.823	0.97
	17	Train 2	2856	117	1556	355	0.97	96.1	81.4	90.3	0.797	0.97
	18	Train 3	2755	161	1662	306	0.97	94.5	84.5	90.4	0.800	0.97
	19	Train 4	2693	247	1599	345	0.95	91.6	82.3	87.9	0.746	0.95
	20	Train 5	2773	194	1729	188	0.97	93.5	90.2	92.2	0.836	0.97
		Avg	2770	174	1649	292	0.97	94.1	85.0	90.5	0.800	0.97
		SD	58	49	71	68	0.01	1.7	3.5	1.6	0.035	0.01
		Validation 1	846	140	453	189	0.87	85.8	70.6	79.8	0.572	0.87
		Validation 2	836	125	405	262	0.86	87.0	60.7	76.2	0.501	0.86
		Validation 3	854	137	422	215	0.86	86.2	66.2	78.4	0.539	0.86
	Validation 4	853	116	433	226	0.87	88.0	65.7	79.0	0.558	0.87	
	Validation 5	798	158	484	188	0.85	83.5	72.0	78.7	0.559	0.85	
	Avg	837.4	135.2	439.4	216.0	0.86	86.1	67.0	78.4	0.545	0.86	
	SD	23	16	30	31	0.01	1.7	4.5	1.3	0.028	0.01	

Test 1	848	140	410	230	0.82	85.8	64.1	77.3	0.515	0.82
Test 2	864	97	402	265	0.85	89.9	60.3	77.8	0.535	0.85
Test 3	860	128	386	254	0.85	87.0	60.3	76.5	0.498	0.85
Test 4	846	140	432	226	0.86	85.8	65.7	77.7	0.529	0.86
Test 5	808	164	450	206	0.85	83.1	68.6	77.3	0.523	0.85
Avg	845.2	133.8	416.0	236.2	0.85	86.3	63.8	77.3	0.519	0.85
SD	22	24	25	23	0.02	2.5	3.6	0.5	0.015	0.02

	Model Number		TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	21	Train 1	2852	83	1672	277	0.98	97.2	85.8	92.6	0.847	0.98
	22	Train 2	2860	84	1736	204	0.99	97.1	89.5	94.1	0.877	0.99
	23	Train 3	2830	135	1796	123	0.98	95.4	93.6	94.7	0.889	0.98
	24	Train 4	2786	150	1834	114	0.98	94.9	94.1	94.6	0.888	0.98
	25	Train 5	2835	102	1740	207	0.98	96.5	89.4	93.7	0.868	0.98
		Avg	2833	111	1756	185	0.98	96.2	90.5	93.9	0.874	0.98
		SD	29	30	62	67	0.00	1.0	3.4	0.8	0.017	0.00
			Validation 1	847	125	446	210	0.88	87.1	68.0	79.4	0.567
		Validation 2	852	138	416	222	0.85	86.1	65.2	77.9	0.528	0.85
		Validation 3	772	170	514	172	0.87	82.0	74.9	79.0	0.569	0.87
		Validation 4	803	170	481	174	0.85	82.5	73.4	78.9	0.560	0.85
		Validation 5	855	131	430	212	0.86	86.7	67.0	78.9	0.552	0.86

Avg	826	147	457	198	0.86	84.9	69.7	78.8	0.555	0.86
SD	37	22	40	23	0.01	2.4	4.2	0.6	0.016	0.01
Test 1	858	130	376	264	0.82	86.8	58.8	75.8	0.481	0.82
Test 2	832	129	429	238	0.85	86.6	64.3	77.5	0.527	0.85
Test 3	820	168	441	199	0.85	83.0	68.9	77.5	0.524	0.85
Test 4	822	164	452	190	0.85	83.4	70.4	78.3	0.542	0.85
Test 5	834	138	426	230	0.84	85.8	64.9	77.4	0.523	0.84
Avg	833	146	425	224	0.84	85.1	65.5	77.3	0.519	0.84
SD	15	19	29	30	0.01	1.8	4.6	0.9	0.023	0.01

	Model Number		TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	
[1000,1000]	26	Train 1	2945	32	1405	502	0.98	98.9	73.7	89.1	0.777	0.98	
	27	Train 2	2864	66	1612	342	0.98	97.7	82.5	91.6	0.828	0.98	
	28	Train 3	2606	329	1918	31	0.99	88.8	98.4	92.6	0.857	0.99	
	29	Train 4	2708	221	1850	105	0.98	92.5	94.6	93.3	0.863	0.98	
	30	Train 5	2863	83	1704	234	0.98	97.2	87.9	93.5	0.864	0.98	
		Avg		2797	146	1698	243	0.98	95.0	87.4	92.0	0.838	0.98
		SD		137	125	203	188	0.00	4.3	9.8	1.8	0.037	0.00
			Validation 1	858	72	362	336	0.86	92.3	51.9	74.9	0.494	0.86
			Validation 2	914	90	355	269	0.85	91.0	56.9	77.9	0.523	0.85
			Validation 3	694	278	530	126	0.85	71.4	80.8	75.2	0.512	0.85

Validation 4	766	214	513	135	0.87	78.2	79.2	78.6	0.564	0.87
Validation 5	864	113	429	222	0.86	88.4	65.9	79.4	0.565	0.86
Avg	819	153	438	218	0.86	84.3	66.9	77.2	0.532	0.86
SD	88	89	82	89	0.01	9.1	12.9	2.0	0.032	0.01
Test 1	916	72	306	334	0.81	92.7	47.8	75.1	0.469	0.81
Test 2	871	90	371	296	0.84	90.6	55.6	76.3	0.505	0.84
Test 3	693	295	515	125	0.84	70.1	80.5	74.2	0.494	0.84
Test 4	767	219	510	132	0.86	77.8	79.4	78.4	0.562	0.86
Test 5	834	138	423	233	0.83	85.8	64.5	77.2	0.519	0.83
Avg	816	163	425	224	0.84	83.4	65.6	76.2	0.510	0.84
SD	88	93	90	94	0.02	9.4	14.4	1.7	0.035	0.02

Table S8. Results comparing model performance for various network architectures at the KCNH2. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC). Averages (Avg) and standard deviations (SD) are shown.

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	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[10]	1	Train 1	2426	19	458	202	99.2	69.4	92.9	0.779	0.98
	2	Train 2	2373	17	513	202	99.3	71.7	92.9	0.795	0.98
	3	Train 3	2422	16	438	229	99.3	65.7	92.1	0.756	0.98
	4	Train 4	2441	18	472	174	99.3	73.1	93.8	0.805	0.98
	5	Train 5	2392	23	563	127	99.0	81.6	95.2	0.857	0.99
		Avg	2411	19	489	187	99.2	72.4	93.4	0.799	0.98
		SD	28	3	50	39	0.1	5.9	1.2	0.038	0.00
		Validation 1	791	10	150	84	98.8	64.1	90.9	0.727	0.98
		Validation 2	786	10	161	78	98.7	67.4	91.5	0.750	0.98
		Validation 3	792	5	150	88	99.4	63.0	91.0	0.736	0.96
		Validation 4	800	6	145	84	99.3	63.3	91.3	0.736	0.97
		Validation 5	813	4	159	59	99.5	72.9	93.9	0.811	0.97
		Avg	796.4	7.0	153.0	78.6	99.1	66.1	91.7	0.752	0.97
		SD	11	3	7	12	0.4	4.2	1.2	0.034	0.01
		Test 1	793	2	151	89	99.7	62.9	91.2	0.745	0.96
		Test 2	846	9	126	54	98.9	70.0	93.9	0.776	0.98
		Test 3	797	9	150	79	98.9	65.5	91.5	0.741	0.98
		Test 4	768	8	173	86	99.0	66.8	90.9	0.750	0.97
	Test 5	797	12	167	59	98.5	73.9	93.1	0.791	0.98	

Avg	800.2	8.0	153.4	73.4	99.0	67.6	92.1	0.760	0.97
SD	28	4	18	16	0.5	4.2	1.3	0.022	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[100]	6	Train 1	2435	21	577	72	99.1	88.9	97.0	0.908	0.99
	7	Train 2	2358	30	651	66	98.7	90.8	96.9	0.912	0.99
	8	Train 3	2410	25	618	52	99.0	92.2	97.5	0.926	0.99
	9	Train 4	2430	22	570	83	99.1	87.3	96.6	0.896	0.99
	10	Train 5	2416	24	575	90	99.0	86.5	96.3	0.889	0.99
		Avg	2410	24	598	73	99.0	89.2	96.9	0.906	0.99
		SD	31	4	35	15	0.2	2.4	0.4	0.014	0.00
		Validation 1	777	13	203	42	98.4	82.9	94.7	0.849	0.98
		Validation 2	784	14	202	35	98.2	85.2	95.3	0.863	0.98
		Validation 3	784	16	207	28	98.0	88.1	95.7	0.877	0.98
		Validation 4	798	15	177	45	98.2	79.7	94.2	0.822	0.98
		Validation 5	785	7	202	41	99.1	83.1	95.4	0.868	0.98
		Avg	785.6	13.0	198.2	38.2	98.4	83.8	95.1	0.856	0.98
		SD	8	4	12	7	0.4	3.1	0.6	0.021	0.00
		Test 1	791	4	197	43	99.5	82.1	95.5	0.870	0.97
		Test 2	842	13	155	25	98.5	86.1	96.3	0.870	0.99
		Test 3	793	13	202	27	98.4	88.2	96.1	0.886	0.98

Test 4	765	11	213	46	98.6	82.2	94.5	0.850	0.98
Test 5	795	14	175	51	98.3	77.4	93.7	0.810	0.98
Avg	797.2	11.0	188.4	38.4	98.6	83.1	95.2	0.857	0.98
SD	28	4	23	12	0.5	4.2	1.1	0.030	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000]	11	Train 1	2396	22	473	214	99.1	68.9	92.4	0.770	0.99
	12	Train 2	2380	14	552	159	99.4	77.6	94.4	0.839	0.98
	13	Train 3	2394	24	558	129	99.0	81.2	95.1	0.853	0.99
	14	Train 4	2446	17	518	124	99.3	80.7	95.5	0.858	0.98
	15	Train 5	2404	19	530	152	99.2	77.7	94.5	0.835	0.98
		Avg	2404	19	526	156	99.2	77.2	94.4	0.831	0.98
		SD	25	4	34	36	0.2	5.0	1.2	0.035	0.01
		Validation 1	822	6	136	71	99.3	65.7	92.6	0.755	0.96
		Validation 2	778	14	178	65	98.2	73.3	92.4	0.779	0.97
		Validation 3	807	10	172	46	98.8	78.9	94.6	0.832	0.97
		Validation 4	792	10	180	53	98.8	77.3	93.9	0.820	0.98
		Validation 5	799	10	166	60	98.8	73.5	93.2	0.794	0.98
		Avg	799.6	10.0	166.4	59.0	98.8	73.8	93.3	0.797	0.97
		SD	16	3	18	10	0.4	5.1	0.9	0.031	0.01
		Test 1	793	2	156	84	99.7	65.0	91.7	0.760	0.96

Test 2	847	8	140	40	99.1	77.8	95.4	0.832	0.98
Test 3	796	10	184	45	98.8	80.3	94.7	0.841	0.98
Test 4	768	8	193	66	99.0	74.5	92.9	0.805	0.97
Test 5	799	10	165	61	98.8	73.0	93.1	0.791	0.98
Avg	800.6	7.6	167.6	59.2	99.1	73.9	93.5	0.805	0.97
SD	29	3	21	18	0.4	5.8	1.5	0.033	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC	
[10,10]	16	Train 1	2428	26	593	58	98.9	91.1	97.3	0.917	0.99	
	17	Train 2	2362	32	655	56	98.7	92.1	97.2	0.919	0.99	
	18	Train 3	2412	20	566	107	99.2	84.1	95.9	0.877	0.99	
	19	Train 4	2426	25	601	53	99.0	91.9	97.5	0.924	0.99	
	20	Train 5	2418	22	594	71	99.1	89.3	97.0	0.910	0.99	
		Avg	2409	25	602	69	99.0	89.7	97.0	0.909	0.99	
		SD	27	5	33	22	0.2	3.3	0.6	0.019	0.00	
			Validation 1	785	7	191	52	99.1	78.6	94.3	0.838	0.98
			Validation 2	785	7	199	44	99.1	81.9	95.1	0.860	0.97
			Validation 3	798	5	176	56	99.4	75.9	94.1	0.826	0.98
			Validation 4	804	10	192	29	98.8	86.9	96.2	0.886	0.99
			Validation 5	778	14	213	30	98.2	87.7	95.7	0.880	0.99
		Avg	790.0	8.6	194.2	42.2	98.9	82.1	95.1	0.857	0.98	
		SD	11	4	13	12	0.4	5.1	0.9	0.026	0.01	

Test 1	790	5	192	48	99.4	80.0	94.9	0.853	0.97
Test 2	843	12	158	22	98.6	87.8	96.7	0.884	0.99
Test 3	797	9	185	44	98.9	80.8	94.9	0.847	0.98
Test 4	765	11	218	41	98.6	84.2	95.0	0.864	0.98
Test 5	793	16	189	37	98.0	83.6	94.9	0.846	0.98
Avg	797.6	10.6	188.4	38.4	98.7	83.1	95.3	0.858	0.98
SD	28	4	21	10	0.5	3.1	0.8	0.015	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[100,100]	21	Train 1	2407	17	647	34	99.3	95.0	98.4	0.952	1.00
	22	Train 2	2373	16	685	31	99.3	95.7	98.5	0.957	1.00
	23	Train 3	2418	15	647	25	99.4	96.3	98.7	0.962	1.00
	24	Train 4	2442	15	628	20	99.4	96.9	98.9	0.966	1.00
	25	Train 5	2400	14	659	32	99.4	95.4	98.5	0.957	1.00
		Avg	2408	15	653	28	99.4	95.8	98.6	0.959	1.00
		SD	25	1	21	6	0.0	0.8	0.2	0.005	0.00
		Validation 1	803	19	187	26	97.7	87.8	95.7	0.866	0.99
		Validation 2	781	16	208	30	98.0	87.4	95.6	0.873	0.98
		Validation 3	791	11	200	33	98.6	85.8	95.7	0.876	0.98
	Validation 4	793	15	196	31	98.1	86.3	95.6	0.868	0.98	
	Validation 5	806	12	180	37	98.5	82.9	95.3	0.853	0.98	

Avg	795	15	194	31	98.2	86.1	95.6	0.867	0.98
SD	10	3	11	4	0.4	1.9	0.2	0.009	0.00
Test 1	791	4	201	39	99.5	83.8	95.8	0.882	0.98
Test 2	846	9	159	21	98.9	88.3	97.1	0.897	0.99
Test 3	790	16	210	19	98.0	91.7	96.6	0.901	0.99
Test 4	764	12	226	33	98.5	87.3	95.7	0.882	0.98
Test 5	795	14	188	38	98.3	83.2	95.0	0.849	0.99
Avg	797	11	197	30	98.6	86.8	96.0	0.882	0.99
SD	30	5	25	9	0.6	3.5	0.8	0.021	0.01

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC	ROC-AUC
[1000,1000]	26	Train 1	2401	26	671	7	98.9	99.0	98.9	0.969	1.00
	27	Train 2	2375	13	703	14	99.5	98.0	99.1	0.976	1.00
	28	Train 3	2394	18	686	7	99.3	99.0	99.2	0.977	1.00
	29	Train 4	2446	8	636	15	99.7	97.7	99.3	0.978	1.00
	30	Train 5	2417	9	662	17	99.6	97.5	99.2	0.975	1.00
		Avg	2407	15	672	12	99.4	98.2	99.1	0.975	1.00
		SD	27	7	25	5	0.3	0.7	0.1	0.003	0.00
		Validation 1	803	16	198	18	98.0	91.7	96.7	0.900	0.99
		Validation 2	786	12	216	21	98.5	91.1	96.8	0.909	0.99
		Validation 3	795	23	199	13	97.2	93.9	96.5	0.895	0.99

Validation 4	797	14	201	23	98.3	89.7	96.4	0.893	0.99
Validation 5	792	14	204	25	98.3	89.1	96.2	0.889	0.99
Avg	795	16	204	20	98.1	91.1	96.5	0.897	0.99
SD	6	4	7	5	0.5	1.9	0.2	0.008	0.00
Test 1	782	13	215	25	98.4	89.6	96.3	0.896	0.98
Test 2	847	8	162	18	99.1	90.0	97.5	0.911	0.99
Test 3	788	18	221	8	97.8	96.5	97.5	0.929	0.98
Test 4	762	14	228	31	98.2	88.0	95.7	0.882	0.99
Test 5	796	13	200	26	98.4	88.5	96.2	0.888	0.99
Avg	795	13	205	22	98.4	90.5	96.6	0.901	0.99
SD	32	4	26	9	0.5	3.4	0.8	0.019	0.01

Table S9. Results comparing model performance for various network architectures at the SLC6A4. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC). Averages (Avg) and standard deviations (SD) are shown.

AChE	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	91.5	91.3	91.4	0.827	0.97	87.2	85.3	86.3	0.722	0.92	84.9	84.1	84.7	0.690	0.91
	2.2	1.7	0.7	0.011	0.00	2.3	3.2	1.3	0.027	0.01	5.0	4.7	1.4	0.019	0.01
[1000,1000]	95.3	96.5	95.8	0.915	0.99	87.9	86.6	87.4	0.744	0.93	84.6	84.1	84.4	0.685	0.92
	2.5	2.0	1.9	0.038	0.00	3.5	3.8	1.8	0.037	0.02	3.8	6.1	1.5	0.027	0.01
ADORA2A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	98.1	93.7	96.6	0.924	0.99	96.8	90.8	94.8	0.883	0.98	96.8	90.3	94.7	0.880	0.98
	0.5	2.3	0.5	0.012	0.00	0.6	1.9	0.5	0.010	0.00	1.7	3.1	1.0	0.023	0.00
[1000,1000]	99.0	78.1	91.7	0.787	1.00	97.3	92.4	95.6	0.903	0.98	96.7	91.3	94.8	0.884	0.98
	0.2	41.6	14.7	0.388	0.00	0.4	1.6	0.5	0.010	0.01	1.3	2.0	0.9	0.018	0.00
AR	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	76.1	99.4	93.2	0.823	0.95	69.2	97.8	90.2	0.740	0.87	68.0	98.1	90.1	0.737	0.87
	2.3	0.3	0.5	0.012	0.01	1.4	0.7	0.7	0.016	0.01	1.6	0.6	1.1	0.023	0.02
[1000,1000]	73.2	99.4	92.5	0.803	0.94	65.9	97.9	89.3	0.718	0.87	64.5	98.2	89.2	0.715	0.87
	8.2	0.4	2.1	0.058	0.03	4.7	1.6	0.7	0.018	0.02	6.7	1.6	1.7	0.034	0.01

KCNH2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.2	90.5	93.9	0.874	0.98	84.9	69.7	78.8	0.555	0.86	85.1	65.5	77.3	0.519	0.84
	1.0	3.4	0.8	0.017	0.00	2.4	4.2	0.6	0.016	0.01	1.8	4.6	0.9	0.023	0.01
[1000,1000]	95.0	87.4	92.0	0.838	0.98	84.3	66.9	77.2	0.532	0.86	83.4	65.6	76.2	0.510	0.84
	4.3	9.8	1.8	0.037	0.00	9.1	12.9	2.0	0.032	0.01	9.4	14.4	1.7	0.035	0.02
SLC6A4	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	99.4	95.8	98.6	0.959	1.00	98.2	86.1	95.6	0.867	0.98	98.6	86.8	96.0	0.882	0.99
	0.0	0.8	0.2	0.005	0.00	0.4	1.9	0.2	0.009	0.00	0.6	3.5	0.8	0.021	0.01
[1000,1000]	99.4	98.2	99.1	0.975	1.00	98.1	91.1	96.5	0.897	0.99	98.4	90.5	96.6	0.901	0.99
	0.3	0.7	0.1	0.003	0.00	0.5	1.9	0.2	0.008	0.00	0.5	3.4	0.8	0.019	0.01
ADRA2A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	93.2	97.9	95.7	0.915	0.99	88.8	92.9	91.1	0.821	0.96	88.3	93.3	90.9	0.817	0.96
	0.3	0.2	0.1	0.003	0.00	3.5	2.7	1.7	0.034	0.01	3.9	2.7	1.4	0.031	0.01
[1000,1000]	95.4	98.7	97.2	0.944	0.99	88.6	93.4	91.2	0.823	0.96	88.4	93.7	91.2	0.822	0.96
	1.1	0.5	0.4	0.007	0.00	1.3	0.6	0.7	0.014	0.01	4.2	1.6	1.9	0.039	0.01

ADRB1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	94.3	91.8	93.1	0.862	0.98	92.8	93.9	93.2	0.864	0.97	92.4	91.5	92.1	0.839	0.96
	0.3	0.5	0.2	0.004	0.00	2.0	1.0	0.8	0.016	0.01	1.9	0.8	0.9	0.018	0.01
[1000,1000]	96.1	93.6	94.9	0.898	0.99	92.1	91.0	91.6	0.831	0.96	92.5	91.5	92.1	0.839	0.97
	0.6	0.8	0.4	0.008	0.00	1.4	1.4	1.4	0.028	0.01	1.7	0.4	1.0	0.021	0.01
ADRB2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	76.8	95.5	86.4	0.739	0.96	69.9	92.3	81.3	0.642	0.89	69.1	92.0	80.7	0.629	0.88
	5.6	0.9	2.1	0.035	0.00	3.5	3.4	1.2	0.025	0.01	5.9	2.5	2.2	0.038	0.01
[1000,1000]	75.1	95.4	85.4	0.722	0.95	68.7	91.9	80.6	0.626	0.88	67.6	92.4	80.4	0.624	0.88
	4.8	1.7	1.7	0.027	0.00	4.8	2.8	1.1	0.010	0.01	6.6	3.4	1.6	0.031	0.02
OPRD1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.6	87.5	94.6	0.869	0.99	96.4	81.7	92.3	0.805	0.97	96.5	81.6	92.3	0.807	0.96
	0.3	1.2	0.2	0.006	0.00	0.8	1.9	0.5	0.013	0.00	1.0	5.7	1.1	0.028	0.01
[1000,1000]	98.2	91.0	96.1	0.905	0.99	96.0	84.2	92.7	0.818	0.97	96.4	82.1	92.3	0.809	0.97
	0.2	1.9	0.5	0.013	0.00	1.1	2.6	0.4	0.012	0.01	1.6	6.3	1.0	0.027	0.01

DRD1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	83.9	98.3	92.5	0.846	0.97	78.4	93.9	87.7	0.742	0.94	78.5	94.8	88.2	0.755	0.93
	1.1	0.3	0.3	0.006	0.01	1.2	0.9	0.7	0.014	0.01	3.5	1.6	1.5	0.028	0.01
[1000,1000]	83.9	97.6	92.1	0.837	0.97	79.3	95.7	89.1	0.774	0.94	78.7	94.0	87.7	0.746	0.93
	1.7	0.3	0.6	0.011	0.00	3.5	0.5	1.3	0.026	0.00	4.4	2.3	1.6	0.029	0.01
DRD2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	99.1	83.6	96.6	0.872	0.99	98.8	79.2	94.8	0.832	0.97	98.8	78.0	95.3	0.824	0.97
	0.2	1.6	0.2	0.009	0.00	0.4	2.6	1.7	0.020	0.01	0.7	5.0	1.1	0.034	0.01
[1000,1000]	99.1	90.7	97.7	0.916	0.99	98.4	83.4	95.9	0.848	0.98	98.3	82.2	95.6	0.838	0.97
	0.2	2.2	0.2	0.012	0.00	0.7	2.5	0.6	0.016	0.00	0.8	4.5	0.8	0.015	0.01
SLC6A3	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.9	97.6	96.7	0.933	0.99	92.1	92.1	92.1	0.840	0.97	91.8	91.8	91.8	0.834	0.96
	0.5	0.7	0.3	0.005	0.00	1.3	1.9	0.9	0.018	0.00	2.0	1.5	1.3	0.025	0.01
[1000,1000]	95.1	96.0	95.5	0.910	0.99	92.3	91.9	92.1	0.841	0.97	91.9	90.7	91.4	0.826	0.97
	1.7	3.1	0.6	0.012	0.00	3.0	4.7	1.3	0.027	0.01	2.2	5.7	1.4	0.029	0.01

EDNRA	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	98.0	96.3	97.2	0.943	0.99	96.3	94.7	95.5	0.910	0.97	96.2	95.4	95.8	0.916	0.97
	0.7	0.2	0.3	0.007	0.00	0.7	2.6	1.3	0.025	0.02	1.9	1.1	1.0	0.020	0.02
[1000,1000]	98.5	96.6	97.6	0.952	0.99	96.8	94.8	95.9	0.918	0.98	96.4	95.2	95.8	0.915	0.97
	0.4	0.7	0.2	0.004	0.01	1.5	0.3	0.8	0.016	0.01	1.7	1.1	1.2	0.024	0.02
NR3C1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	74.4	99.5	91.9	0.809	0.95	69.1	98.9	90.0	0.759	0.90	69.7	98.7	90.0	0.759	0.89
	1.3	0.2	0.3	0.007	0.00	2.3	0.5	0.6	0.012	0.01	4.2	0.7	0.7	0.020	0.01
[1000,1000]	74.9	99.2	91.9	0.807	0.94	69.7	98.2	89.6	0.750	0.89	69.6	98.6	89.8	0.756	0.89
	3.4	0.3	0.8	0.019	0.00	4.2	0.9	0.7	0.017	0.01	3.1	0.9	0.8	0.016	0.02
HRH1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.6	95.2	95.4	0.908	0.99	93.3	91.6	92.4	0.849	0.98	92.0	91.1	91.7	0.832	0.97
	0.8	2.0	0.6	0.012	0.00	1.7	3.3	1.7	0.032	0.01	2.1	4.0	2.7	0.056	0.01
[1000,1000]	97.5	95.8	96.7	0.934	0.99	94.7	91.4	93.2	0.863	0.98	93.6	89.8	91.8	0.835	0.97
	0.6	1.1	0.3	0.006	0.00	1.9	2.6	2.1	0.041	0.01	0.6	4.9	2.2	0.045	0.01

OPRM1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.7	96.7	97.3	0.943	0.99	96.2	91.6	94.4	0.882	0.98	95.6	91.6	94.0	0.874	0.98
	0.6	0.8	0.1	0.001	0.00	1.4	1.7	1.5	0.031	0.00	1.1	1.3	0.4	0.007	0.00
[1000,1000]	97.6	95.8	96.9	0.935	0.99	95.8	90.6	93.8	0.869	0.98	95.2	91.1	93.6	0.865	0.98
	0.4	1.6	0.4	0.009	0.00	1.3	1.5	0.9	0.018	0.00	0.9	1.3	0.1	0.003	0.00
CHRM1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.2	91.4	95.0	0.894	0.99	95.2	85.0	91.2	0.814	0.96	94.5	86.1	91.3	0.814	0.96
	0.5	2.0	0.4	0.010	0.00	1.2	2.8	0.9	0.018	0.01	2.0	2.3	1.3	0.030	0.02
[1000,1000]	98.1	93.5	96.4	0.923	0.99	95.0	87.1	92.0	0.830	0.96	95.2	86.5	91.9	0.826	0.96
	0.6	1.9	0.6	0.014	0.00	1.4	2.4	0.9	0.016	0.01	0.6	3.2	1.3	0.025	0.01
CHRM2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	94.0	97.4	95.9	0.917	0.99	89.1	95.4	92.6	0.850	0.98	87.3	95.2	91.7	0.833	0.97
	2.6	1.1	0.7	0.014	0.00	3.9	1.4	1.5	0.027	0.01	5.2	1.8	1.8	0.036	0.01
[1000,1000]	96.6	97.4	97.0	0.940	0.99	92.7	92.4	92.6	0.852	0.97	91.9	92.7	92.4	0.846	0.97
	1.3	1.5	0.4	0.007	0.00	3.3	2.6	1.1	0.022	0.01	3.0	2.0	1.2	0.024	0.01

CHRM3	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.9	94.3	95.2	0.902	0.99	92.9	89.1	91.3	0.821	0.97	92.9	88.1	90.9	0.813	0.96
	0.6	1.1	0.3	0.005	0.00	1.1	1.5	0.8	0.016	0.01	2.1	3.2	1.1	0.023	0.01
[1000,1000]	96.6	96.8	96.7	0.933	1.00	93.6	89.7	92.0	0.834	0.97	92.4	89.4	91.2	0.820	0.97
	1.2	1.3	0.4	0.007	0.01	1.9	1.6	0.5	0.011	0.01	3.4	3.1	1.2	0.023	0.01
SLC6A2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.5	95.9	95.7	0.911	0.99	94.0	91.4	92.9	0.854	0.97	94.0	91.8	93.2	0.858	0.97
	0.9	0.8	0.3	0.006	0.00	0.5	2.2	1.1	0.023	0.00	2.2	1.9	1.1	0.023	0.00
[1000,1000]	96.1	96.6	96.3	0.924	0.99	94.8	92.6	93.9	0.873	0.97	94.0	92.0	93.2	0.860	0.97
	0.6	0.8	0.2	0.003	0.00	0.6	1.7	0.5	0.011	0.01	2.1	2.1	0.9	0.018	0.01
HTR2A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	99.0	92.8	97.7	0.932	0.99	98.7	88.9	96.7	0.895	0.98	98.5	87.2	96.1	0.882	0.98
	0.1	1.4	0.2	0.007	0.00	0.4	5.0	1.2	0.035	0.01	0.4	2.1	0.6	0.018	0.00
[1000,1000]	99.3	95.4	98.4	0.954	1.00	98.6	88.4	96.5	0.893	0.98	98.5	88.4	96.3	0.890	0.98
	0.2	1.2	0.2	0.004	0.00	0.5	2.7	0.5	0.014	0.01	0.5	2.4	0.5	0.016	0.01

HTR3A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	85.9	99.2	95.3	0.886	0.98	79.6	98.2	92.3	0.821	0.97	78.5	98.2	92.4	0.815	0.96
	6.6	0.6	1.6	0.041	0.01	6.0	1.6	1.4	0.022	0.01	15.2	1.6	3.7	0.090	0.02
[1000,1000]	91.7	99.8	97.3	0.937	0.99	83.9	96.9	93.3	0.830	0.96	82.5	98.1	93.5	0.842	0.97
	2.4	0.1	0.7	0.016	0.00	5.4	0.9	1.3	0.035	0.01	8.1	0.7	2.0	0.050	0.02
LCK	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	98.0	83.9	94.7	0.850	0.98	96.9	78.1	92.6	0.783	0.96	97.1	73.6	91.8	0.758	0.95
	0.5	2.6	0.4	0.011	0.01	0.8	5.3	1.6	0.039	0.02	1.5	3.7	2.3	0.031	0.02
[1000,1000]	98.1	92.3	96.7	0.908	0.99	95.8	83.5	93.1	0.798	0.96	95.6	83.1	93.8	0.805	0.96
	0.6	2.8	0.4	0.008	0.00	1.0	4.6	1.0	0.028	0.01	2.3	9.4	2.4	0.069	0.02
AVPR1A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.6	99.0	98.4	0.967	0.99	95.3	97.0	96.4	0.922	0.99	94.3	97.0	96.1	0.915	0.98
	0.3	0.6	0.3	0.007	0.00	1.8	1.1	1.1	0.025	0.01	3.4	1.3	1.1	0.025	0.01
[1000,1000]	98.3	99.3	98.9	0.977	1.00	96.7	97.1	97.0	0.935	0.99	96.5	97.4	97.0	0.936	0.99
	0.8	0.3	0.3	0.005	0.00	1.3	1.1	0.9	0.019	0.01	1.3	0.7	0.6	0.012	0.00

AGTR1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	87.2	100.0	94.8	0.895	0.99	85.2	99.2	93.6	0.869	0.97	82.6	99.2	92.8	0.849	0.97
	2.2	0.1	0.8	0.016	0.00	2.9	0.6	1.0	0.019	0.01	7.0	0.3	1.8	0.047	0.01
[1000,1000]	91.8	99.9	96.6	0.930	0.99	85.9	98.8	93.7	0.870	0.97	84.4	99.1	93.5	0.861	0.97
	1.9	0.1	0.6	0.013	0.00	3.4	0.8	1.2	0.023	0.01	7.6	0.6	1.9	0.047	0.02
AKT1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.6	92.8	96.1	0.909	0.99	96.3	89.8	94.3	0.866	0.98	95.9	88.7	93.7	0.851	0.97
	0.3	1.3	0.3	0.007	0.01	0.6	3.3	0.9	0.023	0.01	1.2	3.5	1.9	0.038	0.01
[1000,1000]	98.4	94.8	97.3	0.936	0.99	97.3	89.4	95.0	0.878	0.98	96.1	88.9	93.9	0.854	0.97
	0.4	1.2	0.2	0.005	0.00	0.6	2.2	0.7	0.016	0.01	0.9	4.3	1.6	0.035	0.01
BACE1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.8	90.3	94.8	0.877	0.98	95.5	86.8	92.9	0.830	0.97	95.4	85.6	92.5	0.819	0.97
	0.7	1.1	0.2	0.002	0.00	0.8	1.8	0.4	0.010	0.00	0.7	2.9	1.0	0.023	0.01
[1000,1000]	97.7	90.3	95.4	0.891	0.99	96.3	84.5	92.6	0.825	0.97	95.8	84.8	92.6	0.821	0.97
	0.6	2.6	0.5	0.012	0.00	1.2	2.3	0.5	0.011	0.01	1.5	5.1	0.7	0.018	0.00

BCHE	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	85.6	96.8	92.4	0.841	0.97	76.8	93.0	86.7	0.719	0.93	76.1	93.1	86.3	0.713	0.93
	3.1	1.0	0.7	0.015	0.00	4.6	2.5	0.7	0.009	0.01	4.6	1.1	1.8	0.032	0.01
[1000,1000]	89.1	96.7	93.7	0.868	0.98	80.9	93.5	88.5	0.760	0.94	79.4	92.4	87.1	0.732	0.94
	3.3	1.0	0.8	0.016	0.00	5.2	2.2	1.5	0.032	0.02	6.0	2.6	1.9	0.032	0.01
CASP1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	75.5	97.0	90.5	0.770	0.97	68.4	95.2	87.3	0.683	0.90	67.9	94.7	86.6	0.669	0.89
	1.2	0.6	0.6	0.014	0.00	2.5	0.8	1.1	0.024	0.01	2.9	0.9	1.6	0.034	0.02
[1000,1000]	69.2	97.1	88.8	0.724	0.95	65.5	96.0	86.6	0.676	0.90	62.5	96.0	85.9	0.651	0.89
	4.7	0.8	0.8	0.021	0.00	6.4	1.6	1.7	0.037	0.02	6.8	1.3	1.9	0.040	0.02
CASP3	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	85.0	97.4	92.6	0.844	0.98	79.2	95.3	88.9	0.768	0.94	79.4	95.3	89.1	0.769	0.95
	2.0	0.5	0.6	0.012	0.00	3.7	1.1	1.0	0.017	0.01	3.1	2.0	1.5	0.035	0.01
[1000,1000]	84.1	98.3	92.8	0.851	0.99	77.8	96.1	89.0	0.771	0.96	77.5	95.9	88.7	0.763	0.95
	6.8	1.0	2.0	0.039	0.00	10.1	2.3	2.7	0.052	0.02	5.0	1.5	2.2	0.045	0.01

CASP8	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	88.0	98.6	96.2	0.890	0.98	85.4	98.6	95.7	0.872	0.97	86.6	98.2	95.5	0.871	0.96
	1.9	0.2	0.4	0.012	0.00	4.8	0.6	0.6	0.025	0.01	3.3	0.8	1.3	0.035	0.03
[1000,1000]	89.7	98.9	96.9	0.909	0.99	89.0	98.9	96.6	0.903	0.96	88.0	98.3	96.0	0.883	0.97
	2.5	0.2	0.5	0.015	0.00	4.0	1.0	1.2	0.038	0.02	4.8	0.7	1.1	0.037	0.03
CHRM5	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	91.6	98.1	95.6	0.907	0.99	82.5	95.7	90.5	0.802	0.96	83.8	93.9	90.1	0.791	0.96
	3.4	0.2	1.2	0.025	0.00	5.4	2.1	1.4	0.029	0.01	3.3	3.9	2.2	0.042	0.02
[1000,1000]	92.4	98.7	96.3	0.922	0.99	83.0	96.1	91.1	0.811	0.96	80.6	96.1	90.2	0.792	0.96
	1.9	0.4	0.5	0.010	0.00	1.5	1.9	1.0	0.021	0.01	9.5	1.3	3.9	0.080	0.01
CHUK	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	83.9	99.2	95.8	0.877	0.99	74.4	99.0	93.1	0.804	0.99	72.2	99.1	92.9	0.794	0.98
	11.1	0.5	2.1	0.066	0.00	10.8	0.5	2.2	0.064	0.01	16.0	0.6	4.3	0.106	0.01
[1000,1000]	94.4	98.8	97.8	0.936	0.99	85.6	98.4	95.6	0.869	0.99	82.7	97.8	94.5	0.839	0.98
	4.1	0.6	0.8	0.028	0.00	9.2	1.5	2.5	0.075	0.02	7.3	1.6	0.6	0.021	0.01

CSF1R	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.6	98.2	97.9	0.957	1.00	95.2	93.5	94.5	0.888	0.99	95.5	95.0	95.3	0.905	0.99
	0.6	1.2	0.3	0.006	0.00	1.7	1.3	0.6	0.012	0.00	1.7	1.9	1.3	0.027	0.01
[1000,1000]	98.2	97.9	98.1	0.961	1.00	96.3	94.3	95.3	0.907	0.99	95.8	93.1	94.7	0.893	0.99
	0.7	1.8	0.5	0.010	0.00	2.8	2.5	1.3	0.025	0.00	2.4	4.2	1.9	0.038	0.01
CSNK1D	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	94.7	98.8	97.1	0.941	0.99	88.4	94.7	92.2	0.837	0.97	88.6	95.7	92.7	0.850	0.97
	1.2	0.6	0.6	0.012	0.00	4.4	1.2	1.5	0.034	0.01	4.8	1.9	2.4	0.047	0.01
[1000,1000]	89.7	97.5	94.4	0.886	0.99	84.8	94.4	90.4	0.806	0.97	84.8	95.0	90.8	0.813	0.97
	7.7	2.5	1.9	0.037	0.00	6.7	5.6	1.2	0.025	0.01	9.3	3.3	2.6	0.049	0.01
EDNRB	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	94.4	97.6	96.3	0.924	1.00	91.8	96.7	94.9	0.891	0.99	85.4	96.4	91.9	0.830	0.98
	1.9	1.1	0.7	0.014	0.00	2.9	1.2	1.1	0.023	0.00	5.5	2.4	2.7	0.050	0.01
[1000,1000]	97.8	97.5	97.6	0.950	1.00	96.0	94.1	94.9	0.895	0.99	92.6	94.7	93.9	0.870	0.99
	1.3	0.9	0.5	0.011	0.00	1.9	3.7	2.3	0.046	0.01	3.5	2.1	1.6	0.040	0.01

ELANE	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.1	95.0	95.0	0.897	0.99	93.2	91.0	92.4	0.840	0.98	91.5	91.1	91.6	0.824	0.97
	0.9	0.9	0.5	0.010	0.00	1.2	2.8	0.7	0.017	0.00	4.0	2.1	1.5	0.022	0.01
[1000,1000]	94.4	96.1	95.1	0.899	0.99	91.3	92.1	91.6	0.826	0.97	90.6	92.4	91.5	0.824	0.97
	1.3	0.7	0.6	0.012	0.00	2.3	1.6	1.4	0.029	0.01	4.9	2.6	2.2	0.037	0.01
EPHA2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	90.6	99.9	96.9	0.929	1.00	85.1	99.7	94.8	0.885	0.98	82.7	99.8	94.9	0.874	0.98
	0.7	0.2	0.3	0.004	0.01	4.2	0.3	1.8	0.034	0.01	8.0	0.3	1.3	0.045	0.01
[1000,1000]	96.0	99.8	98.6	0.968	1.00	90.9	98.8	96.1	0.913	0.99	89.0	99.0	96.1	0.905	0.98
	1.7	0.2	0.5	0.012	0.00	1.8	0.6	0.7	0.015	0.01	3.7	0.8	0.3	0.012	0.01
FGFR1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.2	93.7	96.0	0.912	0.99	95.6	89.8	93.5	0.860	0.98	95.7	89.3	93.5	0.858	0.98
	0.7	1.9	0.3	0.007	0.00	1.7	2.9	1.0	0.021	0.01	3.0	2.1	2.5	0.042	0.01
[1000,1000]	98.1	92.8	96.2	0.917	0.99	96.5	87.4	93.3	0.852	0.98	96.5	86.9	93.1	0.848	0.97
	0.7	2.5	0.5	0.012	0.00	1.5	1.8	0.5	0.012	0.00	1.5	5.7	3.3	0.061	0.01

FKBP1A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	94.7	98.3	97.4	0.932	0.99	89.5	97.4	95.2	0.879	0.99	93.9	96.0	95.4	0.884	0.99
	3.8	0.9	0.5	0.014	0.01	6.6	2.3	1.4	0.037	0.00	3.4	4.3	2.8	0.068	0.01
[1000,1000]	94.1	97.4	96.2	0.904	1.00	90.6	97.6	95.7	0.886	0.99	89.0	97.5	95.7	0.877	0.99
	3.4	2.9	3.5	0.086	0.01	4.6	1.6	1.1	0.032	0.00	10.1	1.3	2.3	0.085	0.01
FLT1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.6	98.9	97.8	0.950	0.99	91.6	97.8	95.7	0.904	0.98	91.2	97.8	95.6	0.901	0.98
	0.9	0.4	0.1	0.003	0.00	1.7	0.8	0.2	0.004	0.01	2.5	0.9	0.8	0.016	0.01
[1000,1000]	96.2	99.4	98.3	0.963	1.00	91.7	98.2	96.0	0.911	0.99	91.3	97.8	95.5	0.901	0.99
	1.4	0.3	0.3	0.007	0.00	3.5	0.8	0.7	0.016	0.01	4.0	1.1	0.9	0.019	0.01
FLT4	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.1	99.1	97.5	0.948	0.99	90.3	98.0	95.2	0.896	0.98	89.5	96.7	93.8	0.871	0.98
	1.2	0.5	0.3	0.007	0.00	6.6	0.8	2.3	0.049	0.01	3.4	2.0	1.2	0.022	0.01
[1000,1000]	96.3	99.5	98.3	0.964	0.99	88.9	98.3	94.8	0.890	0.98	86.9	97.6	93.4	0.862	0.98
	2.0	0.3	0.7	0.015	0.01	7.3	1.2	2.4	0.052	0.01	3.8	1.1	1.2	0.021	0.01

FYN	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	80.9	99.4	94.4	0.857	0.98	62.6	97.5	87.1	0.682	0.93	58.3	97.2	86.1	0.641	0.92
	4.1	0.2	0.9	0.026	0.01	5.4	1.4	1.6	0.051	0.01	6.5	1.7	2.1	0.035	0.02
[1000,1000]	84.4	99.7	95.4	0.885	0.98	64.3	96.3	87.1	0.672	0.92	65.9	97.0	88.2	0.696	0.93
	3.2	0.3	0.6	0.017	0.01	6.1	2.1	1.0	0.018	0.02	8.1	2.1	1.8	0.051	0.01
GSK3B	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.1	88.9	94.4	0.872	0.98	94.4	80.1	89.8	0.764	0.95	94.8	79.9	89.8	0.767	0.95
	1.0	2.9	1.2	0.027	0.00	1.8	2.4	1.1	0.022	0.01	1.6	5.3	1.6	0.031	0.01
[1000,1000]	98.8	90.6	96.1	0.911	0.99	95.9	78.3	90.1	0.772	0.96	96.2	77.3	89.9	0.769	0.95
	0.3	3.9	1.1	0.024	0.00	1.3	4.3	0.8	0.019	0.01	1.7	4.4	1.6	0.031	0.01
HDAC3	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.2	95.0	96.1	0.921	0.99	94.5	93.9	94.2	0.884	0.98	94.5	93.3	93.9	0.877	0.97
	0.5	0.5	0.1	0.001	0.00	1.0	1.9	1.3	0.026	0.01	1.9	2.0	1.5	0.031	0.01
[1000,1000]	97.1	96.4	96.8	0.935	0.99	94.1	93.8	94.0	0.879	0.97	94.2	93.5	93.8	0.876	0.97
	1.0	1.3	0.3	0.006	0.00	2.8	2.2	0.4	0.010	0.01	1.9	1.5	0.8	0.016	0.01

IGF1R	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.6	95.8	97.1	0.932	0.99	96.3	90.8	94.6	0.874	0.99	95.6	92.4	94.5	0.877	0.98
	0.7	1.4	0.3	0.005	0.01	0.9	2.9	0.4	0.013	0.00	1.4	2.6	1.8	0.032	0.01
[1000,1000]	97.6	98.2	97.7	0.948	1.00	95.4	94.9	95.2	0.892	0.99	94.6	95.2	95.0	0.889	0.98
	0.8	1.0	0.3	0.009	0.00	2.3	2.6	1.6	0.033	0.00	3.3	3.0	2.3	0.036	0.01
INSR	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	94.8	98.6	96.9	0.938	0.99	91.8	96.6	94.4	0.888	0.99	90.0	96.5	93.9	0.872	0.99
	1.8	1.0	0.6	0.012	0.01	3.1	2.0	0.6	0.012	0.00	4.1	1.8	1.4	0.033	0.01
[1000,1000]	98.3	99.0	98.7	0.973	1.00	91.2	96.4	94.1	0.881	0.99	92.6	96.5	94.8	0.891	0.99
	0.7	0.4	0.3	0.007	0.00	2.2	1.4	0.8	0.015	0.01	2.5	2.4	1.7	0.037	0.00
KDR	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.1	73.6	93.2	0.746	0.97	96.7	68.9	91.9	0.702	0.96	96.6	66.5	91.6	0.679	0.95
	0.7	3.6	0.7	0.028	0.01	0.8	4.1	0.7	0.027	0.01	1.0	7.2	0.6	0.037	0.01
[1000,1000]	97.2	91.0	96.1	0.865	0.99	95.6	82.1	93.3	0.769	0.96	95.7	79.2	92.9	0.747	0.95
	1.2	4.2	0.6	0.015	0.00	2.3	6.4	1.1	0.022	0.01	1.6	6.9	0.9	0.030	0.01

LTB4R	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	86.9	99.8	96.6	0.909	0.99	84.5	99.5	95.3	0.883	0.97	81.0	99.6	95.0	0.864	0.97
	3.4	0.2	0.9	0.024	0.00	6.9	0.4	2.7	0.055	0.01	4.7	0.4	0.5	0.024	0.01
[1000,1000]	91.8	99.9	97.9	0.942	1.00	83.7	99.7	95.4	0.883	0.96	84.4	99.8	95.9	0.892	0.97
	1.8	0.1	0.5	0.013	0.01	4.7	0.4	0.9	0.024	0.01	2.8	0.5	0.7	0.015	0.01
LYN	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	90.7	98.8	96.4	0.914	0.99	79.6	97.8	92.3	0.815	0.97	81.5	98.1	93.1	0.833	0.97
	1.4	0.3	0.3	0.009	0.00	2.6	0.8	1.2	0.031	0.01	3.0	0.7	0.7	0.026	0.01
[1000,1000]	91.9	98.6	96.5	0.918	0.99	82.5	97.8	93.2	0.836	0.97	82.5	98.0	93.4	0.839	0.97
	2.8	0.5	0.5	0.013	0.00	7.2	0.8	2.1	0.053	0.01	4.5	0.7	1.1	0.035	0.01
MAPK1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	45.8	99.0	79.9	0.572	0.85	43.4	98.6	78.6	0.543	0.77	42.4	98.4	78.3	0.531	0.77
	5.2	1.0	1.1	0.021	0.01	2.7	1.6	0.6	0.019	0.01	1.9	1.6	0.8	0.037	0.02
[1000,1000]	49.6	97.8	80.4	0.580	0.86	46.4	96.1	78.5	0.527	0.78	45.0	96.2	77.8	0.514	0.77
	9.5	2.6	1.8	0.031	0.01	6.7	4.3	0.9	0.027	0.01	3.1	4.2	1.4	0.054	0.01

MAPK9	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.7	97.6	97.7	0.953	1.00	96.0	93.9	95.0	0.900	0.99	94.3	92.7	93.5	0.870	0.99
	0.5	0.3	0.2	0.005	0.00	1.4	1.4	1.0	0.019	0.01	2.7	2.4	0.8	0.017	0.01
[1000,1000]	98.6	98.9	98.7	0.975	1.00	95.3	94.9	95.1	0.901	0.99	94.2	94.9	94.5	0.891	0.99
	0.6	0.6	0.1	0.002	0.00	0.6	3.2	1.1	0.024	0.00	2.3	2.2	0.4	0.009	0.00
MAPKAPK2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	93.5	96.8	95.4	0.905	0.99	86.6	93.3	90.5	0.803	0.97	85.7	93.6	90.3	0.800	0.96
	2.5	1.1	0.6	0.012	0.00	1.8	1.8	1.1	0.021	0.01	3.5	2.6	1.5	0.023	0.01
[1000,1000]	94.4	96.7	95.8	0.912	0.99	88.1	93.0	90.9	0.815	0.97	86.2	93.3	90.2	0.799	0.96
	1.5	1.3	0.7	0.014	0.00	1.8	1.5	0.4	0.008	0.01	3.0	2.0	1.3	0.019	0.01
MET	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	98.6	94.3	97.3	0.934	1.00	96.7	89.3	94.6	0.867	0.98	97.1	88.8	94.7	0.869	0.98
	0.2	1.2	0.2	0.006	0.01	1.1	2.0	0.4	0.008	0.01	1.2	2.3	0.7	0.012	0.01
[1000,1000]	98.7	95.4	97.8	0.945	1.00	97.9	89.5	95.5	0.889	0.99	97.4	89.6	95.2	0.882	0.98
	0.3	1.1	0.3	0.007	0.00	0.4	2.3	0.8	0.020	0.00	1.1	2.1	0.6	0.011	0.01

MMP13	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	97.8	93.8	96.5	0.919	0.99	96.7	90.1	94.5	0.876	0.98	96.4	90.7	94.6	0.875	0.98
	0.7	1.6	0.1	0.003	0.00	1.5	3.4	0.8	0.017	0.01	1.5	3.7	0.7	0.019	0.01
[1000,1000]	97.8	95.9	97.2	0.935	0.99	95.6	91.7	94.4	0.871	0.98	96.2	91.7	94.7	0.879	0.98
	0.5	1.4	0.2	0.005	0.00	0.8	3.0	1.2	0.029	0.01	1.0	1.4	0.6	0.015	0.01
MMP2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.4	93.7	95.4	0.900	0.99	94.4	89.3	92.5	0.838	0.98	94.0	87.1	91.5	0.816	0.97
	1.2	1.2	0.6	0.014	0.00	0.6	2.9	0.8	0.019	0.01	0.7	3.2	1.3	0.027	0.01
[1000,1000]	96.5	95.0	95.9	0.913	0.99	93.4	90.6	92.4	0.836	0.98	93.0	89.0	91.5	0.818	0.97
	1.2	1.6	0.4	0.008	0.00	1.9	4.1	0.8	0.017	0.01	2.1	3.1	1.5	0.030	0.00
MMP3	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.2	94.4	95.5	0.904	0.99	95.6	91.0	93.9	0.869	0.98	94.9	91.0	93.4	0.857	0.98
	0.7	0.7	0.3	0.007	0.00	1.2	2.7	1.2	0.024	0.01	0.5	1.5	0.7	0.014	0.01
[1000,1000]	96.8	94.5	95.9	0.914	0.99	95.4	93.3	94.7	0.885	0.98	94.5	91.0	93.1	0.852	0.98
	0.9	2.5	0.4	0.010	0.00	2.4	2.5	1.4	0.028	0.01	2.2	4.7	0.8	0.016	0.01

MMP9	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	85.9	94.2	89.3	0.790	0.96	84.4	88.9	86.3	0.725	0.93	83.8	88.8	85.9	0.718	0.92
	1.3	0.7	0.8	0.016	0.00	2.1	1.2	1.2	0.022	0.00	3.0	2.0	1.5	0.026	0.01
[1000,1000]	88.1	93.7	90.4	0.810	0.97	84.4	88.3	86.0	0.720	0.93	83.3	87.3	85.1	0.701	0.93
	1.5	1.3	0.5	0.009	0.00	1.0	2.5	1.3	0.026	0.01	3.5	1.8	1.4	0.020	0.01
NEK2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	83.9	99.4	95.9	0.880	0.99	71.7	98.2	92.7	0.768	0.96	70.7	98.7	92.7	0.773	0.96
	4.2	0.6	0.5	0.016	0.01	5.7	0.8	0.6	0.039	0.02	8.3	0.7	1.7	0.048	0.04
[1000,1000]	89.1	99.5	97.2	0.918	0.99	74.2	98.1	93.0	0.785	0.96	72.1	98.4	92.8	0.776	0.96
	3.6	0.2	0.7	0.019	0.00	7.0	1.4	1.0	0.042	0.01	9.6	1.0	1.2	0.047	0.04
P2RY1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.4	99.4	98.4	0.964	1.00	94.4	98.8	97.3	0.940	0.99	93.6	99.2	97.5	0.941	0.98
	1.0	0.3	0.4	0.009	0.01	1.0	0.2	0.3	0.006	0.00	5.7	0.7	1.5	0.038	0.02
[1000,1000]	97.0	99.3	98.5	0.967	1.00	95.4	99.2	98.0	0.954	0.99	93.8	99.2	97.3	0.940	0.98
	1.9	0.4	0.4	0.010	0.00	3.2	0.6	1.0	0.022	0.01	1.3	1.0	0.7	0.018	0.02

PAK4	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	92.6	99.9	98.0	0.949	0.99	80.7	99.1	94.4	0.850	0.97	79.8	99.0	94.1	0.841	0.97
	2.9	0.1	0.6	0.017	0.00	3.7	0.8	1.6	0.035	0.02	10.2	0.9	2.2	0.060	0.02
[1000,1000]	94.9	99.9	98.6	0.965	0.99	85.5	98.9	95.7	0.881	0.97	83.9	98.5	94.7	0.859	0.97
	2.0	0.1	0.4	0.011	0.01	6.8	1.0	1.1	0.035	0.02	8.1	1.9	2.2	0.058	0.02
PDE4A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	92.3	98.2	95.9	0.914	0.99	88.0	95.8	92.8	0.848	0.96	84.0	95.8	91.5	0.819	0.96
	1.0	0.5	0.3	0.005	0.00	3.8	1.5	1.5	0.031	0.01	9.9	2.0	2.3	0.059	0.01
[1000,1000]	94.9	99.0	97.4	0.946	1.00	88.0	96.8	93.4	0.861	0.97	85.8	96.3	92.5	0.839	0.97
	0.9	0.5	0.4	0.008	0.00	2.7	2.0	0.3	0.007	0.01	8.4	1.0	2.2	0.054	0.01
PDE5A	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	95.6	94.7	95.2	0.903	0.98	92.6	90.0	91.5	0.827	0.96	92.6	89.4	91.1	0.820	0.95
	1.0	1.6	0.5	0.011	0.00	1.3	2.5	0.9	0.017	0.00	2.0	4.3	1.5	0.028	0.03
[1000,1000]	95.9	97.2	96.5	0.929	0.99	92.4	92.7	92.6	0.850	0.97	92.1	91.0	91.6	0.828	0.96
	1.2	1.3	0.3	0.006	0.00	2.6	2.1	0.7	0.011	0.01	2.3	2.9	1.8	0.032	0.02

PIK3CA	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	99.3	93.3	97.5	0.940	0.99	99.0	90.1	96.2	0.911	0.99	99.0	90.6	96.5	0.917	0.99
	0.2	1.5	0.4	0.008	0.01	0.4	2.2	0.6	0.013	0.00	0.7	3.1	0.8	0.019	0.00
[1000,1000]	99.2	95.8	98.2	0.957	1.00	98.4	92.8	96.7	0.922	0.99	98.6	93.1	96.9	0.926	0.99
	0.2	1.0	0.3	0.006	0.00	0.5	1.7	0.6	0.015	0.00	0.5	1.2	0.6	0.013	0.00
PPARG	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	74.7	96.7	88.5	0.754	0.94	71.3	95.5	86.3	0.710	0.90	71.4	95.3	86.4	0.708	0.90
	2.9	1.3	0.6	0.012	0.00	3.6	1.8	0.7	0.016	0.01	2.9	2.1	1.1	0.021	0.01
[1000,1000]	74.0	97.7	88.8	0.763	0.95	71.2	96.1	86.9	0.718	0.91	69.6	96.3	86.3	0.708	0.91
	2.5	0.6	0.7	0.014	0.01	1.6	0.9	0.7	0.012	0.00	1.0	0.8	1.0	0.021	0.01
PTPN1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	87.0	95.5	92.1	0.836	0.98	76.2	90.3	84.7	0.677	0.92	70.4	87.9	80.8	0.595	0.89
	1.8	1.4	0.3	0.005	0.01	3.0	2.0	1.8	0.042	0.02	6.3	1.4	2.3	0.043	0.02
[1000,1000]	85.5	96.3	92.0	0.835	0.98	72.1	90.3	82.7	0.647	0.91	70.2	89.5	82.0	0.619	0.89
	6.5	2.8	1.1	0.021	0.00	9.9	5.1	2.3	0.038	0.01	5.3	4.1	2.8	0.048	0.01

PTPN11	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	66.8	98.8	91.7	0.747	0.97	37.0	96.7	82.6	0.455	0.88	39.2	97.5	84.2	0.492	0.89
	13.5	0.7	2.6	0.086	0.01	9.5	2.6	3.1	0.063	0.02	11.0	1.8	2.2	0.054	0.05
[1000,1000]	77.6	97.9	93.4	0.803	0.97	48.4	95.9	84.8	0.536	0.88	50.0	96.5	85.9	0.556	0.88
	2.5	0.7	1.0	0.027	0.00	1.8	2.2	1.8	0.052	0.03	14.2	1.1	2.9	0.103	0.05
PTPN2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	69.9	99.1	92.9	0.778	0.96	56.1	98.8	88.5	0.667	0.92	47.3	98.9	87.6	0.602	0.92
	3.8	0.2	0.6	0.023	0.01	7.5	0.3	2.0	0.054	0.02	18.9	1.1	3.6	0.129	0.02
[1000,1000]	81.9	99.0	95.3	0.859	0.98	75.0	97.4	92.5	0.770	0.94	64.2	97.7	90.4	0.703	0.93
	2.1	0.5	0.6	0.020	0.00	8.8	1.1	2.1	0.054	0.02	13.7	2.2	2.0	0.075	0.02
RAF1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	98.1	99.0	98.5	0.970	1.00	97.2	96.6	96.9	0.938	0.99	96.8	96.8	96.8	0.934	0.99
	0.5	0.4	0.2	0.005	0.00	0.6	1.6	0.5	0.010	0.01	0.9	2.6	0.8	0.016	0.01
[1000,1000]	98.7	99.4	99.0	0.980	1.00	96.9	97.3	97.1	0.942	1.00	96.2	96.9	96.5	0.929	0.99
	0.6	0.5	0.2	0.004	0.00	1.2	1.2	0.7	0.014	0.00	1.6	2.3	0.3	0.005	0.01

RARA	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	57.5	99.9	95.7	0.735	0.95	53.3	99.9	95.5	0.705	0.90	52.7	99.9	95.3	0.703	0.89
	4.7	0.1	0.5	0.030	0.02	9.0	0.1	0.9	0.062	0.03	7.3	0.1	0.6	0.048	0.03
[1000,1000]	73.0	99.9	97.3	0.835	0.98	64.5	99.8	96.1	0.772	0.91	61.9	99.7	96.0	0.752	0.91
	6.9	0.1	0.5	0.037	0.01	5.9	0.2	0.9	0.045	0.02	2.5	0.1	0.6	0.020	0.03
RARB	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	73.2	100.0	97.8	0.841	0.98	69.4	100.0	97.5	0.815	0.97	70.1	99.9	97.5	0.821	0.97
	13.0	0.0	1.0	0.077	0.01	20.9	0.0	1.7	0.138	0.01	8.1	0.1	0.6	0.048	0.03
[1000,1000]	91.4	99.9	99.2	0.947	0.99	86.7	99.9	98.8	0.919	0.97	85.2	99.8	98.6	0.905	0.96
	1.5	0.1	0.1	0.007	0.00	7.6	0.1	0.7	0.043	0.01	5.4	0.2	0.4	0.028	0.03
ROCK1	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	98.0	96.0	97.0	0.941	0.99	94.2	92.3	93.3	0.866	0.98	95.4	92.5	94.1	0.881	0.98
	0.5	1.1	0.5	0.010	0.01	1.5	1.6	0.9	0.018	0.01	1.3	1.8	0.7	0.015	0.00
[1000,1000]	98.9	96.6	97.9	0.957	1.00	95.7	91.8	93.9	0.877	0.98	95.7	91.6	93.8	0.876	0.98
	0.7	0.8	0.3	0.005	0.00	2.1	2.1	0.7	0.015	0.01	1.8	0.8	1.0	0.019	0.01

RPS6KA5	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	79.6	100.0	96.5	0.873	0.99	60.2	99.9	92.6	0.740	0.96	58.2	99.6	92.2	0.714	0.96
	8.3	0.0	1.3	0.052	0.00	7.1	0.2	1.6	0.043	0.02	8.2	0.6	1.6	0.061	0.01
[1000,1000]	88.8	100.0	98.0	0.931	1.00	65.9	99.8	94.2	0.777	0.96	65.5	99.4	93.5	0.760	0.97
	5.5	0.0	1.0	0.034	0.01	10.1	0.3	1.7	0.067	0.03	13.0	0.8	1.9	0.082	0.01
SIRT2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	78.5	98.9	94.3	0.833	0.98	65.3	97.8	91.1	0.710	0.93	51.7	97.3	87.8	0.593	0.92
	4.7	0.3	0.9	0.028	0.01	9.1	1.0	2.6	0.075	0.02	17.8	1.2	2.6	0.114	0.03
[1000,1000]	83.0	98.5	95.1	0.855	0.98	67.5	96.0	89.8	0.684	0.93	61.8	96.9	89.6	0.663	0.92
	4.5	0.5	0.8	0.029	0.01	9.5	1.9	2.3	0.043	0.02	13.9	0.9	2.1	0.092	0.03
SIRT3	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	79.3	98.9	96.5	0.833	0.97	71.5	98.0	94.9	0.739	0.95	71.1	98.6	95.6	0.761	0.93
	2.6	0.3	0.3	0.007	0.01	7.8	1.0	1.3	0.058	0.02	18.2	1.3	1.5	0.106	0.04
[1000,1000]	78.4	98.8	96.4	0.825	0.98	73.5	98.5	95.5	0.777	0.95	47.2	99.2	92.0	0.599	0.93
	5.4	0.6	0.2	0.015	0.01	17.0	1.1	1.4	0.091	0.03	20.4	0.8	4.5	0.117	0.04

SRC	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.3	91.6	94.6	0.883	0.99	92.5	87.8	90.8	0.803	0.97	92.6	86.8	90.5	0.794	0.96
	1.4	1.4	0.4	0.008	0.00	1.3	3.7	0.6	0.017	0.01	2.0	2.1	1.5	0.027	0.01
[1000,1000]	97.8	94.6	96.6	0.927	0.99	93.3	87.6	91.3	0.811	0.97	93.1	88.0	91.1	0.809	0.97
	0.9	1.9	0.3	0.007	0.00	2.7	2.6	1.4	0.026	0.00	2.0	3.6	0.9	0.014	0.01
TACR2	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	88.8	99.7	96.2	0.913	0.98	86.3	99.2	95.2	0.887	0.97	85.1	99.3	95.0	0.881	0.97
	2.2	0.2	0.5	0.013	0.00	2.5	0.3	0.7	0.020	0.01	3.0	0.7	0.6	0.018	0.01
[1000,1000]	90.2	99.8	96.8	0.926	0.99	87.9	99.3	95.8	0.901	0.97	85.5	99.2	95.1	0.884	0.97
	2.1	0.1	0.6	0.015	0.00	1.9	0.5	0.8	0.016	0.01	4.1	1.0	0.8	0.017	0.01
TBXA2R	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	93.2	97.4	95.9	0.910	0.99	90.9	95.8	94.2	0.870	0.97	90.4	96.0	94.1	0.869	0.97
	1.0	0.6	0.2	0.005	0.01	2.9	1.5	1.0	0.020	0.01	3.1	1.6	0.7	0.015	0.01
[1000,1000]	92.5	98.4	96.4	0.919	0.99	90.6	96.6	94.6	0.881	0.98	89.0	96.7	94.0	0.866	0.97
	2.7	0.9	0.6	0.013	0.00	3.8	2.1	0.6	0.013	0.01	3.5	2.0	0.9	0.020	0.01

TEK	Train					Validation					Test				
	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
[100,100]	96.1	97.7	97.0	0.938	0.99	92.9	96.5	95.1	0.898	0.98	93.2	96.5	95.1	0.897	0.98
	1.1	0.8	0.5	0.010	0.00	1.4	1.2	0.9	0.018	0.01	0.4	2.1	1.1	0.025	0.01
[1000,1000]	97.0	98.8	98.1	0.960	1.00	92.9	96.9	95.3	0.902	0.98	93.3	96.3	95.0	0.896	0.98
	0.3	0.7	0.3	0.007	0.00	2.0	2.0	1.0	0.019	0.01	2.3	1.3	0.9	0.021	0.01
AVERAGE	92.1	96.5	95.8	0.901	0.99	86.9	93.2	92.5	0.822	0.96	86.2	92.9	92.2	0.814	0.96
SD	8.8	4.2	3.1	0.069	0.02	11.7	5.9	4.1	0.091	0.04	12.1	6.5	4.2	0.093	0.04

Table S10. Summary model performance results for each target. In each case standard deviations are shown below averages. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC). The best model was chosen in each case based on Test set performance, with MCC taking preference.

AChE

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	496	0	27	392	100.0	6.4	57.2	0.190
22	Test 2	573	2	21	319	99.7	6.2	64.9	0.180
23	Test 3	499	7	74	335	98.6	18.1	62.6	0.292
24	Test 4	528	2	39	346	99.6	10.1	62.0	0.233
25	Test 5	501	4	68	342	99.2	16.6	62.2	0.292
	Avg	519	3	46	347	99.4	11.5	61.8	0.237
	SD	33	3	24	27	0.5	5.6	2.8	0.054

ADORA2A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	809	8	318	70	99.0	82.0	93.5	0.852
27	Test 2	826	7	280	92	99.2	75.3	91.8	0.807
28	Test 3	686	9	375	135	98.7	73.5	88.0	0.766
29	Test 4	791	11	313	90	98.6	77.7	91.6	0.812
30	Test 5	783	13	295	114	98.4	72.1	89.5	0.765
	Avg	779	10	316	100	98.8	76.1	90.9	0.800
	SD	55	2	36	25	0.3	3.9	2.1	0.036

AR

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	484	56	579	865	89.6	40.1	53.6	0.284
22	Test 2	462	76	859	587	85.9	59.4	66.6	0.403

23	Test 3	407	65	881	631	86.2	58.3	64.9	0.379
24	Test 4	467	102	856	559	82.1	60.5	66.7	0.385
25	Test 5	451	67	913	553	87.1	62.3	68.8	0.433
	Avg	454	73	818	639	86.2	56.1	64.1	0.377
	SD	29	18	135	130	2.7	9.1	6.0	0.056

KCNH2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	972	16	139	501	98.4	21.7	68.2	0.334
22	Test 2	948	13	174	493	98.6	26.1	68.9	0.381
23	Test 3	969	19	189	451	98.1	29.5	71.1	0.404
24	Test 4	986	0	0	642	100.0	0.0	60.6	#DIV/0!
25	Test 5	959	13	156	500	98.7	23.8	68.5	0.361
	Avg	967	12	132	517	98.8	20.2	67.5	#DIV/0!
	SD	14	7	76	73	0.7	11.7	4.0	#DIV/0!

SLC6A4

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	793	2	157	83	99.7	65.4	91.8	0.763
27	Test 2	851	4	122	58	99.5	67.8	94.0	0.780
28	Test 3	798	8	169	60	99.0	73.8	93.4	0.803
29	Test 4	775	1	154	105	99.9	59.5	89.8	0.720
30	Test 5	806	3	108	118	99.6	47.8	88.3	0.633
	Avg	805	4	142	85	99.6	62.8	91.5	0.740

SD	28	3	26	27	0.3	9.9	2.4	0.067
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ADRA2A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	145	3	114	109	98.0	51.1	69.8	0.517
22	Test 2	143	6	120	102	96.0	54.1	70.9	0.518
23	Test 3	168	2	113	88	98.8	56.2	75.7	0.593
24	Test 4	184	5	108	74	97.4	59.3	78.7	0.616
25	Test 5	182	4	103	82	97.8	55.7	76.8	0.591
	Avg	164	4	112	91	97.6	55.3	74.4	0.567
	SD	20	2	6	14	1.0	3.0	3.9	0.046

ADRB1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	254	3	127	84	98.8	60.2	81.4	0.656
27	Test 2	211	3	133	121	98.6	52.4	73.5	0.559
28	Test 3	269	6	114	79	97.8	59.1	81.8	0.641
29	Test 4	254	5	139	70	98.1	66.5	84.0	0.696
30	Test 5	253	2	143	70	99.2	67.1	84.6	0.715
	Avg	248	4	131	85	98.5	61.1	81.1	0.653
	SD	22	2	11	21	0.6	6.1	4.4	0.060

ADRB2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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21	Test 1	388	1	45	357	99.7	11.2	54.7	0.234
22	Test 2	388	2	65	336	99.5	16.2	57.3	0.282
23	Test 3	369	5	44	373	98.7	10.6	52.2	0.191
24	Test 4	355	2	71	363	99.4	16.4	53.9	0.272
25	Test 5	426	7	85	273	98.4	23.7	64.6	0.344
	Avg	385	3	62	340	99.1	15.6	56.5	0.264
	SD	27	3	18	40	0.6	5.3	4.9	0.057

OPRD1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	566	2	113	164	99.6	40.8	80.4	0.554
27	Test 2	605	2	81	157	99.7	34.0	81.2	0.509
28	Test 3	602	10	123	110	98.4	52.8	85.8	0.628
29	Test 4	578	4	119	144	99.3	45.2	82.5	0.585
30	Test 5	636	1	66	142	99.8	31.7	83.1	0.503
	Avg	597	4	100	143	99.4	40.9	82.6	0.556
	SD	27	4	25	21	0.6	8.5	2.1	0.052

DRD1

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
	21	Test 1	251	7	170	240	97.3	41.5	63.0	0.428
[100,100]	22	Test 2	270	15	189	194	94.7	49.3	68.7	0.473
	23	Test 3	274	7	162	225	97.5	41.9	65.3	0.447
0.4	24	Test 4	278	7	157	226	97.5	41.0	65.1	0.443

0.001	25	Test 5	237	4	164	263	98.3	38.4	60.0	0.407
100		Avg	262	8	168	230	97.1	42.4	64.4	0.440
		SD	17	4	12	25	1.4	4.1	3.2	0.025

DRD2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	1081	3	79	203	99.7	28.0	84.9	0.473
27	Test 2	1120	9	118	119	99.2	49.8	90.6	0.639
28	Test 3	1156	4	108	98	99.7	52.4	92.5	0.679
29	Test 4	1173	2	75	116	99.8	39.3	91.4	0.588
30	Test 5	1140	6	117	103	99.5	53.2	92.0	0.676
	Avg	1134	5	99	128	99.6	44.5	90.3	0.611
	SD	36	3	21	43	0.2	10.8	3.1	0.086

SLC6A3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	500	21	207	157	96.0	56.9	79.9	0.595
22	Test 2	468	8	194	215	98.3	47.4	74.8	0.543
23	Test 3	488	11	215	171	97.8	55.7	79.4	0.608
24	Test 4	506	5	202	172	99.0	54.0	80.0	0.619
25	Test 5	497	5	187	196	99.0	48.8	77.3	0.575
	Avg	492	10	201	182	98.0	52.6	78.3	0.588
	SD	15	7	11	23	1.3	4.2	2.2	0.030

EDNRA

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	257	0	158	72	100.0	68.7	85.2	0.733
22	Test 2	220	1	208	58	99.5	78.2	87.9	0.782
23	Test 3	251	1	155	80	99.6	66.0	83.4	0.702
24	Test 4	270	12	135	70	95.7	65.9	83.2	0.662
25	Test 5	268	5	142	72	98.2	66.4	84.2	0.698
	Avg	253	4	160	70	98.6	69.0	84.8	0.715
	SD	20	5	29	8	1.7	5.3	1.9	0.045

NR3C1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	611	45	487	855	93.1	36.3	55.0	0.313
22	Test 2	537	78	935	448	87.3	67.6	73.7	0.507
23	Test 3	499	74	859	566	87.1	60.3	68.0	0.429
24	Test 4	552	61	767	618	90.0	55.4	66.0	0.425
25	Test 5	514	47	704	733	91.6	49.0	61.0	0.377
	Avg	543	61	750	644	89.8	53.7	64.7	0.410
	SD	43	15	172	156	2.6	11.9	7.1	0.072

HRH1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	271	1	107	97	99.6	52.5	79.4	0.615
27	Test 2	253	3	138	82	98.8	62.7	82.1	0.672

28	Test 3	274	4	135	63	98.6	68.2	85.9	0.723
29	Test 4	230	4	146	96	98.3	60.3	79.0	0.631
30	Test 5	228	7	122	119	97.0	50.6	73.5	0.536
	Avg	251	4	130	91	98.5	58.9	80.0	0.636
	SD	22	2	15	21	1.0	7.3	4.6	0.070

OPRM1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	714	8	305	156	98.9	66.2	86.1	0.719
22	Test 2	720	14	307	142	98.1	68.4	86.8	0.725
23	Test 3	739	10	277	157	98.7	63.8	85.9	0.703
24	Test 4	678	5	319	181	99.3	63.8	84.3	0.699
25	Test 5	716	6	302	159	99.2	65.5	86.1	0.719
	Avg	713	9	302	159	98.8	65.5	85.8	0.713
	SD	22	4	15	14	0.5	1.9	0.9	0.012

CHRM1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	362	6	147	136	98.4	51.9	78.2	0.588
27	Test 2	362	3	103	183	99.2	36.0	71.4	0.473
28	Test 3	417	4	103	127	99.0	44.8	79.9	0.565
29	Test 4	431	2	122	96	99.5	56.0	84.9	0.667
30	Test 5	426	1	112	112	99.8	50.0	82.6	0.624
	Avg	400	3	117	131	99.2	47.7	79.4	0.584

SD	35	2	18	33	0.5	7.7	5.2	0.073
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CHRM2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	330	4	223	176	98.8	55.9	75.4	0.589
27	Test 2	317	7	315	94	97.8	77.0	86.2	0.749
28	Test 3	313	5	286	129	98.4	68.9	81.7	0.682
29	Test 4	329	5	275	124	98.5	68.9	82.4	0.691
30	Test 5	317	6	263	147	98.1	64.1	79.1	0.642
	Avg	321	5	272	134	98.3	67.0	81.0	0.671
	SD	8	1	34	30	0.4	7.7	4.0	0.060

CHRM3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	302	1	126	101	99.7	55.5	80.8	0.640
27	Test 2	303	7	132	88	97.7	60.0	82.1	0.647
28	Test 3	322	5	106	97	98.5	52.2	80.8	0.606
29	Test 4	304	0	95	131	100.0	42.0	75.3	0.542
30	Test 5	291	2	128	109	99.3	54.0	79.1	0.616
	Avg	304	3	117	105	99.0	52.8	79.6	0.610
	SD	11	3	16	16	0.9	6.6	2.6	0.042

SLC6A2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	595	7	196	172	98.8	53.3	81.5	0.621
27	Test 2	557	13	236	164	97.7	59.0	81.8	0.639
28	Test 3	571	5	172	222	99.1	43.7	76.6	0.544
29	Test 4	559	6	198	207	98.9	48.9	78.0	0.579
30	Test 5	590	7	176	197	98.8	47.2	79.0	0.572
	Avg	574	8	196	192	98.7	50.4	79.4	0.591
	SD	17	3	25	24	0.6	5.9	2.2	0.039

HTR2A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	753	1	93	111	99.9	45.6	88.3	0.626
27	Test 2	743	2	96	117	99.7	45.1	87.6	0.615
28	Test 3	759	2	68	129	99.7	34.5	86.3	0.532
29	Test 4	753	3	82	120	99.6	40.6	87.2	0.577
30	Test 5	739	2	91	126	99.7	41.9	86.6	0.589
	Avg	749	2	86	121	99.7	41.5	87.2	0.588
	SD	8	1	11	7	0.1	4.5	0.8	0.037

HTR3A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	92	6	142	61	93.9	70.0	77.7	0.598
27	Test 2	100	1	160	40	99.0	80.0	86.4	0.748
28	Test 3	79	3	189	30	96.3	86.3	89.0	0.766
29	Test 4	81	2	171	47	97.6	78.4	83.7	0.687

30	Test 5	78	9	175	39	89.7	81.8	84.1	0.664
	Avg	86	4	167	43	95.3	79.3	84.2	0.693
	SD	10	3	18	12	3.7	6.0	4.2	0.067

LCK

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	362	1	14	74	99.7	15.9	83.4	0.346
27	Test 2	364	0	13	74	100.0	14.9	83.6	0.352
28	Test 3	362	0	7	82	100.0	7.9	81.8	0.253
29	Test 4	344	0	6	101	100.0	5.6	77.6	0.208
30	Test 5	298	1	20	132	99.7	13.2	70.5	0.288
	Avg	346	0	12	93	99.9	11.5	79.4	0.289
	SD	28	1	6	25	0.2	4.5	5.5	0.061

AVPR1A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	131	1	161	42	99.2	79.3	87.2	0.768
27	Test 2	108	2	186	39	98.2	82.7	87.8	0.765
28	Test 3	116	2	183	34	98.3	84.3	89.3	0.794
29	Test 4	139	3	157	36	97.9	81.3	88.4	0.784
30	Test 5	116	1	166	52	99.1	76.1	84.2	0.718
	Avg	122	2	171	41	98.6	80.8	87.3	0.766
	SD	13	1	13	7	0.6	3.2	1.9	0.029

AGTR1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	193	7	164	33	96.5	83.2	89.9	0.805
27	Test 2	157	2	149	89	98.7	62.6	77.1	0.619
28	Test 3	160	10	154	73	94.1	67.8	79.1	0.623
29	Test 4	169	4	172	52	97.7	76.8	85.9	0.743
30	Test 5	99	5	216	77	95.2	73.7	79.3	0.610
	Avg	156	6	171	65	96.4	72.8	82.3	0.680
	SD	35	3	27	22	1.9	8.0	5.4	0.089

AKT1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	614	3	93	87	99.5	51.7	88.7	0.657
27	Test 2	563	7	126	101	98.8	55.5	86.4	0.657
28	Test 3	548	2	122	125	99.6	49.4	84.1	0.626
29	Test 4	518	3	158	118	99.4	57.2	84.8	0.672
30	Test 5	504	3	148	142	99.4	51.0	81.8	0.619
	Avg	549	4	129	115	99.4	53.0	85.2	0.646
	SD	43	2	25	21	0.3	3.3	2.6	0.023

BACE1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	1275	4	164	281	99.7	36.9	83.5	0.539
27	Test 2	1186	6	243	289	99.5	45.7	82.9	0.594

28	Test 3	1166	12	354	192	99.0	64.8	88.2	0.726
29	Test 4	1205	8	283	228	99.3	55.4	86.3	0.667
30	Test 5	1140	14	353	217	98.8	61.9	86.6	0.698
	Avg	1194	9	279	241	99.3	52.9	85.5	0.645
	SD	51	4	80	42	0.4	11.6	2.2	0.077

BCHE

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	267	14	254	174	95.0	59.3	73.5	0.548
27	Test 2	268	1	185	255	99.6	42.0	63.9	0.460
28	Test 3	297	11	251	150	96.4	62.6	77.3	0.606
29	Test 4	275	6	222	206	97.9	51.9	70.1	0.521
30	Test 5	250	11	252	196	95.8	56.3	70.8	0.520
	Avg	271	9	233	196	96.9	54.4	71.1	0.531
	SD	17	5	30	39	1.8	8.0	4.9	0.053

CASP1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	239	14	321	339	94.5	48.6	61.3	0.400
22	Test 2	224	27	388	274	89.2	58.6	67.0	0.429
23	Test 3	269	11	289	344	96.1	45.7	61.1	0.410
24	Test 4	274	17	308	314	94.2	49.5	63.7	0.425
25	Test 5	264	30	315	304	89.8	50.9	63.4	0.392
	Avg	254	20	324	315	92.7	50.7	63.3	0.411

SD	22	8	38	28	3.0	4.8	2.4	0.016
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CASP3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	253	12	202	134	95.5	60.1	75.7	0.576
22	Test 2	241	6	179	175	97.6	50.6	69.9	0.513
23	Test 3	202	1	186	212	99.5	46.7	64.6	0.472
24	Test 4	229	6	159	207	97.4	43.4	64.6	0.447
25	Test 5	226	1	138	236	99.6	36.9	60.6	0.419
	Avg	230	5	173	193	97.9	47.6	67.1	0.486
	SD	19	5	25	39	1.7	8.6	5.9	0.061

CASP8

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	59	6	222	5	90.8	97.8	96.2	0.891
27	Test 2	51	8	218	15	86.4	93.6	92.1	0.768
28	Test 3	64	1	214	13	98.5	94.3	95.2	0.875
29	Test 4	51	4	232	5	92.7	97.9	96.9	0.900
30	Test 5	79	7	193	13	91.9	93.7	93.2	0.839
	Avg	61	5	216	10	92.1	95.4	94.7	0.855
	SD	12	3	14	5	4.3	2.2	2.0	0.054

CHRM5

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	139	1	131	81	99.3	61.8	76.7	0.617
27	Test 2	152	2	115	83	98.7	58.1	75.9	0.598
28	Test 3	127	2	134	89	98.4	60.1	74.1	0.579
29	Test 4	116	2	144	90	98.3	61.5	73.9	0.573
30	Test 5	131	7	155	59	94.9	72.4	81.3	0.660
	Avg	133	3	136	80	97.9	62.8	76.4	0.606
	SD	13	2	15	13	1.7	5.6	3.0	0.035

CHUK

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	70	0	155	52	100.0	74.9	81.2	0.655
27	Test 2	76	1	176	24	98.7	88.0	91.0	0.809
28	Test 3	61	1	169	46	98.4	78.6	83.0	0.659
29	Test 4	45	1	199	32	97.8	86.1	88.1	0.698
30	Test 5	59	2	165	51	96.7	76.4	80.9	0.619
	Avg	62	1	173	41	98.3	80.8	84.8	0.688
	SD	12	1	16	12	1.2	5.9	4.5	0.073

CSF1R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	275	0	126	76	100.0	62.4	84.1	0.699
22	Test 2	269	0	119	89	100.0	57.2	81.3	0.656
23	Test 3	267	2	133	75	99.3	63.9	83.9	0.696
24	Test 4	267	4	113	93	98.5	54.9	79.7	0.615

25	Test 5	250	2	148	77	99.2	65.8	83.4	0.699
	Avg	266	2	128	82	99.4	60.8	82.5	0.673
	SD	9	2	14	8	0.6	4.6	1.9	0.037

CSNK1D

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	144	3	111	89	98.0	55.5	73.5	0.562
22	Test 2	131	1	110	105	99.2	51.2	69.5	0.525
23	Test 3	142	3	119	83	97.9	58.9	75.2	0.587
24	Test 4	139	0	112	96	100.0	53.8	72.3	0.564
25	Test 5	141	4	123	79	97.2	60.9	76.1	0.595
	Avg	139	2	115	90	98.5	56.1	73.3	0.567
	SD	5	2	6	10	1.1	3.9	2.6	0.027

EDNRB

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	218	0	145	46	100.0	75.9	88.8	0.792
27	Test 2	159	0	169	81	100.0	67.6	80.2	0.669
28	Test 3	145	0	200	64	100.0	75.8	84.4	0.725
29	Test 4	167	0	190	52	100.0	78.5	87.3	0.774
30	Test 5	119	1	229	60	99.2	79.2	85.1	0.720
	Avg	162	0	187	61	99.8	75.4	85.1	0.736
	SD	36	0	32	13	0.4	4.6	3.3	0.048

ELANE

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	480	1	60	160	99.8	27.3	77.0	0.446
22	Test 2	438	3	85	175	99.3	32.7	74.6	0.467
23	Test 3	442	0	59	200	100.0	22.8	71.5	0.396
24	Test 4	366	3	128	204	99.2	38.6	70.5	0.483
25	Test 5	400	1	72	228	99.8	24.0	67.3	0.385
	Avg	425	2	81	193	99.6	29.1	72.2	0.435
	SD	44	1	28	26	0.3	6.5	3.8	0.043

EPHA2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	165	2	118	41	98.8	74.2	86.8	0.757
27	Test 2	97	3	204	22	97.0	90.3	92.3	0.836
28	Test 3	78	0	199	49	100.0	80.2	85.0	0.702
29	Test 4	105	2	162	57	98.1	74.0	81.9	0.677
30	Test 5	74	2	212	38	97.4	84.8	87.7	0.732
	Avg	104	2	179	41	98.3	80.7	86.7	0.741
	SD	37	1	39	13	1.2	7.0	3.8	0.061

FGFR1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	536	0	79	59	100.0	57.2	91.2	0.718
22	Test 2	421	1	103	149	99.8	40.9	77.7	0.544

23	Test 3	416	2	89	167	99.5	34.8	74.9	0.487
24	Test 4	394	10	130	140	97.5	48.1	77.7	0.552
25	Test 5	383	0	119	172	100.0	40.9	74.5	0.531
	Avg	430	3	104	137	99.4	44.4	79.2	0.566
	SD	61	4	21	46	1.0	8.6	6.9	0.088

FKBP1A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	83	1	174	14	98.8	92.6	94.5	0.881
22	Test 2	99	2	155	16	98.0	90.6	93.4	0.867
23	Test 3	53	1	174	44	98.1	79.8	83.5	0.649
24	Test 4	61	0	193	18	100.0	91.5	93.4	0.840
25	Test 5	54	0	204	14	100.0	93.6	94.9	0.862
	Avg	70	1	180	21	99.0	89.6	91.9	0.820
	SD	20	1	19	13	1.0	5.6	4.8	0.097

FLT1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	205	1	330	97	99.5	77.3	84.5	0.720
22	Test 2	241	5	296	91	98.0	76.5	84.8	0.727
23	Test 3	220	4	299	110	98.2	73.1	82.0	0.683
24	Test 4	202	2	351	78	99.0	81.8	87.4	0.761
25	Test 5	202	6	347	78	97.1	81.6	86.7	0.745
	Avg	214	4	325	91	98.4	78.1	85.1	0.727

SD	17	2	26	14	0.9	3.7	2.1	0.029
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FLT4

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	149	2	147	53	98.7	73.5	84.3	0.723
22	Test 2	123	0	124	104	100.0	54.4	70.4	0.543
23	Test 3	128	6	159	58	95.5	73.3	81.8	0.670
24	Test 4	133	1	118	99	99.3	54.4	71.5	0.550
25	Test 5	130	2	149	70	98.5	68.0	79.5	0.651
	Avg	133	2	139	77	98.4	64.7	77.5	0.627
	SD	10	2	18	23	1.7	9.7	6.2	0.078

FYN

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	95	6	120	78	94.1	60.6	71.9	0.524
27	Test 2	72	1	143	83	98.6	63.3	71.9	0.532
28	Test 3	78	11	181	29	87.6	86.2	86.6	0.704
29	Test 4	81	9	142	67	90.0	67.9	74.6	0.532
30	Test 5	63	4	140	92	94.0	60.3	67.9	0.454
	Avg	78	6	145	70	92.9	67.7	74.6	0.549
	SD	12	4	22	25	4.2	10.8	7.1	0.093

GSK3B

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	522	1	96	142	99.8	40.3	81.2	0.558
27	Test 2	489	2	56	214	99.6	20.7	71.6	0.367
28	Test 3	490	4	113	154	99.2	42.3	79.2	0.549
29	Test 4	500	2	108	151	99.6	41.7	79.9	0.557
30	Test 5	537	2	85	137	99.6	38.3	81.7	0.542
	Avg	508	2	92	160	99.6	36.7	78.7	0.514
	SD	21	1	23	31	0.2	9.0	4.1	0.083

HDAC3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	209	3	149	77	98.6	65.9	81.7	0.677
22	Test 2	206	3	146	83	98.6	63.8	80.4	0.657
23	Test 3	225	2	135	76	99.1	64.0	82.2	0.680
24	Test 4	183	4	146	105	97.9	58.2	75.1	0.584
25	Test 5	214	2	132	90	99.1	59.5	79.0	0.635
	Avg	207	3	142	86	98.6	62.3	79.7	0.647
	SD	15	1	8	12	0.5	3.3	2.8	0.039

IGF1R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	585	3	72	63	99.5	53.3	90.9	0.675
27	Test 2	470	3	176	74	99.4	70.4	89.3	0.769
28	Test 3	521	2	135	65	99.6	67.5	90.7	0.766
29	Test 4	454	2	187	80	99.6	70.0	88.7	0.764

30	Test 5	435	8	186	94	98.2	66.4	85.9	0.710
	Avg	493	4	151	75	99.2	65.5	89.1	0.737
	SD	61	3	49	13	0.6	7.0	2.0	0.042

INSR

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	255	1	109	31	99.6	77.9	91.9	0.827
27	Test 2	166	2	173	55	98.8	75.9	85.6	0.743
28	Test 3	143	2	165	86	98.6	65.7	77.8	0.628
29	Test 4	139	1	188	68	99.3	73.4	82.6	0.696
30	Test 5	177	1	177	41	99.4	81.2	89.4	0.806
	Avg	176	1	162	56	99.2	74.8	85.5	0.740
	SD	47	1	31	22	0.4	5.8	5.6	0.081

KDR

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	1629	4	21	225	99.8	8.5	87.8	0.244
27	Test 2	1526	20	151	182	98.7	45.3	89.2	0.585
28	Test 3	1576	6	33	264	99.6	11.1	85.6	0.275
29	Test 4	1485	2	44	348	99.9	11.2	81.4	0.292
30	Test 5	1563	5	69	242	99.7	22.2	86.9	0.418
	Avg	1556	7	64	252	99.5	19.7	86.2	0.363
	SD	54	7	52	61	0.5	15.3	3.0	0.141

LTB4R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	52	3	190	31	94.5	86.0	87.7	0.701
27	Test 2	66	5	175	30	93.0	85.4	87.3	0.719
28	Test 3	74	5	168	29	93.7	85.3	87.7	0.738
29	Test 4	71	4	188	13	94.7	93.5	93.8	0.853
30	Test 5	66	4	199	7	94.3	96.6	96.0	0.897
	Avg	66	4	184	22	94.0	89.4	90.5	0.781
	SD	8	1	12	11	0.7	5.3	4.1	0.087

LYN

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	99	3	135	63	97.1	68.2	78.0	0.620
27	Test 2	78	2	167	53	97.5	75.9	81.7	0.655
28	Test 3	90	3	177	30	96.8	85.5	89.0	0.777
29	Test 4	96	2	179	23	98.0	88.6	91.7	0.830
30	Test 5	79	2	164	55	97.5	74.9	81.0	0.647
	Avg	88	2	164	45	97.4	78.6	84.3	0.706
	SD	10	1	18	17	0.5	8.3	5.8	0.092

MAPK1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	1293	31	157	1976	97.7	7.4	41.9	0.108
22	Test 2	1233	12	99	2113	99.0	4.5	38.5	0.096

23	Test 3	1202	0	0	2255	100.0	0.0	34.8	#DIV/0!
24	Test 4	1202	0	21	2234	100.0	0.9	35.4	0.057
25	Test 5	1236	0	0	2221	100.0	0.0	35.8	#DIV/0!
	Avg	1233	9	55	2160	99.3	2.6	37.3	#DIV/0!
	SD	37	14	70	116	1.0	3.3	3.0	#DIV/0!

MAPK9

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	261	0	131	71	100.0	64.9	84.7	0.714
27	Test 2	237	1	173	52	99.6	76.9	88.6	0.789
28	Test 3	240	2	153	68	99.2	69.2	84.9	0.724
29	Test 4	237	0	152	74	100.0	67.3	84.0	0.716
30	Test 5	246	3	169	45	98.8	79.0	89.6	0.802
	Avg	244	1	156	62	99.5	71.4	86.3	0.749
	SD	10	1	17	13	0.5	6.2	2.6	0.043

MAPKAPK2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	161	3	131	102	98.2	56.2	73.6	0.566
22	Test 2	175	2	147	73	98.9	66.8	81.1	0.674
23	Test 3	162	3	108	124	98.2	46.6	68.0	0.491
24	Test 4	133	3	170	91	97.8	65.1	76.3	0.602
25	Test 5	184	3	137	73	98.4	65.2	80.9	0.665
	Avg	163	3	139	93	98.3	60.0	76.0	0.600

SD	19	0	23	21	0.4	8.6	5.5	0.075
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MET

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	601	1	93	108	99.8	46.3	86.4	0.621
27	Test 2	541	0	127	135	100.0	48.5	83.2	0.623
28	Test 3	564	3	126	110	99.5	53.4	85.9	0.656
29	Test 4	580	3	132	88	99.5	60.0	88.7	0.709
30	Test 5	576	2	143	82	99.7	63.6	89.5	0.738
	Avg	572	2	124	105	99.7	54.3	86.7	0.669
	SD	22	1	19	21	0.2	7.4	2.5	0.052

MMP13

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	487	5	124	84	99.0	59.6	87.3	0.691
27	Test 2	465	5	141	89	98.9	61.3	86.6	0.696
28	Test 3	482	4	129	85	99.2	60.3	87.3	0.698
29	Test 4	473	3	105	119	99.4	46.9	82.6	0.597
30	Test 5	462	2	123	113	99.6	52.1	83.6	0.638
	Avg	474	4	124	98	99.2	56.0	85.5	0.664
	SD	11	1	13	17	0.3	6.3	2.2	0.045

MMP2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	602	5	164	152	99.2	51.9	83.0	0.627
27	Test 2	582	10	182	149	98.3	55.0	82.8	0.630
28	Test 3	594	5	205	119	99.2	63.3	86.6	0.711
29	Test 4	567	4	162	190	99.3	46.0	79.0	0.573
30	Test 5	564	5	210	144	99.1	59.3	83.9	0.672
	Avg	582	6	185	151	99.0	55.1	83.0	0.643
	SD	17	2	22	25	0.4	6.7	2.7	0.052

MMP3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	376	5	90	88	98.7	50.6	83.4	0.611
22	Test 2	367	0	80	112	100.0	41.7	80.0	0.565
23	Test 3	370	6	90	93	98.4	49.2	82.3	0.592
24	Test 4	307	1	119	132	99.7	47.4	76.2	0.570
25	Test 5	322	5	93	139	98.5	40.1	74.2	0.500
	Avg	348	3	94	113	99.0	45.8	79.2	0.568
	SD	32	3	15	23	0.7	4.6	3.9	0.042

MMP9

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	548	2	34	302	99.6	10.1	65.7	0.240
22	Test 2	488	1	41	356	99.8	10.3	59.7	0.237
23	Test 3	514	0	24	348	100.0	6.5	60.7	0.196
24	Test 4	517	2	22	345	99.6	6.0	60.8	0.170

25	Test 5	510	0	0	376	100.0	0.0	57.6	#DIV/0!
	Avg	515	1	24	345	99.8	6.6	60.9	#DIV/0!
	SD	21	1	16	27	0.2	4.2	3.0	#DIV/0!

NEK2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	72	1	159	39	98.6	80.3	85.2	0.712
27	Test 2	72	2	130	67	97.3	66.0	74.5	0.564
28	Test 3	53	1	162	55	98.1	74.7	79.3	0.594
29	Test 4	44	0	165	62	100.0	72.7	77.1	0.549
30	Test 5	44	9	175	43	83.0	80.3	80.8	0.538
	Avg	57	3	158	53	95.4	74.8	79.4	0.591
	SD	14	4	17	12	7.0	6.0	4.0	0.071

P2RY1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	109	2	189	32	98.2	85.5	89.8	0.799
22	Test 2	137	0	180	15	100.0	92.3	95.5	0.912
23	Test 3	81	4	216	31	95.3	87.4	89.5	0.764
24	Test 4	123	0	184	25	100.0	88.0	92.5	0.855
30	Test 5	100	4	204	24	96.2	89.5	91.6	0.821
	Avg	110	2	195	25	97.9	88.6	91.7	0.830
	SD	21	2	15	7	2.2	2.5	2.4	0.057

PAK4

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	94	3	169	30	96.9	84.9	88.9	0.779
27	Test 2	64	2	197	33	97.0	85.7	88.2	0.733
28	Test 3	75	3	195	23	96.2	89.4	91.2	0.801
29	Test 4	69	1	185	41	98.6	81.9	85.8	0.707
30	Test 5	66	3	170	57	95.7	74.9	79.7	0.605
	Avg	74	2	183	37	96.9	83.4	86.8	0.725
	SD	12	1	13	13	1.1	5.4	4.4	0.077

PDE4A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	128	3	114	89	97.7	56.2	72.5	0.551
27	Test 2	142	3	139	50	97.9	73.5	84.1	0.717
28	Test 3	108	2	168	56	98.2	75.0	82.6	0.688
29	Test 4	122	7	141	64	94.6	68.8	78.7	0.621
30	Test 5	131	7	157	39	94.9	80.1	86.2	0.739
	Avg	126	4	144	60	96.7	70.7	80.8	0.663
	SD	12	2	20	19	1.8	9.1	5.4	0.077

PDE5A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	280	5	156	104	98.2	60.0	80.0	0.638
27	Test 2	300	5	132	108	98.4	55.0	79.3	0.611

28	Test 3	286	7	137	115	97.6	54.4	77.6	0.588
29	Test 4	346	7	95	97	98.0	49.5	80.9	0.582
30	Test 5	308	7	139	91	97.8	60.4	82.0	0.649
	Avg	304	6	132	103	98.0	55.9	80.0	0.613
	SD	26	1	22	9	0.3	4.5	1.7	0.030

PIK3CA

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	989	5	296	72	99.5	80.4	94.3	0.855
27	Test 2	915	0	359	88	100.0	80.3	93.5	0.856
28	Test 3	858	4	377	123	99.5	75.4	90.7	0.805
29	Test 4	970	3	281	108	99.7	72.2	91.9	0.800
30	Test 5	975	5	311	71	99.5	81.4	94.4	0.861
	Avg	941	3	325	92	99.6	78.0	93.0	0.835
	SD	54	2	41	23	0.2	4.0	1.6	0.030

PPARG

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	854	14	326	1135	98.4	22.3	50.7	0.283
22	Test 2	867	24	465	973	97.3	32.3	57.2	0.354
23	Test 3	770	36	620	903	95.5	40.7	59.7	0.383
24	Test 4	808	51	601	869	94.1	40.9	60.5	0.376
30	Test 5	894	44	590	801	95.3	42.4	63.7	0.416
	Avg	839	34	520	936	96.1	35.7	58.4	0.362

SD	49	15	125	127	1.7	8.5	4.9	0.049
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PTPN1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	302	18	196	214	94.4	47.8	68.2	0.460
27	Test 2	333	5	119	273	98.5	30.4	61.9	0.383
28	Test 3	271	9	155	295	96.8	34.4	58.4	0.364
29	Test 4	287	10	231	202	96.6	53.3	71.0	0.522
30	Test 5	223	13	307	187	94.5	62.1	72.6	0.534
	Avg	283	11	202	234	96.2	45.6	66.4	0.453
	SD	41	5	72	47	1.7	13.2	6.1	0.078

PTPN11

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	75	7	136	95	91.5	58.9	67.4	0.444
27	Test 2	56	9	159	89	86.2	64.1	68.7	0.409
28	Test 3	52	8	167	86	86.7	66.0	70.0	0.418
29	Test 4	55	17	164	77	76.4	68.0	70.0	0.379
30	Test 5	74	1	133	105	98.7	55.9	66.1	0.471
	Avg	62	8	152	90	87.9	62.6	68.4	0.424
	SD	11	6	16	10	8.1	5.1	1.7	0.035

PTPN2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	69	7	196	37	90.8	84.1	85.8	0.680
27	Test 2	62	3	178	66	95.4	73.0	77.7	0.565
28	Test 3	69	2	172	66	97.2	72.3	78.0	0.589
29	Test 4	53	11	190	55	82.8	77.6	78.6	0.513
30	Test 5	60	3	185	61	95.2	75.2	79.3	0.581
	Avg	63	5	184	57	92.3	76.4	79.9	0.586
	SD	7	4	9	12	5.8	4.8	3.4	0.060

RAF1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	276	3	155	53	98.9	74.5	88.5	0.776
22	Test 2	306	1	130	50	99.7	72.2	89.5	0.783
23	Test 3	265	0	119	103	100.0	53.6	78.9	0.621
24	Test 4	269	1	130	87	99.6	59.9	81.9	0.667
30	Test 5	230	0	175	82	100.0	68.1	83.2	0.708
	Avg	269	1	142	75	99.6	65.7	84.4	0.711
	SD	27	1	23	23	0.4	8.7	4.5	0.069

RARA

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	63	25	603	30	71.6	95.3	92.4	0.653
27	Test 2	51	19	622	29	72.9	95.5	93.3	0.645
28	Test 3	57	14	579	71	80.3	89.1	88.2	0.541
29	Test 4	47	15	645	14	75.8	97.9	96.0	0.742

30	Test 5	46	19	591	65	70.8	90.1	88.3	0.483
	Avg	53	18	608	42	74.3	93.6	91.7	0.613
	SD	7	4	26	25	3.9	3.8	3.3	0.102

RARB

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	55	4	642	28	93.2	95.8	95.6	0.765
27	Test 2	52	7	663	7	88.1	99.0	98.1	0.871
28	Test 3	59	4	659	7	93.7	98.9	98.5	0.907
29	Test 4	55	3	663	8	94.8	98.8	98.5	0.902
30	Test 5	52	7	658	12	88.1	98.2	97.4	0.832
	Avg	55	5	657	12	91.6	98.1	97.6	0.855
	SD	3	2	9	9	3.2	1.3	1.2	0.059

ROCK1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	281	1	109	91	99.6	54.5	80.9	0.636
22	Test 2	272	0	131	79	100.0	62.4	83.6	0.695
23	Test 3	237	1	138	106	99.6	56.6	77.8	0.620
24	Test 4	263	0	132	87	100.0	60.3	82.0	0.673
30	Test 5	236	2	162	82	99.2	66.4	82.6	0.692
	Avg	258	1	134	89	99.7	60.0	81.4	0.663
	SD	20	1	19	11	0.3	4.7	2.2	0.034

RPS6KA5

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	47	3	183	19	94.0	90.6	91.3	0.767
27	Test 2	38	2	191	21	95.0	90.1	90.9	0.734
28	Test 3	45	3	156	48	93.8	76.5	79.8	0.571
29	Test 4	44	1	180	27	97.8	87.0	88.9	0.721
30	Test 5	39	2	186	25	95.1	88.2	89.3	0.706
	Avg	43	2	179	28	95.1	86.5	88.0	0.700
	SD	4	1	14	12	1.6	5.8	4.7	0.075

SIRT2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	90	3	163	73	96.8	69.1	76.9	0.593
27	Test 2	62	8	171	88	88.6	66.0	70.8	0.449
28	Test 3	45	11	217	56	80.4	79.5	79.6	0.488
29	Test 4	74	2	168	85	97.4	66.4	73.6	0.538
30	Test 5	60	6	201	62	90.9	76.4	79.3	0.558
	Avg	66	6	184	73	90.8	71.5	76.0	0.525
	SD	17	4	24	14	6.9	6.1	3.8	0.057

SIRT3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	45	3	188	9	93.8	95.4	95.1	0.854
22	Test 2	30	4	200	11	88.2	94.8	93.9	0.769

23	Test 3	12	3	216	14	80.0	93.9	93.1	0.575
24	Test 4	22	5	211	7	81.5	96.8	95.1	0.759
25	Test 5	19	8	213	5	70.4	97.7	94.7	0.717
	Avg	26	5	206	9	82.8	95.7	94.4	0.735
	SD	13	2	12	3	8.9	1.5	0.9	0.102

SRC

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	544	2	115	186	99.6	38.2	77.8	0.525
27	Test 2	506	3	149	189	99.4	44.1	77.3	0.555
28	Test 3	500	0	175	172	100.0	50.4	79.7	0.613
29	Test 4	580	1	174	92	99.8	65.4	89.0	0.748
30	Test 5	562	6	171	108	98.9	61.3	86.5	0.696
	Avg	538	2	157	149	99.6	51.9	82.1	0.627
	SD	35	2	26	46	0.4	11.4	5.4	0.094

TACR2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	169	9	311	69	94.9	81.8	86.0	0.724
27	Test 2	177	11	344	26	94.1	93.0	93.4	0.856
28	Test 3	137	10	361	50	93.2	87.8	89.2	0.756
29	Test 4	128	11	383	36	92.1	91.4	91.6	0.793
30	Test 5	216	8	280	54	96.4	83.8	88.9	0.787
	Avg	165	10	336	47	94.2	87.6	89.8	0.783

SD	35	1	41	17	1.7	4.8	2.8	0.049
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TBXA2R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	210	3	240	128	98.6	65.2	77.5	0.623
22	Test 2	187	3	284	107	98.4	72.6	81.1	0.667
23	Test 3	188	3	252	138	98.4	64.6	75.7	0.597
24	Test 4	169	9	314	89	94.9	77.9	83.1	0.676
25	Test 5	217	13	247	104	94.3	70.4	79.9	0.637
	Avg	194	6	267	113	96.9	70.2	79.4	0.640
	SD	19	5	31	20	2.1	5.5	2.9	0.032

TEK

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	162	5	160	57	97.0	73.7	83.9	0.708
22	Test 2	172	2	137	73	98.9	65.2	80.5	0.664
23	Test 3	153	4	120	107	97.5	52.9	71.1	0.529
24	Test 4	154	1	128	101	99.4	55.9	73.4	0.574
25	Test 5	132	3	170	79	97.8	68.3	78.6	0.634
	Avg	155	3	143	83	98.1	63.2	77.5	0.622
	SD	15	2	21	21	1.0	8.7	5.2	0.071

Table S11. Model test set performance results for each target where a positive probability value of 0.1 was used as the threshold to assign compounds as predicted active or inactive. In each case standard deviations are shown below averages. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC).

AChE

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	185	311	415	4	37.3	99.0	65.6	0.447
22	Test 2	225	350	337	3	39.1	99.1	61.4	0.427
23	Test 3	213	293	403	6	42.1	98.5	67.3	0.473
24	Test 4	258	272	377	8	48.7	97.9	69.4	0.507
25	Test 5	115	390	409	1	22.8	99.8	57.3	0.337
	Avg	199	323	388	4	38.0	98.9	64.2	0.438
	SD	54	47	32	3	9.5	0.7	4.9	0.064

ADORA2A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	674	143	384	4	82.5	99.0	87.8	0.767
27	Test 2	736	97	358	14	88.4	96.2	90.8	0.806
28	Test 3	622	73	491	19	89.5	96.3	92.4	0.849
29	Test 4	696	106	399	4	86.8	99.0	90.9	0.820
30	Test 5	681	115	392	17	85.6	95.8	89.0	0.781
	Avg	682	107	405	12	86.5	97.3	90.2	0.805
	SD	41	26	51	7	2.7	1.6	1.8	0.032

AR

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	219	321	1443	1	40.6	99.9	83.8	0.574
22	Test 2	210	328	1443	3	39.0	99.8	83.3	0.558

23	Test 3	184	288	1512	0	39.0	100.0	85.5	0.572
24	Test 4	210	359	1411	4	36.9	99.7	81.7	0.534
25	Test 5	176	342	1466	0	34.0	100.0	82.8	0.525
	Avg	200	328	1455	2	37.9	99.9	83.4	0.553
	SD	19	26	37	2	2.5	0.1	1.4	0.022

KCNH2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	493	495	572	68	49.9	89.4	65.4	0.404
22	Test 2	481	480	625	42	50.1	93.7	67.9	0.461
23	Test 3	435	553	610	30	44.0	95.3	64.2	0.425
24	Test 4	470	516	604	38	47.7	94.1	66.0	0.440
25	Test 5	482	490	600	56	49.6	91.5	66.5	0.428
	Avg	472	507	602	47	48.2	92.8	66.0	0.432
	SD	22	29	19	15	2.5	2.4	1.4	0.021

SLC6A4

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	703	92	227	13	88.4	94.6	89.9	0.759
27	Test 2	796	59	176	4	93.1	97.8	93.9	0.822
28	Test 3	684	122	225	4	84.9	98.3	87.8	0.731
29	Test 4	698	78	250	9	89.9	96.5	91.6	0.805
30	Test 5	737	72	223	3	91.1	98.7	92.8	0.822
	Avg	724	85	220	7	89.5	97.2	91.2	0.788

SD	45	24	27	4	3.1	1.7	2.4	0.041
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ADRA2A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	83	65	221	2	56.1	99.1	81.9	0.643
22	Test 2	79	70	221	1	53.0	99.5	80.9	0.627
23	Test 3	90	80	200	1	52.9	99.5	78.2	0.607
24	Test 4	110	79	182	0	58.2	100.0	78.7	0.637
25	Test 5	112	74	184	1	60.2	99.5	79.8	0.648
	Avg	95	74	202	1	56.1	99.5	79.9	0.632
	SD	15	6	19	1	3.2	0.3	1.5	0.016

ADRB1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	201	56	201	10	78.2	95.3	85.9	0.735
27	Test 2	128	86	251	3	59.8	98.8	81.0	0.651
28	Test 3	200	75	188	5	72.7	97.4	82.9	0.696
29	Test 4	144	115	207	2	55.6	99.0	75.0	0.586
30	Test 5	127	128	209	4	49.8	98.1	71.8	0.532
	Avg	160	92	211	5	63.2	97.7	79.3	0.640
	SD	38	29	24	3	11.9	1.5	5.8	0.082

ADRB2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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21	Test 1	178	211	400	2	45.8	99.5	73.1	0.540
22	Test 2	128	262	398	3	32.8	99.3	66.5	0.431
23	Test 3	98	276	415	2	26.2	99.5	64.9	0.386
24	Test 4	134	223	429	5	37.5	98.8	71.2	0.476
25	Test 5	67	366	358	0	15.5	100.0	53.7	0.277
	Avg	121	268	400	2	31.6	99.4	65.9	0.422
	SD	42	61	27	2	11.5	0.4	7.6	0.099

OPRD1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	460	108	271	6	81.0	97.8	86.5	0.744
27	Test 2	457	150	221	17	75.3	92.9	80.2	0.618
28	Test 3	431	181	231	2	70.4	99.1	78.3	0.622
29	Test 4	407	175	261	2	69.9	99.2	79.1	0.641
30	Test 5	517	120	203	5	81.2	97.6	85.2	0.698
	Avg	454	147	237	6	75.6	97.3	81.9	0.665
	SD	41	32	28	6	5.5	2.6	3.7	0.055

DRD1

	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
	21	Test 1	105	153	408	2	40.7	99.5	76.8	0.534
[100,100]	22	Test 2	123	162	382	1	43.2	99.7	75.6	0.546
	23	Test 3	83	198	387	0	29.5	100.0	70.4	0.442
0.4	24	Test 4	125	160	382	1	43.9	99.7	75.9	0.551

0.001	25	Test 5	111	130	424	3	46.1	99.3	80.1	0.579
100		Avg	109	161	397	1	40.7	99.7	75.7	0.530
		SD	17	24	19	1	6.5	0.3	3.5	0.052

DRD2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	993	91	266	16	91.6	94.3	92.2	0.792
27	Test 2	987	142	215	22	87.4	90.7	88.0	0.673
28	Test 3	911	249	203	3	78.5	98.5	81.6	0.586
29	Test 4	1057	118	175	16	90.0	91.6	90.2	0.689
30	Test 5	1000	146	208	12	87.3	94.5	88.4	0.686
	Avg	990	149	213	14	87.0	94.0	88.1	0.685
	SD	52	60	33	7	5.0	3.1	4.0	0.073

SLC6A3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	335	186	359	5	64.3	98.6	78.4	0.637
22	Test 2	364	112	400	9	76.5	97.8	86.3	0.750
23	Test 3	335	164	378	8	67.1	97.9	80.6	0.662
24	Test 4	396	115	372	2	77.5	99.5	86.8	0.764
25	Test 5	362	140	373	10	72.1	97.4	83.1	0.698
	Avg	358	143	376	7	71.5	98.2	83.0	0.702
	SD	25	32	15	3	5.7	0.8	3.6	0.055

EDNRA

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	139	118	225	5	54.1	97.8	74.7	0.568
22	Test 2	123	98	262	4	55.7	98.5	79.1	0.614
23	Test 3	207	45	231	4	82.1	98.3	89.9	0.811
24	Test 4	111	171	205	0	39.4	100.0	64.9	0.463
25	Test 5	146	127	204	10	53.5	95.3	71.9	0.519
	Avg	145	112	225	5	56.9	98.0	76.1	0.595
	SD	37	46	24	4	15.5	1.7	9.3	0.133

NR3C1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	312	344	1340	2	47.6	99.9	82.7	0.612
22	Test 2	248	367	1382	1	40.3	99.9	81.6	0.563
23	Test 3	179	394	1424	1	31.2	99.9	80.2	0.492
24	Test 4	197	416	1384	1	32.1	99.9	79.1	0.495
25	Test 5	207	354	1434	3	36.9	99.8	82.1	0.538
	Avg	229	375	1393	2	37.6	99.9	81.2	0.540
	SD	53	30	38	1	6.7	0.1	1.5	0.050

HRH1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	190	82	201	3	69.9	98.5	82.1	0.689
27	Test 2	164	92	219	1	64.1	99.5	80.5	0.666

28	Test 3	193	85	194	4	69.4	98.0	81.3	0.675
29	Test 4	165	69	241	1	70.5	99.6	85.3	0.735
30	Test 5	177	58	238	3	75.3	98.8	87.2	0.764
	Avg	178	77	219	2	69.8	98.9	83.3	0.706
	SD	14	14	21	1	4.0	0.7	2.8	0.042

OPRM1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	532	190	455	6	73.7	98.7	83.4	0.709
22	Test 2	585	149	443	6	79.7	98.7	86.9	0.761
23	Test 3	632	117	424	10	84.4	97.7	89.3	0.794
24	Test 4	529	154	493	7	77.5	98.6	86.4	0.755
25	Test 5	598	124	454	7	82.8	98.5	88.9	0.793
	Avg	575	147	454	7	79.6	98.4	87.0	0.762
	SD	44	29	25	2	4.3	0.4	2.3	0.035

CHRM1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	226	142	280	3	61.4	98.9	77.7	0.627
27	Test 2	262	103	276	10	71.8	96.5	82.6	0.687
28	Test 3	294	127	213	17	69.8	92.6	77.9	0.598
29	Test 4	305	128	213	5	70.4	97.7	79.6	0.644
30	Test 5	288	139	218	6	67.4	97.3	77.7	0.618
	Avg	275	128	240	8	68.2	96.6	79.1	0.635

SD	32	15	35	6	4.1	2.4	2.1	0.034
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CHRM2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	261	73	393	6	78.1	98.5	89.2	0.793
27	Test 2	159	165	406	3	49.1	99.3	77.1	0.579
28	Test 3	189	129	413	2	59.4	99.5	82.1	0.666
29	Test 4	206	128	397	2	61.7	99.5	82.3	0.676
30	Test 5	200	123	401	9	61.9	97.8	82.0	0.657
	Avg	203	124	402	4	62.0	98.9	82.5	0.674
	SD	37	33	8	3	10.4	0.7	4.3	0.077

CHRM3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	153	150	226	1	50.5	99.6	71.5	0.546
27	Test 2	179	131	220	0	57.7	100.0	75.3	0.602
28	Test 3	226	101	200	3	69.1	98.5	80.4	0.664
29	Test 4	227	77	221	5	74.7	97.8	84.5	0.722
30	Test 5	192	101	229	8	65.5	96.6	79.4	0.638
	Avg	195	112	219	3	63.5	98.5	78.2	0.634
	SD	32	29	11	3	9.5	1.4	5.0	0.066

SLC6A2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	1668	62	1118	62	96.4	94.7	95.7	0.912
27	Test 2	1684	67	1115	44	96.2	96.2	96.2	0.921
28	Test 3	1677	92	1099	42	94.8	96.3	95.4	0.905
29	Test 4	1689	76	1095	50	95.7	95.6	95.7	0.910
30	Test 5	1654	97	1122	37	94.5	96.8	95.4	0.906
	Avg	1674	79	1110	47	95.5	95.9	95.7	0.911
	SD	14	15	12	10	0.9	0.8	0.3	0.006

HTR2A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	668	86	194	10	88.6	95.1	90.0	0.753
27	Test 2	619	126	208	5	83.1	97.7	86.3	0.705
28	Test 3	702	59	192	5	92.2	97.5	93.3	0.825
29	Test 4	663	93	198	4	87.7	98.0	89.9	0.760
30	Test 5	633	108	211	6	85.4	97.2	88.1	0.734
	Avg	657	94	201	6	87.4	97.1	89.5	0.755
	SD	32	25	8	2	3.4	1.2	2.6	0.044

HTR3A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	35	63	202	1	35.7	99.5	78.7	0.509
27	Test 2	59	42	200	0	58.4	100.0	86.0	0.695
28	Test 3	18	64	219	0	22.0	100.0	78.7	0.412
29	Test 4	33	50	217	1	39.8	99.5	83.1	0.555

30	Test 5	29	58	214	0	33.3	100.0	80.7	0.512
	Avg	35	55	210	0	37.8	99.8	81.5	0.537
	SD	15	9	9	1	13.3	0.3	3.1	0.103

LCK

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	237	126	83	5	65.3	94.3	71.0	0.474
27	Test 2	253	111	87	0	69.5	100.0	75.4	0.553
28	Test 3	305	57	77	12	84.3	86.5	84.7	0.616
29	Test 4	261	83	103	4	75.9	96.3	80.7	0.623
30	Test 5	202	97	144	8	67.6	94.7	76.7	0.590
	Avg	252	95	99	6	72.5	94.4	77.7	0.571
	SD	37	26	27	4	7.7	4.9	5.2	0.061

AVPR1A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	108	24	202	1	81.8	99.5	92.5	0.848
27	Test 2	72	38	225	0	65.5	100.0	88.7	0.748
28	Test 3	52	66	215	2	44.1	99.1	79.7	0.560
29	Test 4	102	40	193	0	71.8	100.0	88.1	0.771
30	Test 5	99	18	217	1	84.6	99.5	94.3	0.877
	Avg	87	37	210	1	69.6	99.6	88.7	0.761
	SD	24	19	13	1	16.2	0.4	5.7	0.124

AGTR1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	151	49	197	0	75.5	100.0	87.7	0.778
27	Test 2	127	32	238	0	79.9	100.0	91.9	0.839
28	Test 3	128	42	227	0	75.3	100.0	89.4	0.797
29	Test 4	135	38	224	0	78.0	100.0	90.4	0.817
30	Test 5	66	38	293	0	63.5	100.0	90.4	0.750
	Avg	121	40	236	0	74.4	100.0	90.0	0.796
	SD	32	6	35	0	6.4	0.0	1.6	0.035

AKT1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	542	75	177	3	87.8	98.3	90.2	0.775
27	Test 2	445	125	221	6	78.1	97.4	83.6	0.687
28	Test 3	432	118	230	17	78.5	93.1	83.1	0.668
29	Test 4	427	94	272	4	82.0	98.6	87.7	0.769
30	Test 5	404	103	281	9	79.7	96.9	85.9	0.737
	Avg	450	103	236	8	81.2	96.9	86.1	0.727
	SD	54	20	42	6	4.0	2.2	3.0	0.048

BACE1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	1133	146	407	38	88.6	91.5	89.3	0.750
27	Test 2	985	207	504	28	82.6	94.7	86.4	0.726

28	Test 3	846	332	530	16	71.8	97.1	79.8	0.641
29	Test 4	870	343	491	20	71.7	96.1	78.9	0.620
30	Test 5	768	386	561	9	66.6	98.4	77.1	0.614
	Avg	920	283	499	22	76.3	95.6	82.3	0.670
	SD	142	101	58	11	9.0	2.7	5.3	0.063

BCHE

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	115	166	428	0	40.9	100.0	76.6	0.543
27	Test 2	133	136	439	1	49.4	99.8	80.7	0.610
28	Test 3	85	223	401	0	27.6	100.0	68.5	0.421
29	Test 4	132	149	427	1	47.0	99.8	78.8	0.586
30	Test 5	117	144	443	5	44.8	98.9	79.0	0.559
	Avg	116	164	428	1	42.0	99.7	76.7	0.544
	SD	19	35	16	2	8.6	0.5	4.8	0.073

CASP1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	0	253	660	0	0.0	100.0	72.3	#DIV/0!
22	Test 2	0	251	662	0	0.0	100.0	72.5	#DIV/0!
23	Test 3	57	223	631	2	20.4	99.7	75.4	0.376
24	Test 4	0	291	622	0	0.0	100.0	68.1	#DIV/0!
25	Test 5	0	294	619	0	0.0	100.0	67.8	#DIV/0!
	Avg	11	262	639	0	4.1	99.9	71.2	#DIV/0!

SD	25	30	21	1	9.1	0.1	3.2	#DIV/0!
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CASP3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	104	161	336	0	39.2	100.0	73.2	0.515
22	Test 2	73	174	350	4	29.6	98.9	70.4	0.418
23	Test 3	79	124	397	1	38.9	99.7	79.2	0.538
24	Test 4	101	134	362	4	43.0	98.9	77.0	0.538
25	Test 5	75	152	374	0	33.0	100.0	74.7	0.485
	Avg	86	149	364	2	36.7	99.5	74.9	0.499
	SD	15	20	23	2	5.4	0.6	3.4	0.050

CASP8

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	16	49	227	0	24.6	100.0	83.2	0.450
27	Test 2	10	49	233	0	16.9	100.0	83.2	0.374
28	Test 3	22	43	227	0	33.8	100.0	85.3	0.533
29	Test 4	2	53	237	0	3.6	100.0	81.8	0.172
30	Test 5	46	40	205	1	53.5	99.5	86.0	0.657
	Avg	19	47	226	0	26.5	99.9	83.9	0.437
	SD	17	5	12	0	18.7	0.2	1.7	0.182

CHRM5

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	38	102	212	0	27.1	100.0	71.0	0.428
27	Test 2	71	83	197	1	46.1	99.5	76.1	0.561
28	Test 3	62	67	222	1	48.1	99.6	80.7	0.598
29	Test 4	27	91	234	0	22.9	100.0	74.1	0.406
30	Test 5	14	124	213	1	10.1	99.5	64.5	0.234
	Avg	42	93	216	1	30.9	99.7	73.3	0.445
	SD	24	21	14	1	16.1	0.3	6.0	0.144

CHUK

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	18	52	206	1	25.7	99.5	80.9	0.434
27	Test 2	14	63	200	0	18.2	100.0	77.3	0.372
28	Test 3	28	34	213	2	45.2	99.1	87.0	0.593
29	Test 4	12	34	231	0	26.1	100.0	87.7	0.477
30	Test 5	15	46	216	0	24.6	100.0	83.4	0.450
	Avg	17	46	213	1	27.9	99.7	83.2	0.465
	SD	6	12	12	1	10.1	0.4	4.4	0.081

CSF1R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	207	68	202	0	75.3	100.0	85.7	0.750
22	Test 2	191	78	208	0	71.0	100.0	83.6	0.719
23	Test 3	177	92	208	0	65.8	100.0	80.7	0.675
24	Test 4	193	78	206	0	71.2	100.0	83.6	0.719

25	Test 5	139	113	225	0	55.2	100.0	76.3	0.606
	Avg	181	86	210	0	67.7	100.0	82.0	0.694
	SD	26	17	9	0	7.8	0.0	3.7	0.056

CSNK1D

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	75	72	200	0	51.0	100.0	79.3	0.612
22	Test 2	70	62	215	0	53.0	100.0	82.1	0.642
23	Test 3	63	82	202	0	43.4	100.0	76.4	0.556
24	Test 4	65	74	207	1	46.8	99.5	78.4	0.578
25	Test 5	64	81	202	0	44.1	100.0	76.7	0.561
	Avg	67	74	205	0	47.7	99.9	78.6	0.590
	SD	5	8	6	0	4.2	0.2	2.3	0.036

EDNRB

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	131	87	191	0	60.1	100.0	78.7	0.643
27	Test 2	125	34	249	1	78.6	99.6	91.4	0.826
28	Test 3	84	61	261	3	57.9	98.9	84.4	0.664
29	Test 4	71	96	242	0	42.5	100.0	76.5	0.552
30	Test 5	55	65	287	2	45.8	99.3	83.6	0.593
	Avg	93	69	246	1	57.0	99.6	82.9	0.655
	SD	33	24	35	1	14.2	0.5	5.8	0.105

ELANE

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	344	137	215	5	71.5	97.7	79.7	0.643
22	Test 2	303	138	260	0	68.7	100.0	80.3	0.670
23	Test 3	306	136	258	1	69.2	99.6	80.5	0.670
24	Test 4	236	133	331	1	64.0	99.7	80.9	0.672
25	Test 5	225	176	298	2	56.1	99.3	74.6	0.586
	Avg	283	144	272	2	65.9	99.3	79.2	0.648
	SD	51	18	44	2	6.1	0.9	2.6	0.037

EPHA2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	153	14	159	0	91.6	100.0	95.7	0.918
27	Test 2	78	22	226	0	78.0	100.0	93.3	0.843
28	Test 3	51	27	248	0	65.4	100.0	91.7	0.768
29	Test 4	77	30	219	0	72.0	100.0	90.8	0.796
30	Test 5	34	42	250	0	44.7	100.0	87.1	0.619
	Avg	79	27	220	0	70.3	100.0	91.7	0.789
	SD	46	10	37	0	17.3	0.0	3.2	0.111

FGFR1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	445	91	137	1	83.0	99.3	86.4	0.702
22	Test 2	273	149	246	6	64.7	97.6	77.0	0.612

23	Test 3	319	99	253	3	76.3	98.8	84.9	0.730
24	Test 4	175	229	270	0	43.3	100.0	66.0	0.484
25	Test 5	214	169	289	2	55.9	99.3	74.6	0.586
	Avg	285	147	239	2	64.6	99.0	77.8	0.623
	SD	105	56	59	2	15.9	0.9	8.3	0.098

FKBP1A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	0	84	188	0	0.0	100.0	69.1	#DIV/0!
22	Test 2	0	101	171	0	0.0	100.0	62.9	#DIV/0!
23	Test 3	11	43	217	1	20.4	99.5	83.8	0.387
24	Test 4	12	49	211	0	19.7	100.0	82.0	0.400
25	Test 5	3	51	218	0	5.6	100.0	81.3	0.212
	Avg	5	66	201	0	9.1	99.9	75.8	#DIV/0!
	SD	6	25	21	0	10.2	0.2	9.3	#DIV/0!

FLT1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	94	112	427	0	45.6	100.0	82.3	0.601
22	Test 2	147	99	386	1	59.8	99.7	84.2	0.685
23	Test 3	136	88	407	2	60.7	99.5	85.8	0.697
24	Test 4	83	121	429	0	40.7	100.0	80.9	0.563
25	Test 5	92	116	425	0	44.2	100.0	81.7	0.589
	Avg	110	107	415	1	50.2	99.9	83.0	0.627

SD	29	13	18	1	9.3	0.2	2.0	0.060
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FLT4

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	38	113	199	1	25.2	99.5	67.5	0.389
22	Test 2	59	64	228	0	48.0	100.0	81.8	0.612
23	Test 3	49	85	217	0	36.6	100.0	75.8	0.513
24	Test 4	54	80	217	0	40.3	100.0	77.2	0.543
25	Test 5	52	80	219	0	39.4	100.0	77.2	0.537
	Avg	50	84	216	0	37.9	99.9	75.9	0.519
	SD	8	18	11	0	8.3	0.2	5.2	0.082

FYN

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	27	74	198	0	26.7	100.0	75.3	0.441
27	Test 2	15	58	225	1	20.5	99.6	80.3	0.384
28	Test 3	11	78	210	0	12.4	100.0	73.9	0.300
29	Test 4	12	78	209	0	13.3	100.0	73.9	0.312
30	Test 5	6	61	232	0	9.0	100.0	79.6	0.266
	Avg	14	70	215	0	16.4	99.9	76.6	0.341
	SD	8	10	14	0	7.2	0.2	3.1	0.071

GSK3B

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	396	127	229	9	75.7	96.2	82.1	0.668
27	Test 2	418	73	246	24	85.1	91.1	87.3	0.739
28	Test 3	341	153	258	9	69.0	96.6	78.7	0.629
29	Test 4	308	194	250	9	61.4	96.5	73.3	0.556
30	Test 5	362	177	207	15	67.2	93.2	74.8	0.549
	Avg	365	145	238	13	71.7	94.7	79.2	0.628
	SD	44	47	20	7	9.1	2.5	5.7	0.080

HDAC3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	127	85	218	8	59.9	96.5	78.8	0.610
22	Test 2	95	114	223	6	45.5	97.4	72.6	0.508
23	Test 3	114	113	209	2	50.2	99.1	73.7	0.558
24	Test 4	117	70	251	0	62.6	100.0	84.0	0.699
25	Test 5	116	100	219	3	53.7	98.6	76.5	0.588
	Avg	114	96	224	4	54.4	98.3	77.1	0.593
	SD	12	19	16	3	7.0	1.4	4.5	0.071

IGF1R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	542	46	132	3	92.2	97.8	93.2	0.814
27	Test 2	350	123	249	1	74.0	99.6	82.8	0.700
28	Test 3	424	99	200	0	81.1	100.0	86.3	0.736
29	Test 4	366	90	259	8	80.3	97.0	86.4	0.746

30	Test 5	320	123	278	2	72.2	99.3	82.7	0.701
	Avg	400	96	224	3	79.9	98.7	86.3	0.740
	SD	88	32	59	3	7.8	1.3	4.3	0.046

INSR

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	203	53	140	0	79.3	100.0	86.6	0.758
27	Test 2	128	40	228	0	76.2	100.0	89.9	0.805
28	Test 3	99	46	251	0	68.3	100.0	88.4	0.760
29	Test 4	86	54	256	0	61.4	100.0	86.4	0.712
30	Test 5	106	72	218	0	59.6	100.0	81.8	0.669
	Avg	124	53	219	0	68.9	100.0	86.6	0.741
	SD	47	12	47	0	8.7	0.0	3.0	0.052

KDR

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	1323	310	239	7	81.0	97.2	83.1	0.580
27	Test 2	905	641	321	12	58.5	96.4	65.2	0.420
28	Test 3	1385	197	273	24	87.5	91.9	88.2	0.669
29	Test 4	1174	313	375	17	79.0	95.7	82.4	0.629
30	Test 5	1299	269	295	16	82.8	94.9	84.8	0.630
	Avg	1217	346	301	15	77.8	95.2	80.8	0.586
	SD	191	171	51	6	11.2	2.0	9.0	0.098

LTB4R

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	36	19	221	0	65.5	100.0	93.1	0.776
27	Test 2	39	32	205	0	54.9	100.0	88.4	0.689
28	Test 3	42	37	197	0	53.2	100.0	86.6	0.669
29	Test 4	27	48	201	0	36.0	100.0	82.6	0.539
30	Test 5	18	52	206	0	25.7	100.0	81.2	0.453
	Avg	32	38	206	0	47.1	100.0	86.4	0.625
	SD	10	13	9	0	15.9	0.0	4.8	0.128

LYN

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	64	38	198	0	62.7	100.0	87.3	0.726
27	Test 2	39	41	220	0	48.8	100.0	86.3	0.641
28	Test 3	29	64	206	1	31.2	99.5	78.3	0.473
29	Test 4	30	68	201	1	30.6	99.5	77.0	0.464
30	Test 5	24	57	219	0	29.6	100.0	81.0	0.485
	Avg	37	54	209	0	40.6	99.8	82.0	0.558
	SD	16	14	10	1	14.7	0.3	4.7	0.119

MAPK1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	358	966	2133	0	27.0	100.0	72.1	0.431
22	Test 2	290	955	2212	0	23.3	100.0	72.4	0.403

23	Test 3	348	854	2255	0	29.0	100.0	75.3	0.458
24	Test 4	298	904	2255	0	24.8	100.0	73.9	0.421
25	Test 5	361	875	2221	0	29.2	100.0	74.7	0.458
	Avg	331	911	2215	0	26.7	100.0	73.7	0.434
	SD	34	49	50	0	2.6	0.0	1.4	0.024

MAPK9

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	200	61	201	1	76.6	99.5	86.6	0.762
27	Test 2	167	71	224	1	70.2	99.6	84.4	0.725
28	Test 3	166	76	220	1	68.6	99.5	83.4	0.709
29	Test 4	197	40	224	2	83.1	99.1	90.9	0.830
30	Test 5	156	93	214	0	62.7	100.0	79.9	0.661
	Avg	177	68	217	1	72.2	99.5	85.1	0.737
	SD	20	20	10	1	7.9	0.3	4.1	0.063

MAPKAPK2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	90	74	229	4	54.9	98.3	80.4	0.616
22	Test 2	84	93	219	1	47.5	99.5	76.3	0.570
23	Test 3	85	80	232	0	51.5	100.0	79.8	0.619
24	Test 4	34	102	261	0	25.0	100.0	74.3	0.424
25	Test 5	63	124	210	0	33.7	100.0	68.8	0.460
	Avg	71	95	230	1	42.5	99.6	75.9	0.538

SD	23	20	19	2	12.7	0.7	4.7	0.090
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MET

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	536	66	196	5	89.0	97.5	91.2	0.800
27	Test 2	439	102	260	2	81.1	99.2	87.0	0.757
28	Test 3	487	80	230	6	85.9	97.5	89.3	0.780
29	Test 4	457	126	217	3	78.4	98.6	83.9	0.694
30	Test 5	447	131	224	1	77.3	99.6	83.6	0.695
	Avg	473	101	225	3	82.4	98.5	87.0	0.745
	SD	40	28	23	2	5.0	1.0	3.3	0.048

MMP13

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	360	132	205	3	73.2	98.6	80.7	0.656
27	Test 2	363	107	229	1	77.2	99.6	84.6	0.722
28	Test 3	372	114	211	3	76.5	98.6	83.3	0.694
29	Test 4	414	62	222	2	87.0	99.1	90.9	0.818
30	Test 5	345	119	228	8	74.4	96.6	81.9	0.671
	Avg	371	107	219	3	77.7	98.5	84.3	0.712
	SD	26	27	11	3	5.5	1.1	4.0	0.064

MMP2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	449	158	313	3	74.0	99.1	82.6	0.693
27	Test 2	382	210	324	7	64.5	97.9	76.5	0.606
28	Test 3	341	258	321	3	56.9	99.1	71.7	0.553
29	Test 4	428	143	348	4	75.0	98.9	84.1	0.719
30	Test 5	354	215	348	6	62.2	98.3	76.1	0.603
	Avg	391	197	331	5	66.5	98.6	78.2	0.635
	SD	47	47	16	2	7.8	0.5	5.1	0.069

MMP3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	231	150	176	2	60.6	98.9	72.8	0.562
22	Test 2	186	181	192	0	50.7	100.0	67.6	0.511
23	Test 3	245	131	180	3	65.2	98.4	76.0	0.600
24	Test 4	191	117	248	3	62.0	98.8	78.5	0.635
25	Test 5	217	110	228	4	66.4	98.3	79.6	0.651
	Avg	214	138	205	2	61.0	98.9	74.9	0.592
	SD	25	29	32	2	6.2	0.7	4.8	0.057

MMP9

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	228	322	333	3	41.5	99.1	63.3	0.448
22	Test 2	244	245	390	7	49.9	98.2	71.6	0.531
23	Test 3	234	280	372	0	45.5	100.0	68.4	0.510
24	Test 4	270	249	364	3	52.0	99.2	71.6	0.546

25	Test 5	252	258	375	1	49.4	99.7	70.8	0.538
	Avg	246	271	367	3	47.7	99.3	69.1	0.515
	SD	16	32	21	3	4.2	0.7	3.5	0.040

NEK2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	25	48	198	0	34.2	100.0	82.3	0.525
27	Test 2	32	42	197	0	43.2	100.0	84.5	0.597
28	Test 3	22	32	217	0	40.7	100.0	88.2	0.596
29	Test 4	11	33	227	0	25.0	100.0	87.8	0.467
30	Test 5	3	50	218	0	5.7	100.0	81.5	0.215
	Avg	19	41	211	0	29.8	100.0	84.9	0.480
	SD	12	8	13	0	15.2	0.0	3.1	0.158

P2RY1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	77	34	221	0	69.4	100.0	89.8	0.775
22	Test 2	73	64	195	0	53.3	100.0	80.7	0.633
23	Test 3	53	32	244	3	62.4	98.8	89.5	0.713
24	Test 4	69	54	209	0	56.1	100.0	83.7	0.668
30	Test 5	76	28	228	0	73.1	100.0	91.6	0.807
	Avg	70	42	219	1	62.8	99.8	87.0	0.719
	SD	10	16	19	1	8.4	0.5	4.6	0.072

PAK4

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	28	69	199	0	28.9	100.0	76.7	0.463
27	Test 2	27	39	230	0	40.9	100.0	86.8	0.591
28	Test 3	28	50	218	0	35.9	100.0	83.1	0.540
29	Test 4	33	37	226	0	47.1	100.0	87.5	0.636
30	Test 5	34	35	227	0	49.3	100.0	88.2	0.653
	Avg	30	46	220	0	40.4	100.0	84.5	0.577
	SD	3	14	13	0	8.3	0.0	4.8	0.077

PDE4A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	70	61	202	1	53.4	99.5	81.4	0.632
27	Test 2	93	52	188	1	64.1	99.5	84.1	0.701
28	Test 3	44	66	223	1	40.0	99.6	79.9	0.544
29	Test 4	66	63	204	1	51.2	99.5	80.8	0.616
30	Test 5	48	90	196	0	34.8	100.0	73.1	0.488
	Avg	64	66	203	1	48.7	99.6	79.9	0.596
	SD	20	14	13	0	11.6	0.2	4.1	0.082

PDE5A

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	153	132	245	15	53.7	94.2	73.0	0.518
27	Test 2	249	56	238	2	81.6	99.2	89.4	0.805

28	Test 3	184	109	249	3	62.8	98.8	79.4	0.647
29	Test 4	261	92	191	1	73.9	99.5	82.9	0.702
30	Test 5	190	125	225	5	60.3	97.8	76.1	0.599
	Avg	207	103	230	5	66.5	97.9	80.2	0.654
	SD	46	30	23	6	11.2	2.1	6.3	0.108

PIK3CA

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	910	84	358	10	91.5	97.3	93.1	0.843
27	Test 2	769	146	443	4	84.0	99.1	89.0	0.788
28	Test 3	723	139	486	14	83.9	97.2	88.8	0.784
29	Test 4	827	146	387	2	85.0	99.5	89.1	0.782
30	Test 5	712	268	380	2	72.7	99.5	80.2	0.649
	Avg	788	157	411	6	83.4	98.5	88.0	0.769
	SD	82	67	52	5	6.8	1.2	4.7	0.072

PPARG

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	409	459	1438	23	47.1	98.4	79.3	0.567
22	Test 2	256	635	1436	2	28.7	99.9	72.6	0.443
23	Test 3	309	497	1518	5	38.3	99.7	78.4	0.529
24	Test 4	202	657	1469	1	23.5	99.9	71.7	0.401
30	Test 5	251	687	1376	15	26.8	98.9	69.9	0.396
	Avg	285	587	1447	9	32.9	99.4	74.4	0.467

SD	79	102	52	9	9.7	0.7	4.2	0.077
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PTPN1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	46	274	408	2	14.4	99.5	62.2	0.278
27	Test 2	101	237	388	4	29.9	99.0	67.0	0.410
28	Test 3	73	207	437	13	26.1	97.1	69.9	0.350
29	Test 4	56	241	433	0	18.9	100.0	67.0	0.348
30	Test 5	34	202	494	0	14.4	100.0	72.3	0.320
	Avg	62	232	432	4	20.7	99.1	67.7	0.341
	SD	26	29	40	5	7.0	1.2	3.8	0.048

PTPN11

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	9	73	231	0	11.0	100.0	76.7	0.289
27	Test 2	1	64	248	0	1.5	100.0	79.6	0.111
28	Test 3	8	52	251	2	13.3	99.2	82.7	0.281
29	Test 4	0	72	241	0	0.0	100.0	77.0	#DIV/0!
30	Test 5	1	74	238	0	1.3	100.0	76.4	0.101
	Avg	4	67	242	0	5.4	99.8	78.5	#DIV/0!
	SD	4	9	8	1	6.2	0.4	2.7	#DIV/0!

PTPN2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
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26	Test 1	17	59	232	1	22.4	99.6	80.6	0.403
27	Test 2	11	54	244	0	16.9	100.0	82.5	0.372
28	Test 3	6	65	238	0	8.5	100.0	79.0	0.258
29	Test 4	6	58	245	0	9.4	100.0	81.2	0.275
30	Test 5	16	47	246	0	25.4	100.0	84.8	0.462
	Avg	11	57	241	0	16.5	99.9	81.6	0.354
	SD	5	7	6	0	7.6	0.2	2.2	0.086

RAF1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	191	88	208	0	68.5	100.0	81.9	0.694
22	Test 2	212	95	180	0	69.1	100.0	80.5	0.672
23	Test 3	197	68	222	0	74.3	100.0	86.0	0.754
24	Test 4	203	67	217	0	75.2	100.0	86.2	0.758
30	Test 5	146	84	256	1	63.5	99.6	82.5	0.686
	Avg	190	80	217	0	70.1	99.9	83.4	0.713
	SD	26	12	27	0	4.8	0.2	2.6	0.040

RARA

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	26	62	633	0	29.5	100.0	91.4	0.519
27	Test 2	12	58	651	0	17.1	100.0	92.0	0.397
28	Test 3	32	39	650	0	45.1	100.0	94.6	0.652
29	Test 4	11	51	659	0	17.7	100.0	92.9	0.406

30	Test 5	34	31	655	1	52.3	99.8	95.6	0.695
	Avg	23	48	650	0	32.4	100.0	93.3	0.534
	SD	11	13	10	0	15.9	0.1	1.8	0.137

RARB

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	51	8	670	0	86.4	100.0	98.9	0.924
27	Test 2	13	46	670	0	22.0	100.0	93.7	0.454
28	Test 3	31	32	666	0	49.2	100.0	95.6	0.685
29	Test 4	38	20	671	0	65.5	100.0	97.3	0.798
30	Test 5	29	30	670	0	49.2	100.0	95.9	0.686
	Avg	32	27	669	0	54.5	100.0	96.3	0.709
	SD	14	14	2	0	23.7	0.0	1.9	0.173

ROCK1

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	175	107	200	0	62.1	100.0	77.8	0.636
22	Test 2	140	132	210	0	51.5	100.0	72.6	0.562
23	Test 3	155	83	243	1	65.1	99.6	82.6	0.692
24	Test 4	134	129	216	3	51.0	98.6	72.6	0.547
30	Test 5	119	119	243	1	50.0	99.6	75.1	0.573
	Avg	145	114	222	1	55.9	99.6	76.1	0.602
	SD	21	20	20	1	7.1	0.6	4.2	0.060

RPS6KA5

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	11	39	202	0	22.0	100.0	84.5	0.429
27	Test 2	4	36	212	0	10.0	100.0	85.7	0.292
28	Test 3	13	35	204	0	27.1	100.0	86.1	0.481
29	Test 4	2	43	207	0	4.4	100.0	82.9	0.192
30	Test 5	10	31	211	0	24.4	100.0	87.7	0.461
	Avg	8	37	207	0	17.6	100.0	85.4	0.371
	SD	5	4	4	0	9.8	0.0	1.8	0.124

SIRT2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	49	44	236	0	52.7	100.0	86.6	0.666
27	Test 2	14	56	259	0	20.0	100.0	83.0	0.406
28	Test 3	6	50	273	0	10.7	100.0	84.8	0.301
29	Test 4	12	64	252	1	15.8	99.6	80.2	0.333
30	Test 5	9	57	263	0	13.6	100.0	82.7	0.335
	Avg	18	54	257	0	22.6	99.9	83.5	0.408
	SD	18	8	14	0	17.2	0.2	2.4	0.149

SIRT3

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
21	Test 1	0	48	197	0	0.0	100.0	80.4	#DIV/0!
22	Test 2	0	34	211	0	0.0	100.0	86.1	#DIV/0!

23	Test 3	0	15	230	0	0.0	100.0	93.9	#DIV/0!
24	Test 4	0	27	218	0	0.0	100.0	89.0	#DIV/0!
25	Test 5	0	27	218	0	0.0	100.0	89.0	#DIV/0!
	Avg	0	30	215	0	0.0	100.0	87.7	#DIV/0!
	SD	0	12	12	0	0.0	0.0	4.9	#DIV/0!

SRC

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	424	122	290	11	77.7	96.3	84.3	0.709
27	Test 2	332	177	330	8	65.2	97.6	78.2	0.628
28	Test 3	340	160	338	9	68.0	97.4	80.0	0.653
29	Test 4	377	204	262	4	64.9	98.5	75.4	0.591
30	Test 5	369	199	274	5	65.0	98.2	75.9	0.598
	Avg	368	172	299	7	68.1	97.6	78.8	0.636
	SD	36	33	34	3	5.5	0.8	3.6	0.048

TACR2

Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
26	Test 1	132	46	378	2	74.2	99.5	91.4	0.803
27	Test 2	114	74	370	0	60.6	100.0	86.7	0.711
28	Test 3	103	44	411	0	70.1	100.0	92.1	0.796
29	Test 4	86	53	419	0	61.9	100.0	90.5	0.741
30	Test 5	173	51	332	2	77.2	99.4	90.5	0.810
	Avg	122	54	382	1	68.8	99.8	90.3	0.772

		SD	33	12	35	1	7.3	0.3	2.1	0.044
TBXA2R										
	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
	21	Test 1	59	154	368	0	27.7	100.0	73.5	0.442
	22	Test 2	103	87	388	3	54.2	99.2	84.5	0.649
	23	Test 3	84	107	388	2	44.0	99.5	81.2	0.575
	24	Test 4	33	145	403	0	18.5	100.0	75.0	0.369
	25	Test 5	100	130	351	0	43.5	100.0	77.6	0.563
		Avg	76	125	380	1	37.6	99.7	78.4	0.520
		SD	30	28	20	1	14.3	0.4	4.5	0.112
TEK										
	Model Number		TP	FN	TN	FP	SE	SP	ACC	MCC
	21	Test 1	102	65	217	0	61.1	100.0	83.1	0.686
	22	Test 2	118	56	210	0	67.8	100.0	85.4	0.732
	23	Test 3	118	39	227	0	75.2	100.0	89.8	0.801
	24	Test 4	90	65	229	0	58.1	100.0	83.1	0.673
	25	Test 5	50	85	249	0	37.0	100.0	77.9	0.525
		Avg	96	62	226	0	59.8	100.0	83.9	0.683
		SD	28	17	15	0	14.3	0.0	4.3	0.101

Table S12. Model performance results for each target where a positive probability value of 0.9 was used as the threshold to assign compounds as predicted active or inactive. In each case standard deviations are shown below averages. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC).

Target Gene	SE			SP			ACC			MCC		
	DNN	Δ SA	Δ RF	DNN	Δ SA	Δ RF	DNN	Δ SA	Δ RF	DNN	Δ SA	Δ RF
AChE	88.4	6.6	-3.2	85.3	-4.6	7.5	87.0	1.6	1.6	0.737	0.024	0.030
ADORA2A	97.6	2.8	-0.5	93.2	2.0	4.2	96.1	2.5	1.1	0.912	0.054	0.024
ADRA2A	91.3	11.2	2.0	93.9	-1.2	-1.2	92.7	4.3	0.2	0.853	0.084	0.004
AR	66.5	-0.8	1.1	99.1	1.4	1.2	90.5	0.8	1.2	0.749	0.026	0.036
ADRB1	92.7	7.0	0.3	89.5	-2.5	1.5	91.2	2.5	0.9	0.823	0.046	0.017
ADRB2	72.9	-2.3	-3.3	89.9	2.2	1.4	81.6	0.0	-0.9	0.639	0.004	-0.014
OPRD1	97.1	1.1	-1.2	81.0	-0.3	4.5	92.4	0.7	0.4	0.813	0.018	0.011
DRD1	77.4	0.9	-3.7	96.6	1.5	4.3	89.2	1.4	1.2	0.773	0.030	0.028
DRD2	98.3	1.9	-1.0	84.8	5.7	7.8	96.1	2.5	0.5	0.855	0.091	0.021
SLC6A3	89.9	1.3	-3.1	94.5	1.9	4.9	91.8	1.5	0.2	0.837	0.032	0.010
EDNRA	93.8	-0.6	-3.4	95.6	1.7	4.8	94.6	0.4	0.4	0.893	0.010	0.009
NR3C1	74.5	2.3	0.7	96.9	0.1	0.6	90.1	0.7	0.6	0.760	0.018	0.015
KCNH2	84.4	15.7	-8.6	70.9	-11.5	17.4	79.1	5.0	1.6	0.558	0.059	0.036
HRH1	95.2	8.0	-0.6	88.4	-5.3	0.7	92.0	1.7	0.0	0.840	0.032	-0.001
OPRM1	94.8	1.2	-1.1	94.5	1.7	3.2	94.7	1.4	0.6	0.889	0.030	0.014
CHRM1	96.6	6.4	0.9	83.3	-2.9	0.7	91.7	2.9	0.8	0.821	0.062	0.019
CHRM2	93.9	2.9	0.0	94.5	1.1	3.2	94.2	1.9	1.8	0.883	0.039	0.035
CHRM3	91.9	3.4	-3.2	93.8	1.8	5.8	92.8	2.8	0.8	0.854	0.053	0.017
SLC6A2	94.9	4.2	-0.2	92.5	-1.0	1.0	93.9	2.0	0.3	0.875	0.039	0.008
HTR2A	99.1	2.4	-0.4	88.2	-0.4	6.1	96.7	1.8	1.0	0.901	0.051	0.030
HTR3A	89.4	5.7	-1.0	98.2	-0.4	0.4	95.8	1.3	0.0	0.893	0.034	0.000
SLC6A4	98.4	2.7	-0.3	89.0	2.1	6.3	96.3	2.5	1.2	0.892	0.070	0.037
LCK	95.5	3.7	0.2	79.8	-2.6	-0.9	92.3	2.5	0.0	0.763	0.054	-0.002

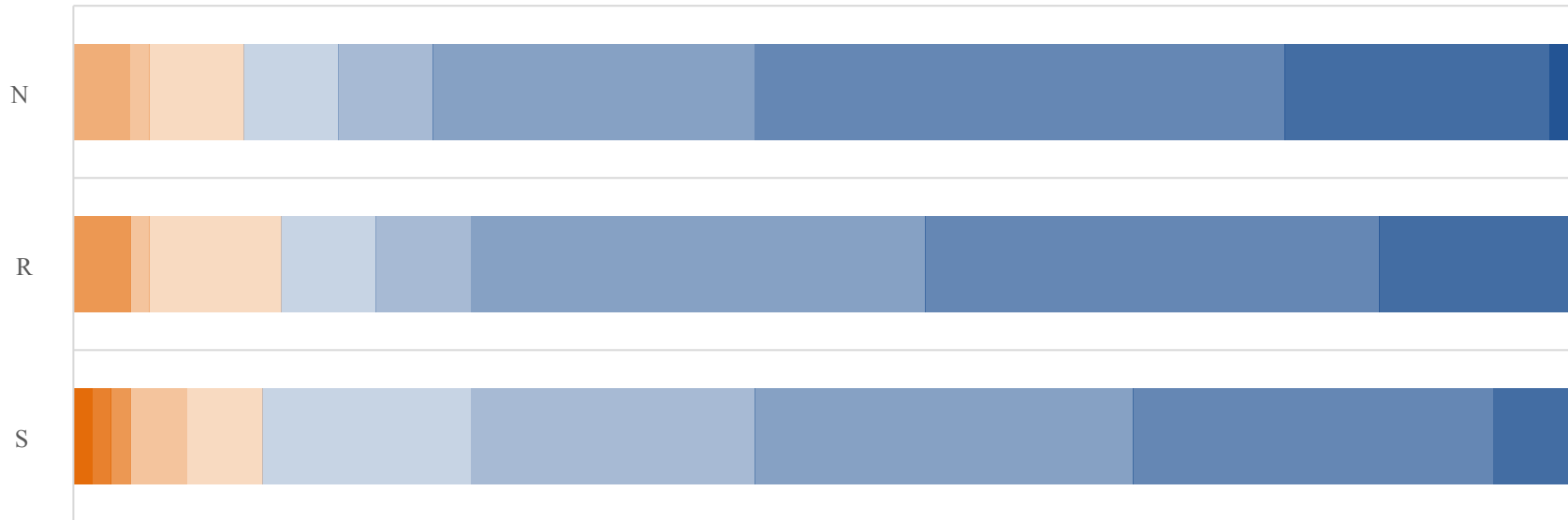
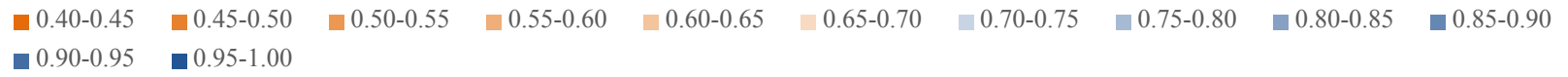
AVPR1A	93.9	1.9	0.6	99.3	1.5	4.8	97.2	1.6	3.2	0.941	0.034	0.068
AGTR1	87.3	0.0	3.4	99.3	1.0	1.9	94.5	0.6	2.6	0.888	0.014	0.054
AKT1	95.4	1.0	-1.4	91.3	4.4	6.6	94.1	2.1	1.1	0.864	0.049	0.028
BACE1	92.0	-1.1	-5.7	93.5	5.7	14.1	92.5	0.9	0.1	0.827	0.028	0.016
BCHE	85.6	7.1	-0.9	93.6	0.6	4.7	90.4	3.3	2.5	0.799	0.067	0.048
CASP1	69.1	5.3	-1.9	94.7	-0.1	-0.1	86.5	1.5	-0.8	0.680	0.039	-0.018
CASP3	84.8	3.4	3.7	94.9	-1.1	-1.1	91.0	0.6	0.7	0.809	0.013	0.015
CASP8	86.8	-4.9	-2.5	95.4	-2.1	-2.8	92.1	-4.1	-4.1	0.832	-0.060	-0.059
CHRM5	87.4	3.6	-4.2	95.3	1.5	4.0	92.3	2.3	0.9	0.835	0.048	0.015
CHUK	88.8	5.7	-3.3	97.4	0.4	0.0	95.2	1.7	-0.9	0.871	0.047	-0.024
CSF1R	94.3	5.9	-2.4	97.0	0.8	3.1	95.5	3.7	0.0	0.910	0.070	0.001
CSNK1D	91.4	12.4	3.8	94.8	-1.6	2.0	93.4	4.4	2.8	0.864	0.085	0.056
EDNRB	96.1	2.0	-0.5	94.4	-0.4	-0.7	95.1	0.6	-0.6	0.899	0.013	-0.012
ELANE	90.9	-0.4	-5.2	93.8	0.2	5.8	92.1	-0.1	-0.8	0.839	-0.001	-0.012
EPHA2	87.2	0.0	-0.7	99.6	1.1	1.8	95.4	0.7	1.0	0.899	0.018	0.023
FGFR1	96.8	5.9	0.8	92.0	-2.8	1.4	95.1	2.8	1.0	0.892	0.054	0.021
FKBP1A	88.1	-3.0	-6.9	97.4	-0.4	1.5	94.8	-1.1	-0.9	0.869	-0.028	-0.025
FLT1	91.6	1.6	-3.0	99.0	0.9	2.5	96.2	1.2	0.4	0.919	0.024	0.008
FLT4	91.9	10.7	0.0	96.5	-0.4	1.2	94.5	4.3	0.6	0.888	0.086	0.014
FYN	77.8	5.1	-3.0	98.2	0.4	1.5	92.7	1.6	0.3	0.809	0.044	0.006
GSK3B	96.8	12.2	-1.1	78.3	-5.2	2.5	90.4	6.2	0.1	0.785	0.121	0.001
HDAC3	94.1	2.3	0.3	94.8	1.5	2.7	94.5	2.0	1.6	0.890	0.039	0.032
IGF1R	94.6	-1.0	-2.1	95.5	1.3	5.1	94.9	-0.2	0.3	0.889	-0.003	0.011
INSR	91.7	1.7	-3.1	98.9	1.2	1.9	95.5	1.4	-0.5	0.912	0.028	-0.007

KDR	97.4	2.8	-0.3	73.1	-9.7	9.2	93.5	0.8	1.2	0.748	0.005	0.058
LTB4R	91.4	4.3	2.2	98.8	0.0	1.2	96.8	1.2	1.5	0.918	0.030	0.038
LYN	89.1	10.9	-1.8	98.0	2.7	2.7	95.4	5.2	1.4	0.888	0.127	0.030
MAPK1	43.5	-4.4	2.3	99.2	4.0	-0.2	79.3	1.0	0.6	0.557	0.043	0.013
MAPK9	95.5	3.5	-2.9	97.7	2.2	7.9	96.5	2.9	2.0	0.931	0.058	0.040
MAPKAPK2	86.9	5.1	-3.3	94.1	1.4	2.5	91.0	3.0	0.0	0.816	0.062	-0.001
MET	97.7	4.3	-1.0	91.9	3.2	8.4	95.9	4.0	1.9	0.904	0.091	0.045
MMP13	94.9	1.5	-2.1	94.7	3.3	10.6	94.8	2.1	2.3	0.887	0.045	0.054
MMP2	95.5	1.7	0.0	89.2	-3.6	6.0	93.2	-0.2	2.1	0.852	-0.006	0.048
MMP3	94.7	1.8	-1.7	92.4	1.2	8.8	93.8	1.5	2.1	0.868	0.033	0.047
MMP9	81.6	-0.2	-5.0	88.8	-1.5	6.9	84.6	-0.8	0.0	0.696	-0.016	0.011
NEK2	77.0	9.4	-2.7	98.5	0.7	1.0	94.0	2.6	0.3	0.813	0.085	0.007
P2RY1	92.7	-2.4	-2.4	100.0	1.5	3.4	97.7	0.3	1.5	0.947	0.007	0.035
PAK4	89.4	7.0	-4.7	99.3	0.8	1.1	96.9	2.2	-0.3	0.914	0.064	-0.009
PDE4A	90.8	2.9	-1.1	94.9	-0.4	0.5	93.1	1.0	-0.3	0.859	0.020	-0.005
PDE5A	90.1	3.4	-4.8	96.5	2.8	7.3	93.0	3.1	0.6	0.862	0.062	0.016
PIK3CA	98.9	1.5	-0.4	93.3	-1.5	4.6	97.2	0.6	1.2	0.934	0.014	0.027
PPARG	69.5	-0.8	-2.9	96.1	3.4	2.0	86.0	1.8	0.2	0.702	0.041	0.006
PTPN1	76.6	9.5	-3.9	89.7	-2.6	3.1	84.7	2.0	0.4	0.673	0.046	0.005
PTPN11	64.8	26.2	14.8	91.9	-3.4	-3.4	85.7	3.4	0.8	0.584	0.153	0.052
PTPN2	67.9	2.5	2.5	96.0	-1.7	2.3	90.1	-0.7	2.4	0.687	-0.022	0.069
RAF1	99.7	4.2	0.0	95.2	-1.1	1.5	97.7	1.8	0.7	0.954	0.038	0.013
RARA	63.1	1.9	1.9	99.4	1.8	0.0	95.2	1.9	0.3	0.742	0.092	0.013
RARB	85.9	11.3	5.6	99.9	1.1	0.0	98.8	1.9	0.5	0.913	0.137	0.033

ROCK1	94.3	5.4	-2.5	92.0	-3.6	1.1	93.2	1.2	-0.9	0.864	0.021	-0.018
RPS6KA5	73.7	12.3	0.0	100.0	1.5	2.7	95.3	3.4	2.2	0.835	0.135	0.080
SIRT2	70.8	2.3	5.6	95.2	-0.6	-1.6	89.8	0.0	0.0	0.692	0.003	0.006
SIRT3	76.7	-2.4	-4.7	98.5	0.8	0.8	95.4	0.3	0.0	0.802	0.010	-0.005
SRC	94.7	4.6	-2.7	88.7	0.7	8.1	92.4	3.1	1.5	0.839	0.064	0.029
TACR2	87.6	-1.6	-4.4	100.0	2.4	2.4	96.0	1.1	0.2	0.910	0.029	0.008
TBXA2R	88.8	-0.4	-2.1	94.9	-0.4	1.4	93.0	-0.4	0.3	0.838	-0.010	0.003
TEK	89.9	2.5	-4.1	97.8	2.6	1.9	94.5	2.6	-0.6	0.887	0.053	-0.013

Table S13. A comparison between DNNs and previously published structural alert (SA) and random forest (RF) models trained on the same training data and evaluated on the same test data. Test data results are shown here, including the change in result from models previously published in Wedlake *et al.*³⁸ (Δ). These are coloured blue or orange, to show increased or decreased performance respectively. Full results can be found in Table S14. SE=sensitivity, SP=specificity, ACC=accuracy, MCC=Matthews correlation coefficient.

D o M V



D o A

73-76 76-79 79-82 82-85 85-88 88-91 91-94 94-97 97-100

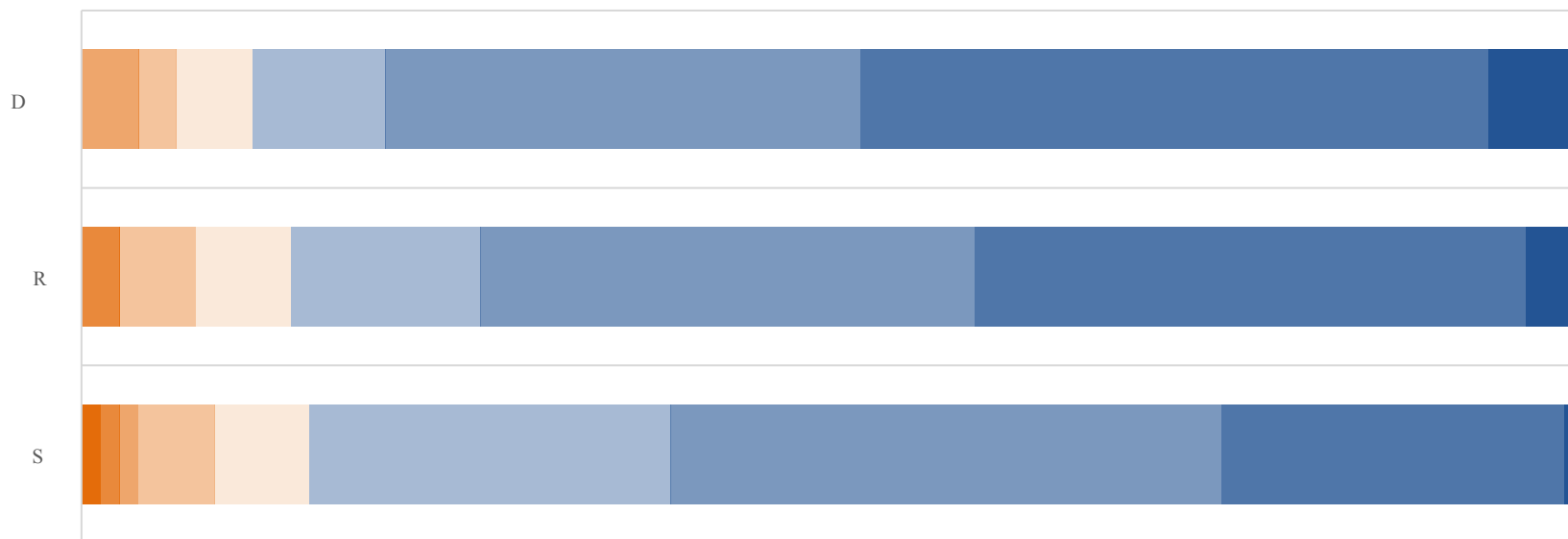


Figure S1. Comparison charts for the distribution of test accuracy and MCC values between DNNs and previously published structural alert (SA) and random forest (RF) models trained on the same training data and evaluated on the same test data. Numbers on each category indicate the number of models falling into that class.

Target Gene	Training Set									
	TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
AChE	1878	126	1344	123	0.98	93.7	91.6	92.8	0.853	0.98
ADORA2A	2911	46	1545	37	1.00	98.4	97.7	98.2	0.960	1.00
ADRA2A	615	34	758	11	0.99	94.8	98.6	96.8	0.936	0.99
AR	1397	592	5441	28	0.94	70.2	99.5	91.7	0.784	0.94
ADRB1	936	24	745	61	0.99	97.5	92.4	95.2	0.903	0.99
ADRB2	1146	316	1432	69	0.95	78.4	95.4	87.0	0.750	0.95
OPRD1	2197	43	820	84	0.99	98.1	90.7	96.0	0.901	0.99
DRD1	831	198	1462	22	0.97	80.8	98.5	91.2	0.823	0.97
DRD2	4220	42	796	59	0.99	99.0	93.1	98.0	0.929	0.99
SLC6A3	1773	97	1404	41	0.99	94.8	97.2	95.8	0.916	0.99
EDNRA	932	30	834	25	0.99	96.9	97.1	97.0	0.939	0.99
NR3C1	1773	501	5146	97	0.93	78.0	98.1	92.0	0.809	0.93
KCNH2	3463	154	2190	231	0.98	95.7	90.5	93.6	0.867	0.98
HRH1	938	25	792	30	1.00	97.4	96.4	96.9	0.938	1.00
OPRM1	2600	61	1685	38	0.99	97.7	97.8	97.7	0.953	0.99
CHRM1	1465	19	859	78	0.99	98.7	91.7	96.0	0.916	0.99
CHRM2	1187	38	1468	38	0.99	96.9	97.5	97.2	0.944	0.99
CHRM3	1141	49	821	18	0.99	95.9	97.9	96.7	0.933	0.99
SLC6A2	2145	78	1388	61	0.99	96.5	95.8	96.2	0.921	0.99
HTR2A	2775	22	726	45	1.00	99.2	94.2	98.1	0.944	1.00
HTR3A	329	19	775	3	1.00	94.5	99.6	98.0	0.954	1.00
SLC6A4	3041	16	830	22	1.00	99.5	97.4	99.0	0.971	1.00

LCK	1259	24	377	28	0.99	98.1	93.1	96.9	0.915	0.99
AVPR1A	448	8	782	5	1.00	98.2	99.4	99.0	0.977	1.00
AGTR1	555	46	878	1	0.99	92.3	99.9	96.8	0.935	0.99
AKT1	2022	50	865	35	0.99	97.6	96.1	97.1	0.933	0.99
BACE1	4211	263	1881	94	0.99	94.1	95.2	94.5	0.874	0.99
BCHE	900	138	1556	57	0.98	86.7	96.5	92.6	0.845	0.98
CASP1	736	274	2366	62	0.97	72.9	97.4	90.2	0.759	0.97
CASP3	776	105	1296	58	0.98	88.1	95.7	92.7	0.847	0.98
CASP8	802	79	1303	51	0.99	91.0	96.2	94.2	0.878	0.99
CHRM5	475	37	795	15	0.99	92.8	98.1	96.1	0.917	0.99
CHUK	211	16	794	10	0.99	93.0	98.8	97.5	0.926	0.99
CSF1R	970	30	782	7	1.00	97.0	99.1	97.9	0.959	1.00
CSNK1D	499	25	762	14	0.99	95.2	98.2	97.0	0.938	0.99
EDNRB	595	9	905	26	1.00	98.5	97.2	97.7	0.953	1.00
ELANE	1488	106	987	31	0.99	93.4	97.0	94.8	0.893	0.99
EPHA2	374	13	829	0	1.00	96.6	100.0	98.9	0.975	1.00
FGFR1	1593	43	857	63	0.99	97.4	93.2	95.9	0.910	0.99
FKBP1A	240	13	728	13	1.00	94.9	98.2	97.4	0.931	1.00
FLT1	748	41	1576	20	0.99	94.8	98.7	97.4	0.942	0.99
FLT4	473	15	816	13	0.99	96.9	98.4	97.9	0.954	0.99
FYN	295	26	805	1	1.00	91.9	99.9	97.6	0.941	1.00
GSK3B	1905	28	846	84	0.99	98.6	91.0	96.1	0.910	0.99
HDAC3	769	26	846	43	0.99	96.7	95.2	95.9	0.918	0.99
IGF1R	1822	55	807	14	1.00	97.1	98.3	97.4	0.941	1.00

INSR	647	11	825	4	1.00	98.3	99.5	99.0	0.980	1.00
KDR	5730	101	1003	198	0.99	98.3	83.5	95.7	0.846	0.99
LTB4R	235	22	784	1	0.99	91.4	99.9	97.8	0.940	0.99
LYN	330	14	787	6	1.00	95.9	99.2	98.2	0.958	1.00
MAPK1	2121	2579	8294	59	0.84	45.1	99.3	79.8	0.572	0.84
MAPK9	894	22	818	5	1.00	97.6	99.4	98.4	0.969	1.00
MAPKAPK2	567	48	843	30	0.99	92.2	96.6	94.8	0.892	0.99
MET	2143	36	807	28	1.00	98.3	96.6	97.9	0.947	1.00
MMP13	1762	62	787	23	0.99	96.6	97.2	96.8	0.926	0.99
MMP2	2119	66	1158	103	0.99	97.0	91.8	95.1	0.894	0.99
MMP3	1247	62	740	36	0.99	95.3	95.4	95.3	0.900	0.99
MMP9	1711	229	1280	104	0.96	88.2	92.5	90.0	0.799	0.96
NEK2	199	25	779	6	0.99	88.8	99.2	96.9	0.910	0.99
P2RY1	420	17	829	7	1.00	96.1	99.2	98.1	0.958	1.00
PAK4	279	16	831	1	0.99	94.6	99.9	98.5	0.961	0.99
PDE4A	454	26	773	10	1.00	94.6	98.7	97.1	0.939	1.00
PDE5A	1129	69	869	19	0.99	94.2	97.9	95.8	0.915	0.99
PIK3CA	3514	28	1462	85	1.00	99.2	94.5	97.8	0.947	1.00
PPARG	2424	853	5343	160	0.94	74.0	97.1	88.5	0.754	0.94
PTPN1	1004	133	1559	79	0.98	88.3	95.2	92.4	0.842	0.98
PTPN11	238	28	903	12	0.98	89.5	98.7	96.6	0.902	0.98
PTPN2	215	43	897	11	0.99	83.3	98.8	95.4	0.862	0.99
RAF1	1004	13	800	15	1.00	98.7	98.2	98.5	0.969	1.00
RARA	169	84	2465	0	0.99	66.8	100.0	96.9	0.804	0.99

RARB	208	19	2524	0	0.98	91.6	100.0	99.3	0.954	0.98
ROCK1	952	28	813	30	0.99	97.1	96.4	96.8	0.936	0.99
RPS6KA5	154	13	777	0	1.00	92.2	100.0	98.6	0.952	1.00
SIRT2	243	29	946	31	0.98	89.3	96.8	95.2	0.859	0.98
SIRT3	87	21	801	10	0.98	80.6	98.8	96.6	0.831	0.98
SRC	2034	46	1078	62	0.99	97.8	94.6	96.6	0.926	0.99
TACR2	549	77	1384	1	0.99	87.7	99.9	96.1	0.910	0.99
TBXA2R	715	55	1376	34	0.98	92.9	97.6	95.9	0.910	0.98
TEK	540	49	854	7	0.99	91.7	99.2	96.1	0.921	0.99

Target Gene	Test									
	TP	FN	TN	FP	ROC-AUC	SE	SP	ACC	MCC	ROC-AUC
AChE	539	71	423	73	0.92	88.4	85.3	87.0	0.737	0.92
ADORA2A	962	24	467	34	0.98	97.6	93.2	96.1	0.912	0.98
ADRA2A	179	17	230	15	0.97	91.3	93.9	92.7	0.853	0.97
AR	431	217	1798	17	0.88	66.5	99.1	90.5	0.749	0.88
ADRB1	279	22	247	29	0.94	92.7	89.5	91.2	0.823	0.94
ADRB2	352	131	461	52	0.89	72.9	89.9	81.6	0.639	0.89
OPRD1	744	22	255	60	0.98	97.1	81.0	92.4	0.813	0.98
DRD1	250	73	490	17	0.93	77.4	96.6	89.2	0.773	0.93
DRD2	1410	24	239	43	0.98	98.3	84.8	96.1	0.855	0.98
SLC6A3	576	65	446	26	0.97	89.9	94.5	91.8	0.837	0.97
EDNRA	303	20	280	13	0.97	93.8	95.6	94.6	0.893	0.97
NR3C1	554	190	1676	54	0.91	74.5	96.9	90.1	0.760	0.91

KCNH2	1078	200	585	240	0.85	84.4	70.9	79.1	0.558	0.85
HRH1	298	15	251	33	0.97	95.2	88.4	92.0	0.840	0.97
OPRM1	901	49	553	32	0.98	94.8	94.5	94.7	0.889	0.98
CHRM1	513	18	254	51	0.96	96.6	83.3	91.7	0.821	0.96
CHRM2	386	25	498	29	0.98	93.9	94.5	94.2	0.883	0.98
CHRM3	319	28	258	17	0.97	91.9	93.8	92.8	0.854	0.97
SLC6A2	654	35	455	37	0.97	94.9	92.5	93.9	0.875	0.97
HTR2A	951	9	232	31	0.99	99.1	88.2	96.7	0.901	0.99
HTR3A	93	11	272	5	0.95	89.4	98.2	95.8	0.893	0.95
SLC6A4	970	16	252	31	0.99	98.4	89.0	96.3	0.892	0.99
LCK	429	20	95	24	0.94	95.5	79.8	92.3	0.763	0.94
AVPR1A	153	10	270	2	0.98	93.9	99.3	97.2	0.941	0.98
AGTR1	179	26	301	2	0.98	87.3	99.3	94.5	0.888	0.98
AKT1	662	32	293	28	0.98	95.4	91.3	94.1	0.864	0.98
BACE1	1419	123	590	41	0.97	92.0	93.5	92.5	0.827	0.97
BCHE	310	52	498	34	0.95	85.6	93.6	90.4	0.799	0.95
CASP1	248	111	730	41	0.91	69.1	94.7	86.5	0.680	0.91
CASP3	251	45	450	24	0.96	84.8	94.9	91.0	0.809	0.96
CASP8	257	39	452	22	0.97	86.8	95.4	92.1	0.832	0.97
CHRM5	146	21	262	13	0.97	87.4	95.3	92.3	0.835	0.97
CHUK	79	10	259	7	0.98	88.8	97.4	95.2	0.871	0.98
CSF1R	317	19	256	8	0.99	94.3	97.0	95.5	0.910	0.99
CSNK1D	170	16	238	13	0.97	91.4	94.8	93.4	0.864	0.97
EDNRB	197	8	288	17	0.99	96.1	94.4	95.1	0.899	0.99

ELANE	491	49	335	22	0.97	90.9	93.8	92.1	0.839	0.97
EPHA2	123	18	272	1	0.98	87.2	99.6	95.4	0.899	0.98
FGFR1	510	17	265	23	0.99	96.8	92.0	95.1	0.892	0.99
FKBP1A	89	12	260	7	0.99	88.1	97.4	94.8	0.869	0.99
FLT1	274	25	479	5	0.99	91.6	99.0	96.2	0.919	0.99
FLT4	171	15	245	9	0.98	91.9	96.5	94.5	0.888	0.98
FYN	77	22	266	5	0.94	77.8	98.2	92.7	0.809	0.94
GSK3B	597	20	256	71	0.96	96.8	78.3	90.4	0.785	0.96
HDAC3	241	15	239	13	0.98	94.1	94.8	94.5	0.890	0.98
IGF1R	574	33	298	14	0.99	94.6	95.5	94.9	0.889	0.99
INSR	211	19	261	3	0.99	91.7	98.9	95.5	0.912	0.99
KDR	1934	51	277	102	0.97	97.4	73.1	93.5	0.748	0.97
LTB4R	85	8	244	3	0.97	91.4	98.8	96.8	0.918	0.97
LYN	98	12	251	5	0.97	89.1	98.0	95.4	0.888	0.97
MAPK1	657	852	2701	23	0.77	43.5	99.2	79.3	0.557	0.77
MAPK9	298	14	260	6	0.99	95.5	97.7	96.5	0.931	0.99
MAPKAPK2	186	28	269	17	0.97	86.9	94.1	91.0	0.816	0.97
MET	676	16	285	25	0.99	97.7	91.9	95.9	0.904	0.99
MMP13	535	29	286	16	0.99	94.9	94.7	94.8	0.887	0.99
MMP2	719	34	372	45	0.98	95.5	89.2	93.2	0.852	0.98
MMP3	426	24	242	20	0.98	94.7	92.4	93.8	0.868	0.98
MMP9	524	118	413	52	0.91	81.6	88.8	84.6	0.696	0.91
NEK2	57	17	271	4	0.97	77.0	98.5	94.0	0.813	0.97
P2RY1	114	9	267	0	0.99	92.7	100.0	97.7	0.947	0.99

PAK4	76	9	269	2	0.99	89.4	99.3	96.9	0.914	0.99
PDE4A	157	16	222	12	0.97	90.8	94.9	93.1	0.859	0.97
PDE5A	318	35	278	10	0.98	90.1	96.5	93.0	0.862	0.98
PIK3CA	1169	13	503	36	0.99	98.9	93.3	97.2	0.934	0.99
PPARG	754	331	1707	70	0.91	69.5	96.1	86.0	0.702	0.91
PTPN1	256	78	488	56	0.92	76.6	89.7	84.7	0.673	0.92
PTPN11	57	31	273	24	0.90	64.8	91.9	85.7	0.584	0.90
PTPN2	55	26	289	12	0.90	67.9	96.0	90.1	0.687	0.90
RAF1	333	1	256	13	1.00	99.7	95.2	97.7	0.954	1.00
RARA	65	38	779	5	0.90	63.1	99.4	95.2	0.742	0.90
RARB	61	10	823	1	0.96	85.9	99.9	98.8	0.913	0.96
ROCK1	297	18	253	22	0.99	94.3	92.0	93.2	0.864	0.99
RPS6KA5	42	15	263	0	0.95	73.7	100.0	95.3	0.835	0.95
SIRT2	63	26	296	15	0.89	70.8	95.2	89.8	0.692	0.89
SIRT3	33	10	260	4	0.94	76.7	98.5	95.4	0.802	0.94
SRC	592	33	347	44	0.97	94.7	88.7	92.4	0.839	0.97
TACR2	219	31	532	0	0.99	87.6	100.0	96.0	0.910	0.99
TBXA2R	206	26	469	25	0.96	88.8	94.9	93.0	0.838	0.96
TEK	179	20	265	6	0.98	89.9	97.8	94.5	0.887	0.98

Table S14. Model performance results for each target on the training/test split used to compare model performance to structural alert and random forest models. Performance statistics are shown for the training set first, followed by the test set. Model performances are reported as sensitivity (SE), specificity (SP), accuracy (ACC), Matthews correlation coefficient (MCC) and area under receiver operating characteristic curve (ROC-AUC).

t-Test: Paired Two Sample for Means - Accuracy

	SA vs DNN		RF vs DNN	
	SA	DNN	RF	DNN
Mean	92.81	93.73	93.76	93.73
Variance	12.31	9.82	10.75	9.82
Observations	79	79	79	79
Pearson Correlation	0.91		0.95	
Hypothesized Mean Difference	0		0	
df	78		78	
t Stat	-5.65		0.25	
	1.25861E-			
P(T<=t) one-tail	07		0.400478763	
t Critical one-tail	1.66		1.66	
	2.51722E-			
P(T<=t) two-tail	07		0.800957526	
t Critical two-tail	1.99		1.99	

t-Test: Paired Two Sample for Means - MCC

	SA vs DNN		RF vs DNN	
	SA	DNN	RF	DNN
Mean	0.7903	0.8321	0.8146	0.8321
Variance	0.0093	0.0079	0.0083	0.0079
Observations	79	79	79	79
Pearson Correlation	0.9196		0.9648	
Hypothesized Mean Difference	0		0	
df	78		78	
t Stat	-9.8296		-6.4893	
	1.3414E-			
P(T<=t) one-tail	15		3.62582E-09	
t Critical one-tail	1.6646		1.6646	
	2.68279E-			
P(T<=t) two-tail	15		7.25164E-09	
t Critical two-tail	1.9908		1.9908	

Z score test - Accuracy

	SA vs DNN		RF vs DNN	
	SA	DNN	RF	DNN
Mean	92.81	93.73	93.76	93.73
Variance	12.31	9.82	10.75	9.82
Z	-3.87		-1.49	
p	0.0000550		0.0679810	

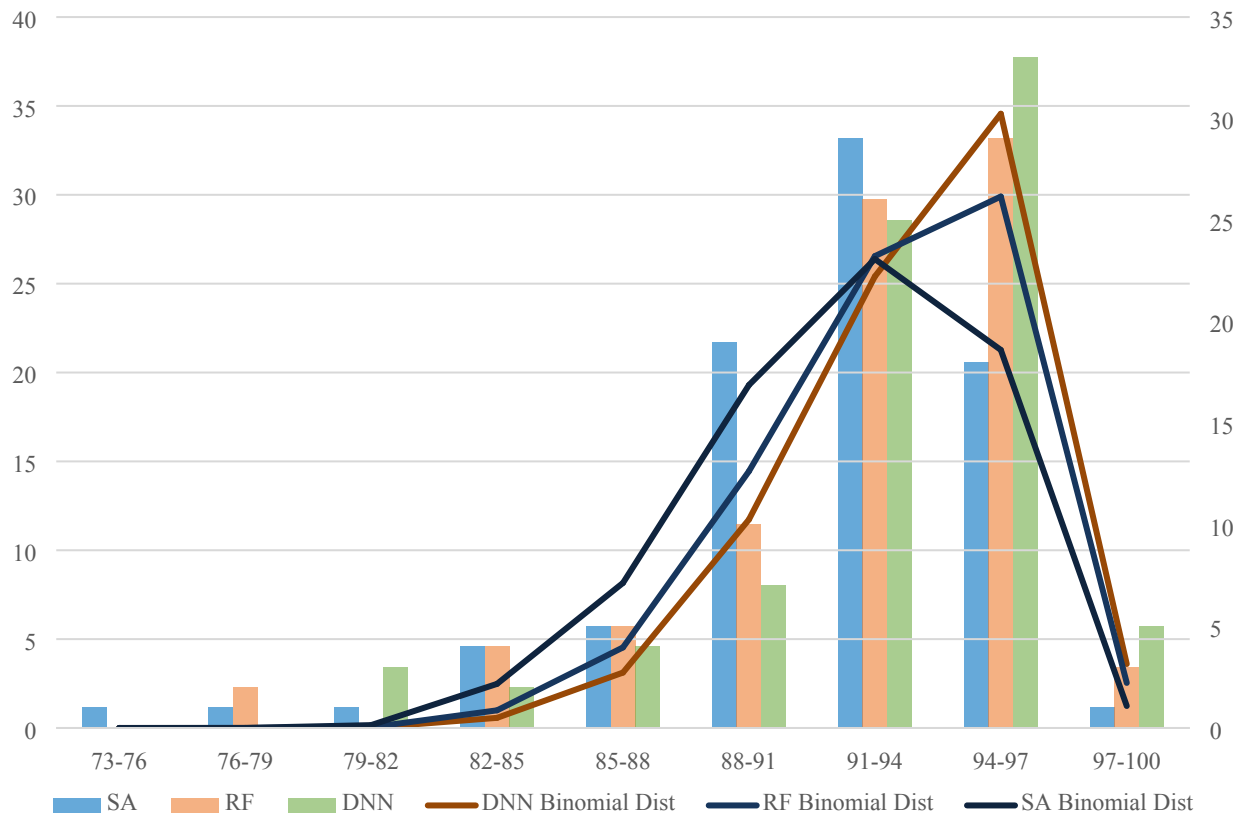
Z score test - MCC

	SA vs DNN		RF vs DNN	
	SA	DNN	RF	DNN

Mean	0.7903	0.8321	0.8146	0.8321
Variance	0.0093	0.0079	0.0083	0.0079
Z	-4.1936		-1.7595	
p	0.000014		0.03929	

Table S15. p-value analysis to show statistical significance between statistical performance for DNN models vs Sa and RF models. At $\alpha=0.05$ DNNs show statistically significant performance increase in accuracy and MCC over SAs and statistically significant performance increase in MCC over RFs.

Accuracy Model Comparison Histogram with Binomial Distributions



MCC Model Comparison Histogram with Binomial Distributions

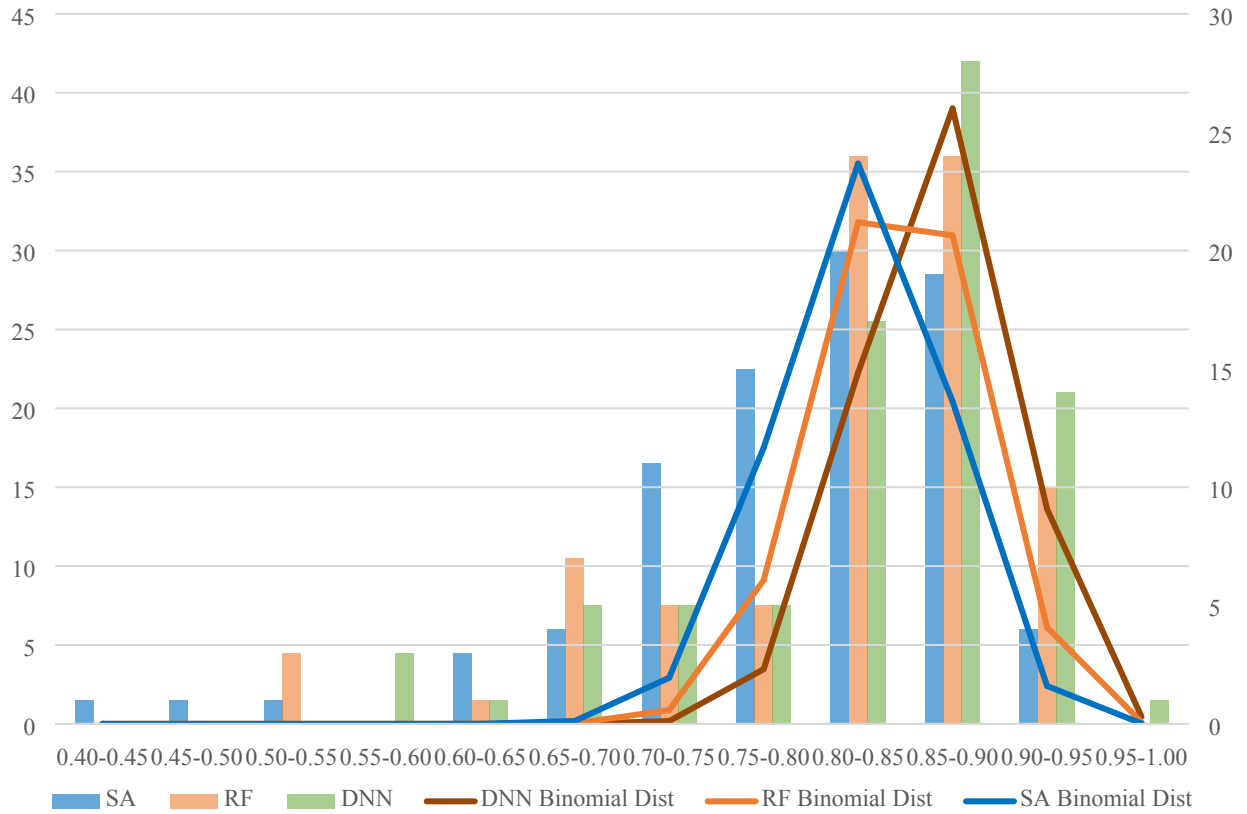


Figure S2. Histograms showing the distribution of test set model performance across the three modelling approaches overlaid with binomial distributions fitted to them. Accuracy binomial distributions are fit to probability values of 0.925 (SA), 0.935 (RF) and 0.94 (MCC) and MCC binomial distributions are fit to probability values of 0.83 (SA), 0.85 (RF) and 0.87 (MCC).

