

Table S2: Prediction performance of SVM models trained on a data set of one ligand and tested on the other. Please note that all data of a given category was trained, allowing to over-learn on itself and hence self-prediction values (trained and test data being the same), all models showed 100% correct predictions. This is in contrast to cross-validation performance results in Table 3 (in the manuscript).

Trained	Tested	Accuracy (%)	Sensitivity (%)	Specificity (%)	F-measure (%)	AUC (%)
AMP	AMP	100.0	100.0	100.0	100.0	100.0
AMP	ADP	91.5	28.7	94.9	25.5	73.3
AMP	ATP	89.0	41.3	91.7	28.7	74.9
AMP	GMP	93.2	23.6	97.0	26.3	72.8
AMP	GDP	83.6	54.7	84.9	22.7	75.1
AMP	GTP	86.1	47.7	88.4	27.7	76.3
AMP	CAMP	84.7	43.8	87.5	26.5	75.4
AMP	PCG	86.1	32.0	89.9	23.0	62.9
ADP	AMP	96.2	25.3	98.1	26.0	81.1
ADP	ADP	100.0	100.0	100.0	100.0	100.0
ADP	ATP	96.2	41.9	99.2	54.0	86.2
ADP	GMP	84.3	47.5	86.3	23.7	72.8
ADP	GDP	95.5	27.2	98.7	34.8	80.3
ADP	GTP	90.3	35.6	93.6	29.1	77.6
ADP	CAMP	84.3	40.4	87.2	24.4	73.6
ADP	PCG	88.3	46.0	91.3	33.8	74.5
ATP	AMP	96.5	31.3	98.3	32.6	85.3
ATP	ADP	96.0	45.2	98.7	53.1	86.4
ATP	ATP	100.0	100.0	100.0	99.9	100.0
ATP	GMP	84.0	52.5	85.7	25.2	73.9
ATP	GDP	94.7	20.0	98.2	25.1	78.2
ATP	GTP	90.5	39.1	93.6	31.5	78.6
ATP	CAMP	91.8	23.3	96.4	26.4	73.2
ATP	PCG	92.0	46.0	95.2	42.6	74.7
GMP	AMP	83.9	42.5	85.0	12.4	73.1
GMP	ADP	83.8	36.3	86.3	18.4	70.0
GMP	ATP	84.5	35.7	87.3	19.9	71.1
GMP	GMP	100.0	100.0	100.0	100.0	100.0
GMP	GDP	83.8	48.0	85.4	20.7	74.2

GMP	GTP	80.4	47.4	82.4	21.3	71.2
GMP	CAMP	77.4	55.4	78.9	23.6	75.0
GMP	PCG	83.8	38.0	87.0	23.3	61.3
GDP	AMP	82.3	49.5	83.2	13.0	75.6
GDP	ADP	92.0	26.6	95.5	25.0	75.6
GDP	ATP	86.1	38.3	88.9	22.9	73.9
GDP	GMP	94.6	29.3	98.1	35.9	85.2
GDP	GDP	100.0	100.0	100.0	99.8	100.0
GDP	GTP	95.2	26.7	99.3	38.4	80.9
GDP	CAMP	81.6	39.6	84.4	21.3	70.3
GDP	PCG	91.5	38.0	95.2	36.5	70.6
GTP	AMP	82.3	49.5	83.2	13.0	74.4
GTP	ADP	91.1	25.8	94.6	22.6	74.3
GTP	ATP	84.5	43.6	86.8	23.2	74.1
GTP	GMP	80.9	40.9	83.1	18.1	67.3
GTP	GDP	95.5	33.3	98.4	39.7	83.3
GTP	GTP	100.0	100.0	100.0	99.9	100.0
GTP	CAMP	67.2	57.9	67.8	18.2	66.7
GTP	PCG	81.6	36.0	84.8	20.2	59.7
CAMP	AMP	76.9	48.3	77.6	10.0	70.2
CAMP	ADP	78.2	44.8	80.0	17.2	69.8
CAMP	ATP	76.0	50.6	77.4	18.5	70.2
CAMP	GMP	74.6	52.9	75.8	17.6	67.0
CAMP	GDP	78.6	51.8	79.8	17.5	69.2
CAMP	GTP	77.7	56.1	79.0	21.9	70.9
CAMP	CAMP	100.0	100.0	100.0	100.0	100.0
CAMP	PCG	95.3	76.0	96.7	67.9	91.2
PCG	AMP	66.7	57.6	67.0	8.5	64.9
PCG	ADP	65.1	58.1	65.5	14.4	65.0
PCG	ATP	62.4	64.0	62.3	15.5	64.6
PCG	GMP	60.2	68.6	59.7	15.0	62.6
PCG	GDP	71.2	55.7	71.9	14.5	66.1
PCG	GTP	68.6	60.0	69.1	17.6	65.6
PCG	CAMP	92.5	30.0	96.6	33.3	77.8
PCG	PCG	100.0	100.0	100.0	100.0	100.0