

Comparison of cross-validated results of ML models on validation dataset

A set of the best hyperparameters was found for the selected ML models. These models were then trained on a training dataset with 10-fold cross-validation. The following plot and table show these results to compare the performance of the selected models.

Table: Mean of MSE ten-fold cross-validated results for prediction of Docking Score values used for model selection

MODEL	CHEMPLP_1DB1	london_1DB1	ASE_1DB1	AHB_1DB1	AdG_1DB1	CHEMPLP_3KPZ	london_3KPZ	ASE_3KPZ	AHB_3KPZ	AdG_3KPZ
KR	83.01	1.2	5.59	87.89	3.26	6.01	1.18	5.4	105.49	3.38
MLP	37.65	0.67	2.36	55.18	2.26	2.8	0.67	2.3	66.52	2.48
SVR	41.1	0.61	2.26	57.3	2.08	2.73	0.61	2.04	58.52	2.16
RF	45.56	0.66	3.12	51.02	2.32	3.17	0.65	2.84	61.6	2.54

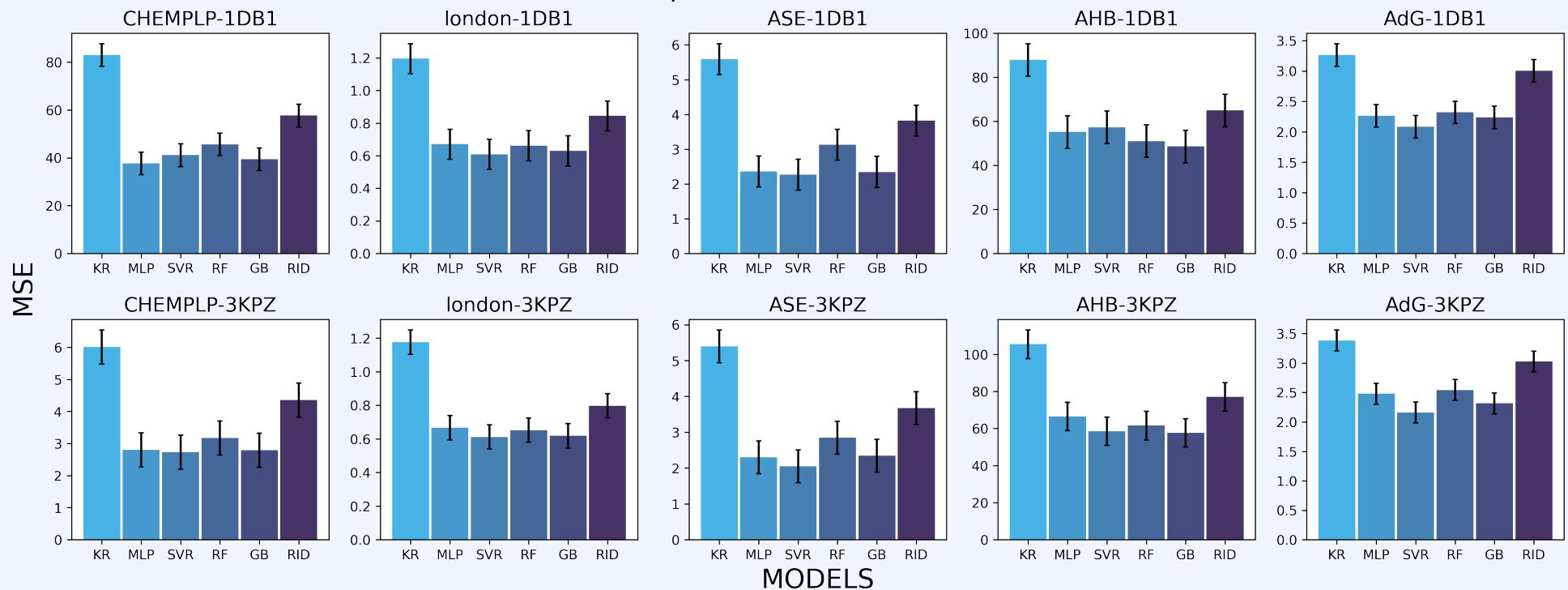
GB	39.39	0.63	2.34	48.62	2.24	2.79	0.62	2.34	57.67	2.32
RID	57.65	0.84	3.82	64.95	3.0	4.35	0.8	3.67	77.08	3.03

**Table: MSE testset results for prediction of Docking Score values,
final model, that will be used for new, neverseen data.**

MODEL	CHEMPLP_1DB1	london_1DB1	ASE_1DB1	AHB_1DB1	AdG_1DB1	CHEMPLP_3KPZ	london_3KPZ	ASE_3KPZ	AHB_3KPZ	AdG_3KPZ
83.01	1.2	5.59	87.89	3.26	6.01	1.18	5.4	105.49	3.38	KR
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41.1	0.61	2.26	57.3	2.08	2.73	0.61	2.04	58.52	2.16	SVR
45.56	0.66	3.12	51.02	2.32	3.17	0.65	2.84	61.6	2.54	RF
39.39	0.63	2.34	48.62	2.24	2.79	0.62	2.34	57.67	2.32	GB
57.65	0.84	3.82	64.95	3.0	4.35	0.8	3.67	77.08	3.03	RID

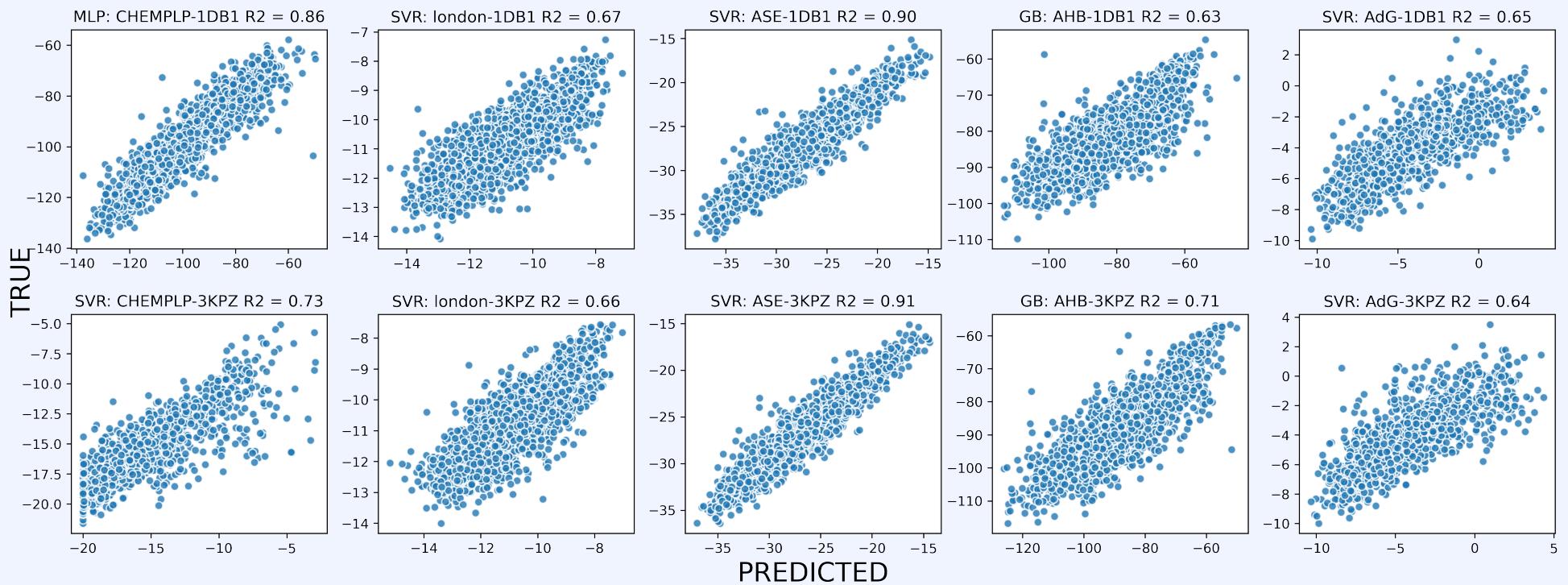
Plots: Mean of MSE with std ten-fold cross-validated results for prediction of Docking Score values

VDR-ML, comparison of models - MSE, cv=10



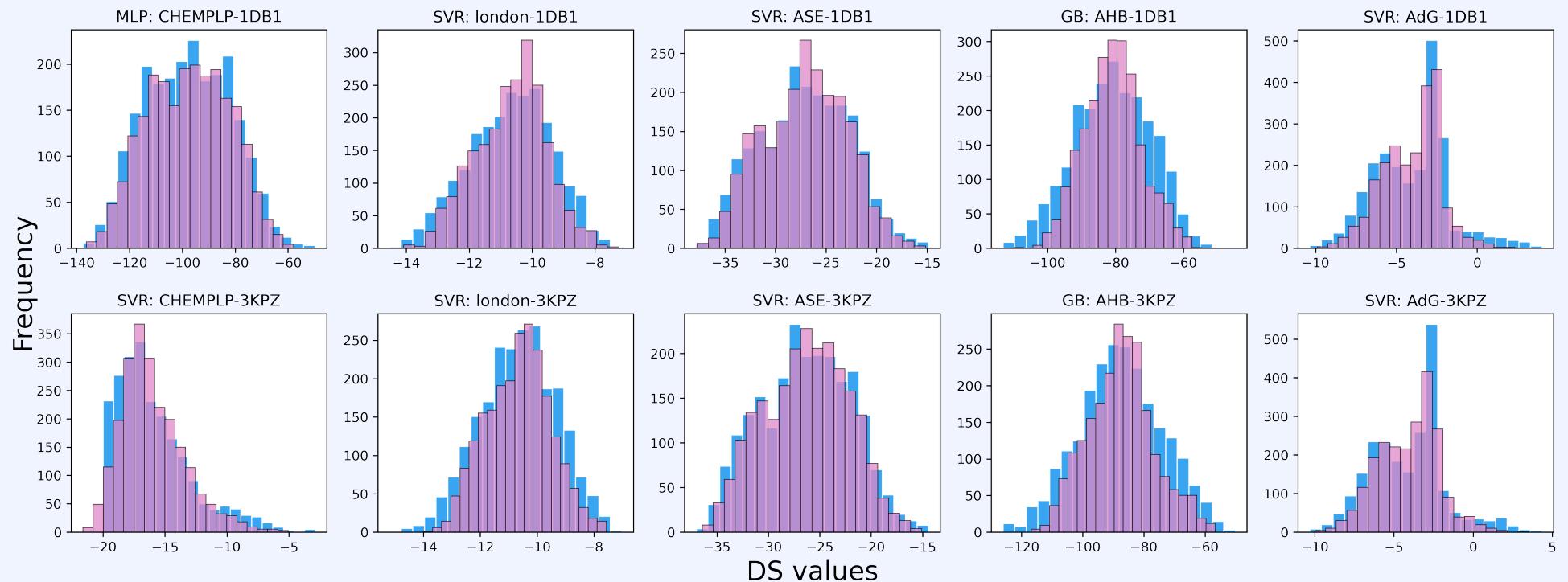
Plots: MSE testset best performing models correlations of true and predicted ds values

VDR-ML, correlations of true and predicted values, test set



Plots: Histograms of the docking scores values for the best performing models

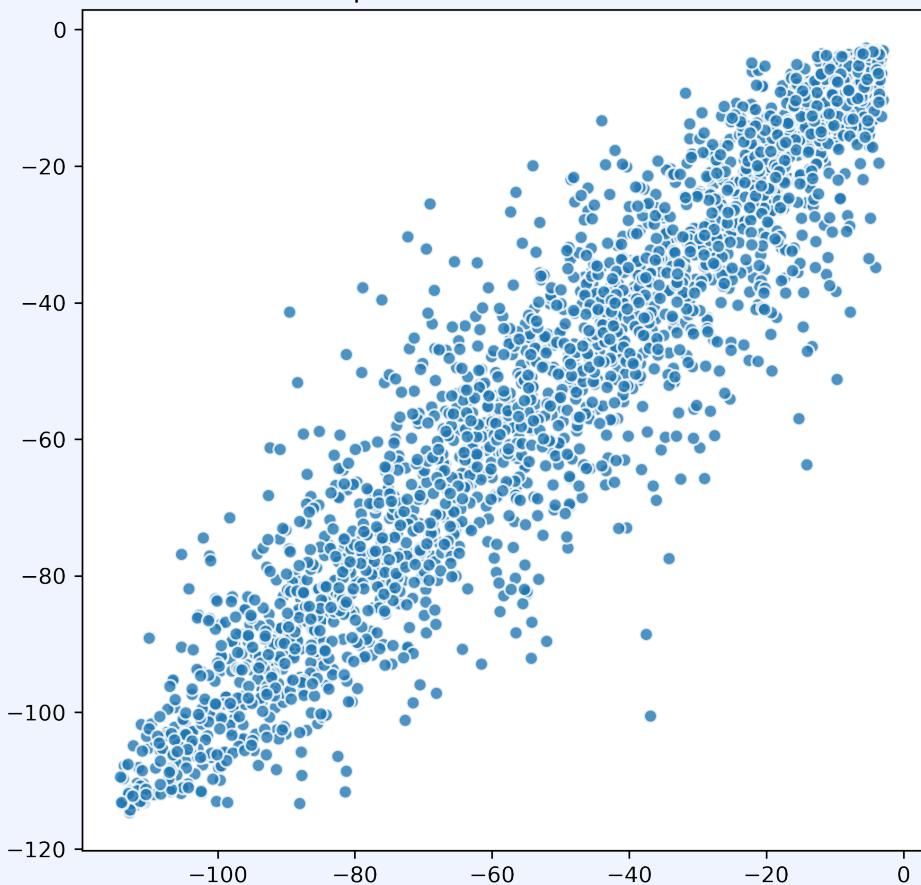
VDR-ML, histograms of true and predicted values, test set, best models



Plots: Correlation of ECR computed from testset predicted values best performing models with R2 > 0.7 vs true ECR

ECR VDR-ML dataset, best_models

ECR 1DB1 predicted vs true: r2 score 0.89



ECR 3KPZ predicted vs true: r2 score 0.61

