

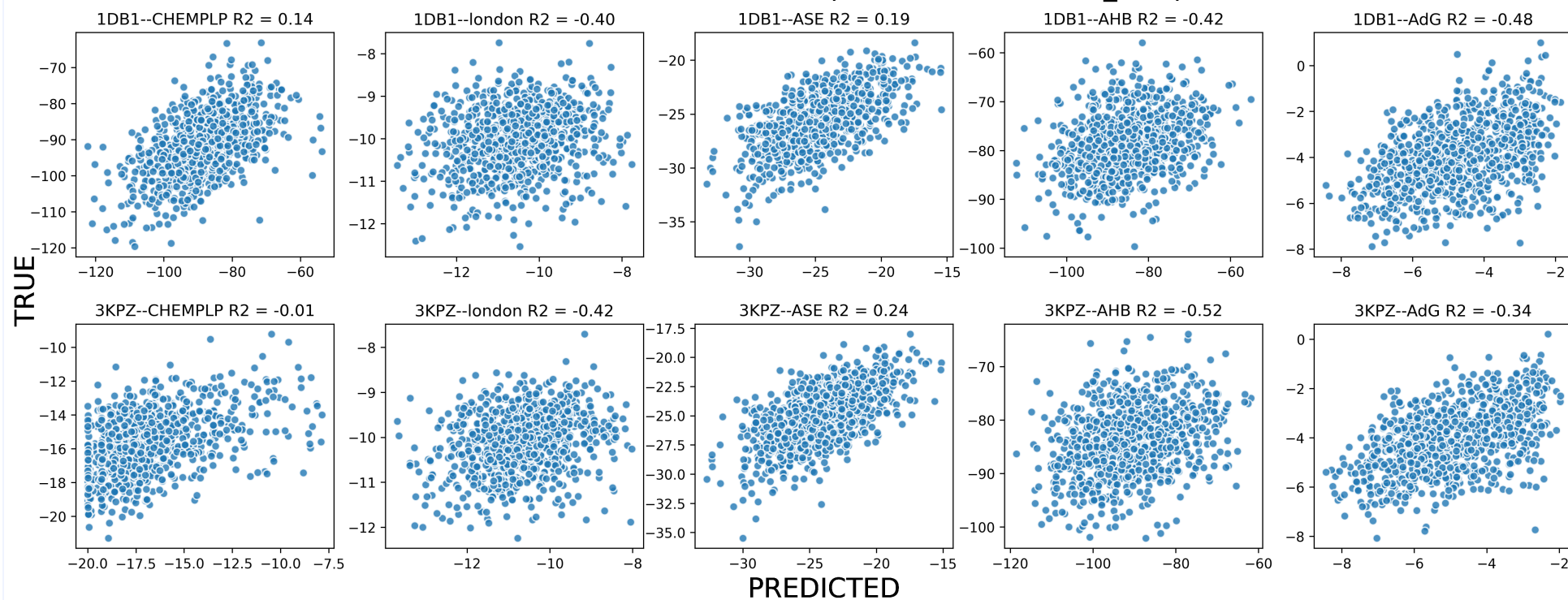
Result tables and figures for predicted docking score values

Table: MSE, MAE, R2 score results for prediction of Docking Score values

1DB1_ds_CHEMPLP1DB1_ds_london	1DB1_ds_ASE	1DB1_ds_AHB	1DB1_ds_AdG	3KPZ_ds_CHEMPLP3KPZ_ds_london	3KPZ_ds_ASE	3KPZ_ds_AHB	3KPZ_ds_AdG		
93.54	1.45	7.36	123.94	2.68	6.24	1.4	6.64	152.36	2.61
7.57	0.93	2.17	8.86	1.33	2.03	0.92	2.08	10.01	1.33
0.14	-0.4	0.19	-0.42	-0.48	-0.01	-0.42	0.24	-0.52	-0.34

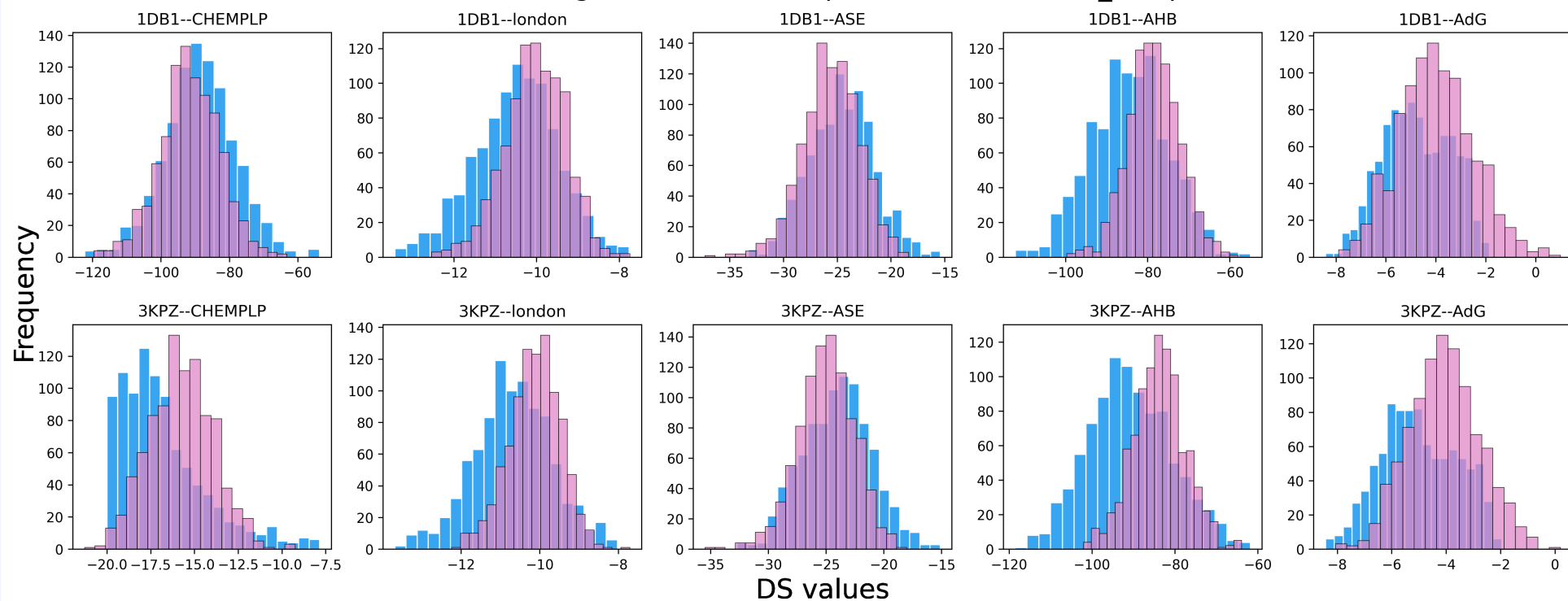
Plots: Correlations of true and predicted ds values

VDR-ML, correlations of true and predicted values, 1k_sample



Plots: Comparison of histograms of the docking scores values

VDR-ML, histograms of true and predicted values, 1k_sample



Plots: Correlation of ECR computed from True and predicted values with $R^2 > 0.7$

ECR VDR-ML dataset, 1k_sample

