

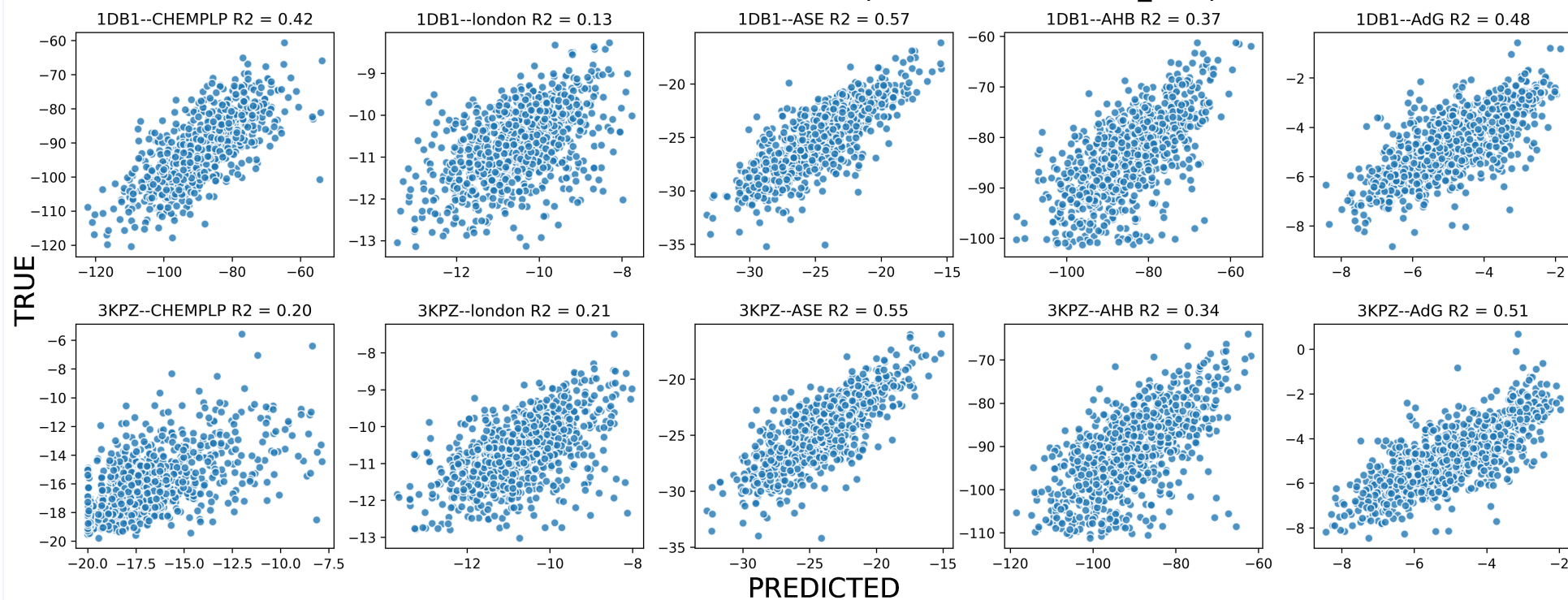
Result tables and figures for predicted docking score values

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		
63.03	0.9	3.9	54.76	0.93	4.9	0.77	3.91	66.64	0.96
6.13	0.72	1.51	5.74	0.72	1.69	0.66	1.54	6.29	0.74
0.42	0.13	0.57	0.37	0.48	0.2	0.21	0.55	0.34	0.51

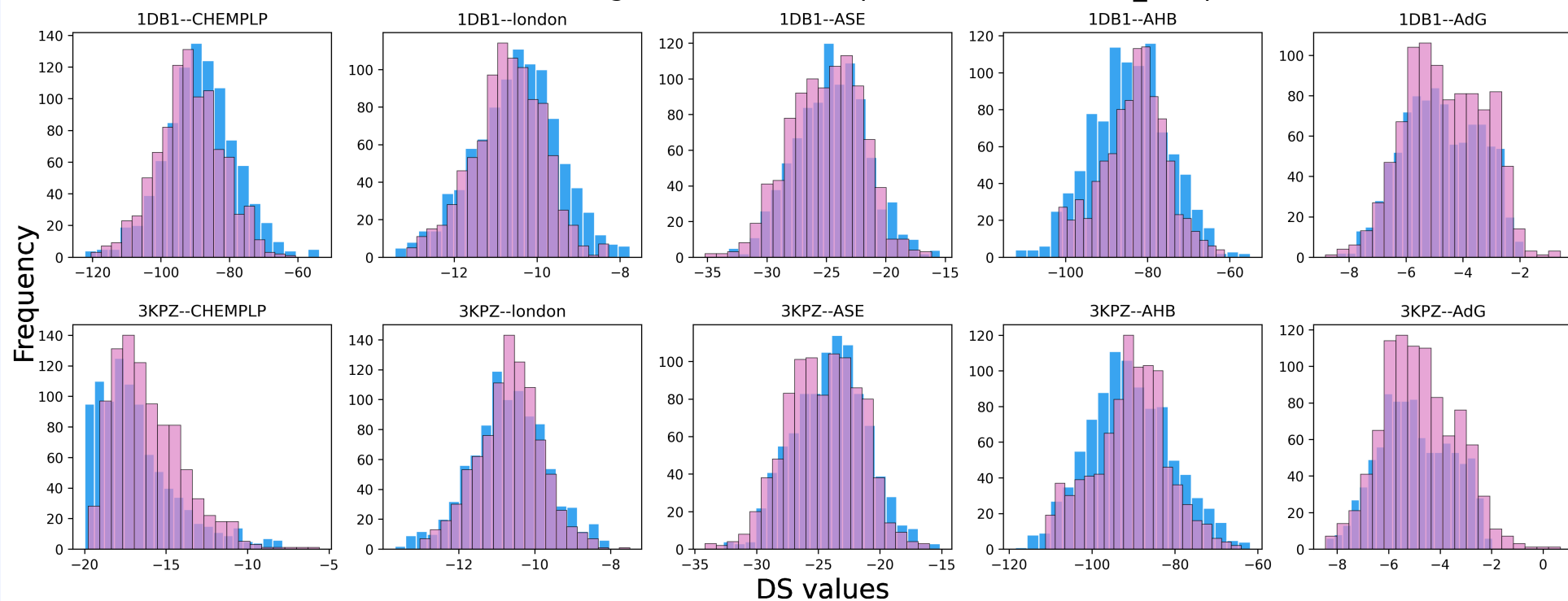
Plots: Correlations of true and predicted ds values

VDR-TRF-ada, correlations of true and predicted values, 1k_sample



Plots: Comparison of histograms of the docking scores values

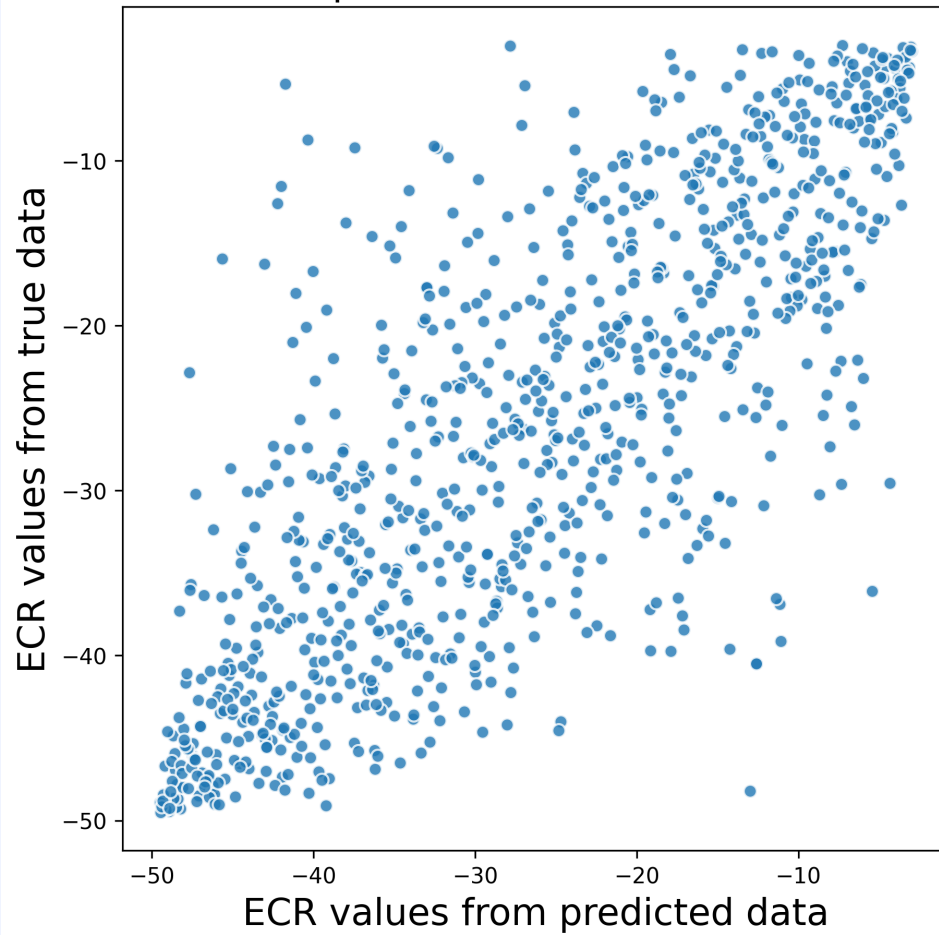
VDR-TRF-ada, histograms of true and predicted values, 1k_sample



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

ECR VDR-TRF-ada dataset, 1k_sample

ECR 1DB1 predicted vs true: r2 score 0.57



ECR 3KPZ predicted vs true: r2 score 0.30

