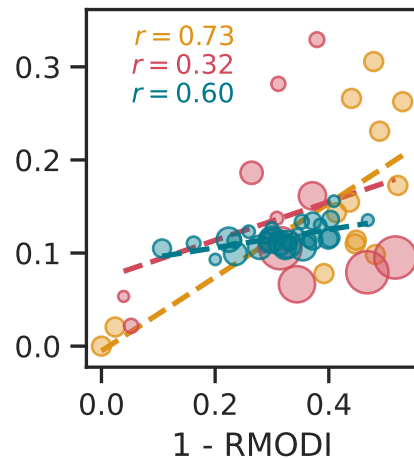
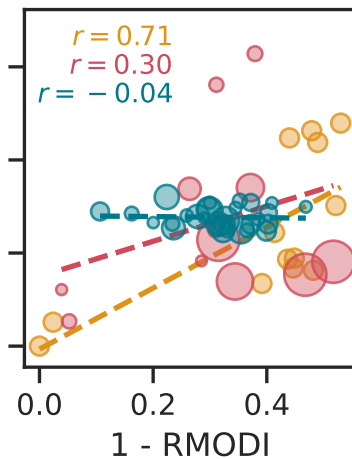


Fingerprints
Relative RMSE

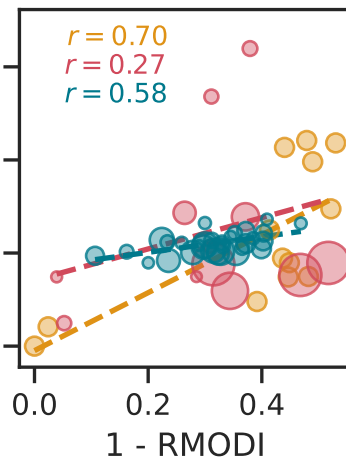
KNN



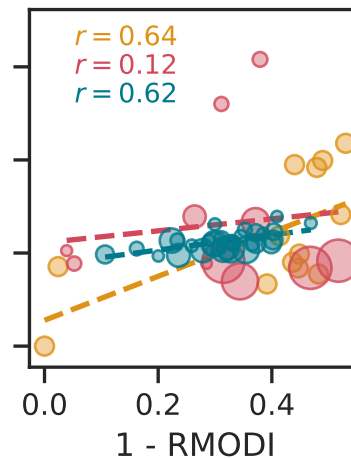
PLS



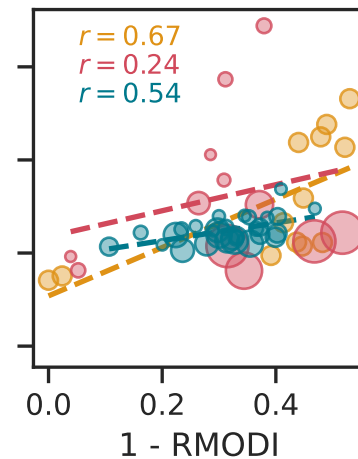
RF



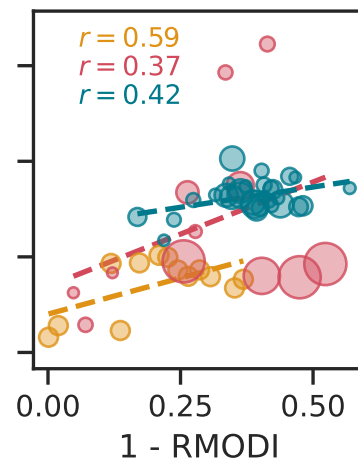
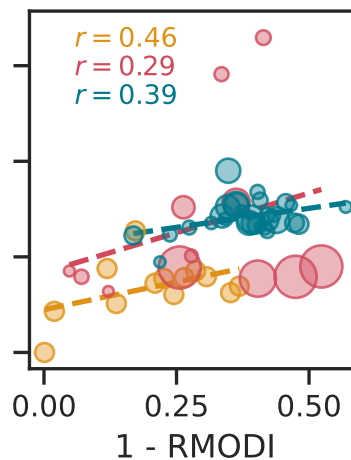
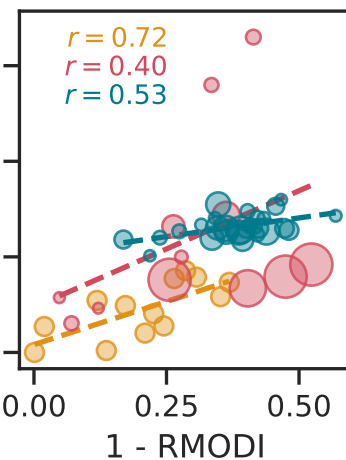
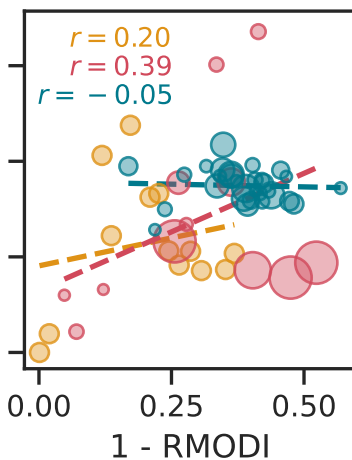
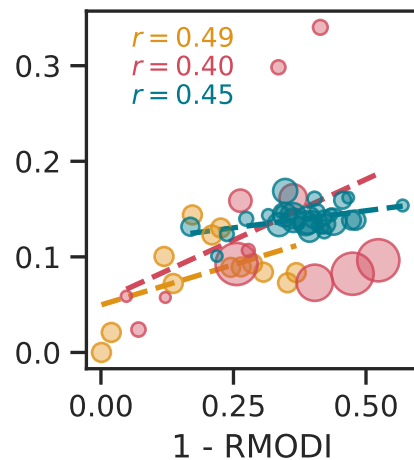
SVR



MLP



Descriptors
Relative RMSE



● ZINC+GuacaMol

● TDC

● ChEMBL