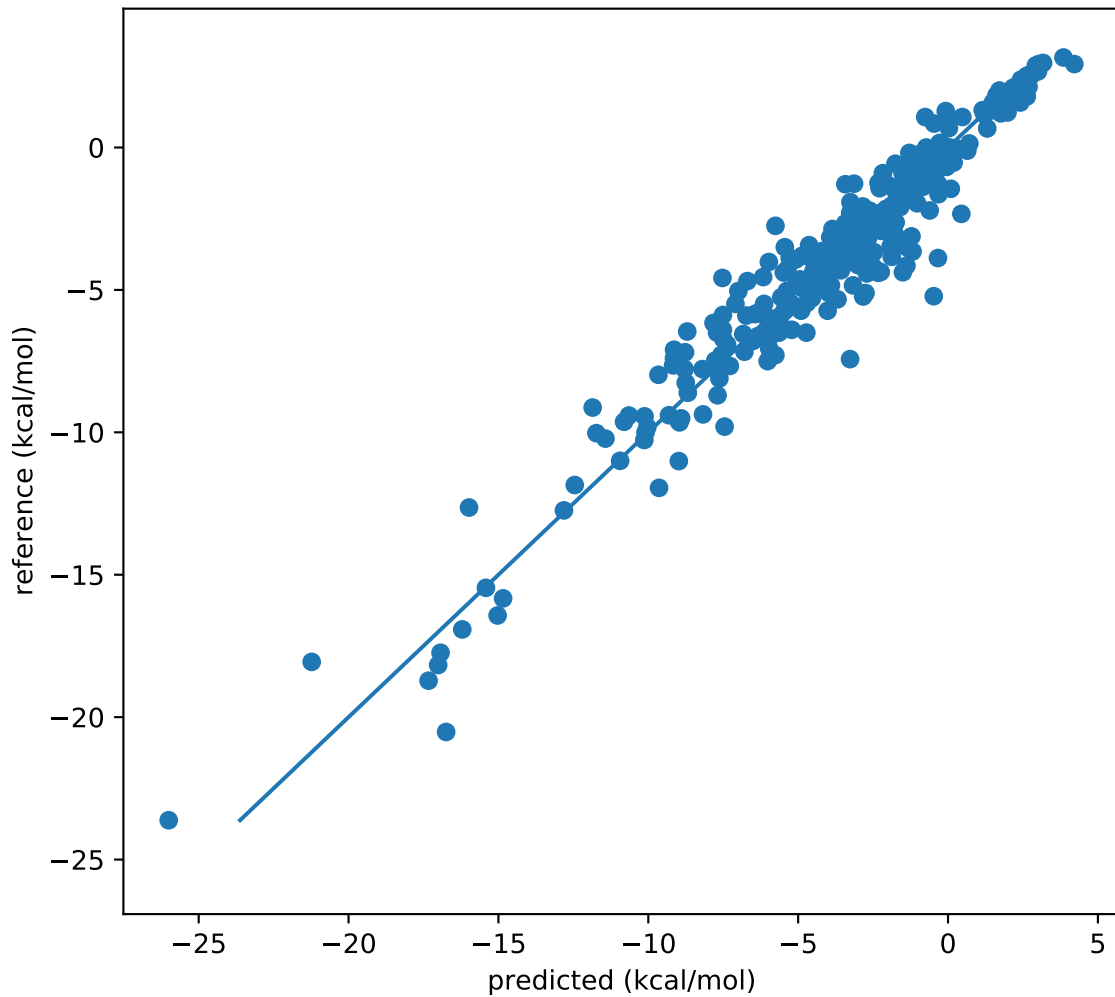


GBSA hydration free energies  
FreeSolv 50:50 (n=321)  
(training set: RMSE=1.112 kcal/mol)



GBSA hydration free energies  
FreeSolv 50:50 (n=321)  
(validation set: RMSE=nan kcal/mol)

