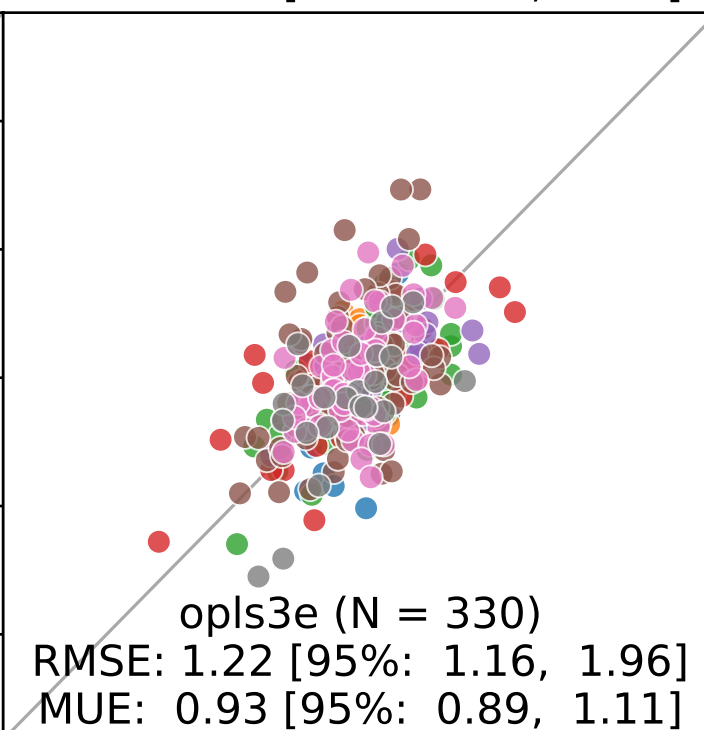
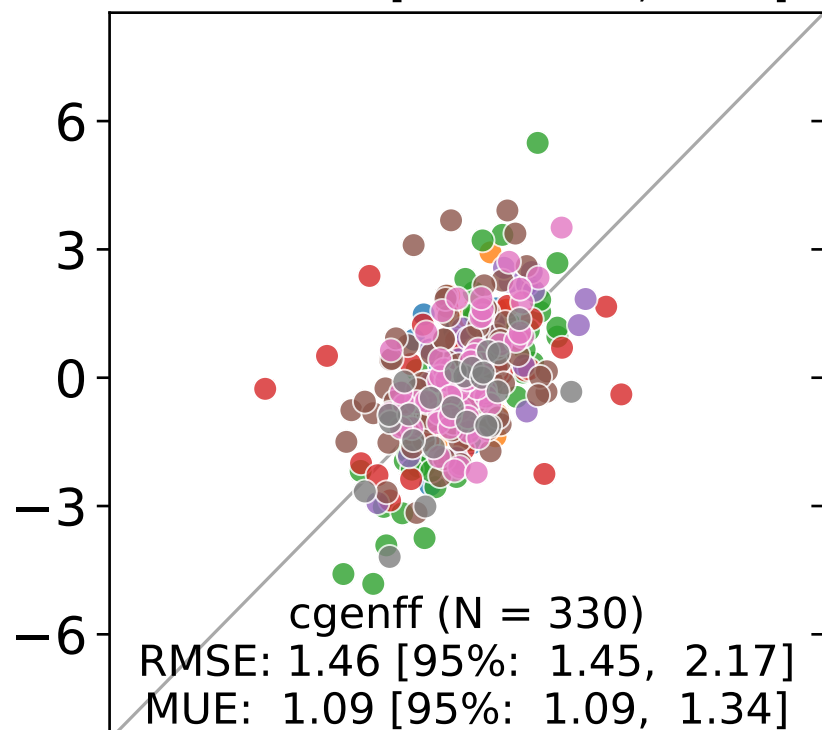


# $\Delta\Delta G$ [kcal/mol]

parsley-1.0.0 (N = 330)  
RMSE: 1.33 [95%: 1.34, 2.11]  
MUE: 1.02 [95%: 1.01, 1.26]

gaff-2.1 (N = 330)  
RMSE: 1.19 [95%: 1.23, 2.03]  
MUE: 0.92 [95%: 0.94, 1.16]

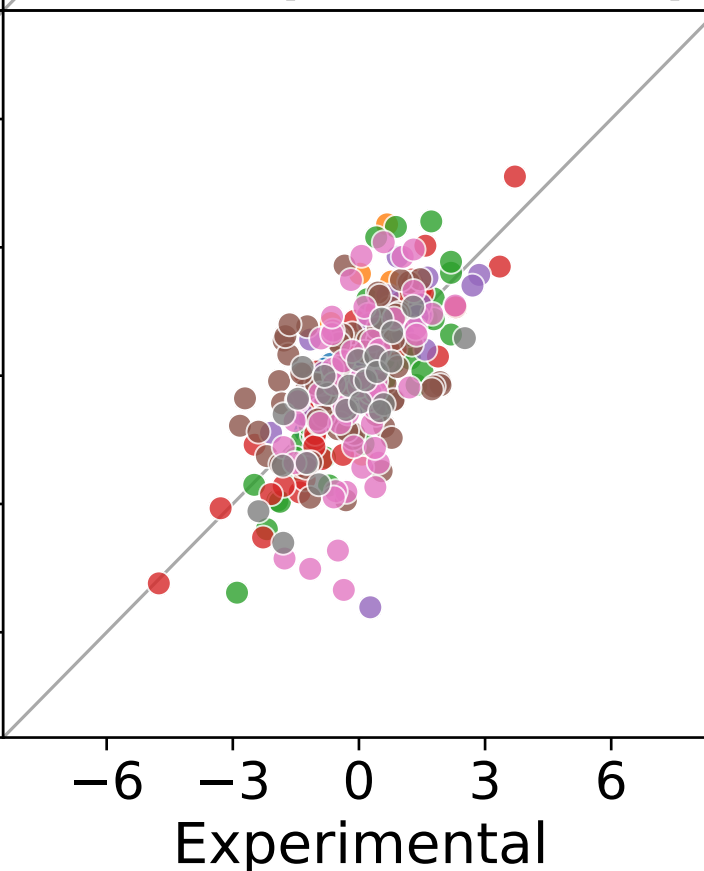
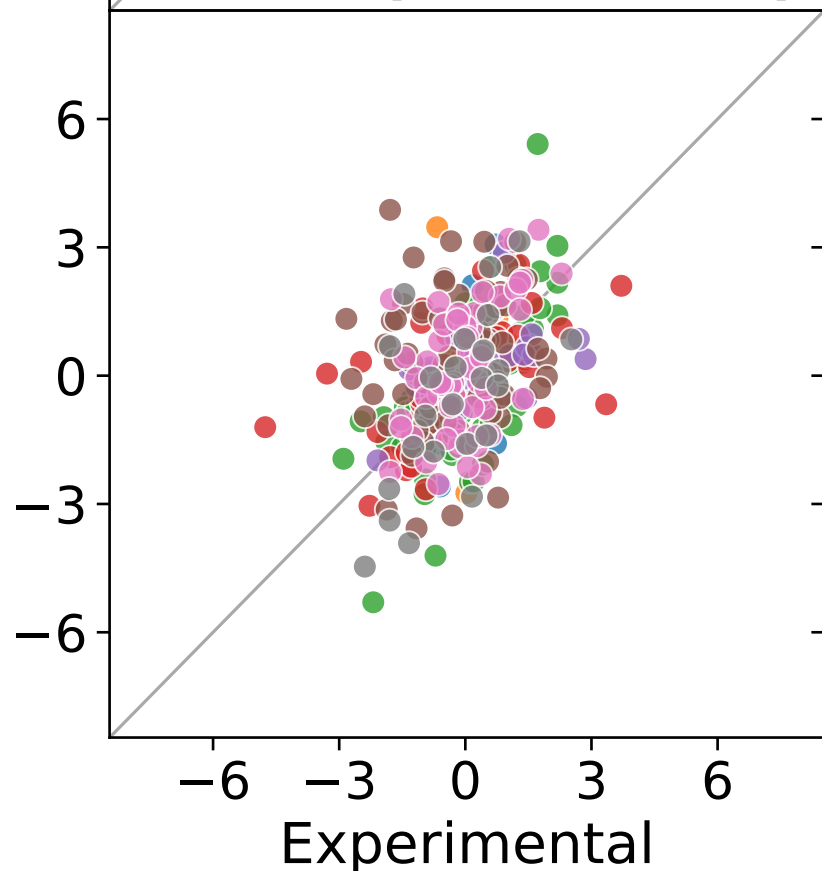
Predicted



Target

- jnk1
- thrombin
- p38
- ptp1b
- cdk2
- mcl1
- bace
- tyk2

Predicted



Experimental

Experimental