

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

parsley-1.0.0 (N = 329)  
RMSE: 1.33 [95%: 1.33, 2.09]  
MUE: 1.02 [95%: 1.01, 1.27]

gaff-2.1 (N = 330)  
RMSE: 1.19 [95%: 1.23, 2.01]  
MUE: 0.92 [95%: 0.95, 1.16]

Predicted

6  
3  
0  
-3  
-6

cgenff (N = 330)  
RMSE: 1.46 [95%: 1.45, 2.20]  
MUE: 1.09 [95%: 1.08, 1.35]

opls3e (N = 330)  
RMSE: 1.22 [95%: 1.15, 1.94]  
MUE: 0.93 [95%: 0.89, 1.10]

Predicted

6  
3  
0  
-3  
-6

-6 -3 0 3 6

Experimental

-6 -3 0 3 6

Experimental

Target

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