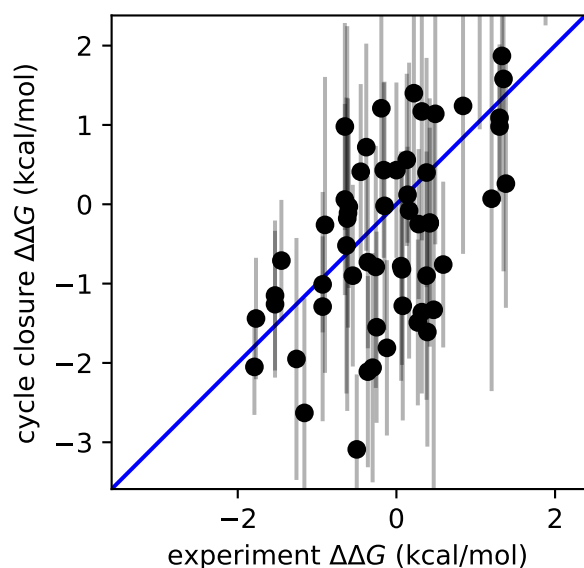
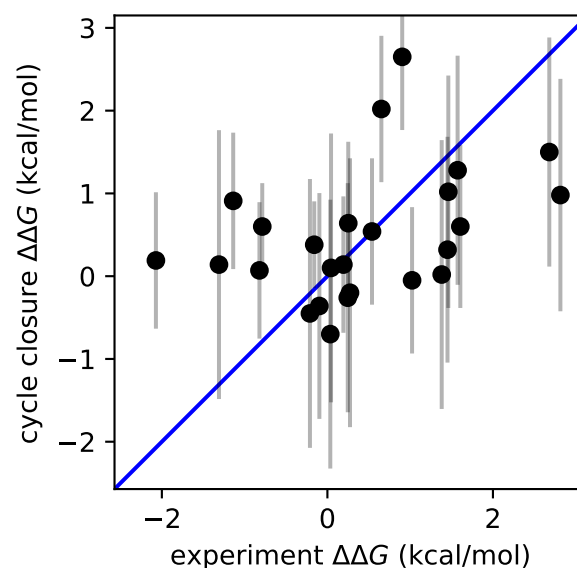


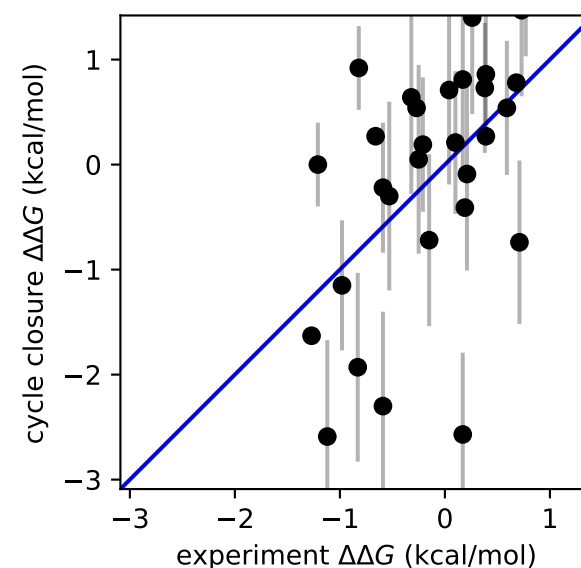
BACE (N = 58)
RMSE 1.0 [95%: 0.9, 1.2] kcal/mol
MUE 0.8 [95%: 0.7, 1.0] kcal/mol



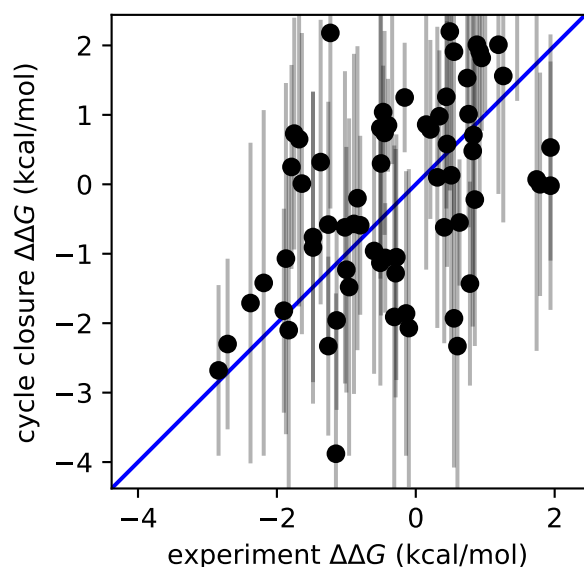
CDK2 (N = 25)
RMSE 1.1 [95%: 0.9, 1.3] kcal/mol
MUE 0.9 [95%: 0.7, 1.2] kcal/mol



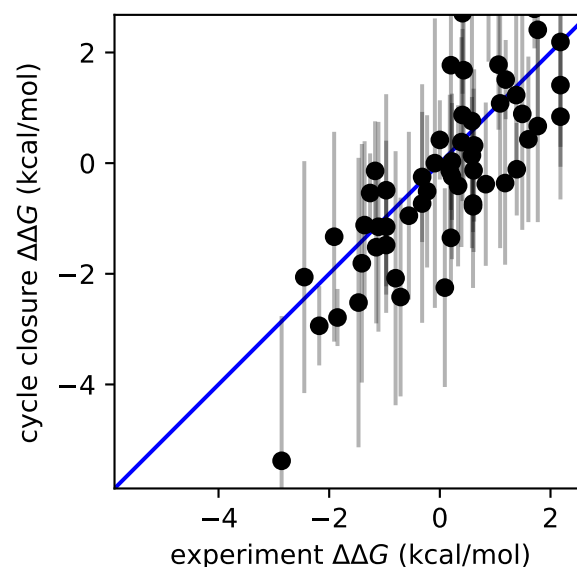
JNK1 (N = 31)
RMSE 1.0 [95%: 0.7, 1.3] kcal/mol
MUE 0.8 [95%: 0.6, 1.0] kcal/mol



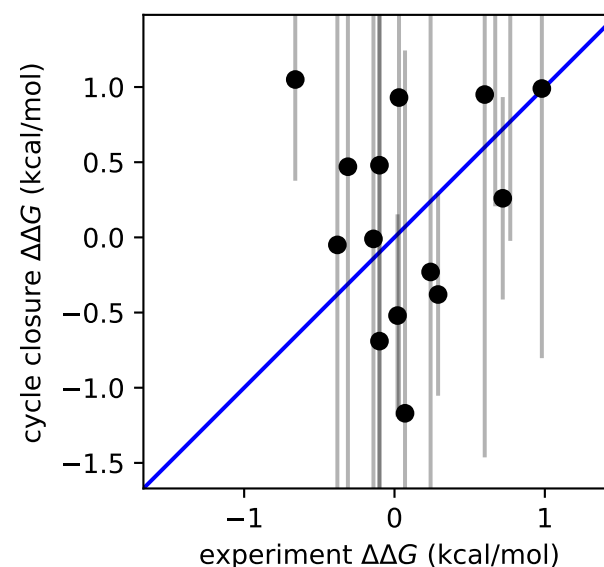
MCL1 (N = 71)
RMSE 1.4 [95%: 1.2, 1.6] kcal/mol
MUE 1.2 [95%: 1.0, 1.3] kcal/mol



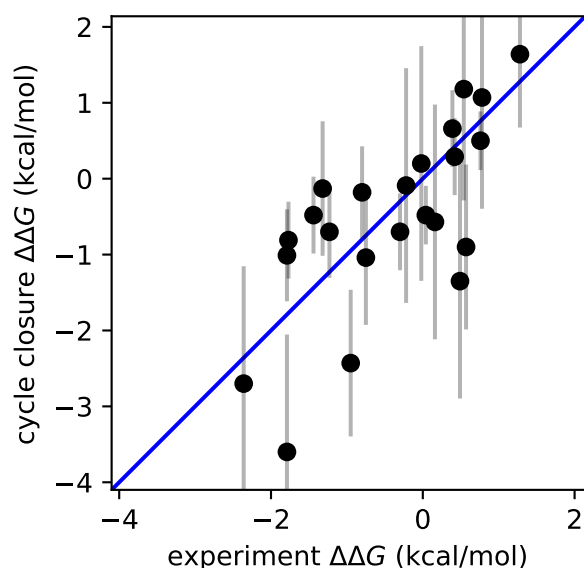
P38 (N = 56)
RMSE 1.0 [95%: 0.8, 1.2] kcal/mol
MUE 0.8 [95%: 0.6, 1.0] kcal/mol



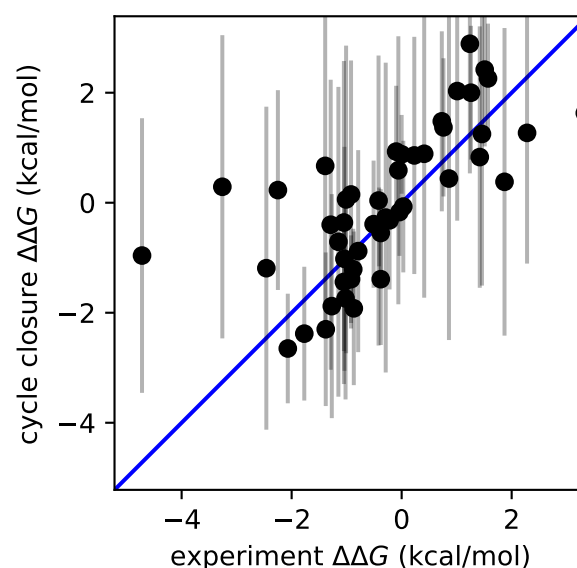
Thrombin (N = 16)
RMSE 0.9 [95%: 0.6, 1.2] kcal/mol
MUE 0.8 [95%: 0.5, 1.0] kcal/mol



Tyk2 (N = 24)
RMSE 0.9 [95%: 0.7, 1.1] kcal/mol
MUE 0.8 [95%: 0.5, 1.0] kcal/mol



PTP1B (N = 49)
RMSE 1.2 [95%: 0.9, 1.5] kcal/mol
MUE 0.9 [95%: 0.7, 1.1] kcal/mol



all (N = 330)
RMSE 1.1 [95%: 1.1, 1.2] kcal/mol
MUE 0.9 [95%: 0.8, 1.0] kcal/mol

