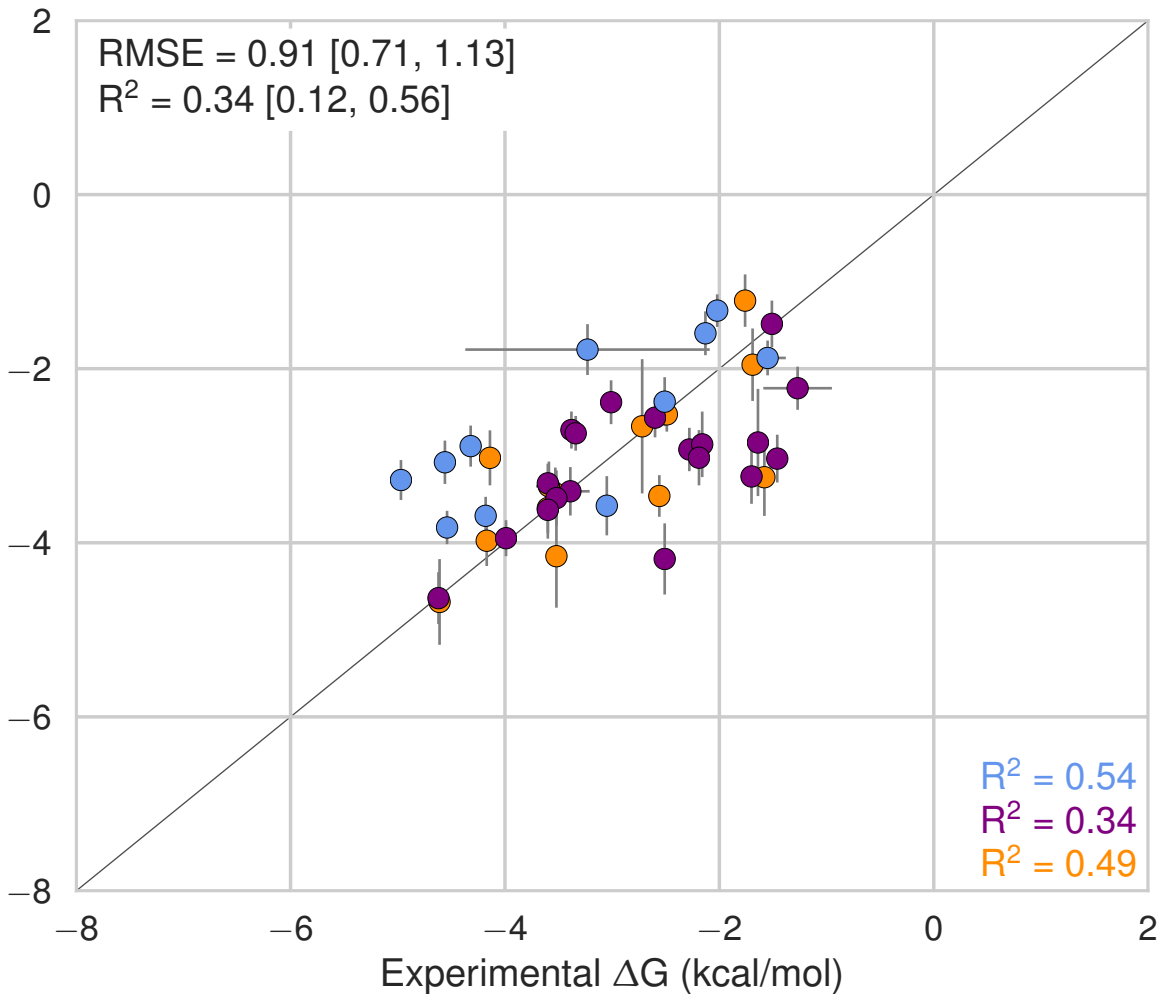


SMIRNOFF99Frosst  $\Delta G$  (kcal/mol)

RMSE = 0.91 [0.71, 1.13]  
 $R^2 = 0.34$  [0.12, 0.56]



$R^2 = 0.54$

$R^2 = 0.34$

$R^2 = 0.49$