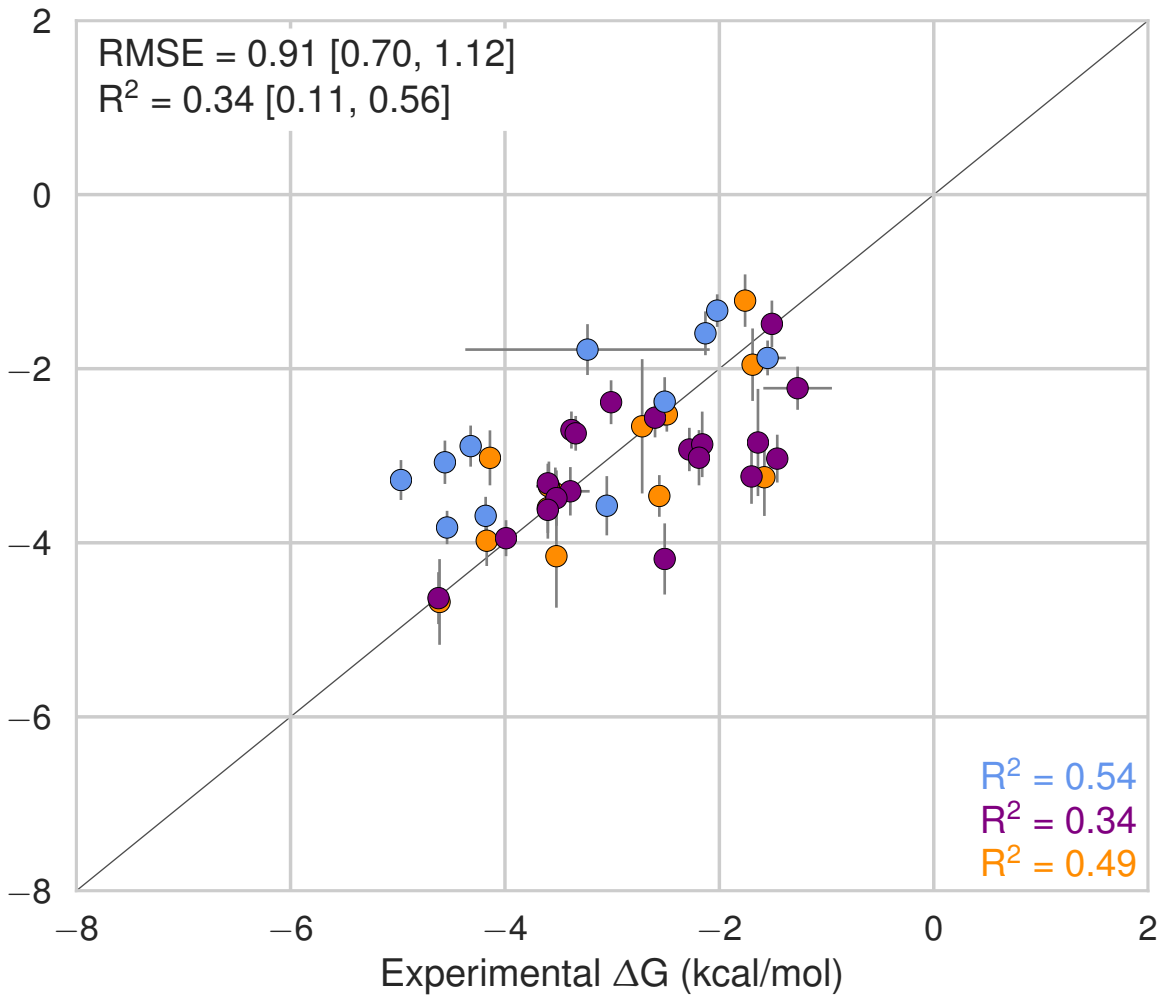


SMIRNOFF99Frosst ΔG (kcal/mol)

RMSE = 0.91 [0.70, 1.12]
 $R^2 = 0.34$ [0.11, 0.56]



$R^2 = 0.54$

$R^2 = 0.34$

$R^2 = 0.49$