

GAFF v2.1  $\Delta G$  (kcal/mol)

RMSE = 1.68 [1.51, 1.85]  
 $R^2 = 0.82$  [0.61, 0.92]

$R^2 = 0.73$  [0.19, 0.98]

$R^2 = 0.81$  [0.61, 0.93]

$R^2 = 0.93$  [0.83, 0.98]

Experimental  $\Delta G$  (kcal/mol)

