

MSE =  $2.94e+01$   $^{3.3e+01}_{2.6e+01}$  kcal/mol

RMSE =  $5.43e+00$   $^{5.7e+00}_{5.1e+00}$  kcal/mol

$R = 9.22e-01$ ,  $R_S = 0.91$ ,  $n = 500$

