

MSE =  $1.90e+01$  $^{2.2e+01}_{1.7e+01}$  kcal/mol

RMSE =  $4.36e+00$  $^{4.7e+00}_{4.1e+00}$  kcal/mol

$R = 9.44e-01$ ,  $R_S = 0.94$ ,  $n = 500$

