

MSE =  $8.19e+00$  $^{9.1e+00}_{7.4e+00}$  kcal/mol

RMSE =  $2.86e+00$  $^{3.0e+00}_{2.7e+00}$  kcal/mol

$R = 9.77e-01$ ,  $R_S = 0.97$ ,  $n = 500$

