

MSE =  $3.00e+01$  <sup>$3.3e+01$</sup>  <sub>$2.6e+01$</sub>  kcal/mol

RMSE =  $5.48e+00$  <sup>$5.7e+00$</sup>  <sub>$5.1e+00$</sub>  kcal/mol

$R = 9.19e-01$ ,  $R_S = 0.91$ ,  $n = 500$

