

MSE =  $2.72e+01$  <sup>$3.1e+01$</sup>  <sub>$2.4e+01$</sub>  kcal/mol

RMSE =  $5.22e+00$  <sup>$5.6e+00$</sup>  <sub>$4.9e+00$</sub>  kcal/mol

$R = 9.33e-01$ ,  $R_S = 0.93$ ,  $n = 500$

