

MSE =  $2.34e+02$  <sup>$2.5e+02$</sup> / <sub>$2.2e+02$</sub>  kcal/mol

RMSE =  $1.53e+01$  <sup>$1.6e+01$</sup> / <sub>$1.5e+01$</sub>  kcal/mol

$R = 9.97e-01$ ,  $R_S = 1.00$ ,  $n = 500$

