

MSE = $2.51e+01$ $\frac{2.8e+01}{2.3e+01}$ kcal/mol

RMSE = $5.01e+00$ $\frac{5.3e+00}{4.8e+00}$ kcal/mol

$R = 9.27e-01$, $R_S = 0.92$, $n = 500$

