

MSE = $1.01\text{e}+03$ $\frac{1.1\text{e}+03}{9.6\text{e}+02}$ kcal/mol

RMSE = $3.18\text{e}+01$ $\frac{3.3\text{e}+01}{3.1\text{e}+01}$ kcal/mol

$R = 9.46\text{e}-01$, $R_S = 0.94$, $n = 500$

