

$$\text{MSE} = 1.01\text{e}+03 \frac{1.1\text{e}+03}{9.7\text{e}+02} \text{ kcal/mol}$$

$$\text{RMSE} = 3.18\text{e}+01 \frac{3.2\text{e}+01}{3.1\text{e}+01} \text{ kcal/mol}$$

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

