

MSE = $1.05\text{e}+02$ $^{1.1\text{e}+02}_{9.5\text{e}+01}$ kcal/mol

RMSE = $1.02\text{e}+01$ $^{1.1\text{e}+01}_{9.7\text{e}+00}$ kcal/mol

$R = 9.26\text{e}-01$, $R_S = 0.92$, $n = 500$

