

MSE = $2.42e+01$ $^{2.8e+01}_{2.1e+01}$ kcal/mol

RMSE = $4.92e+00$ $^{5.3e+00}_{4.6e+00}$ kcal/mol

$R = 9.35e-01$, $R_S = 0.93$, $n = 500$

