

MSE = $2.94e+01$ $^{3.4e+01}_{2.6e+01}$ kcal/mol

RMSE = $5.43e+00$ $^{5.8e+00}_{5.1e+00}$ kcal/mol

$R = 9.22e-01$, $R_S = 0.91$, $n = 500$

