

MSE = $2.11e+01$ $^{2.4e+01}_{1.9e+01}$ kcal/mol

RMSE = $4.59e+00$ $^{4.9e+00}_{4.3e+00}$ kcal/mol

$R = 9.38e-01$, $R_S = 0.94$, $n = 500$

