

MSE = $1.66e+01$ $^{1.9e+01}_{1.5e+01}$ kcal/mol

RMSE = $4.08e+00$ $^{4.4e+00}_{3.9e+00}$ kcal/mol

$R = 9.59e-01$, $R_S = 0.96$, $n = 500$

