

MSE = $1.33e+01$ $^{1.6e+01}_{1.2e+01}$ kcal/mol

RMSE = $3.65e+00$ $^{4.0e+00}_{3.5e+00}$ kcal/mol

$R = 9.93e-01$, $R_S = 0.99$, $n = 500$

