

MSE = $1.67e+01$ $^{1.9e+01}_{1.5e+01}$ kcal/mol

RMSE = $4.09e+00$ $^{4.3e+00}_{3.9e+00}$ kcal/mol

$R = 9.58e-01$, $R_S = 0.96$, $n = 500$

