

MSE = $1.01e+01$ $^{1.1e+01}_{8.8e+00}$ kcal/mol

RMSE = $3.17e+00$ $^{3.3e+00}_{3.0e+00}$ kcal/mol

$R = 9.71e-01$, $R_S = 0.97$, $n = 500$

