

MSE = $4.53e+03$ ^{$4.6e+03$} _{$4.4e+03$} kcal/mol

RMSE = $6.73e+01$ ^{$6.8e+01$} _{$6.6e+01$} kcal/mol

$R = 9.46e-01$, $R_S = 0.94$, $n = 500$

