

MSE = $7.87e+03$ ^{$8.2e+03$} / _{$7.6e+03$} kcal/mol

RMSE = $8.87e+01$ ^{$9.0e+01$} / _{$8.7e+01$} kcal/mol

$R = 8.19e-01$, $R_S = 0.79$, $n = 500$

