

MSE = $2.91e+03$ ^{$3.0e+03$} _{$2.8e+03$} kcal/mol

RMSE = $5.40e+01$ ^{$5.5e+01$} _{$5.3e+01$} kcal/mol

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

