

MSE = $3.21e+03$ ^{$3.4e+03$} _{$3.1e+03$} kcal/mol

RMSE = $5.67e+01$ ^{$5.8e+01$} _{$5.6e+01$} kcal/mol

$R = 9.75e-01$, $R_S = 0.97$, $n = 500$

