

MSE = $2.64e+01$ ^{$3.0e+01$} _{$2.3e+01$} kcal/mol

RMSE = $5.14e+00$ ^{$5.5e+00$} _{$4.8e+00$} kcal/mol

$R = 9.22e-01$, $R_S = 0.91$, $n = 500$

