

MSE = $3.09e+01$ ^{$3.5e+01$} _{$2.8e+01$} kcal/mol

RMSE = $5.56e+00$ ^{$5.9e+00$} _{$5.3e+00$} kcal/mol

$R = 9.29e-01$, $R_S = 0.93$, $n = 500$

