

MSE = $8.28e+02$ ^{$8.6e+02$} / _{$8.0e+02$} kcal/mol

RMSE = $2.88e+01$ ^{$2.9e+01$} / _{$2.8e+01$} kcal/mol

$R = 9.14e-01$, $R_S = 0.90$, $n = 500$

