

MSE = $7.69e+02$ ^{$8.0e+02$} / _{$7.4e+02$} kcal/mol

RMSE = $2.77e+01$ ^{$2.8e+01$} / _{$2.7e+01$} kcal/mol

$R = 9.12e-01$, $R_S = 0.90$, $n = 500$

