

MSE = $2.06e+02$ ^{$2.3e+02$} _{$1.8e+02$} kcal/mol

RMSE = $1.43e+01$ ^{$1.5e+01$} _{$1.3e+01$} kcal/mol

$R = 8.56e-01$, $R_S = 0.84$, $n = 500$

