

MSE = $1.34e+02$ ^{$1.5e+02$} / _{$1.2e+02$} kcal/mol

RMSE = $1.16e+01$ ^{$1.2e+01$} / _{$1.1e+01$} kcal/mol

$R = 9.03e-01$, $R_S = 0.89$, $n = 500$

