

MSE = $2.59e+01$ ^{$2.9e+01$} / _{$2.3e+01$} kcal/mol

RMSE = $5.09e+00$ ^{$5.4e+00$} / _{$4.8e+00$} kcal/mol

$R = 9.26e-01$, $R_S = 0.92$, $n = 500$

