

MSE = $9.56e+01$ ^{$1.1e+02$} _{$8.3e+01$} kcal/mol

RMSE = $9.78e+00$ ^{$1.0e+01$} _{$9.1e+00$} kcal/mol

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

