

MSE = $2.82e+01$ ^{$3.2e+01$} _{$2.5e+01$} kcal/mol

RMSE = $5.31e+00$ ^{$5.7e+00$} _{$5.0e+00$} kcal/mol

$R = 9.32e-01$, $R_S = 0.93$, $n = 500$

