

MSE = $3.00e+01$ $^{3.5e+01}_{2.6e+01}$ kcal/mol

RMSE = $5.47e+00$ $^{5.9e+00}_{5.1e+00}$ kcal/mol

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

