

MSE = 1.05×10^2 $^{1.2 \times 10^2}_{9.6 \times 10^1}$ kcal/mol

RMSE = 1.02×10^1 $^{1.1 \times 10^1}_{9.8 \times 10^0}$ kcal/mol

$R = 9.26 \times 10^{-1}$, $R_S = 0.92$, $n = 500$

