

all within-target pairs  $\Delta\Delta G$  (N = 5620)  
RMSE: 0PLS2.1 1.37 [95%: 1.34, 1.39] kcal/mol  
MUE : 0PLS2.1 1.09 [95%: 1.07, 1.11] kcal/mol  
R2 : 0PLS2.1 0.10 [95%: 0.06, 0.15] kcal/mol  
rho : 0PLS2.1 0.73 [95%: 0.72, 0.74] kcal/mol

