all within-target pairs $\Delta\Delta G$ (N = 5620) RMSE: OPLS3 1.37 [95%: 1.34, 1.39] kcal/mol MUE: OPLS3 1.09 [95%: 1.07, 1.11] kcal/mol R2 0PLS3 0.10 [95%: 0.06, 0.15] kcal/mol 0PLS3 rho : 0.73 [95%: 0.72, 0.74] kcal/mol

