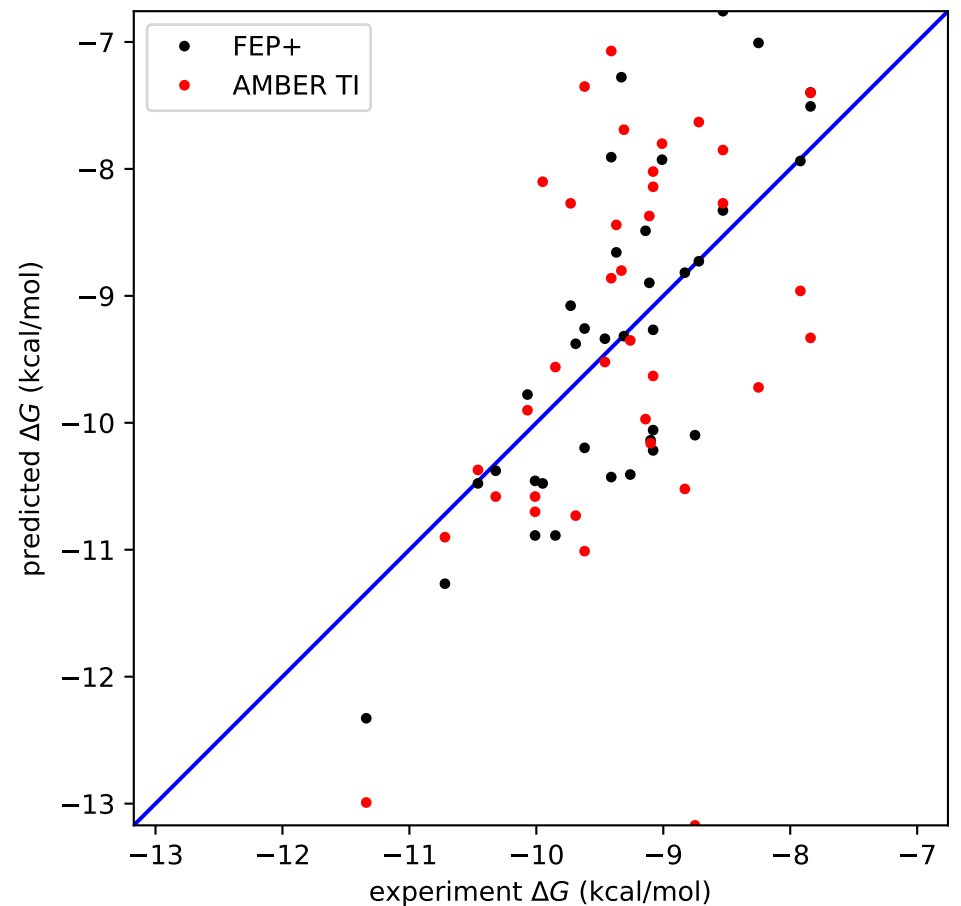
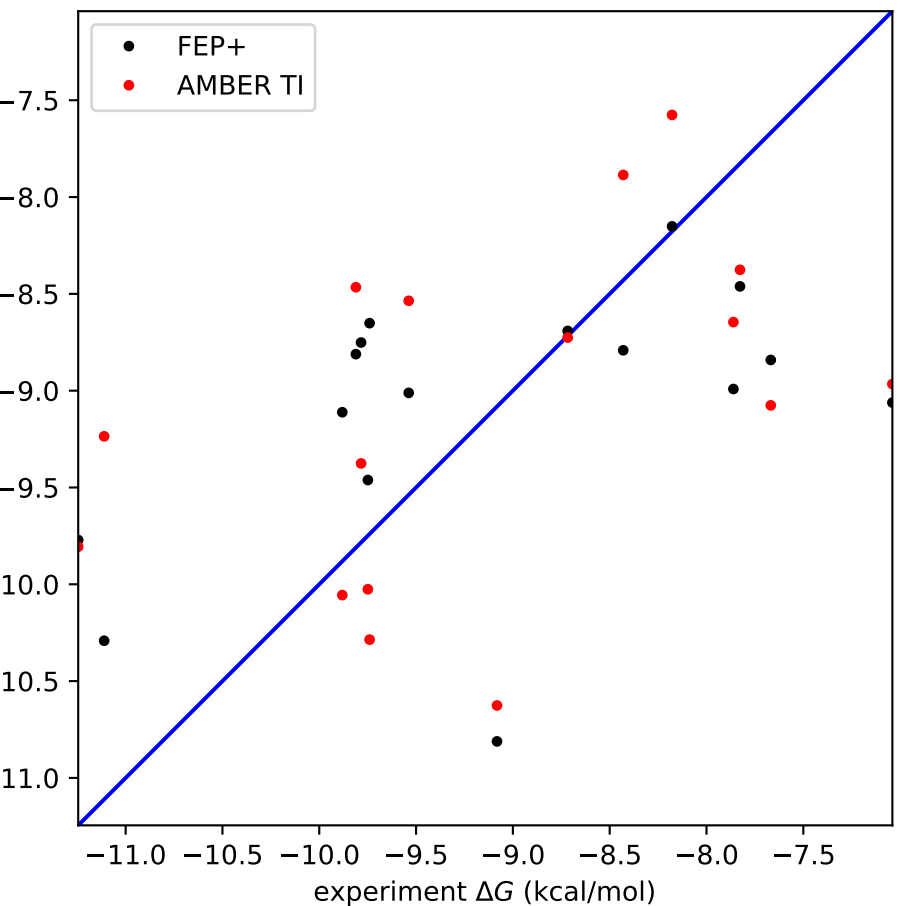


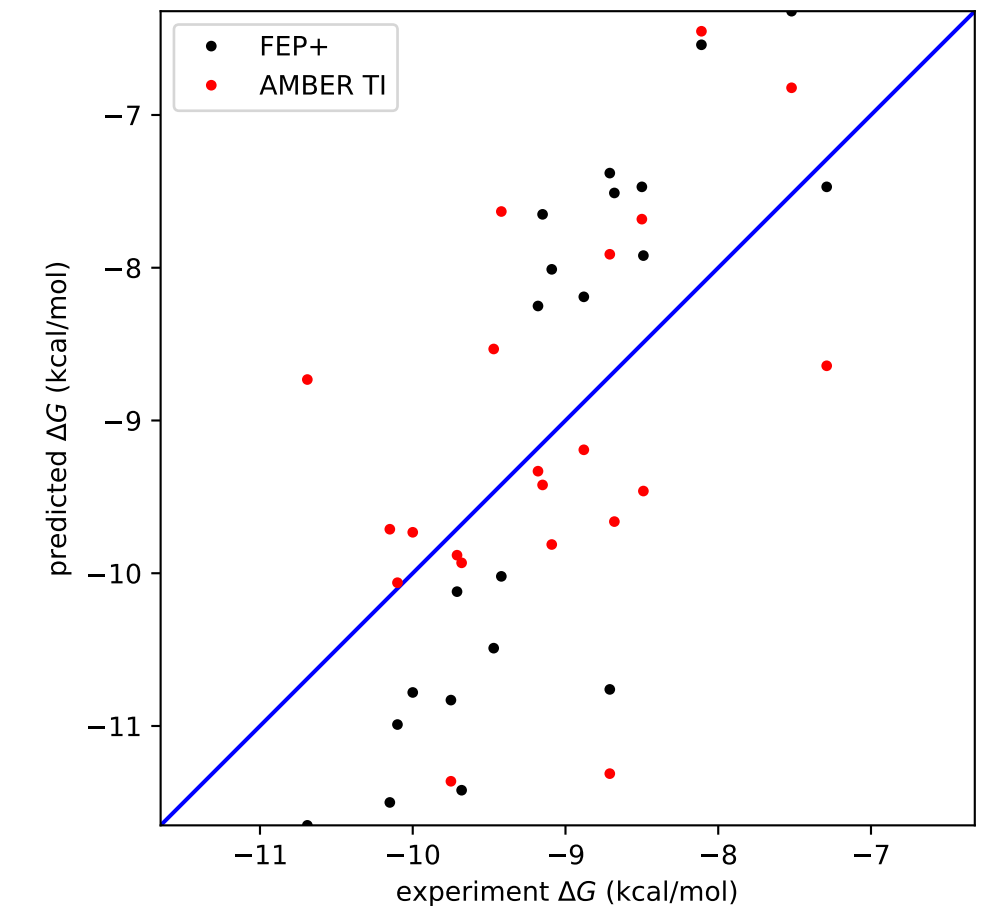
RMSE: FEP+ 0.85 [95%: 0.66, 1.03] kcal/mol  
RMSE: AMBER TI 1.32 [95%: 0.97, 1.71] kcal/mol  
MUE : FEP+ 0.66 [95%: 0.50, 0.84] kcal/mol  
MUE : AMBER TI 1.03 [95%: 0.79, 1.33] kcal/mol  
R2 : FEP+ -0.23 [95%: -1.56, 0.37] kcal/mol  
R2 : AMBER TI -1.98 [95%: -6.21, -0.31] kcal/mol  
rho : FEP+ 0.78 [95%: 0.61, 0.89] kcal/mol  
rho : AMBER TI 0.43 [95%: 0.06, 0.72] kcal/mol



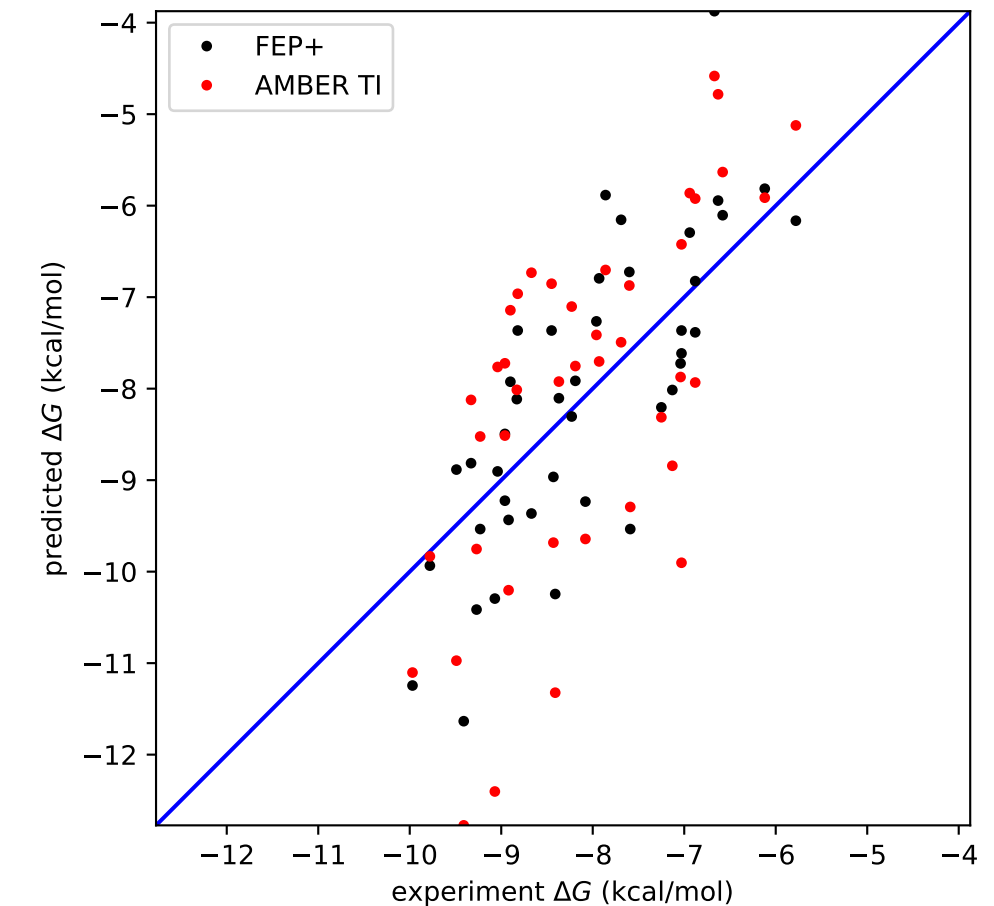
RMSE: FEP+ 1.04 [95%: 0.76, 1.29] kcal/mol  
RMSE: AMBER TI 1.08 [95%: 0.76, 1.34] kcal/mol  
MUE : FEP+ 0.88 [95%: 0.60, 1.17] kcal/mol  
MUE : AMBER TI 0.90 [95%: 0.61, 1.21] kcal/mol  
R2 : FEP+ 0.22 [95%: -0.55, 0.51] kcal/mol  
R2 : AMBER TI 0.16 [95%: -0.46, 0.40] kcal/mol  
rho : FEP+ 0.48 [95%: 0.07, 0.82] kcal/mol  
rho : AMBER TI 0.47 [95%: 0.20, 0.70] kcal/mol



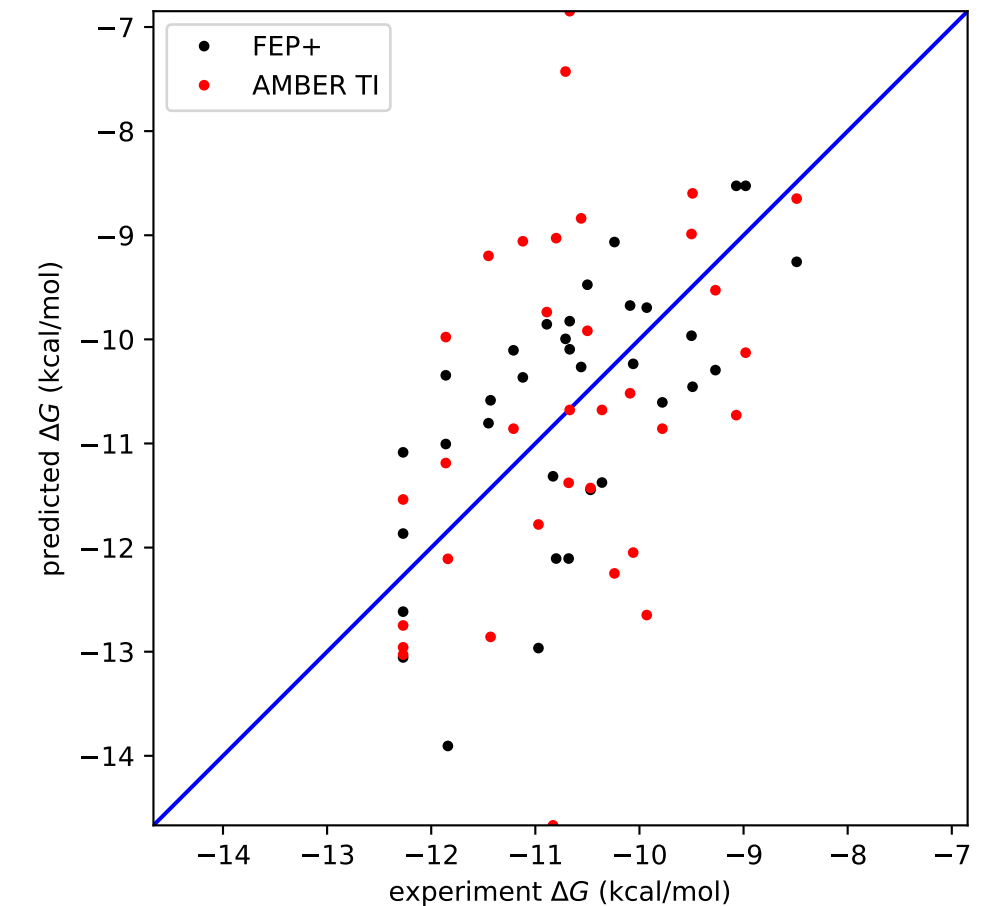
RMSE: FEP+ 1.14 [95%: 0.95, 1.32] kcal/mol  
RMSE: AMBER TI 1.13 [95%: 0.80, 1.43] kcal/mol  
MUE : FEP+ 1.05 [95%: 0.86, 1.22] kcal/mol  
MUE : AMBER TI 0.90 [95%: 0.61, 1.20] kcal/mol  
R2 : FEP+ -0.84 [95%: -3.27, 0.01] kcal/mol  
R2 : AMBER TI -0.80 [95%: -3.32, 0.17] kcal/mol  
rho : FEP+ 0.84 [95%: 0.70, 0.95] kcal/mol  
rho : AMBER TI 0.47 [95%: 0.05, 0.75] kcal/mol



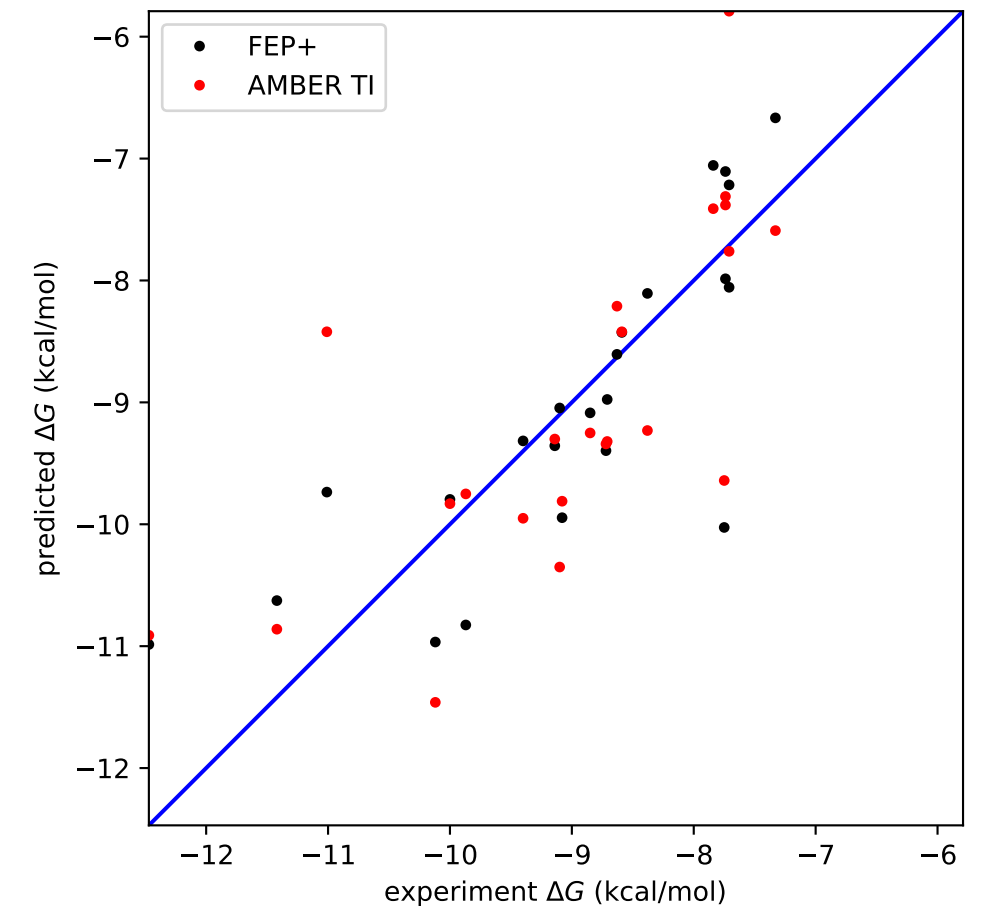
RMSE: FEP+ 1.04 [95%: 0.81, 1.28] kcal/mol  
RMSE: AMBER TI 1.48 [95%: 1.20, 1.75] kcal/mol  
MUE : FEP+ 0.84 [95%: 0.66, 1.04] kcal/mol  
MUE : AMBER TI 1.24 [95%: 0.99, 1.49] kcal/mol  
R2 : FEP+ 0.02 [95%: -0.70, 0.48] kcal/mol  
R2 : AMBER TI -0.97 [95%: -2.22, -0.17] kcal/mol  
rho : FEP+ 0.77 [95%: 0.66, 0.86] kcal/mol  
rho : AMBER TI 0.65 [95%: 0.45, 0.78] kcal/mol



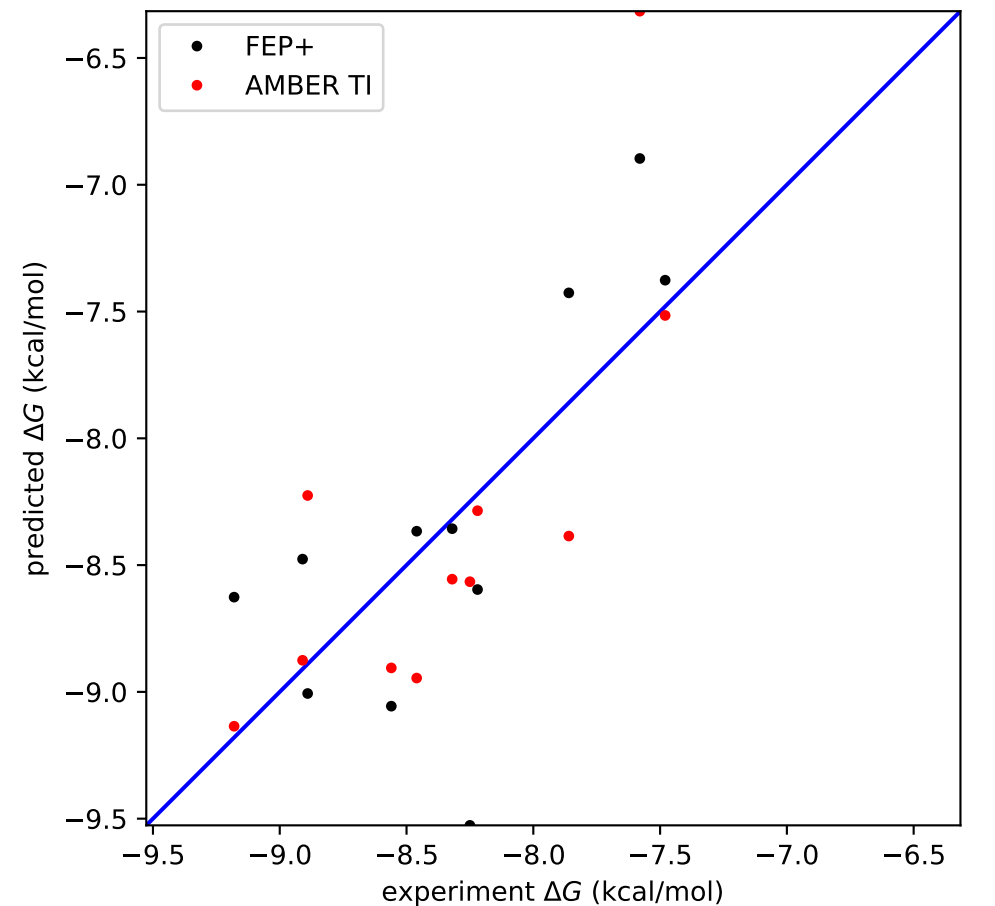
RMSE: FEP+ 0.97 [95%: 0.79, 1.15] kcal/mol  
RMSE: AMBER TI 1.62 [95%: 1.24, 1.98] kcal/mol  
MUE : FEP+ 0.86 [95%: 0.72, 1.00] kcal/mol  
MUE : AMBER TI 1.28 [95%: 0.96, 1.61] kcal/mol  
R2 : FEP+ 0.05 [95%: -0.81, 0.44] kcal/mol  
R2 : AMBER TI -1.66 [95%: -4.96, -0.20] kcal/mol  
rho : FEP+ 0.65 [95%: 0.46, 0.78] kcal/mol  
rho : AMBER TI 0.38 [95%: 0.13, 0.61] kcal/mol



RMSE: FEP+ 0.80 [95%: 0.52, 1.06] kcal/mol  
RMSE: AMBER TI 1.01 [95%: 0.67, 1.33] kcal/mol  
MUE : FEP+ 0.60 [95%: 0.41, 0.83] kcal/mol  
MUE : AMBER TI 0.76 [95%: 0.50, 1.05] kcal/mol  
R2 : FEP+ 0.62 [95%: 0.03, 0.79] kcal/mol  
R2 : AMBER TI 0.39 [95%: -0.40, 0.72] kcal/mol  
rho : FEP+ 0.80 [95%: 0.60, 0.92] kcal/mol  
rho : AMBER TI 0.71 [95%: 0.47, 0.88] kcal/mol



RMSE: FEP+ 0.54 [95%: 0.31, 0.76] kcal/mol  
RMSE: AMBER TI 0.51 [95%: 0.25, 0.74] kcal/mol  
MUE : FEP+ 0.42 [95%: 0.24, 0.63] kcal/mol  
MUE : AMBER TI 0.37 [95%: 0.18, 0.60] kcal/mol  
R2 : FEP+ -0.08 [95%: -3.29, 0.65] kcal/mol  
R2 : AMBER TI 0.04 [95%: -1.62, 0.78] kcal/mol  
rho : FEP+ 0.71 [95%: 0.14, 0.93] kcal/mol  
rho : AMBER TI 0.76 [95%: 0.30, 0.94] kcal/mol



RMSE: FEP+ 0.57 [95%: 0.32, 0.80] kcal/mol  
RMSE: AMBER TI 1.13 [95%: 0.76, 1.47] kcal/mol  
MUE : FEP+ 0.44 [95%: 0.28, 0.62] kcal/mol  
MUE : AMBER TI 0.89 [95%: 0.57, 1.23] kcal/mol  
R2 : FEP+ 0.79 [95%: 0.50, 0.92] kcal/mol  
R2 : AMBER TI 0.19 [95%: -0.96, 0.61] kcal/mol  
rho : FEP+ 0.89 [95%: 0.72, 0.97] kcal/mol  
rho : AMBER TI 0.57 [95%: 0.18, 0.84] kcal/mol

