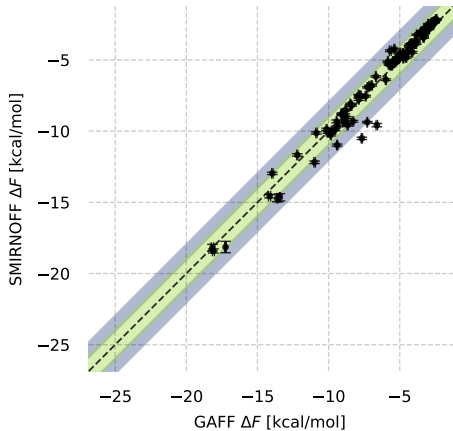
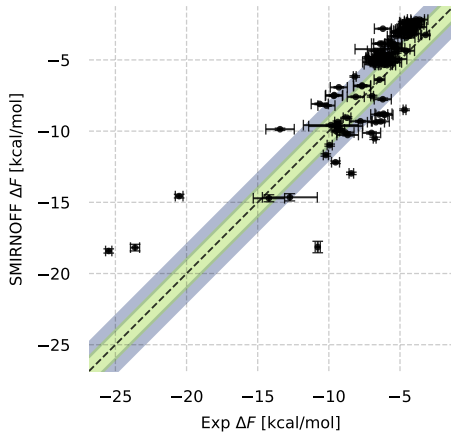


$R^2$ : 0.974 [ 0.951, 0.989]  
MU diff: -0.063 [-0.173, 0.060] kcal/mol  
RMS diff: 0.629 [ 0.449, 0.805] kcal/mol



$R^2$ : 0.717 [ 0.639, 0.811]  
MUE: -0.836 [-1.199, -0.453] kcal/mol  
RMSE: 2.156 [ 1.809, 2.513] kcal/mol



$R^2$ : 0.728 [ 0.635, 0.830]  
MUE: -0.774 [-1.115, -0.432] kcal/mol  
RMSE: 2.016 [ 1.623, 2.395] kcal/mol

