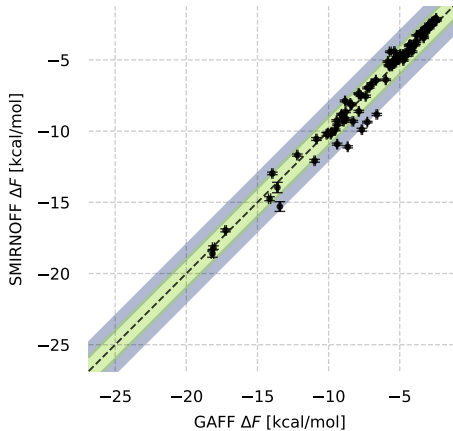
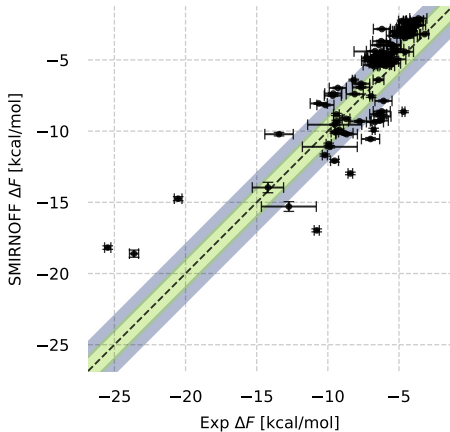


R^2 : 0.975 [0.957, 0.988]
MD: -0.055 [-0.161, 0.066] kcal/mol
RMS diff: 0.615 [0.461, 0.765] kcal/mol



R^2 : 0.726 [0.649, 0.813]
ME: -0.829 [-1.185, -0.466] kcal/mol
RMSE: 2.112 [1.793, 2.439] kcal/mol



R^2 : 0.728 [0.630, 0.834]
ME: -0.774 [-1.123, -0.420] kcal/mol
RMSE: 2.016 [1.636, 2.404] kcal/mol

