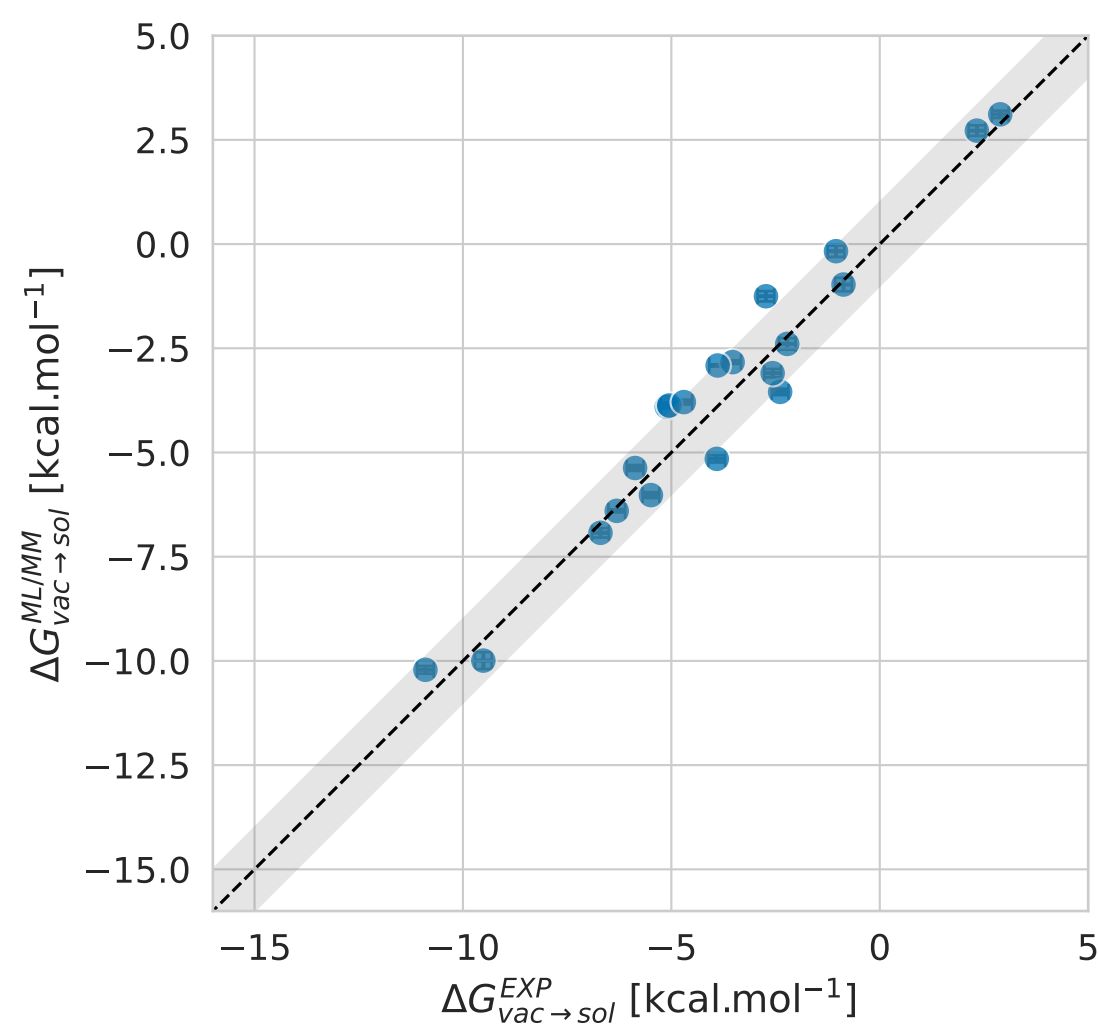
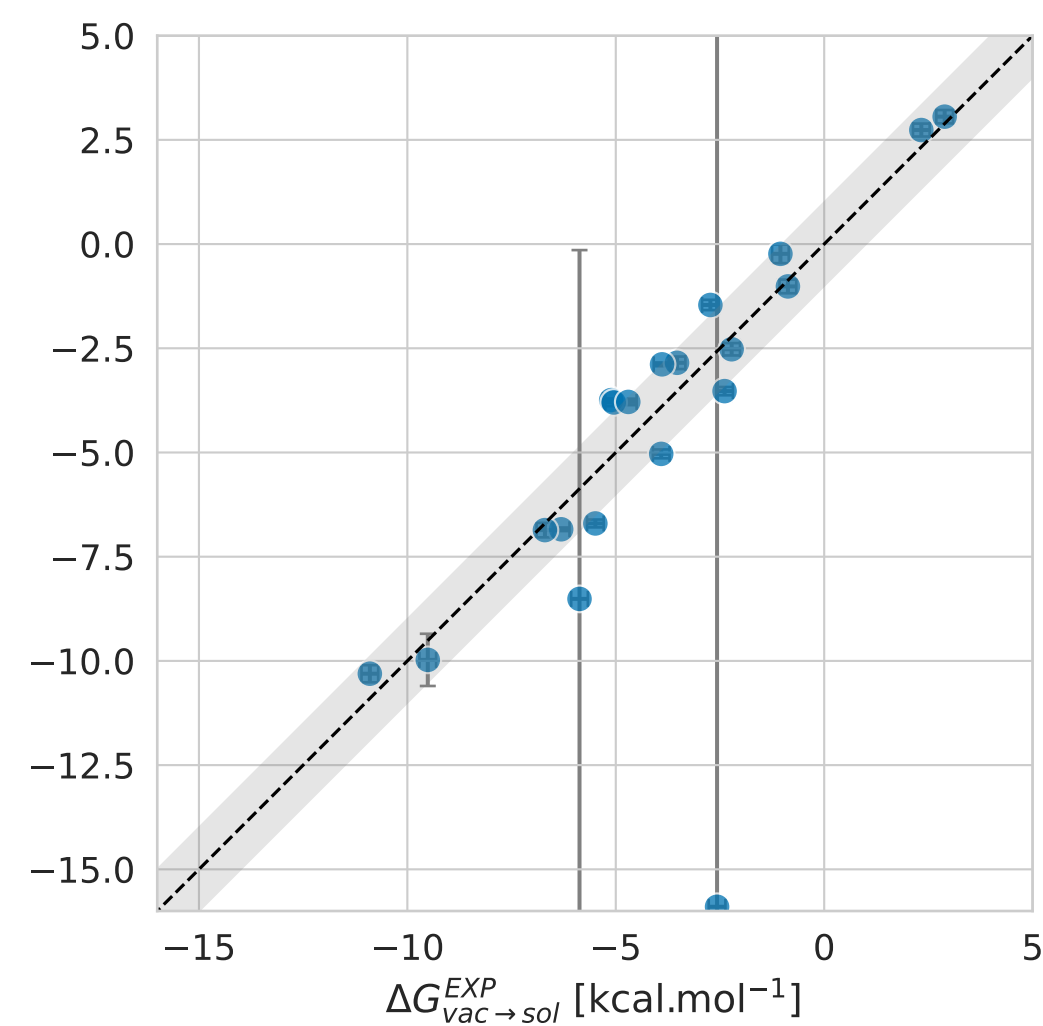


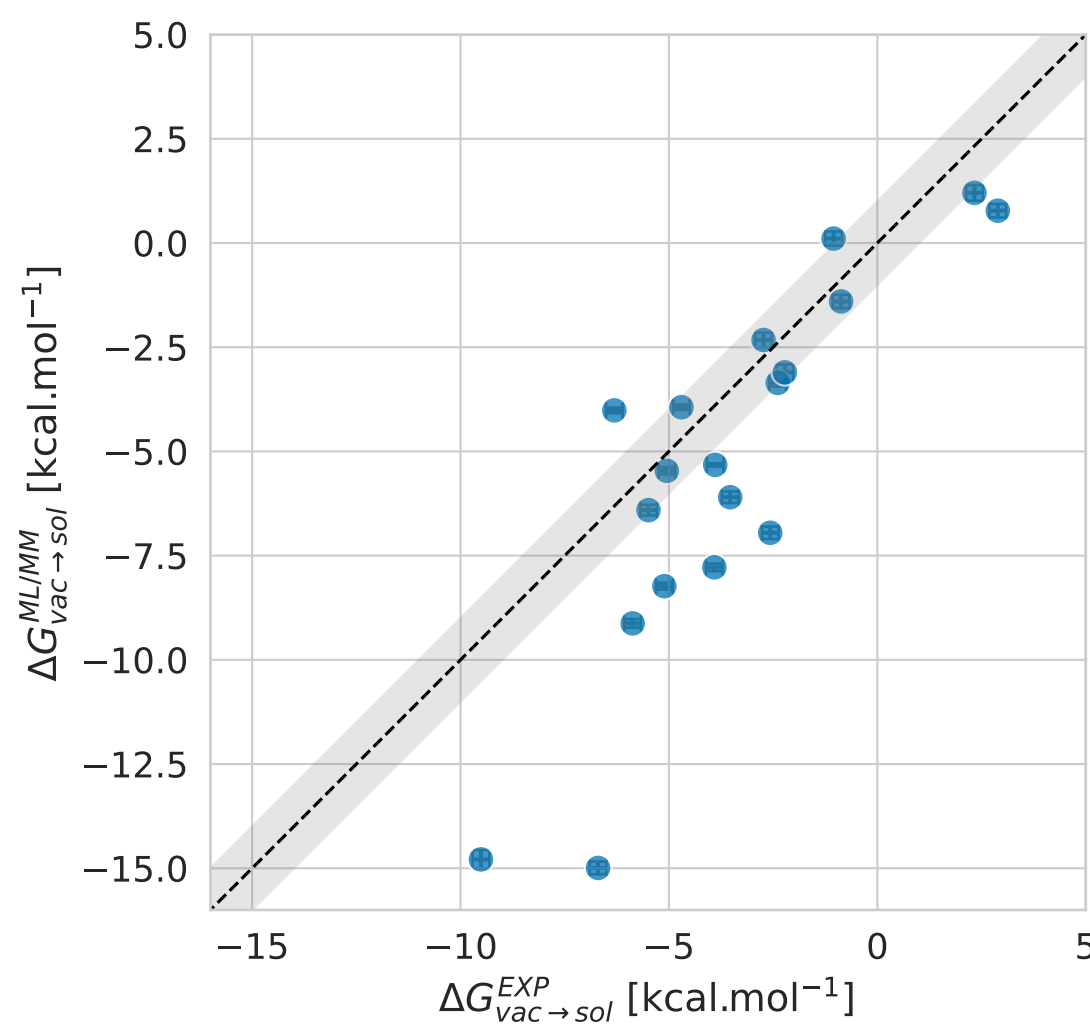
OpenFF/TIP3P
 R^2 : 0.95 [0.75, 0.98]
RMSE: 0.80 [0.61, 1.01]
MUE: 0.68 [0.46, 0.89]
MSE: 0.23 [-0.19, 0.71]
 ρ : 0.97 [0.92, 0.99]
 τ : 0.86 [0.72, 0.98]



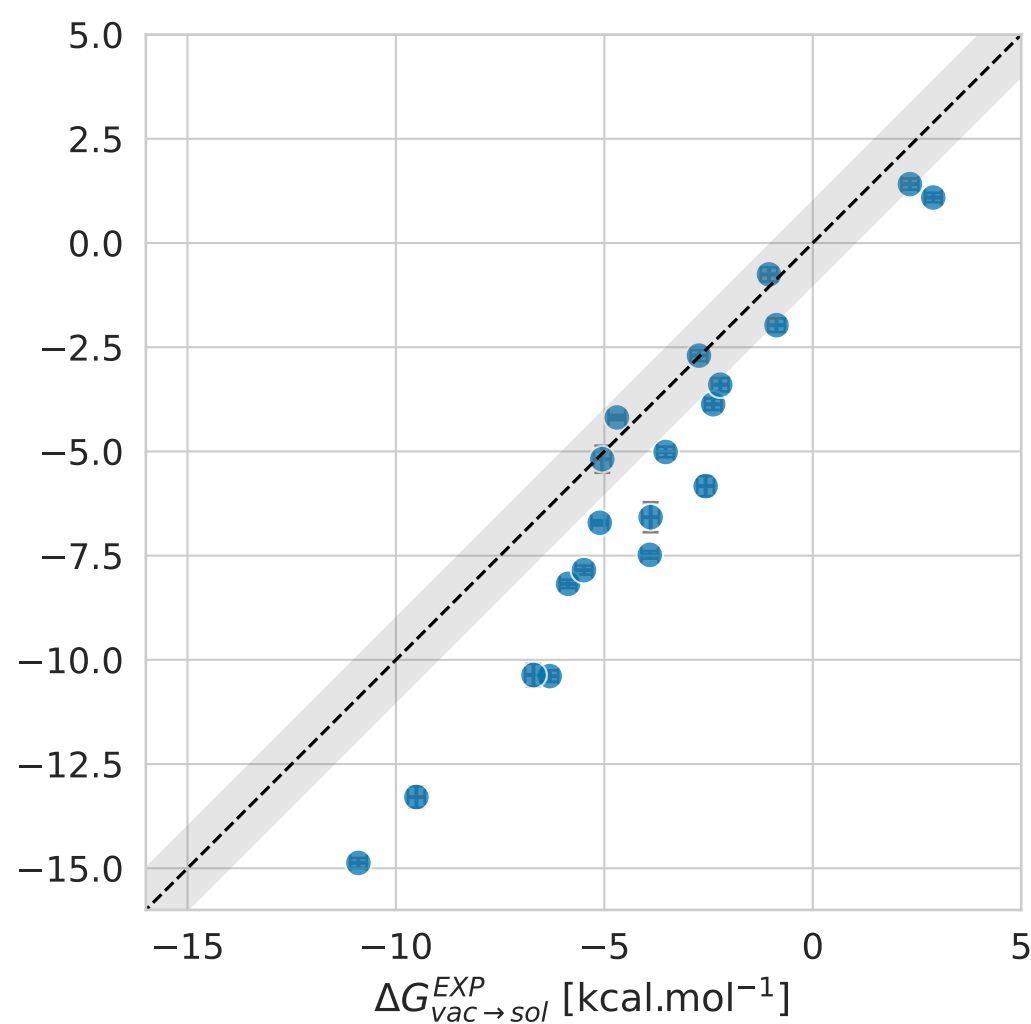
ML/MM (MM Embedding)
 R^2 : 0.51 [0.01, 0.96]
RMSE: 3.15 [0.79, 6.07]
MUE: 1.48 [0.67, 2.85]
MSE: -0.63 [-1.95, 0.34]
 ρ : 0.71 [0.34, 0.98]
 τ : 0.74 [0.43, 0.96]



General Model
 R^2 : 0.78 [0.61, 0.94]
RMSE: 3.20 [2.15, 4.16]
MUE: 2.46 [1.45, 3.42]
MSE: -2.00 [-3.28, -0.85]
 ρ : 0.89 [0.74, 0.97]
 τ : 0.72 [0.45, 0.90]



Bespoke Model
 R^2 : 0.92 [0.75, 0.97]
RMSE: 2.40 [1.88, 2.87]
MUE: 2.01 [1.57, 2.66]
MSE: -1.93 [-2.47, -1.22]
 ρ : 0.96 [0.87, 0.98]
 τ : 0.84 [0.71, 0.96]



Patched Model
 R^2 : 0.95 [0.91, 0.98]
RMSE: 1.63 [1.26, 1.94]
MUE: 1.41 [1.00, 1.81]
MSE: -1.39 [-1.75, -0.89]
 ρ : 0.98 [0.95, 0.99]
 τ : 0.88 [0.77, 0.98]

