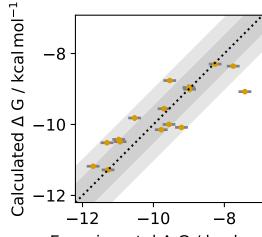
ML/MM: openff-1.0.0 ANI-2x (N = 16) RMSE: 0.65 [95%: 0.43, 0.93] MUE: 0.50 [95%: 0.34, 0.74] R2: 0.76 [95%: 0.50, 0.90] rho: 0.87 [95%: 0.68, 0.95] $\frac{1}{2}$



Experimental Δ G / kcal mol⁻¹