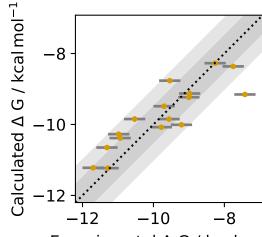
ML/MM: openff-1.0.0 ANI-2x (N = 16) RMSE: 0.65 [95%: 0.46, 0.98] MUE: 0.52 [95%: 0.38, 0.80] R2: 0.76 [95%: 0.48, 0.90] rho: 0.87 [95%: 0.70, 0.94] $\frac{1}{6}$



Experimental Δ G / kcal mol⁻¹