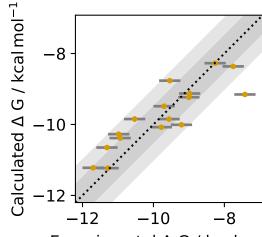ML/MM: openff-1.0.0
ANI-2x
(N = 16)

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]