ANI-2x (N = 16)RMSE: 0.47 [95%: 0.37, 0.75] MUE: 0.35 [95%: 0.28, 0.63] 0.86 [95%: 0.60, 0.94] R2: 0.93 [95%: 0.76, 0.97] rho: Calculated Δ G / kcal mol $^{-1}$ 10 -12-10-8 Experimental Δ G / kcal mol⁻¹

ML/MM:

openff-1.0.0