(N = 16)RMSE: 0.47 [95%: 0.32, 0.68] MUE: 0.35 [95%: 0.24, 0.55] 0.86 [95%: 0.65, 0.95] R2: 0.93 [95%: 0.80, 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

ANI-2x