

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]

