

ML/MM: openff-1.0.0

ANI-2x

(N = 16)

RMSE: 0.47 [95%: 0.32, 0.68]

MUE: 0.35 [95%: 0.24, 0.55]

R2: 0.86 [95%: 0.65, 0.95]

rho: 0.93 [95%: 0.80, 0.97]

