

ML/MM: openff-1.0.0

ANI-2x

(N = 16)

RMSE: 0.47 [95%: 0.37, 0.75]

MUE: 0.35 [95%: 0.28, 0.63]

R2: 0.86 [95%: 0.60, 0.94]

rho: 0.93 [95%: 0.76, 0.97]

