

MM: openff-1.0.0

(N = 16)

RMSE: 0.97 [95%: 0.71, 1.29]

MUE: 0.77 [95%: 0.56, 1.13]

R2: 0.42 [95%: 0.08, 0.76]

rho: 0.65 [95%: 0.27, 0.87]

