

MM: openff-1.0.0

(N = 16)

RMSE: 0.97 [95%: 0.69, 1.26]

MUE: 0.77 [95%: 0.52, 1.10]

R2: 0.42 [95%: 0.07, 0.76]

rho: 0.65 [95%: 0.26, 0.88]

