n: td OpenFF Gen 2 Torsion Set 4 eMolecules Discrepancy 2 101 C14Cl2F 10.0 QM **MM Current** MM Initial 7.5 5.0 Energy (kcal/mol) 2.5 0.0 -2.5-5.0**-**7.5

100

50

Dihedral (degree)

150

-150

-100

-50

Torsion profile: iteration 1