Torsion profile: iteration 0 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 -150-100-50100 150 50

Dihedral (degree)