m: td OpenFF Gen 2 Torsion Set 4 eMolecules Discrepancy 2 098 C11H7 15.0 QM MM Initial 12.5 10.0 Energy (kcal/mol) 7.5 5.0 2.5 0.0 -2.5

50

Dihedral (degree)

100

150

-150

-100

-50

Torsion profile: iteration 0