m: td OpenFF Gen 2 Torsion Set 4 eMolecules Discrepancy 2 113 C14H1 30 QM **MM** Current **MM** Initial 25 20 Energy (kcal/mol) 15 10 5

50

Dihedral (degree)

100

150

0

-150

-100

-50

Torsion profile: iteration 0