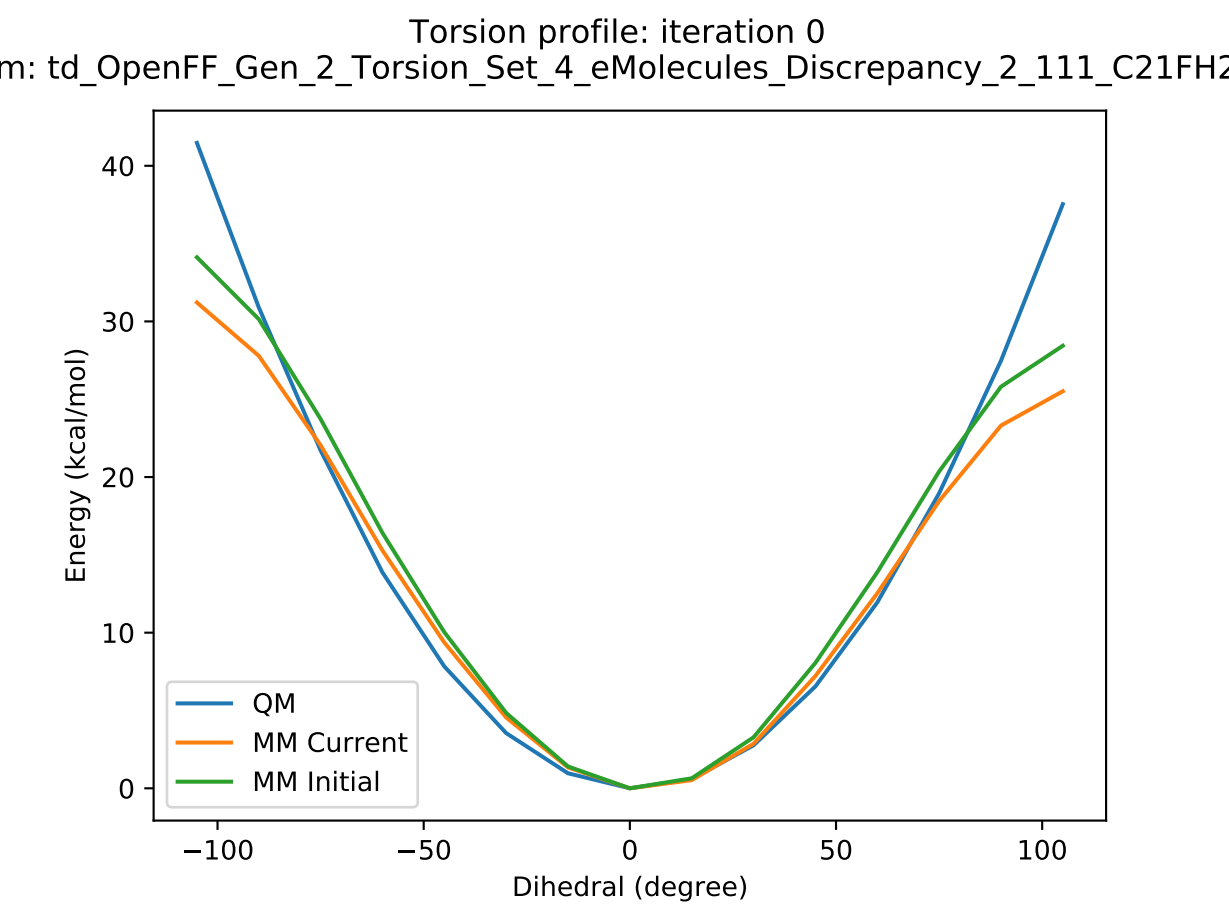
Torsion profile: iteration 0
m: td_OpenFF_Gen_2_Torsion_Set_4_eMolecules_Discrepancy_2_111_C21FH2
Energy (kcal/mol)
Dihedral (degree)
QM
MM Current
MM Initial
40
30
20
10
0
−100
−50
0
50
100