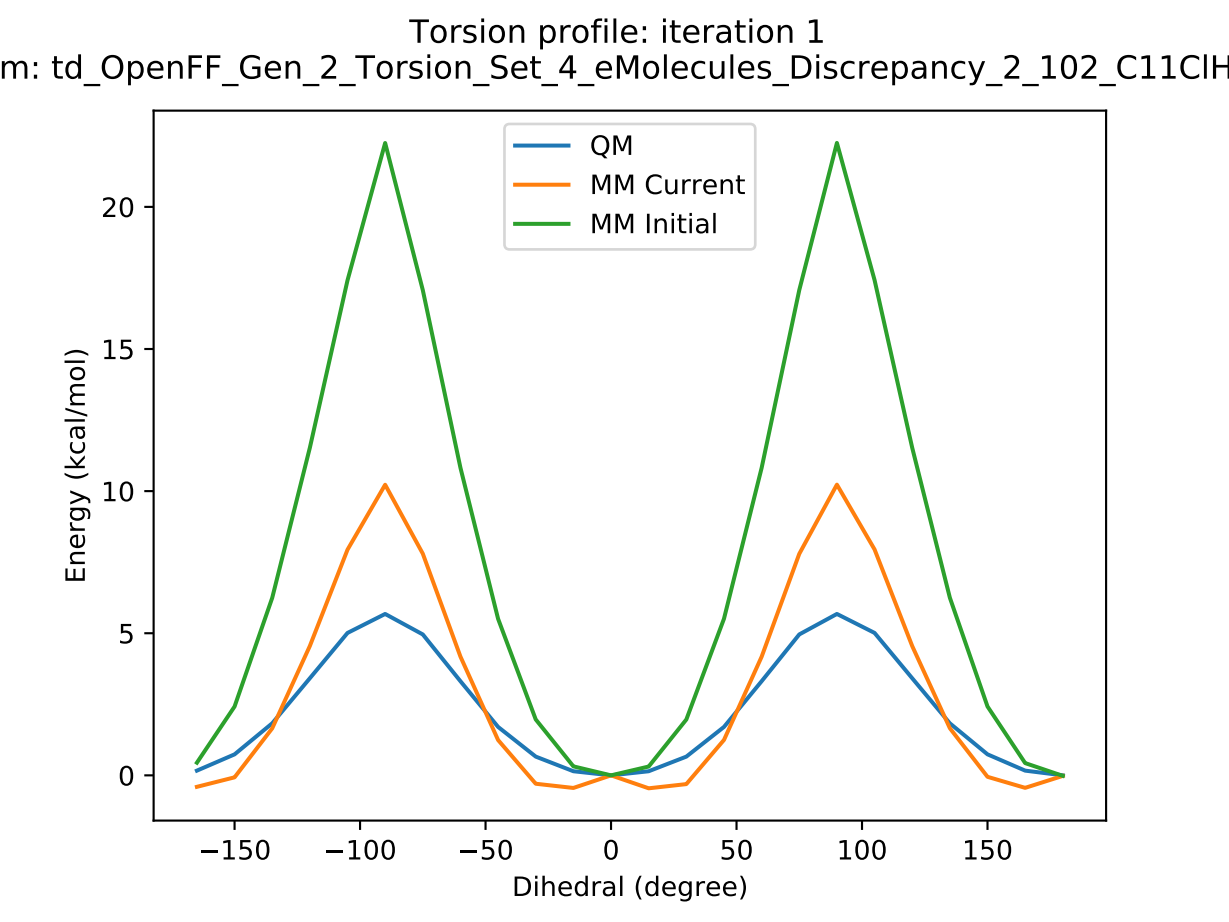
Torsion profile: iteration 1
m: td_OpenFF_Gen_2_Torsion_Set_4_eMolecules_Discrepancy_2_102_C11ClH
QM
MM Current
MM Initial
Energy (kcal/mol)
20
15
10
5
0
−150
−100
−50
0
50
100
150
Dihedral (degree)