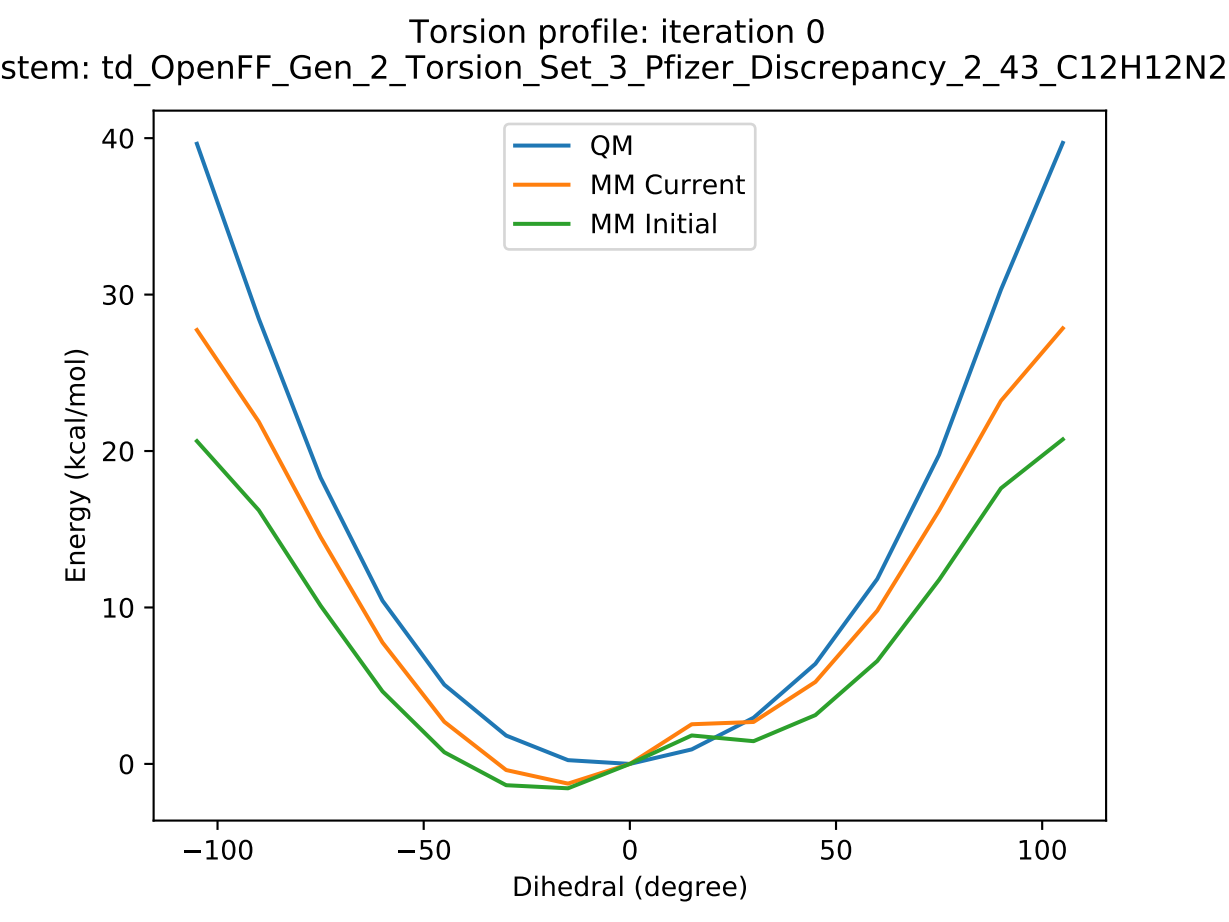
Torsion profile: iteration 0
stem: td_OpenFF_Gen_2_Torsion_Set_3_Pfizer_Discrepancy_2_43_C12H12N2
QM
MM Current
MM Initial
Energy (kcal/mol)
40
30
20
10
0
−100
−50
0
50
100
Dihedral (degree)