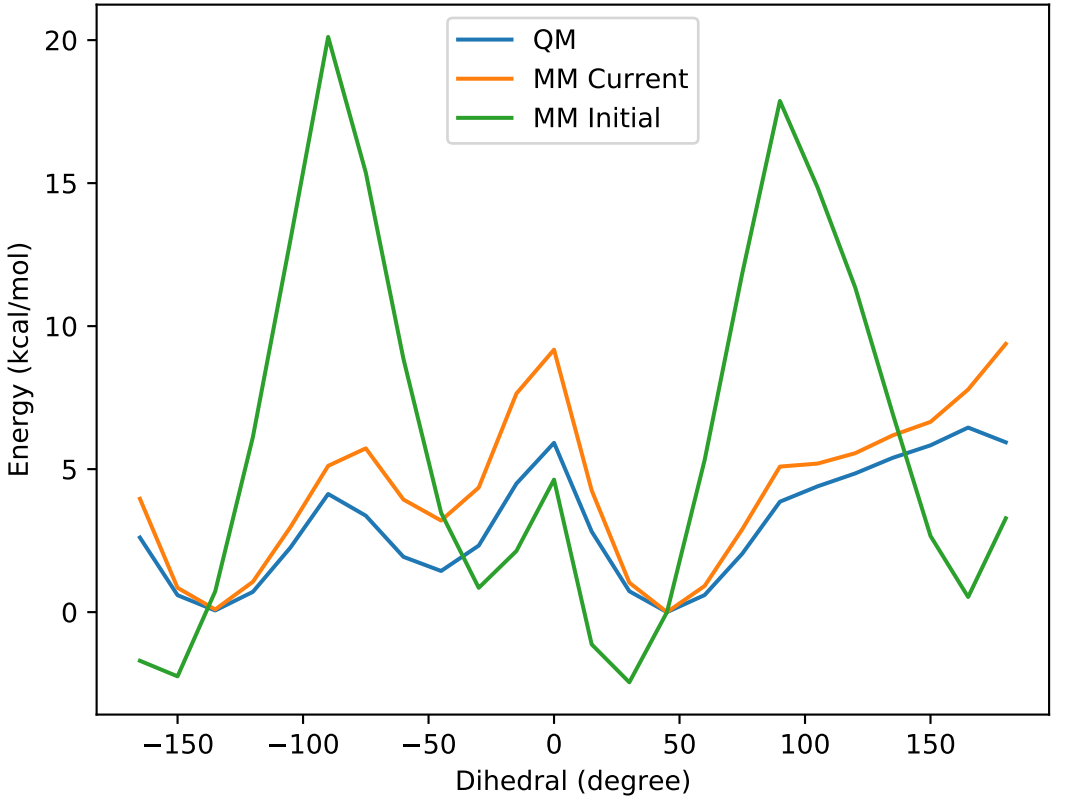
Torsion profile: iteration 1
System: td_OpenFF_Gen_2_Torsion_Set_5_Bayer_2_066_C26H27NO2
QM
MM Current
MM Initial
Energy (kcal/mol)
20
15
10
5
0
−150
−100
−50
0
50
100
150
Dihedral (degree)