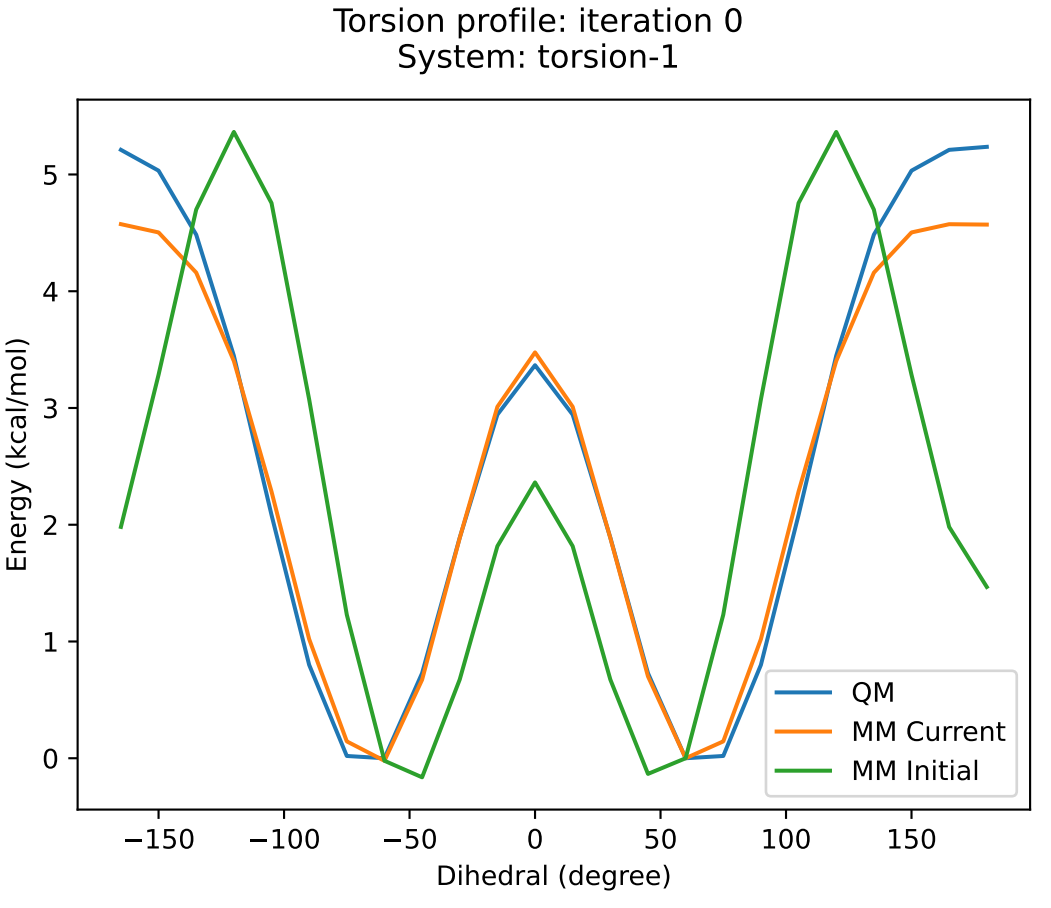
Torsion profile: iteration 0
System: torsion-1
Energy (kcal/mol)
Dihedral (degree)
QM
MM Current
MM Initial
5
4
3
2
1
0
−150
−100
−50
0
50
100
150