Torsion profile: iteration 0 ystem: td OpenFF Gen 2 Torsion Set 3 Pfizer Discrepancy 2 44 C9H8N2C 30 25 Energy (kcal/mol) 20 15 10 5 QM **MM** Current MM Initial 0 -150-100-5050 100 150

Dihedral (degree)