Torsion Explorer

Molecule Set Up:

- Generate SMILE string
- Use OpenBabel to convert to PDB and XYZ files

  (Use generate 3D Coordinates)
- Check the connectivity of PDB file

(OpenBabel does not always deal well with heteroaromatics in these molecule types.)

Optimisation with PSI4:

Template file

```
memory 500 mb

set globals basis cc-pVDZ
set optking opt_coordinates cartesian

molecule{
1 1
***xyz file coordinate data***
}

optimise('b3lyp')
```

Command line

```
psi4 molecule.in molecule.out
```

TorsionDrive Set Up:

If running on Eddie needs to be done on an interactive session

Requires 2 input files:

1. Dihedrals
2. Molecule Data

- Original PDB file requires amending with the final optimised geometry from the psi4 **molecule.out** file

(Generating the PDB file from the optimised geometry can lead to incorrect bond coordination. I think because it generates the bonds based solely on distance.)

Dihedrals.txt

```
# Dihedral Definition By Atom Indicies Starting From 1
# i     j     k     l
  11    10    9     8
```

Command line

```
#to run TorsionDrive
torsiondrive-launch Dihedrals.txt moleucule.pdb -g 30 -v

#to generate plot once completed
torsiondrive-plot1d
```

Molecular Dynamics Simulation:

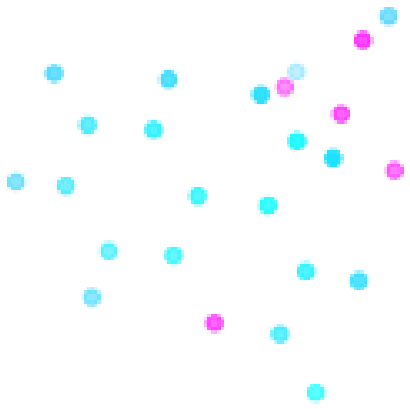
Pemberton Data:

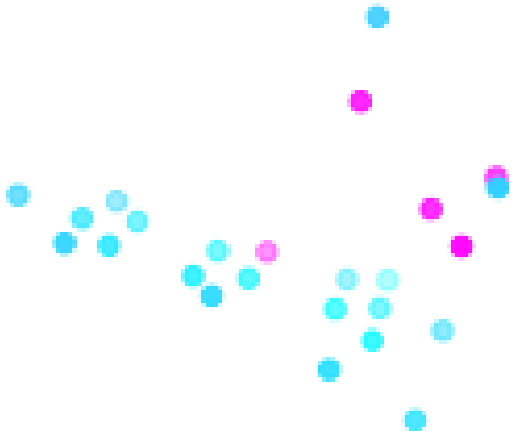
J. Med. Chem. 2019, 62, 18, 8480–8496

Publication Date:September 4, 2019

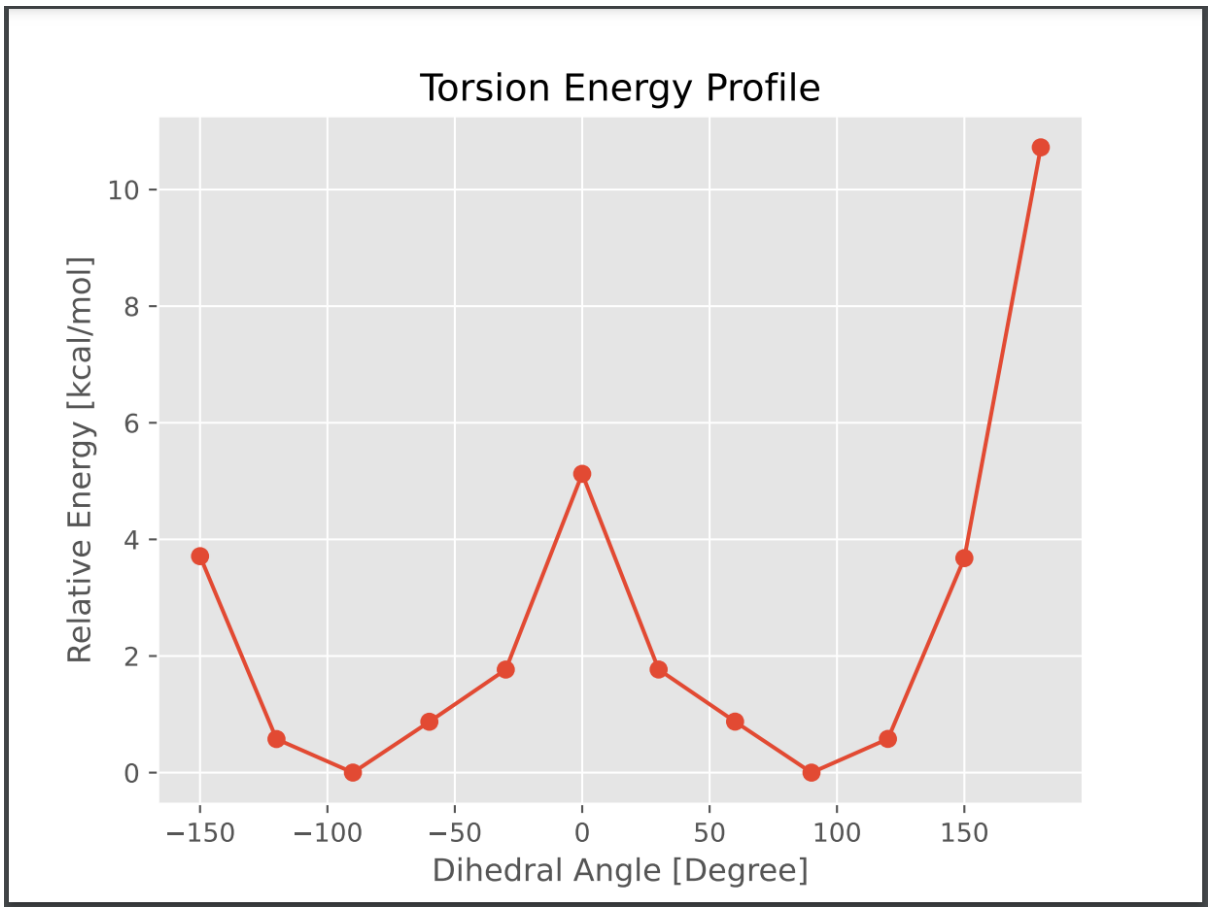
https://doi.org/10.1021/acs.jmedchem.9b00728

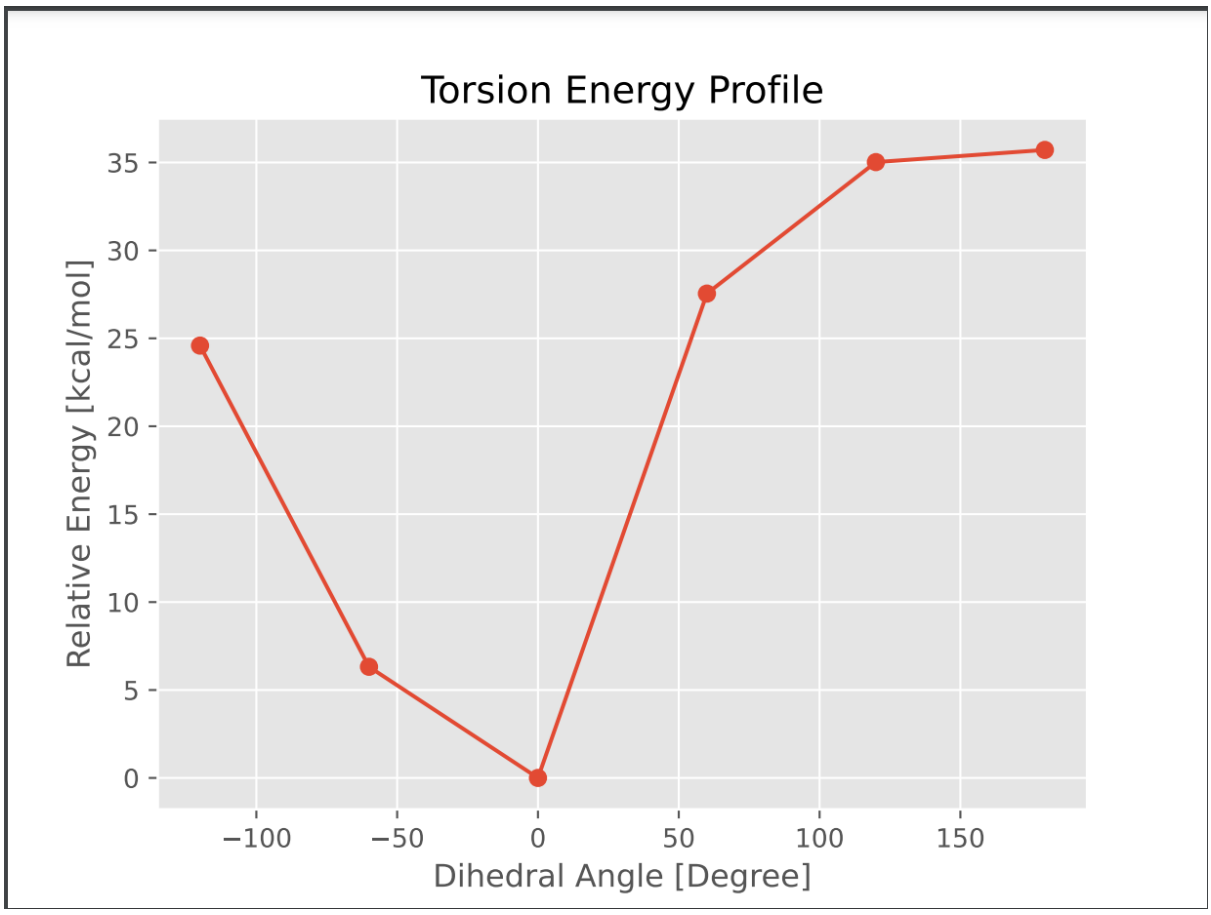
Base molecule:





Oxygens are highlighted in purple


Torsion Energy Profile
Relative Energy [kcal/mol]
0
2
4
6
8
10
−150
−100
−50
0
50
100
150
Dihedral Angle [Degree]



TorsionDrive plots