

A.

```
# Sample the peptide space, interval 10°
$ puckers --peptide 37
#> #      PHI      PSI      X      Y
#>    0.000    0.000    0.000    0.000
#>    0.000    10.000   0.000   10.000
#>    0.000    20.000   0.000   20.000
#>    0.000    30.000   0.000   30.000
#>    0.000    40.000   0.000   40.000
#>    0.000    50.000   0.000   50.000
#>    0.000    60.000   0.000   60.000
#>    0.000    70.000   0.000   70.000
#>    0.000    80.000   0.000   80.000
#>    0.000    90.000   0.000   90.000
#>    0.000   100.000   0.000  100.000

# Sample the fivering space, interval 6°
$ puckers --fivering 21
#> #      NU1      NU3      Zx      Zy
#>   13.274    83.808   -60.000  -60.000
#>   16.801    80.281   -60.000  -54.000
#>   20.327    76.755   -60.000  -48.000
#>   23.854    73.228   -60.000  -42.000
#>   27.381    69.701   -60.000  -36.000
#>   30.907    66.175   -60.000  -30.000
#>   34.434    62.648   -60.000  -24.000
#>   37.961    59.121   -60.000  -18.000
#>   41.488    55.594   -60.000  -12.000
#>   45.014    52.068   -60.000   -6.000
#>   48.541    48.541   -60.000   0.000

# Sample the sixring space, approximate 632 points
$ puckers --sixring 630
#> #    ALPHA1    ALPHA2    ALPHA3      RHO    THETA    PHI
#>   139.882    146.537    139.882    0.670    0.071    0.000
#>   139.882    139.882    146.537    0.670    0.071    2.094
#>   146.537    139.882    139.882    0.670    0.071    4.189
#>   136.202    155.698    136.202    0.670    0.214    0.000
#>   130.303    153.337    144.349    0.670    0.214    0.628
#>   129.352    147.008    151.586    0.670    0.214    1.257
#>   133.826    138.827    155.430    0.670    0.214    1.885
#>   141.583    131.823    154.634    0.670    0.214    2.513
#>   149.450    129.028    149.450    0.670    0.214    3.142
#>   154.633    131.824    141.585    0.670    0.214    3.770
#>   155.429    138.828    133.828    0.670    0.214    4.398
```

B.

```
from puckepy.formalism import CP5, AS
from puckepy.formalism import Pdb

# Parse the pdb file for atomnames and coordinates
fiveringPdb = Pdb(filename="dna_adenosine.pdb")
# Mutates variable in place
fiveringPdb.parse()

# Calculate Cremer-Pople coordinates from a pdb file
# Calculate by querying the atom names
# => return a tuple of (amplitude, phase angle)
cp5_amplitude, cp5_phaseangle = CP5().from_atomnames(
    pdb=fiveringPdb,
    query_names=["04'", "C1'", "C2'", "C3'", "C4'"]
)

# Calculate Altona Sundaralingam coordinates from a pdb file
# Calculate by querying the atom indices
# => return a tuple of (amplitude, phase angle)
as_amplitude, as_phaseangle = AS().from_indices(
    coordinates=fiveringPdb.coordinates,
    indices=[7, 8, 26, 24, 5]
)
```

C.

```
from puckepy.formalism import CP5, write_to_pdb

# Make a set of Cremer-Pople coordinate for five-membered rings
# and invert to the coordinates of the abstracted conformer
inverted_coordinates = CP5(0.35, 90.).invert()

# Write out to a pdb file
write_to_pdb(
    fname="inverted_fivering.pdb",
    coordinates=inverted_coordinates,
    residuename="FIV"
)
```

D.

```
from puckepy.confssampling import Fivering, FiveringAxes

# Example using the Fivering() class
fivering, axes = Fivering(21), FiveringAxes(21)

for zx, zy, nu1, nu3 in zip(axes.zx,
                           axes.zy,
                           fivering.nu1,
                           fivering.nu3):
    print(" %8.3f %8.3f %8.3f %8.3f" % (zx,
                                       zy,
                                       nu1,
                                       nu3)
          )
```

E.

```
from puckepy.formalism import Xyz
from puckepy.geometry import dihedral

# Read from xyz file and parse the coordinates
xyz_coordinates = Xyz("dna_adenosine.xyz").parse()

# Calculate specific dihedrals of interest
chi_angle = dihedral(
    xyz_coordinates[8], #04'
    xyz_coordinates[10], #C1'
    xyz_coordinates[11], #N9
    xyz_coordinates[23], #C4
)
```