File modification

1. Create library using IBM with benzylic tribromide + peptide chain + thiol. – Completed

2. Use Monte Carlo Multiple Minimum for conformational sampling. – Completed

3. Modify format of MCMM output to match Protein Data Bank and overlay cyclic peptides with protein backbones. Find low RMSD values.

4. Align with Kirtzer hot loops to find possible mimics

Steps for file modification

- Convert maegz to mol2. Completed
- Convert mol2 to PDB file format. Almost completed

Completed: Changing Atom ID

The script involved changing the carbon atoms to the corresponding bonding information and removing numbers from other elements.

```
if atom_id > 21 and atom_id < file_listFirstRingLength * 5 + 20 + 5 + 1:
    if (atom_id - 2 )% 5 == 0:
        data1 = txt[j].replace('N'+str(atom_id),'N  ')
        output.write(data1)
    if (atom_id - 3 )% 5 == 0:
        data1 = txt[j].replace('C'+str(atom_id),'C  ')
        output.write(data1)
    if (atom_id - 4 )% 5 == 0:
        data1 = txt[j].replace('O'+str(atom_id),'O  ')
        output.write(data1)
    if (atom_id )% 5 == 0:
        data1 = txt[j].replace('C'+str(atom_id),'CA ')
        output.write(data1)
    if (atom_id - 6 )% 5 == 0:
        data1 = txt[j].replace('C'+str(atom_id),'CB ')
        output.write(data1)
```

```
@<TRIPOS>MOLECUL
3R82
147   149    1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 CA
      2 C
      3 O
      4 N
      5 CA
      6 C6
      7 S7
      8 C8
      9 C9
     10 C10
     11 C11
     12 C12
     13 C13
     14 C14
     15 C15
     16 S16
     17 C17
     18 CA
     19 C
```

```
@<TRIPOS>MOLECULE
3R82
147   149    1
SMALL
USER_CHARGES


@<TRIPOS>ATOM
      1 C1
      2 C2
      3 O3
      4 N4
      5 C5
      6 C6
      7 S7
      8 C8
      9 C9
     10 C10
     11 C11
     12 C12
     13 C13
     14 C14
     15 C15
     16 S16
     17 C17
     18 C18
     19 C19
```

Progress Update

Previously, the script did not function properly due to certain bicyclic peptides having different atom order.

The main difference was that some would have a N at 19 and some would start with a C at 19. After noticing this pattern was due to if the bicyclic started on the larger ring or shorter ring, a new set of parameters were made.

```
@<TRIPOS>ATOM
      1 CA        48.0935   54.0207   20.7930 C.3       0 UNK         -0.1987
      2 C         49.0134   53.3344   19.7934 C.2       0 UNK          0.4824
      3 O         49.1263   53.7961   18.6577 O.2       0 UNK         -0.5319
      4 N         49.6563   52.2368   20.2170 N.am      1 UNK         -0.4339
      5 CA        50.5357   51.3600   19.4338 C.3       1 UNK          0.0266
      6 C6        51.8112   52.0741   18.9073 C.3      10 UNK          -0.1344
      7 C7        52.7389   52.6450   19.9971 C.3      10 UNK          -0.0346
      8 S8        53.4508   51.3955   21.1100 S.3      10 UNK          -0.3574
      9 C9        54.9072   52.2583   21.7876 C.3      10 UNK           0.0206
     10 C10       54.5439   53.3561   22.7786 C.ar     10 UNK          -0.0827
     11 C11       54.5137   53.0758   24.1476 C.ar     10 UNK          -0.1180
     12 C12       54.2364   54.0883   25.0632 C.ar     10 UNK          -0.1071
     13 C13       53.9830   55.3857   24.6110 C.ar     10 UNK          -0.0732
```

Progress Update

- Currently, the script seems to work fine. The residue ID is also updating, and the atom id is changing correctly. Right now, mol2 files from mobxterm are being downloaded and converted to pdb file type.