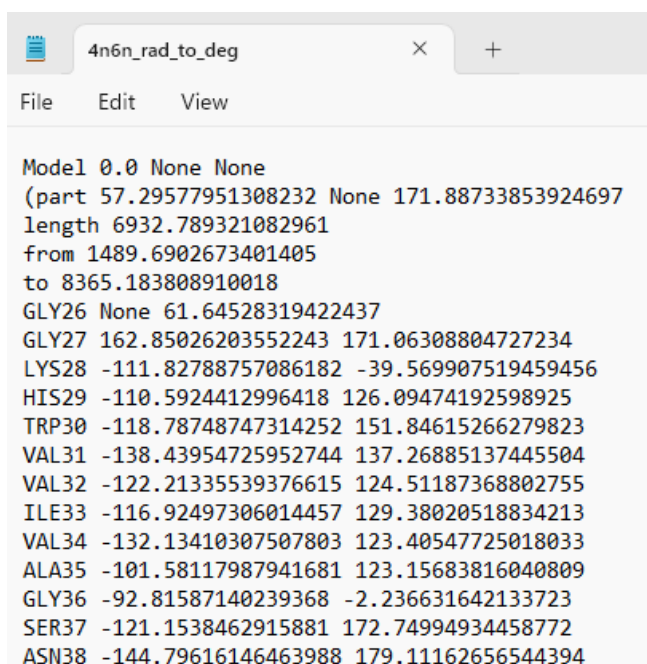


This is a continuation of the process from the “dihedral_angle_radians_to_degrees” repository, where you will find instructions on how to create a .txt file in the proper format for this secondary structure prediction module.

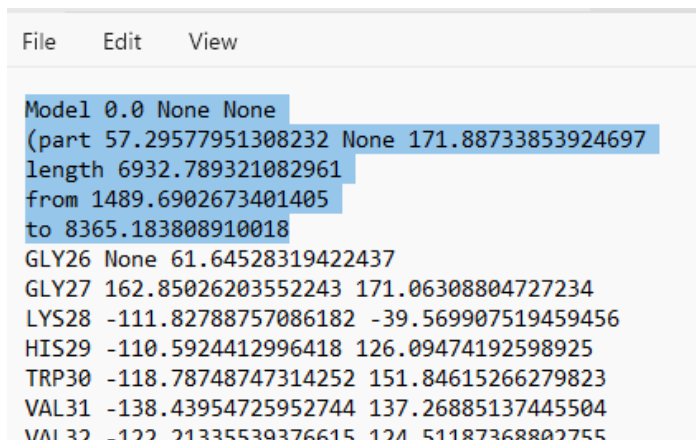
To find the secondary structure of your protein of interest, input a .txt file of the dihedral angles in degrees format to the “deg_2_sec.py” module. (You can find the modules to do this in the “dihedral_angle_radians_to_degrees” repository found here: https://github.com/sstonya/dihedral_angle_radians_to_degrees.git).

Your .txt file should look like this:



```
Model 0.0 None None
(part 57.29577951308232 None 171.88733853924697
length 6932.789321082961
from 1489.6902673401405
to 8365.183808910018
GLY26 None 61.64528319422437
GLY27 162.85026203552243 171.06308804727234
LYS28 -111.82788757086182 -39.569907519459456
HIS29 -110.5924412996418 126.09474192598925
TRP30 -118.78748747314252 151.84615266279823
VAL31 -138.43954725952744 137.26885137445504
VAL32 -122.21335539376615 124.51187368802755
ILE33 -116.92497306014457 129.38020518834213
VAL34 -132.13410307507803 123.40547725018033
ALA35 -101.58117987941681 123.15683816040809
GLY36 -92.81587140239368 -2.236631642133723
SER37 -121.1538462915881 172.74994934458772
ASN38 -144.79616146463988 179.11162656544394
```

You will need to remove sections of the radian output file which do not format as ({residue}, (coordinates)). For example, the first 5 rows of the document do not follow this format (see highlighted area in the example below).



```
File Edit View
Model 0.0 None None
(part 57.29577951308232 None 171.88733853924697
length 6932.789321082961
from 1489.6902673401405
to 8365.183808910018
GLY26 None 61.64528319422437
GLY27 162.85026203552243 171.06308804727234
LYS28 -111.82788757086182 -39.569907519459456
HIS29 -110.5924412996418 126.09474192598925
TRP30 -118.78748747314252 151.84615266279823
VAL31 -138.43954725952744 137.26885137445504
VAL32 -122.21335539376615 124.51187368802755
```

Remove the highlighted area for every part in which you see a similar formatting. Save your edited .txt file.

Copy the path to your .txt file and paste it in the “input_file_path” sections of the “deg_2_sec.py” module. This module will convert the degree coordinates into secondary structures (Note: you can change the angle (phi, psi) number values).

```
1  #Dihedral angle to secondary structure converter
2
3  def second_struc(phi,psi):
4      if phi is None or psi is None:
5          return 'None'
6      elif (-60 <= phi <= -40 and -70 <= psi <= -50):
7          return "Right-handed Alpha-helix"
8      elif (40 <= phi <= 70 and 30 <= psi <= 60):
9          return "Left-handed Alpha-helix"
10     elif (-150 <= phi <= 30 and 120 <= psi <= 140):
11         return "Beta-sheet"
12     else:
13         return "Other"
14
15 def convert_degs_to_sec(input_file_path, output_file_path):
16     with open(input_file_path, 'r') as input_file:
17         lines = input_file.readlines()
18
19     convert_coords = []
20
21     for line in lines:
22         parts = line.strip().split(' ')
23         residue_name = parts[0]
24         phi = float(parts[1]) if parts[1].upper().lower() != 'none' else None
25         psi = float(parts[2]) if parts[2].upper().lower() != 'none' else None
26
27         converted_coords = [second_struc(phi, psi)]
28
29         converted_line = ' '.join([residue_name] + converted_coords)
30
31         convert_coords.append(converted_line)
32
33     with open(output_file_path, 'w') as output_file:
34         output_file.write('\n'.join(convert_coords))
35
36 input_file_path = r"C:\Users\Tania\Documents\rad_2_deg.txt"
37 output_file_path = r"C:\Users\Tania\Documents\4n6n_sec_struc.txt"
38 convert_degs_to_sec(input_file_path, output_file_path)
39
```

You will receive an output like this:

```
GLY26 None
GLY27 Other
LYS28 Other
HIS29 Beta-sheet
TRP30 Other
VAL31 Beta-sheet
VAL32 Beta-sheet
ILE33 Beta-sheet
VAL34 Beta-sheet
ALA35 Beta-sheet
GLY36 Other
SER37 Other
ASN38 Other
GLY39 Other
TRP40 Other
TYR41 Other
ASN42 Other
TYR43 Other
ARG44 Other
HIS45 Other
GLN46 Other
ALA47 Other
ASP48 Right-handed Alpha-helix
ALA49 Other
CYS50 Other
HIS51 Other
ALA52 Other
TYR53 Other
```

This .txt file predicts the secondary structures of the PDB protein.