GSoC 2019 Project Proposal

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BioShell

A New Activity for Sugar

My Introduction

- I am Manan Goel, a sophomore at the International Institute of Information Technology - Hyderabad pursuing a B.Tech. in Computer Science followed by an M.S. in Computational Natural Sciences.
- My first language is Hindi but I am also fluent in English.
- My email is manangoel1999@gmail.com and this is the link(manangoel99) to my GitHub profile.
- I am placed in Hyderabad, Telangana, India (+5:30 GMT).

Previous Projects and Open Source Contributions

- I have to admit that I haven't contributed a lot to large scale open source projects like sugar. I have made a few pull requests which are listed below -
  - https://github.com/sugarlabs/www-sugarlabs/pull/292
  - https://github.com/sugarlabs/www-sugarlabs/pull/291
- I have worked quite a bit on a lot of solo projects which I made using different frameworks in different programming languages. The following is a list of my personal projects that I've worked on over the past two years -
  - The following are my versions of existing games that I made using OpenGL and WebGL
    - https://github.com/manangoel99/SubwaySurfer
    - https://github.com/manangoel99/FlightSimulator
    - https://github.com/manangoel99/JetpackJoyride

- This is a web-based billing system I worked on for a catering start-up company in my hometown
  - https://github.com/manangoel99/BestBhojv2
- A quizzing web app with its front end created using ReactJS and back end written in GoLang.
  - https://github.com/manangoel99/QuizPortal
- A web app clone of the Android app SplitWise made in Flask and BootStrap was used for the Front End.
  - https://github.com/manangoel99/LetsSplit
- As a part of an internship, I did last year I worked on creating a proxy rotator for a web scraper created using BeautifulSoup and Selenium and also optimize the amount of data collected along with the time taken to do it.

Motivation

- **My motivation for taking part in the Google Summer of Code:**
  - My major motivation for being a part of Google Summer of Code starts with a little story. During my last two years of school, I was one of the very few students who pursued computer science and at the time there was a persistent thought in my mind that writing code for these basic algorithms has to mean something. Writing code can't just stop at sorting an array of numbers. When I got into college I found open source to be what I was looking for, something which brought people together to work as a community to build something that affects so many.

    As a first year, I was never confident enough about my skills and was hence, too shy leading to the fact that I couldn't effectively communicate with the people of different open source communities.

    I believe that GSoC is an amazing platform to get involved with open source communities since it provides a single place through which a person can get in touch with the world of open source.

- ## Why I chose Sugar Labs:

    - I came to know about Sugar Labs through GSoC organisations while I was searching for different projects I could start working on. The first thing that made me want to work with Sugar Labs was that almost all the projects were built using Python, a language I believe I'm extremely proficient in.

      I grew up in a small town in interior Haryana where the idea of getting educated from a computer-based platform is extremely new, so I felt that Sugar Labs brings something to children which I did not have for a long time and I would love to contribute to that.

      I found the Sugar Labs community to be amazing with prompt replies from mentors who are extremely helpful. Moreover, I also loved the fact that it is a meritocracy where I could start working on different issues and projects as soon as I could.

- ## Why I want to work on this project:

    - I am pursuing a B. Tech. in Computer Science which will be followed by an M.S. in Computational Natural Science where we study how Computer Science techniques like Machine Learning, probabilistic simulations can be applied in Natural Science Problems like Protein Folding which has baffled scientists for centuries now.

      My passion for this project comes from my passion for Bioinformatics which is, in my opinion, a beautiful amalgamation of the two fields. There are some amazing bioinformatics algorithms which help us gain insight into different biological problems like how we differ from other organisms on a DNA level and from the same data we can also find out how genetically close we are to different organisms.

When I first saw these algorithms in action, it blew my mind and I would like to give a similar experience to children but at a much earlier stage than I did.

- **My Expectations from Sugar Labs:**
  - During :
    - I understand that molecular biology may not be the field of expertise for my mentors but I would like that they read about a few very basic concepts like Phylogenetic Trees and the Ramachandran Plot which I can also help them with.
    - I would like the mentors to be supportive just like they have been till now but also not shy away from giving me constructive criticism since that would help me in making a great project.
  - After :
    - There are a lot of other molecular biology-based concepts which I won't be able to include in the activity during the course of GSoC 2019. I would like to keep working on this project even after GSoC ends and I would love to have the support of the organisation in doing the same.

Project Details

1. Overview

"BioShell" is a new activity for the Sugar platform through which I hope to help students get a better understanding of different molecular biology problems. As a student in school, I very quickly lost interest in molecular biology because when I studied the concepts of DNA sequences, Protein Structures, Transcription and Translation etcetera, I could not understand how they worked and of the significance, they had in the real world. Last year, I took a course in college which introduced me to these concepts from the perspective of a computer science student.

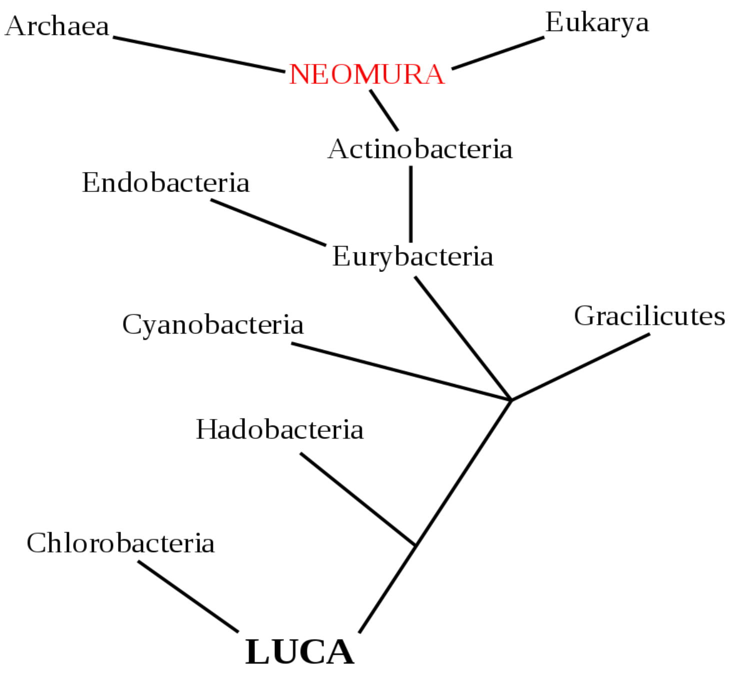
Of these concepts, the activity will include the construction on Phylogenetic Trees using DNA sequences of different organisms which are also available online, Analyzing protein structures described in .pdb files which are also available online and Translation process which involves creating a Protein in accordance with RNA which can be obtained from DNA.

The activity will open with a home screen where the user can choose between using the Phylogenetic Tree Construction and Protein Analysis modules.

This activity is aimed at students in and above the 10th grade who get an introduction to molecular biology and the concepts that I'm presenting.

2. Construction of Phylogenetic Trees

A phylogenetic tree is a tree showing evolutionary relationships between different species upon similarities and differences in their genetic characteristics.

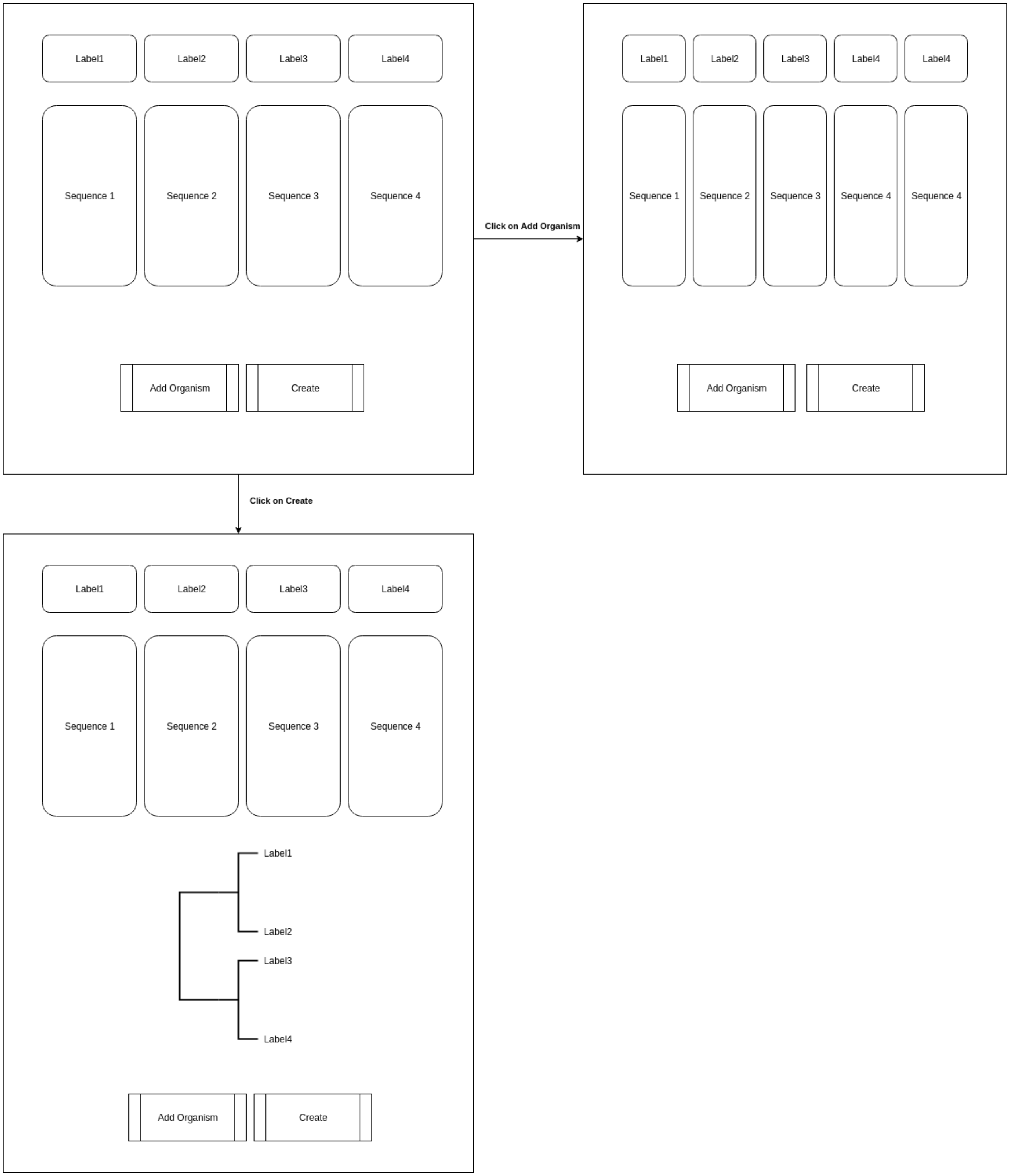


The DNA sequence of each known organism is comprised by repetition of four compounds namely Adenine, Guanine, Tyrosine and Cytosine which are simply known as A, G, T and C respectively. The DNA sequence for an organism can be represented as a string of A, T, G and Cs. For Example - The following string is the DNA sequence found in insulin in humans.

“ATGGCCCTGTGGATGCGCCTCCTGCCCCTGCTGGCGCTGCTGGCCCTCTGGGGACCTGACCCAGCCGCAGCCTTTGTGAACCAACACCTGTGCGGCTCACACCTGGTGGAAGCTCTCTACCTAGTGTGCGGGGAACGAGGCTTCTTCTACACACCCAAGACCCGCCGGGAGGCAGAGGACCTGCAGGTGGGGCAGGTGGAGCTGGGCGGGGGCCCTGGTGCAGGCAGCCTGCAGCCCTTGGCCCTGGAGGGGTCCCTGCAGAAGCGTGGCATTGTGGAACAATGCTGTACCAGCATCTGCTCCCTCTACCAGCTGGAGAACTACTGCAACTAG”

Using the DNA sequences input by the user along with a few DNA sequences kept as a part of the database in the activity I plan to construct a phylogenetic tree using a distance-matrix method called UPGMA (unweighted pair group method with arithmetic mean) which calculates the genetic distance from multiple sequence alignments. In UPGMA, at each step, we create a similarity/dissimilarity matrix to show how close/far two organisms are. We then combine the two closest organisms to form a higher level cluster. This is a link to a working example of the algorithm.

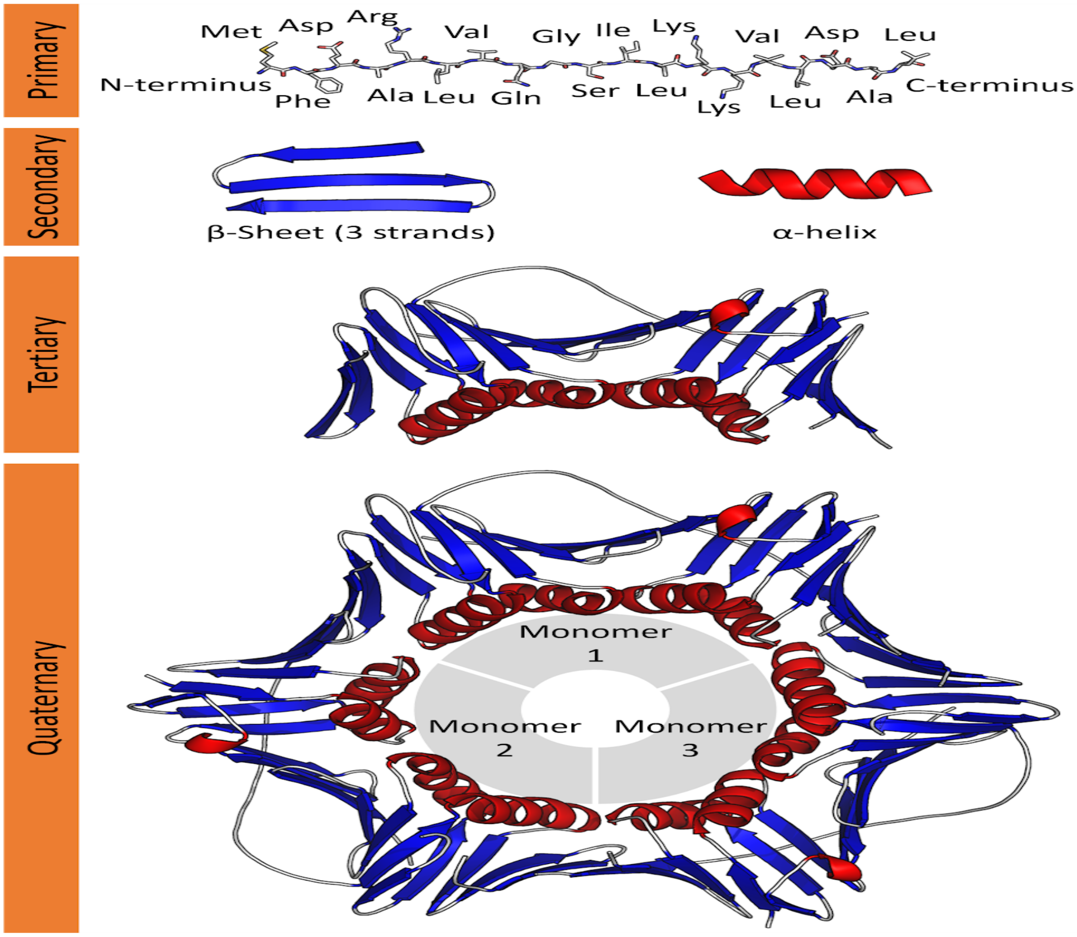
In the activity, there’ll be multiple text boxes along with labels in which the user can input the DNA sequences for different organisms along with their labels. On hitting the “Create” button, the activity will run UPGMA on the given sequences and construct the phylogenetic tree which will then be displayed on the screen. The following is a very basic model of what the layout would look like.


Label1
Label2
Label3
Label4
Sequence 1
Sequence 2
Sequence 3
Sequence 4
Add Organism
Create
Click on Add Organism
Label1
Label2
Label3
Label4
Label4
Sequence 1
Sequence 2
Sequence 3
Sequence 4
Sequence 4
Add Organism
Create
Click on Create
Label1
Label2
Label3
Label4
Sequence 1
Sequence 2
Sequence 3
Sequence 4
Label1
Label2
Label3
Label4
Add Organism
Create

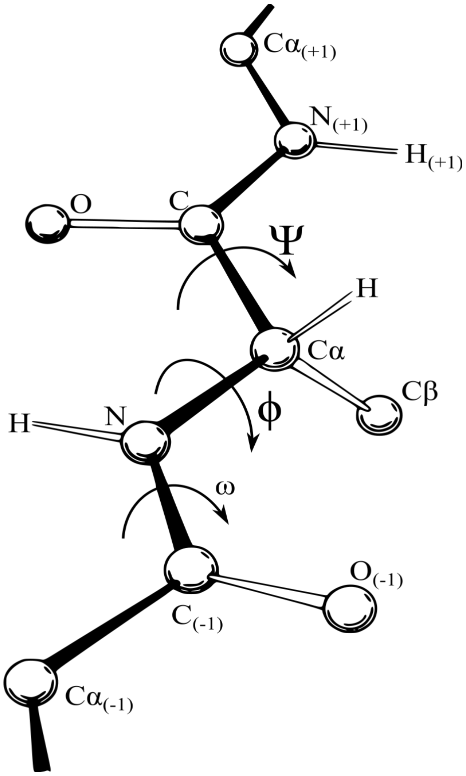
3. Protein Structures

The whole body of an organism is constituted by proteins and for any person working in practically any area of molecular biology, Proteins form some of the most interesting problems which still go unsolved. However, in spite of the fact that we can't make too many theoretical deductions, there are certain things that can be seen across different protein structures.

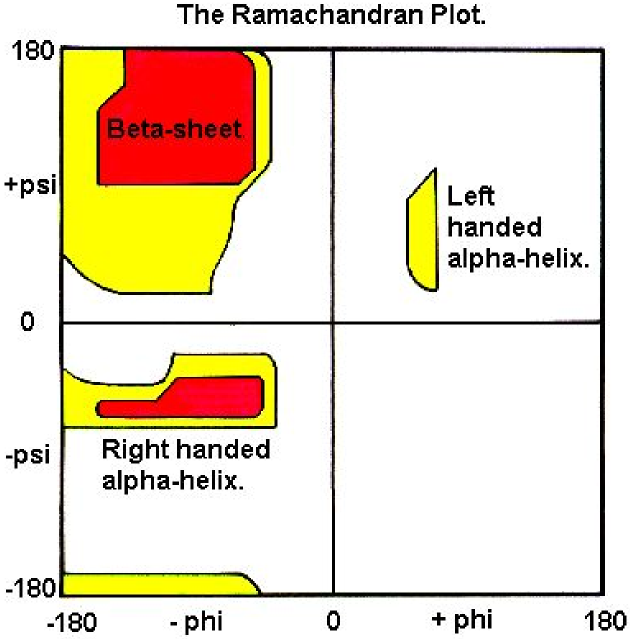
First off, we look at different kinds of protein structures -



The first of these being a pattern in dihedral angles for a protein which was first observed by G. N. Ramachandran, C. Ramakrishnan, and V. Sasisekharan using which they developed the Ramachandran Plot. The dihedral angles are named Φ, Ψ and ω.

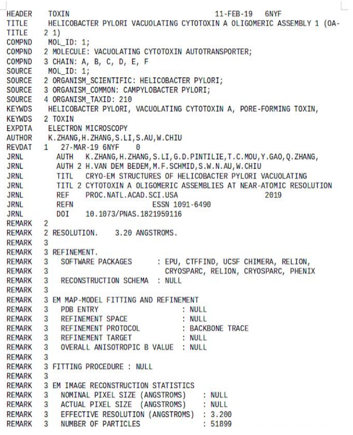


According to the plot, certain dihedral angles can exist only in specific secondary structures.



The description of different protein structures is openly available to all in the form of the Protein Data Bank(PDB) where each discovered protein has a unique code corresponding to which there exists a file which describes the position of all the atoms present in the protein.

These are a couple of screenshot of the PDB file for 6YNF -



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TITLE    2 1)
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: VACUOLATING CYTOTOXIN AUTOTRANSPORTER;
COMPND   3 CHAIN: A, B, C, D, E, F
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HELICOBACTER PYLORI;
SOURCE   3 ORGANISM_COMMON: CAMPYLOBACTER PYLORI;
SOURCE   4 ORGANISM_TAXID: 210
KEYWDS    HELICOBACTER PYLORI, VACUOLATING CYTOTOXIN A, PORE-FORMING TOXIN,
KEYWDS   2 TOXIN
EXPDTA    ELECTRON MICROSCOPY
AUTHOR    K.ZHANG,H.ZHANG,S.LI,S.AU,W.CHIU
REVDAT   1   27-MAR-19 6NYF    0
JRNL        AUTH   K.ZHANG,H.ZHANG,S.LI,G.D.PINTILIE,T.C.MOU,Y.GAO,Q.ZHANG,
JRNL        AUTH 2 H.VAN DEM BEDEM,M.F.SCHMID,S.W.N.AU,W.CHIU
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JRNL        TITL 2 CYTOTOXIN A OLIGOMERIC ASSEMBLIES AT NEAR-ATOMIC RESOLUTION
JRNL        REF    PROC.NATL.ACAD.SCI.USA                     2019
JRNL        REFN                   ESSN 1091-6490
JRNL        DOI    10.1073/PNAS.1821959116
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REMARK   2 RESOLUTION.    3.20 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
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REMARK   3                            CRYOSPARC, RELION, CRYOSPARC, PHENIX
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REMARK   3 FITTING PROCEDURE : NULL
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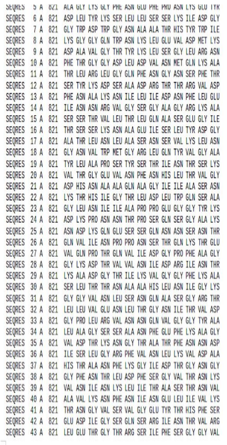

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SEQRES   9 A  821  ASP ALA VAL GLY THR TYR LYS LEU SER GLY LEU ARG ASN
SEQRES  10 A  821  PHE THR GLY GLY ASP LEU ASP VAL ASN MET GLN LYS ALA
SEQRES  11 A  821  THR LEU ARG LEU GLY GLN PHE ASN GLY ASN SER PHE THR
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SEQRES  30 A  821  SER LEU THR THR ASN ALA ALA HIS LEU ASN ILE GLY LYS
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SEQRES  33 A  821  GLY PRO LEU ARG VAL ASN ASN GLN VAL GLY GLY TYR ALA
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SEQRES  36 A  821  ILE SER LEU GLY ARG PHE VAL ASN LEU LYS VAL ASP ALA
SEQRES  37 A  821  HIS THR ALA ASN PHE LYS GLY ILE ASP THR GLY ASN GLY
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SEQRES  41 A  821  THR ASN GLY VAL SER VAL GLY GLU TYR THR HIS PHE SER
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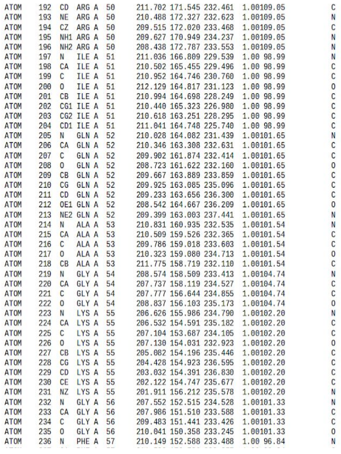

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```

My plan for the activity is that the user inputs the PDB code(in which case the activity will automatically fetch the file from the internet) for the protein or fetch it from a local file. Then the activity automatically opens the file and fetches data from it. This data will include the length of the protein molecule, the total number of chains present in the protein, ratio of the number of occurrences of a specific amino acid with the total number of amino acid residues, the ligand molecules in the protein and finally the dihedral angles at a few points in the structure and their position on the Ramachandran Plot to show that experimental data is in accordance with the hypothesis presented in the Plot.

4. Technologies Used
   - Language - Python
   - Framework for GUI - PyGtk+3
   - Framework for fetching PDB file - BeautifulSoup
   - Sugar Artworks

Timeline

Dates	Target
May 6 - May 27 (Community Bonding Period)	● Work with my mentor and the community in order to develop communication and find my way around the workings of the organisation. ● Setting up the repositories and creating the working environment. ● Researching and talking to the mentors and finding the best way to implement the features along with explaining the concepts used to the mentors.
May 28 - June 4 (Week 1)	● Creating the UI for the home screen which displays a menu for choosing between the different features in the activity. ● Connect each option with the required module which will be empty for now.

June 5 - June 12 (Week 2)	● Create the GUI for the Phylogenetic Tree Construction section of the activity including the textboxes, labels for each organism and buttons for adding an organism and Creating the tree. ● Connect the Create Tree button to the module in which UPGMA will be written. ● Write the logic for Adding a new label textbox and a DNA sequence textbox on pressing the Add Organism button.
June 13 - June 20 (Week 3)	● Implement the UPGMA module which will run the algorithm on the data input in the textboxes and construct the tree. ● Return the constructed tree to the parent module for drawing on the GUI.
June 21 - June 24 (Week 4)	● Implement the logic for drawing the tree on the canvas in a way which is most easily understandable by the user.
June 24 - June 28 (1st Evaluation)	● 1st Evaluation ○ Deliverable: A working GUI with working Phylogenetic Tree Construction with modules connected appropriately.
June 29 - July 6 (Week 5)	● Create a GUI for the Protein Structure Analysis module which will consist of a textbox which will take the PDB code for the protein. ● Also, add a browse button through which the user can open a local PDB file for analysis. ● Write a web scraping script which can fetch the PDB file according to the code provided from RCSB.
July 7 - July 14 (Week 6)	● Write the script for analyzing the protein file in order to fetch all the required data. ● Return the obtained data to the parent module for display to the user.
July 15 - July 22 (Week 7)	● Display the basic data to the user. ● Create the Ramachandran Plot on which I will plot some of the data points from the lost of dihedral angles.
July 22 - July 26 (2nd Evaluation)	● 2nd Evaluation ○ Deliverable: A standalone GUI with working modules for Phylogenetic Tree Construction,

	Protein Structure Analysis and seamless integration between the modules.
July 27 - August 3 (Week 8)	● Review the existing code for the first 3 days in order to find and fix bugs (if any). ● Conversion of Project to Sugar Activity which includes creating a toolbar and porting it to sugar.
August 4 - August 11 (Week 9)	● Testing and Code Review to check for bugs and if all use cases are being satisfied correctly. ● Use the Sugar Artwork to make the activity look like a part of the sugar environment.
August 12 - August 19 (Week 10)	● Test Run of the activity and fix bugs (if any). ● Final Code Review and writing the project report.
August 19 - August 26 (Final Submission)	● Final Evaluation: ○ Deliverables: Completed Activity -> BioShell along with the Project Report.
After August 26 (Post GSoC)	● Keep working on the activity to add more features and other sugar projects.

The time I will be Able to Give to The Project

I'll be able to give 30-35 hours a week of solid work to the project to create a neat and clean activity. I would also like to stay ahead of schedule so that I can research on how to improve the project while it is in progress and also work on other Sugar projects.

References

- Phylogenetic Tree Diagram - https://en.wikipedia.org/wiki/Phylogenetic_tree#/media/File:Neomuratree.svg
- UPGMA - https://en.wikipedia.org/wiki/UPGMA
- Protein Structures - https://en.wikipedia.org/wiki/File:Protein_structure_(full).png

- Dihedral Angle Diagram - https://en.wikipedia.org/wiki/Dihedral_angle#/media/File:Protein_backbone_PhiPsiOmega_drawing.svg
- Ramachandran Plot Diagram - http://www.cryst.bbk.ac.uk/PPS95/course/3_geometry/rama.gif
- 6YNF.pdb - https://www.rcsb.org/structure/6NYF