User Manual

Clone Git Repository

1. Open your terminal or command prompt.
2. Clone the repository using the following link:
   ```
   git clone
   https://github.com/meshi-m/3D-Data-Processing-In-Structural
   -Biology.git
   ```

Install Required Packages

Ensure you have the following Python packages installed. You can install them using `pip`:

```
pip install torch esm sklearn numpy pandas matplotlib scipy
```

(if installing esm won't work, try fair-esm)

Run the Program

1. Navigate to the cloned repository directory:
   ```
   cd 3D-Data-Processing-In-Structural-Biology/hackathon
   ```
2. Run the program:
   ```
   python esm_embeddings.py
   ```

Using the Program

When the program is running, you have two options:

1. **Enter a Peptide Sequence**: Type a peptide sequence into the terminal to get the prediction if positive or negative.
2. **Exit the Program**: Type `exit` to close the program.