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PROTEIN STRUCTURE AND FUNCTION

MEMBERS

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INTRODUCTION

A protein is a biological molecule made of amino acids that performs many functions in the body — like enzymes, hormones, and structural components. It is coded by DNA and has a sequence, a structure, and a function.

Relationship between biopython and protein: Biopython is a powerful Python library for;

Working with protein sequences (FASTA, UniProt). Analyzing 3D structures (PDB files).Extracting features like helices, sheets, motifsLinking to biological databases like UniProt, NCBI, PDB.

```
###basic example
!pip install biopython
```

```
Collecting biopython
  Downloading biopython-1.85-cp311-cp311-manylinux_2_17_x86_64.manylinux2014_x86
Requirement already satisfied: numpy in /usr/local/lib/python3.11/dist-packages
Downloading biopython-1.85-cp311-cp311-manylinux_2_17_x86_64.manylinux2014_x86_6
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 3.3/3.3 MB 35.0 MB/s eta 0:00
Installing collected packages: biopython
Successfully installed biopython-1.85
```

```
from Bio import SeqIO

record = SeqIO.read("/content/rcsb_pdb_1AEK.fasta", "fasta")
print("Protein ID:", record.id)
print("Sequence:", record.seq)
print("Length:", len(record.seq))
```

```
Protein ID: 1AEK_1|Chain
Sequence: MKTLVHVASVEKGRSYEDFQKVYNAIALKLREDDEYDNYIGYGPVLVRLAWHISGTWDKHDNTGGSYGGT
Length: 294
```

PROTEIN STRUCTURE AND FUNCTION

Proteins are essential biomolecules that perform a wide variety of functions within living organisms, including catalyzing biochemical reactions, providing structural support, and facilitating cellular communication. Understanding the structure and function of proteins is crucial for fields such as bioinformatics, molecular biology, and drug design. Biopython, a powerful open-source bioinformatics library in Python, provides tools to retrieve, analyze, and visualize protein sequences and structures.

PARSE AND PDB FILE: The Protein Data Bank (PDB) file format is a widely used standard for representing 3D structures of proteins and other biological macromolecules. These files contain detailed atomic-level information about the spatial arrangement of atoms in a protein, including coordinates, chains, residues, and more. In Biopython, the Bio.PDB module allows users to parse PDB files and extract structural information efficiently. Parsing a PDB file means reading its content and converting it into a structured format that can be analyzed programmatically.

Steps involves in protein structure and function:

I) adding code to the structure

```
from Bio.PDB import PDBList, PDBParser

# Download structure
pdb_id = "1AKE"
pdbl = PDBList()
pdbl.retrieve_pdb_file(pdb_id, pdir='.', file_format='pdb')

# Parse the structure
parser = PDBParser()
structure = parser.get_structure(pdb_id, f"pdb{pdb_id.lower()}.ent")

# View basic info
print(f"Structure ID: {structure.id}")
for model in structure:
    print(f"Model ID: {model.id}")
```

```
    for chain in model:
        print(f"Chain ID: {chain.id}")
```

```
Downloading PDB structure '1ake'...
Structure ID: 1AKE
Model ID: 0
Chain ID: A
Chain ID: B
/usr/local/lib/python3.11/dist-packages/Bio/PDB/StructureBuilder.py:100: PDBCons
  warnings.warn(
/usr/local/lib/python3.11/dist-packages/Bio/PDB/StructureBuilder.py:100: PDBCons
  warnings.warn(
/usr/local/lib/python3.11/dist-packages/Bio/PDB/StructureBuilder.py:100: PDBCons
  warnings.warn(
/usr/local/lib/python3.11/dist-packages/Bio/PDB/StructureBuilder.py:100: PDBCons
  warnings.warn(
```

II) listing of residue and atom

```
for model in structure:
    for chain in model:
        for residue in chain:
            print(f"Residue: {residue.resname} {residue.id}")
            for atom in residue:
                print(f"  Atom: {atom.name}, Coord: {atom.coord}")
```

```
Residue: MET (' ', 1, ' ')
  Atom: N, Coord: [26.981 53.977 40.085]
  Atom: CA, Coord: [26.091 52.849 39.889]
  Atom: C, Coord: [26.679 52.163 38.675]
  Atom: O, Coord: [27.02  52.865 37.715]
  Atom: CB, Coord: [24.677 53.31  39.58 ]
  Atom: CG, Coord: [23.624 52.189 39.442]
  Atom: SD, Coord: [21.917 52.816 39.301]
  Atom: CE, Coord: [21.93  53.926 37.91 ]
Residue: ARG (' ', 2, ' ')
  Atom: N, Coord: [26.861 50.841 38.803]
  Atom: CA, Coord: [27.437 49.969 37.786]
  Atom: C, Coord: [26.336 48.959 37.429]
  Atom: O, Coord: [25.745 48.313 38.312]
  Atom: CB, Coord: [28.653 49.266 38.349]
  Atom: CG, Coord: [29.87  50.188 38.416]
  Atom: CD, Coord: [31.033 49.532 39.173]
  Atom: NE, Coord: [32.318 50.244 39.125]
  Atom: CZ, Coord: [33.462 49.75  39.679]
  Atom: NH1, Coord: [33.522 48.572 40.308]
  Atom: NH2, Coord: [34.61  50.427 39.597]
Residue: ILE (' ', 3, ' ')
  Atom: N, Coord: [26.039 48.836 36.139]
  Atom: CA, Coord: [24.961 47.988 35.671]
  Atom: C, Coord: [25.374 47.08  34.537]
  Atom: O, Coord: [26.029 47.614 33.642]
  Atom: CB, Coord: [23.802 48.88  35.202]
  Atom: CG1, Coord: [23.317 49.724 36.378]
```

```
      Atom: CG2, Coord: [22.66  48.01  34.642]
      Atom: CD1, Coord: [22.436 50.89  35.992]
    Residue: ILE (' ', 4, ' ')
      Atom: N, Coord: [25.062 45.774 34.541]
      Atom: CA, Coord: [25.194 44.925 33.36 ]
      Atom: C, Coord: [23.804 44.715 32.751]
      Atom: O, Coord: [22.824 44.536 33.484]
      Atom: CB, Coord: [25.789 43.561 33.72 ]
      Atom: CG1, Coord: [27.206 43.753 34.233]
      Atom: CG2, Coord: [25.829 42.65  32.463]
      Atom: CD1, Coord: [27.967 42.486 34.621]
    Residue: LEU (' ', 5, ' ')
      Atom: N, Coord: [23.655 44.874 31.424]
      Atom: CA, Coord: [22.428 44.503 30.712]
      Atom: C, Coord: [22.668 43.134 30.012]
      Atom: O, Coord: [23.614 42.932 29.232]
      Atom: CB, Coord: [22.088 45.547 29.675]
      Atom: CG, Coord: [22.076 47.021 30.069]
      Atom: CD1, Coord: [21.735 47.848 28.817]
      Atom: CD2, Coord: [21.088 47.249 31.193]
    Residue: LEU (' ', 6, ' ')
      Atom: N, Coord: [21.787 42.178 30.248]
      Atom: CA, Coord: [21.933 40.811 29.752]
      Atom: C, Coord: [20.711 40.529 28.87 ]
      Atom: O, Coord: [19.602 40.977 29.22 ]
      Atom: CB, Coord: [21.919 39.891 30.945]
      Atom: CG, Coord: [22.847 38.789 31.103]
      Atom: CD1, Coord: [24.254 39.345 31.21 ]
      Atom: CD2, Coord: [22.465 38.042 32.355]
    Residue: GLY (' ', 7, ' ')
```

III) Distance between two atoms

```
from Bio.PDB import NeighborSearch

atoms = list(structure.get_atoms())
ns = NeighborSearch(atoms)

# Example: find atoms within 5Å of a chosen atom
close_atoms = ns.search(atom.coord, 5.0)
print(f"Nearby atoms: {len(close_atoms)}")
```

```
Nearby atoms: 6
```

IV) stability, solubility and potential environment

```
from Bio.SeqUtils import ProtParam
from Bio.PDB.Polypeptide import PPBuilder

ppb = PPBuilder()
for pp in ppb.build_peptides(structure):
    seq = pp.get_sequence()
    print("Sequence:", seq)
```

```
    analysis = ProtParam.ProteinAnalysis(str(seq))
    print("Molecular weight:", analysis.molecular_weight())
    print("Aromaticity:", analysis.aromaticity())
    print("Instability index:", analysis.instability_index())
```

```
Sequence: MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
Molecular weight: 23585.735300000008
Aromaticity: 0.05607476635514019
Instability index: 19.56355140186915
Sequence: MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKE
Molecular weight: 23585.735300000008
Aromaticity: 0.05607476635514019
Instability index: 19.56355140186915
```

ALPHA HELICES, BETA SHEETS AND MOTIFS:

1. *Alpha Helix (α-Helix)*:
    - A spiral structure stabilized by hydrogen bonds between amino acids.
    - Common in proteins, contributing to stability and function.
2. *Beta Sheets (β-Sheets)*:
    - Flat, pleated structures formed by beta strands connected by hydrogen bonds.
    - Can be parallel or antiparallel, influencing protein stability.
3. *Motifs*:
    - Short, conserved sequences or structures with specific functions.
    - Examples include zinc fingers (DNA binding) and beta barrels (membrane proteins).

```
!Sudo apt install dssp
```

```
/bin/bash: line 1: Sudo: command not found
```

```
!brew install dssp
```

```
/bin/bash: line 1: brew: command not found
```

```
dssp = {}  # Define dssp as an empty dictionary
alpha_helices = []
beta_sheets = []

# Now you can populate dssp with your data
# For example:
dssp[('A', (1, 'ALA'))] = ['atom', 'A', 'H']
dssp[('A', (2, 'GLY'))] = ['atom', 'G', 'E']

for key, value in dssp.items():
    chain_id = key[0]
    residue_number = key[1][0]  # Assuming key[1] is a tuple with residue number first
```

```
    aa = value[1]  # Single-letter amino acid code
    ss = value[2]  # Secondary structure

    if ss == 'H':
        alpha_helices.append((chain_id, residue_number, aa))
    elif ss == 'E':
        beta_sheets.append((chain_id, residue_number, aa))

print("Alpha helices:", alpha_helices)
print("Beta sheets:", beta_sheets)
```

```
Alpha helices: [('A', 1, 'A')]
Beta sheets: [('A', 2, 'G')]
```

```
from itertools import groupby
from operator import itemgetter

def group_consecutive(residues):
    groups = []
    for k, g in groupby(enumerate(residues), lambda x: x[0] - x[1][0]):
        group = list(map(itemgetter(1), g))
        groups.append(group)
    return groups

# Extract just positions
helix_positions = [res[0] for res in alpha_helices]
sheet_positions = [res[0] for res in beta_sheets]

# Group them
helix_groups = group_consecutive(list(enumerate(helix_positions)))
sheet_groups = group_consecutive(list(enumerate(sheet_positions)))

# Print motif segments
print("\nAlpha Helix Segments:")
for group in helix_groups:
    print(group)

print("\nBeta Sheet Segments:")
for group in sheet_groups:
    print(group)
```

```
Alpha Helix Segments:
[(0, 'A')]

Beta Sheet Segments:
[(0, 'A')]
```

SEQUENCE WITH 3D STRUCTURE

Key aspects:

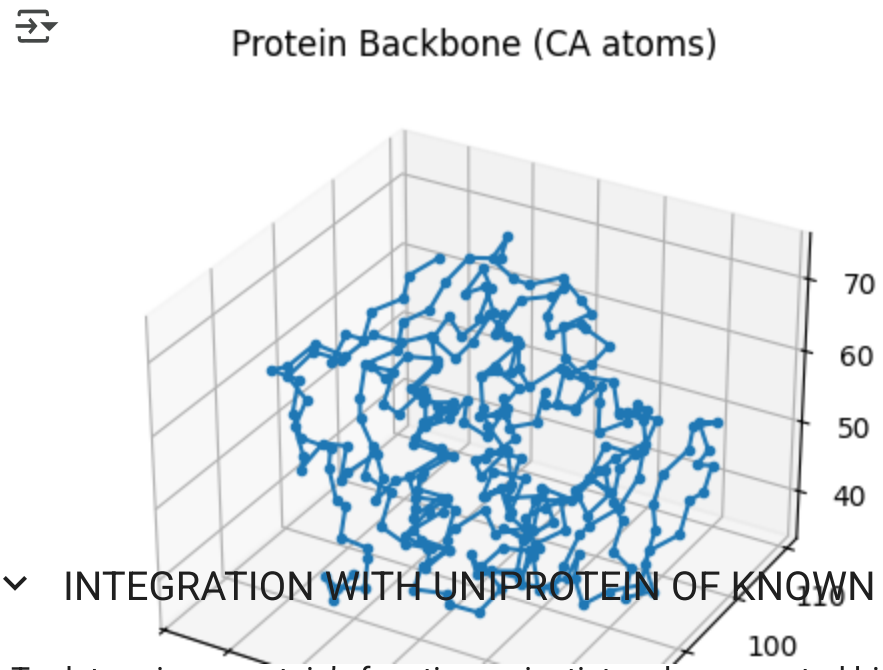
1. *PDB files*: Contain atomic coordinates for proteins.
2. *BioPython's PDB module*: Parse PDB files, extract data, and analyze structures.
3. *Structure visualization*: Use libraries like Matplotlib or PyMOL for 3D visualization.

```
from Bio.PDB import PDBParser
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

# Load structure and get CA atoms
parser = PDBParser()
structure = parser.get_structure("protein", "/content/1aek (3).pdb")
ca_atoms = [atom for atom in structure.get_atoms() if atom.name == 'CA']

# Extract coordinates
coords = [atom.coord for atom in ca_atoms]
x, y, z = zip(*coords)

# Create 3D plot
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.plot(x, y, z, 'o-', markersize=3)
ax.set_title("Protein Backbone (CA atoms)")
plt.show()
```



INTEGRATION WITH UNIPROTEIN OF KNOWN FUNCTION

To determine a protein's function, scientists rely on curated biological databases. UniProt (Universal Protein Resource) is one of the most comprehensive and reliable protein databases available. It provides detailed information on protein sequences, functions, structures, domains, and evolutionary data. Providing a detailed functional description of the protein, Listing biological processes it's involved in, Showing its subcellular location, structure, and sequence, Linking to experimental data, literature, and 3D models.

```
import requests

uniprot_id = "P00519"  # or your protein's UniProt ID
url = f"https://rest.uniprot.org/uniprotkb/{uniprot_id}.json"

response = requests.get(url)
data = response.json()
```

```
# Function info path
function_info = data["comments"]

for comment in function_info:
    if comment["commentType"] == "FUNCTION":
        print("Function:", comment["texts"][0]["value"])
```

```
Function: Non-receptor tyrosine-protein kinase that plays a role in many key pro
```

```
!pip install nglview==3.0.8
```

```
Collecting nglview==3.0.8
  Downloading nglview-3.0.8.tar.gz (6.8 MB)
     ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 6.8/6.8 MB 35.0 MB/s eta 0:
  Installing build dependencies ... done
  Getting requirements to build wheel ... done
  Preparing metadata (pyproject.toml) ... done
Requirement already satisfied: ipywidgets>=7 in /usr/local/lib/python3.11/dist-p
Requirement already satisfied: jupyterlab_widgets in /usr/local/lib/python3.11/d
Requirement already satisfied: numpy in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: ipykernel>=4.5.1 in /usr/local/lib/python3.11/dis
Requirement already satisfied: ipython-genutils~=0.2.0 in /usr/local/lib/python3
Requirement already satisfied: traitlets>=4.3.1 in /usr/local/lib/python3.11/dis
Requirement already satisfied: widgetsnbextension~=3.6.0 in /usr/local/lib/pytho
Requirement already satisfied: ipython>=4.0.0 in /usr/local/lib/python3.11/dist-
Requirement already satisfied: debugpy>=1.0 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: jupyter-client>=6.1.12 in /usr/local/lib/python3.
Requirement already satisfied: matplotlib-inline>=0.1 in /usr/local/lib/python3.
Requirement already satisfied: nest-asyncio in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: packaging in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: psutil in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: pyzmq>=17 in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: tornado>=6.1 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: setuptools>=18.5 in /usr/local/lib/python3.11/dis
Collecting jedi>=0.16 (from ipython>=4.0.0->ipywidgets>=7->nglview==3.0.8)
  Downloading jedi-0.19.2-py2.py3-none-any.whl.metadata (22 kB)
Requirement already satisfied: decorator in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: pickleshare in /usr/local/lib/python3.11/dist-pac
Requirement already satisfied: prompt-toolkit!=3.0.0,!=3.0.1,<3.1.0,>=2.0.0 in /
Requirement already satisfied: pygments in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: backcall in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: pexpect>4.3 in /usr/local/lib/python3.11/dist-pac
Requirement already satisfied: notebook>=4.4.1 in /usr/local/lib/python3.11/dist
Requirement already satisfied: parso<0.9.0,>=0.8.4 in /usr/local/lib/python3.11/
Requirement already satisfied: jupyter-core>=4.6.0 in /usr/local/lib/python3.11/
Requirement already satisfied: python-dateutil>=2.1 in /usr/local/lib/python3.11
Requirement already satisfied: jinja2 in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: argon2-cffi in /usr/local/lib/python3.11/dist-pac
Requirement already satisfied: nbformat in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: nbconvert>=5 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: Send2Trash>=1.8.0 in /usr/local/lib/python3.11/di
Requirement already satisfied: terminado>=0.8.3 in /usr/local/lib/python3.11/dis
Requirement already satisfied: prometheus-client in /usr/local/lib/python3.11/di
Requirement already satisfied: nbclassic>=0.4.7 in /usr/local/lib/python3.11/dis
Requirement already satisfied: ptyprocess>=0.5 in /usr/local/lib/python3.11/dist
```

```
Requirement already satisfied: wcwidth in /usr/local/lib/python3.11/dist-package
Requirement already satisfied: platformdirs>=2.5 in /usr/local/lib/python3.11/di
Requirement already satisfied: notebook-shim>=0.2.3 in /usr/local/lib/python3.11
Requirement already satisfied: beautifulsoup4 in /usr/local/lib/python3.11/dist-
Requirement already satisfied: bleach!=5.0.0 in /usr/local/lib/python3.11/dist-p
Requirement already satisfied: defusedxml in /usr/local/lib/python3.11/dist-pack
Requirement already satisfied: jupyterlab-pygments in /usr/local/lib/python3.11/
Requirement already satisfied: markupsafe>=2.0 in /usr/local/lib/python3.11/dist
Requirement already satisfied: mistune<4,>=2.0.3 in /usr/local/lib/python3.11/di
Requirement already satisfied: nbclient>=0.5.0 in /usr/local/lib/python3.11/dist
Requirement already satisfied: pandocfilters>=1.4.1 in /usr/local/lib/python3.11
Requirement already satisfied: fastjsonschema>=2.15 in /usr/local/lib/python3.11
Requirement already satisfied: jsonschema>=2.6 in /usr/local/lib/python3.11/dist
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.11/dist-packag
```

```
!pip install bio
```

```
Collecting bio
  Downloading bio-1.8.0-py3-none-any.whl.metadata (5.7 kB)
Requirement already satisfied: biopython>=1.80 in /usr/local/lib/python3.11/dist
Collecting gprofiler-official (from bio)
  Downloading gprofiler_official-1.0.0-py3-none-any.whl.metadata (11 kB)
Collecting mygene (from bio)
  Downloading mygene-3.2.2-py2.py3-none-any.whl.metadata (10 kB)
Requirement already satisfied: pandas in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: pooch in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: requests in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: tqdm in /usr/local/lib/python3.11/dist-packages (
Requirement already satisfied: numpy in /usr/local/lib/python3.11/dist-packages
Collecting biothings-client>=0.2.6 (from mygene->bio)
  Downloading biothings_client-0.4.1-py3-none-any.whl.metadata (10 kB)
Requirement already satisfied: python-dateutil>=2.8.2 in /usr/local/lib/python3.
Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: tzdata>=2022.7 in /usr/local/lib/python3.11/dist-
Requirement already satisfied: platformdirs>=2.5.0 in /usr/local/lib/python3.11/
Requirement already satisfied: packaging>=20.0 in /usr/local/lib/python3.11/dist
Requirement already satisfied: charset-normalizer<4,>=2 in /usr/local/lib/python
Requirement already satisfied: idna<4,>=2.5 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: urllib3<3,>=1.21.1 in /usr/local/lib/python3.11/d
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.11/d
Requirement already satisfied: httpx>=0.22.0 in /usr/local/lib/python3.11/dist-p
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: anyio in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: httpcore==1.* in /usr/local/lib/python3.11/dist-p
Requirement already satisfied: h11>=0.16 in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: sniffio>=1.1 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: typing_extensions>=4.5 in /usr/local/lib/python3.
Downloading bio-1.8.0-py3-none-any.whl (321 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 321.1/321.1 kB 6.0 MB/s eta 0
Downloading gprofiler_official-1.0.0-py3-none-any.whl (9.3 kB)
Downloading mygene-3.2.2-py2.py3-none-any.whl (5.4 kB)
Downloading biothings_client-0.4.1-py3-none-any.whl (46 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 46.7/46.7 kB 2.7 MB/s eta 0:0
Installing collected packages: gprofiler-official, biothings-client, mygene, bio
Successfully installed bio-1.8.0 biothings-client-0.4.1 gprofiler-official-1.0.0
```

```
!pip install "ipywidgets>=7,<8"
```

```
Requirement already satisfied: ipywidgets<8,>=7 in /usr/local/lib/python3.11/dis
Requirement already satisfied: ipykernel>=4.5.1 in /usr/local/lib/python3.11/dis
Requirement already satisfied: ipython-genutils~=0.2.0 in /usr/local/lib/python3
Requirement already satisfied: traitlets>=4.3.1 in /usr/local/lib/python3.11/dis
Requirement already satisfied: widgetsnbextension~=3.6.0 in /usr/local/lib/pytho
Requirement already satisfied: ipython>=4.0.0 in /usr/local/lib/python3.11/dist-
Requirement already satisfied: jupyterlab-widgets>=1.0.0 in /usr/local/lib/pytho
Requirement already satisfied: debugpy>=1.0 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: jupyter-client>=6.1.12 in /usr/local/lib/python3.
Requirement already satisfied: matplotlib-inline>=0.1 in /usr/local/lib/python3.
Requirement already satisfied: nest-asyncio in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: packaging in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: psutil in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: pyzmq>=17 in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: tornado>=6.1 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: setuptools>=18.5 in /usr/local/lib/python3.11/dis
Requirement already satisfied: jedi>=0.16 in /usr/local/lib/python3.11/dist-pack
Requirement already satisfied: decorator in /usr/local/lib/python3.11/dist-packa
Requirement already satisfied: pickleshare in /usr/local/lib/python3.11/dist-pac
Requirement already satisfied: prompt-toolkit!=3.0.0,!=3.0.1,<3.1.0,>=2.0.0 in /
Requirement already satisfied: pygments in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: backcall in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: pexpect>4.3 in /usr/local/lib/python3.11/dist-pac
Requirement already satisfied: notebook>=4.4.1 in /usr/local/lib/python3.11/dist
Requirement already satisfied: parso<0.9.0,>=0.8.4 in /usr/local/lib/python3.11/
Requirement already satisfied: jupyter-core>=4.6.0 in /usr/local/lib/python3.11/
Requirement already satisfied: python-dateutil>=2.1 in /usr/local/lib/python3.11
Requirement already satisfied: jinja2 in /usr/local/lib/python3.11/dist-packages
Requirement already satisfied: argon2-cffi in /usr/local/lib/python3.11/dist-pac
Requirement already satisfied: nbformat in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: nbconvert>=5 in /usr/local/lib/python3.11/dist-pa
Requirement already satisfied: Send2Trash>=1.8.0 in /usr/local/lib/python3.11/di
Requirement already satisfied: terminado>=0.8.3 in /usr/local/lib/python3.11/dis
Requirement already satisfied: prometheus-client in /usr/local/lib/python3.11/di
Requirement already satisfied: nbclassic>=0.4.7 in /usr/local/lib/python3.11/dis
Requirement already satisfied: ptyprocess>=0.5 in /usr/local/lib/python3.11/dist
Requirement already satisfied: wcwidth in /usr/local/lib/python3.11/dist-package
Requirement already satisfied: platformdirs>=2.5 in /usr/local/lib/python3.11/di
Requirement already satisfied: notebook-shim>=0.2.3 in /usr/local/lib/python3.11
Requirement already satisfied: beautifulsoup4 in /usr/local/lib/python3.11/dist-
Requirement already satisfied: bleach!=5.0.0 in /usr/local/lib/python3.11/dist-p
Requirement already satisfied: defusedxml in /usr/local/lib/python3.11/dist-pack
Requirement already satisfied: jupyterlab-pygments in /usr/local/lib/python3.11/
Requirement already satisfied: markupsafe>=2.0 in /usr/local/lib/python3.11/dist
Requirement already satisfied: mistune<4,>=2.0.3 in /usr/local/lib/python3.11/di
Requirement already satisfied: nbclient>=0.5.0 in /usr/local/lib/python3.11/dist
Requirement already satisfied: pandocfilters>=1.4.1 in /usr/local/lib/python3.11
Requirement already satisfied: fastjsonschema>=2.15 in /usr/local/lib/python3.11
Requirement already satisfied: jsonschema>=2.6 in /usr/local/lib/python3.11/dist
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.11/dist-packag
Requirement already satisfied: argon2-cffi-bindings in /usr/local/lib/python3.11
```

```
    Requirement already satisfied: webencodings in /usr/local/lib/python3.11/dist-pa
    Requirement already satisfied: tinycss2<1.5,>=1.1.0 in /usr/local/lib/python3.11
    Requirement already satisfied: attrs>=22.2.0 in /usr/local/lib/python3.11/dist-p
    Requirement already satisfied: jsonschema-specifications>=2023.03.6 in /usr/loca
    Requirement already satisfied: referencing>=0.28.4 in /usr/local/lib/python3.11/
    Requirement already satisfied: rpds-py>=0.7.1 in /usr/local/lib/python3.11/dist-
    Requirement already satisfied: jupyter-server<3,>=1.8 in /usr/local/lib/python3.
```

```
!jupyter-nbextension enable nglview --py --sys-prefix
```

```
Enabling notebook extension nglview-js-widgets/extension...
    Paths used for configuration of notebook:
            /usr/etc/jupyter/nbconfig/notebook.json
    Paths used for configuration of notebook:

          - Validating: OK
    Paths used for configuration of notebook:
            /usr/etc/jupyter/nbconfig/notebook.json
```

```
from Bio.PDB import PDBParser

parser = PDBParser()
structure = parser.get_structure("1AKE", "/content/1aek (3).pdb")
```

```
import nglview as nv
```

```

```

```
view=nv.show_biopython (structure)
```

```
view
```

```
NGLWidget()
```

CONCLUSION

Understanding the structure and function of proteins is fundamental to modern biology, biotechnology, and medicine. A protein's three-dimensional (3D) structure directly influences how it interacts with other molecules and performs its biological functions. Through computational tools and databases like Biopython, DSSP, and UniProt, we can analyze protein sequences, predict or explore secondary structures (such as alpha helices and beta sheets), and annotate functions.

In conclusion, the combination of sequence analysis, structural modeling, and functional annotation provides a powerful framework for exploring proteins, helping us decode their roles in complex biological systems.