Université Paris Cité

ASSIGNMENT AND DETECTION OF TRANSMEMBRANE PARTS OF A PROTEIN

PROJECT REPORT - 2022 - MASTER BIO-INFORMATICS

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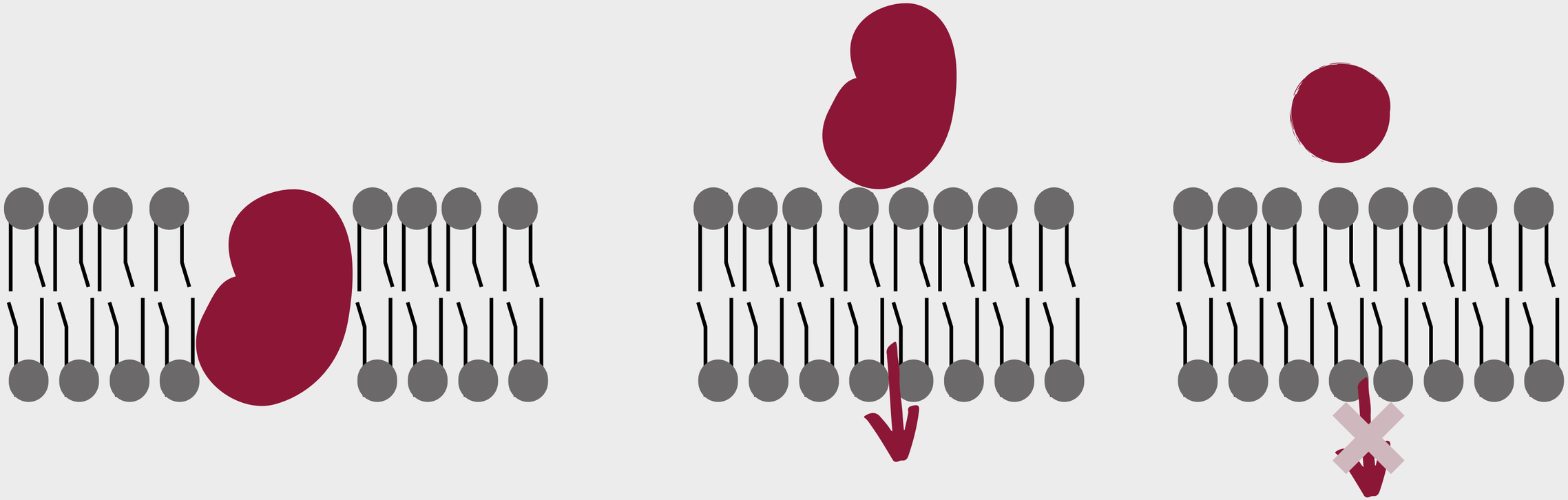
Transmembrane protein



Missing information on the lipid bilayer

- Made w/ detergent
- Position of the membrane

Environment

- Aqueous environment
- w/ detergent

Size

- TMP are larger
- Determine by NMR

Crystallisation

Building an algorithm

detects transmembrane part
predicts membrane position

Algorithm main steps

Calculate accessibility score

Using DSSP

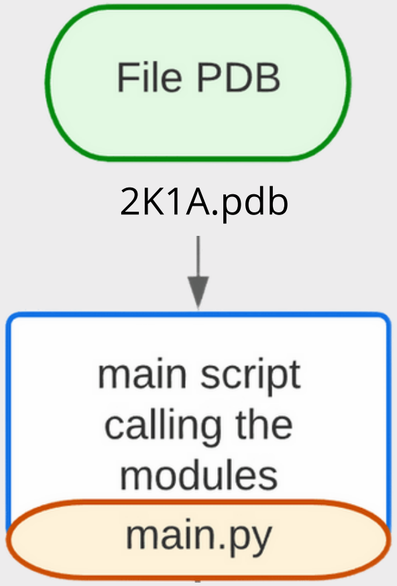
Recovering solvent-accessible AC

Scanning the protein

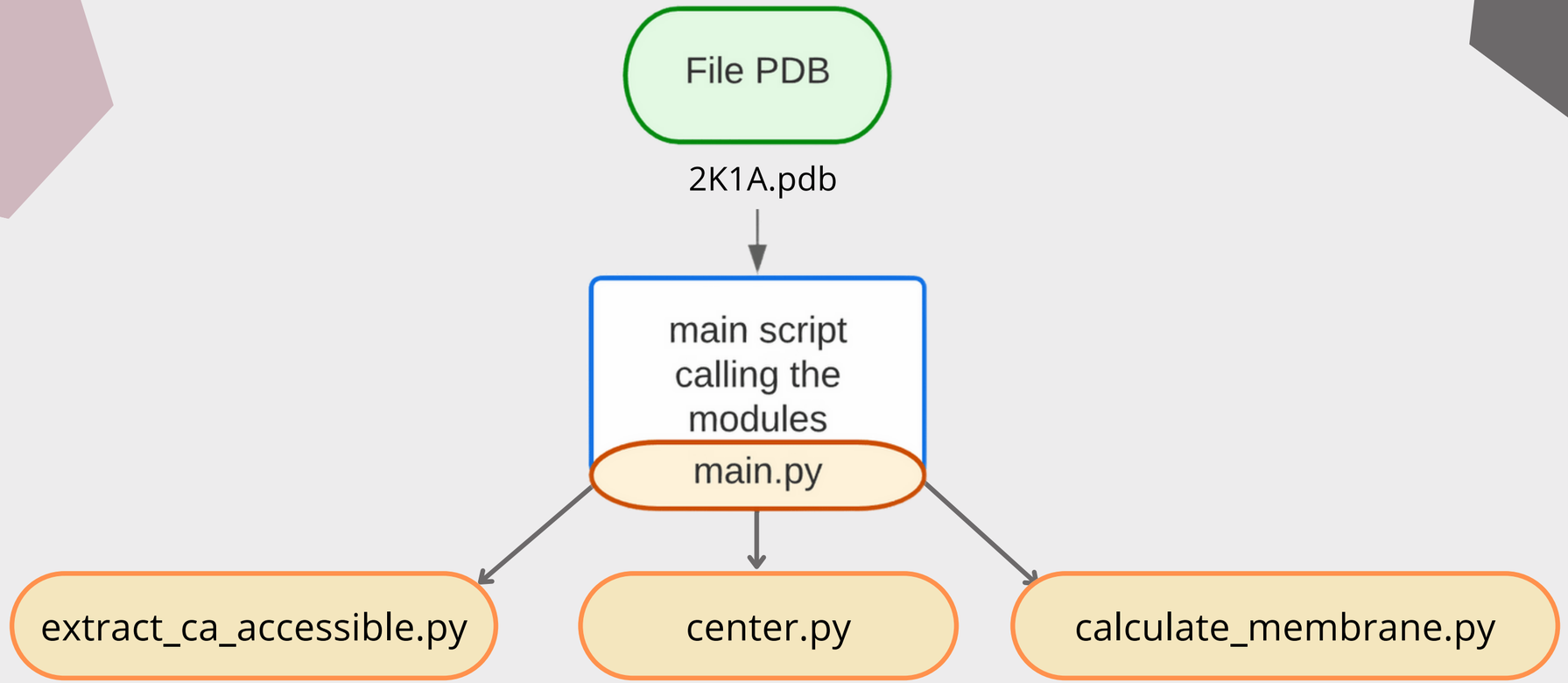
Via a sphere

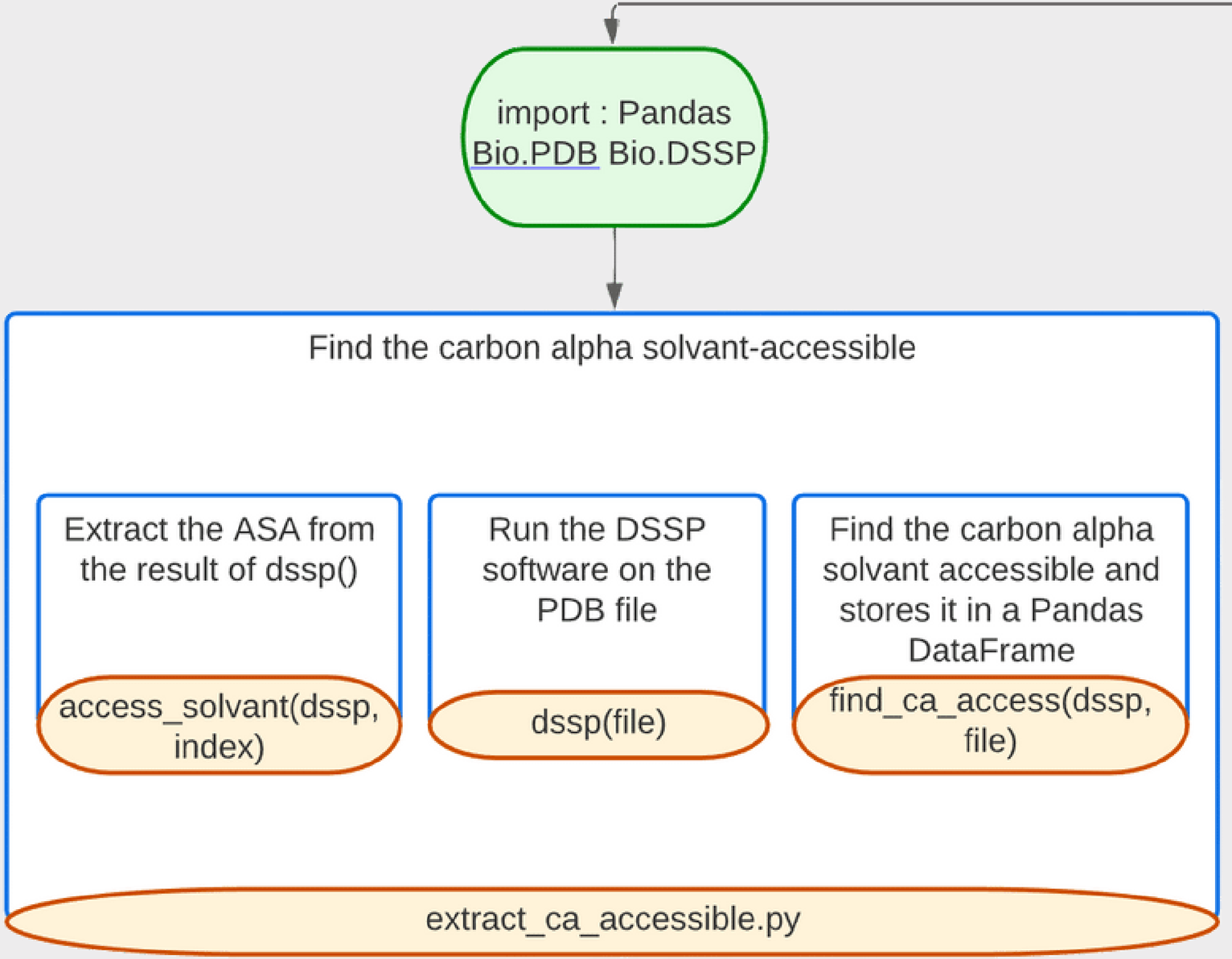
Predicting the position of the membrane

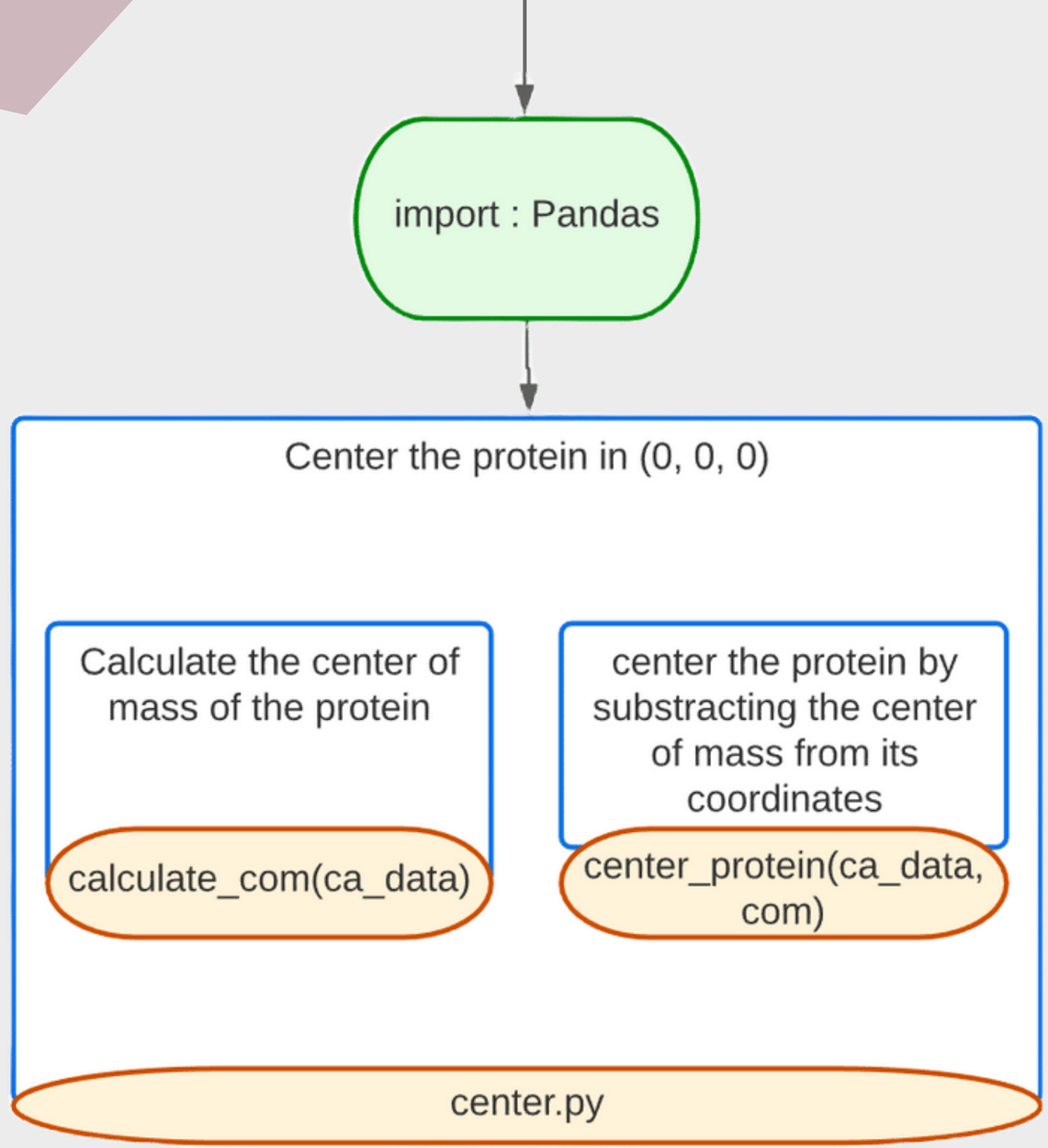
With a score

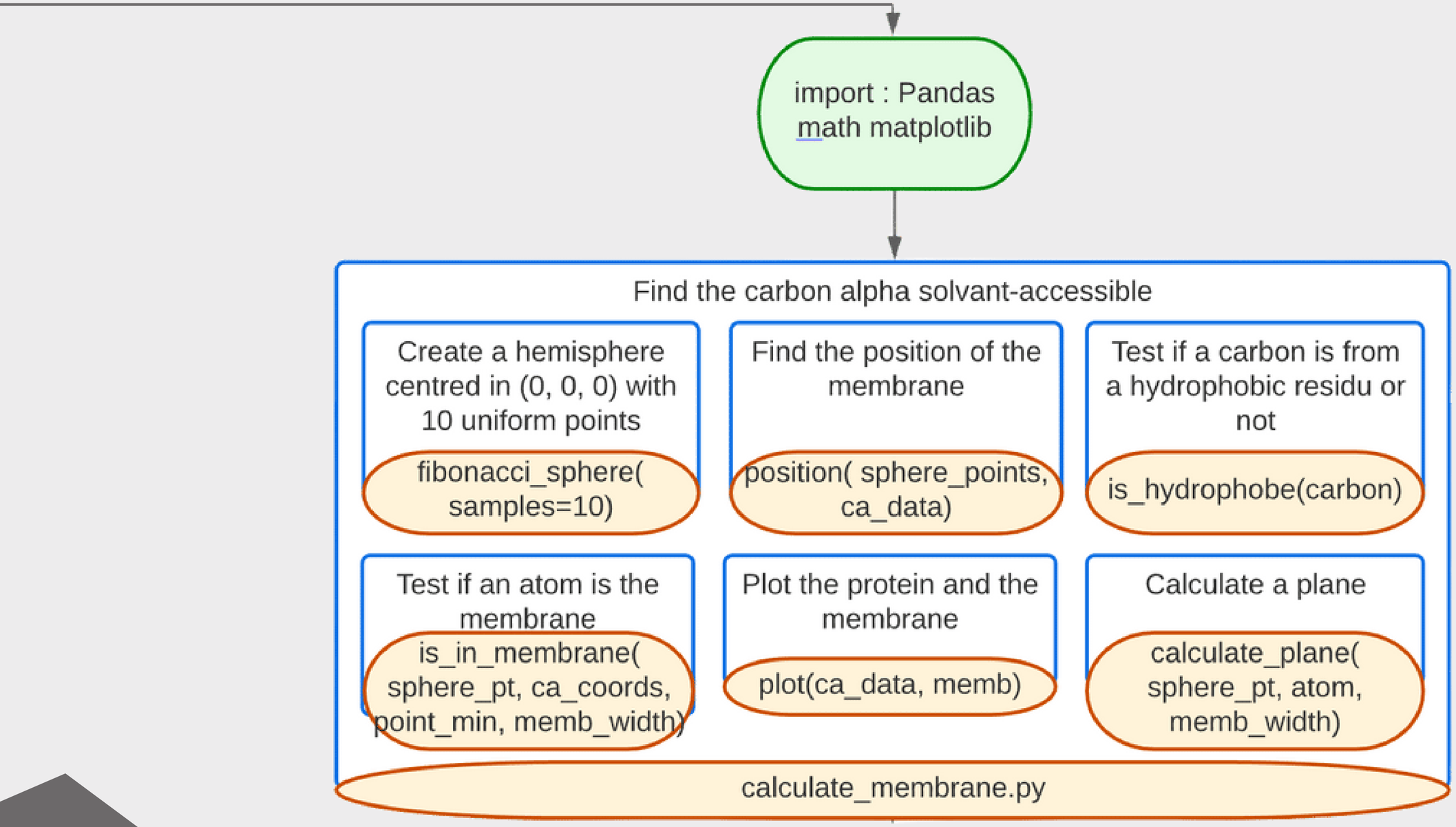


python3 src/main.py data/2k1a.pdb

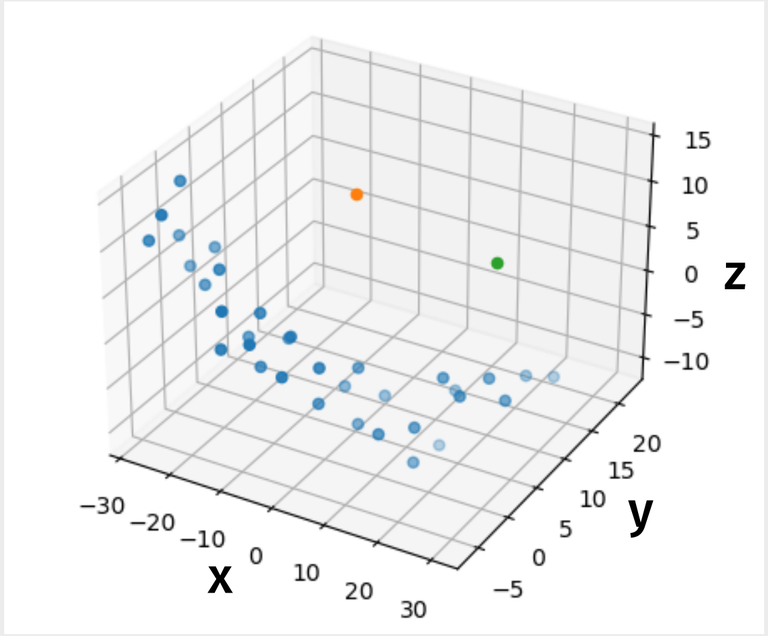

File PDB
2K1A.pdb
main script calling the modules
main.py
extract_ca_accessible.py
center.py
calculate_membrane.py

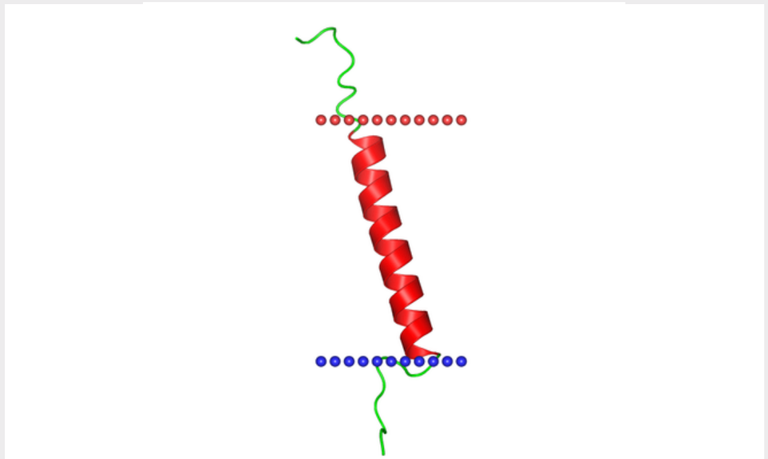

import : Pandas Bio.PDB Bio.DSSP
Find the carbon alpha solvant-accessible
Extract the ASA from the result of dssp()
access_solvant(dssp, index)
Run the DSSP software on the PDB file
dssp(file)
Find the carbon alpha solvant accessible and stores it in a Pandas DataFrame
find_ca_access(dssp, file)
extract_ca_accessible.py


import : Pandas
Center the protein in (0, 0, 0)
Calculate the center of mass of the protein
calculate_com(ca_data)
center the protein by substracting the center of mass from its coordinates
center_protein(ca_data, com)
center.py

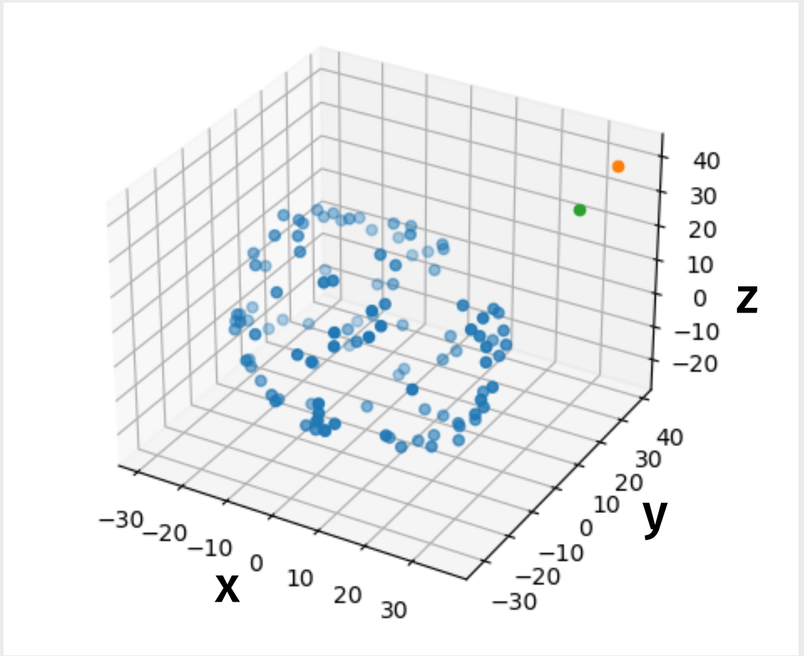

import : Pandas
math matplotlib
Find the carbon alpha solvant-accessible
Create a hemisphere centred in (0, 0, 0) with 10 uniform points
fibonacci_sphere(samples=10)
Find the position of the membrane
position(sphere_points, ca_data)
Test if a carbon is from a hydrophobic residu or not
is_hydrophobe(carbon)
Test if an atom is the membrane
is_in_membrane(sphere_pt, ca_coords, point_min, memb_width)
Plot the protein and the membrane
plot(ca_data, memb)
Calculate a plane
calculate_plane(sphere_pt, atom, memb_width)
calculate_membrane.py

Transmembrane protein 2K1A





Globular protein 1SI4



Visualisation

Membrane width variation

Parallelisation

to position the mebrane

increasing the number of points

For a better prediction

Thank you !

Any questions ?