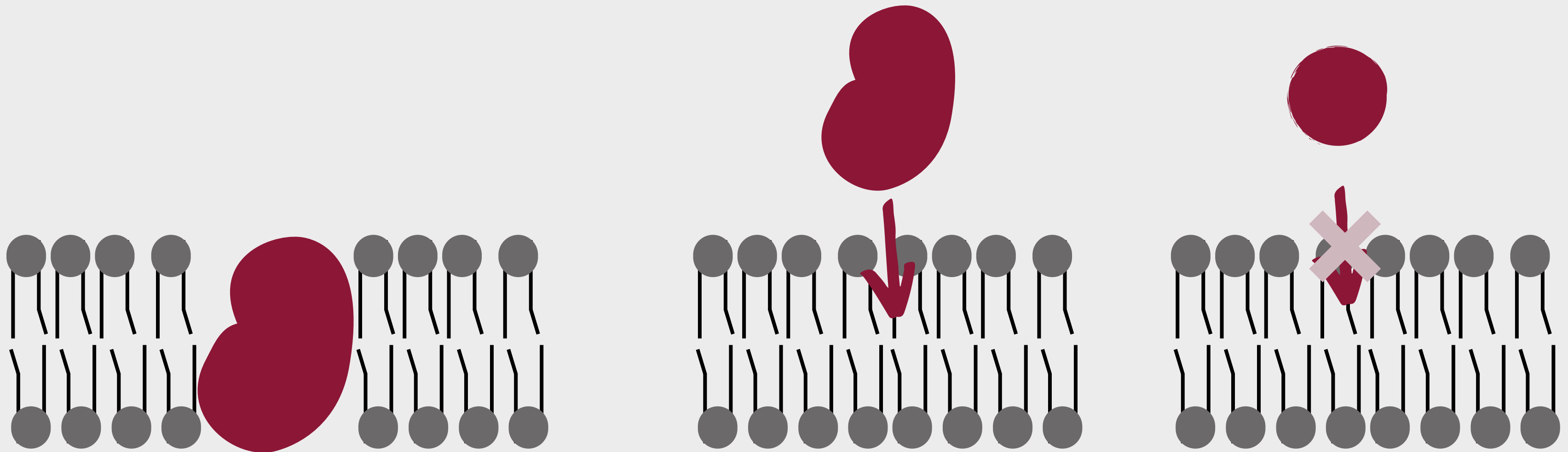


# **ASSIGNMENT AND DETECTION OF TRANSMEMBRANE PARTS OF A PROTEIN**

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

File PDB

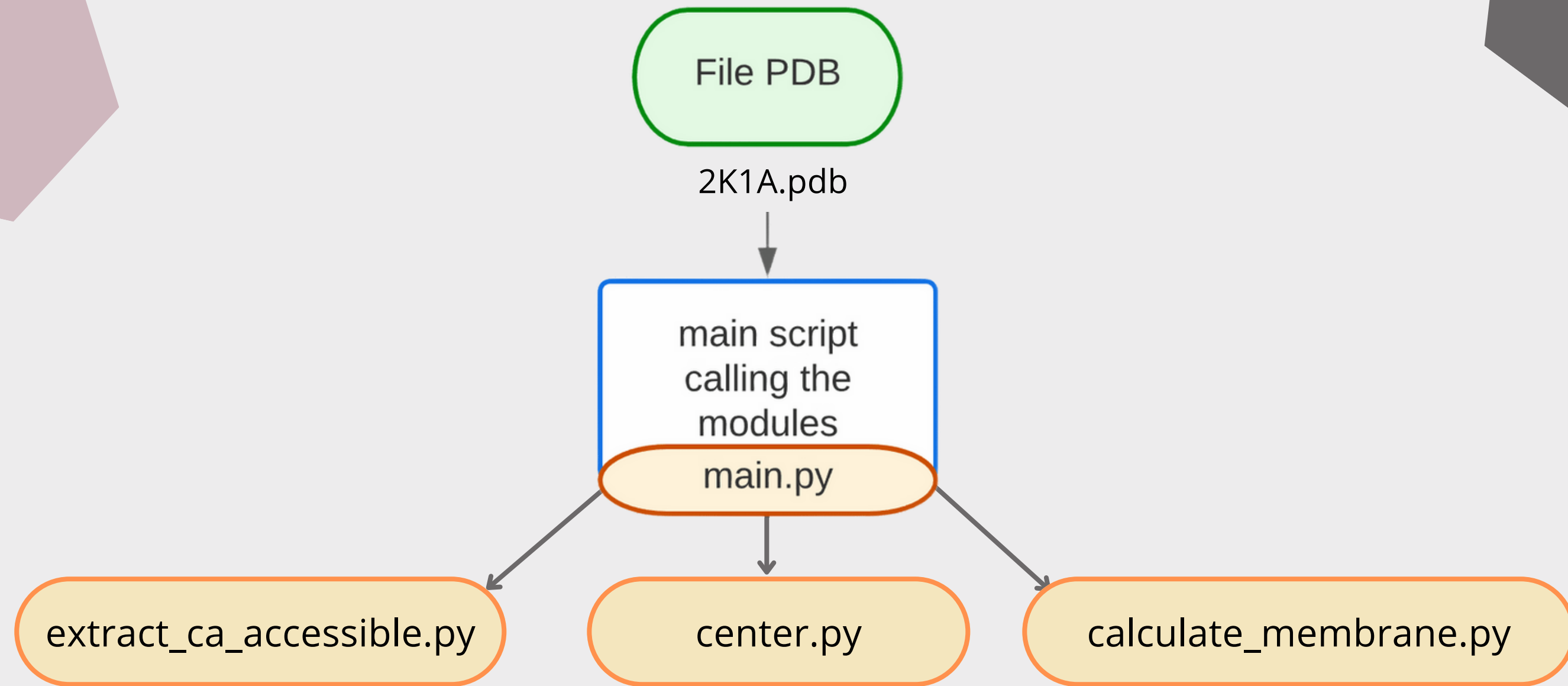
2K1A.pdb



main script  
calling the  
modules

main.py

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



import : Pandas  
Bio.PDB Bio.DSSP

Find the carbon alpha solvent-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  
solvent 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  
subtracting the center  
of mass from its  
coordinates

`center_protein(ca_data,  
com)`

`center.py`

import : Pandas  
math matplotlib

Find the carbon alpha solvent-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

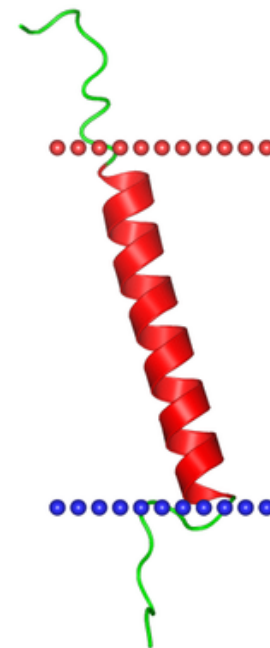
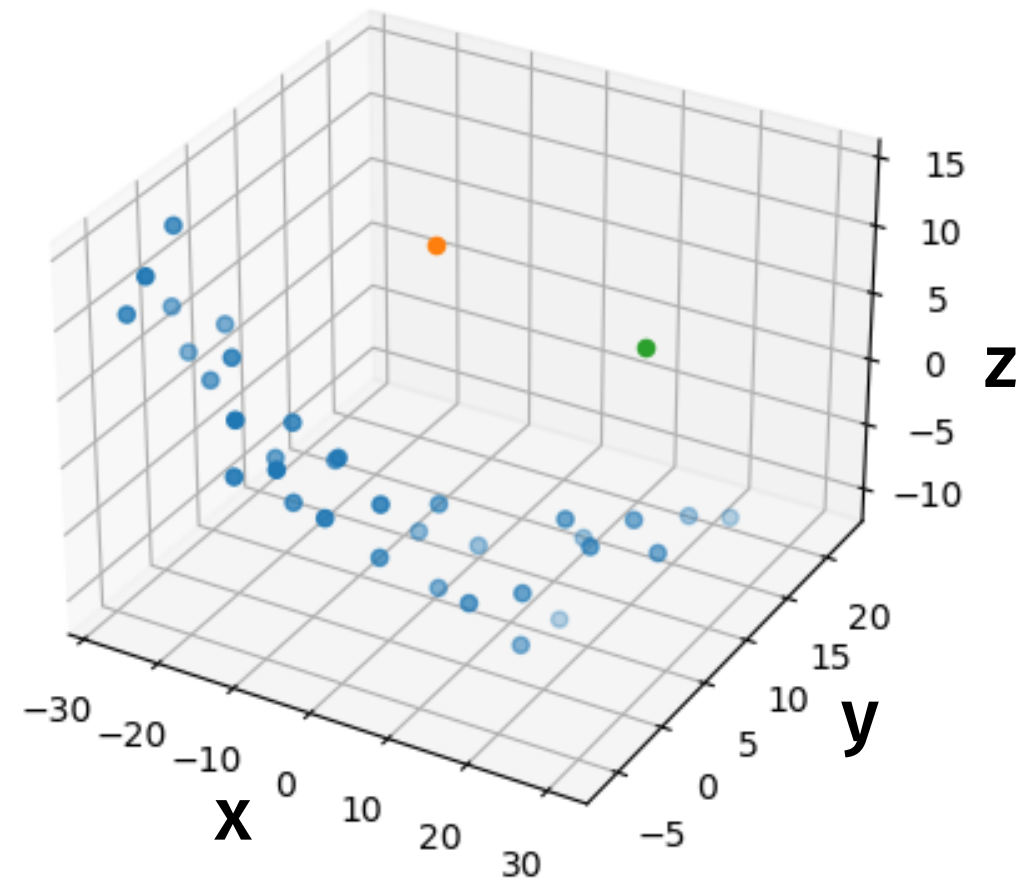
plot(ca\_data, memb)

Calculate a plane

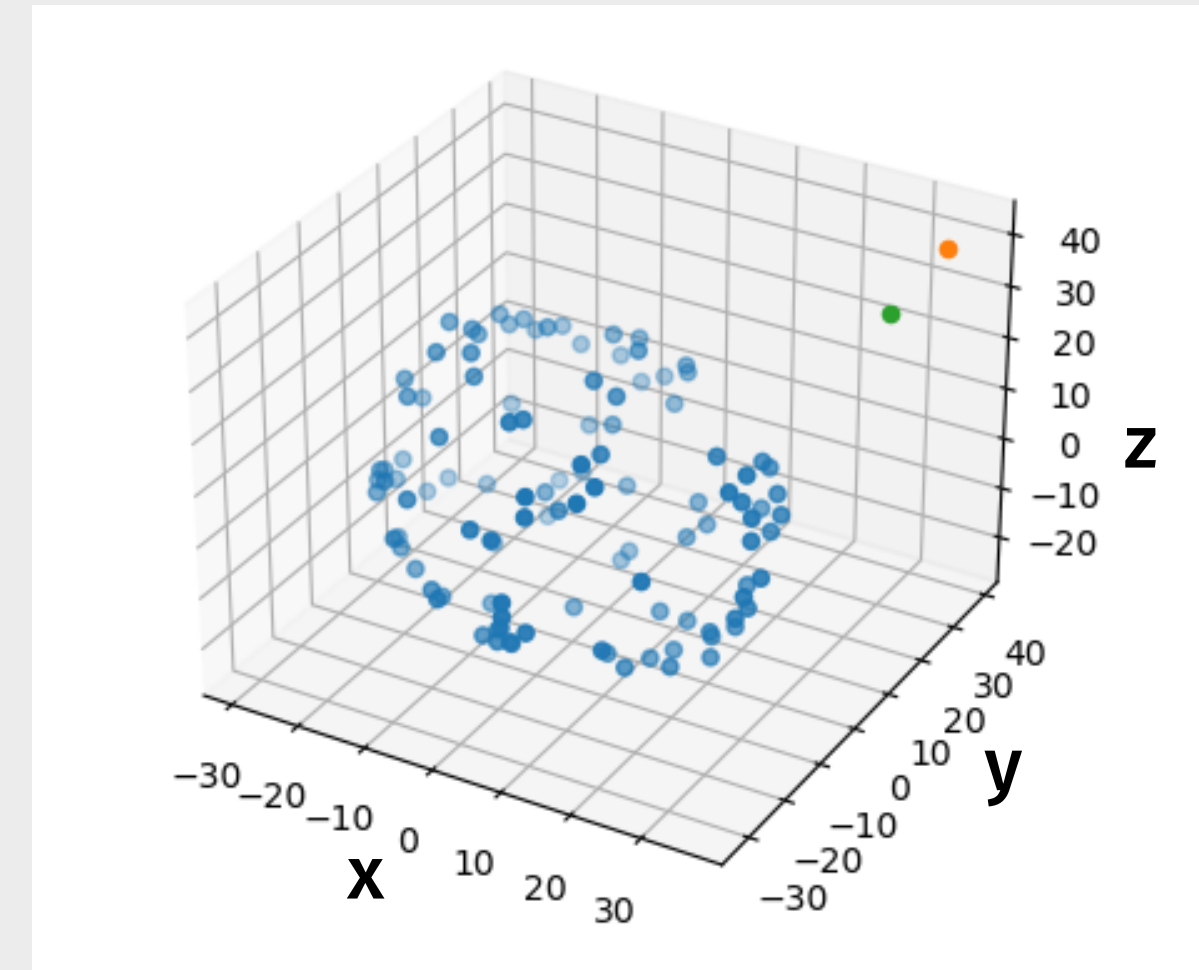
calculate\_plane(  
sphere\_pt, atom,  
memb\_width)

calculate\_membrane.py

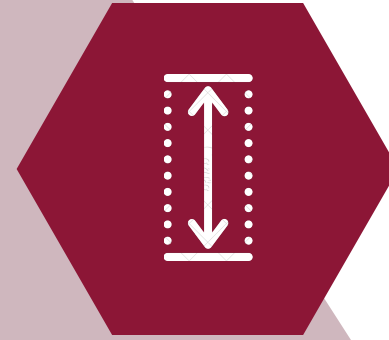
Transmembrane protein 2K1A



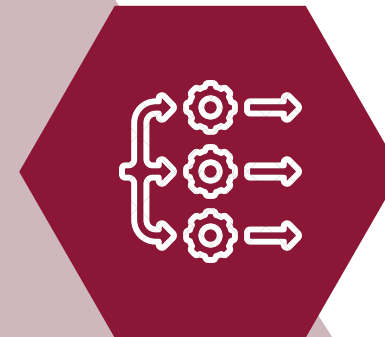
Globular protein 1SI4



Visualisation



## Membrane width variation



## Parallelisation

to position the mebrane



## increasing the number of points

For a better prediction



# Thank you !

Any questions ?