Remarks:

* ***You have learnt about protein structures and how it looks when projected into a 3D space.***
* ***How is it related to your project?***

1. No more than 100 words per answer!!!
2. Use your own words or drawings to answer the questions
3. Insert picture(s) in the space provided for hand-drawn figures (either pictures of pencil-and-paper drawings or digital drawings are ok)
4. Submit the e-copy of your answer via electronic means

**3. Practical usage of free computational chemistry-related resources for academic usage**

**3.1. Reason of small-molecule design:** *find the background information of your project*

*Recommended readings/information sources:*

* Ask your supervisor(s), mentor(s), coworkers, classmates, friends...
* Look for related scientific publications. You may search on Google to start with.
* The Uniprot database of protein information <https://www.uniprot.org>.

|  |  |
| --- | --- |
| Q3.1.1 | What is the name of the receptor(s) you are going to work on?  Is it a protein, a DNA/RNA or other types of biomolecules? |
| Ans |  |

|  |  |
| --- | --- |
| Q3.1.2 | From what species can this protein be found? |
| Ans |  |

|  |  |
| --- | --- |
| Q3.1.3 | What you want to do to the receptor? Inhibit or activate? |
| Ans |  |

|  |  |
| --- | --- |
| Q3.1.4 | What is the function of your target biomolecule? Why you want to alter its function? |
| Ans |  |

**3.2. The protein databank**

* As we are working on structure-based drug design, we need to have the STRUCTURE INFORMATION.
* Required by major scientific journals, experimental structures of proteins would be deposited onto the protein databank.
* Such information can be freely accessed at the website of RCSB PDB <https://rcsb.org>

|  |  |
| --- | --- |
| Q3.2.1 | Search for your target protein on the RCSB PDB. If it is a popular protein, you may need to add a species filter. Copy the list of PDB identifiers from your query here.  *Hint:* |
| Ans |  |

3.2.2. Selection of experimental structure for inhibitor design

|  |  |
| --- | --- |
| Q3.2.2 | Specify the ID of structure you want to use for inhibitor design (include the chain ID if possible) and give the reason. Common reasons of choosing the experimental structure can be:   * *High resolution (the smaller the value, the better the resolution)* * *Resolving all the atomic position of important residues, e.g. at the catalytic pocket.* * *Protein being a certain mutant of interest or without any mutations* * *Protein in a certain functional form that you want to inhibit/activate.* * *Protein is complexed with a ligand that you use as the lead structure.*   You can discuss with your coworkers who are more familiar to this project for more hints! |
| Ans | |  |  | | --- | --- | | PDB ID |  | | Chain  (e.g. A, B, C…) |  | | Missing residues?  If yes, list them. |  | | Mutation?  If yes, list them. |  | | Reason |  | |

**3.2. Installation of protein-ligand modelling tools for this project**

Please refer to “demo0-install.pdf” for installation instructions.

3.2.1. Installation of computational chemistry programs

3.2.1.1. Anaconda/miniconda

3.2.1.2. Install everything in the same conda environment

3.2.1.3. Optional manual install

|  |  |
| --- | --- |
| Q3.2 | As a proof of your successful installation and for the ease of debugging in the future, please fill in the following form. |
| Ans | |  |  | | --- | --- | | PyMOL version   * In the menu bar of PyMOL:   *Help -> About PyMOL* |  | | Whether you can start the Optimize plugin:   * In the menu bar of PyMOL:   *Plugin ->Legacy Plugins -> Optimize* | Yes/No | |

**3.3. Other free online resources that will be discussed later**

3.3.1. pubchem <https://pubchem.ncbi.nlm.nih.gov/> [ex2-3]

3.3.2. PDB2PQR server [ex1-3]

3.3.3. (pdb quick screen/swisssimilarity/pharmit/zinc) [ex3]