Remarks:

* ***From the previous exercise you now have a target protein of your choice, and a set of software ready to use.***
* ***But how to use them? What kind of information they can provide us?***
* ***In the step-by-step tutorial provided, you will learn how to quicky obtain an initial model of a protein-ligand complex, and how to interpret the results.***

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

**4. Exercise 1: warm-up exercise and limits of quick computational model.**

**4.1. Fundamental of science: control test to validate your protocol**

*Don’t trust the computer-generated results blindly! Always validate with known experimental data.*

|  |  |
| --- | --- |
| Q4.1.1 | For the protein you would like to target, is there any experimental data available for you to validate your computational method and/or to serve as the reference? |
| Ans | |  |  | | --- | --- | | **Experimental structure**   * Put the PDB code here (if available) * Describe the complex |  | | **If an experimental structure exist, which one you would choose for modelling?** |  | | Any MISSING residues in the experimental structure WITHIN the targeted region? |  | | Any MUTATED residues in the experimental structure WITHIN the targeted region? |  | | **Experimental activity/affinity data**   * e.g. Kd, IC50, EC50 |  | | **Others** |  | | **Will you be able to validate your model experimentally after you get the preliminary computational results?** | Yes/No | |

**4.2. Tutorial 1: Manual fitting of ligand and quick evaluation**

*Follow the tutorial in “demo1-manual-fit-eval.pdf”.*

|  |  |
| --- | --- |
| Q4.2.1 | Render a high-quality image of your protein-ligand complex, either of lig1, the reference compound, your own design, or both.   * Paste the image here * Tell us what is in the picture in “Title” * Describe the interaction pattern (e.g. hydrogen bond between x and y) |
| Ans | |  |  | | --- | --- | | **Image** |  | | **Title** |  | | **Description** |  | |

|  |  |
| --- | --- |
| Q4.2.2 | Copy the data in one of the \*summary.csv file(s) here. Which protein-ligand complex score the best? Which one score the worst? Try to explain the score based on visual inspection of the interaction mode! |
| Ans | |  |  | | --- | --- | | **File** | \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_.csv | | **Data** | |  |  | | --- | --- | | **Complex** | **Score** | |  |  | |  |  | |  |  | | | **Ranking** | Best complex:  Worst complex: | | **Explanation** |  | |

* **Congratulations**, now you have an idea of what the project is and had some hands-on experience with the provided tools.
* **Try to apply this workflow on the protein you would like to study!** 
  + You may refer to the “summary” section (green box) in the tutorial pdf file.
  + Remember to take notes of your procedures so it would be easier for writing reports in the future!
* *If you are interested in some more efficient workflow for protein-ligand binding prediction which is more commonly used, please try the next set(s) of tutorial materials! Stay tuned! (Still working on it…)*