M1 ISDD - BI

PROTEIN DOCKING COURSE

February 2018

PROJECT ASSIGNMENT

/home/sdv/all/protdocking/project/

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The project will be evaluated based on: *i)* your technical skills on the docking tools we have learned, *ii)* your capacity to identify, run and analyse a docking problem, and *iii)* your understanding of the different aspects that we have seen during the classes.

1) You will be assigned a docking case from the Benchmark 5.0:

http://zlab.umassmed.edu/benchmark/

2) The goal is to run docking simulations on the unbound coordinates of the subunits (from the benchmark). You will design and run your own docking protocol, based on the docking tools you have learned in class. You may choose any tool and use additional information or data (min. 2 tools: e.g. rigid-body & scoring; rigid-body & refinement; flexible docking & interface prediction, etc.).

3) You have to describe the docking calculations and analyze the results (comparing to the reference structure).

4) You have to provide the PDB files for the docking solutions that you consider as the 10 best ones according to your calculations.

These are some ideas you should include in your report:

- Describe your system (PDB names for the files used for docking, reference complex, etc.)
- Explain the preparation of the files for docking (if any)
- Justify the chosen tools
- Explain the docking simulations you have run, with all the parameters you selected.
- Explain any additional tool or data you have used (if any)
- Explain the results, and compare the docking solutions with the reference structure (use tables, graphic plots or molecular images to explain your analysis)
- Discuss the success of the predictions for this case. Was your docking protocol appropriate? Would it have been better with a different protocol?

You may add anything you consider important for your docking case, any comment, ideas, suggestions to improve the results, etc.

NOTE: the report will NOT be evaluated based on the SUCCESS of docking. It will be evaluated based on your docking skills, justification of the used techniques, interpretation of results, capacity to solve possible problems during docking, etc.

HINTS: some of the questions listed in the practical tutorials may help you to analyse and discuss your docking case

IMPORTANT:

- THE ASSIGNMENT IS PERSONAL, IT WILL NOT BE ACCEPTABLE TO FIND TWO PERSONS WITH EXACTLY THE SAME DOCKING PROTOCOL, PARAMETERS AND ANALYSES. COPYING EACH OTHER WOULD INVOLVE THE INVALIDATION OF THE SUBJECT FOR THIS YEAR.

SEND THE REPORT (max. 5 pages) AND THE PDB FILES FOR THE TOP 10 PREDICTIONS TO:

- email to me (juanf@bsc.es) (cc Prof. Camproux)

Deadline: 19-March