Università
della
Svizzera
italiana

Facoltà
di
scienze
biomediche

Final project

Structure-based virtual screening

Deadline

Final Project submission: 15th January

Assignment: 40%

Final Project: 60%

Tasks

1. Describe all the known structures for the target attached to the final project (primary, secondary, etc.). Also describe the chemical and physical properties of the residues present in the putative binding site. (10 points)

2. Provide results and detailed description of the docking procedure between the target and the given molecule. (20 points)

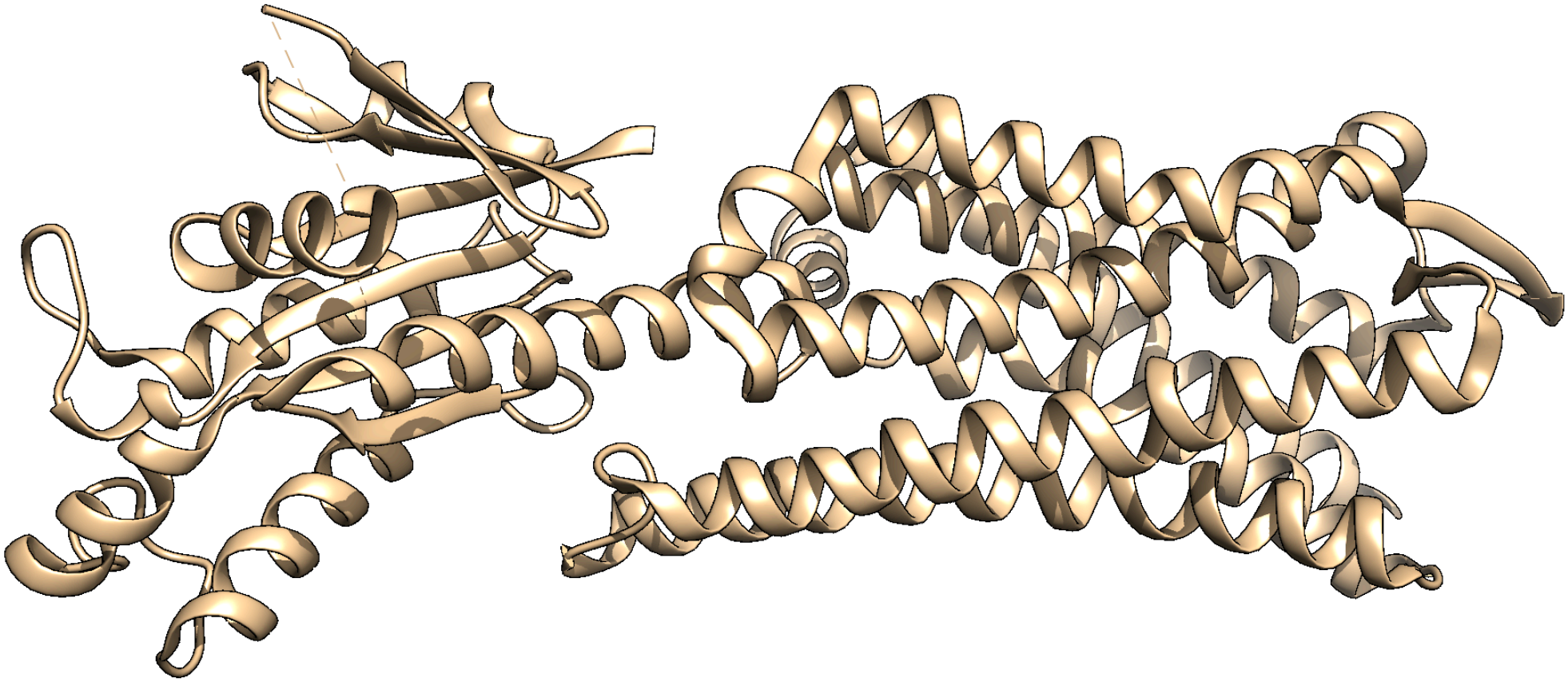
3. Plan a structure-based virtual screening in order to create a more powerful drug than the suggested scaffold. (70 points)

COMPULSORY

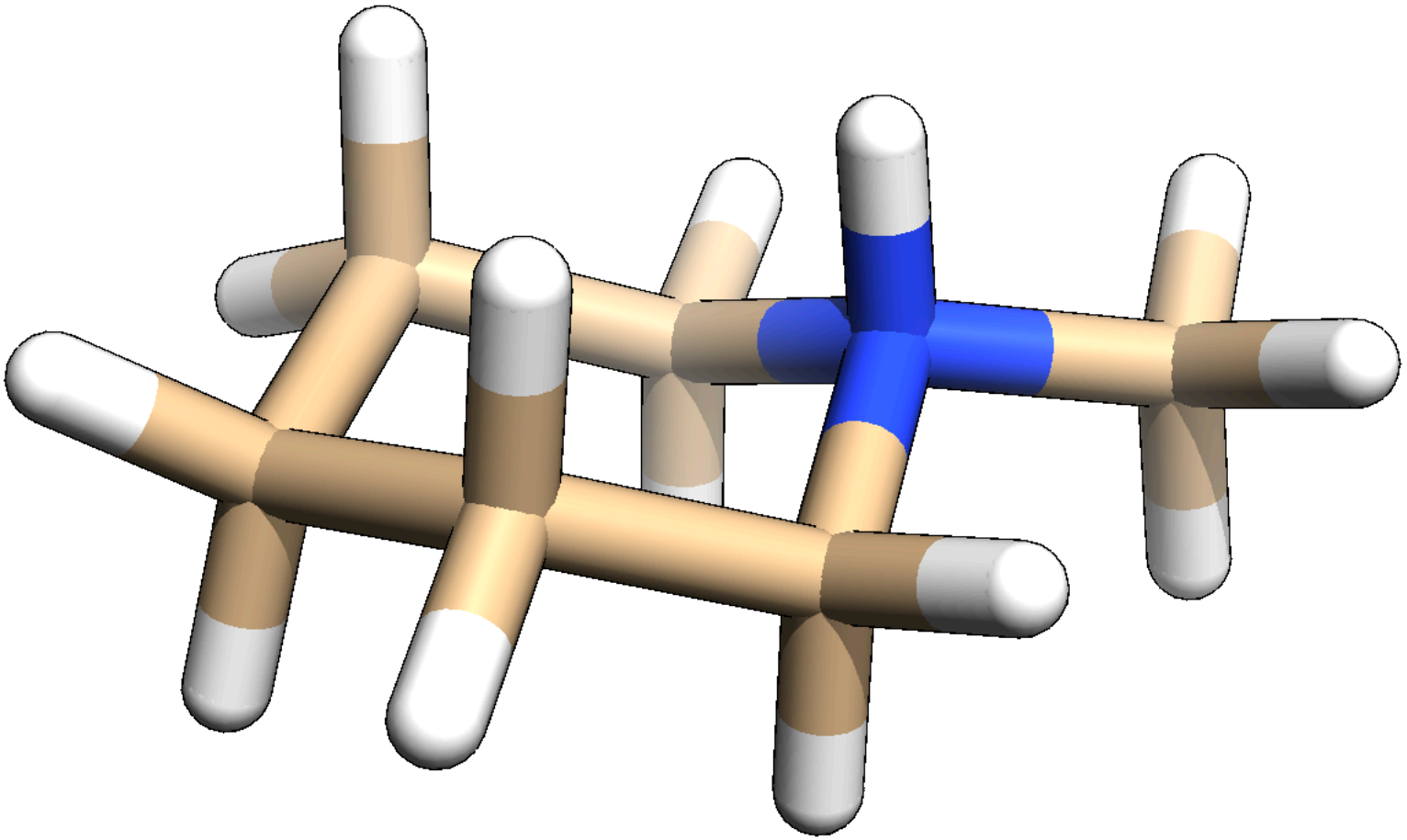
Whatever procedure you follow, docking must be explained as seen during lesson (both theoretically and practically). Uploading only the results of docking will be considered as blank.

The virtual screening procedure requires for you to develop your own molecule and check the new structure with other docking procedures. There is no limit to the step that you can take, but each one of them must be well described and the previous point apply also for all the docking in the virtual screening phase.

Target



Ligand



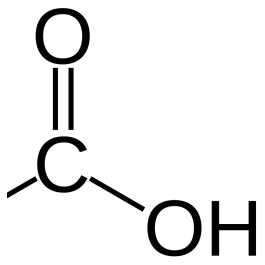
Guideline

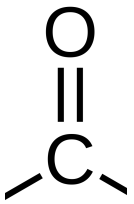
1. There is a drug coming from this scaffold, can you find it?

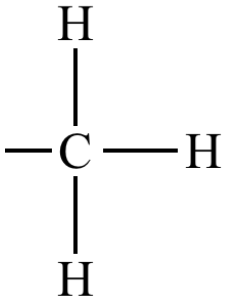
2. Target weight: around 350 Da.

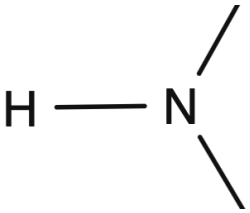
3. Your drug must be deliverable through intravenous, intramuscular, and oral administration.

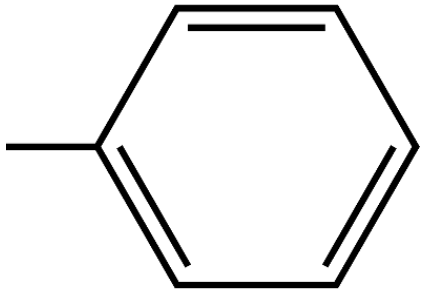
Possible functional groups

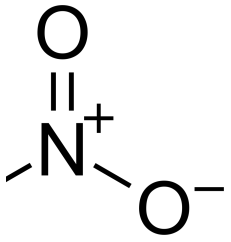


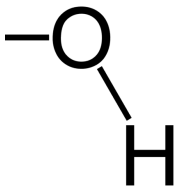


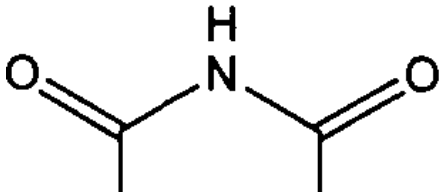


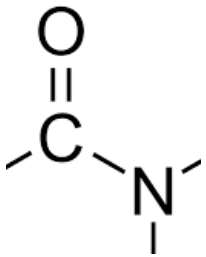












Atom modifications and much more….