# Bioinformatics project 7.5 ECTS; Assignment 1.

### THIS FORM MUST BE UPLOADED IN ABSALON WITHIN THE FIRST WEEK OF THE BLOK

### (OTHERWISE THE PROJECT MAY NOT BE ELIGIBLE FOR EXAMINATION)

#### Name of binf/DIKU supervisor:

#### Amelie Stein Co-supervisor: Marion Lucia Silvestrini (Postdoc)

#### External supervisor(s), if any: None

#### Title and short abstract of project:

Stability predictions with Rosetta and DynamicBind of inhibitors bound to HIV

A previous student project established and demonstrated the possibility of applying Rosetta for stability prediction on inhibitors bound to HIV. The aim of this project is to broaden the understanding of stability effects on inhibitor binding to HIV. Drug fold resistance effects are gathered from the Stanford HIV Drug Resistance Database (HIVDB), specifically for the PI HIV inhibition drug class. Within the PU HIV inhibition drug class, the drug fold of the inhibitors: ATV, IDV, LPV and NFV will be looked into. These drug folds will be compared to the predicted Rosetta and DynamicBind cLDDT to establish prediction accuracy. Python will be used for data management and previously established pipelines will be used for predictions. The goal is to include more drugs to further HIV inhibition prediction understanding.

#### Name of student (For group projects, please give names of fellow students):

Rasmus Willsleff Andersen

KU-id: fvt270

#### Any comments or extra information can be supplied here:

Doing the project in parallel with Nicholas Scott Raiken – not together, but in parallel.

### After uploading the assignment 1, the student must send an e-mail to the internal supervisor and ask him/her to approve the assignment in ABSALON.