

Exercise Sheet 6

Aim: Visualising of protein structures and of protein-ligand interactions, Evaluation of homology models

Protein structure: Homology modelling

For the interactive material for this exercise follow this link:

https://www-cbi.cs.uni-saarland.de/wp-content/uploads/Softwarewerkzeuge_Teil_2/start2a.html

Exercise 6.1: Homology modelling

The follow the link

1. Punktmutationen in cAPK

- (1) From which organism does the sequence originate?
- (2) Which organism was used for the expression of the protein?
- (3) What is the reported maximum (best) resolution of the X-ray structure?
- (4) Which other (non-protein) molecules are present in the structure?
- (5) Determine the corresponding UniProt accession number of this protein.

Investigate 1ATP.pdb (using a Visualisation program of your choice or directly on the website via 3D View)

- (6) Find the active centre
- (7) What is „chain E“ and what is „chain I“ ?
- (8) Which consequences would you expect upon the exchange of Asp166 by Ala?
Carry out this mutation on the corresponding FASTA sequence using a text editor.
- (9) Compare the obtained homology model to that of the wild-type. Please note that the numbering of the residues might have changed if the first amino acid within the X-ray did not start at 1. Are there are crucial changes notable in the structure of the protein?

Remark: For the second project you will need a program to visualize protein structures (.pdb files), such as VMD, PyMol, USCF Chimera, SWISS-PDB Viewer / DeepView,...

To start VMD on the CIP-Pool computers first open a terminal window or console, and enter following comand line (press the enter key):

```
vmd or /usr/local/bin/vmd
```