

**Exercises to the Lecture ``Protein Prediction``  
Summer Term 2010**

**Sheet 1**

General information

- Our course homepage, containing lecture slides, video, and exercise sheets:  
<http://rostlab.informatik.tu-muenchen.de/cms/pp/>
- Time and place of the exercise: **Friday, 14:30 – 16:00**, room **01.08.021** (practical room)
- Groups of 2-3 people
- Grading („Schein“):  
40% exercise (programming), 60% final exam (lecture content), probably July 2, 14:30
- Contact: [hamp@rostlab.org](mailto:hamp@rostlab.org), [schaefer@rostlab.org](mailto:schaefer@rostlab.org)

Exercise 1: Dogma of Molecular Biology

- a) What is a genome and what information does it contain?
- b) What is the relation between genes and proteins?
- c) Describe the different structural levels found in proteins.
- d) Give a few examples of protein functions.
- e) Describe the relation between proteins and evolution.

Exercise 2: Protein Interactions

- a) What is the relationship between protein function and protein interaction?
- b) Name a few types of protein interactions.

### Exercise 3: Visualization of 1EJA

- a) Find the pdb entry for the structure 1EJA. What actual structure does it represent?
- b) Take a look at the pdb file of that structure (hint: Click 'Display Files' in the upper right corner of the pdb web page). Which basic entries do you see? Which ones are responsible for the definition of the three dimensional structure? What do the several fields stand for?
- c) Visualize the structure with the tool SRS3D ([www.srs3d.org](http://www.srs3d.org)).
- d) Familiarize yourself with the basic settings.
- e) What does the blue ball represent?
- f) Select an atom and push the "up-arrow" key multiple times. What happens?
- g) For each chain, select all residues which are closer than 6 Å to the other chain.
- h) Copy and paste the selection into a text file and save it.

### Exercise 4: Visualisation of 1AIP

- a) Follow steps a) to c) from the last exercise for the structure 1AIP.
- b) Describe the symmetry of the complex.
- c) Assuming you wanted to create a set of unique protein-protein interfaces, which interfaces of this complex would you consider?
- d) For each chain contributing to one of the interfaces above, repeat steps g) and h) of Exercise 3.

### Exercise 5: Application of the PPI prediction tool ISIS

- a) Familiarize yourself with the command line options of `profisis` (`man profisis`).
- b) For each chain found in the structures above, predict the PPI hotspots by the use of `profisis`. You find the necessary input files for `profisis` in  
`/mnt/home/rost/hampt/exercise01`.
- c) Assume that the output from SRS3D is our gold standard. Write a tool which parses the output of SRS3D and ISIS and measures the accuracy of `profisis`.