Softwarewerkzeuge der Bioinformatik

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Exercise Sheet 1

Sequence Analysis: Biological Databases

Learning objective: The goal is to learn how to use databases to find information about speicfic genes, proteins and organisms, such as sequences, IDs, mutations, protein families, genome positions, transport mechanisms, drug targets etc.

Exercise 1.1: NCBI and UniProtKB

Use NCBI (http://www.ncbi.nlm.nih.gov) and UniProtKB (http://www.uniprot.org/) to answer questions about a protein. The accession number of the protein in the UniProtKB/Swiss-Prot database is Q38856.

- a) What is the protein?
- b) What is the name of the organism?
- c) What is its function?
- d) In which cellular compartment can it be found?
- e) Have mutations been found for this protein that affect its function? If so, which ones (position and amino acid exchange) and what are the functional consequences?
- f) What is the name of the corresponding gene and on which chromosome is it located?
- g) Save the protein sequence in FASTA format.
- h) To which protein family does the protein belong?
- i) Find one more protein of the same family in the same organism. Name the accession number.
- j) Find another protein from the organism *Oryza sativa* with the same function, cellular compartment and family as **Q38856**. Write down the *accession number*.

Exercise 1.2: TCDB - Transporter Classification Database

In this exercise you use TCDB (http://www.tcdb.org) to classify protein Q38856 of the previous exercise.

Hint: The transporter classification ID (TC–ID) is comprised of five components X.A.Y.Z.V, where X, Y, Z and V are number and A a letter.

- X: transporter class
- A: transporter subclass
- Y: transporter (super)family
- Z: transporter subfamily
- a) What is the TC-ID of the protein?
- b) What is the name of the transporter class to which the protein belongs?

- c) What is the name of the transporter family?
- d) Describe the structural similarities of proteins in this family.
- e) Which substrates are transported by proteins of this family?
- f) What is known about the transport mechanism? What is the different to ATP based transport?

Exercise 1.3: PATRIC - Pathosystems Resource Integration Center

In this exercise you use PATRIC (http://patricbrc.org/) to find information about the species Staphylococcus.

- a) What can you find out about the lineage of staphylococci?
- b) The following is about antibiotic resistances and drug targets in the bacterium *Staphylococcus* aureus, specifically *Staphylococcus* aureus subsp. aureus N315.
 - i. Which databases are accessed by PATRIC regarding antibiotic resistance?
 - ii. How many genes associated with antibiotic resistance are listed? Name some examples.
 - iii. What is the function of mecA or of the corresponding protein?
 - iv. Which drug targets can you find and from which databases?