Homology modelling demo

At the beginning we try to run demo provided by Modeller developers (prediction of *Peptococcus aerogenes* ferredoxin based on *Azotobacter vinelandii* ferredoxin). Login to the computer. Create a new directory in your home directory. Then go to the directory **`/usr/lib/modeller9.14/examples/automodel`** find files **`alignment.ali`** and **`model-default.py`** and copy them to the directory you created. In the directory **`/usr/lib/ modeller9.14/examples/atom_files`** find the file **`pdb5fd1.ent`** and copy it to the directory you created. The homology modelling procedure can be started by typing:

```
python model-default.py
```

Model building can take several seconds, no more than one minute. You can watch files being created during the procedure in the directory.

Structural-palaeontology tutorial

Try to predict 3D structure of the subunit 1 of cytochrom-*c* oxidase (EC 1.9.3.1) of Siberian mammoth *Mammuthus primigenius*. Go to the web site of the European Bioinformatics Institute (EBI, http://www.ebi.ac.uk). Type the Latin name of genus *Mammuthus* and press Search. From the list of query results select Protein Sequences and then the first subunit of cytochrom-*c* oxidase (**`COX1_MAMPR`**). Scroll down the record of the protein to sequence field and click to FASTA. Copy the sequence to the clipboard.

Now go to the BLAST service (http://www.ebi.ac.uk/Tools/sss/ncbiblast/), deselect the database UniProt Knowledgebase, select the database Protein Structure Sequences, select the PROTEIN query, paste the sequence and submit. This will find proteins with known 3D structure similar to mammoth cytochrom-*c* oxidase. Download selected PDB file and copy it to the Linux computer. Copy the alignment to the Linux computer to the file **`alignment.ali`**. Then remove middle consensus lines, numbers and blank spaces and separate query and sequence records. Finally replace ferredoxin sequences for sequences of cytochrome-*c* oxidases. Place query (mammoth) to the record **`sequence`** and sequence (selected PDB) to the record **`structureX`**. Update PDB IDs, residue numbers and chains. Update PDB IDs in the file **`model-default.py`** and run:

```
python model-default.py
```

In couple of seconds, no more then one minute, you obtain a PDB file with the model of mammoth cytochrome-*c* oxidase.