

## Problem set 2 (Hand in by April 24)

### Problem 1

**Protein synthesis.** Bacteria divide every 20 min. Estimate the synthesis rate of ribosomes in units amino acids per seconds assuming that there are about  $20 \cdot 10^3$  ribosomes at work. (Hint: estimate the size of bacteria (see problem set 1!); estimate then the total amount of protein and the average molecular mass of an amino acid).

### Problem 2

**Protein conformations and sizes.**

- Find an approximative formula for the radius of a globular protein ( $R$ ) as a function of its molecular weight ( $MW$ ). Take bold averages for the properties of an amino acid.
- What would be the contour length (i.e. total extended length) of a protein with 40 kDalton ?
- How many different sequences of amino acids exist theoretically for such a protein?

### Problem 3

**Exploring the 3D structure of proteins.** The aim of this exercise is to familiarize yourself with a molecular viewer, a program that allows you to display, visualize, and manipulate the 3D structures of macromolecules.

- Download and install a molecular viewer of your choice on your computer - or find a computer with a viewer already installed. Popular choices are Klaus Schulten's (who is currently a visiting professor at the LMU) **Visual Molecular Dynamics**, VMD for short, **RasMol**, or **PyMol**. Follow the instructions on the respective websites for installation on your computer.  
VMD: <http://www.ks.uiuc.edu/Research/vmd/>  
RasMol: <https://www.umass.edu/microbio/rasmol/getras.htm>  
PyMol: <http://www.pymol.org>
- Myoglobin was the very first protein for which an X-ray crystal structure was determined. It is critical for the transport of oxygen. Download a file that has the 3D structure information for the protein myoglobin. You can obtain the file by going to the website of the **Protein Data Bank (PDB)**: <http://www.rcsb.org>. To find the myoglobin structure, enter the four character structure identifier for myoglobin 1MBN into the search field. On the page with the myoglobin entry, you

can find a lot of information. On the top right, you find a menu with download options (“Download Files”). Select “PDB File (Text)” and save the file to your computer.

- c) Open the PDB file with the molecular viewer. In VMD, this is accomplished by opening the “File” menu, selecting “New Molecule”, “Browse” for the PDB file that you have downloaded, and click on “Load”. Render the myoglobin structure in a way that you can inspect the  $\alpha$ -helices; for example, use the cartoon representation for the  $\alpha$ -helices (in VMD, select the “Graphics” menu, open “Representations”, and select “Cartoon” from the “Drawing Method” tab). How many  $\alpha$ -helices are there?
- d) Render the heme of myoglobin (in the “Graphical Representations” window, select “Create Rep” and type “not protein” into the “Selected Atoms” field; select for example “Drawing Method” “Licorice”) and the hydroxide ion in the oxygen binding site (create another representation for the atom selection “resid 154” and select for example “VDW” as “Drawing Method”). Is the oxygen in the plane of the heme?
- e) Select one other molecule from Jane and David Richardson’s article *Biophysical Highlights from 54 Years of Macromolecular Crystallography* (Biophysical Journal, 2014; the article is available on the course website). Include a nice rendering of your molecule of choice with the solution of your problem set.