Problem set 1
(Hand in by April 15)

Problem 1

Quantifying *E. coli*. One of the most common model organisms for research and a key player in biotechnology is *Escherichia coli*, a simple rod-shaped bacterium. In the following, you can approximate *E. coli* cells as cylinders with 1 μm diameter and 2 μm length. You can round to the nearest order of magnitude.

a) What is the volume (in μm^3 and L) of an *E. coli* cell?

b) What is the concentration, if there is one molecule of a certain kind in one *E. coli* cell?

c) How many molecules of a certain kind are in one *E. coli* cell, if their concentration is 1 μM? 1 mM?

d) If we assume that molecules are very approximately on a cubic lattice, what is the spacing between molecules at 1 nM? 1 μM? 1 mM?

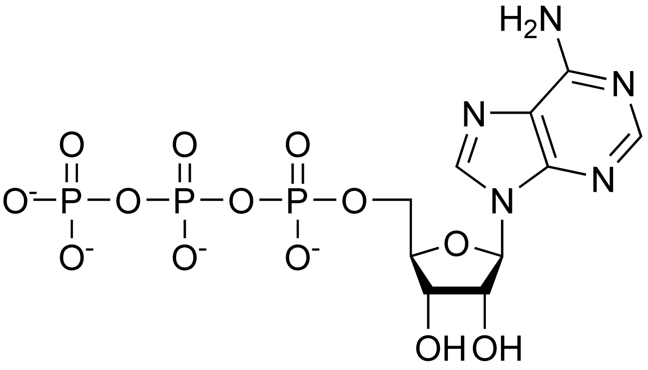
e) What is the mass of an *E. coli* cell, if we assume that it roughly has the same density as water?

f) What is the surface area of an *E. coli* cell?

g) The cellular membranes are assembled from lipid molecules. If we take into consideration that *E. coli* is enclosed by an inner and outer membrane and that each of these membranes is a lipid *double layer*, how many lipid molecules are there in one *E. coli* cell? You can assume that each lipid molecule covers a surface area in the membrane of 0.5 nm^2.

Problem 2

ATP hydrolysis. Adenosine triphosphate (or ATP for short) is the "energy currency" of the cell. The energy is stored in the spatial arrangement of three negatively charged phosphate groups, see figure. The energy is release when the last phosphate group (also called the γ-phosphate) is broken off or released, i.e. when ATP is *hydrolyzed* to ADP (adenosine diphosphate). You can compute a simple estimate of the energy released upon ATP hydrolysis by considering the electrostatic energy of the phosphate groups. You can treat the phosphate groups as point charges on a line, with the γ-phosphate having a charge of $-2e$ and the other two each with a charge of $-1e$, separated by a distance of 0.3 nm between phosphate groups, and use Coloumb's law to compute the potential energy.



a) What is the energy difference between ATP and ADP, if you assume that the released phosphate moves infinitely far away and that the reaction takes place in vacuum?

b) How does the results from the previous question change, if the reaction takes place in water?

Problem 3

Lennard-Jones potential. The (non-electrostatic and non-covalent) interactions between atoms are often modeled with a so-called Lennard-Jones or “12-6” potential. The energy as a function of the distance between the atoms r is given by the functional form

$$E(r) = 4\epsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right) \tag{1}$$

a) For what distance is the interaction energy minimal? What is the energy at the minimum?

b) Draw (by hand or, better, by using a software of your choice) the potential for parameters $\epsilon = 1.66 \cdot 10^{-21}$ J and $\sigma = 3.4 \cdot 10^{-10}$ m.

c) Can you think of a molecular interpretation of the two terms in the energy function?