Molecular, Cellular & Tissue Biomechanics, Fall 2006

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Problem Set # 1

Problem 1: ATP is the $20 bill of energy units in the cell, ~20 times the thermal energy kT. When we look up the standard free energy for ATP, it is listed at 7kcal/mole. If you convert 7kcal/mole to kT units you see something is wrong, it doesn't lead to our value of 20kT. Do this conversion. Remember we need to modify the free energy to include the typical concentrations of the reactants, ATP, and products ADP and free Phosphate. Use the fact that the free concentration of these species in a typical cell is found to be ~1mM for ATP, 10μm for ADP and ~1mM for phosphate to show that the "20 bucks" rule holds.

Problem 2: a.) Get familiar with the protein data bank. From the books on protein structures we see that the linear distance/residues of peptides arranged in an α-helix is 1.5 Angstroms. Check this out with the protein data bank on a real structure. Download the structure 1K40, the FAT domain of Focal Adhesion Kinase. Calculate the linear distance/residue found in one of the helix structures and compare to the 1.5Angstrom value.

b.) Look up the structure for the photosynthetic reaction center, 2RCR, with authors Kabbani, Chang, Tiede, J. Norris and Schiffer. What is the dominant secondary structure of this membrane protein? What paper is referenced for this structure? The "Special Pair" is a pair of bacteriochlorophyll molecules whose planar structures are particularly close. Note this forms the photon "trap" or sink that is responsible for photosynthesis. Which molecules form the special pair? (The possibilities are: BCL 300, BCL350, BCL 400, BCL450) A straightforward way to do this is to cut out these molecules from the .pdb file using a notepad or text editor. Save this portion with a .pdb file extension and open with a viewer. You should only see the atoms that are in your file subset.

For fun, but not required for this homework set, you can calculate how parallel these chlorophyll molecules are and the distanced between them. Note photon energy is stored in a dipole spanning the nitrogen atoms in the chlorophyll molecules. Energy transfer probabilities depend on the distance ($1/r^6$) and orientation between these dipoles. The "special pair" is so close that it actually shares electrons and can be considered one molecule not two.

Problem 3: Use of some simple back of the envelope estimates: assume E-coli is a cylindrical like cell about 2 μm long and 0.8 μm in diameter.

a) Estimating that E-coli is 70 percent water by mass and 30% other stuff of which half is protein. Calculate a ballpark total number of proteins found in e-coli, assume the proteins are our typical 300aa (30kD) protein.

b) What is the cellular protein concentration in mg/ml (standard units of protein concentration)?

c) Now we have some outside information that there are 15,000 ribosomes in E-coli making proteins. What is the average spacing between these? Would you say things are crowded or not?

d) If E-coli doubles every 3,000 seconds in minimal media, estimate the typical amount of time it takes a ribosome to make a protein? Compare your result to the measured value of 25aa/second.

e) If we assume the energetic cost to make the amino acids found in these proteins is 4ATP, what is our minimal energy budget, in J and glucose molecules, for creating the proteins for each new E-coli cell?

Problem 4: Use a kinetic energy model to estimate the speed of a water molecule moving freely in between collisions. Note that for this problem, we assume a water molecule moves independently. In reality water molecules are connected to each other through hydrogen bonds where at any instant there might be 7 or so molecules linked to each other. Estimate the speed of your typical 300aa protein in between collisions?

Problem 5: What is the force due to gravity of our typical 300aa protein in air? Calculate for your e-coli cell (problem 3 above) in solution. Assume the density of protein and other stuff is 1.38 that of water.

Updated values for physical properties of our "Typical Protein" 300aa long

mass ~30kD
mass 4.8×10^{-23}kg
density 1.38×10^{3} kg/m^3
volume 34.8 nm^3
radius 2.02 nm

100kD protein (see Howard Chapter 2)

mass 100kD
mass 166×10^{-24}kg
density 1.38×10^{3} kg/m^3
volume 120 nm^3
radius 3 nm