Tutorial 2

To be discussed during the tutorial on Friday, 15 Feb 2008. Your contributions toward the discussion are strongly encouraged and will be evaluated.

1. The pH of pure water is not a universal constant; rather, it depends on the temperature: At 0°C, it’s 7.5, whereas at 40°C, it’s 6.8. Explain this phenomenon and comment on why your explanation is numerically reasonable.

2. From experimental data, we found the amino acid compositions of a peptide are below:

<table>
<thead>
<tr>
<th>Amino acid</th>
<th>number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serine</td>
<td>3</td>
</tr>
<tr>
<td>Glycine</td>
<td>2</td>
</tr>
</tbody>
</table>

   a. Calculate the total number of possible sequences which can be built from the amino acids.
   b. Indicate the possible positions of glycine in the sequences.

3. The amino acids His 31 and Asp 70 are separated by ~ 0.35 nm in T4 lysozyme. Calculate the Columbic potential between the two charged side chains (make the assumption that these are point charges in a dielectric medium of 40\(\epsilon_0\)). Estimate the \(pK_a\) of the His residue in this ion pair (\(pK_a\) of the His in water is 6.0).

4. The optimum distance for the van der Waals interaction between two carbonyl oxygen atom is \(r_0 = 0.353\) nm. The energy for this interaction is -20.78 kJ/mol.
   a. Estimate the repulsive parameter A and dispersion parameter B for the Lennard-Jones 6-12 potential.
   b. Calculate the energy at \(r = 0.33\) nm and \(r = 0.4\) nm, using the parameters in a.

5. Derive the force functions for a Coulombic interaction, a dipole-dipole interaction, and a van der Waals interaction.

6. (a) Compare the similarities and differences of hydrogen bond with covalent bond/van der Waals interaction and polar-polar interaction. Discuss the role of hydrogen bond in stabilizing the secondary structure of DNA and protein.
   (b) Explain the influence of solvent on the strength of hydrogen bond and the stability of DNA and protein structures.