Review
Chemistry of Life

I. Atoms
   A. Periodic table of elements
   B. Atoms
      1. nucleus
      2. shell (s) = cloud (s)

II. Molecules
   A. covalent bound
   B. ionic bound
   C. hydrogen bound
   D. functional group

III. Bio-molecules
   A. DNA
   B. RNA
   C. Protein
   D. Carbohydrates
   E. Lipids
Periodic table of elements
# Chemical Composition of Human Body

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Element</th>
<th>Percentage of Human Body Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>Oxygen</td>
<td>65.0</td>
</tr>
<tr>
<td>C</td>
<td>Carbon</td>
<td>18.5</td>
</tr>
<tr>
<td>H</td>
<td>Hydrogen</td>
<td>9.5</td>
</tr>
<tr>
<td>N</td>
<td>Nitrogen</td>
<td>3.3</td>
</tr>
<tr>
<td>Ca</td>
<td>Calcium</td>
<td>1.5</td>
</tr>
<tr>
<td>P</td>
<td>Phosphorus</td>
<td>1.0</td>
</tr>
<tr>
<td>K</td>
<td>Potassium</td>
<td>0.4</td>
</tr>
<tr>
<td>S</td>
<td>Sulfur</td>
<td>0.3</td>
</tr>
<tr>
<td>Na</td>
<td>Sodium</td>
<td>0.2</td>
</tr>
<tr>
<td>Cl</td>
<td>Chlorine</td>
<td>0.2</td>
</tr>
<tr>
<td>Mg</td>
<td>Magnesium</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Trace elements (less than 0.01%): boron (B), chromium (Cr), cobalt (Co), copper (Cu), fluorine (F), iodine (I), iron (Fe), manganese (Mn), molybdenum (Mo), selenium (Se), silicon (Si), tin (Sn), vanadium (V), and zinc (Zn).
I. Atoms found in life

- **Hydrogen (H)**
  - Atomic number = 1

- **Carbon (C)**
  - Atomic number = 6

- **Nitrogen (N)**
  - Atomic number = 7

- **Oxygen (O)**
  - Atomic number = 8
# Molecules

## Table 2.8: Alternative Ways to Represent Molecules

<table>
<thead>
<tr>
<th>Molecular Formula</th>
<th>Electron Configuration</th>
<th>Structural Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td><img src="image" alt="Hydrogen" /></td>
<td>H–H Single bond</td>
</tr>
<tr>
<td>O₂</td>
<td><img src="image" alt="Oxygen" /></td>
<td>O=O Double bond</td>
</tr>
<tr>
<td>CH₄ Methane</td>
<td><img src="image" alt="Methane" /></td>
<td>H–C–H</td>
</tr>
<tr>
<td>H₂O Water</td>
<td><img src="image" alt="Water" /></td>
<td>O–H</td>
</tr>
</tbody>
</table>
II. Molecules

A. Molecular bonds
   1. covalent bonds
      a. number of bonds and molecular stability
      b. polar and nonpolar covalent bonds
II. Molecules

2. Ionic bonds

\[ \text{Na}^+ + \text{Cl}^- \rightarrow \text{NaCl} \]

oxidized \hspace{1cm} \text{reduced}

Oxidation-reduction Rx (redox)
II. Molecules

B. Hydrogen bonds
# Functional groups

A small group of atoms that impart specific properties to the molecules to which they are attached.

<table>
<thead>
<tr>
<th>Functional group</th>
<th>Class of compounds</th>
<th>Structural formula</th>
<th>Example</th>
<th>Ball-and-stick model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydroxyl (-OH)</td>
<td>Alcohols</td>
<td>R—OH</td>
<td>Ethanol</td>
<td><img src="image" alt="Ethanol" /></td>
</tr>
<tr>
<td>Carbonyl (-CHO)</td>
<td>Aldehydes</td>
<td>R—O</td>
<td>Acetaldehyde</td>
<td><img src="image" alt="Acetaldehyde" /></td>
</tr>
<tr>
<td>Carbonyl (-CO)</td>
<td>Ketones</td>
<td>R—C=O</td>
<td>Acetone</td>
<td><img src="image" alt="Acetone" /></td>
</tr>
<tr>
<td>Carboxyl (-COOH)</td>
<td>Carboxylic acids</td>
<td>R—C=O—OH</td>
<td>Acetic acid</td>
<td><img src="image" alt="Acetic acid" /></td>
</tr>
<tr>
<td>Amino (-NH₂)</td>
<td>Amines</td>
<td>R—NH₂</td>
<td>Methylamine</td>
<td><img src="image" alt="Methylamine" /></td>
</tr>
<tr>
<td>Phosphate (-PO₃²⁻)</td>
<td>Organic phosphates</td>
<td>R—O—P—O⁻</td>
<td>3-Phosphoglyceric acid</td>
<td><img src="image" alt="3-Phosphoglyceric acid" /></td>
</tr>
<tr>
<td>Sulphhydryl (-SH)</td>
<td>Thiols</td>
<td>R—SH</td>
<td>Mercaptoethanol</td>
<td><img src="image" alt="Mercaptoethanol" /></td>
</tr>
</tbody>
</table>
Organic and Biochemistry

I. Introduction
II. Nucleic acids
   A. 3 functions
   B. Nucleotides
   C. DNA/RNA
   D. ATP
III. Proteins
   A. multiple functions
   B. amino acids
   C. Protein structure
      1. globular and fibrous
      2. four levels of structure
IV. Carbohydrates
   A. Monosaccharides
   B. Disaccharides
   C. Polysaccharides
V. Lipids
   A. Triglycerides
      1. glycerol and fatty acids
      2. saturated vs. unsaturated
   B. Lipoproteins
   C. Phospholipids
   D. Steroids
C. Biological molecules

1. 4 main classes
2. Monomers
3. Condensation and hydrolysis reactions
4. Functional groups

- carbohydrates
- lipids
- proteins
- nucleic acids
2. Monomers

<table>
<thead>
<tr>
<th>Carbohydrates</th>
<th>monosaccharides</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lipids</td>
<td>fatty acids</td>
</tr>
<tr>
<td>Proteins</td>
<td>amino acids</td>
</tr>
<tr>
<td>Nucleic acids</td>
<td>nucleotides</td>
</tr>
</tbody>
</table>

Monosaccharides

Fatty acids

Dimers

Polymers

Polarity?
V. Nucleic Acids

A. 3 functions

B. Nucleotides
C. DNA/RNA
D. ATP

A. 3 functions of nucleic acids carriers

1. information
2. energy
3. electrons

NADH

DNA/ RNA

ATP
B. Nucleotides

Phosphate, 5 carbon sugar, and nitrogenous base
ribose or deoxyribose
A, T or U, C, G

C. DNA/ RNA

Deoxyribose nucleic acid

Ribose nucleic acid
Protein

- A sequence from 20 amino acids
  
  ![Protein Structure]

- Adopts a stable 3D structure that can be measured experimentally
  
  ![Protein Structure]
IV. Proteins

A. Multiple functions
B. Amino acids
C. Protein structure
   1. globular and fibrous
   2. four levels of structure

Myosin and actin

Structural
Enzymes
Hormones
Lipoproteins

HDL/ LDL/ VLDL
hemoglobin
fibrin
Protein Structure Space

http://www.nigms.nih.gov/psi/
B. Amino acids

Leucine (hydrophobic)

Serine (hydrophilic)
Side Chain Structures

Alanine (A)
[Cys]

Cysteine (C)
[His]

Histidine (H)

Methionine (M)

Threonine (T)

Asparagine (N)
[Glu]

Glutamic Acid (E)

Leucine (L)

Proline (P)

Tyrosine (Y)

Valine (V)

Arginine (R)

Glutamine (Q)

Isoleucine (I)

Phenylalanine (F)

Tryptophan (W)

Aspartic Acid (D)

Glycine (G)

Lysine (K)

Serine (S)

[ Ala ]

[ Cys ]

[ His ]

[ Met ]

[ Thr ]

[ Asn ]

[ Gin ]

[ Ile ]

[ Phe ]

[ Trp ]

[ Arg ]

[ Glu ]

[ Leu ]

[ Pro ]

[ Tyr ]

[ Asp ]

[ Gly ]

[ Lys ]

[ Ser ]

[ Val ]
Amino acids & side chains

- nonpolar and hydrophobic
- polar and hydrophilic
- acidic
- basic
Bonds

- Protein folding is influenced by many bonds.
- Many of the covalent bonds in a long chain of amino acids allow free rotation of the atoms they join, so that the polypeptide backbone can in principle fold in an enormous number of ways.
- Each folded chain will be constrained by many different sets of weak non-covalent bonds formed by atoms – hydrogen bonds, ionic bonds, and van der Waals attractions.
- Individual non-covalent bonds are weak compared to covalent bonds, so that it takes many non-covalent bonds to hold two regions of a polypeptide chain together.
Peptide bonds

Amino acid + Amino acid → Dipeptide

Dehydration synthesis
Polypeptide backbone can in principle fold in an enormous number of ways

- Two bonds within the backbone can rotate to allow different shapes to be formed.
- The angles of these bonds determine the backbone conformation ($\varphi$ and $\psi$).
- Shape or conformation of protein is determined by peptide chain backbone.
Hydrogen Bonds

- Some atoms (esp. O and N) can draw electrons away from surrounding hydrogens
- This creates a partial charge
- These partial charges can interact to form hydrogen bonds

- Hydrogen bonds form:
  - between main chain polar groups in the core of the protein
  - amino acid side chain and main chain atoms and water on the surface of the protein
Each folded chain is constrained by many non-covalent bonds
Principles of protein structure

Primary amino acid sequence

Secondary structure: $\alpha$ helices, $\beta$ sheets

Tertiary structure: from X-ray, NMR

Quaternary structure: multiple subunits
Protein secondary structure

- Secondary structure describes the way the chain folds
- Local structure of consecutive amino acids
- Common regular secondary structures
  - α Helix
  - β Sheet
  - β turn
**α-helices**

- The commonest secondary structural elements
- Generated by local hydrogen bonding between C=O and N-H groups close together
- O of each residue (n) accepts a hydrogen bond from four residues further along (n+4).
- The alpha helix has 3.6 residues per turn, corresponding to a rotation of 100 degree per residue, so that side chains project out from the helical axis at 100 degree intervals.
\(\alpha\)-helices

Myoglobin (John Kendrew, 1958)

Myoglobin is an example of a protein having many \(\alpha\)-helices. These are formed by amino acid stretches 4-40 residues in length.

The view down the helix axis

Side chains project out from the helical axis.
Beta sheet

- Beta sheet involves hydrogen bonds between backbone groups from residues distant from each other.
- Two or more strands that may be widely separated in the protein sequence are arranged side by side, with hydrogen bonds between the strands.
- The strands can run in the same direction (parallel beta sheet) or antiparallel direction (name); mixed sheets are also possible.
**β sheets**

Thioredoxin from *E. coli* is an example of a protein with many β sheets, formed from β strands composed of 5-10 residues. They are arranged in parallel or antiparallel orientations.

*Thioredoxin*
beta turn

- The simplest secondary structure element usually involves four residues but sometimes requires only three.
- It consists of a hydrogen bond between the carbonyl oxygen of one residue (n) and the amide N-H of residue n + 3, reversing the direction of the chain.
- This turn element is called a beta turn or reverse turn or hairpin turn.
Tertiary structure

- In a folded protein, the secondary structure elements fold into a compact and nearly solid object stabilized by weak interactions involving both polar and nonpolar groups.
- The resulting compact folded form is called the tertiary structure of the protein.
- One way to characterize tertiary structure is by the topological arrangement of the various secondary structure elements as they pack together.
- One effect of tertiary structure is to create a complex surface topography that enables a protein to interact specifically either with small molecules that may bind in clefts, or with other macromolecules, with which it may have regions of complementary topology and charge.
Beta barrel

- In this retinol-binding protein (PDB 1rlb), a large antiparallel beta sheet curves all the way around so that the last strand is hydrogen bonded to the first, forming a closed cylinder. The interior of this beta barrel is lined with hydrophobic side chains; nonpolar molecules can bind inside
Tertiary structure

- Two proteins with similar secondary structure elements may have different tertiary structures.
- Approximately the same secondary structure elements can be arranged in more than one way.
- Both TIM (left) and DHFR (right) consist of eight beta strands with connecting alpha helices, yet the 3D structures are quite different.
Program for Visualization

- **RASMOL** (authored by Roger A. Sayle) is one of the most frequently used software.
  - Available for most of computer systems PC/Windows, Macintosh, Unix
  - Easy to operate and generate nice pictures.

- **Swiss PDB Viewer** (authored by Nicolus Guex, etc)
  - Complex but provides more computational functions.

- **PyMOL**
Different representation of structure

- There is a variety of representation methods for structure, which are suitable for different purposes.
  - Spacefill
  - Ball and stick
  - Cartoons
  - Others
3. Polysaccharides
II. Carbohydrates

A. Monosaccharides

B. Disaccharides

\[ C_6H_{12}O_6 \]

Polarity (1:2:1)

Monosaccharide

Disaccharide

Isomers

\( \alpha \)-Glucose

\( \beta \)-Fructose

Sucrose

\( \beta \)-Galactose

\( \beta \)-Lactose
Glucose
III. Lipids

A. Triglycerides

1. glycerol and fatty acids
2. saturated vs. unsaturated

Saturated versus unsaturated