# Fundamentals

BIOS 1006

17 June 2025

## Objectives

- Know all definitions.
- Know the basic atoms that comprise biological systems. (CHNOPS)
- Describe why carbon is ideal for forming the skeleton of biomolecules.
- Name and draw the common functional groups found in biomolecules.
- Recognize different molecular representations and draw abbreviated and expanded structural formulae.
- Describe the four basic building that comprise biological systems, their different sub-classifications, and the four major classes of biomolecules that they form. Identify to which class of the four basic building blocks a small molecule belongs or is related.
- Describe the properties of water that make it an ideal solute for life.
- Describe the properties of hydrogen bonds and what is required for them to be formed.
- Describe the three types of "weak" interactions, the types of groups that participate in these interactions and the role they play in solvation and biomolecular structure.
- Describe Lennard-Jones plots and use them to describe and predict interactions between molecules.
- Describe the hydrophobic effect and van der Waals interactions and describe their different roles in biomolecular structure.
- Describe the properties and principles of buffers and buffering capacity.
- Calculate the pH from the concentration of $H^+$ and vice versa.
- Calculate the pH, pKa or the amounts of acid and conjugate base using the Henderson-Hasselbalch equation.
- Predict protonation state of a group based on it pKa and the buffer pH.
- Describe the physiologically important buffers.

# Definitions

**electrostatic** involves charges

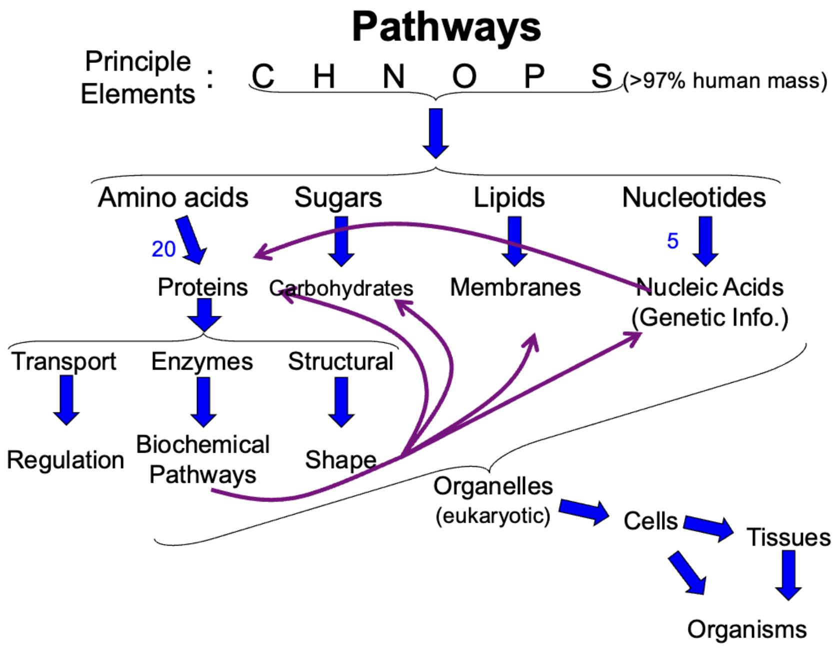
**functional groups** specific groups of atoms within molecules that are responsible for the molecule's characteristic chemical reactions

**solute** in a solution, dissolved in a solvent

**solvent** in a solution, dissolves the solute

**weak interactions** weaker, transient interactions that are additive and can become stronger

## The biological building blocks




### Functional groups

(R denotes a generic hydrocarbon chain)

Memorize!

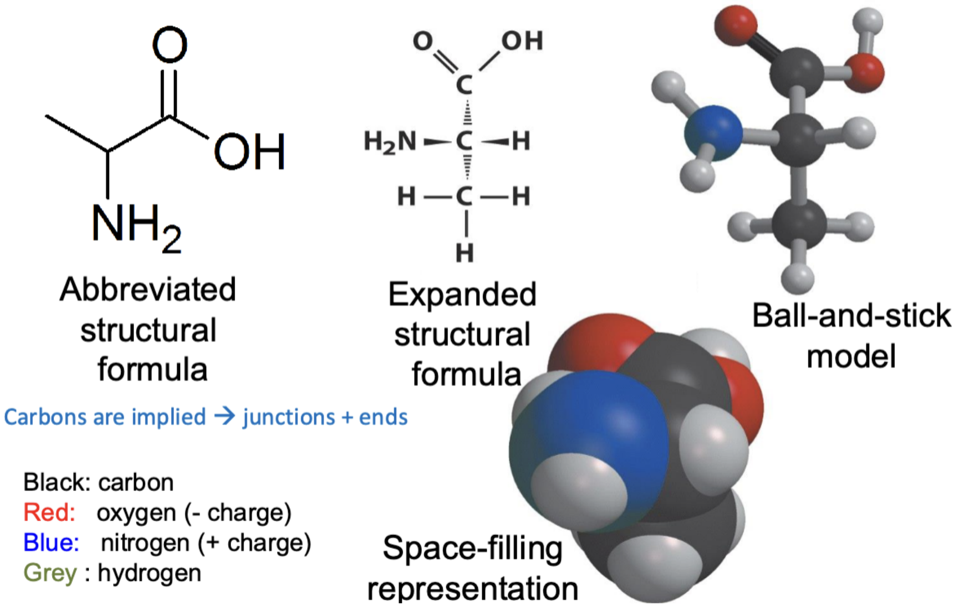
| Family Name | Group Structure | Group Name | Significance |
|---|---|---|---|
| Alcohol | R—OH | Hydroxyl | Polar (and therefore water-soluble), forms hydrogen bonds |
| Aldehyde | R—C(=O)—H | Carbonyl | Polar, found in some sugars |
| Ketone | R—C(=O)—R′ | Carbonyl | Polar, found in some sugars |
| Acids | R—C(=O)—OH | Carboxyl | Weakly acidic, bears a negative charge when it donates a proton |
| Amine | R—$NH_2$ | Amino | Weakly basic, bears a positive charge when it accepts a proton |
| Amide | R—C(=O)—$NH_2$ | Amido | Polar but does not bear a charge |
| Thiol | R—SH | Thiol | Easily oxidized; can form —S—S— (disulfide) bonds readily |
| Ester | R—C(=O)—O—R′ | Ester | Found in certain lipid molecules |
| Alkene | RCH═CHR′ | Double bond | Important structural component of many biomolecules (e.g., found in lipid molecules) |

+ **phosphate** ($PO_4^{3-}$)

- **Hydroxyl + carbonyl → carboxyl**

- **Amine + carbonyl → amide**
- **Aldehyde** has carboxyl at the **end**; **ketone** has it in the **middle**

## Representations of molecules




## The four major classes

### Amino acids

- Hundreds of naturally occurring forms
- Defined by the presence of amine and carboxylic acid groups
- Classified based on the proximity of these groups
- Three different classes: $\alpha$, $\beta$, and $\gamma$ based on which carbon is attached to the amine (closest to the central carbon is $\alpha$, next is $\gamma$, etc.)
- $\alpha$ amino acid (most common): **amine** attached to $\alpha$ **carbon** (1 away from the central carbon), carboxyl and an **R group** (side chain, 20 different common types)
- **Peptide** or **amide** bonds link amino acids together (form amide group with the carboxyl group + amine group)

### Sugars (carbohydrates)

- Molecules containing carbonyl and hydroxyl functional groups
- Two classes: **ketose** and **aldose** sugars (carbonyl in the middle = ketose, at the end = aldose, same as functional groups)
- Hydrated carbons
- Very hydrophilic

**Lipids**

- Soluble in hydrophobic solutions
- Do not polymerize but form higher order structures
- Fatty acids

**Nucleotides**

- 3 basic components: phosphate group(s), ribose, nitrogenous base
- Polymerize into: DNA (deoxyribose, adenosine, cytosine, guanine, thymine); RNA (ribose, adenosine, cytosine, guanine, uracil)
- **Purines** (2 rings) and **pyrimidines** (1 ring)
- Mnemonics: “Pure As Gold” (adenine and guanine are purines) and “CUT the Py” (cytosine, thymine, and uracil are pyrimidines)

# Water ($H_2O$): the biological solvent

## Physical properties of water

- Solvent characteristics
- Non-compressible
- Chemical stability
- Biochemical reactant
- Hydration of molecules
- Participates in biomolecular interactions
- Ice floats
- High boiling and freezing temperatures
- High heat of vaporization
- High specific heat capacity
- High surface tension
- Dissolves molecules with ionizable or polarizable functional groups but cannot dissolve nonpolar or hydrophobic molecules

## Molecular properties of water

- **Tetrahedral** electron geometry (104.5 degrees), $sp^3$ hybridized, 0.99 Å from H to O
- Electronegativity results in the formation of **polar bonds**
- Forms **hydrogen bonds** (hydrogen is attracted to the lone pair electrons of an oxygen from another molecule)

## Properties of hydrogen bonds

- Hydrogen bonds in between casual interaction and covalent interaction in terms of proximity
- Both covalent and electrostatic properties
- Collinear orientation (present in a straight line)
- Other orientations possible but not as strong
- Electrostatic interaction
- Atoms involved share electrons
- In liquid water, 3.4 neighbors on average (4 in ice)

## Weak interactions

- Weak interactions are constantly being formed and broken between biomolecules (more transient)
- Additive (can become strong)
- Essential for rapid communication
- Allows for flexibility
- Three types of weak electrostatic interactions
  - **Salt bridges** (ionic)
  - **Van der Waals interactions**
  - **Hydrogen bonds**

## Relative strengths of interactions

Strongest to weakest

- Int**ra**molecular forces
  - Ionic bonds
  - Covalent bonds
- Int**er**molecular forces (IMFs)
  - Ionic interactions and salt bridges
  - Van der Waals forces
  - Hydrogen bonds
  - Dipole-dipole interactions
  - London dispersion forces (LDFs)

### Salt bridges and ionic interactions

- One positive interacting with one negative with full electrical charges (ionic bonds are NOT salt bridges)
- Interaction strength calculated from Coulomb's law:

$$F = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{\varepsilon_r r^2}$$

  - $F$ is interaction strength
  - $q_1$ and $q_2$ are signed charges
  - $r$ is the distance between centers
  - $\varepsilon_r$ is the dielectric constant
  - All others are constants

- Water is good at breaking ionic bonds
- **Hydration shells** prevent ionic bonds from reforming