Biological and Bioorganic Chemistry
Some useful material will be announced ...
What shall we do?

Feb 19

Mar 4

Mar 18
Carbonyl compounds – aldehydes and ketones. Carbohydrates.

Apr 1

Apr 15
Amines, aminoacids, peptides. Heterocyclic compounds and their biological activity.
Amines
The amino group

Bond angles in ammonia: 107°

- Ammonia
- Methylamine
- Ethylamine
Amines are organic compounds and functional groups that contain a basic nitrogen atom with a lone electronic pair.
Amines classification

Secondary Amine

Tertiary Amine

Quaternary Ammonium Chloride

Secondary Amine

Primary Amine
Naming aliphatic amines

- Dimethylamine
- Trimethylamine
- Tetramethylammonium Chloride
- N,N-dimethylpropylamine
- Benzylamine (phenylmethylnamine)
Naming aliphatic amines

- Methanamine (methylamine)
- Propan-1-amine (n-propyl amine)
- Propan-2-amine (isopropyl amine)

- N-methylethanamine
- N-ethyl-N-methylpropanamine

IUPAC nomenclature
Isomerism of amines

ISOMERISM

- Structural Isomerism
  - Chain Isomerism
  - Position Isomerism
  - Functional Isomerism
- Stereoisomerism or space isomerism (Geometrical isomerism)
- Metamerism
Synthesis of amines

\[
\text{CH}_3\text{(CH}_2\text{)_6CH}_2\text{Br} + \text{NH}_3 \rightarrow \text{CH}_3\text{(CH}_2\text{)_6CH}_2\text{NH}_2 \quad 45\% \\
\rightarrow [\text{CH}_3\text{(CH}_2\text{)_6CH}_2\text{]}_2\text{NH} \quad 43\% \\
\rightarrow [\text{CH}_3\text{(CH}_2\text{)_6CH}_2\text{]}_3\text{N} \quad \text{Trace} \\
\rightarrow [\text{CH}_3\text{(CH}_2\text{)_6CH}_2\text{]}_4\text{N}^+\text{Br}^- \quad \text{Smaller Trace}
\]
Synthesis of amines

\[ \text{CH}_3(\text{CH}_2)_6\text{CH}_2\text{Br} \quad \rightarrow \quad \text{CH}_3(\text{CH}_2)_6\text{CH}_2\text{N}=\text{N} \quad \text{N} \]

+ NaN₃

2. LiAlH₄

\[ \text{CH}_3(\text{CH}_2)_6\text{CH}_2\text{NH}_2 \]

\[ \text{H}_2\text{N-R} \]

\[ \text{R-X} \]

KOH

\[ \text{H}^+/\text{H}_2\text{O} \]
Synthesis of amines
Synthesis of amines

The Hofmann rearrangement...

The Curtius rearrangement...
Basicity of amines

\[
\text{NH}_2 + \text{HCl} \rightarrow \text{NH}_3^+\text{Cl}^-
\]

phenylammonium chloride
Basicity of amines

- $R \rightarrow \text{N}^\text{+}$
- $R \rightarrow \text{N}^\text{+}$
- $R \rightarrow \text{N}^\text{+}$

$\rightarrow$ basic character increases

More basic
- $\text{NH}_2$
- $\delta^-$
- $\delta^-$
- $\delta^-$
- $\text{OH}$

Less basic
- $\text{NH}_2$
- $\delta^+$
- $\delta^+$

Less basic
- $\text{NH}_2$
- X

$\text{ortho effect}$

$\text{e}^-$ donating group

$\text{e}^-$ withdrawing group
Reactions of amines

Chemical reaction diagram showing the interaction between two compounds.
Reactions of amines

\[
\begin{align*}
\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3\text{SO}_2\text{Cl} & \rightarrow \text{a sulfonamide} \\
\end{align*}
\]
Reactions of amines

Hofmann elimination
Biologically active amines

Examples of Pharmaceuticals Containing α-Chiral Amines

- **Amikacin** (Amikin, BMS) antibiotic
- **Sitagliptin** (Januvia, Merck) type 2 diabetes
- **Oseltamivir** (Tamiflu, Gilead) anti-viral
- **Chloroquine** (Aralen) anti-malarial
- **Sertraline** (Zoloft, Pfizer) Serotonin Reuptake Inhibitor
Amino acids structure

Unionized (1) and zwitterionic (2) structures of amino acids
Standard amino acids

- Alanin (Ala)
- Arginin (Arg)
- Asparagin (Asn)
- Asparaginsäure (Asp)
- Cysteine (Cys)
- Glutaminsäure (Glu)
- Glutamin (Gln)
- Glycin (Gly)
- Histidin (His)
- Isoleucin (Ile)
- Leucin (Leu)
- Lysin (Lys)
- Methionin (Met)
- Phenylalanin (Phe)
- Prolin (Pro)
- Serin (Ser)
- Threonin (Thr)
- Tryptophan (Trp)
- Tyrosin (Tyr)
- Valin (Val)
Standard amino acids
Peptide bond formation

Amino acid (1) + Amino acid (2) → Peptide bond → Dipeptide + Water
Polypeptides

Peptides - are short chains of **amino acid** monomers (< 20) linked by **peptide** (amide) bonds.
Like other biological macromolecules such as polysaccharides and nucleic acids, proteins are essential parts of organisms and participate in virtually every process within cells. Many proteins are enzymes that catalyze biochemical reactions and are vital to metabolism. Proteins also have structural or mechanical functions, such as actin and myosin in muscle and the proteins in the cytoskeleton, which form a system of scaffolding that maintains cell shape. Other proteins are important in cell signaling, immune responses, cell adhesion, and the cell cycle. Proteins are also necessary in animals' diets, since animals cannot synthesize all the amino acids they need and must obtain essential amino acids from food. Through the process of digestion, animals break down ingested protein into free amino acids that are then used in metabolism.
Proteins - are large biological molecules, or macromolecules, consisting of one or more chains of amino acid residues.
Biologically active heterocycles
Carboxylic acids derivatives

- Pyrroldine
- Tetrahydrothiophene
- Tetrahydrofuran
- Piperdine
- Pyran
- Dioxan
- Morpholine
- Pyrrole
- Thiophene
- Furan
- Pyridine
- Pyrimidine
- Pyrazine
- Triazine
- Imidazole
- Thiazole
- Oxazole
- Indole
- Purine
- Pyrone
- Pyridone
- Quinoline
- Isoquinoline
Pyrrole derivatives - porphyrins

Chemical structure of the Fe(II)-protoporphyrin IX heme group in myoglobin and hemoglobin.
Indole derivatives – tryptophan and LSD
Pyridine derivatives – vitamin B6, nicotine, cocaine
Imidazole and pyrazole derivatives – histamine, analgin
Drugs activity and danger

Active/Lethal Dose Ratio and Dependence Potential of Psychoactive Drugs

- Narcotics
- Depressants
- Stimulants
- Anesthetics
- Hallucinogens
- Cannabis

Drugs are classified based on their Active Dose / Lethal Dose ratio and Dependence Potential.
Caffeine – an everyday narcotic
Nucleic acids are polymeric macromolecules, or large biological molecules, essential for all known forms of life.

The Swiss scientist Friedrich Miescher discovered nucleic acids (DNA) in 1869. Later, he raises the idea that they could be involved in heredity.
Deoxyribonucleic acid (DNA)
Deoxyribonucleic acid (DNA) is a molecule that encodes the genetic instructions used in the development and functioning of all known living organisms and many viruses. DNA is a nucleic acid.
Thank you for your attention!