

Bioinformatics III

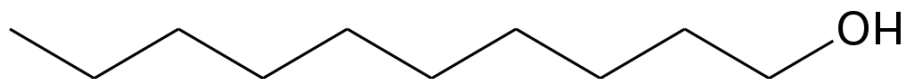
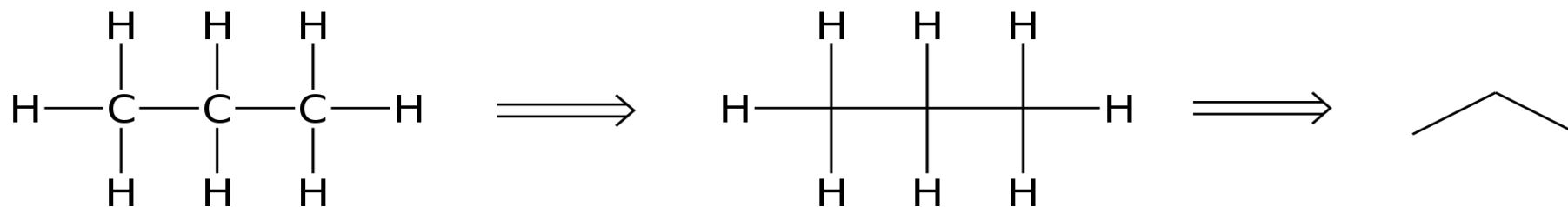
Analysis and prediction of 3D structures of biomolecules

Lecture 6 - biochemistry - a reminder

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2023 m.

Chemical formulae

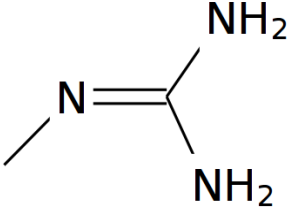
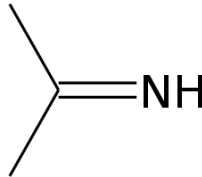
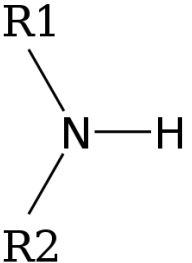
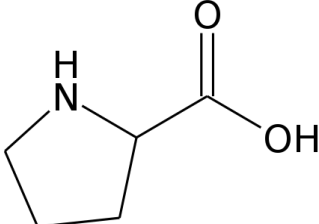
In organic chemistry structural formulae, bonds are depicted as lines and their intersections are carbon atoms; hydrogen atoms are usually implicit:



Functional groups

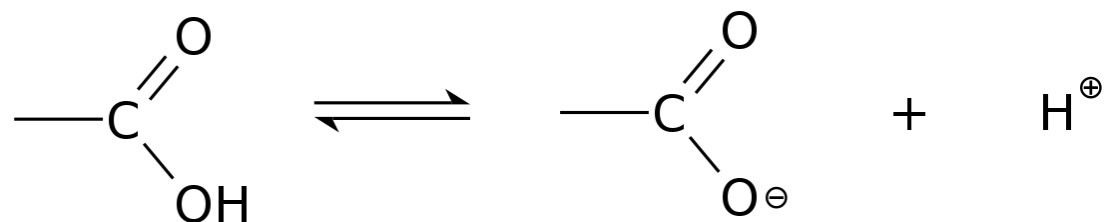
Formula	Name	Compounds	Properties
—OH	hydroxyl	alcohols	do not dissociate easily
—NH_2	amino	amines (primary)	basic
$\begin{array}{c} \text{O} \\ // \\ \text{—C} \\ \backslash \\ \text{OH} \end{array}$	carboxyl	organic acids	acidic
$\begin{array}{c} \text{O} \\ // \\ \text{—C} \\ \backslash \\ \text{NH}_2 \end{array}$	amido-	amides	very weak bases
$\begin{array}{c} \text{O} \\ // \\ \text{—C} \\ \backslash \\ \text{N—} \\ \\ \text{H} \end{array}$		secondary amides, peptides	

Functional groups (cont.)

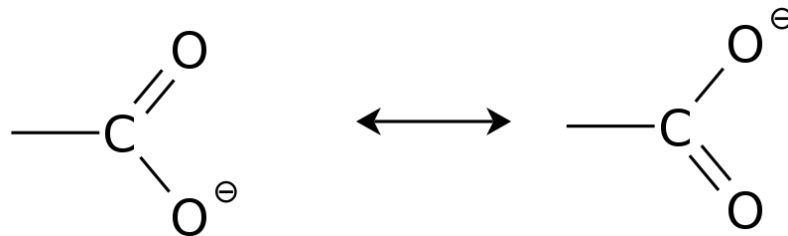
Formula	Name	Compounds	Properties
—SH	thiol, sulfo	thioalcohols, mercaptanes	hard to dissociate, easily oxidised
	guanidino-	guanidine derivatives	basic
	imino-	imines	
	secondary amino-	secondary amines	basic
	amino (imino) acid proline (Pro)		

Properties of organic acids

Dissociate in water:

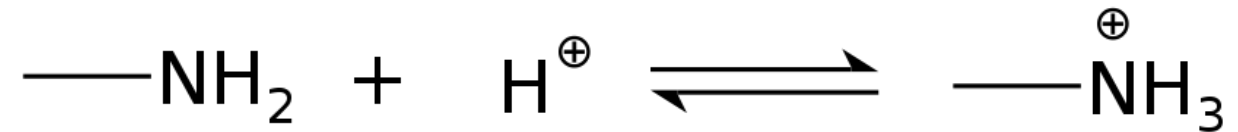


Carboxyle ion has a resonance structure:

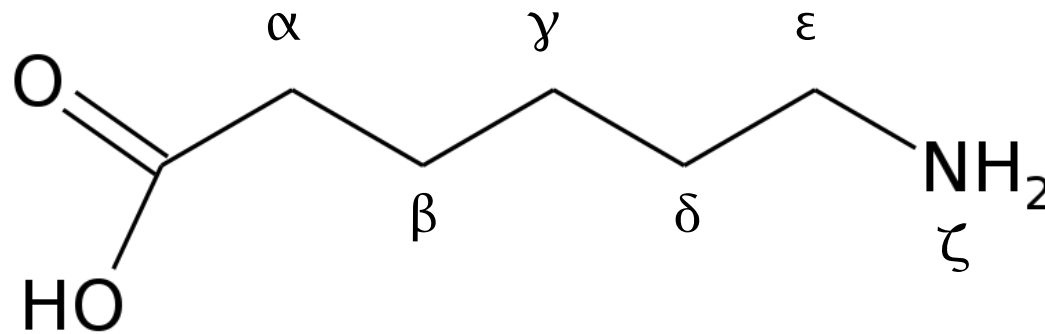


Properties of amino groups

Amines are basic (i.e. they can bind a proton):



Amino acids, biochemical nomenclature



αβγδε(ε)ζηθ(θ)ικλμνξοπρσ(ς)τυφ(φ)χψω

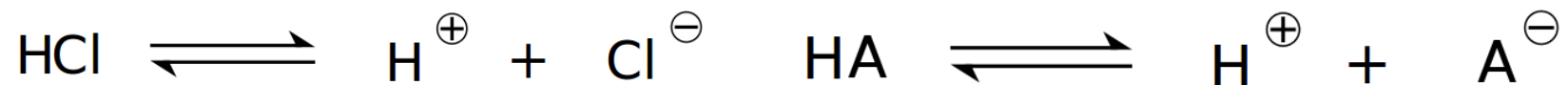
pH, buffers, ionisation constant



$$K = \frac{[\text{H}^+][\text{OH}^-]}{[\text{H}_2\text{O}]} = \text{const} \quad [\text{H}_2\text{O}] \gg [\text{H}^+] \Rightarrow [\text{H}_2\text{O}] = \text{const}$$

In a neutral medium:

$$[\text{H}^+][\text{OH}^-] = \text{const} = 10^{-14} \text{ M}^2 \quad \text{pH} = -\log_{10}[\text{H}^+] = 7$$

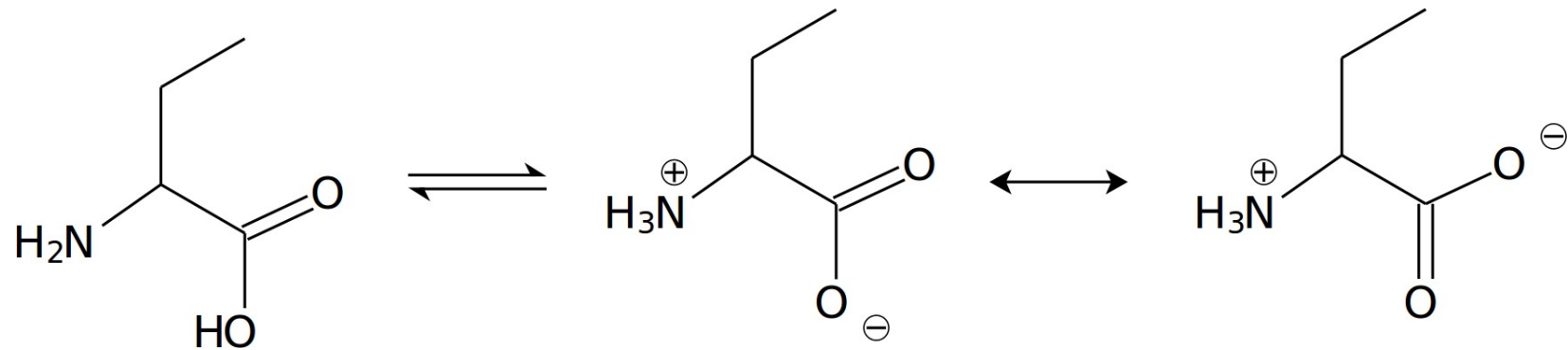


Henderson–Hasselbalch equation:

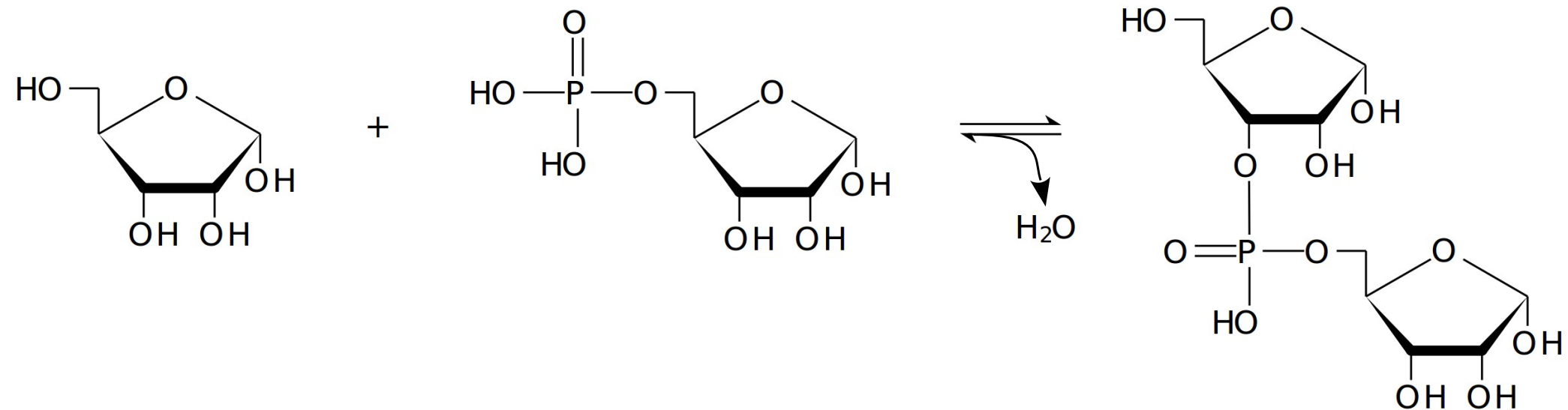
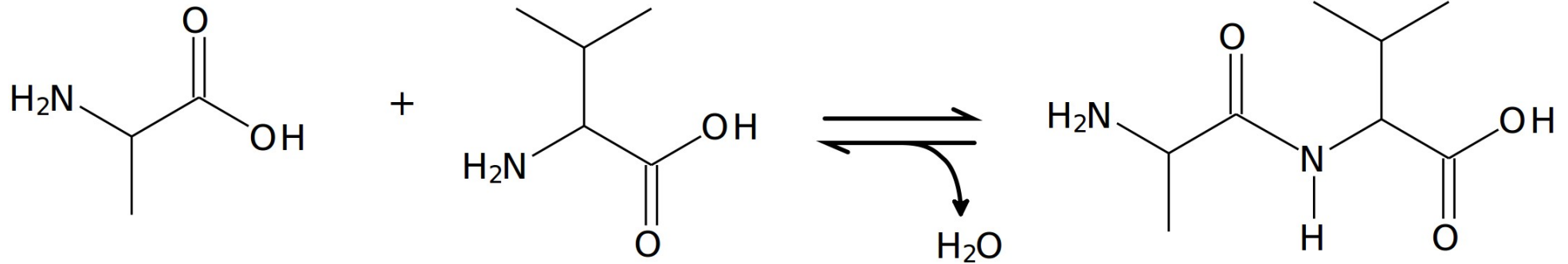
$$\text{pH} = \text{p}K_a + \log_{10} \frac{[\text{A}^-]}{[\text{HA}]}$$

Zwitterions

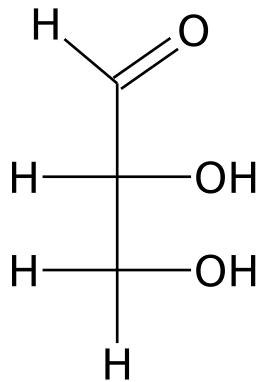
Amino acids have both of their groups ionised:



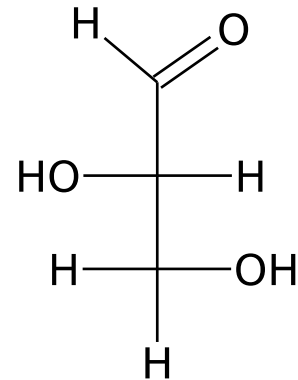
(Poli)condensation



Hydrocarbons. Glycerol aldehyde

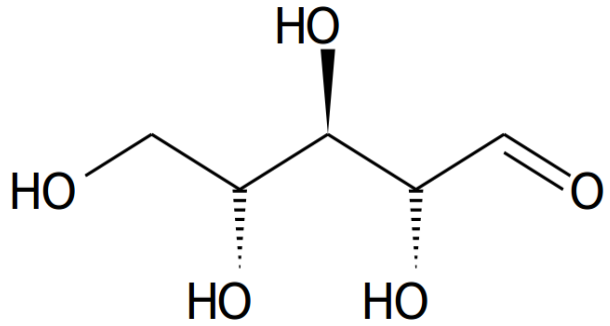


D-glyceraldehyde
(R)-glyceraldehyde
(+)-glyceraldehyde

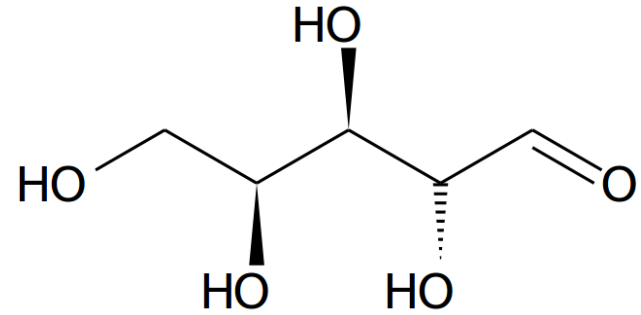


L-glyceraldehyde
(S)-glyceraldehyde
(-)-glyceraldehyde

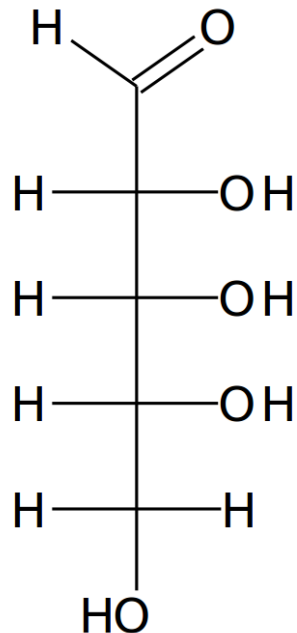
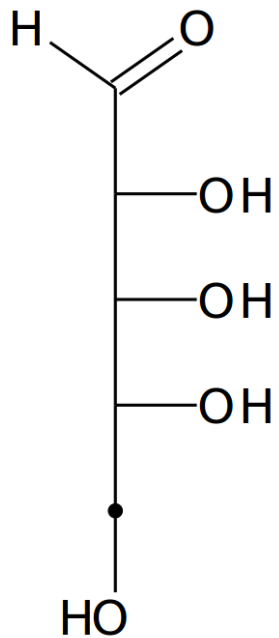
Sugars (saccharides)



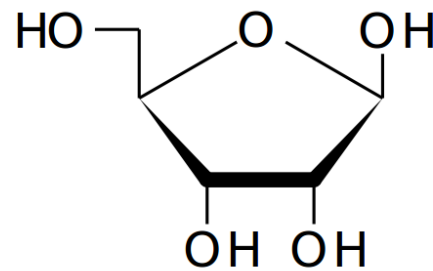
D-Ribose – linear form



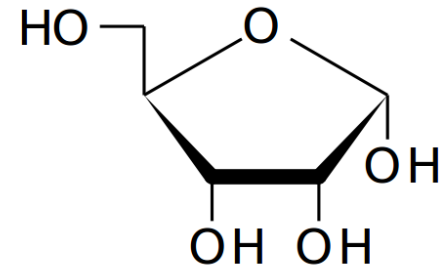
Another pentose



Fisher projections



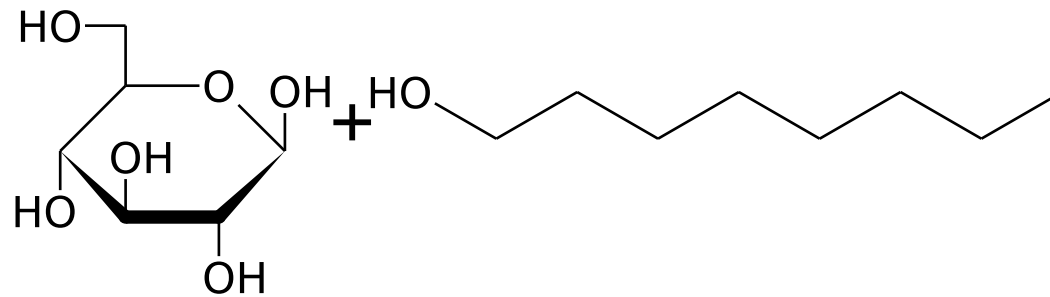
beta



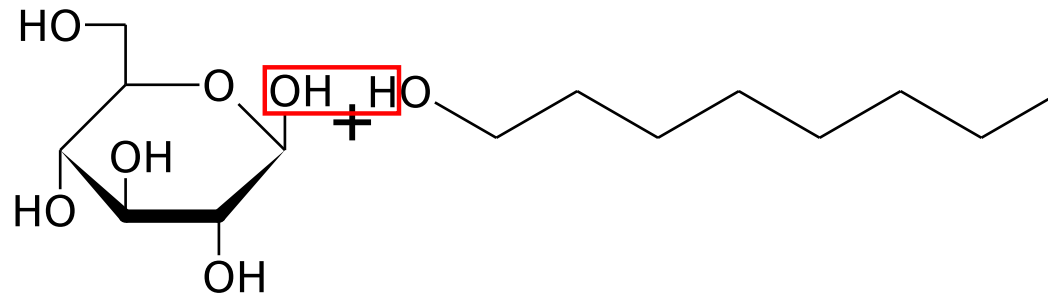
alpha

Ribofuranose

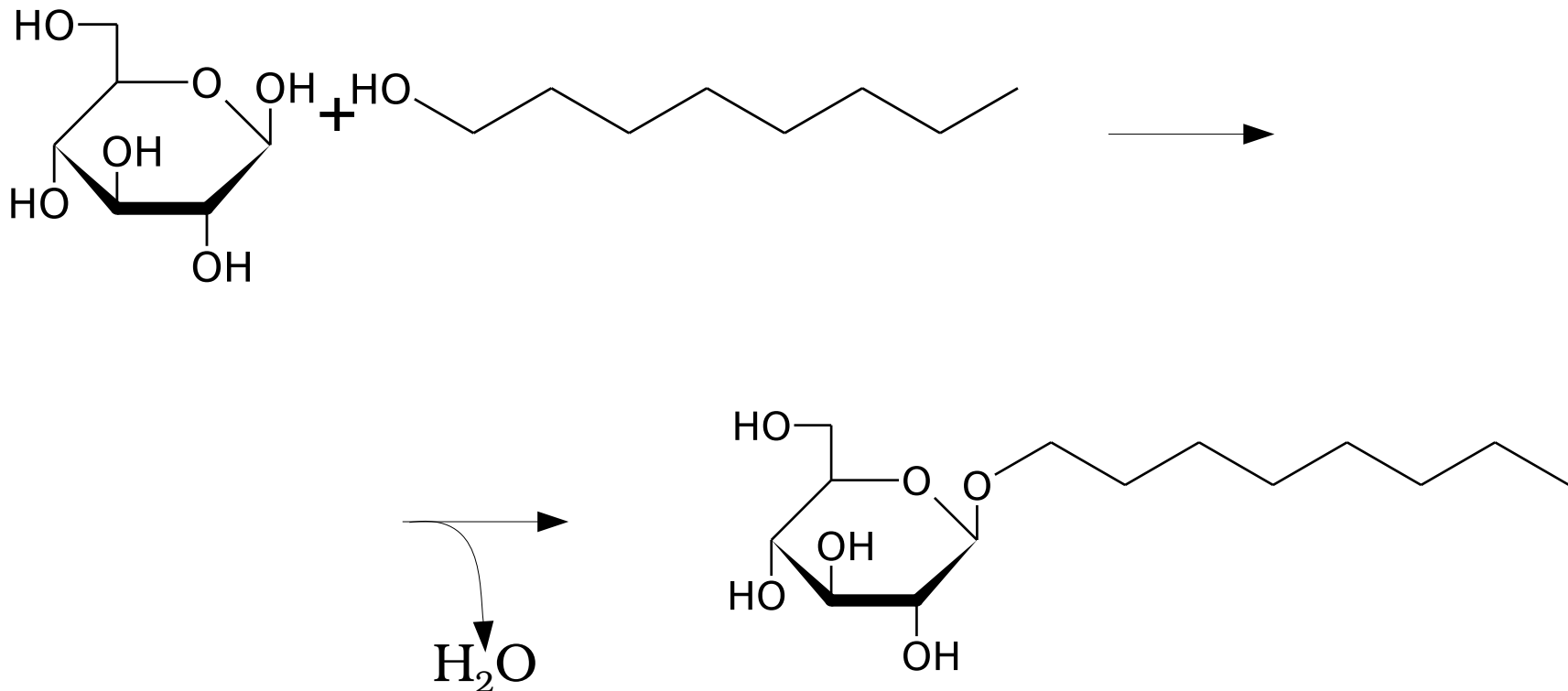
Glycosides



Glycosides

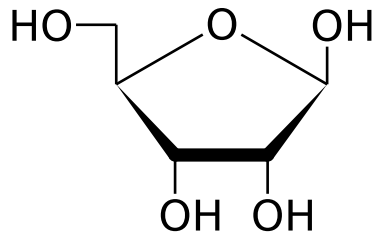


Glycosides

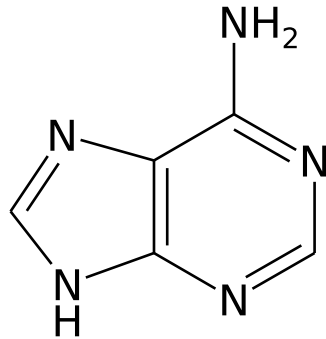


Octyl glucoside (n-octyl- β -D-glucoside)

Glycosides (Nucleosides)

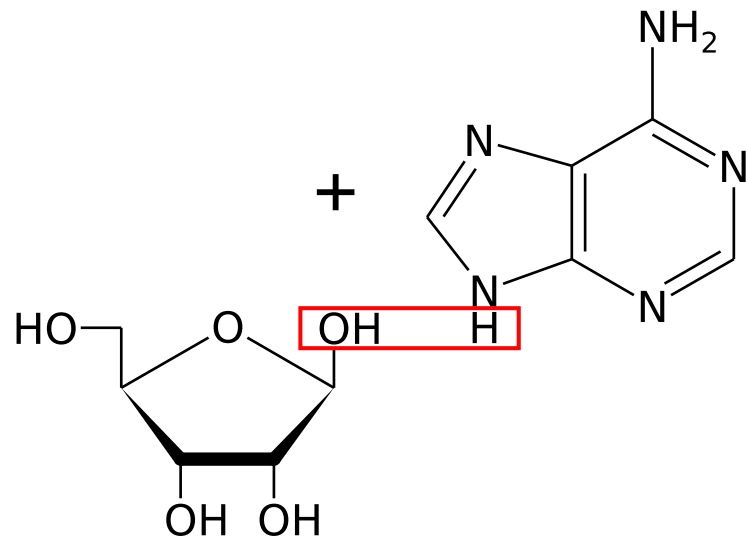


Ribose

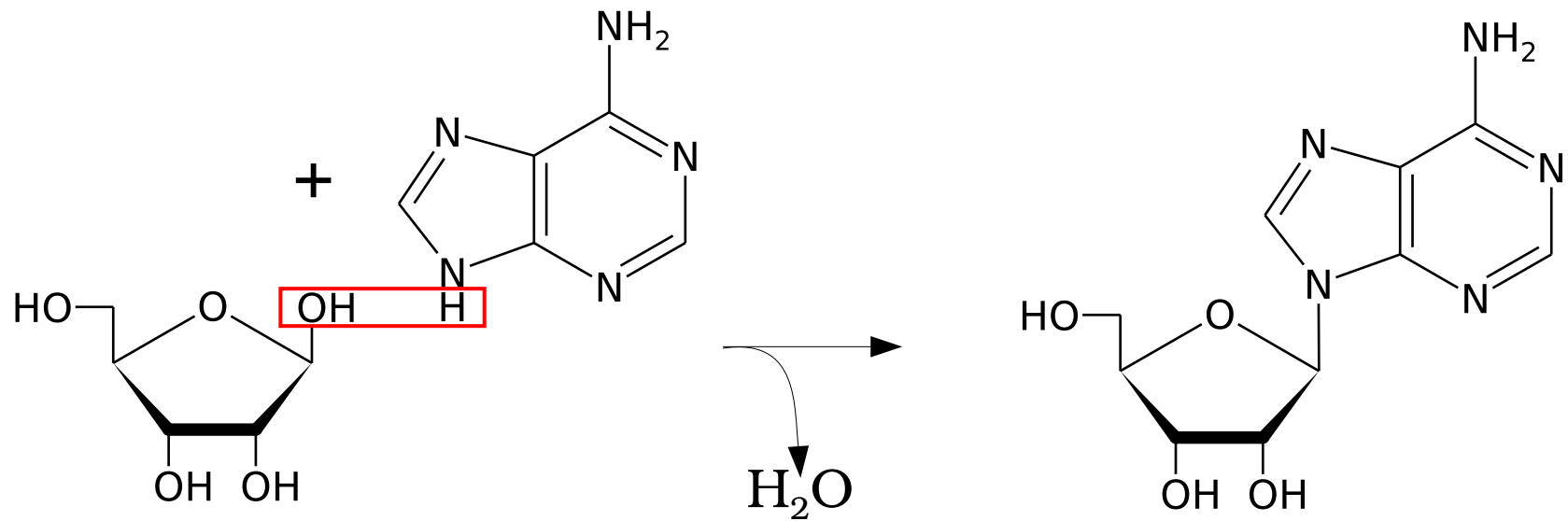


Adenine

Glycosides (Nucleosides)

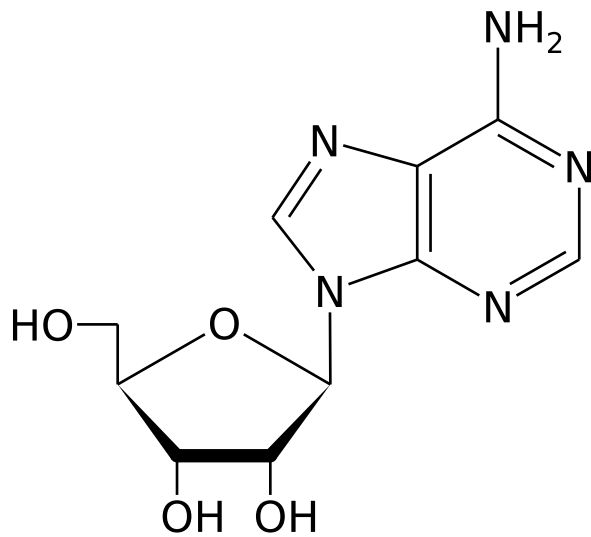


Glycosides (Nucleosides)

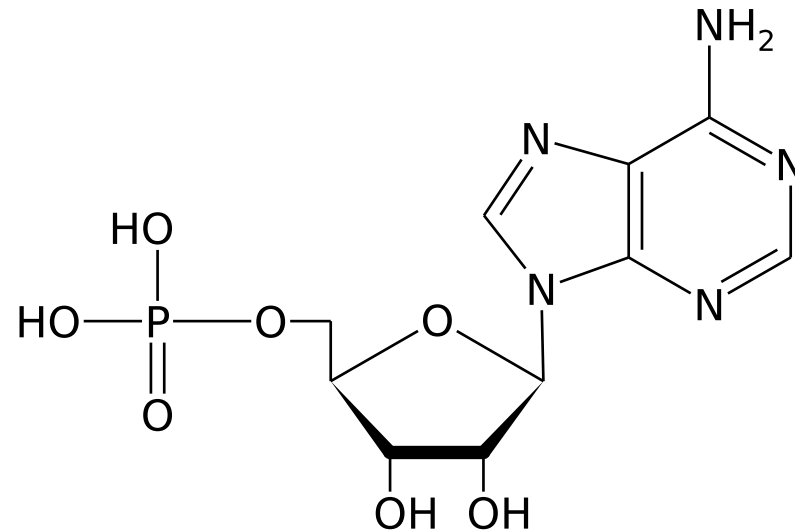


Adenosinas
(nukleozidas)

Nukleoides ir nukleotides

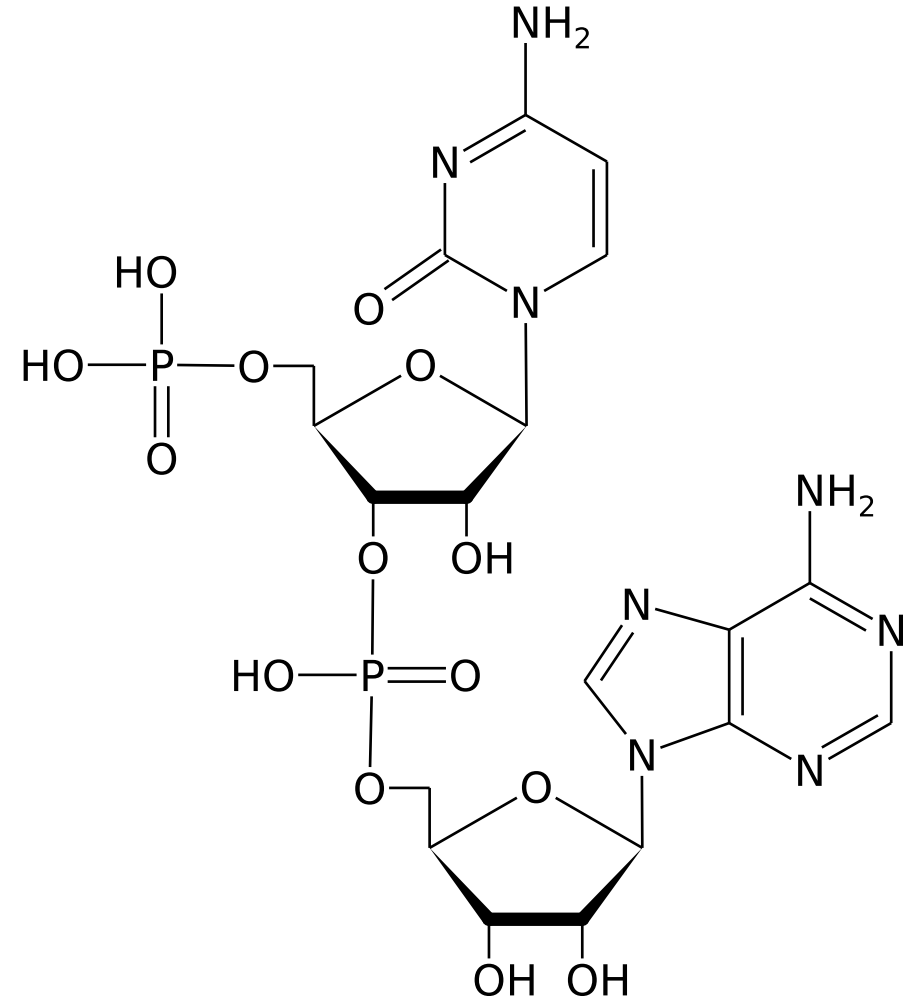
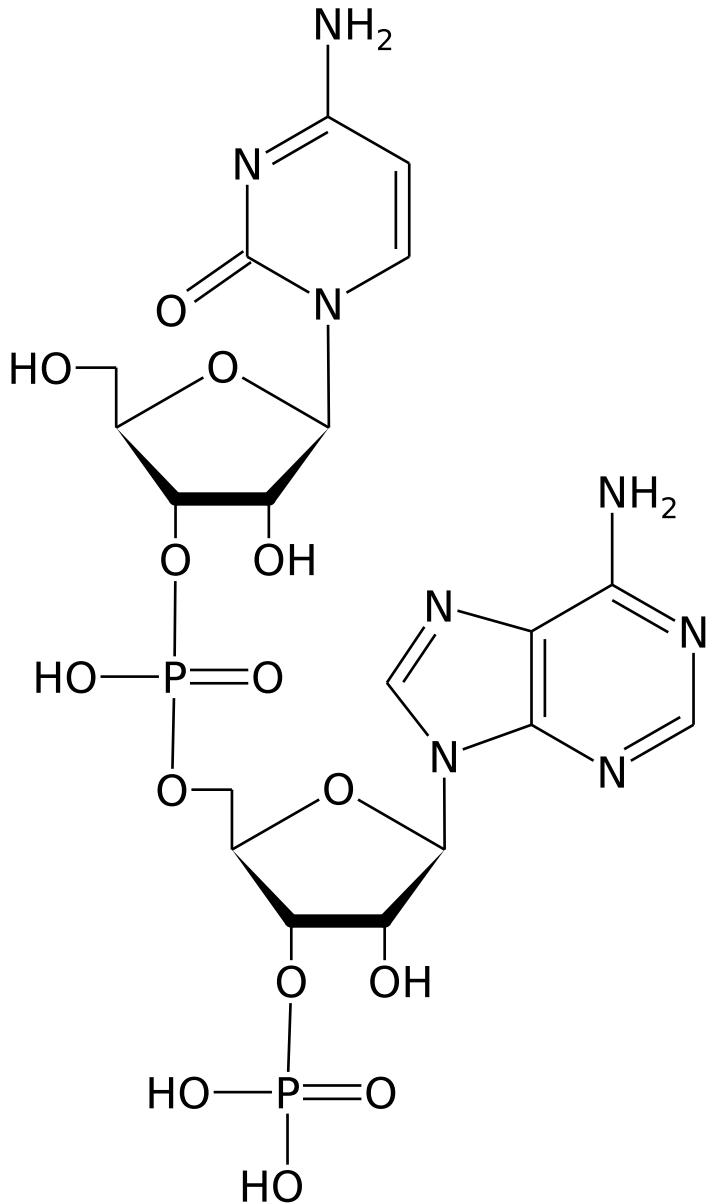


Adenosine
(nucleoside)

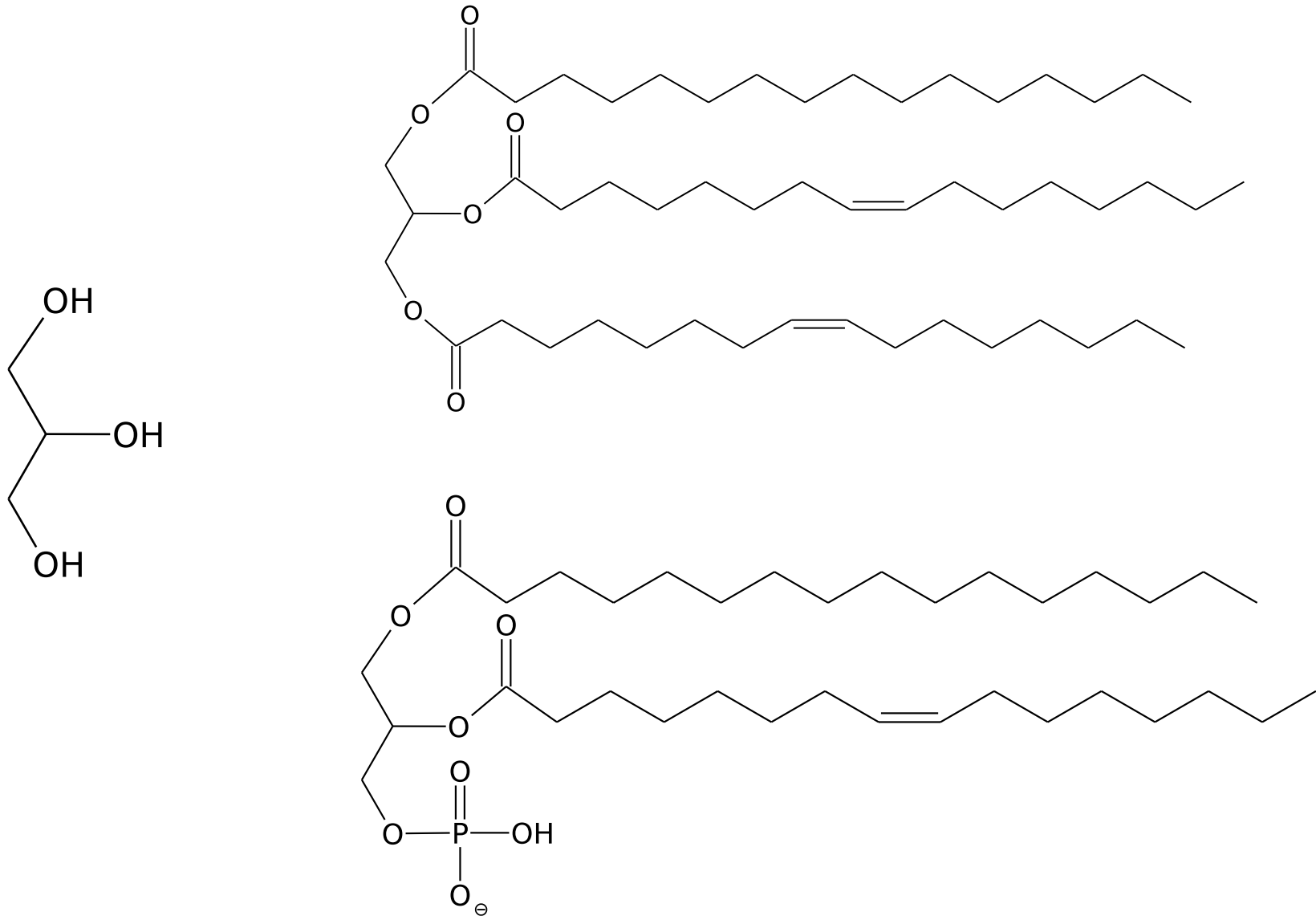


Adenosine phosphate
(nucleotide)

Nucleic acids



(Phospho-)lipids



Basic topics

- ✓ zwitterions
- ✓ policondensation
- ✓ el. dissociation
- ✓ acidity constant
- ✓ equilibrium
- ✓ pH & buffers
- ✓ sugars
- ✓ glycosides
- ✓ nucleotides
- ✓ nucleic acids
- ✓ (phospho-)lipids