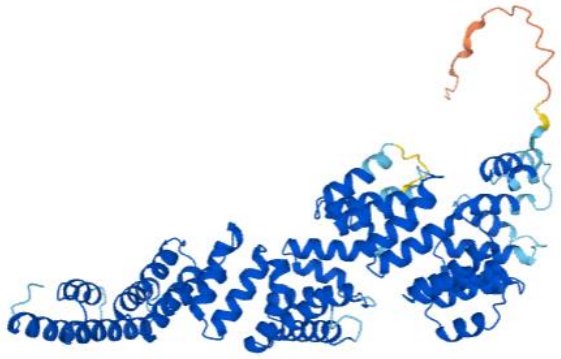
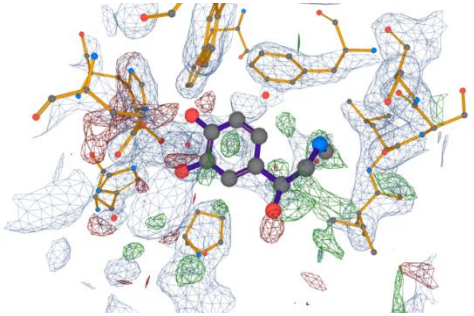
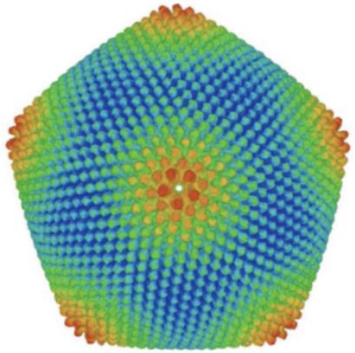
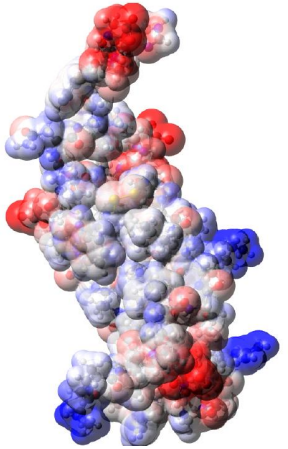
Molecular descriptors



Radka Svobodová

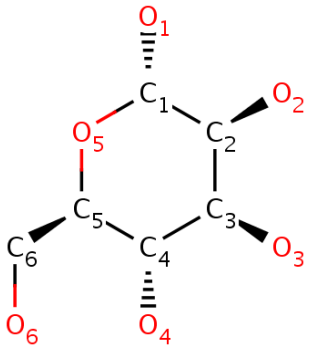


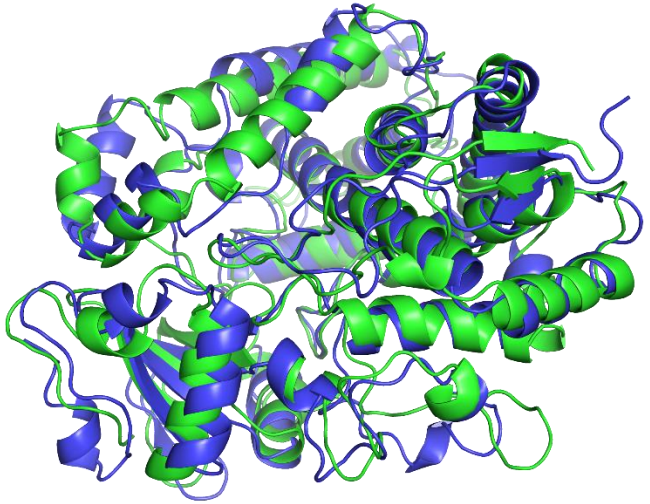




Content

- **Introduction:** concept of chemoinformatics, content of the subject, history of the field
- **Computer model of a molecule:** 1D, 2D and 3D structure, molecule representation using graph and matrix
- **2D structure (topology) of a molecule:**
  - writing a molecule using a string (SMILES, InChi, InChiKey)
  - **Molecular graphs:** Isomorphism and canonical indexing

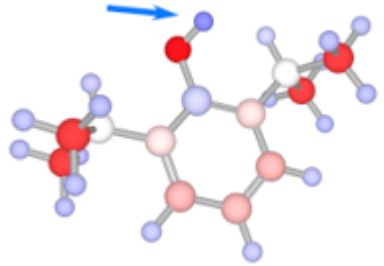


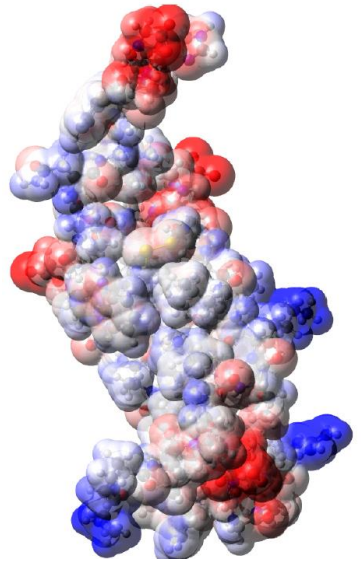


Content

Basic chemoinformatics tasks:

- **Molecular descriptors:** 1D, 2D and 3D descriptors, their application
- **Similarity of molecules:** similarity comparison, similarity coefficients
- **QSAR and QSPR models:** Models for studying quantitative relationships between structure and activity/property of
- **Databases** of small and large molecule structures, searching them





3D structure (geometry) of the molecule:

- representation using Cartesian and internal coordinates, data formats, geometry comparison
- **Visualization** of structures of molecules and molecular fragments, models for visualization of molecules
- **Generation of molecule structures** using AI algorithms

Introduction to descriptors

Molecule → **Numerical characteristics** (descriptors) → **property = function (descriptors)**

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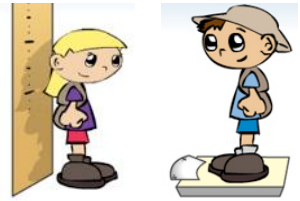
Example from life

Human body →



Height and weight →

BMI = weight / height^2

BMI (Body Mass Index):

Malnutrition: BMI < 18,5

Obesity: BMI > 30

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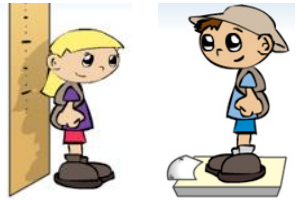

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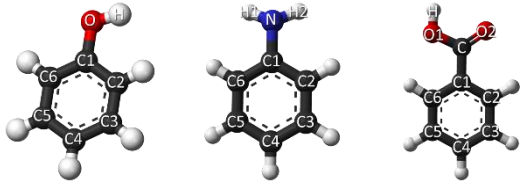
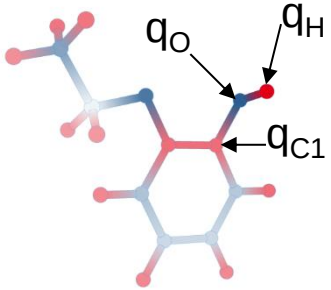
Chemoinformatics



Structure of a molecule

→



Charges on atoms

→

$pK_a = c_H.q_H + c_O.q_O + c_{C1}.q_{C1}$

where c_H, c_O and c_{C1} are parameters