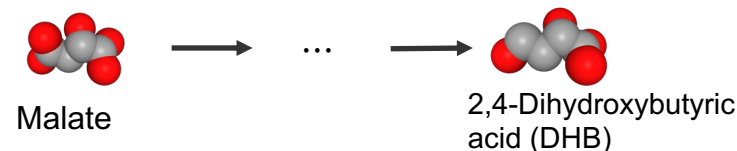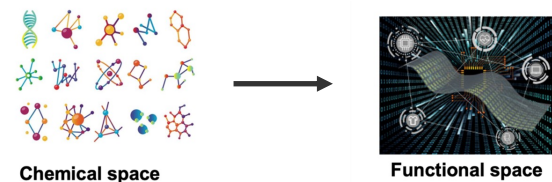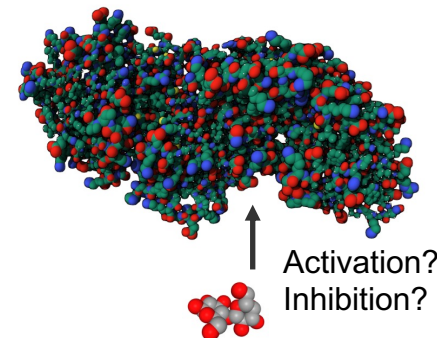# Why do we want to make predictions for molecules?

Motivation

- Molecules are the building blocks of life
  - Understanding their functions and interactions is relevant for many different natural sciences
    - Biology
    - Biochemistry
    - Medicine
    - Environmental Sciences
  - It has also many import industrial applications
    - Designing new materials with desired properties
    - Designing new pathways of chemical reactions for the synthesis of different substances
      - Drugs
      - Biofuels
      - Chemicals

Activation?
Inhibition?

Chemical space

Functional space

Malate

...

2,4-Dihydroxybutyric acid (DHB)

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Methods to determine molecule properties

- Experiments
  - ➕ Advantage: Usually very accurate
  - ➖ Disadvantages: Often time-consuming, difficult, and expensive

- Non-ML computational methods:
 Simulate the behavior of molecules using theoretical principles, empirical data, and statistical analysis
  - ➕ Advantages: Speed, Costs, Accessibility
  - ➖ Disadvantages: Accuracy, Complexity Limits, Data Requirement

- Machine Learning models:
  - ➕ Advantages: Handling Complexity, Detecting Patterns, Speed, Flexibility
  - ➖ Disadvantages: Accuracy, Data Dependency, Overfitting

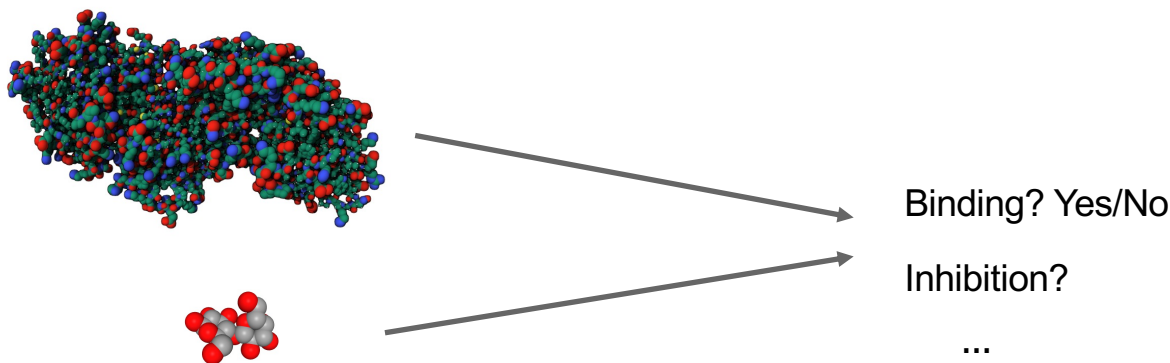# Examples for predicting molecule properties

- Protein property prediction:

→ Optimal pH

→ Effect of mutations

→ ...
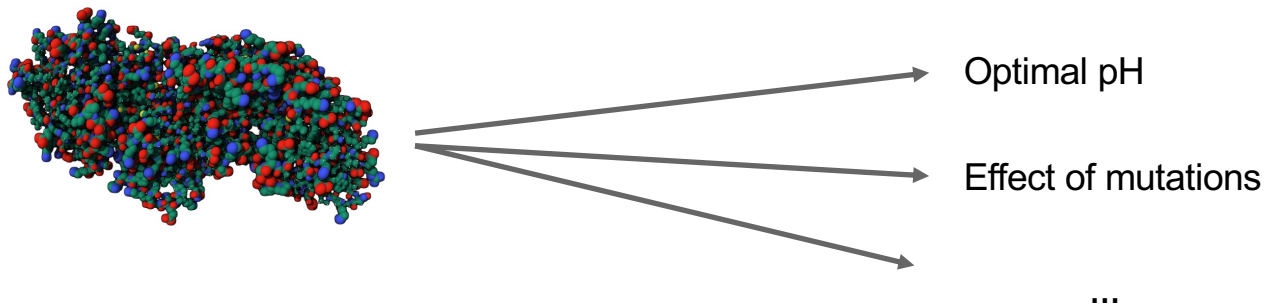
- Small molecule property prediction:

→ Toxicity

→ ...

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Examples for predicting molecule properties (2)

■ Protein-small molecule interaction predictions:

Binding? Yes/No

Inhibition?

...

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On what kind of molecules will we focus?

- We will mostly focus on biomolecules:
    - Micromolecules (Small Molecules):
        - Vitamins
        - Amino Acids
        - Monosaccharides
        - Nucleotides

    - Macromolecules
        - **Proteins**
        - Nucleic Acids (DNA and RNA)
        - Polysaccharides

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