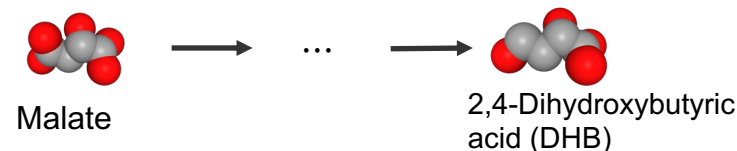
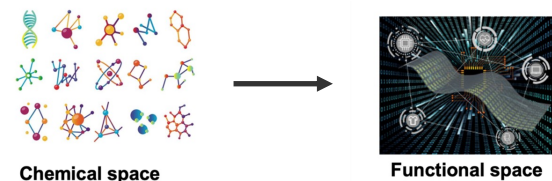
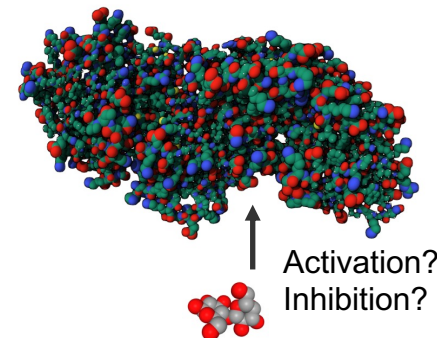


Why do we want to make
predictions for molecules?

- 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



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

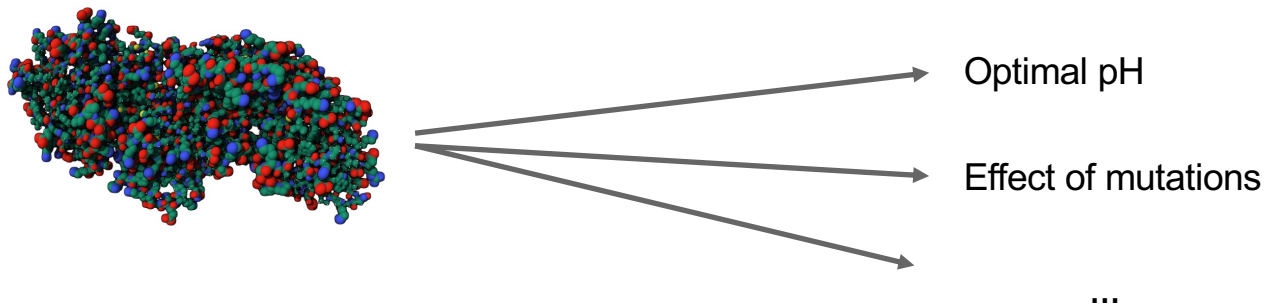
- ➕ Advantages: Speed, Costs, Accessibility
- ➖ Disadvantages: Accuracy, Complexity Limits, Data Requirement

■ Machine Learning models:

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

Examples for predicting molecule properties

■ Protein property prediction:

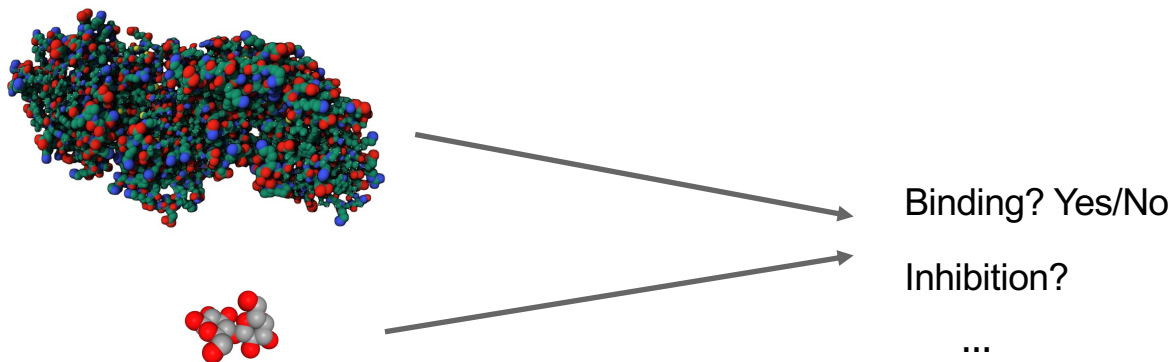


■ Small molecule property prediction:



Examples for predicting molecule properties (2)

- Protein-small molecule interaction predictions:



On what kind of molecules will we focus?

- We will mostly focus on biomolecules:

- Micromolecules (Small Molecules):

- Inorganic Ions
 - Vitamins
 - Amino Acids
 - Monosaccharides
 - Nucleotides



- Macromolecules

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

