Course content

This course introduces students to the complex and multidisciplinary process of drug discovery, focusing on the application of artificial intelligence (AI) methods in drug development. The course aims to familiarize students with the key stages of drug discovery, including the identification and optimization of drug candidates. Topics such as physicochemical properties, drug likeness, and drug safety are discussed, with an emphasis on how AI can accelerate these processes and improve the predictability of drug design.

Key topics covered include:

1. Overview of drug discovery: the drug development process, from identifying initial compounds to optimization.
2. The role of ADME-Tox (Absorption, Distribution, Metabolism, Excretion, Toxicity) in drug design.
3. Machine learning applications in drug discovery: understanding the data generated throughout the development process.
4. Artificial intelligence in drug target discovery and compound optimization.
5. AI-based prediction of drug safety, efficacy, and clinical outcomes.

Course objectives

Knowledge

1. Understand the basic stages and challenges of the drug discovery process, from early-stage screening to optimization.
2. Learn the key factors that determine a drug molecule's potential, such as physicochemical properties, drug likeness, and safety.
3. Gain insight into the historical development of drug design and the role of AI in transforming this field.
4. Familiarize with machine learning methods, including Random Forest and Deep Learning, used in drug target identification and optimization.

Skills

1. Apply machine learning techniques to predict drug properties and optimize drug candidates.
2. Analyze and utilize large datasets from drug development processes, including physicochemical properties, drug interactions, and clinical trial data.
3. Develop and apply AI tools for drug target discovery and the prediction of drug efficacy and safety.

Competencies

1. Enhance critical thinking skills in the context of drug discovery, particularly the application of AI methods to solve complex problems.
2. Improve problem-solving abilities by working with multidisciplinary data from chemistry, biology, and computer science.
3. Gain proficiency in the practical use of machine learning algorithms for drug design and optimization.