EPFL

CH-604 **Medicinal chemistry: concepts and case studies from the pharmaceutical industry**

Quancard Jean

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	1
Session	
Exam	Oral
Workload	30h
Hours	**14**
Lecture	10
Exercises	4
Number of positions	**25**

Frequency

Every 2 years

Summary

We will cover key concepts of Medicinal Chemistry, from identification of active chemical starting points to how they are optimized to deliver drug candidates. We will use real case studies from the pharmaceutical industry. Students will design compounds to solve Medicinal Chemistry problems.

Content

The course will focus on the science of Medicinal Chemistry which aims to identify small molecules to treat human disease.

We will cover the different phases of drug discovery. Starting from how to identify a starting point with activity on a target, we will then discuss how to optimize it towards a drug candidate. A small molecule needs to have many properties to become a drug. To name a few: it needs to bind to a target to elicit a biological effect; when taken as a pill it needs to be absorbed and reach the diseased tissue to have a therapeutic effect; it also needs to be safe for the patient... This means the medicinal chemist needs to optimize a wide range of properties to get to a drug candidate and importantly understand the relationship between the chemical structure and its properties.

These concepts will be introduced together with real case studies from the pharmaceutical industry. Students will also work on common problems that medicinal chemists face and will have the opportunity to design compounds with the aim to improve properties of a molecule.

The expectation is that this course will give students the basic knowledge that is needed to be an effective medicinal chemist at the start of their career.

Concepts that will be covered specifically:

-Introduction to the phases of drug discovery and development
-Hit generation: how to identify chemical starting points
-Molecular recognition: interactions between a small molecule and its target
-Properties in drug discovery: physico-chemical properties, ADME, tox
-The use of in silico models to predict compound properties
-Bioisosteres in drug design
-Hit to lead and lead optimization
-Phenotypic drug discovery: how to find a drug without a target
-Fragment based drug discovery
-Structure based design
-Recent approaches: targeted protein degradation by small molecules; targeting RNA

Learning Prerequisites

Required courses

Organic chemistry

Learning Outcomes

By the end of the course, the student must be able to:
- Apply common strategies to modify a chemical structure to optimize these properties
- Recognize understand key concepts of medicinal chemistry and the properties of drug candidates

Resources

Bibliography

Important literature references will be provided.