Master's programme in Drug Discovery and Safety

Specialization Computational Medicinal Chemistry and Toxicology

Study programme

General description

In the specialization Computational Medicinal Chemistry and Toxicology you will utilize state-of-the-art computational approaches to study new molecules and to predict their properties and interactions with biological molecules. You will explore the fascinating structures of proteins and other drug targets using methods such as molecular docking, molecular dynamics, ab initio studies and free-energy calculations. Even before a molecule has been created and tested, you will be able to predict whether it is likely to have medicinal applications.

Programme components (EC)

The Master's programme in Drug Discovery and Safety is a two-year programme starting in September. The specialization Computational Medicinal Chemistry and Toxicology contains the following components (EC):

- Compulsory courses (36)
- Major research project (42)
- Literature thesis and colloquium (12)
- Ethics and academic skills (6)
- Elective: minor research project; traineeship abroad/company; optional courses (24)

Course overview

Period	Month	Course (EC)	Category
1	Sep – Oct	Chemical biology (6)	Compulsory course
		ADME processes and toxic side effects (6)	Compulsory course
		Principles of pharmacochemistry (6)	Introductory course*
2	Nov – Dec	Computer-aided drug design and virtual screening (6)	Compulsory course
3	Jan	Drug action (6)	Compulsory course
4	Feb – Mar	Computational design and synthesis of drugs (6)	Compulsory course
5	Apr – May	Biomolecular simulation in medicinal chemistry and toxicology (6)	Compulsory course
6	Jun		

More information: www.vu.nl/dds

This overview can be subjected to alterations.
Every part of the programme, including the choice of optional courses, has to be discussed and agreed upon with the Master's coordinator and approved by the examination board.

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*Compulsory course only for students without prior background in pharmaceutical sciences

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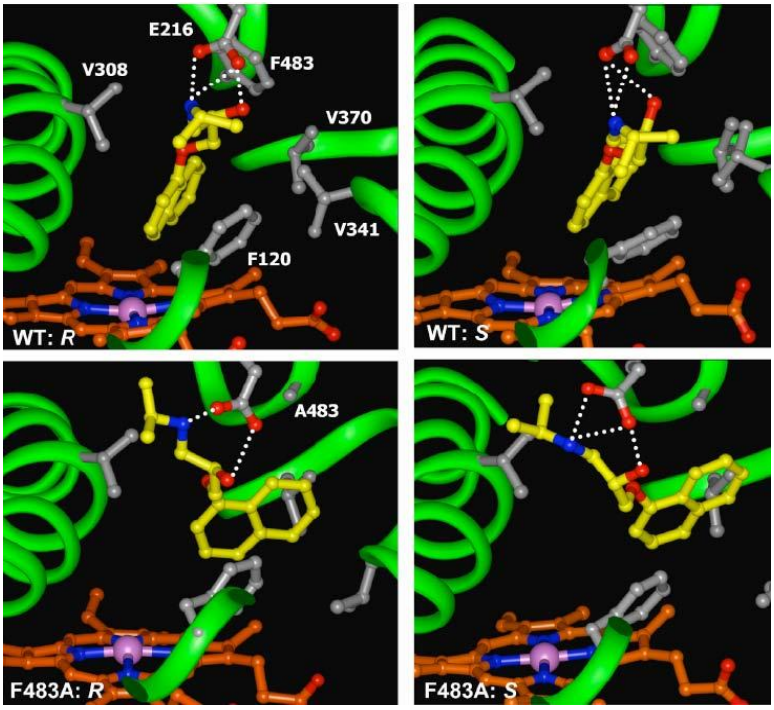
Research topics



Computer simulations to better understand drug action, activity and toxicology

As computational chemists, we use computer simulations to investigate the structure and dynamics of proteins such as Cytochrome P450 enzymes. Moreover, we explore the interactions between these important metabolic proteins and smaller molecules. We utilize different methods to *e.g.* calculate the essential binding free energy for these interactions. The interdisciplinary character of the Master's programme in Drug Discovery and Safety allows computational chemists to closely collaborate with experimental laboratory researchers. With this approach, we aim to obtain a better understanding of the activity and toxicology of drugs and drug-like compounds.