

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 (core) courses (30-36)
- Major research project (42-60)
- Literature thesis and colloquium (12)
- Ethics and academic skills (6)
- Elective: minor research project; traineeship abroad/company; optional courses (6-30)

Course overview

Period	Month	Course (EC)	Category
1	Sep – Oct	Chemical biology (6)	Compulsory core course*
		ADMET (6)	Compulsory core course*
		Principles of pharmacology (6)	Introductory course**
2	Nov – Dec	Computer-aided drug design and virtual screening (6)	Compulsory course
3	Jan	Ethics and academic skills courses (6 total)	
4	Feb – Mar	Computational design and synthesis of drugs (6),	Compulsory core course
		Drug action (6)	Compulsory core course*
5	Apr – May	Biomolecular simulation in medicinal chemistry and toxicology (6)	Compulsory course
6	Jun-	Traineeship, literature study, optional course	

More information: www.vu.nl/dds

* Computational Design and Synthesis of Drugs is compulsory for this specialization. At least 2 out of 3 other compulsory core courses are obligatory.

** *Principles of pharmacology* only compulsory for students without prior background in pharmaceutical sciences.

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.

Master's coordinator: **Dr. D. Geerke**

Phone: +31 20 59 87606 E-mail: d.p.geerke@vu.nl

Molecular and Computational Toxicology: Dr. Daan Geerke

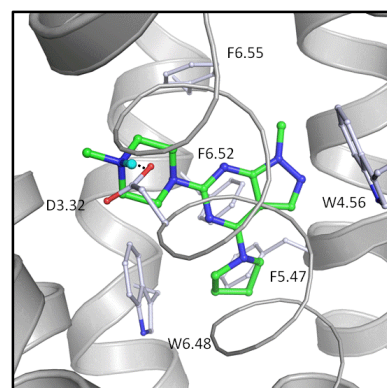
Computer simulations to better understand drug action, activity and toxicology

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.

Medicinal Chemistry: Prof. Dr. Iwan de Esch

Computational modeling of organic compounds and their interaction with protein targets

Our computational chemists use protein sequences, protein crystal structures, molecular dynamics and conformations of organic molecules to generate three-dimensional models of protein-ligand complexes with state-of-the-art computational chemistry technologies. These *in silico* models lead to a better molecular understanding of ligand-protein interactions. In turn, this enables virtual screening for new organic ligands, paving the way for improved medicines.



Efficiently traveling in 'chemical space': Fragment-Based Drug Discovery (FBDD)

In FBDD, the synergy between computational design and organic synthesis is at its finest. Small molecules (fragments) that bind to the biological target are identified and the fragments are grown step-by-step into new efficient ligands through an intimate design and synthesis process. We apply FBDD to a variety of protein targets (G-protein coupled receptors, kinases, ion channels, etc.) that are important in a range of therapeutic areas (inflammation, cancer, neglected third-world diseases, flu and antibiotics).

