

Specialization Drug Design and Synthesis

Study programme

General description

Truly being about chemistry in an interdisciplinary drug context, in the specialization Drug Design and Synthesis you will focus on computer-aided drug design and organic synthesis of novel biologically active compounds. You will work with state-of-the-art computational approaches and the newest synthesis, purification and compound characterization equipment. Your classes will reveal how to reap the fruits of life science research and will guide you along the way to become an innovative computational designer and/or medicinal synthetic chemist. Uniquely, you can choose to devote your main attention to organic synthesis, to computational design, or to a combination of both.

Programme components (EC)

The Master's programme in Drug Discovery and Safety is a two-year programme starting in September. The specialization Drug Design and Synthesis 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 <small>1st/2nd year</small>	Chemical biology (6)	Compulsory course
		ADME processes and toxic side effects (6)	Compulsory course
		Physical-organic chemistry (6)	Compulsory course
		Principles of pharmacochimistry (6)	Introductory course*
2	Nov – Dec	Synthetic approaches in medicinal chemistry (6)	Compulsory course
		Computer-aided drug design and virtual screening	Optional course
3	Jan	Drug action (6)	Compulsory course
4	Feb – Mar	Computational design and synthesis of drugs (6)	Compulsory course
5	Apr – May		
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.

Master's coordinator: **Dr. Maikel Wijtmans**

Phone: +31 20 59 87603 E-mail: m.wijtmans@vu.nl

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

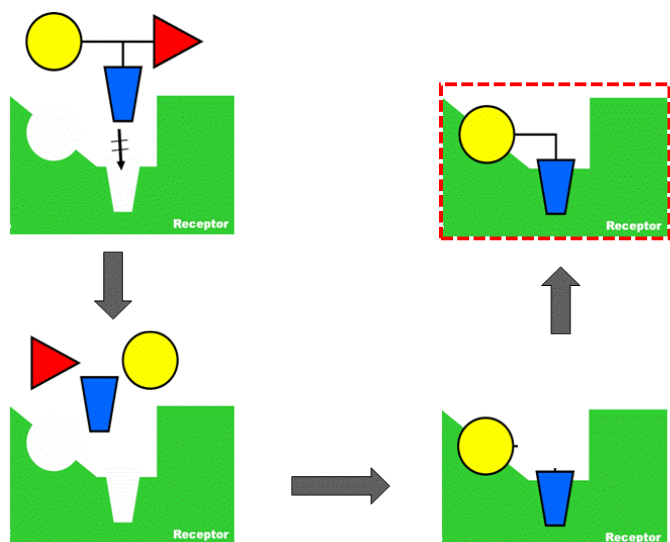
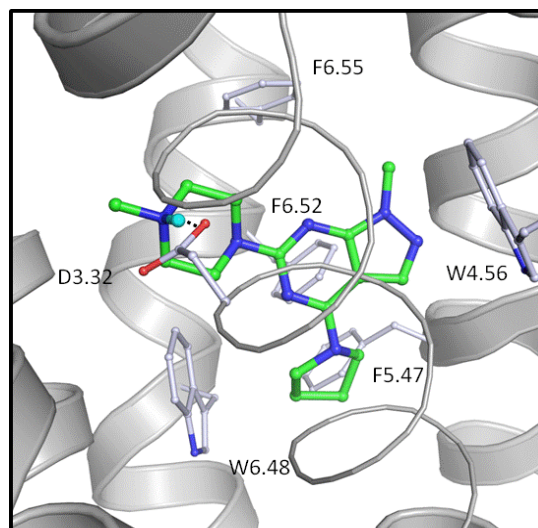
Dr. Chris de Graaf; Dr. Maikel Wijtmans; Dr. Iwan de Esch

Synthesis of organic compounds for fundamental and applied medicinal research

Our synthetic chemists use state-of-the-art synthetic equipment and a large diversity of reaction types to prepare novel organic molecules, many of which are heterocyclic compounds. Collaborations with pharmacologists allow elucidation of the biological activity of these compounds. The resulting insights pave the way to further synthesis of exciting new organic compounds that help in unraveling cell processes and may serve as potential medicines.

Computational modeling of organic compounds and their interaction with protein targets

Our computational chemists use protein sequences, protein crystal structures 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 this emerging drug discovery approach, the synergy between computational design and organic synthesis is at its finest. In FBDD, 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).