

Program of Studies:	Master Program Bioinformatics
Name of the module:	Medicinal Chemistry & Drug Design for Bioinformaticians
Abbreviation:	B-M-11
Subtitle:	-
Modules:	Lecture and tutorial
Semester:	Every summer term
Responsible lecturer:	PD Dr. Martin Empting
Lecturer:	PD Dr. Martin Empting, PD Dr. Matthias Engel, Dr. Walid Elgaher
Language:	English
Level of the unit/ Mandatory or not:	Graduate course / mandatory elective
Course type/weekly hours:	V2 Ü1
Total workload:	150 h = 45 h of classes and 105 h private study and assignments
Credits:	5
Entrance requirements:	basic knowledge in biochemistry, protein structure and organic chemistry
Aims/Competences to be developed:	
Content:	The lecture series will tackle the fundamentals of modern medicinal chemistry including an overview on common pharmaceutical drug targets, pharmacodynamics, structure-activity relationships as well as considerations regarding pharmacokinetics (ADME-T; Absorption, Distribution, Metabolism, Excretion, Toxicology). The students will learn about the different types of assay systems for determining pharmacodynamics and pharmacokinetic parameters. A special focus is the core principles medicinal chemistry optimization applied in the hit-identification, lead generation and lead optimization phases. These include various kinds of hit-finding and screening methodologies, specific effects and characteristics of frequent substituents, bioisosterism, ringtransformations, binding modes, as well as ligand- and structure-based approaches. Finally, methods for quantifying drug-target interactions will be covered. In addition to the lecture series, an exercise course will be provided to train and reiterate on the subject matter and prepare the students for the written exam.

Assessment/Exams:	written exam
Literature:	Graham L. Patrick "An introduction to medicinal chemistry"