

<b>Program of Studies:</b>	<b>Master Program Bioinformatics</b>
<b>Name of the module:</b>	<b>Special Lecture Bioinformatics: Modern Methods in Drug Discovery</b>
<b>Abbreviation:</b>	<b>BI-BM-1</b>
<b>Subtitle:</b>	-
<b>Modules:</b>	Lecture: 2 h (weekly) Tutorial: 1 h
<b>Semester:</b>	1st semester/ yearly during the winter term
<b>Responsible lecturer:</b>	PD Dr. Michael Hutter
<b>Lecturer:</b>	PD Dr. Michael Hutter
<b>Language:</b>	English/German
<b>Level of the unit/ Mandatory or not :</b>	Graduate course / mandatory elective
<b>Course type/weekly hours:</b>	Lecture: 2 h (weekly) Tutorial: 1 h (weekly)
<b>Total workload:</b>	150 h = 48 h of classes and 102 h private study and assignments
<b>Credits:</b>	5
<b>Entrance requirements:</b>	<ul style="list-style-type: none"> <li>▪ basic knowledge of Organic Chemistry and Genetics</li> <li>▪ scope of the lectures: <ul style="list-style-type: none"> <li>Bioinformatik I + II</li> <li>Computational Chemistry, Softwarewerkzeuge der Bioinformatik</li> </ul> </li> </ul> <p>Students need to have successfully passed one of the following courses to be admitted:</p> <ul style="list-style-type: none"> <li>Bioinformatik II</li> <li>Bioinformatics III (Master program Bioinformatics)</li> <li>Computational Chemistry</li> <li>Softwarewerkzeuge der Bioinformatik</li> </ul>
<b>Aims/Competences to be developed:</b>	<p>During the course the students will get familiar with current methods of bioinformatics and chemoinformatics in the development of pharmaceutical drugs and their molecular targets also on the level of genes. Subsequently, the students should be able to set their mark within interdisciplinary research groups.</p> <p>The combination of knowledge from bioinformatics and other natural and life sciences is a demanding aspect of this course. Focus is the applicability of bioinformatical knowledge onto the field of pharmaceutically relevant tasks. The exercises play an important role in deepening the understanding:</p> <ul style="list-style-type: none"> <li>- about half of the exercises consist of application of computer programs onto selected biological systems and virtual screening issues.</li> <li>- the other half serves the consolidation and extension of special knowledge</li> </ul>

	In total, the emphasis is set on critical evaluation and interpretation of results in order to allow subsequent independent research and to strengthen scientific communication skills.
<b>Content:</b>	<p>The main point of the course is set on the computer-assisted prediction of suitable pharmaceutical drugs and the search for new potential target in the human genome.</p> <p>Following topics are covered:</p> <ol style="list-style-type: none"> <li>(1) molecular causes of typical diseases and mechanism of action of pharmaceutical drugs</li> <li>(2) virtual compound libraries and search strategies</li> <li>(3) <i>in silico</i> eADMET-models and filters, bioavailability</li> <li>(4) statistics and QSAR-methods</li> <li>(5) metabolism, toxicology and adverse side effects with respect to biomarkers</li> <li>(6) polymorphism und susceptible genes</li> <li>(7) indentification of orthologue genes for deriving new targets and model organisms</li> <li>(8) current trends and strategies</li> </ol>
<b>Assessment/Exams:</b>	<p>Autonomous processing of 6 examination sheets that are handed out biweekly as homework.</p> <p>Admission to the final exam: at least 50% of points from the homework achieved. After failure to pass the final exam there is the possibility to pass an oral exam.</p> <p>This course is marked: yes</p> <p>The mark confers to the mark of the final exam.</p>
<b>Used media:</b>	<p>The lecture will be presented predominately using electronic slides.</p> <p>Some excercises require access to internet and publically available online databases.</p>
<b>Literature:</b>	<p>Electronic slides of the lectures will be made available on the web side of the course (<a href="https://www-cbi.cs.uni-saarland.de/teaching/ws-1920/mddd-ws-1920/">https://www-cbi.cs.uni-saarland.de/teaching/ws-1920/mddd-ws-1920/</a>)</p> <p>The original publications quoted are recommended for further self studies. Furthermore, a precompiled set of textbooks is available in the library.</p> <p>A.R. Leach, V. Gillet: An Introduction to Chemoinformatics, Springer 2007</p> <p>G. Klebe: Wirkstoffdesign, Spektrum Akad. Verlag 2009</p>