Modulhandbuch

für den Masterstudiengang

Life Science Informatics

Der

Rheinischen Friedrich-Wilhelms-Universität Bonn

und

Und der Rheinisch-Westfalischen Technischen Hochschule Aachen

Überarbeitet, Stand: 19.08.2019

Information and/und Abbreviations/Abkürzungen

Duration of each module is **one semester**.
Lecture (L): Vorlesung
Seminar (S): Seminar
Lab course (LC): Praktikum
Exercise (E): Übung
CP (Credit point[s]): Leistungspunkte
Example/Beispiel: A two-hours-lecture with a one-hour-exercise is abbreviated as/ Eine Vorlesung mit zwei Semesterwochenstunden und einer Stunde Übung wird folgendermaßen ausgedrückt: L2 + E1
Hours per week (HPW): Semesterwochenstunden (SWS)

***** The classes marked with an asterik **(*)** are introductory classes. They are assigned individually to incoming students in the following manner:

To ensure that **students with different backgrounds in computer science or the life sciences** have comparable interdisciplinary knowledge and skills, mandatory bridging courses in computer Science/mathematics (CSMA) and biology/chemistry (BIOCHEM) are offered during the first term. For students with a degree in computer science, BIOCHEM is mandatory and CSMA is optional.

For students with a degree in the life sciences, CSMA is mandatory and BIOCHEM is optional.

Within the first month of the semester, the head of the programme and the committee will assign each new student to and inform each student about the mandatory and optional introductory classes.

Module	Module 1
Level	Master
Abbreviation of the module	ICS
Course title	Computer Science for Life Scientists *
Semester of study	1st semester, Winter Semester
Staff member in charge of module	Prof. Dr.-Ing. Thomas Schultz
Staff member	Prof. Dr.-Ing. Thomas Schultz
Language	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	L5+E2/ 6 hours per week
Work load	Lecture: Contact hours 50, self-study 50 Exercises: Contact hours 70, self-study 100
Credit points	11
Mandatory requirements	Background knowledge as specified in Section 3 of examination regulations.
Requirements	No other requirements.
Learning outcomes	**Knowledge** of concepts from imperative and object oriented programming; algorithms for sorting, searching, graph, and numerical algorithms, as well as data structures for dynamic sets; fundamental facts from theoretical computer science. **Skills.** Ability to design, implement, debug, and test computer programs, including basic object-oriented analysis and design. Ability to design and analyse algorithms based on different design techniques, including divide-and-conquer, greedy algorithms, and dynamic programming. **Competences.** Productive work in small teams, self-dependent solution of practical problems, presentation of solution strategies and implementations, self management.
Contents	Comprehensive introduction to aspects of practical computer science that are required to pursue work in the area of Life Science Informatics. This includes concepts of imperative and object oriented programming; techniques for algorithm design and analysis, including divide-and-conquer, greedy algorithms, and dynamic programming; examples of algorithms and data structures for tasks including sorting, searching, efficient data storage and retrieval, graph analysis; foundations of numerical algorithms and theoretical computer science.
Assemessment (Studienleistungen)	The grading results from 100% of the written final exam of this module. To be admitted to the exam, students have to hand in weekly assignments in written form. As will be clearly indicated, some will have to be done individually, others can be handed in in groups of up to three. In any case, each student has to be able to explain the solution to the tutors upon request to obtain the points. There will be 12 assignment sheets, which will be grouped into three sets of four sheets. Students have to achieve at least 50% of the points overall, and at least 35% for each set of four sheets.
Media used in the course	Projector, Whiteboard
References	Robert Sedgewick, Kevin Wayne: Computer Science. An Interdisciplinary Approach. Addison-Wesley, 2016 Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, Clifford Stein: Introduction to Algorithms. MIT Press, 3rd edition, 2009 Mitchell L. Model: Bioinformatics Programming Using Python. O'Reilly, 2009

Module	Module 2
Level	Master
Abbreviation of the module	IMA
Course title	Mathematics for Life Scientists *
Semester of study	1st semester, Winter Semester
Staff member in charge of module	PD. Dr. Martin Vogt
Staff member	PD. Dr. Martin Vogt
Language	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	L1+E1/ 2 hours per week
Work load	40 hours, 20 hours in class, 20 hours self-study
Credit points	3
Mandatory requirements	Mandatory
Requirements	none
Learning outcomes	**Knowledge** Basic mathematical concepts from logic and naïve set theory Practical linear algebra and analysis Basic concepts of probability theory and statistics **Skills** Proficiency in mathematical calculations and manipulations for problem solving in the life sciences and computer science **Competences** Familiarity with mathematical descriptions and formulations of life science-based theories, models, and observations Ability to apply mathematical formalisms to models in life sciences and computer science
Contents	- Basic Mathematical concepts - Review of linear algebra, analysis, ordinary differential equations - Introduction to probability theory and statistics
Assemessment (Studienleistungen)	Exam
Media used in the course	Slides, handouts, exercise sheets
References	Course handouts

Module :	Module 3
Level:	Master
Abbreviation of the module:	ICB
Course:	Chemistry and Biology for LSI *
Semester of study:	1st semester, Winter Semester
Staff member in charge of the module	Dr. Alexandra Reitelmann
Staff member:	Dr. Alexandra Reitelmann
Language:	English
Assignment to curriculum	Mandatory
Type of course/hours per week	L4 + E1/ 5 hours per week
Work load	Lecture: Contact hours 50, self-study 50 Exercises: Contact hours 70, self-study 100
Credit points:	7
Mandatory requirements:	None
Recommended requirements	Proficiency in English
Learning outcomes:	**Knowledge** Students will be made familiar with substantial foundations in Chemistry and Biology **Skills** Students will learn –based on the knowledge provided in the course- how to easily applies this knowledge to problems they have to solve. **Competences** Students will be able to apply the contents of the lecture easily to problems from the field of Life Science Informatics
Contents:	• Atoms, models, electron configuration • Chemical bonds and redox reactions • Aromaticity, stereochemistry, carbonyl compounds • Introduction to the molecular structure of the cell and selected cellular and organ systems (cell membrane, cell organells, cell nucleus, specialised cells [nerve cells and immune cells], immune system)
Course achievement/ type of exam:	Written exam
Media used in the course:	Powerpoint slides (PDF), teaching laptop with internet access, exercises
References:	Reece et al: Campbell Biology, current edition

Module:	Module 4
Level	Master, Biological Databases
Abbreviation of the module	BDB, 1st semester, Winter Semester
Semester of study:	1st semester, Winter Semester
Staff member in charge of the module:	Professor Dr. Martin Hofmann-Apititus
Staff member:	Professor Dr. Martin Hofmann-Apititus
Language:	English
Assignment to curriculum	Mandatory
Type of course/hours per week	L4 / 4 hours per week,
Work load	Estimate: 180 hours, 80 hours contact time, 100 hours self-study
Credit points:	6
Mandatory requirements:	keine
Recommended requirements	• Good proficiency in English • Basic knowledge in biology, chemistry, computer science
Learning outcomes:	**Knowledge** The module introduces students to modern concepts for the representation of biological, chemical, pharmacological and medical data and knowledge in information systems **Skills** Foundations of meaningful and effective knowledge about and use of biological, chemical and pharmacological data, databases and information systems. **Competences** Biomedical knowledge management has a key role in pharmaceutical industry and biotechnology. With our module we lay the foundation for the ability to ➢ Understand what biologists, chemists and medical researchers need from a specialist in life science informatics ➢ Communicate, as a life science informatics specialist, with biologists, chemists and medical researchers about data and databases ➢ Translate scientific questions from the empirical, experimental sciences into IT-based, model-driven approaches involving biological databases Work in a data-driven, pharmaceutical research environment

Contents:	• Setting the scene; setting expectations; definition of goals
	• Overview on biological (and related) databases
	• Introduction to classes of biological databases;
	  • bibliographic databases (e.g. PubMed)
	  • gene and genome databases (e.g. ENSEMBL)
	  • genetic variation databases (e.g. dbSNP)
	  • gene expression databases (e.g. ArrayExpress)
	  • protein databases (e.g. UniProt)
	  • protein-protein interaction databases
	  • pathway databases
	  • eCRFs and clinical study planning tools
	  • tranSMART as an example for a multi-omics translational database
	• role of ontologies for shared semantics / annotations
	• FAIR data and FAIR principles
	• Reproducibility crisis; provenance; interoperability and re-usability of data

Course achievement/ type of exam:	Lecture, written examination
Media used in the course:	No slides; no powerpoint. Plain talk and – sometimes – a quick “guided tour” life through the database currently discussed
References:	• https://www.ebi.ac.uk; https://www.ncbi.nlm.nih.gov

Module	Module 5
Level	Master
Abbreviation of the module	BI1
Course	Introduction to Bioinformatics
Semester of study	1st semester, Winter Semester
Staff member in charge of the module	Prof. Dr. Thomas Berlage
Staff member	Prof. Dr. Thomas Berlage
Language	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	L1+E1/ 2 hours per week
Work load	90 hours in total: 20 hours contact time, 20 hours self study, excersise: 20 hours contact time, 30 hours self-.study
Credit points	3
Mandatory requirements	none
Requirements	none
Learning outcomes	**Knowledge:** Interdisciplinary thinking knowledge: Understanding informatics solutions/contributions to biological approaches,in particular molecular biology (genomics, proteomics, expression analysis, network analysis) **Skills:** Modeling natural phenomena Understanding probabilistic approaches **Comptetences:** Understanding trade-offs and limitations inherent in algorithmic approaches Enhanced analytical and logical skills Benefits for future professional life: Important application field
Contents	Genome and Sequences (DNA sequences, Algorithms for sequence comparison, Sequence databases, Patterns and motifs, Phylogenetic trees) Proteins and Structures (3D modelling, Protein databases, Protein structure analysis and prediction) Protein Expression and Function (DNA chip technology, Gene expression analysis, Clustering, Proteomics) Pathways and Systems (Metabolic networks, Pathway analysis, Cell simulation)
Assessment	Klausur, Übungsaufgaben
Media used in the course	Folien, Übungsaufgaben, BSCW Workspace
References	• Reinhard Rauhut, Bioinformatik. Sequenz - Struktur - Funktion. Wiley-VCH, 2001. • Richard Durbin, A. Krogh, G. Mitchison, S. Eddy, Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids. Cambridge University Press, 1999. • Joao Carlos Setubal, Joao Meidanis, Introduction to Computational Molecular Biology. PWS Publishing, 1997. • Minoru Kanehisa, Post-Genome Informatics. Oxford University Press, 2000.

Module :	Module 6
Level:	Master
Abbreviation of the module:	MDL
Course:	Molecular Modeling and Drug Design
Semester of study:	2^{nd} semester, Summer Semester
Staff member in charge of the module:	Professor Dr. Jürgen Bajorath
Staff member:	Professor Dr. Jürgen Bajorath
Language:	English
Assignment to curriculum	Mandatory
Type of course/hours per week	L3 + E2/ 5 hours per week
Work load	Estimate: 180 hours in total, 80 contact time, 100 self-study
Credit points:	6
Mandatory requirements:	none
Recommended requirements	Module 3 (ICB)
Learning outcomes:	**Knowledge** Understand computational drug design and molecular modelling methods **Skills** Mathematical and computational methods to analyze protein-ligand interactions and design biologically active compounds Modeling and molecular properties and biological activities of small molecules; basic drug design concepts, interdisciplinary communication skills **Compentences** Preparation for basic and applied interdisciplinary computational research
Contents:	• Molecular structure, properties, and representation • Molecular mechanics, conformational analysis, bioactive conformation modeling • Pharmacophore and QSAR analysis • Structure-based drug design
Course achievement/ type of exam:	Written Exam
Media used in the course:	Interactive Teaching Program Molecular Conceptor
References:	Molecular Conceptor

Module	Module 7
Level	Master
Abbreviation of the module	BI2
Course title	Visual Computing in the Life Sciences
Semester of study	2nd semester, Summer Semester
Staff member in charge of module	Prof. Dr.-Ing. Thomas Schultz
Staff member	Prof. Dr.-Ing. Thomas Schultz
Language	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	L3+E1/ 4 hours per week
Work load	Lecture: Contact hours 45, self-study 45 Exercises: Contact hours 15, self-study 75
Credit points	6
Mandatory requirements	None
Requirements	Strongly recommended: Computer Science for Life Scientists
Learning outcomes	**Knowledge:** of algorithms and techniques for the visualization of multi-dimensional data and graphs, of foundations of human visual perception and rules for visualization design; knowledge of methods for biomedical image analysis, including filtering, registration, segmentation, and statistical inference. **Skills:** Ability to design, create, and interpret visualizations of data from the life sciences. Ability to process and analyse images from life science applications, to select and use image processing and analysis algorithms, and independently implement basic methods. **Competences:** Productive work in small teams, self-dependent solution of problems in the area of visualization and image analysis in the life sciences; presentation of solution strategies and implementations, critical reflection of conclusions drawn from data visualization and automated image analysis.
Contents	Introduction to principles and methods from visual computing, in particular data visualization and image analysis, as they relate to the area of Life Science Informatics. This includes techniques for visualizing multidimensional data and graphs, dimensionality reduction, human perception and guidelines for visualization design; biomedical image acquisition, filtering, registration, segmentation, and use within hypothesis testing and predictive modeling.
Assemessment (Studienleistungen)	The grading results from 100% of the written final exam of this module. To be admitted to the exam, students have to hand in six assignments in written form. Assignments can be handed in in groups of up to three, but each student has to be able to explain the solution to the tutors upon request to obtain the points. Students have to achieve at least 50% of the points overall.
Media used in the course	Projector, Whiteboard
References	M. Ward et al., Interactive Data Visualization: Foundations, Techniques, and Applications. CRC Press, 2010 T. Munzner, Visualization Analysis and Design, A K Peters, 2015 B. Preim, C. Botha, Visual Computing for Medicine: Theory, Algorithms, and Applications. Morgan Kaufmann, 2014 C. Bishop, Pattern Recognition and Machine Learning. Springer, 2006

Module	Module 7
Level	Master
Abbreviation of the module	BI2
Course title	Programming Lab 1
Semester of study	2nd semester, Summer Semester
Staff member in charge of module	Professor Dr. –Ing. Thomas Schulz
Staff member	PD Dr. Martin Vogt
Language	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	LC4/ 4 hours per week
Work load	Estimate: 70-80, 40 hours in class, 30-40 hours self study
Credit points	8
Mandatory requirements	None
Requirements	Computer Science for Life Scientists
Learning outcomes	**Knowledge** In depth practical knowledge of one programming/scripting language (Python) in the context of bio- and chemoinformatic applications. Understanding and implementation of relevant algorithmic concepts. **Skills** Practical programming and implementation. Efficient and effective programming. Problem solving. **Competences** Programming skills for automation of workflows. Ability to solve of computational and algorithmic challenges in interdisciplinary research and applications.
Contents	- General programming exercises (Python) - Implementation of basic bioinformatic algorithms - Algorithmic approaches to problem solving
Assemessment (Studienleistungen)	Evaluation of programming assignments (weekly/biweekly)
Media used in the course	Computers, handouts, slides
References	Course handouts

Module :	Module 8
Level:	Master
Abbreviation of the module:	KND
Course:	Life Science Knowledge Discovery
Semester of study:	2nd semester, Summer Semester
Staff member in charge of the module	Professor Dr. Martin Hofmann-Apitius
Staff members:	Professor Dr. Martin Hofmann-Apitius
Language:	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	L4/ 4 hours per week
Work load	Estimate: 180 hours in total, 70 hours contact time, 110 hours self-study
Credit points:	6
Mandatory requirements:	None
Recommended requirements	Good proficiency in English, basic knowledge in statistics and computer science
Learning outcomes:	**Knowledge** The module introduces students to modern concepts for knowledge discovery in the life sciences. The lecture leads from an introduction to knowledge discovery (Fayyad) via statistical modelling, information retrieval and machine learning to named entity recognition and relationship mining in unstructured information sources. **Skills** The students are provided with an understanding and introduced to a meaningful application of relevant data mining strategies in the Life Sciences. **Competences:** Biomedical knowledge discovery encompasses a broad spectrum of technologies with high relevance for the pharmaceutical and biotechnology industry. In particular, this lecture and exercise enables students to 1. design mining strategies suited to support the analysis of high dimensional data, 2.to implement simple unstructured information mining strategies based on named entity recognition, 3.to apply modern technologies for information fusion and information aggregation, 3. to use text mining as one of the fundamental approaches towards knowledge discovery in the life science, 4. to apply data mining strategies and technologies effectively in teams. 5. “translating” life science problems into meaningful data mining approaches
Contents:	1. Introduction to knowledge discovery as defined by Fayyad et al.(1998), Formal representation of knowledge, 2. Use of ontologies in semantic mining, 3. Relationship mining and natural language processing, 4. Statistical modelling, Fundamentals of classification and correlation, 5. Introduction to machine learning, Named entity recognition methods, 6. Text mining and its application in life science informatics, 7. Hypothesis generation by data fusion and data aggregation.
Course achievement/ type of exam:	Lecture, written examination, participation in exercises with compulsory attendance and a quota of 50% of the exercises solved
Media used in the course:	No slides, no powerpoint. Plain talk and sometimes (more exceptionally: YouTube tutorials on selected topics)
References:	• Knowledge discovery in databases: An overview; Fayyad; Springer 2001

Module :	Module 8
Level:	Master
Abbreviation of the module:	KND
Course:	Scientific Presentation I
Semester of study:	2nd semester, Summer Semester
Staff member in charge of the module	Professor Dr. Martin Hofmann-Apitius
Staff member:	Dr. Alexandra Reitelmann
Language:	English
Assignment to curriculum	Mandatory
Type of course/ Type of course/ hours per week	S2/ 2 hours per week,
Work load	Estimate: 120 hours in total: 60 hours contact time, 60 hours self-study
Credit points:	4
Mandatory requirements:	None
Recommended requirements	Proficiency in English, Chemistry and Biology for LSI
Learning outcomes:	**Knowledge** Students will be made familiar with several forms of oral scientific communication. **Skills** Students will learn –based on the knowledge provided in the course- how to quickly and effectively communicate to students, lecturers. **Competences** Students will be introduced to effectively communicate scientific topics in a written and oral way on an advanced level.
Contents:	• Time management/ self management • Structure of an oral presentation • Slide Design (slide templates, amount of text on slides) • The essentials of oral communication: voice, body language, mimics, interaction with the audience – practised in examples with individual feedback, may -but does not have- to include video-taped presentations of students. • Video training
Course achievement/ type of exam:	• Oral assignments/presentation
Media used in the course:	Powerpoint slides (PDF), teaching laptop with internet access, computer pool for supervised learning, video camera
References:	• Nature and Science, other research journals

Module :	Module 9
Level:	Master
Abbreviation of the module	CHI
Course:	Chemoinformatics
Semester of study:	3rd semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member:	Professor Dr. Jürgen Bajorath
Language:	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	L3+E1, 4 hours per week
Work load	Estimate: 180 hours in total, 80 contact time, 100 self-study
Credit points:	6
Mandatory requirements:	none
Recommended requirements	Lecture Molecular Modeling and Drug Design
Learning outcomes:	**Knowledge** Understand concepts and methods in chemoinformatics **Skills** Study of data structures and algorithms to understand selected chemoinformatics methods and their practical application Understanding and applying chemoinformatics methods; interdisciplinary communication skills **Competences** Preparation for interdisciplinary computational research and applications
Contents:	• Molecular descriptors and chemical spaces • Graph comparison • Compound classification algorithms • Molecular similarity methods • Machine learning algorithms • Diversity design • Virtual screening
Course achievement/ type of exam:	Klausur
Media used in the course:	Slides
References:	• Script with exercises, • Leach/Gillet: “Introdution to Chemoinformatics”

Module	Module 9
Level	Master
Abbreviation of the module	CHI
Course title	Programming Lab II
Semester of study	3rd Semester, Winter Semester
Staff member in charge of module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Martin Hofmann-Apitius
Language	English
Assignment to curriculum	Mandatory
Type of course/ hours per week	LC4/ 4 hours per week
Work load	Estimate: 240, 100 hours in class, 140 hours self study
Credit points	8
Mandatory requirements	Lecture: Computer Science for Life Scientists
Requirements	none
Learning outcomes	**Knowledge** • In depth practical knowledge of one programming language (Java) in the context of bioinformatic applications. • Understanding and implementation of relevant algorithmic concepts. **Skills** • Practical programming and implementation. • Efficient and effective programming. • Problem solving. **Competences** • Programming skills for automation of workflows. • Ability to solve of computational and algorithmic challenges in interdisciplinary research and applications.
Contents	• General programming exercises (Java) • Implementation obioinformatic algorithms • Algorithmic approaches to problem solving
Assemessment (Studienleistungen)	Evaluation of programming assignments
Media used in the course	Computers, handouts, slides
References	Course handouts

Module :	Module 10
Level:	Master
Abbreviation of the module:	LSI
Course:	LSI Tutorial I
Semester of study:	1st semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member:	Dr. Alexandra Reitelmann
Language:	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC4/ 4 hours per week,
Work load	Estimate: 180 hours in total: 90 hours contact time, 90 hours self-study
Credit points:	6
Mandatory requirements:	None
Recommended requirements	Proficiency in English
Learning outcomes:	**Knowledge** Introduction to Programming in Python **Skills** Application of Python skills to solve Life Science problems **Competences** Students gain confidence in their ability to solve Life Science problems. Students learn to effectively collaborate on programming projects.
Contents:	• Variables • Data structures (simple and complex) • Focus: Dictionaries in Python for Life Science Problems • Data Input and Output (files, screen, key board and other input devices) • Control elements (for-loops, if-/while- statements) • Procedures, functions and methods • Coding own functions • Regular Expressions for Life Scientists • Introduction to GUIs
Course achievement/ type of exam:	Programming assignments
Media used in the course:	Powerpoint slides (PDF), teaching laptop with internet access, students' laptops with internet access, Computer Pool (Computer Lab)
References:	Jones, Martin: Python for Biologists, current edition (Print on demand or eBook).

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Introduction to Machine Learning Tutorial
Semester of study	2nd semester, Summer Semester
Staff member in charge of Module	Professor Dr. Jürgen Bajorath
Staff member	Dr. Alexandra Reitelmann
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC4/ 4 hours per hours per week
Work load	180 hours /90 hours contact time and 90 hours self study
Credit points	6 Credit points
Mandatory requirements	none
Requirements	none
Learning outcomes	**Knowledge** Overview about Machine Learning Algorithms often used in solving problems in the Life Sciences. **Skills** Successful application of Machine Learning Algorithms for problem solving in the Life Sciences **Competences** • Students collaborate effectively together in programming tasks. • Students hone their programme solving-skills. • Students strengthen their creative programming skills. • Students communicate their results effectively.
Contents	• kNN in the Life Sciences • SVM in the Life Sciences • K-means clustering in the Life Sciences • Other ML methods relevant in the Life Sciences • Data pre-processing techniques in the Life Sciences
Assemessment (Studienleistungen)	Programming assignments throughout the class
Media used in the course	Slides, Jupyter Notebooks
References	• Aurelien Geron Hands-on Machine Learning with Scikit-Learn & TensorFlow O'Reilly (7-12-2018, tenth release)

Module :	Module 10
Level:	Master
Abbreviation of the module:	LSI
Course:	Computational Systems Biology
Semester of study:	3rd semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member:	Professor Dr. Hofmann-Apitius, Dr. Alexandra Reitelmann
Language:	English
Assignment to curriculum	Optional
Type of course/ hours per week	S2, 2 hours per week,
Work load	Estimate: 120 hours, 60 hours contact-time, 60 hours self-study
Credit points:	4
Mandatory requirements:	none
Recommended requirements	Excellent proficiency in English, basic knowledge in statistics, life sciences and computer science
Learning outcomes:	**Knowledge** The seminar introduces students to current concepts of systems biology taking dementia and ageing as examples. **Skills** The seminar will educate the student to understand biology as an informational science. The students will be introduced to understand and apply approaches of systems theory or other models to the analysis of biological, often molecular) networks. **Compentences** The seminar will educate the student read and understand papers from the field of systems biology. Moreover the student will be trained to apply discussed models to new problems and to communicate and discuss scientific results or scientific factual information effectively.
Contents:	• Introduction to Systems Biology • Integrating technology, biology and computation, Silicon cell • Metabolic control analysis • Kinetic modelling, mechanistic and modular approaches to modelling and inference of cellular regulatory networks, integration of modelling and signalling networks • Emergent functionalities, properties,Modelling of signalling pathways, Complex brain networks: graph theoretical analysis of structural and functional systems, impact of systems biology to predictive an personalised medicine
Course achievement/ type of exam:	Regular attendance (80% minimum), contributions to discussions after presentations and the presentation of an original research paper taken from a relevant journal in the field.
Media used in the course:	Slides (Powerpoint, PDF), Internet: Pubmed (to determine the number of publications from the field of the paper the student will present and to infer the research intensity in the field discussed)
References:	• Kriete, Eils: *Computational Systems Biology,* 2nd edition; Elsevier • Original research articles

Module :	Module 10
Level:	Master
Abbreviation of the module:	LSI
Course:	Molecular Modeling and Drug Design
Semester of study:	3rd semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member:	Professor Dr. Jürgen Bajorath
Language:	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC4/ 4 hours per week
Work load	Estimate: 240 hours in total, 100 hours contact time and 140 hours self-study
Credit points:	8
Mandatory requirements:	Lecture Molecular Modeling and Drug Design
Recommended requirements	Lecture Chemoinformatics
Learning outcomes:	**Knowledge** Understand computational drug design and molecular modelling methods **Skills** • Practical computational exercises in molecular modelling and ligand- and structure-based drug design • Modeling and predicting properties and biological activities of small molecules; interdisciplinary communication skills **Competences** Preparation for interdisciplinary computational research and applications
Contents:	• Molecule generation and representation, conformational analysis, energy minimization • Pharmacophore and QSAR modeling • Protein-ligand docking
Course achievement/ type of exam:	Protocol, test
Media used in the course:	Computer, MOE Molecular Modeling Program
References:	Script, MOE documentation, original literature

Module :	Module 10
Level:	Master
Abbreviation of the module:	LSI
Course:	Chemoinformatics
Semester of study:	3rd semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member:	Professor Dr. Jürgen Bajorath
Language:	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC4 / 4 hours per week
Work load	Estimate: 240 hours, 100 hours contact time, 140 hours self-study
Credit points:	8
Mandatory requirements:	Lecture and Exercise Chemoinformatics
Recommended requirements	Lecture Molecular Modeling and Drug Design
Learning outcomes:	**Knowledge** Understand and apply concepts and methods in chemoinformatics **Skills** • Practical computational exercises to apply informatics methods to problems in organic and medicinal chemistry • Applying chemoinformatics methods; implementation of simple algorithms; • interdisciplinary communication skills **Competences** Preparation for interdisciplinary computational research and applications
Contents:	Fingerprint generation, similarity searching, cluster analysis, partitioning, virtual screening, chemoinformatics application scripting
Course achievement/ type of exam:	Protocol, test
Media used in the course:	Computer, MOE Chemionformatics Software, Handouts
References:	Script, MOE documentation, original literature

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Data Mining and Machine Learning in the Life Sciences
Semester of study	3rd semester, Winter Semester
Staff member in charge of Module	Professor Dr. Jürgen Bajorath
Staff member	Hon.-Prof. Dr. Holger Fröhlich
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	L4 / 4 hours per week
Work load	90 hours: 40 hours contact time, 50 hours self-study
Credit points	6
Mandatory requirements	None
Requirements	None
Learning outcomes	**Knowledge** • Knowledge and understanding of a variety of commonly used data science techniques that are relevant in life science applications • **Skills** • Understanding the pre-requisites for building a good model • Ability to judge when to best use which method • Understanding of advantages and limitations of discussed techniques • **Competences** • Students should learn to see data science in an interdisciplinary and application oriented context. They should see the potential of data mining and machine learning approaches, but also critically see their limitations and prerequisites.
Contents	• Introduction and statistical basics • Cluster analysis • Classical supervised machine learning methods • Deep learning approaches
Assemessment (Studienleistungen)	Exam
Media used in the course	Powerpoint
References	- Hastie, Tibshirani, Friedman, The Elements of Statistical Learning, Springer, 2001 - Duda, Hart, Stork, Pattern Classification, Wiley Interscience, 2001 - Hinton, Salakhutdinov, Reducing the Dimensionality of Data with Neural Networks, Science, 313:504-507, 2006 - Kingma, Welling, Auto-encoding Variational Bayes, NIPS 2013

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Seleted Chapters of Molecular Cell Biology
Semester of study	3rd Semester, Winter Semester
Staff member in charge of Module	Professor Dr. Jürgen Bajorath
Staff member	Dr. Alexandra Reitelmann
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	S2, 2 hours per week
Work load	120 hours, 40 hours contact time, 70 hours self study
Credit points	4
Mandatory requirements	none
Requirements	English
Learning outcomes	**Knowledge** Providng in-depth knowledge about the involvement of the immune system in diseases. **Skills** • Students will learn to effectively read original and review scientific papers. • Students will learn to effectively communicate their insights to others • Students will broaden their understanding of the role **Competences** • Students will learn collobarate and communicate effectively to broaden their understanding of the immune system's role in diseases.
Contents	• Immune System • Cancer • Nervous System and Neurodegenerative Diseases • And other diseases
Assemessment (Studienleistungen)	• Paper presentation
Media used in the course	Slides, teaching laptop with internet access
References	Research magazines such as for example Nature and Science

Module :	Module 10
Level:	Master
Abbreviation of the module:	LSI
Course:	Scientific Presentation II
Semester of study:	3rd semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member:	Dr. Alexandra Reitelmann
Language:	English
Assignment to curriculum	Optional
Type of course/hours per week	S2/ 2 hours per week,
Work load	Estimate: 120 hours in total: 50 hours contact time, 70 hours self-study
Credit points:	4
Mandatory requirements:	None
Recommended requirements	Proficiency in English, Biology Bridging Course
Learning outcomes:	**Knowledge** Students will be made familiar with several forms of written scientific communication. **Skills** Students will learn –based on the knowledge provided in the course- how to quickly and effectively communicate in written form. **Competences** Students will be introduced to effectively communicate scientific topics in a written way on an advanced level.
Contents:	• Time management/ self management • Structure of written presentations • Different forms of written presentations • Writing techniques • Prevention of the writer's block
Assessment	Writing assignments
Media used in the course:	Powerpoint slides (PDF), teaching laptop with internet access
References:	

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course	Visualistics
Semester of study	3rd semester, Winter Semester
Modulveranstwortlicher	Professor Dr. Jürgen Bajorath
Staff member	Prof. Dr. Thomas Berlage
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	S2 / 2 hours per week
Work load	Estimate: 120 hours, 50 hours contact time, 70 hours self-study
Credit points	4
Mandatory requirements	none
Recommended requirements	None
Learing Outcomes	**Knowledge:** Student will learn to understand different visualization methods, their biomedical applications and benefits/trade-offs. **Skills** Abstraction, modeling and structuring of scientific knowledge Design of presentations and scientific papers **Competences** Students will learn to prepare presentations supported by slides, will be involved interdisciplinary discussions. This will enhance their abilities to communicate scientific results effectively. Students will learn necessary skills for a scientific career and interdisciplinary team work.
Contents	• Biomedical visualization, • Applications in medicine, genomics, proteomics and imaging • Visualization techniques • Zooming and navigation • Visual data mining • Visualization and cognition
Assessment	Seminar
Media used in the course	Powerpoint, papers
References	• 20 topics with about 2-4 papers each

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course	High Content Screening
Semester of study	3rd semester, Winter Semester
Staff member in charge of the module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Thomas Berlage
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	S2/ 2 hours per week
Work load	Estimate: 120 hours, 50 hours contact time, 70 hours self-study
Credit points	4
Mandatory requirements	None
Recommended requirements	None
Learing Outcomes	**Knowledge:** Image-based high content screening techniques, trainable image analysis, Scientific image and data analysis **Skills** Data analysis tool configuration and interpretation of results Discussion about underlying validity of data and results, Training image analysis, scripting, statistical analysis and visual presentation with Excel **Competences** Familiarity with computer-based analysis of high throughput automated experiments. Students will learn to prepare presentations supported by slides, will be involved interdisciplinary discussions. This will enhance their abilities to communicate scientific results effectively. Students will learn necessary skills for scientific career and interdisciplinary team work and will be introduced to scientific work.
Contents	High content screening Cellular analysis Trainable image analysis (object recognition, object classification) Statistical analysis of high content screening Sources of variation and error Presentation and discussion of results
Assessment	Initial lecture, software demonstration Experimental work at the computer Parallel competition of teams getting different results each Result discussion and presentation
Media used in the course	Power point, Excel Zeta software, Image datasets
References	References taken from scientific journals and conference proceedings

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Modeling, Simulation and Visualization: Computer course in modern computational biology
Semester of study	3rd semester, Winter Semester
Staff member in charge of module	Professor Dr. Jürgen Bajorath
Staff member	Prof. Dr. Andreas Weber
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC4 / 4 hours per week,
Work load	Estimate: 240 hours in total; 100 hours contact time and 140 hours self-study
Credit points	8
Mandatory requirements	Basic knowledge in Mathematics for the Life Science, Fundamental programming experiences,
Requirements	none
Learning outcomes	**Knowledge** The module provides basic knowledge of modelling approaches in modern computational biology and practical experience with relevant simulation and visualization techniques. The students will perform computer simulations of selected mathematical models for typical processes and phenomena appearing in the modern Life Sciences, for example: 1. Regulation of gene expression and the control of circadian rhythm, 2 Computing parameter domains for bistability in signalling networks; 3. Analyzing the oscillatory and chaotic structure in epidemic models; The aim of each selected 'project' is to understand the basic biological principles by developing and/or applying appropriate simulation algorithms, performing statistical analysis of corresponding 'numerical experiments' and visually presenting the results on the screen (mostly 'on-line') **Skills** Ability to handle a programming language such as Python and its simulation and visualization tools to investigate biological hypothesis and to perform simulation experiments. **Competences** Gaining profound knowledge in modeling of complex biological systems as well as practical experiences in computer simulation and visualization tools; learning to formulate scientific hypotheses and to communicate scientific results.
Contents	Proto-typical problems will be presented as 'projects' (or 'case studies') and treated at the computer working places, usually by a small group of students, depending on the number of participants and available computers. Important will be, that each participant gets enough time to conceive and implement self-written program modules.
Assemessment (Studienleistungen)	Final report and presentation of project results, regular participation in the practical computer lab course, collection of performed simulations and visualizations (as printed protocols or finished and stored computer demonstrations)
Media used in the course	Preparing powerpoint slides, computer demonstrations, basic calculations at the front table, participating the forum discussions.
References	E.S. Allman & J.A. Rhodes "Mathematical Models in Biology" Cambr.Univ.Press 2004; G. deVries et al. "A Corse in Mathematical Biology" SIAM, Philadelphia 2006

Module	Modul 10
Level	Master
Abbreviation of the module	LSI
Course title	Mechanism Enrichment using NeuroMMSig
Semester of study	3rd semester, Winter Semester
Staff member in charge of module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Martin Hofmann-Apitius
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC2/ 2 hours per week
Work load	120 hours in total: 50 hours contact time, 70 hours self-study
Credit points	4
Mandatory requirements	none
Recommended requirements	Lecture Life Science Knowledge Discovery
Learning outcomes	**Knowledge** Students are made familiar with methods to interprete signals through computable knowledge-based models and will learn to analyse complex clinical data (mechanism-based stratification of patient data). **Skills** Students will learn to apply the above mentioned methods effectively. **Competences** Students will learn to work in teams and communicate scientifical results effectively
Contents	Methods of information extraction in the biomedical field, knowledge-based models, algorthms for the functional interpretation of data of given knowledge based models
Assemessment (Studienleistungen)	Lab report
Media used in the course	Slides, computer, Jupyter Notebooks
References	

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Introduction into Medicinal Chemistry
Semester of study	3rd semester, Winter Semester
Staff member in charge of Module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Diana Imhof
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	L2/ 2 hours per week, lecture contains practical exercises that are an integral part of the lecture
Work load	Estimate: 90 h int total: 60 h contact time, 30 h self-study
Credit points	3
Mandatory requirements	Lecture Introduction to Chemistry and Biology
Requirements	Good proficiency in English; basic knowledge of natural sciences, e.g. chemistry, biology, physics, and mathematics; basic knowledge of computer programs
Learning outcomes	**Knowledge** This module will give an introduction into general concepts and modern methods in medicinal chemistry and drug development with an emphasis on computer-aided drug design strategies. The students will learn how to use open access softwares, platforms and online servers. **Skills** Students will be made familiar with the appropriate application of relevant concepts in drug design and development. Specific examples will be given. **Competences** Interdisciplinary knowledge will be conveyed. Students will be qualified to recognize correlations with other modules of the program. In particular, a transfer of theoretical concepts and techniques into practice will be performed due to the practical course.
Contents	Structures of biomolecules, drug targets, general mode of drug action, stereochemistry and drug action, properties of drugs, lead structures, quantitative structure-activity relationships, molecular modelling and docking approaches for large and small molecules, molecular dynamic simulation: principle, purpose and limitations, use of relevant databases, structure-based drug design approaches, drug metabolism, drug synthesis and development in industry
Assemessment (Studienleistungen)	Written exam
Media used in the course	PowerPoint, CIP-Pool, script, textbooks on Medicinal Chemistry, publications
References	Biochemistry and Medicinal Chemistry Textbooks (e.g. 2018 Medicinal Chemistry Reviews, Vol. 53), selected publications (provided), database cross citations

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Longitudinal modelling of disease progression
Semester of study	3rd semester, Winter Semester
Person in charge of module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Martin Hofmann-Apitius
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC2/ 2 hours per week in the semester
Work load	120 hours, 40 hours contact time, 80 hours self-study
Credit points	4
Mandatory requirements	none
Recommended requirements	none
Learning outcomes	**Knowledge** Methods of longitudinal modelling of complex biomedical data **Skills** Students learn how to apply these methods effectively. **Competences** Students learn to work effectively in teams and to communicate results in an appropriate manner.
Contents	Mutlivariate methods, longitudinal omics modelling, mixed models, random effects, conditional models, flexible baysian joint models and other state-of-the-art-methods
Assemessment (Studienleistungen)	Oral presentation
Media used in the course	Slides, original research papers
References	

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Current Trends in Applied Life Science Informatics
Semester of study	3rd semester, Winter Semester
Staff member in charge of module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Martin Hofmann-Apitius
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	S2/ 2 hours per week
Work load	120 hours int total: 40 hours contact time, 80 self-study
Credit points	4
Mandatory requirements	none
Recommended requirements	none
Learning outcomes	**Knowledge** Students will acquire knowledge about data mining/text mining and knowledge discovery in the biomedical field. **Skills** Of-Students will learn state-art methods from the above mentioned field. **Competences** Students will learn to collaborate effectively in teams and communicate results effectively. Students will learn to effectively read and analyse original papers in a highly dynamic research area.
Contents	Life Scince Knowledge discovery, Machine Learning methods in the field of the biomedical sciences´, text mining data ming in the biomedical research field
Assemessment (Studienleistungen)	Oral presentation
Media used in the course	Slides, original literature, research articles
References	

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Biomedical Databases - Design, Implementation, Optimisation
Semester of study	2nd semester, Summer Semester
Person in charge of Module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Martin Hofmann-Apitius,
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	LC2/ 2 hours per week
Work load	120 in total: 40 hours contact time, 80 hours self-study
Credit points	4
Mandatory requirements	Lecture: Biological Dabases
Requirements	none
Learning outcomes	**Knowledge** Students will be made familiar with current Biological Database technologies. **Skills** Students will learn to successfully apply current Biological Dabase technologies in pracital Life Science problems. **Competences** Students will learn to collaborate successfully in international teams applying current Biolocial Database technologies to Life Science problems.
Contents	1. Biological Databases 2. Database Technologies 3. Development of a software library 4. Version management of software projects with git 5. Project management with SCRUM 6. Development of suitable algorithms to identify relevant disease causing genes
Assemessment (Studienleistungen)	Oral presentation and lab report
Media used in the course	Slides, whiteboard, videos, hand-outs
References	

Module	Module 10
Level	Master
Abbreviation of the module	LSI
Course title	Knowledge Assembly, Data Integration and Modeling in Systems and Networks Biology
Semester of study	3rd semester, Winter Semester
Staff member in charge of module	Professor Dr. Jürgen Bajorath
Staff member	Professor Dr. Martin Hofmann-Apitius
Language	English
Assignment to curriculum	Optional
Type of course/ hours per week	S2/ 2 hours per week
Work load	120 hours in total: 40 hours contact time, 80 hours self-study
Credit points	4
Mandatory requirements	Lecture Biological Dabases
Requirements	None
Learning outcomes	**Knowledge** Students will learn to read, understand, compile and present a paper from the filed of Systems and Network Biology. **Skills** Students will understand worksflows from data to knowledge representation that will lead to new scientific insights. **Competences** Students will learn to compile and present highly complex knowedge gained from original literature to a group of peers and seniors.
Contents	1. Protein-protein interaction networks 2. Gene regulatory networks 3. Metabolic networks 4. Signaling networks 5. Neuronal and networks 6. Disease networks 7. Interactome 8. Metabolome
Assemessment (Studienleistungen)	Oral presentation
Media used in the course	Slides
References	Original research literature