



Description of the degree program

# Artificial Intelligence for Molecular Sciences (Master) PO 1

Date: 26.09.2025

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<b>Foundations</b>	<b>26 ECTS</b>
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<b>Title</b>	Introduction to AIMS		
<b>Number</b>	1498110 AM-P-1	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	Institut für Physikal. und Theoretische Chemie
<b>Hours per Week / ECTS</b>	3 / 5,0	<b>Module owner</b>	Prof. Dr. Christoph Jacob
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>			
<b>Course achievement</b>	presentation (Referat, SL)		
<b>Contents</b>			
<p><b>Lecture Series:</b> introduction to research data in molecular sciences: molecular representations, protein structure data, spectroscopic data, genomic databases, proteomics and other -omics data; research data management in different fields of the molecular sciences.</p> <p><b>Seminar:</b> student presentations of current topics and challenges related to artificial intelligence in molecular sciences (chemistry, pharmacy, biology)</p>			
<b>Objective qualification</b>			
Students have an overview of current topics and challenges in the research field "Artificial Intelligence in Molecular Sciences". They are familiar with different types of research data generated in the molecular sciences and are able to carry out simple analyses of such data sets. They are familiar with the methods and tools of research data management in the molecular sciences.			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Introduction to AIMS		Lecture	english
Introduction to AIMS		Seminar	english

<b>Title</b>	Mathematics for Engineers A		
<b>Number</b>	1294250	<b>Module version</b>	V2
<b>Shorttext</b>	MAT-STD7-25	<b>Language</b>	english
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Carl-Friedrich-Gauß-Fakultät
<b>Module duration</b>	1	<b>Institution</b>	Institut für Partielle Differentialgleichungen
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Studiendekan der Mathematik
<b>Workload (h)</b>	240		
<b>Class attendance (h)</b>	112	<b>Self studying (h)</b>	128
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	1 written exam (180 minutes) After approval by the examination board mathematics (Prüfungsausschuss Mathematik), the examiner can also choose the take-home exam as the form of examination.		
<b>Course achievement</b>			
<b>Contents</b>			
<p>Mathematics for engineering students A (Calculus 1)</p> <p>1 sequences and limit: definitions and concepts, e.g. monotony and bounds, convergence criteria of comparison and of monotony, typical limits, Euler's number <math>e</math>, accumulation point, limit superior, Bachmann-Landau notation, supremum, Cauchy sequence, basic properties of real numbers</p> <p>2 series: convergence and absolute convergence, geometric, harmonic and exponential series, comparison test, ratio test, root test, alternating series test with proofs</p> <p>3 functions: concepts, standard functions including hyperbolic and area functions, relation to trigonometric functions, inverse function, rational functions and partial fraction decomposition, graphical representation</p> <p>4 limits of functions and continuity: definition, properties of continuous functions, classification of discontinuities, intermediate value theorem, extreme value theorem with proof</p> <p>5 differentiation: difference and differential quotient, <math>C^n</math>-spaces and norms, product and chain rule, derivatives of standard functions, derivatives of inverse functions, mean value theorem, de l'Hospital's rule with proof, extreme values, curvature Taylor polynomials and series</p> <p>6 integration: definit and indefinit integral (Riemann), fundamental theorem of calculus with proof, integration by parts, integration by substitution, integrals of standard functions, integrals of rational functions and power series, improper integrals, Gamma-unction</p> <p>Mathematics for engineering students A (Linear Algebra)</p> <p>1 algebraic structures: number domains, group, field, modulo, complex numbers, cartesian and polar form, Euler's identity, roots of complex numbers, polynomial division, linear factor decomposition, fundamental theorem of algebra without proof</p> <p>2 vectors and vector spaces: linear independence, sub-space, basis, dimension, norm, scalar product, projection, ortho-normal basis, Cauchy Schwarz inequality</p> <p>3 linear maps and matrices: definition of general linear maps, kernel, image, rank, inverse matrix, transposition, determinant, matrix norm</p> <p>4 Gaussian algorithm: trapezoid form, underdetermined systems and parameter-dependent solutions, inverse matrix</p> <p>5 eigenvalues and eigenvectors: diagonalizable matrices, eigenvalues and -vectors of symmetric matrices, Jordan form, similarity</p> <p>6 vectors in geometry: lines and planes, Hesse normal form, vector product, triple product, transformation of coordinates</p>			

<b>Objective qualification</b>
The students combine the learnt mathematical methods of univariate calculus and linear algebra in the description and investigation of applied problems in the engineering sciences. They choose appropriate calculation techniques and appropriate methods of proof for the discussion of the mathematical fundamentals in the applied and engineering sciences, and they apply these techniques and methods. The students explain the formation of mathematical concepts and they derive the motivation of these concepts from applications and from the mathematical specification and delimitation of terms and definitions. The students reproduce and explain basic proofs and ideas of proofs in univariate calculus and linear algebra. They are able to identify and to test relations between the learnt concepts. The students are able to analyse mathematical problems occurring in applications and engineering lectures, to extract and to solve treatable sub-problems and to identify continuative difficulties. Finally, students use constructively modern tools for the treatment of computational problems.
<b>Literature</b>
Text books and lecture notes on calculus, linear algebra, mathematics for engineers, e.g. * Burg, Haf, Wille, Meister: Höhere Mathematik für Ingenieure, Band I & II, SpringerVieweg * Ansorge, Oberle, Rothe, Sonar: Mathematik in den Ingenieur- und Naturwissenschaften, Band I, Wiley * Langemann, Sommer: So einfach ist Mathematik, zwölf Herausforderungen im ersten Semester, SpringerSpektrum



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
You can attend lectures in German or English. Participation in the small exercises is voluntary.			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Mathematics for Engineers A (Analysis 1)	1,0	Exercise	german
Mathematics for Engineers A (Analysis 1)	1,0	Exercise, small group	german
	2,0	Lecture/Exercise	german
	1,0	Exercise, small group	german
	2,0	Lecture/Exercise	english
	1,0	Exercise	english
	1,0	Exercise, small group	english
	2,0	Lecture/Exercise	english
	1,0	Exercise	english
	1,0	Exercise, small group	english

Mathematics for Engineers A (Linear Algebra)	1,0	Exercise	german
Mathematics for Engineers A (Linear Algebra)	2,0	Lecture/Exercise	german
Mathematics for Engineers	6,0	Lecture/Exercise	english german

<b>Title</b>	Programming in Python and Python Lab		
<b>Number</b>	1498130 AM-P-3	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	Institut für Physikal. und Theoretische Chemie
<b>Hours per Week / ECTS</b>	5 / 8,0	<b>Module owner</b>	Prof. Dr. Christoph Jacob
<b>Workload (h)</b>	240 h		
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>			
<b>Course achievement</b>	team-based development and documentation of a data science software tool (Comp- Prog, SL)		
<b>Contents</b>			
<p><b>Programming in Python:</b> This seminar covers an introduction to Python. The most important functionalities are presented, including matplotlib, numpy, scipy, and pandas. The planning, execution, documentation, and deposition of programming projects is explained.</p> <p><b>Python Lab:</b></p> <ul style="list-style-type: none"> <li>• Introduction to explorative data analysis in Python</li> <li>• Statistical data analysis</li> <li>• Unsupervised machine learning</li> <li>• Supervised machine learning</li> <li>• Critical assessment of machine learning</li> </ul>			
<b>Objective qualification</b>			
<p>After successful completion of this module, students will have the competence to apply Python for designing and implementing small to medium software projects and analytic workflows with a focus on statistics and machine learning. During an interactive learning phase during which the students will be able to apply common packages such as scikit-learn, and they will be able to synthesize analysis workflows for diverse data science questions. These workflows will be presented and discussed in a mini-conference among the students. After the mini-conference, students will form small teams to develop data science software tools which will be presented during the closing event. They will gain the competence to critically evaluate machine learning workflows.</p>			
<b>Literature</b>			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Python Lab	3,0	Internship	english
	1,0	Colloquium	english
Programming in Python	1,0	Course	english

<b>Title</b>	Scientific Software Engineering – Lab		
<b>Number</b>	3325000040 AM-P-4	<b>Module version</b>	
<b>Shorttext</b>	AM-P-4	<b>Language</b>	english
<b>Frequency of offer</b>		<b>Teaching unit</b>	Fakultät Architektur, Bauingenieurwesen und Umweltwissenschaften
<b>Module duration</b>	1	<b>Institution</b>	Institut für rechnergestützte Modellierung im Bauingenieurwesen
<b>Hours per Week / ECTS</b>	/ 5,0	<b>Module owner</b>	
<b>Workload (h)</b>	150 h		
<b>Class attendance (h)</b>	56	<b>Self studying (h)</b>	94
<b>Compulsory requirements</b>			
<b>Recommended requirements</b>	Algorithms & Programming (Lab)		
<b>Expected performance/ Type of examination</b>	written exam (60 min) or oral exam (30 min)		
<b>Course achievement</b>	Homework according to examiners specifications		
<b>Contents</b>			
Software Design Principles, Design Patterns, Software Quality Metrics, Agile Software Development, Test Driven Development (TDD)			
<b>Objective qualification</b>			
Students will be able to develop sustainable software solutions in the scientific contexts for moderately complex engineering problems using advanced design and implementation approaches. Furthermore, they will be able to evaluate software designs with respect to various quality aspects and to make independent design decisions and implement corresponding solutions.			
<b>Literature</b>			
Lecture script, scientific papers, books			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
	4,0	Laboratory	english

<b>Advanced Area</b>		<b>15 ECTS</b>	
<b>Title</b>	Machine Learning for Data Science		
<b>Number</b>	4229000050	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english german
<b>Frequency of offer</b>	irregular	<b>Teaching unit</b>	Carl-Friedrich-Gauß-Fakultät
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	3 / 5,0	<b>Module owner</b>	Prof. Dr. Michel Bes-serve
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	42	<b>Self studying (h)</b>	108
<b>Compulsory requirements</b>			
<b>Recommended requirements</b>	The lectures and exercises require a good command of the knowledge from Bachelor level "Linear Algebra" and "Analysis" courses, and a background knowledge on probability theory and the python programming language is recommended.		
<b>Expected performance/ Type of examination</b>	1 examination: written exam, 90 minutes or oral exam, 30 minutes or take-home exam		
<b>Course achievement</b>	1 academic achievement: 50% of the exercises must be passed		
<b>Contents</b>			
<ul style="list-style-type: none"> <li>- Supervised Learning Algorithms</li> <li>- Model Selection</li> <li>- Unsupervised Learning Algorithms</li> <li>- Deep Neural network architectures for data science</li> <li>- Self-supervised learning and foundation models</li> <li>- Uses and limitations of ML in data science projects</li> </ul>			
<b>Objective qualification</b>			
After successfully completing this module, students should be able to <ul style="list-style-type: none"> <li>- understand and correctly apply basic concepts of machine learning algorithm design,</li> <li>- master elementary tools for analyzing the performance of machine learning approaches,</li> <li>- identify the most suited ML approaches for a particular application.</li> </ul>			
<b>Literature</b>			
<ul style="list-style-type: none"> <li>- Machine Learning, A Probabilistic Perspective, Murphy, 2012</li> <li>- Deep Learning, Goodfellow et al., 2016</li> <li>- Mathematics for Machine Learning, Deisenroth et al., 2020</li> </ul>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Machine Learning for Data Science	3,0	Lecture/Exercise	english

<b>Title</b>	Pattern Recognition		
<b>Number</b>	2424690	<b>Module version</b>	
<b>Shorttext</b>	ET-NT-69	<b>Language</b>	
<b>Frequency of offer</b>	every term	<b>Teaching unit</b>	Fakultät für Elektrotechnik, Informationstechnik, Physik
<b>Module duration</b>	1	<b>Institution</b>	Institut für Nachrichtentechnik
<b>Hours per Week / ECTS</b>	4 / 5,0	<b>Module owner</b>	Prof. Dr. Tim Fingscheidt
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	56	<b>Self studying (h)</b>	94
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	Oral exam 30 min. or written exam 90 min.		
<b>Course achievement</b>			
<b>Contents</b>			
<ul style="list-style-type: none"> <li>- Bayesian decision rule</li> <li>- Quality metrics in pattern recognition</li> <li>- Supervised learning with parametric distributions</li> <li>- Supervised learning with non-parametric distributions, classification</li> <li>- Linear discriminant functions, single-layer perceptron</li> <li>- Support vector machines (SVMs)</li> <li>- Multi-layer perceptron, neural networks (NNs)</li> <li>- Deep learning</li> <li>- Unsupervised learning, clustering methods</li> </ul> <p>Note: For pattern recognition using hidden Markov models (HMMs), a separate more in-depth module, Spoken Language Processing (ET-NT-68), is offered in the summer semester.</p>			
<b>Objective qualification</b>			
Upon completion of this module, students gain fundamental knowledge about methods and algorithms for classification of data. They are capable to select the appropriate means for real-world problems, to design a solution and to evaluate it.			
<b>Literature</b>			
<ul style="list-style-type: none"> <li>- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001</li> <li>- C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006</li> </ul>			
<b>Remark</b>			
Basic knowledge of statistics, such as acquired in the module "Probability Theory and Statistics", facilitates the understanding of the lecture.			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
	2,0	Lecture	english german
<b>Literature</b>			
<ul style="list-style-type: none"> <li>- R. O. Duda, P. E. Hart, D. G. Stork: Pattern Classification, Wiley, 2001</li> <li>- C. M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006</li> </ul>			
	2,0	Seminar	english german
<b>Literature</b>			
<ul style="list-style-type: none"> <li>- Vorlesungsfolien</li> <li>- R. O. Duda, P. E. Hart, D. G. Stork: Pattern Classification, Wiley, 2001</li> <li>- C. M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006</li> </ul>			

<b>Title</b>	Computer Lab Pattern Recognition		
<b>Number</b>	2424000020	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	every term	<b>Teaching unit</b>	Fakultät für Elektrotechnik, Informationstechnik, Physik
<b>Module duration</b>	1	<b>Institution</b>	Institut für Nachrichtentechnik
<b>Hours per Week / ECTS</b>	4 / 5,0	<b>Module owner</b>	Prof. Dr. Tim Fingscheidt
<b>Workload (h)</b>			
<b>Class attendance (h)</b>	56	<b>Self studying (h)</b>	94
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>			
<b>Course achievement</b>			
<b>Contents</b>			
<p>The course consists of hands-on programming tasks that are solved by the participants and subsequently evaluated in a semi-automated way. In total, seven units from the sub-fields (i) basics of hands-on application of machine learning methods, (ii) image processing (computer vision) and (iii) time series analysis have to be completed. The seven units are:</p> <ul style="list-style-type: none"> <li>• Interactive introduction to Python fundamentals using Jupyter notebooks, fundamentals of data processing, preparation and visualization.</li> <li>• Use of single-layer machine learning models to solve a two-class problem: Support vector machines (based on libsvm) and neural networks. Splitting and use of datasets, application of appropriate metrics for evaluation, use of high-level machine learning libraries such as SciKit-Learn</li> <li>• Use of deep neural networks to solve a multi-class classification problem, introduction to recognized academic datasets such as MNIST and CIFAR-10, introduction to the use of deep learning libraries PyTorch and Tensorflow, usage and adaptation of pre-trained models</li> <li>• Use of convolutional neural networks to solve more challenging image processing problems such as semantic segmentation and depth estimation, use of regularization methods in training</li> <li>• Use of diverse cost functions to optimize neural networks, implementation of generative models such as Generative Adversarial Networks (GANs)</li> <li>• Use of recurrent neural networks to solve problems based on time series data, application of concepts for anomaly detection</li> <li>• Use of recurrent neural networks for speech processing, e.g., for noise reduction, analysis of neural networks with respect to their complexity (FLOPs, number of parameters)</li> </ul> <p>Six out of the seven units have to be successfully passed for the entire computer lab module to be passed, among these unit 4 (convolutional neural networks) and unit 7 (recurrent neural networks in speech processing).</p>			
<b>Objective qualification</b>			
<p>In this course, students acquire the competencies to independently select and apply appropriate machine learning and deep learning methods for complex problems. The students ...</p>			

- ... master the programming language Python as well as the basics of the deep learning libraries PyTorch and Tensorflow.
- ... evaluate the effectiveness of simple machine learning models and neuronal networks for classification and regression problems.
- ... evaluate the quality of deep learning models on appropriate data (sub)sets with meaningful metrics
- ... know and use different types of neural networks for problems in the areas of image processing, time series processing and generative problems
- ... know and use different strategies for data preprocessing and data augmentation
- ... know and use different training and regularization methods for the optimization of neural networks
- ... evaluate the complexity of a neural network on the basis of various parameters

**Literature**

- Christopher M. Bishop, Nasser M. Nasrabadi, "Pattern Recognition and Machine Learning", Springer 2006
- Ian Goodfellow, Yoshua Bengio, Aaron Courville, "Deep Learning", MIT Press 2016



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Computer Lab Pattern Recognition	3,0	Internship	english german
<b>Literature</b>			
<ul style="list-style-type: none"> <li>• Christopher M. Bishop, Nasser M. Nasrabadi, "Pattern Recognition and Machine Learning", Springer 2006</li> <li>• Ian Goodfellow, Yoshua Bengio, Aaron Courville, "Deep Learning", MIT Press 2016</li> </ul>			
Computer Lab Pattern Recognition	1,0	Colloquium	english german
<b>Literature</b>			
<ul style="list-style-type: none"> <li>• Christopher M. Bishop, Nasser M. Nasrabadi, "Pattern Recognition and Machine Learning", Springer 2006</li> <li>• Ian Goodfellow, Yoshua Bengio, Aaron Courville, "Deep Learning", MIT Press 2016</li> </ul>			

<b>Title</b>	Deep Learning Lab		
<b>Number</b>	2424750	<b>Module version</b>	
<b>Shorttext</b>	ET-NT-75	<b>Language</b>	english german
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Elektrotechnik, Informationstechnik, Physik
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	4 / 5,0	<b>Module owner</b>	Prof. Dr. Tim Fingscheidt
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	56	<b>Self studying (h)</b>	94
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>			
<b>Course achievement</b>			
<b>Contents</b>			
<b>Objective qualification</b>			
<b>Literature</b>			
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001 - C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006 - I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
	3,0	Internship	german
<b>Literature</b>			
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001 - C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006 - I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016			

	1,0	Colloquium	german
<b>Literature</b>			
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001 - C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006 - I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016			

<b>Title</b>	Methods of Uncertainty Analysis and Quantification		
<b>Number</b>	2540420 AM-V-5	<b>Module version</b>	
<b>Shorttext</b>	AM-V-5	<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Maschinenbau
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	3 / 5,0	<b>Module owner</b>	Prof. Dr. Sabine Langer
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	42	<b>Self studying (h)</b>	108
<b>Compulsory requirements</b>			
<b>Recommended requirements</b>	Basic knowledge of the finite element method, numerical procedures for quadrature and polynomial approximation as well as probability theory and statistics are helpful. Attending the course "Unsicherheiten in technischen Systemen" is not a requirement.		
<b>Expected performance/ Type of examination</b>	1 examination element: Written exam (90 min) or oral exam (30 min)		
<b>Course achievement</b>			
<b>Contents</b>			
Probability and random variables, advanced Monte Carlo methods, stochastic quadrature, stochastic spectral methods, global sensitivity analysis, data-driven uncertainty quantification			
<b>Objective qualification</b>			
Students can formulate and name elementary rules of probability theory and different ways to describe probability distributions. They can model technical/physical systems in a stochastic way using random variables. The students are further able to apply Monte Carlo and stochastic spectral methods to quantify uncertainties and also to assess the impact and propagation of uncertainties in models through global sensitivity analysis. Moreover, they are able to evaluate the numerical efficiency of the aforementioned methods. The students are also able to outline the principles of data-driven approaches to uncertainty analysis.			
<b>Literature</b>			
<ul style="list-style-type: none"> <li>• O. Le Maitre, O.M. Knio: Spectral Methods for Uncertainty Quantification, Springer Netherlands, 2010</li> <li>• D. Xiu: Numerical Methods for Stochastic Computations: A Spectral Method Approach, Princeton University Press, 2010</li> <li>• G. J. Lord, C.E. Powell, T. Shardlow: An introduction to computational stochastic PDEs, Cambridge University Press, 2014</li> </ul>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
	2,0	Lecture	english
	1,0	Exercise	english

<b>Profile Area Chemical Synthesis And Drug Design</b>	<b>37 ECTS</b>
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<b>Title</b>	Reaction Mechanisms		
<b>Number</b>	1498570 AM-A-1	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	3 / 4,0	<b>Module owner</b>	Prof. Dr. Christopher Teskey
<b>Workload (h)</b>	120		
<b>Class attendance (h)</b>	42	<b>Self studying (h)</b>	78
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	oral or written exam (PL) nach BPO §5 (3)		
<b>Course achievement</b>	none		
<b>Module grade composition</b>	see expected performance		
<b>Contents</b>			
<p><b>Lecture:</b> Orbitals and stereochemistry, enolate chemistry, radical reactions, photochemical reactions, pericyclic reactions, rearrangements, transition metal-catalyzed cross-coupling, C-H activation, metathesis, organocatalysis, photoredox catalysis, methods to elucidate reaction mechanisms, kinetics of organic chemical reactions.</p> <p><b>Exercise:</b> Deepening and consolidating the material presented in the lecture, working on exercises.</p>			
<b>Objective qualification</b>			
The students understand the chemical reactivity of organic molecules and are able to apply chemical reactions specifically to modify molecules. They are able to formulate and classify the underlying organic chemical reaction mechanisms. With their help, they are able to make meaningful statements about the success of planned reaction paths from the starting molecule to the target molecule and to explain the main and by-products. The students know methods to explain reaction mechanisms and can assess and discuss their range of application and significance.			
<b>Literature</b>			
information in the courses			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
none			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Reaction mechanisms	2,0	Lecture	english
Reaction mechanisms	1,0	Exercise	english

<b>Title</b>	Organometallic Chemistry		
<b>Number</b>	1498590 AM-A-2	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	3 / 4,0	<b>Module owner</b>	Prof. Dr. Matthias Tamm
<b>Workload (h)</b>	120		
<b>Class attendance (h)</b>	42	<b>Self studying (h)</b>	78
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Oral or Written Exam		
<b>Course achievement</b>	none		
<b>Module grade composition</b>	see expected performance		
<b>Contents</b>			
<p><b>Lecture:</b> Coordination chemistry of transition metals, central atoms and ligand types, coordination numbers, geometries of complexes, bonding in transition metal complexes (valence bond theory, crystal field theory, molecular orbital theory), isolobal principle, carbonyl complexes, substitution and redox reactions, transition metal hydrides and dihydrogen complexes, iso(valence)-electronic ligands to CO, metal-alkyl complexes, catalytic elementary reactions (oxidative addition, reductive elimination, insertions, hydride eliminations), catalytic processes (hydroformylation, acetic acid preparation, olefin polymerization, hydrogenations, Wacker process), carbene (alkylidene) and carbyne (alkylidyne) complexes, olefin and alkyne metathesis, complexes with <math>\pi</math>-ligands (olefin, alkyne, allyl, cyclopentadienyl, arene complexes), sandwich compounds, spectroscopic methods for structure elucidation in organometallic chemistry (IR, NMR), occurrence and biological functions of inorganic elements, especially the trace elements Co, Fe, Cu and Zn, cobalamins, hemoproteins, FeS clusters and non-heme iron, copper and zinc proteins.</p> <p><b>Exercise:</b> Consolidation of the lecture material by examples and exercises, exam preparation</p>			
<b>Objective qualification</b>			
Students will master advanced concepts in the chemistry of metals, coordination chemistry, and organometallic chemistry. They understand the role of metals in nature and are familiar with the fundamentals of bioinorganic and bioorganometallic chemistry. They can discuss and predict the structure and properties of metal complexes using modern bonding concepts and have knowledge of the use of transition metal complexes in industrial processes. They know the principles of homogeneous and heterogeneous catalysis and are able to combine important elementary reactions into catalytic cycles and formulate them.			
<b>Literature</b>			
information in the courses			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
none			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Organometallic Chemistry	2,0	Lecture	english
Organometallic Chemistry	1,0	Exercise	english

<b>Title</b>	Catalysis		
<b>Number</b>	1498750 AM-A-3	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Prof. Dr. Marc Walter
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	84	<b>Self studying (h)</b>	156
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Lab work (PL, expA, 25% of overall module mark) Lectures: oral or written exam according to BPO §5 (3) (PL, 75% of overall module mark)		
<b>Course achievement</b>	none		
<b>Module grade composition</b>	see expected performance		
<b>Contents</b>			
<p><b>Lecture Applied homogeneous catalysis:</b> Societal relevance, metal-organic basics of catalysis, elementary reactions, catalytic cycles, industrial applications (Wacker process, acetic acid preparation, hydroformylation, hydrocyanation, hydrogenation, carbonylations, oligomerisation and polymerization of olefins and dienes, copolymerization of CO and olefins), recent developments (C-C cross-couplings, CH activation and functionalization, oxidation reactions, asymmetric catalysis, alkane, olefin and alkyne metathesis), contributions of homogeneous catalysis to sustainable and resource-efficient development of chemistry, elucidation of reaction mechanisms.</p> <p><b>Lecture Applied Heterogeneous Catalysis and Catalytic Polymer Syntheses:</b> Fundamentals of heterogeneous catalysis, adsorption and kinetics, theoretical concepts, preparation and characterization of catalysts, deactivation, mass transfer, reactors for catalysts, industrial catalysis, polymerization with transition metal complexes, Ziegler-Natta polymerization, Phillips catalysts, metallocene and postmetallocene catalysts, metathesis polymerizations.</p> <p><b>Practical course:</b> Work on two projects; a) synthesis, characterization and use of a catalyst in homogeneous catalysis; b) synthesis of a polymer by metal catalysis.</p>			
<b>Objective qualification</b>			
The students master the basic principles of homogeneous catalysis and the differentiation to heterogeneous catalysis and can confidently apply the underlying elementary reactions to catalytic processes. They have an overview of the most important metal-catalyzed industrial processes as well as of current developments and modern aspects of catalysis research. The students are familiar with methods of metal-catalyzed polymer synthesis and are able to evaluate and discuss the advantages of these methods compared to classical non-catalytic methods. They are familiar with methods for the characterization of polymers as well as their fields of application and are able to evaluate these methods.			
<b>Literature</b>			
information in the courses			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
none			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Applied homogeneous catalysis	2,0	Lecture	german
Applied heterogeneous catalysis and catalytic polymer synthesis	2,0	Lecture	german
Lab Course metal catalysis	2,0	Internship	german

<b>Title</b>	Advanced Inorganic Chemistry		
<b>Number</b>	1499710 AM-A-4	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english german
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Prof. Dr. Martin Bröring
<b>Workload (h)</b>	240		
<b>Class attendance (h)</b>	84	<b>Self studying (h)</b>	156
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Presentation (PL, 25 % of overall module grade) Oral Exam or Written Exam (PL, 75 % of overall module grade) nach BPO §5 (3)		
<b>Course achievement</b>	none		
<b>Module grade composition</b>	see expected performance		
<b>Contents</b>			
<p>The module offers a versatile selection of topics, which are treated in a balanced way in lectures and exercises and prepare the students for independent research activities. The lecture block 'Advanced Inorganic Chemistry' is composed of two of the following components, which change annually:</p> <p><b>Lecture Modern Aspects of Coordination Chemistry:</b> Ligand Field Theory: Strong field approach, weak field approach, atomic terms, correlation diagrams, interpretation of optical transitions, molecular magnetism, spin-only formula, orbital moments, orbital moment cancellation, spin-orbit coupling, trends in 3d and 4f elements, spin crossover, spin dynamics, magnetic communication, super-exchange, spin polarisation, spin delocalisation, double exchange, high spin molecules, zero field splitting, magnetic tunnelling, non-innocence, spectroscopy.</p> <p><b>Lecture Supramolecular Coordination Chemistry:</b> Classes of non-covalent interactions, energetics, dynamic and static behaviour, ordering principles, networks, MOFs (Metal Organic Frameworks), co-ordination polymers, brick-and-mortar processes, complex-as-ligand approach, molecules-to-materials, solvothermal syntheses, template syntheses, stacked compounds, surface functionalisation, aurophilicity as a control tool, nanostructuring.</p> <p><b>Lecture Bioinorganic Model Systems:</b> Historical overview of metalloproteins, mechanistic models, biogenic ligands, classification of model systems (speculative model, structural model, functional model), biological and chemical modelling, bioisomorphic substitution, site-specific mutagenesis, model complexes for iron sequestration, hydrolases, light collection, oxygen management, electron transfer, ni-trogen cycle, hydrogenases.</p> <p><b>Lecture Synthesis of Inorganic Molecular Compounds:</b> Symmetry, structure and bonding properties of molecules, hydrides of elements, polyhedral boranes and carboranes, silanes and hydrosilylation, car-bene, alkene and alkyne analogues of main group elements (element-element multiple bonds), coordination numbers &gt; 4 for main group elements (hypervalency), Supramolecular chemistry (weak interactions), inorganic rings, chains and clusters, elementorganic compounds in organic synthesis and catalysis, frustrated Lewis acid-base pairs, modern methods for functionalisation of main group elements.</p> <p><b>Lecture Structural Chemistry:</b> History, overview of general methods for structure determination, description and models, ionic compounds (Madelung constants, radii quotients), sphere packing as a structural fea-</p>			

ture (Hume-Rothery and Laves phases, alloys), polyhedra as a structural feature, symmetry as an ordering principle (group-subgroup relationships, phase transformations), physical properties of solids.

**Lecture Chemistry of the f-elements:** History; occurrence and separation; physical and chemical properties; differentiation from d-transition metals and s-block elements; chemical binding and role of f-orbitals; magnetism; current developments in coordination and organic metal chemistry; applications in technology, medicine, organic synthesis and small molecule activation.

**Seminar:** Recording, evaluation and processing of EPR and Mössbauer spectra as well as magnetic measurements on selected paramagnets; interpretation of the electronic structures in the synopsis of all the measurement data obtained; recording of the results and presentation in lecture form.

#### Objective qualification

The students are able to specifically build up inorganic molecular compounds and structures and to interpret and modify them with regard to their structure-activity relationships. Their understanding of the function of inorganic compounds in the biosphere as well as in supramolecular aggregates allows the students to discuss novel model compounds, switches, magnets and catalysts based on main group- and transition metals. Unusual structural and bonding relationships are competently evaluated. Students also have knowledge of interpreting and modelling spectra of paramagnetic compounds, and apply these independently.

#### Literature

information in the courses



#### Related courses

##### Rules for the choice of courses

The following courses must be taken:

- Lectures with a minimum of 4 SWS
- Seminar Analysis of Paramagnetic Compounds **or** Seminar Practical X-Ray Structure Analysis

!The Seminar Analysis of Paramagnetic Compounds can only be taken in combination with the lecture "Modern Aspects of Coordination Chemistry!"

##### Compulsory attendance

Name of the course	SWS	Eventtype	Language
Molecular Main Group Chemistry	2,0	Lecture	english german
Pigments of Life	2,0	Lecture	english
Structural Chemistry	2,0	Lecture	english
Bioinorganic Model Systems	2,0	Lecture	english
Modern Aspects of Coordination Chemistry	2,0	Lecture	english
Paramagnetic Compunds	2,0	Seminar	english german
Seminar Paramagnets	2,0	Seminar	english

<b>Title</b>	Organic Synthesis Planning		
<b>Number</b>	1499160 AM-A-5	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	irregular	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	3 / 4,0	<b>Module owner</b>	Prof. Dr. Thomas Lindel
<b>Workload (h)</b>	120		
<b>Class attendance (h)</b>	42	<b>Self studying (h)</b>	78
<b>Compulsory requirements</b>	keine		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	oral or written exam (PL)		
<b>Course achievement</b>	none		
<b>Module grade composition</b>	see expected performance		
<b>Contents</b>			
<b>Lecture:</b> Reaction databases, retrosynthesis, functional group conversions, chemoselectivity, protecting group chemistry, atom-economic synthesis, multi-step sequences, biomimetic synthesis, natural product synthesis, current examples from the literature.			
<b>Objective qualification</b>			
Based on database-assisted retrosynthetic analysis, students are able to propose multi-step synthesis sequences for complex organic compounds, especially for natural and active ingredients.			
<b>Literature</b>			
information in the courses			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
none			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Organic Synthesis Planning	2,0	Lecture	english

Organic Synthesis Planning	1,0	Exercise	english
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<b>Title</b>	Enzyme Engineering		
<b>Number</b>	1601250 AM-A-6	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	9 / 10,0	<b>Module owner</b>	Prof. Dr. Anett Schallmey
<b>Workload (h)</b>	300 h		
<b>Class attendance (h)</b>	148 h	<b>Self studying (h)</b>	162 h
<b>Compulsory requirements</b>			
<b>Recommended requirements</b>	Participants need to have basic knowledge in molecular biology/genetics and protein biochemistry.		
<b>Expected performance/ Type of examination</b>	Oral examination (50 min) or written exam (200 min.) according to BPO §5 (3)		
<b>Course achievement</b>	Practical Exercise including experimental work.		
<b>Module grade composition</b>	Oral examination or written exam (PL) according to BPO §5 (3). <del>Written exam: 20 min. written exam or 25 min. oral exam; exam can also be</del>		
<b>Contents</b>			
(en) Lecture: General principles and methods for enzyme engineering via protein design and directed evolution using literature examples; introduction of computational tools for identification of mutational hotspots; discussion of different genetic methods for the generation of mutant libraries and suitable assay systems for library screening. Practical exercise: Promoting a deeper understanding of lecture contents, application of selected computational tools for enzyme engineering, practical skills for generating and screening mutant libraries.			
<b>Objective qualification</b>			
The students know different genetic and bioinformatics methods for targeted adaptation of enzyme-specific characteristics via enzyme engineering. Starting from the amino acid sequence of an enzyme, they are able to predict mutational hotspots using computational tools, to generate corresponding mutant libraries, and to select suitable assay systems for library screening. After completing the module, students will be able to - explain various genetic and bioinformatic methods for the targeted modification of enzyme-specific properties. - select suitable mutations based on the amino acid sequence of an enzyme to improve a desired enzyme property using digital tools. - practically create mutant libraries using molecular biology methods. - select and practically apply suitable assay systems for screening mutant libraries. - carry out computer-aided modelling.			

- assess the presentation of scientific results (protocols) of others in the context of a peer review.

**Literature**



**Related courses**

**Rules for the choice of courses**

**Compulsory attendance**

Attendance is compulsory for the practical exercise.

Name of the course	SWS	Eventtype	Language
Enzyme Engineering (Bt-MM 11, Bt-MB 12, AM-A-6, CM-A-5)	2,0	Lecture	german
Enzyme Engineering (Bt-MM 11, Bt-MB 12, AM-A-6, CM-A-5)	7,0	Practical exercise	english

<b>Title</b>	Fundamentals of Protein Structure Analysis		
<b>Number</b>	1399640 AM-A-7	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	9 / 10,0	<b>Module owner</b>	Prof. Dr. Wulf Blankenfeldt
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	126	<b>Self studying (h)</b>	174
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	written exam (ca. 200 min.)		
<b>Course achievement</b>	<ul style="list-style-type: none"> <li>- experimental work</li> <li>- successful participation in the seminar</li> <li>- presentation (45 minutes in groups or two or three students)</li> </ul>		
<b>Contents</b>			
<p>Lecture: Protein structures, common principles of protein structures, methods in structural biology, protein crystallization, characterization of crystals, X-ray diffraction data collection, the phase problem and its solutions, model building and refinement, interpretation of protein structures.</p> <p>Practical course: Protein crystallization, X-ray diffraction data collection, protein structure analysis (molecular replacement), model building, refinement and validation, protein structure analysis and interpretation.</p> <p>Seminar: Recent publications in structural biology.</p>			
<b>Objective qualification</b>			
<p>After completing this module students will be able to</p> <ul style="list-style-type: none"> <li>- name forces that lead to the formation of the stable three-dimensional structures of proteins.</li> <li>- name methods that can be used to determine three-dimensional structures and to explain their underlying physical principles.</li> <li>- name the most important steps in structure determination with crystallographic methods and to explain their background.</li> <li>- judge the quality of published protein structures.</li> <li>- suggest subsequent experiments that utilize the information contained in three-dimensional structures.</li> <li>- plan scientific projects in the field of structural biology.</li> <li>- grasp the content of scientific publications in the field of structural biology.</li> <li>- critically analyze the content of scientific publications in the field of structural biology.</li> <li>- search, present and discuss relevant scientific content.</li> <li>- contribute to controversial discussions of scientific topics.</li> </ul>			
<b>Literature</b>			

- Rupp, Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, Garland Science
- Rhodes, Crystallography Made Crystal Clear, Academic Press
- Klostermeier & Rudolph, Biophysical Chemistry, CRC Press

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Fundamentals of Protein Structure Analysis (Bio-BB 22, Bio-SB 22, Bt-MM 05, AM-A-7)	1,0	Lecture	english
Fundamentals of Protein Structure Analysis (Bio-BB 22, Bio-SB 22, AM-A-7)		Seminar	english
Fundamentals of Protein Structure Analysis (Bio-BB 22, Bio-SB 22, Bt-MM 05, AM-A-7)		Internship	

<b>Title</b>	Biomolecular Modelling		
<b>Number</b>	1499680 AM-A-8	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Prof. Dr. Christoph Jacob
<b>Workload (h)</b>	240		
<b>Class attendance (h)</b>	84	<b>Self studying (h)</b>	156
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Oral or written exam+ (30% of the practical work mark are taken into account in the overall module mark)		
<b>Course achievement</b>	Practical work (marked)		
<b>Module grade composition</b>	see expected performance		
<b>Contents</b>			
<p><b>Lecture:</b> Introduction to the basics of simulations of biomacromolecules - BornOppenheimer approximation, potential energy surface, basics of statistical thermodynamics, empirical force fields and their efficient implementation - geometry optimization, molecular dynamics methods, thermodynamic and static description of (bio)chemical processes, analysis of molecular dynamics simulations, calculation of free energies, multiscale simulation methods - implicit solvent models, coarsegrained models, hybrid QM/MM methods, quantum-chemical embedding methods.</p> <p><b>Computer Lab:</b> Use of force field programs, visualization of crystal structures, geometry optimization, molecular dynamics and normal mode analysis of polypeptides, simulation of (bio)molecules) with different computational methods and their analysis, analysis of dynamical and entropic effects.</p> <p><b>Project Lab:</b> Molecular Dynamics Simulations of Biomolecules.</p>			
<b>Objective qualification</b>			
The students are familiar with modern methods for modelling the structure of biomacromolecules and for simulating their thermodynamic properties. They know empirical force field methods, methods for performing molecular dynamics simulations, as well as modern multiscale simulation methods. The students are able to judge the applicability and the limitations of such methods, to choose suitable simulation methods for their own research projects and to perform, analyze, and evaluate molecular dynamics simulations.			
<b>Literature</b>			
information in the courses			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
none			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Biomolecular Modelling	2,0	Lecture	english german
Computer Lab Biomolecular Modelling	2,0	Exercise	english german
Project Lab Biomolecular Modelling	2,0	Internship	english

<b>Title</b>	Advanced Theoretical Chemistry		
<b>Number</b>	1499170 AM-A-9	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	irregular	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Prof. Dr. Christoph Jacob
<b>Workload (h)</b>	240		
<b>Class attendance (h)</b>	84	<b>Self studying (h)</b>	156
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	Oral or Written Exam+ (20% of the coursework and 20% of the practical work mark are taken into account in the overall module mark)		
<b>Course achievement</b>	Solve coursework problems (unmarked) Practical work (marked)		
<b>Contents</b>			
<p>Lecture and Computer Lab Advanced Quantum Chemistry: Mathematical Foundations of quantum-chemical methods, Hartree-Fock theory, perturbation theory and configuration interaction, coupled-cluster theory, density-functional theory.</p> <p>Lecture and Computer Lab Theoretical Spectroscopy: Time-dependent quantum mechanics, interaction of electromagnetic radiation with molecules, basics of Hartree-Fock and density-functional theory, quantum-chemical calculation of spectroscopic data (Infrared and Raman spectroscopy, UV/Vis spectroscopy, ESR and NMR, simulation of spectra.</p> <p>Lecture and Computer Lab Artificial Molecular Intelligence: Molecular quantum mechanics in a nutshell: Hartree-Fock (HF) theory, post-HF methods, density functional theory; Molecular machine learning in a nutshell: molecular representations, deep learning and kernel methods, generative models, uncertainty quantification, active learning; Applications: structure-property relationships, chemical space exploration, molecular design.</p> <p>Project Lab Theoretical Biophysical Chemistry: Introduction to scientific programming and in-depth study of selected quantum-chemical methods. Application of quantum-chemical methods that usually cannot be used as "black-box" methods in own independent projects.</p>			
<b>Objective qualification</b>			
The students have acquired knowledge on modern methods of quantum chemistry. They are familiar with the foundations of important methods and possess an overview of commonly used quantum-chemical methods, their implementation in scientific software, and their use in chemistry. They are able to judge the applicability and the limits of different quantum-chemical methods and to use suitable methods for their own research projects, to perform quantum-chemical calculations and to analyse, evaluate, and assess their results.			
<b>Literature</b>			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<p>To complete the module one out of the three lectures and the associated exercise must be completed as well as the project lab.</p> <p>One of the three lectures and the associated exercise is offered every winter term. The project lab is offered every winter term.</p>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Advanced Quantum Chemistry	3,0	Lecture	english german
Computer Lab Advanced Quantum Chemistry	1,0	Exercise	english
Project Lab Advanced Quantum Chemistry	2,0	Internship	english

<b>Title</b>	Machine Learning in Computational Chemistry		
<b>Number</b>	1499180 AM-A-10	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Prof. Dr. Jonny Proppe
<b>Workload (h)</b>	240 h		
<b>Class attendance (h)</b>	84	<b>Self studying (h)</b>	156
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	oral or written exam+ (PL, 20% of the coursework and 20% of the practical work mark are taken into account in the overall module grade)		
<b>Course achievement</b>	solve coursework problems (ÜbA, SL unmarked) practical work (expA, SL marked)		
<b>Contents</b>			
<p><b>Lecture and Computer Lab Artificial Molecular Intelligence:</b> Molecular quantum mechanics in a nutshell: Hartree–Fock (HF) theory, post-HF methods, density functional theory; molecular machine learning in a nutshell: molecular representations, deep learning and kernel methods, generative models, uncertainty quantification, active learning; Applications: structure–property relationships, chemical space exploration, molecular design.</p> <p><b>Project Lab:</b> In-depth study of molecular machine learning methods, application of methods of artificial molecular intelligence in own independent projects.</p>			
<b>Objective qualification</b>			
The students have acquired knowledge on modern methods of molecular machine learning and molecular artificial intelligence. They are familiar with the foundations of important methods and possess an overview of commonly used methods, their implementation, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose and apply suitable methods for their own research projects and to analyse, evaluate, and assess their results.			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Machine Learning in Computational Chemistry	3,0	Lecture	english
Computer Lab Machine Learning in Computational Chemistry	1,0	Exercise	english
Project Lab Machine Learning in Computational Chemistry	2,0	Internship	english

<b>Title</b>	Research Lab Chemical Synthesis and Drug Design		
<b>Number</b>	1499230 AM-A-RP	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	every term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	/	<b>Module owner</b>	Prof. Dr. Marc Walter
<b>Workload (h)</b>	360 - 510		
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	study research project including report and presentation (StA)		
<b>Course achievement</b>			
<b>Contents</b>			
<p><b>Research Lab:</b> Conduction and scientific documentation of (parts of) a current research project. The duration of the research project depends on the number of required credit points.</p> <p><b>Seminar:</b> Participation in scientific colloquia, presentation and discussion of current research results</p>			
<b>Objective qualification</b>			
<p>Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.</p>			
<b>Literature</b>			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
the number of credit points assigned for this module depends on the duration of the research project: 13 LP = 390 h 14 LP = 420 h 15 LP = 450 h 16 LP = 480 h 17 LP = 510 h			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Research Lab Chemical Synthesis and Drug Design		Internship	english
Seminar Research Lab Artificial Intelligence for Molecular Sciences		Seminar	english

<b>Profile Area Spectroscopy and Imaging</b>	<b>37 ECTS</b>
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<b>Title</b>	Molecular Spectroscopy		
<b>Number</b>	1498560 AM-B-1	<b>Module version</b>	1
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	4 / 5,0	<b>Module owner</b>	Prof. Dr. Peter Jomo Walla
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	56	<b>Self studying (h)</b>	94
<b>Compulsory requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Oral exam or written exam (PL) nach BPO §5 (3)		
<b>Course achievement</b>	Completing Exercises (SL)		
<b>Contents</b>			
<p>Lecture: Introduction to quantum mechanical description of chemical bonding, transition dipole moment and density. Selection rules, symmetry of orbitals, theory of atomic and molecular spectra, modern experimental techniques in spectroscopy (UV-VIS spectroscopy, fluorescence spectroscopy, IR, Raman and nonlinear spectroscopy).</p> <p>Excercise: Reinforcement and consolidating the material presented in the lecture, working on exercises.</p>			
<b>Objective qualification</b>			
<p>Students understand the concept of chemical bonding on a quantum chemical basis and are able to explain the structure of molecules. They understand the influence of alternating electromagnetic fields on atoms and molecules and are able to make independent quantitative statements about the absorption and emission of light using transition dipole moments and densities. They will have a thorough theoretical understanding of the spectroscopic properties of atoms and molecules and of modern spectroscopic techniques, and will be able to plan and evaluate their use to determine molecular structures.</p>			
<b>Literature</b>			
Wird über Stud.IP vor Vorlesungsbeginn bekannt gegeben.			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Molecular Spectroscopy	3,0	Lecture	english
Exercise Molecular Spectroscopy	1,0	Exercise	english

<b>Title</b>	Biophysical Chemistry		
<b>Number</b>	1498670 AM-B-2	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	4 / 8,0	<b>Module owner</b>	Prof. Dr. Peter Jomo Walla
<b>Workload (h)</b>	240		
<b>Class attendance (h)</b>	66	<b>Self studying (h)</b>	174
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	oral exam or written exam (PL) nach BPO §5 (3)		
<b>Course achievement</b>	completing exercises (SL)		
<b>Contents</b>			
<p>Lecture Biophysical Chemistry: Brief review of biochemical and microbiological basics, traditional methods such as fluorescence and absorption spectroscopy, light scattering, Raman spectroscopy, NMR, ESR and mass spectrometry on biomolecules. Modern methods such as fluorescence microscopy, single molecule detection, nonlinear and ultrafast spectroscopy or nanotechnology to study biomolecules. Prospects for industrial applications and drug discovery.</p> <p>Exercise: Independent calculation and answering of questions with corrections by instructors and assistants, discussion of solution methods in the exercise.</p> <p>Applied Biophysical Chemistry: In this course, the knowledge gained will be deepened through guest lectures on concrete examples of industrial research, e.g. in combination with an excursion to a pharmaceutical company, or from basic research, e.g. at Max Planck Institutes.</p>			
<b>Objective qualification</b>			
The students know the basics of the most important physicochemical methods for the elucidation of biomolecular interactions and structures and are able to decide which modern or traditional method is most efficient to answer such biochemical questions. They know the limitations and dynamic range of these methods and the importance of structure and dynamics of biomolecules for their function. Students will be able to classify which methods are suitable for studying biomolecules and answering biomolecular questions in the different environments of industrial or basic research.			
<b>Literature</b>			
Wird über Stud.IP vor Vorlesungsbeginn bekannt gegeben.			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Biophysical Chemistry	3,0	Lecture	english german
Biophysical Chemistry	1,0	Exercise	english german
Applied Biophysical Chemistry	0,7	Seminar	english german

<b>Title</b>	Modern Optical Methods and Imaging		
<b>Number</b>	1499190 AM-B-3	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>		<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	0 / 8,0	<b>Module owner</b>	
<b>Workload (h)</b>			
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>			
<b>Course achievement</b>			
<b>Contents</b>			
<b>Objective qualification</b>			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Modern Optical Methods and Imaging	2,0	Lecture	english
	1,0	Exercise	english
Modern Optical Methods and Imaging - Lecture/Demonstration/Course Microscopy	1,0	Lecture	english

<b>Title</b>	Solar and Chemical Energy Conversion		
<b>Number</b>	1497800 AM-B-4	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	irregular	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	8 / 8,0	<b>Module owner</b>	Prof. Dr. Stefanie Tschierlei
<b>Workload (h)</b>	240		
<b>Class attendance (h)</b>	112	<b>Self studying (h)</b>	128
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	Oral exam (marked, 30 minutes) or written exam (marked, 90 minutes)		
<b>Course achievement</b>	Practical work including written report and oral exam (unmarked)		
<b>Contents</b>			
<p>Selected Aspects of Energy Conversion: The lecture covers fundamental areas of physical chemistry (such as thermodynamics, transport processes, fluid mechanics, electrochemistry) and connects them with the main renewable energies (biomass, wind, thermosolar, photovoltaic) and their conversion, transport and storage techniques. The lecture may have different emphases: Hydrogen applications, fuel cells, chemical energy storage, hydrogen economics, natural and artificial light harvesting systems.</p> <p>Molecular design: Artificial intelligence and data science methods will be introduced, in particular machine learning, sequential optimization, and inverse design. It will be discussed how these methods can be applied in a fully automated fashion to design functional molecules and materials on a computer. The search for reactive species and catalysts for the activation of small molecules such as CO<sub>2</sub> and N<sub>2</sub> defines the focus of this lecture.</p> <p>Artificial Photosynthesis and CO<sub>2</sub> Activation: Introduction and working principle of molecular photosensitizers and catalysts, mechanisms of electron and energy transfer processes, artificial photosynthesis, solar fuels, molecular water splitting and CO<sub>2</sub> activation, photoelectro-chemistry, structure-activity relationships.</p> <p>Spectroscopic Methods: Methods for the investigation of light-driven processes and the activation of CO<sub>2</sub>, time-resolved and stationary spectroscopy (e.g. X-ray, UV/vis, IR, Raman), spectroelectrochemistry, spectra evaluation using theory, overview of current spectra analysis methods.</p> <p>Practical course: Work on a practical project related to the respective lecture or seminar content.</p>			
<b>Objective qualification</b>			
Students will be enabled to understand and competently discuss current research and application areas of solar and chemical energy conversion. They will further be enabled to recognize the interactions and synergies of the topics represented and to establish interdisciplinary references. Finally, the students are able to read scientific publications in the field of solar and chemical energy conversion and to classify and evaluate experiments and calculations described therein.			
<b>Literature</b>			

Wird über Stud.IP vor Vorlesungsbeginn bekannt gegeben.



### Related courses

#### Rules for the choice of courses

Choose from a-d with a combined workload of 240 h / 8 CP:

- a) Selected aspects of energy conversion (2 LP)
- b) Molecular design + Lab course on molecular design (1 + 2 LP)
- c) Artificial photosynthesis and CO<sub>2</sub> activation + Lab course on artificial photosynthesis (2 + 1 LP)
- d) Spectroscopic Methods + Lab course on spectroscopic methods (1 + 2 LP)

Note: It is recommended to attend the lab courses associated with the selected theoretical courses. A lab course can only be completed in combination with the corresponding lecture.

#### Compulsory attendance

Name of the course	SWS	Eventtype	Language
Selected aspects of energy conversion	2,0	Lecture	english german
Molecular Design	1,0	Lecture	english german
Lab Course on Molecular Design	2,0	Internship	english german
Artificial photosynthesis and CO <sub>2</sub> activation	2,0	Lecture	english german
Lab course on artificial photosynthesis	1,0	Internship	english german
Spectroscopic Methods	1,0	Lecture	english german
Lab course on spectroscopic methods	2,0	Internship	english german

<b>Title</b>	Physical Biology of the Cell		
<b>Number</b>	1398890 AM-B-5	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1 Semester	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	8 / 10,0	<b>Module owner</b>	Prof. Dr. Christian Sieben
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	112 h	<b>Self studying (h)</b>	188 h
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	successfully finished modules Bio-IB 21 or Bio-IB 23		
<b>Expected performance/ Type of examination</b>	<ul style="list-style-type: none"> <li>- Seminar presentation (1, ca. 15 min)</li> <li>- Course report (1)</li> </ul>		
<b>Course achievement</b>	<ul style="list-style-type: none"> <li>- Experimental work in the practical course</li> <li>- Successful participation in exercise and seminar</li> </ul>		
<b>Contents</b>			
<p>Lecture: Students get practical-oriented insights into the field of cell biophysics. The lecture series provides a broad overview of various topics in quantitative biology and cell biophysics. At the beginning, basic concepts, scales and principles of cellular organization (tissue, cells, organelles) will be considered. In addition, the cellular components and their properties are discussed not only biochemically, but also from a biophysical perspective (e.g. polymers such as DNA or the cytoskeleton). In addition, topics such as membranes, diffusion, electrophysiology, structural biology as well as mechanics and kinetics of cell biological processes are covered in depth. A biophysical approach will be chosen in order to understand and predict processes using models. In order to provide a practical perspective, examples from primary literature will be presented alongside content from textbooks. In particular, topics from cell and infection biology will be used.</p> <p>Practical course: Cell biological processes such as diffusion, cell mobility and the cell cycle are investigated using various model systems. Both bacteria and mammalian cells will be examined using various spectroscopic and microscopic methods. The students should plan, carry out and analyze their experiments themselves. The protocols should be prepared in the form of a short publications according to scientific standards.</p> <p>Seminar: During the seminar, students will present and compare both classical (seminal papers) and current publications. We will compare the scientific methods in both cases in order to give students the opportunity to recognize the appeal of a classical (historical) approach as well.</p> <p>Exercise: During the exercise, students will work through a publication independently in preparation for the upcoming lecture.</p>			
<b>Objective qualification</b>			
<p>After completing the module, students will be able to</p> <ul style="list-style-type: none"> <li>- Understand fundamental orders of magnitude of cellular processes and from this develop their own intuition towards the measurable framework in which biological processes take place.</li> <li>- understand basic terms and concepts of biophysics in cellular and molecular biological systems.</li> </ul>			

- develop interdisciplinary approaches to specific experimental problems from the quantitative methods learned in cell biophysics.
- deal intensively with data analysis up to the generation of computer models. Apply quantitative methods to cell biological preparations, analyze structures and kinetics and make predictions based on biophysical models.
- measure and analyze the function of specific cellular components.
- document, analyze and critically discuss their own results

**Literature**

- Phillips, R., Kondev, J., Theriot, J., Garcia, H.G. and Orme, N., 2012. Physical biology of the cell. Garland Science
- Bornschlögl, T. and Dietz, H., Biophysik in der Zelle
- Aktuelle Publikationen aus der Zell- und Infektionsbiologie, Biophysik in englischer Sprache (Zur Vorlesung und den Seminarvorträgen)



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Physical Biology of the Cell (Bio-ZB 26, Bio-ZN 32, Bt-MZ 05, AM-B-5)	2,0	Lecture	english german
Physical Biology of the Cell (Bio-ZB 26, Bio-ZN 32, Bt-MZ 05, AM-B-5)	1,0	Seminar	english
Physical Biology of the Cell (Bio-ZB 26, Bio-ZN 32, Bt-MZ 05, AM-B-5)	5,0	Internship	english german

<b>Title</b>	Sophisticated Imaging		
<b>Number</b>	1301260 AM-B-6	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	10 / 10,0	<b>Module owner</b>	Manfred Rohde
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	140	<b>Self studying (h)</b>	160
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	- Seminar presentation (1, approx. 20 min) and lab report (1) - The report summarizes the background (from the lecture) and the results of the practical work during the internship		
<b>Course achievement</b>	- Experimental work in the practical course - successful participation in seminar The lecture conveys all contents that are important for the successful completion of the practical course including the protocol.		
<b>Contents</b>			
<p>Lecture: The lecture series provides an overview of the most important imaging and analysis methods in the life sciences. The physical basics of these techniques as well as many application examples from infection biology are taught. One focus is on the presentation of light and electron-optical methods and the corresponding sample preparation. In particular, fluorescence microscopy, confocal microscopy, super-resolution microscopy and high-resolution transmission (TEM) and field emission scanning electron microscopy (FESEM) are covered. In LM, a strong focus is placed on live cell imaging for tracking dynamic processes, as well as the various super-resolution microscopy methods and their areas of application. FESEM and TEM are treated as the methods that allow us to penetrate into the submicroscopic range. Special applications such as the immuno-gold detection of proteins as well as recent developments in the field of cryo-EM will be presented. In addition to visualization methods, the lecture will also cover the acquisition, evaluation and further processing of images and films in order to show which methods are suitable or unsuitable for further processing of images taken with fluorescence and confocal microscopy and to optimize the quality of the images without violating current good scientific practice with regard to image processing. In addition to these techniques, laser dissection microscopy will also be presented, a method that can be used to precisely isolate specific cell components or individual cells from mixed populations. This technique allows target structures to be precisely defined under the microscope and then extracted using a laser beam, which is particularly used in cellular and molecular research.</p> <p>Practical course: Easy-to-perform experiments are chosen to focus on the operation and functionality of the available equipment. The students will independently acquire images at different magnification levels and process them with the help of various image processing tools learned in the practical course. The focus is on the visualization of pathogens (TEM) and host-pathogen interactions (LM/FESEM). In TEM, students will learn how to prepare samples and visualize bacteria, viruses and proteins using the negative-staining method. In addition, a self-conducted infection experiment is designed to illustrate the correlation of LM and FESEM technologies. Immunolabelled samples will also be examined. In LM, mammalian cells are first examined structurally and then infected in order to visualize infected cells and affected organelles. Both high-resolution and super-resolution microscopy methods will be used. In addition to super-resolution and high-resolution microscopy, students will have the opportunity to experience the principles and techniques</p>			

of laser microdissection in practical applications and learn how to use this method to isolate specific cells or cell regions for subsequent molecular analysis.

Seminar: In the accompanying seminar, the latest microscopic techniques that are not available in the module will be presented in seminar lectures.

**Objective qualification**

- After completing the module, students will be able to
- apply basic and advanced knowledge of modern light microscopy (LM), fluorescence microscopy, photo-manipulation and electron microscopy (EM) to their scientific questions.
  - understand which relevant questions in the life sciences they can best work on with which imaging or analysis method.
  - recognize and assess the advantages and disadvantages of a method.
  - recognize what new insights can be gained by combining imaging methods with different resolution and magnification ranges (cross-technology) (correlative microscopy).
  - present and discuss scientific content.
  - engage controversially with scientific topics and issues in a group discussion.

**Literature**

current microscopy-oriented publications in English to accompany the seminar lectures



**Related courses**

**Rules for the choice of courses**

**Compulsory attendance**

Name of the course	SWS	Eventtype	Language
Sophisticated Imaging (Bio-IB 27, Bio-MI 34, AM-B-6)		Lecture	german
Sophisticated Imaging (Bio-IB 27, Bio-MI 34, AM-B-6)		Internship	german
Sophisticated Imaging (Bio-IB 27, Bio-MI 34, AM-B-6)		Seminar	german

<b>Title</b>	Chemometrics		
<b>Number</b>	4011200 AM-B-7	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>		<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	3 / 5,0	<b>Module owner</b>	
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	42	<b>Self studying (h)</b>	108
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	oral exam (30 min)		
<b>Course achievement</b>	project report on practical course		
<b>Contents</b>			
Chemical data and their statistical data analysis; Data pretreatment; Dimensionality reduction; Univariate and multivariate regression and calibration; Validation of univariate and multivariate calibration; Design of experiments applied to chemical data; Univariate and multivariate statistical process control.			
<b>Objective qualification</b>			
Knowledge, understanding and application of chemometric methods to pharmaceutical engineering. Critical evaluation of the performance of chemometric methods in practice.			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Introduction to Chemometrics	2,0	Lecture	english german
Introduction to Chemometrics	1,0	Internship	english german

<b>Title</b>	Theoretical Spectroscopy		
<b>Number</b>	1498120 AM-B-8	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	irregular	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	Institut für Physikal. und Theoretische Chemie
<b>Hours per Week / ECTS</b>	/ 8,0	<b>Module owner</b>	Prof. Dr. Christoph Jacob
<b>Workload (h)</b>			
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	oral or written exam+ (PL, 20% of the coursework and 20% of the practical work mark are taken into account in the overall module grade)		
<b>Course achievement</b>	solve coursework problems (ÜbA, SL unmarked) practical work (expA, SL marked)		
<b>Contents</b>			
<p><b>Lecture and Computer Lab Theoretical Spectroscopy:</b> Time-dependent quantum mechanics, interaction of electromagnetic radiation with molecules, basics of Hartree-Fock and density-functional theory, quantum-chemical calculation of spectroscopic data (Infrared and Raman spectroscopy, UV/Vis spectroscopy, ESR and NMR), simulation of spectra.</p> <p><b>Project Lab:</b> Introduction to scientific programming and in-depth study of selected quantum-chemical methods. Application of quantum-chemical methods that usually cannot be used as "black-box" methods in own independent projects.</p>			
<b>Objective qualification</b>			
<p>The students have acquired knowledge in time-dependent quantum mechanics and on modern methods of theoretical spectroscopy. They are familiar with the foundations of important methods and possess an overview of commonly used quantum-chemical methods in theoretical spectroscopy, their implementation in scientific software, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose suitable methods for their own research projects, to perform calculations and to analyse, evaluate, and assess their results.</p>			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Theoretical Spectroscopy	3,0	Lecture	english german
Computer Lab Theoretical Spectroscopy	1,0	Exercise	english
Project Lab Theoretical Spectroscopy	2,0	Internship	english

<b>Title</b>	Machine Learning in Computational Chemistry		
<b>Number</b>	1499180 AM-A-10	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 8,0	<b>Module owner</b>	Prof. Dr. Jonny Proppe
<b>Workload (h)</b>	240 h		
<b>Class attendance (h)</b>	84	<b>Self studying (h)</b>	156
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	oral or written exam+ (PL, 20% of the coursework and 20% of the practical work mark are taken into account in the overall module grade)		
<b>Course achievement</b>	solve coursework problems (ÜbA, SL unmarked) practical work (expA, SL marked)		
<b>Contents</b>			
<p><b>Lecture and Computer Lab Artificial Molecular Intelligence:</b> Molecular quantum mechanics in a nutshell: Hartree–Fock (HF) theory, post-HF methods, density functional theory; molecular machine learning in a nutshell: molecular representations, deep learning and kernel methods, generative models, uncertainty quantification, active learning; Applications: structure–property relationships, chemical space exploration, molecular design.</p> <p><b>Project Lab:</b> In-depth study of molecular machine learning methods, application of methods of artificial molecular intelligence in own independent projects.</p>			
<b>Objective qualification</b>			
The students have acquired knowledge on modern methods of molecular machine learning and molecular artificial intelligence. They are familiar with the foundations of important methods and possess an overview of commonly used methods, their implementation, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose and apply suitable methods for their own research projects and to analyse, evaluate, and assess their results.			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Machine Learning in Computational Chemistry	3,0	Lecture	english
Computer Lab Machine Learning in Computational Chemistry	1,0	Exercise	english
Project Lab Machine Learning in Computational Chemistry	2,0	Internship	english

<b>Title</b>	Research Lab Spectroscopy and Imaging		
<b>Number</b>	1499240 AM-B-RP	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	every term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	/	<b>Module owner</b>	Prof. Dr. Marc Walter
<b>Workload (h)</b>	360 - 510		
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	study research project including report and presentation (StA)		
<b>Course achievement</b>			
<b>Contents</b>			
<p><b>Research Lab:</b> Conduction and scientific documentation of (parts of) a current research project. The duration of the research project depends on the number of required credit points.</p> <p><b>Seminar:</b> Participation in scientific colloquia, presentation and discussion of current research results</p>			
<b>Objective qualification</b>			
<p>Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.</p>			
<b>Literature</b>			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
the number of credit points assigned for this module depends on the duration of the research project: 12 LP = 360 h 13 LP = 390 h 14 LP = 420 h 15 LP = 450 h 16 LP = 480 h			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Research Lab Spectroscopy and Imaging		Internship	english
Seminar Research Lab Artificial Intelligence for Molecular Sciences		Seminar	english

<b>Profile Area Data-Driven Biology</b>	<b>37 ECTS</b>
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<b>Title</b>	Molecular Microbial Evolution and Diversity		
<b>Number</b>	1399900 AM-C-1	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	9 / 10,0	<b>Module owner</b>	Dr. Jörn Petersen
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	126	<b>Self studying (h)</b>	174
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	written exam (ca. 200 min.)		
<b>Course achievement</b>	- experimental work - protocol (1) - written exam (ca. 90 min.)		
<b>Contents</b>			
<p>Lectures:                      Functional diversity of bacterial communities and relevance for global element cycling, ways to quantify microbial diversity, methods of comparative genomics, population genetics and speciation, the polyphasic bacterial species concept, phylogenetic concepts, evolution of the prokaryotic and eukaryotic cell, multicellularity, symbiosis and pathogenesis, biodiversity informatics, organization of sequence databases, biotechnological utilization of microbial diversity, microbiological resource centers.</p> <p>Practical Course:                      Work in the accompanying practical course focuses on the application of a suite of laboratory methods and is supervised by resident scientists at the Leibniz Institute DSMZ. The methods introduced comprise molecular biological techniques (high throughput sequencing, PCR, cloning), epifluorescence microscopy, bioinformatics (annotations, sequence comparisons, different phylogenetic analyses), state-of-the-art methods for the high-throughput cultivation of novel types of bacteria, chemotaxonomical methods (fatty acid profiles, cell wall chemistry), and the long-term conservation of bacterial strains.</p>			
<b>Objective qualification</b>			
After completing the module, students are able to <ul style="list-style-type: none"> <li>- determining and interpreting microbial diversity based on high throughput sequence datasets</li> <li>- analyzing microbial functional diversity by culture-independent approaches (including field methods)</li> <li>- cultivating and isolating bacterial strains from complex communities, determining their 16S rRNA gene sequences and evaluating the taxonomy of the isolates</li> <li>- characterizing bacterial isolates by physiological and chemotaxonomical methods</li> <li>- conducting phylogenetic analyses and interpreting their results</li> </ul>			

- interpreting morphological, physiological, and phylogenetic diversity in the context of existing information from genome sequence
- quantifying mutation rates and interpret their implications for bacterial evolution
- elucidating the role of accessory genes under natural conditions (by plasmid curing, competition experiments)
- integrating heterogenous datasets from own experiments, literature searches and bioinformatic analysis
- contextualize the integrated data considering the actual state of scientific knowledge.

**Literature**

Madigan et al., Brock Biology of Microorganisms, 2014



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Molecular Microbial Evolution and Diversity (Bio-MI 22, Bio-BD 22, AM-C-1)		Lecture	
Molecular Microbial Evolution and Diversity (Bio-MI 22, Bio-BD 22, AM-C-1)		Internship	english

<b>Title</b>	Immunometabolism		
<b>Number</b>	1398590 AM-C-2	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	8 / 10,0	<b>Module owner</b>	Prof. Dr. Karsten Hiller
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	112	<b>Self studying (h)</b>	188
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	- term paper - oral presentation		
<b>Course achievement</b>	Successful participation in the practical course and seminar		
<b>Module grade composition</b>	The module grade corresponds to the grade for the examination performance.		
<b>Contents</b>			
<p>The seminar gives an introduction into the metabolism of macrophages and how to analyze it by using isotope-labeling experiments and modeling. Especially the role of itaconic acid, ROS, NO and glutathione is discussed. Afterwards, different analytical methods for studying the Immunometabolism of different cell lines will be presented by the students. The students will plan themselves the workflow for the practical course to answer different biological questions. The students will present their work by using different presentation concepts (talk, poster, etc).</p> <p>Practical course: Students will apply their theoretical knowledge to answer different biological questions by using the methods discussed in the seminar. The students will apply several methods, covering cell cultivation, metabolite extraction, seahorse measurements, GC-MS measurements and data analysis, metabolic flux analysis with stable isotopes, etc.</p>			
<b>Objective qualification</b>			
<p>After completing the module, students are able to</p> <ul style="list-style-type: none"> <li>- explain the importance of the metabolism of immune cells during infection/inflammation.</li> <li>- apply modern analytical techniques, such as isotope labelling, mass spectrometry and metabolic flux analysis - evaluate and interpret GC-MS data.</li> <li>- interpret the energy metabolism by means of respiration measurements.</li> <li>- develop concepts for solving systems biology problems with the help of different methods.</li> <li>- present and discuss scientific work.</li> <li>- discuss controversial scientific topics and questions.</li> </ul> <ul style="list-style-type: none"> <li>- search, present and discuss relevant scientific content.</li> <li>- contribute to controversial discussions of scientific topics.</li> <li>- work successfully and independently in a team, organize a team and communicate efficiently with different target groups.</li> <li>- carry out advanced practical and scientific work independently and analyze experimental data.</li> <li>- apply in-depth foreign language skills (usually English).</li> </ul>			

<b>Literature</b>

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
Attendance is compulsory for practicals, exercises, seminars, and excursions.			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Immunmetabolism (Bio-BB 31, Bio-SB 31, AM-C-2)		Seminar	english german
Immunmetabolism (Bio-BB 31, Bio-SB 31, AM-C-2)		Practical exercise	english german

<b>Title</b>	Applied bioinformatics: biomarkers for diagnosis		
<b>Number</b>	1303600 AM-C-3	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	/ 10,0	<b>Module owner</b>	Prof. Dr. Karsten Hiller
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	188	<b>Self studying (h)</b>	112
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	written exam (ca. 200 min.)		
<b>Course achievement</b>	- Successful participation in the seminar - Experimental work		
<b>Module grade composition</b>	The module grade corresponds to the grade for the examination performance.		
<b>Contents</b>			
<p>Seminar:                      1 week course "Introduction to R".                      Integrated Lecture, computational Workshops and Experimental course (whole semester, 4h per week):                      Lecture, Workshops: Introduction into mass-spectrometry driven metabolome analysis, understanding the selection of suitable mass units to ensure reproducible measurements, understanding the relevance of measurement traceability and uncertainty for data interpretation. Introduction to algorithms for machine learning based biomarker prediction, correction for multiple testing, basics of logistic regression and neuronal networks, training and evaluating a machine learning based prediction model, receiver operating characteristics, data normalization. Understanding the relevance of quality controls for data backup and safety. Designing a crossover intervention study.</p> <p>Experimental course: Isolation of metabolites from saliva and/or blood followed by analysis via mass spectrometry. The method will be optimized for specific metabolites and quantification of these performed via isotope dilution. Acquisition of different methods for optimization of sample withdrawal and sample processing as well as data analysis. Determination of biomarker signatures, e.g. based on saliva samples to distinguish whether donor was case or control.</p>			
<b>Objective qualification</b>			
<p>After completing the module, students are able to</p> <ul style="list-style-type: none"> <li>- Perform a simple crossover intervention study and collect samples</li> <li>- Perform metabolome analyses of human saliva and/or blood samples by mass spectrometry</li> <li>- Analyze the raw data with the help of bioinformatics to determine quantitative and semi-quantitative metabolite concentrations</li> <li>- Identify biomarker signatures by application of machine learning algorithms (logistic regression, lasso (least absolute shrinkage and selection operator)</li> <li>- Quantify selected biomarkers with high precision and reproducibility</li> <li>- Apply basic concepts of metrology and standardization</li> <li>- Perform statistical analyses in R.</li> </ul>			

- Understand the relevance of standardization for experimental design and performance.
- Understand the concept of a clinical crossover study / trial to evaluate the efficacy or effects of a drug.
- search, present and discuss relevant scientific content.
- contribute to controversial discussions of scientific topics.
- work successfully and independently in a team, organize a team and communicate efficiently with different target groups.
- carry out advanced practical and scientific work independently and analyze experimental data.
- apply in-depth foreign language skills (usually English).

**Literature**

will be announced in the lecture



**Related courses**

**Rules for the choice of courses**

**Compulsory attendance**

Attendance is compulsory for practicals, exercises, seminars, and excursions.

Name of the course	SWS	Eventtype	Language
Navigating the Metabolic Maze: Machine Learning for Biomarker Detection and Quantification (Bio-BB 32, Bio-SB 32, AM-C-3)		Seminar	english
Navigating the Metabolic Maze: Machine Learning for Biomarker Detection and Quantification (Bio-BB 32, Bio-SB 32, AM-C-3)		Internship	english

<b>Title</b>	Network Biology		
<b>Number</b>	4217840	<b>Module version</b>	V2
<b>Shorttext</b>	INF-MI-84	<b>Language</b>	english
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Carl-Friedrich-Gauß-Fakultät
<b>Module duration</b>	1	<b>Institution</b>	Peter L. Reichertz Institut für Medizinische Informatik
<b>Hours per Week / ECTS</b>	4 / 5,0	<b>Module owner</b>	Prof. Dr. Tim Kacprowski
<b>Workload (h)</b>	150		
<b>Class attendance (h)</b>	56	<b>Self studying (h)</b>	94
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	1 graded work: written exam, 90 minutes, or oral exam, 30 minutes or Take-Home-Exam.		
<b>Course achievement</b>	1 non-graded work: 50% of exercises must be passed		
<b>Contents</b>			
<ul style="list-style-type: none"> <li>- Introduction graph theory</li> <li>- Biological networks</li> <li>- Biological network databases</li> <li>- Statistical network analysis</li> <li>- Graph algorithms</li> <li>- Graph-based machine learning</li> </ul>			
<b>Objective qualification</b>			
After successful completion of this module, students will have a basic understanding of graph theory and its applications for the analysis of biomedical data. They will be able to use network biology tools and critically assess network analyses. They will be capable to devise new graph-based strategies for the analysis of biomedical data.			
<b>Literature</b>			
wird noch bekanntgegeben			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

Network Biology	2,0	Lecture	english
<b>Literature</b>			
to be announced			
	2,0	Exercise	english

<b>Title</b>	Molecular Phylogenetics and Taxonomy		
<b>Number</b>	1398930 AM-C-5	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	10 / 10,0	<b>Module owner</b>	
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	100	<b>Self studying (h)</b>	200
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	written Exam (ca. 200 min.)		
<b>Course achievement</b>	- Successful completion of exercises - Laboratory journal - Presentation (final presentation of one's own research project) (1, approximately 30 minutes)		
<b>Contents</b>			
<p>Lecture:                      Provides fundamental knowledge about the reconstruction of evolutionary history using molecular features (molecular phylogenetics) through various statistical methods, as well as the application of principles of phylogeography and molecular taxonomy.</p> <p>Lab Practical:                      In the lab practical, all aspects of classical Sanger sequencing are performed, including DNA isolation, PCR amplification, sequencing, as well as computer-assisted processing of chromatograms and alignment of sequences.</p> <p>Exercises:                      The exercises focus on bioinformatic data analysis. This includes sequence comparisons using local and internet-based BLAST analyses, estimation of substitution models, phylogenetic analyses using Maximum Likelihood and Bayesian Inference, and the creation of haplotype networks. In the exercises, students apply these methods to the DNA sequences obtained in the lab practical and thus work on small research projects in groups within the module, from laboratory work to evaluation. Exemplary exercises on the phylogenetic analysis of data derived from modern high-throughput techniques are also conducted (Phylotranscriptomics/Phylogenomics).</p>			
<b>Objective qualification</b>			
After completing the module, students will be able to <ul style="list-style-type: none"> <li>- sequence DNA using the Sanger method and review and align sequence chromatograms.</li> <li>- explain and understand the methodological foundations of systematics and phylogenetic reconstruction primarily using molecular features.</li> <li>- theoretically understand the basic principles of phylogenetic analysis (Maximum Parsimony, Maximum Likelihood, Bayesian Inference, and other methods) and practically apply relevant bioinformatic software.</li> </ul>			

- search DNA databases and use them for sequence comparison (BLAST).
- conceptually and practically delimit species based on molecular genetic evidence.
- independently conduct a research project, from organizing practical laboratory work to documenting data, bioinformatic analysis, interpretation, and presenting the results.

**Literature**

- Fachbuch: "Gene und Stammbäume"
- Artikel: aktuelle Publikationen (englisch) zu Themen der Phylogenetik, Phylogeographie und Populationsgenetik
- Fachjournale (englisch): Molecular Ecology, Molecular Phylogenetics and Evolution, Trends in Ecology and Evolution, Systematic Biology

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Molecular Phylogenetics (Bio-GE 25, AM-C-5)		Lecture	german
Molecular Phylogenetics (Bio-GE 25, AM-C-5)		Internship	german

<b>Title</b>	Data Literacy and Genome Research		
<b>Number</b>	1398900 AM-C-6	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	10 / 10,0	<b>Module owner</b>	Prof. Dr. Boas Pucker
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	180	<b>Self studying (h)</b>	120
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Written exam (ca. 200 min.)		
<b>Course achievement</b>	- Experimental work - Protocol (1) - Presentation (in international symposium, ca. 15 min)		
<b>Contents</b>			
<p>With the emergence of next generation sequencing and the recent addition of long read sequencing technologies the amount of genomic data has increased significantly. To enable students to handle these big data sets, it is important to further their understanding in data management and data literacy. This module sets out to teach students all skills necessary to plan, perform, and analyse their own big data sequencing project. It consists of three main parts:</p> <p>Lecture: Sequencing technologies (Sanger, Illumina, Single Molecule Real Time, Nanopore) and general strategies for plant genome projects will be presented. This covers the combination of sequencing data with genetic linkage and HiC data sets.</p> <p>The rapid technological development during the last two decades will be highlighted. A particular focus will be on strategies to reuse existing data sets for new projects. Genome research is traditionally characterized by big data sets and also leading in terms of open access. The concept of read mapping and variant calling as well as recent pangenomic approaches will be introduced. The concept of FAIR data and recent developments towards 'open science' will be explained. Specific tools and file formats will be presented to prepare for hands-on exercises.</p> <p>Exercise:</p> <ul style="list-style-type: none"> <li>- Planning a sequencing experiment including the calculation of required materials and data, identification of the best plant material, and development of a suitable DNA extraction workflow.</li> <li>- Extraction of DNA from plant material in several iterations to achieve optimal results</li> <li>- Control of the DNA quality prior to sequencing (NanoDrop measurement, agarose gel, Qubit measurement)</li> <li>- Performing a complete nanopore sequencing experiment including DNA repair, library preparation, sequencing, and basecalling</li> <li>- Bioinformatic analyses: assembly and annotation of a novel genome sequence, retrieving and integrating public data sets, read mapping and variant calling, annotation of sequence variants, interpretation of obtained results</li> <li>- Integration of public data sets for comparative genomic studies and functional annotation</li> <li>- Peer Review Process: the results of the exercise will be summarised and presented in the style of a scientific paper. To simulate the peer-review process, each student will be assigned papers written by fellow stu-</li> </ul>			

dents to review in form of a report. This enables students to gain insights into the importance and process of peer reviews and fosters cooperative learning.

- International Symposium: Results will be presented in front of an international audience and decisions made during the project will be discussed.

**Objective qualification**

After completing this module students will be able to

- use online resources to find and retrieve genomic information.
- work with different biological databases and data types.
- plan their own sequencing project and workflow.
- extract the genetic material needed for nanopore sequencing.
- perform long read sequencing using a portable MinION.
- work in a terminal on Linux operating systems.
- install bioinformatics tools.
- utilize latest bioinformatic tools for long read analyses.
- analyse and visualise big data.
- work in a cloud-based environment.
- critically interpret the results and summarize these in a scientific report.
- give constructive criticism during of a peer-review process.
- give a scientific talk in front of an international audience.
- communicate the results of a big data project to different target audiences.

**Literature**



**Related courses**

**Rules for the choice of courses**

**Compulsory attendance**

Name of the course	SWS	Eventtype	Language
Data Literacy and Genome Research (Bio-BB 35, Bio-GE 37, AM-C-6)		Lecture	german
Data Literacy and Genome Research (Bio-BB 35, Bio-GE 37, AM-C-6)		Exercise	german

<b>Title</b>	Applied Plant Transcriptomics		
<b>Number</b>	1398800 AM-C-7	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	10 / 10,0	<b>Module owner</b>	Prof. Dr. Boas Pucker
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	150	<b>Self studying (h)</b>	150
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	written exam (ca. 200 min.)		
<b>Course achievement</b>	<ul style="list-style-type: none"> <li>- Successful participation in the practical course</li> <li>- Protocols (1)</li> <li>- Oral presentation (1, 20 min.)</li> </ul>		
<b>Contents</b>			
<p>Lecture: The concepts of various steps in an RNA-seq workflow from experiment design to interpretation of the results are presented. This covers frequently applied tools and databases for the data analysis.</p> <p>Seminar: Recent publications about plant transcriptomics projects will be discussed. Each student will present one scientific publication with a particular focus on the applied methods. Students will take turns as chair of the seminar. Additional studies will be discussed with respect to their quality. Students will learn how to recognize publications with substantial issues in the data analysis.</p> <p>Exercise: Students will conduct a complete RNA-seq experiment with plant data sets. Experimental design, de novo transcriptome assembly, quality control, transcriptome annotation, data processing, statistical analysis, GO/KEGG enrichment studies, data visualization (heatmaps, phylogenetic trees), and interpretation of the results are part of this exercise.</p>			
<b>Objective qualification</b>			
<p>After completing this module students are able to</p> <ul style="list-style-type: none"> <li>- design experiments to study gene expression.</li> <li>- conduct de novo transcriptome assembly.</li> <li>- perform a quality control on RNA-seq data sets.</li> <li>- analyze gene expression based on RNA-seq.</li> <li>- perform functional annotations with the application of transcriptome annotation tools.</li> <li>- create heatmaps and graphs using R.</li> <li>- create phylogenetic trees.</li> <li>- interpret the results of RNA-seq experiments.</li> <li>- recognize flawed publications.</li> </ul>			
<b>Literature</b>			
Open access journals			



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Applied Plant Transcriptomics (Bio-GE 33, Bt-MM 12, AM-C-7)		Lecture	english
Applied Plant Transcriptomics (Bio-GE 33, Bt-MM 12, AM-C-7)		Seminar	english
Applied Plant Transcriptomics (Bio-GE 33, Bt-MM 12, AM-C-7)		Exercise	english

<b>Title</b>	Functional Genomics in Infection Biology		
<b>Number</b>	1398580 AM-C-8	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	0 / 10,0	<b>Module owner</b>	Prof. Dr. Susanne Engelmann
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	140	<b>Self studying (h)</b>	160
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	Oral presentation (1)		
<b>Course achievement</b>	<ul style="list-style-type: none"> <li>- Successful participation in the practical course</li> <li>- Protocols (1)</li> <li>- Oral presentation (1)</li> </ul>		
<b>Contents</b>			
<p>Lecture:                      The Lecture will provide an overview of the potential of functional genomics in infection biology, as well as its limitations.                      Further topics are:</p> <ul style="list-style-type: none"> <li>- Detailed overview of functional genomics methods (genome sequencing, mutagenesis, mutation analysis, transcriptomics, proteomics, metabolomics).</li> <li>- Introduction to systems biology models of infection biology and microbial pathophysiology (e.g. stochastic models of gene expression, thermodynamic models of metabolism).</li> <li>- Introduction to complex omics datasets and their analysis (standard methods of genome reconstruction, annotation, comparative genome analysis and differential gene expression analysis).</li> <li>- Examples of how functional genomics can be used to gain a more complex understanding of host-pathogen interactions.</li> <li>- Microbiome structure and physiology.</li> <li>- Biomarkers as diagnostic tools.</li> </ul> <p>Practical course:</p> <ul style="list-style-type: none"> <li>- Provide skills for designing experiments in genomics, transcriptomics and proteomics</li> <li>- Present analysis strategies using local and web-based databases and analysis tools</li> </ul> <p>Seminar:</p> <ul style="list-style-type: none"> <li>- Presentation of a talk on a current topic in functional genomics</li> <li>- Experience in advanced literature review</li> <li>- Acquisition of knowledge in the independent development of a limited, scientifically relevant topic from functional genome research on the basis of original works in English, in order to give an overview of the current state of research and to present and critically discuss it in a clearly structured lecture of approx. 30 minutes duration with appropriate visualisations.</li> </ul>			

<b>Objective qualification</b>
<p>After completing this module students are able to</p> <ul style="list-style-type: none"> <li>- understand the concepts of functional genomics. In particular, they will be able to recognise the potential and limitations of molecular genetic methods and OMICs technologies in basic and applied research and medical diagnostics.</li> <li>- apply a wide range of infection genetics and functional genomics techniques to study host-pathogen interactions.</li> <li>- design experiments to comprehensively answer a scientific question.</li> <li>- critically analyse the advantages and disadvantages of a method and the results obtained.</li> <li>- place results in a scientific context.</li> <li>- present and discuss researched scientific content.</li> <li>- discuss controversial scientific topics and issues in a group discussion.</li> </ul>
<b>Literature</b>
wird in der Vorlesung bekanntgegeben.



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Functional Genomics in Infection Biology (Bio-IB 28, Bio-MI 33, AM-C-8)		Lecture	english
Functional Genomics in Infection Biology (Bio-IB 28, Bio-MI 33, AM-C-8)		Internship	

<b>Title</b>	Microbial Proteomics		
<b>Number</b>	1301290 AM-C-9	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	
<b>Frequency of offer</b>	only in the summer term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	6 / 10,0	<b>Module owner</b>	Prof. Dr. Susanne Engelmann
<b>Workload (h)</b>	300		
<b>Class attendance (h)</b>	148	<b>Self studying (h)</b>	152
<b>Compulsory requirements</b>	none		
<b>Recommended requirements</b>	none		
<b>Expected performance/ Type of examination</b>	presentation (ca. 40 min.)		
<b>Course achievement</b>	- Experimental work - Successful participation in the seminar - protocol (1) - presentation (ca. 30 min.)		
<b>Contents</b>			
<p>Lecture:                      The lecture "Microbial Proteomics" provides an overview of proteomics methods and their application in microbiology. Based on an introduction to methods for the identification and quantification of proteins in highly complex protein mixtures, modern experimental approaches for the qualitative and quantitative characterisation of the entirety of proteins (proteome) of a microorganism or a community of microorganisms (metaproteome) will be presented. In addition, possibilities for the detection of protein modifications and the visualisation of protein complexes will be demonstrated.</p> <p>Practical course:                      In the practical course "Microbial Proteomics", students should apply the methods taught in the lecture under supervision to answer a question in the field of physiology of microorganisms, infection biology or the elucidation of the mode of action of antibacterial natural products.</p> <p>Seminar:                      In the 'Microbial Proteomics' seminar, students are required to independently analyse recent publications on research in this field, present them in a short talk, and critically question and discuss them.</p>			
<b>Objective qualification</b>			
After completing the module, students are able to <ul style="list-style-type: none"> <li>- describe the basic principles of proteomic methods and critically evaluate the advantages and disadvantages of the methods.</li> <li>- identify and quantify proteins from complex protein mixtures.</li> <li>- analyse large data sets and visualise the results.</li> <li>- design experiments to comprehensively answer a scientific question.</li> <li>- critically analyse the advantages and disadvantages of a method and the results obtained.</li> <li>- place results in a scientific context.</li> </ul>			

- present and discuss researched scientific content.
- discuss controversial scientific issues in a group.

**Literature**

- H. Rehm und T. Letzel, Der Experimentator Proteinbiochemie/Proteomics
- F. Lottspeich und J. W. Engels, Bioanalytik
- aktuelle englischsprachige Fachliteratur



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Microbial Proteomics (Bio-MI 26, Bio-SB 35, AM-C-9)		Lecture	english
Microbial Proteomics (Bio-MI 26, Bio-SB 35, AM-C-9)		Seminar	english
Microbial Proteomics (Bio-MI 26, Bio-SB 35, AM-C-9)		Internship	english

<b>Title</b>	Research Lab Data-Driven Biology		
<b>Number</b>	1499250 AM-C-RP	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>	every term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	/	<b>Module owner</b>	Prof. Dr. Marc Walter
<b>Workload (h)</b>	360 - 510		
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	study research project including report and presentation (StA)		
<b>Course achievement</b>			
<b>Contents</b>			
<p><b>Research Lab:</b> Conduction and scientific documentation of (parts of) a current research project. The duration of the research project depends on the number of required credit points.</p> <p><b>Seminar:</b> Participation in scientific colloquia, presentation and discussion of current research results</p>			
<b>Objective qualification</b>			
<p>Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.</p>			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
the number of credit points assigned for this module depends on the duration of the research project: 12 LP = 360 h 13 LP = 390 h 14 LP = 420 h 15 LP = 450 h 16 LP = 480 h 17 LP = 510 h			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Research Lab Data-Driven Biology		Internship	english
Seminar Research Lab Artificial Intelligence for Molecular Sciences		Seminar	english

<b>Key Qualifications</b>			<b>12 ECTS</b>
<b>Title</b>	Ethics and Epistemology		
<b>Number</b>	4411440 AM-KQ-1	<b>Module version</b>	
<b>Shorttext</b>	GE-Phil-44	<b>Language</b>	
<b>Frequency of offer</b>	only in the winter term	<b>Teaching unit</b>	Fakultät für Geistes- und Erziehungswissenschaften
<b>Module duration</b>	1	<b>Institution</b>	
<b>Hours per Week / ECTS</b>	2 / 5,0	<b>Module owner</b>	Prof. Dr. Hans-Christoph Schmidt am Busch
<b>Workload (h)</b>	Präsenzzeit: 30 h Selbststudium: 120 h Gesamtworkload: 150 h		
<b>Class attendance (h)</b>	30	<b>Self studying (h)</b>	120
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	1 graded examination (Prüfungsleistung): written exam, 120 minutes		
<b>Course achievement</b>	1 non graded examination (Studienleistung): Protokoll, 2 pages		
<b>Contents</b>			
<p>This course provides students with philosophical knowledge in order to reason thoughtfully, judge effectively and act morally in the field of data science. Students learn to differentiate between concepts, phenomena and actions, which is relevant for understanding the presuppositions and implications of machine ethics. This new field is, on the one hand, concerned with established ethical approaches (Kant, Utilitarianism); on the other hand, with giving machines ethical principles, i.e. programs and operations for discovering a way to resolve ethical dilemmas they might encounter. Whereas enabling machines to function in an ethically responsible manner through their own ethical decision making is a long wished-for in AI and robotics, philosophers and society highlight basic questions still in need for an answer; for example: can machines be moral agents? When adopting norms and values, who should they take as paradigmatic role model? Who has the right to judge about that, and why? Students will learn the preconditions and limits of modeling the world according to machines. Not last, which kind of world machines face by means of artificial sensory perception matters for understanding the difficult questions of embodiment, and really being in the world instead of only having one.</p>			
<b>Objective qualification</b>			
<p>The course:</p> <ul style="list-style-type: none"> <li>• provides a philosophical framework and moral compass for guiding the judgement of students regarding data science and its applications (artificial intelligence, robotics, etc.).</li> <li>• aims to develop communication skills, social and civic competences,</li> <li>• reassures students on the limits of machines, machinery settings, and machine ethics,</li> <li>• strengthens personal development in the light of digit(al)ization and related claims of social change.</li> </ul> <p>The students will be able to recognize and interpret social and technical problems in technology and information processing based in classical and recent position in theoretical and practical philosophy. They will be able to interpret these problems ethically and support their position with arguments from machine ethics.</p>			
<b>Literature</b>			
Anderson, Michael/Anderson, Susan Leigh (eds.): Machine Ethics, 2011			

Misselhorn, Catrin: Grundfragen der Maschinenethik, 3rd ed. 2018  
 Nagel, Thomas: What is it like to be a Bat? Englisch/Deutsch, Reclam 2016



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>
Ethics and Epistemology	2,0		english german
<b>Literature</b>			
Literatur: <ul style="list-style-type: none"> <li>• Misselhorn, Catrin: Grundfragen der Maschinenethik, 3rd ed. 2018</li> <li>• Anderson, Michael/Anderson, Susan Leigh (eds.): Machine Ethics, 2011</li> <li>• Nagel, Thomas: What is it like to be a Bat? Englisch/Deutsch, Reclam 2016</li> </ul>			

<b>Title</b>	Professionalization		
<b>Number</b>	1499410	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english german
<b>Frequency of offer</b>	every term	<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	/ 7,0	<b>Module owner</b>	Prof. Dr. Marc Walter
<b>Workload (h)</b>			
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	The examination modalities vary depending on the selected courses, see BPO.		
<b>Course achievement</b>	The examination modalities vary depending on the selected courses, see BPO.		
<b>Contents</b>			
The interdisciplinary courses can be selected from the overall program, see also BPO.			
<b>Objective qualification</b>			
<p>The learning outcomes of the interdisciplinary courses related to key qualifications are divided into three sub-areas:</p> <p><b>Overarching reference: Embedding the subject of study:</b> Students are enabled to embed their subject of study in social, historical, legal or professional contexts (depending on the focus of the course). They are able to recognize, analyze and evaluate overarching subject-related connections and their significance. The students gain an insight into the networking possibilities of the subject and application possibilities of their field of study in professional life.</p> <p><b>Scientific cultures:</b> Students become familiar with the theories and methods of other scientific cultures, learn to deal and work interdisciplinarily with students from other fields of study, can discuss and evaluate current controversies from individual disciplines, recognize the importance of cultural framework conditions for different scientific understandings and applications, know gender-related perspectives on different subject areas and the effects of gender differences, and can deal intensively with application examples from foreign disciplines.</p> <p><b>Action-oriented courses:</b> Students are enabled to apply theoretical knowledge in an action-oriented manner. They acquire procedural knowledge (knowledge of procedures and courses of action, application criteria for certain procedures and courses of action) as well as metacognitive knowledge (including knowledge of their own strengths and weaknesses).</p> <p>Depending on the focus of the course, students acquire the ability to</p> <ul style="list-style-type: none"> <li>• impart knowledge and apply communication techniques,</li> <li>• conduct discussions and negotiations effectively, reflect on themselves and evaluate themselves appropriately,</li> <li>• work cooperatively in a team, manage conflicts,</li> <li>• lead teams,</li> <li>• use information and communication media or</li> <li>• express themselves in another language.</li> </ul>			

The action-oriented courses enable students to use knowledge acquired in other areas more effectively, to work more easily and constructively with other people and thus to facilitate the acquisition and development of new knowledge. They acquire key qualifications that facilitate their entry into professional life and contribute to success in all professional situations.

**Literature**



<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

<b>Master's Thesis</b>	<b>30 ECTS</b>
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<b>Title</b>	Master's Thesis		
<b>Number</b>	1499420	<b>Module version</b>	
<b>Shorttext</b>		<b>Language</b>	english
<b>Frequency of offer</b>		<b>Teaching unit</b>	Fakultät für Lebenswissenschaften
<b>Module duration</b>		<b>Institution</b>	
<b>Hours per Week / ECTS</b>	/ 30,0	<b>Module owner</b>	
<b>Workload (h)</b>			
<b>Class attendance (h)</b>		<b>Self studying (h)</b>	
<b>Compulsory requirements</b>			
<b>Expected performance/ Type of examination</b>	master thesis (see APO §14 and BPO §8)		
<b>Course achievement</b>			
<b>Contents</b>			
The topic of the master's thesis must address an issue from the field of "Artificial Intelligence for Molecular Sciences" in the broader sense and should be chosen in such a way that it matches the chosen specialization.			
<b>Objective qualification</b>			
Students are able to work independently on a scientific question from a sub-field of "Artificial Intelligence for Molecular Sciences" within a specified period of time and to present their research results adequately in written form. They are familiar with the relevant conventions of their field of research and have an insight into current topics of research.			
<b>Literature</b>			

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<b>Related courses</b>			
<b>Rules for the choice of courses</b>			
<b>Compulsory attendance</b>			
<b>Name of the course</b>	<b>SWS</b>	<b>Eventtype</b>	<b>Language</b>

