E – Characteristics of the study course

Name of the course	Organic Chemistry III (natural products)				
Type of the course	compulsory			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	2,6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture

Other requirements on student

Other subjects as prerequisites, etc.

Lecturer

Norbert Müller (coordinator, there may be guest lecturers involved)

Brief annotation of the course

Structure, synthesis and biosynthesis of important natural products
(excluding peptides, proteins, and nucleic acids, which are part of other courses)

(0) General principles of natural product synthesis and comparison to biosynthetic pathways
(1) Carbohydrates
(2) Steroids
(3) Alkaloids
(4) Pyrrole pigments
(5) Lipids
(6) Coenzymes

Study literature and study tools

Chemistry of Natural Products, Bhat, S.V., Nagasampagi, B.A., Sivakumar, M.
Natural Product Chemistry at a Glance, Stephen P. Stanforth
Natural product synthesis I: Targets, Methods, Concepts, Johann Mulzer, Thorsten Bach
Natural product synthesis II: Targets, Methods, Concepts, Johann Mulzer, Thorsten Bach, Uwe Beifuss

E – Characteristics of the study course

Name of the course	Physical Chemistry II				
Type of the course	compulsory			**recom. year / semester**	1/1
Total hours of the course	42	**hours per week**	3	**ECTS**	3.9
Other expression of the size					
Form of exam	oral			**Form of tuition**	lecture
Other requirements on student					

Lecturer

o.Univ.Prof. Dr. Niyazi Serdar Sariciftci

Brief annotation of the course

- Thermodynamics of ideal gases
- Statistical mechanics of gases
- Laws of thermodynamics and their statistical interpretations
- Reaction Kinetics and Catalysis
- Quantum chemisty of H-Atom
- Quantum chemistry of molecular bonding
- Spectroscopy
- Symmetry

Study literature and study tools

Gordon Barrow, Physical Chemistry
Atkins, Physical Chemistry
Engl and Reid, Physical Chemistry

E – Characteristics of the study course

Name of the course	Preparative Chemistry Laboratory for Biological Chemists				
Type of the course	compulsory			**recom. year / semester**	1/2
Total hours of the course	70	**hours per week**	5	**ECTS**	6
Other expression of the size					
Form of exam	combined			**Form of tuition**	laboratory
Other requirements on student					

Other subjects as prerequisites, etc.: Basic Knowledge in Inorganic, Organic Chemistry and Spectroscopy

Lecturer	N. Müller + G. Knör

Brief annotation of the course

Multi-step synthesis of organic and inorganic compounds of biological relevance

The interdisciplinary approach involves planning (by retro-synthetic approach) of the synthesis, literature search and preparation as well as purification and characterisation of the products

Study literature and study tools

Specific literature will be made available for the individual syntheses

Top Drugs: Top Synthetic Routes (Oxford Chemistry Primer) by John Saunders
Synthetic Coordination and Organometallic Chemistry by Boris I. Kharisov

E – Characteristics of the study course

Name of the course	Industrial Biotechnology				
Type of the course	compulsory			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2.6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					

Lecturer

Coordinator: Norbert Müller; course will be held by industrial Biotechnologists from industry

Brief annotation of the course

(0) Introduction to Biotechnology
(1) Enzyme Technology
(2) Microorganisms in Biotechnolgy
(3) Cell & Tissue Culture Technology
(4) Renewable Resources
(5) Process Technology
(6) Exemplary Process Breakdown
(7) Excursion to a biotech production plant

Study literature and study tools

Modern Industrial Microbiology and Biotechnology, 2007, Nduka Okafor, ISBN 978-1-57808-513-2

E – Characteristics of the study course

Name of the course	Biochemical Technology				
Type of the course	compulsory			**recom. year / semester**	1/2
Total hours of the course	15	**hours per week**	1	**ECTS**	
Other expression of the size	n/a				
Form of exam	Combined (oral and written)			**Form of tuition**	lecture
Other requirements on student					

Lecturer

Stefan Howorka

Brief annotation of the course

Biochemical technology

- Definition and industrial applications of biochemical technology
- Definition I: biopolymers (protein, DNA, carbohydrates. lipids) are subjected to chemical modification or genetic engineering to enhance their functional properties and tailor them to specific applications in industry or healthcare
- Definition II: generation of enzymes that are used as tools for the bio-assisted industrial synthesis of vitamins or oligosaccharides

Proteins

- Peptide synthesis (review)
- Synthesis of semisynthetic proteins (expressed protein ligation)
- Genetic strategies for protein engineering
- Chemical tools for targeted modifications of proteins
- Industrial application: PEGylation of therapeutic proteins
- Industrial application: Generation of engineered lipases for application in detergents

Nucleic Acids

- Solid Phase Oligonucleotide Synthesis (chemical differences to biosynthesis)
- Chemical synthesis of RNA
- Industrial application: Synthesis of modified bases carrying fluorophores and chemical tags for immobilization of relevance in DNA microarrays and sequencing technology

Lipids

- Application: Biofuels

Study literature and study tools

Original papers/scripts will be distributed during the course

E – Characteristics of the study course

Name of the course	Spectroscopy & Structure Elucidation II				
Type of the course	compulsory			**recom. year / semester**	1/2
Total hours of the course	14	**hours per week**	1	**ECTS**	1,3
Other expression of the size	weeks per semester, etc.				
Form of exam	written			**Form of tuition**	lecture

Other requirements on student

Other subjects as prerequisites, etc.

Lecturer

Christian Klampfl

Brief annotation of the course

The course provides in depth information on modern, state-of-the-art techniques in mass spectrometry. These include various ionization methods for liquids, solids and gaseous samples, new high resolution mass analyzers as well as some basic knowledge about the interpretation of mass spectra.

Study literature and study tools

Power point slides will be provided by the lecturer

E – Characteristics of the study course

Name of the course	Advanced Instrumental Analysis				
Type of the course	compulsory			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2.4
Other expression of the size					
Form of exam	combined			**Form of tuition**	lab
Other requirements on student					

Lecturer

o.Univ.Prof. Dr. Wolfgang Buchberger

Brief annotation of the course

Hyphenation of high-performance liquid chromatography and mass spectrometry for determination of drugs in blood plasma.
Determination of biomarkers by gas chromatography and mass spectrometric detection.
Application of capillary zone electrophoresis for analysis of biological samples.
Glycoprotein analysis by liquid chromatography and fluorescence spectroscopy.

Study literature and study tools

Not available

E – Characteristics of the study course

Name of the course	Gender Awareness in Science & Technology				
Type of the course	compulsory			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	3
Other expression of the size					
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					

Lecturer	N.N.

optional provided by accredited state agency

Brief annotation of the course

A course addressing issues of “gender problems” is contained in all Master curricula as a binding legal requirement and provided by the “Institut für Frauen- und Geschlechterforschung”.

Study literature and study tools

E – Characteristics of the study course

Name of the course	Patent Law + IP				
Type of the course	compulsory			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	2,6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					

Lecturer

Elvira Landgraf

Brief annotation of the course

History
Treaties
Intellectual Property Rights

- Definitions, Theories
- General
- Selected IPs (focus: “technical” Ips)

Patents

- Conventions (including comparison of patent systems)
- Definitions (state of the art, invention, novelty, inventive step ….)
- Requirements
- Strategies for patenting
- Infringement
- Examples (focusing on chemical, biochemical, biotechnological patents)

Study literature and study tools

E – Characteristics of the study course

Name of the course	Inorganic Chemistry III				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	2.6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					

Other subjects as prerequisites, etc.: Basic Knowledge in Inorganic, Organic and Physical Chemistry and Spectroscopy

Lecturer	G. Knör

Brief annotation of the course

Modern Aspects of Inorganic Chemistry

Metal Complexes and Coordination Compounds

Catalysis and Inorganic Reaction Mechanisms

Bioinorganic Chemistry

Organometallic Chemistry

Structure and Function of Inorganic Materials

Selected Case Studies and Applications

Study literature and study tools

C. Housecroft, A. G. Sharpe, "Inorganic Chemistry", Pearson, 2nd Ed. , 2005

D. F. Shriver, P. W. Atkins, "Inorganic Chemistry", Oxford Univ. Press, 4th Ed, 2006

I. Bertini, H. B. Gray, E. Stiefel, J. Valentine, "Biological Inorganic Chemistry – Structure and Reactivity", University Science Books, 2007

Selected review literature to be announced / provided in the course

E – Characteristics of the study course

Name of the course	Biospecific Detection (and Biosensing)				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2.6
Other expression of the size	-				
Form of exam	combined			**Form of tuition**	lecture

Other requirements on student

Students should be familiar with biomolecules (proteins, nucleic acids) and have basic knowledge in physical chemistry (thermodynamics, chemical kinetics, electrochemistry)

Lecturer

Hermann J. Gruber

Brief annotation of the course

Biospecific detection methods allow to estimate the concentrations of particular molecules of interest (termed "analytes") in complex sample mixtures, usually without separation of the sample mixture into individual components. Biospecific detection is based (1) on specific recognition of analyte molecules (e.g. antigens, genes, enzyme substrate) by complementary probe molecules (e.g. antibodies, oligonucleotides, enzymes) and (2) on experimental conditions which lead to a measurable signals (e.g. fluorescence, color, voltage, etc.). In this lecture, we will address homogeneous assays (binding and enzyme assays), heterogeneous assays (e.g. blots, arrays, ELISA), and biosensors (biocatalysis and binding). The lecture will expand the students' knowledge not only in bioanalytics but also in areas of biotechnology and bionanotechnology.

Study literature and study tools

Handouts with all graphic materials and with explanatory text are available in parallel to the lecture. Further literature is cited in the handouts.

E – Characteristics of the study course

Name of the course	Exercise in Spectroscopy & Structure Elucidation II				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	14	**hours per week**	1	**ECTS**	1,6
Other expression of the size					
Form of exam	combined			**Form of tuition**	Exercises
Other requirements on student					
Lecturer	Ch. Klampfl				

Brief annotation of the course

Application examples of MS, IR, UV-vis spectroscopy
Students will solve structures given spectroscopic data.

Study literature and study tools

Handouts from the corresponding lecture course

Mass Spectrometry: Instrumentation, Interpretation, and Applications (Wiley-Interscience Series in Mass Spectrometry) (Gebundene Ausgabe), by Jerzy Silberring, Ann M. Brinkmalm, Rolf Ekman

E – Characteristics of the study course

Name of the course	Photochemistry				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	2.6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student	Interest in Transdisciplinary Aspects				

Other subjects as prerequisites, etc.: Basic Knowledge in Inorganic, Organic and Physical Chemistry and Spectroscopy

Lecturer	G. Knör

Brief annotation of the course

Interaction of radiation with matter
Difference between thermal and photochemical processes
Fundamental Laws of photochemistry
Jablosnski diagram depicting various processes occuring in the exited sate
qualitative description of fluorescence, phosphorescence, non-radiative processes
(internal conversion, intersystem crossing)
Quantum yield, Photosensitized reactions, Energy and Photoinduced Electron transfer processes
Photochemistry of Coordination Compounds
Supramolecular Photochemistry
Some Practical Aspects and Case Studies
Selected Examples (Bioinorganic and Biomimetic Photochemistry, Photosensitization, Photocatalysis, Solar Energy Conversion, Molecular Photomedicine, Photobiology, Sensory Photoreceptors, Applications of Photochemical Key-Steps in Modern Science)

Study literature and study tools

N. J. Turro, V. Ramamurthy, J. C. Scaiano “Principles of Molecular Photochemistry – An Introduction”, University Science Books 2009

P. Suppan “Chemistry and Light”, Royal Society of Chemistry, 1994

Selected review literature to be announced in the course

E – Characteristics of the study course

Name of the course	Stereochemistry				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	2.6
Other expression of the size					
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					
Lecturer	N. Müller (coordinator)/ M. Waser (to be employed)				

Brief annotation of the course

Fundamentals of stereochemistry: diastereomers & enantiomers
Symmetry
Configuration
Stereochemical nomenclature
Pro-stereoisomers and pro-chirality
Physical Properties and Stereisomerism (including spectroscopy and chiroptical properties)
Conformation
Separation of stereoisomers
Stereoselective synthesis

Study literature and study tools

Basic Organic Stereochemistry, by Ernest L. Eliel, Samuel H. Wilen, Michael P. Doyle

E – Characteristics of the study course

Name of the course	Practical Photochemistry				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2.4
Other expression of the size					
Form of exam	combined			**Form of tuition**	laboratory
Other requirements on student					
Lecturer	G. Knör				

Brief annotation of the course

Introduction to practical photochemistry in the lab
Safety considerations
Preparative photochemistry
Determination of quantum yields

Study literature and study tools

A course script will be provided to the students

E – Characteristics of the study course

Name of the course	Seminar on Biomimetic Systems				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	14	**hours per week**	1	**ECTS**	1.6
Other expression of the size					
Form of exam	combined			**Form of tuition**	seminar

Other requirements on student

Good knowledge in inorganic, organic and bio-chemistry

Lecturer	G. Knör/ N. Müller

Brief annotation of the course

Current literature on biomimetic systems (journal club)

Study literature and study tools

Up-to-date research articles will be provided individually to the students

E – Characteristics of the study course

Name of the course	Physical chemistry III (Kinetics and thermodynamic of macromolecular systems)				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/1
Total hours of the course	42	**hours per week**	3,0	**ECTS**	3,9
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture

Other requirements on student

Other subjects as prerequisites, etc.

Lecturer

Sabine Hild

Brief annotation of the course

The course will teach the basics in the physical chemistry of macromolecular materials
Introduction in the terminology and basic classification of macromolecules
Chain strucutre and conformation
Macromolecules in solution and melt
Amorphous and crystalline state
Thermal and, mechanical porperiets
Colliods and liquid crystal

Study literature and study tools

Introduction to soft matter, Ian. W. Hamley, Wiley, 2007
Physical chmeistry of macromolecules, S. F. Sun, Wiley, 2004

E – Characteristics of the study course

Name of the course	Practicum Macromolecular systems				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2,6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	laboratory

Other requirements on student

Other subjects as prerequisites, etc.

Lecturer

Sabine Hild, Alois Schausberger, Gerhard Eder

Brief annotation of the course

Basic experiments on polymer synthesis and characterization
1) Polymerisation of styrene
2) Determiantion of molecular weight
3) Melt flow index
4) Thermal condction
5) Diffusion
6) Miscibilty gap
7) Mol polarisation
8) Viscosimetry
9) Crystallization and melting of macromolecules

Study literature and study tools

Instruction manual will be provided in the course

E – Characteristics of the study course

Name of the course	Biophysics III				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	3
Other expression of the size					
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					
Lecturer	P. Pohl				

Brief annotation of the course

- Mechanical characteristics of biological membranes
- Mechanosensitive channels (MscL, MscS, OTRPC4, TRPA1)
- Structure and function of the mammalian ear/auditory sensory cells
- Cytoskeleton (actin, intermediate filaments, microtubules)
- Molecular motors (ATPases, myosin, kinesin, dynein)
- Cell movement

Study literature and study tools

David Boal: Mechanics of the Cell;
Dennis Bray: Cell Movements: From Molecules to Motility
Jonathon Howard: Mechanics of Motor Proteins and the Cytoskeleton
Manfred Schliwa: Molecular Motors

E – Characteristics of the study course

Name of the course	Biophysics Laboratory II				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/1
Total hours of the course	28	**hours per week**	2	**ECTS**	3
Other expression of the size					
Form of exam	combined			**Form of tuition**	laboratory
Other requirements on student					
Lecturer	Koordinator P. Pohl (with P. Hinterdorfer)				

Brief annotation of the course

It is the aim of this course to enable the experimental approach for the observation of single molecules and to quantify single molecular properties. For this we will use (i) fluorescence microscopy to follow the mobility of lipids in supported lipd bilayers, (ii) Förster resonance energy transfer to study the interaction of proteins in living cells, and (iii) atomic force microscopy for the investigation of 2-D protein crystals and molecular interaction forces.

Study literature and study tools

Practicum script available, hands-on on fluorescence and force microscopes

E – Characteristics of the study course

Name of the course	Practical Atomic Force Microscopy					
Type of the course	Compulsory dep. on module choice			**recom. year / semester**		1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2.4	
Other expression of the size						
Form of exam	combined			**Form of tuition**	laboratory	
Other requirements on student						
Lecturer	S. Hild , P. Pohl					

Brief annotation of the course

In scanning force microscopy (SFM) the force between a tip and the sample was used to image the surface topography. The SFM can be operated in a number of modes, depending on the application. In general, possible imaging modes are divided into static (also called Contact) modes and a variety of dynamic (or non-contact) modes where the cantilever is vibrated. In the course, the different basic imaging modes will be used to investigate organic samples. Besides this, a brief introduction to materials sensitive techniques and force spectroscopy will be given.
Topics:
Topograghy imaging:
Contact mode
Dynamical modes (Non-contact, Magnetic mode, Pulsed force mode)
Materials sensitive cahracterization
Friction force microscopy
Magnetic force microscopy
Force modulation
Force spectroscopy
Adhesive force measurement

Study literature and study tools

Roland Bennewitz, Hans Josef Hug, Ernst Meyer; Scanning Probe Microscopy: The Lab on a Tip, Springer, Berlin; Auflage: 1 (27. August 2003)
Bhanu P. Jena J. K. Heinrich Horber; Force Microscopy: Applications in Biology and Medicine; Wiley & Sons; Auflage: 1 (18. Juli 2006)

E – Characteristics of the study course

Name of the course	Bioinformatics III: Structural Bioinformatics and Gene Analysis				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2,6
Other expression of the size	Ca. 14 weeks per semester				
Form of exam	written			**Form of tuition**	lecture

Other requirements on student

Basics in Molecular Biology

Lecturer

Prof. Dr. Sepp HOCHREITER / DI Noura CHELBAT

Brief annotation of the course

Contents:

Data bases for 3D structures, Molecular Viewers, Structure prediction, Threading, ab initio prediction, molecular dynamics, structural alignments, protein folding, protein classification, Motif search, gene expression profiles, Microarray technique, Single Nucleotide Polymorphism, Gene selection, Epigenomics, Pathways, etc.

Motivation:

The course "Bioinformatic III" gives an introduction to two main topics of bioinformatics: Structural Bioinformatics and Microarray technique together with gene expression profiles. A main topic in structural bioinformatics is the prediction of the 3D structure. This could be done from the sequences obtained from the genome sequences which would mean that the function of the genes in the genome can be inferred. The Microarray technique is currently the major source of information about the working of the cell and evolved to one of the major topics in Bioinformatics.

In Structural Bioinformatics, the 3D structure of proteins, DNA and RNA is analyzed and predicted from the primary structure. Topics include structural alignments, protein folding, prediction of 2D/3D structures, 3D viewer and molecular dynamics. One of the goals of Structural Bioinformatics is to give computational approaches to predict and analyze the spatial structure of macromolecules like proteins and nucleic acids. Understanding their 3D structure is crucial for understanding their function. Direct applications could be oriented to medical fields and pharmacological research. Especially for drug design, one of the most important goals is to determine which groups of ligands bind to a particular part of a protein and which do not, which properties are these proteins sharing, which proteins could be used as target, which drugs could be constructed and be used as virus inhibitors, etc. Homology and comparative modelling can be used for the detection of 3D structure and hence for function inference, so similar structure can imply similar function. Aspects of protein functions can be obtained by molecular mechanics and molecular dynamics like force-field. When no detections are raised by sequences comparisons then approaches like sequences-to-structure-fitness should be used which is called threading.

In the field of Microarray technique and gene expression profiles the expression states of genes in cell is the focus of interest. The gene expression profile reports how much mRNA is found in the cell which tells what proteins and how many are currently produced in the cell. This in turn tells what the cell is doing currently. Microarrays are the biotechnological tools to measure gene expression profiles. The DNA Microarray Technologies such as cDNA arrays and oligonucleotide arrays provide means of measuring tens of thousands of genes simultaneously (a snapshot of the cell) as a large scale high-throughput method for molecular biology experimentation. Topics in microarray analysis include normalization and summarization algorithms, statistical approaches, biotechnical background knowledge, SNP arrays and topics in gene expression profile analysis covering gene selection, classification and prediction based on the gene expression profile, spurious correlations, pathway extraction, etc. One of the goals of Microarray Technology is the detection of genes that are differentially expressed in tissue samples like healthy and cancerous tissues to see which genes are relevant for cancer. It has important applications in pharmaceutical and clinical research and helps in understanding gene regulation and interactions. The information obtained by recognizing genes that share patterns of expression and hence might be regulated together could be used to draw genetic pathways.

Study literature and study tools

- David W. Mount. Bioinformatics – Sequence and Genome Analysis. Cold Spring Harbor Labaratory Press, Cold Spring Harbor, New York, USA, 2004.
- Philip E. Bourne and HelgeWeissig. Structural Bioinformatics. Wiley-Liss, Hoboken, New Jersey, USA, 2003.
- Michael J. E. Sternberg. Protein Structure Prediction. Oxford University Press, 1996.
- Steen Knudsen. Guide to Analysis of DNA Microarray Data. John Wiley & Sohns, Hoboken, New Jersey, USA, 2004.
- ErnstWit and John McClure. Statistics for Microarrays. JohnWiley & Sohns Ltd., England, 2004.
- Pierre Baldi and G. Wesley Hatfield. DNA Microarrays and Gene Expression – From Experiments to Data Analysis and Modeling. Cambridge University Press, United Kingdom, 2002.
- Geoffry J. McLachlan, Kim-Anh Do, and Christophe Ambroise. Analyzing Microarray Gene Expression Data. John Wiley & Sohns Inc., Hoboken, New Jersey, USA, 2004.
- Jerome K. Percus. Mathematics of Genome Analysis. Cambridge University Press, United Kingdom, 2002.

E – Characteristics of the study course

Name of the course	Seminar computational biology				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	14	**hours per week**	1	**ECTS**	1,6
Other expression of the size	Ca. 14 weeks per semester				
Form of exam	combined			**Form of tuition**	seminar

Other requirements on student

None.

Lecturer

Prof. Dr. Norbert Müller / Prof. Dr. Sepp Hochreiter

Brief annotation of the course

Molecular dynamics

Molecular dynamics (MD) simulates a system by the electrostatic interactions and van der Waals forces of its atoms and molecules based on statistical mechanics. Using these interactions, MD computes the change of the system (movement of atoms) over time.
Advantage of MD over real experiments is that an experiment is made in slow-motion on a computer and can be visualized to observe interactions. Interactions between atoms can experimentally not be measured or inferred; therefore the system cannot be understood. The simulation can be stopped at every time point in order to analyze the current state of the system. Local energy minima and typical motion paths of the system can be identified.

Because of the huge number of interactions and forces, the change of the system cannot be computed analytically. Therefore physical forces are approximated by grouping together atoms which occur very often in a specific constellation. Instead of computing interactions of all single atoms, the interaction between atom groups are computed with MD.

The atom groups and their interactions are described by so-called "force fields".

Still MD is computationally demanding if large molecules are considered or if the molecules move within a liquid like water, where all surrounding molecules have to be simulated as well as their interactions. This is the challenge for computer scientist, where numerical methods are applied and the simulations are often parallelized.

MD is used to predict, to determine, or to refine protein structures obtained by X-ray crystallography and NMR.
MD can allow to observe interaction on an atomic level and is applied to analyze thin film growth and ion sub-plantation or to invent nanotechnological devices.

Study literature and study tools

Literature:

- Philip E. Bourne and Helge Weissig. Structural Bioinformatics. Wiley-Liss, Hoboken, New Jersey, USA, 2003. Chapter 21 ‘Electrostatic Interactions’ pp. 427-440.
- Michael J. E. Sternberg. Protein Structure Prediction. Oxford University Press, 1996, Chapter 10 ‘Modelling protein conformation by molecular mechanics and dynamics’, pp.229-261.
- Volker A. Eyrich, Daron M. Standley, and Richard A. Friesner. *Ab Initio* Protein Structure Prediction Using a Size-dependent Tertiary Folding Potential, in Computational Methods for Protein Folding. Advances in Chemical Physics Vol.120, Richard E. Friesner (ed.), John Wiley & Sons, USA, 2002.
- John L. Klepeis, Heather D. Schafroth, Karl M. Westerberg, Christodoulos A. Floudas. Deterministic Global Optimization and *Ab Initio* Approaches for the Structure Prediction of Polypeptides, Dynamics of Protein Folding, and Protein-Protein Interactions, in Computational Methods for Protein Folding. Advances in Chemical Physics Vol.120, Richard E. Friesner (ed.), John Wiley & Sons, USA, 2002.

Software:

- Tinker
- Gromacs
- MMTK

E – Characteristics of the study course

Name of the course	Exercises in Spectroscopy & Structure Elucidation I					
Type of the course	Compulsory dep. on module choice			**recom. year / semester**		1/1
Total hours of the course	14	**hours per week**	1	**ECTS**	1.6	
Other expression of the size						
Form of exam	combined			**Form of tuition**	exercises	
Other requirements on student						

Knowledge in NMR-spectroscopy, organic chemistry and biochemistry

Lecturer	N. Müller (Coordinator) with assitant(s)

Brief annotation of the course

Structure elucidation based on NMR spectroscopic data is trained on a set of exercise spectra increasing in complexity over the duration of the course. The main information will be contained in one- and two-dimensional NMR data. Other spectroscopic and chemical information will also be provided. Main emphasis is on developing the student's skill in approaching structural problems and avoiding biased approaches. The compound classes used as examples range from simple organic molecules via complex drugs to oligopeptides.

Study literature and study tools

Material is distributed in the lecture.

Organic Structures from Spectra, L. D. Field, S. Sternhell, J. R. Kalman

NMR. From Spectra to Structures. An Experimental Approach, by Burkhard Costisella (Autor), Terence N. Mitchell

E – Characteristics of the study course

Name of the course	Advanced NMR				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	14	**hours per week**	1	**ECTS**	1.3
Other expression of the size					
Form of exam	combined			**Form of tuition**	lecture
Other requirements on student					

Knowledge in NMR-spectroscopy, math, organic chemistry and biochemistry

Lecturer	N. Müller

Brief annotation of the course

(1)The theoretical framework of multi-dimensional, multi-nuclear pulsed NMR(product operators, coherence pathway selection)
(2) Analysis of pulse NMR techniques
(3) Techniques and strategies for resonance assignment and structure elucidation by NMR
(4) Molecular dynamics and NMR

Study literature and study tools

P.J. Hore, J.A. Jones, and S. Wimperis, NMR: The Toolkit, Oxford University Press, Oxford, 2000
T.C. Pochapsky and S.S. Pochapsky: NMR for Physical and Biological Scientists, Garland Science, 2007

E – Characteristics of the study course

Name of the course	Practical Biomolecular NMR				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2.4
Other expression of the size					
Form of exam	combined			**Form of tuition**	laboratory
Other requirements on student					

Knowledge in NMR-spectroscopy and biochemistry

Lecturer	N. Müller with assistants

Brief annotation of the course

(0) Sample preparation
(1) Basic operation of an NMR-spectrometer
(2) Standard experiments
(3) Calibration experiments
(4) Parameter optimisation
(5) Advanced experiments
(6) Special processing techniques

Hands on exercises on the spectrometers and processing stations in a small group

Study literature and study tools

Spectrometer manuals, handouts

E – Characteristics of the study course

Name of the course	Strucutre and properties of biological materials				
Type of the course	Compulsory dep. on module choice			**recom. year / semester**	1/2
Total hours of the course	28	**hours per week**	2	**ECTS**	2,6
Other expression of the size	weeks per semester, etc.				
Form of exam	combined			**Form of tuition**	lecture

Other requirements on student

Other subjects as prerequisites, etc.

Lecturer

Sabine Hild

Brief annotation of the course

Basic knowlegde of the principles of construction and proecsses of hierarchical structure formation of biological materiala (Biopolymer, composites, active systems –muscle-) which should lead to a basic understanding of the influence of the microstructure in in the physical properties of the biological materials. To understand materials optimization the material have to be characterized on different levels of hierarchy which requires basics in different experimental techniques. Therefore besides microscopic techniques (optical, electron and scanning probe), diffraction techniques (X-ray, neutron elctron scattering) as well as spectroscopic techniques will be explained.

1.Introduction
2. Structural biomaterials
2.1 Cellulose
2.2 Chitin
2.3 Spider silk
2.4 Collagen
3. Composite materials
3.1 Shells
3.2 Crustacean cuticle
3.3. Bone
4. Active materials
4.1 Membrane
4.2 Muscle
5. Surface properties
5.1 Lotus effect
5.2 Gecko foot

Study literature and study tools

Literature will be provided based on the actual literature