M4409 Molecular Biophysics

Coordinator (responsible lecturer)
Prof. Dr. Dieter Willbold (dieter.willbold@uni-duesseldorf.de)

Lecturers
Prof. Dr. H. Heise, PD Dr. R. Batra-Safferling, PD Dr. J. Granzin, PD. Dr. O.H. Weiergräber, Dr. M. Stoldt

Contact and organization
Dr. Matthias Stoldt (m.stoldt@fz-juelich.de)

Workload	Credit points	Contact time	Self-study	Duration
420 h	14 CP	300 h	120 h	1 semester

Course components	Frequency	Group size
Practicals: 18 PPW Lectures: 2 PPW	Summer semester	16 students

Learning outcomes/skills:
Students can explain and evaluate the principles and the fundamental concepts of NMR spectroscopy and X-ray structural analysis, the two most important structural biological methodologies (also in relation/comparison to each other), and use these on biological systems (focusing on proteins).

Forms of teaching
Lecture, practical, documenting procedures, preparation of seminar presentations

Content
– Liquid NMR: General basics of the NMR spectroscope, use of the NMR spectroscope in biological questions. Spin quantum numbers, energy levels, population ratios, chemical shifts, FT NMR, 1D experiment, line form, relaxation, Fourier transformation, spectral parameters, scalar and dipolar coupling, structure of an NMR spectrometer.
Recording of 1D experiments (ethanol, amino acids, proteins), processing and evaluation of the spectra. From 1D to 2D experiment, principle of the indirect dimension, homonuclear and heteronuclear experiments.
Basics of triple resonance experiments, recording, processing, allocation strategy (for example: HNCACB, HNCO). Spinal allocation, allocation of 3D NOE spectra, extraction of structure-defining parameters.
Molecular dynamics, strategy of “simulated annealing”, experimental data for structure calculation, example structure calculations, quality parameters, further methods, other applications of NMR in biology.
Visualisation of protein structures and complexes, secondary structures, hydrophobic core, tertiary contacts, electrostatic potential.
– Solid-state NMR General basics of solid-state NMR spectroscopy, formulation of questions that can be dealt with using these methodologies, various methods of achieving high resolution despite anisotropic line broadening: magic angle spinning and macroscopic orientation. Structural information in solid states: torsion angle, dipolar couplings and chemical shift anisotropy. Simulation software: SIMPSON and MATLAB, analysis software: nmrPipe, nmrDraw, CCPN.
Test objects: individual amino acids in solid phase and smaller model peptides.
– X-ray 1. General crystallography (crystal symmetry, crystal optics, polarisation microscopy, use of Bragg’s Law, reciprocal grid, Ewald construction, symmetry elements, point group, Laue group, space group); 2. Crystallisation of proteins (crystallisation methods, microscopy, polarisation and fluorescence); 3. Measurement of diffraction data (x-ray sources, detectors, determination of elementary cells and the space group, data acquisition); 4. Phase

determination (molecular and isomorphic substitution, Patterson methods, heavy atom derivatives); 5. Creation of an atomic model (interpretation of an electron map and model building); 6. Refinement, validation, architecture of proteins (improvement of conformity of the atomic model with the diffraction data, R factor, Ramachandran plot, primary, secondary, tertiary and quaternary structure); 7. Structure and function.

Requirements for admission

Formal: None

With regards to content: Basic knowledge of physical chemistry and basics of biochemistry are a prerequisite. An interest in structural biology and physico-chemical relationships is required.

Examination types

(1) Skill area – Knowledge (65% of the grade): written examination (generally) on the content of the lecture and the practical course

(2) Skill area – Documentation (20% of the grade): protocol (presentation of subject, execution, evaluation and discussions of scientific experiments)

(3) Skill area – Scientific presentation (15% of the grade): seminar presentation (preparation of material, graphical presentation of content, lecture, discussion)

Requirements for the award of credit points for this module

(1) Pass grade in the skill area – Knowledge

(2) Regular and active participation in the practical course

(3) Submission of a protocol complying with the requirements of scientific documentation

(4) Holding a seminar presentation complying with minimum standards

Relevant for following study programmes/major (only MSc programme)

M.Sc. Biology

M.Sc. Biology International;

Compatibility with other curricula

None

Significance of the mark for the overall grade

The mark given will contribute to the final grade in proper relation to its credits.

M.Sc. Biology International: 14/44 CP

Course language

English

Additional information

Registration for the practical is made via the LSF

Module takes place in the Forschungszentrum Jülich (a shuttle bus will transport students between the HHU Düsseldorf campus and the FZ Jülich)