Module Name Advanced Structural Biology: Crystallography, BioNMR, and Predictive Modeling

Identification Number	Workload	Credit Points	Term	Offered Every	Duration
MN-BC-BSM05	360 h	12 CP	1st or 2nd term	Summer Term, 2nd half	7 weeks

1	Course Type	Contact Times	Self-Study Times	Group Size*
	a) Lectures	24 h	48 h	max. 16
	b) Practical/Lab	154 h	108 h	max. 16
	c) Seminar	8 h	24 h	max. 16

2 Module Objectives and Skills to be Acquired

Students who successfully complete this module will:

- Gain expertise in principles and practical application of macromolecular crystallography, NMR of proteins, and computational modeling for studying protein structures.
- Be proficient in setting up crystallization screens, analyzing crystals by X-ray diffraction, and solving protein structures using relevant software.
- Acquire foundational knowledge and hands-on experience with BioNMR techniques to analyze protein dynamics, folding, and interactions.
- Develop skills in predictive modeling of protein structures using state-of-the-art tools like AlphaFold and perform docking simulations to explore molecular interactions.
- Learn to integrate data from experimental methods (e.g., crystallography, NMR) with computational predictions to assess the quality and biological relevance of protein structures.
- Analyze, visualize, and interpret 3D structures of biological macromolecules using molecular viewers and specialized software tools.
- Independently conduct small research projects combining experimental and computational approaches.
- Critically evaluate scientific literature and effectively present findings in professional oral and written formats.
- Apply these interdisciplinary skills to broader fields of biochemistry, and molecular biology.

3 Module Content

- Visualization and analysis of protein structures.
- Crystallographic techniques: theory and practice of X-ray diffraction, crystallization experiments, data collection, and structure determination.
- BioNMR basics: principles, sample preparation, data acquisition, and analysis of protein dynamics and interactions.
- Computational modeling: protein structure prediction (AlphaFold), molecular docking, and integration with experimental data.
- Software tools: ChimeraX, AlphaFold, Phenix, CCP4, Coot, CCPN, TopSpin and docking software like Haddock.
- Critical reading of scientific publications in structural biology and computational modeling.

4 Teaching Methods

- Lectures (theoretical foundations of crystallography, BioNMR, and modeling). Practical work (crystallization, X-ray diffraction, BioNMR experiments, and computational analysis). Focus: Crystallography (65%), BioNMR (25%), and Modeling (10%). Includes guided exercises, independent project work (1 week), and a seminar for discussing research papers.

5 Prerequisites

	Enrolment in the Master´s degree course “Biological Sciences”, in the Master´s degree course “Biochemistry and Molecular Medicine” or in the Master´s degree course “Chemistry”
6	**Type of Examinations** The final examination consists of two parts: A written examination about topics of the lectures and the practical/lab part (50 % of the total module mark) and an oral presentation of a self-chosen structural biology paper (50 % of the total module mark)
7	**Credits Awarded** Regular and active participation; Each examination part at least “sufficient” (see appendix of the examination regulations for details)
8	**Compatibility with other Curricula** Elective module in the Master´s degree course “Chemistry”, Subject module of the Master´s degree course “Biological Sciences”
9	**Proportion of Final Grade** 10%
10	**Module Coordinator** Prof. Dr. Ulrich Baumann, phone 470-3208, e-mail: ubaumann@uni-koeln.de
11	**Additional Information** Focus of research: (B) Biochemistry, Biotechnology and Biophysics Participating faculty: Prof. Dr. U. Baumann, Dr. J. Gebauer, Dr. Daniel Friedrich Further information: https://px.uni-koeln.de/teaching/structuralbiology Literature: • Rupp, B. (2010) Biomolecular Crystallography. Garland Science • Blow, D. (2002) Outline of Protein Crystallography for Biologists. Oxford University Press • Branden, C.I., Tooze, J. (1998) Introduction to Protein Structure. 2nd edition, Taylor and Francis • Liljas, A., Liljas, L., Piskur, J., Lindblom, G., Nissen, P., Kjeldgaard, M. (2009) Textbook on Structural Biology. World Scientific • Hore, P.J. (2015) Nuclear Magnetic Resonance. Oxford University Press • Engels, J.W., Lottspeich, F. (2018) Bioanalytics - Analytical Methods and Concepts in Biochemistry and Molecular Biology. Wiley-VCH [Chapter 18] • Cavanagh. J. (2007) Protein NMR Spectroscopy. Elsevier • Online resources: CCPN (https://ccpn.ac.uk/); ChimeraX (https://www.rbvi.ucsf.edu/chimerax/); Phenix (https://phenix-online.org) • Additional material and subject specific literature will be provided *ad hoc* **General time schedule:** *WEEK 1-4*: (Mo-Fr) Lectures at approx. 9:00-10:30 a.m. (three times a week), following experimental/computational work till 5 p.m. (including lunch break, the exact times of lectures and practical work may vary according to the laboratory needs). *WEEK 5:* self-organised project work (best performed in the computer lab of the institute). *WEEK 6:* Preparation and presentation of seminar talk; *WEEK 7*: Preparation for the written examination Note: The module contains hand-on laboratory work conducted by small groups of students and is taught in course rooms and research laboratories. The module contains computer-based practicals/research as a main component.

* Max. 4 students from the Master´s degree course “Biological Sciences”, 8 students from the Master’s degree course “Biochemistry and Molecular Medicine” and 4 students from the Master´s degree course “Chemistry”.