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

Type of Module	**Module Code**
o Advanced Module	Crystallography

Identification Number	**Workload**	**Credit Points**	**Term**	**Offered Every**	**Start**	**Duration**
MN-B-SM (GA 4)	360 h	12 CP	2nd term of studying	Summer term, 2nd half	Summer term only	7 weeks

1	**Course Types**	**Contact Time**	**Private Study**
	a) Lectures	24 h	48 h
	b) Practical/Lab	154 h	108 h
	c) Seminar	8 h	24 h

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 (for the Module)** Enrollment in the Master's of Science degree course "Genetics and Biology of Aging and Regeneration" or in the Master's degree course "Computational Biology" or in the Master's degree course "Biochemistry and Molecular Medicine" **Additional academic requirements:** None
6	**Type of Examination** The final examination consists of two parts: One hour 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*** Optional compulsory module in the Master's degree course "Biochemistry and Molecular Medicine"
9	**Proportion of Final Grade** 12.0 %
10	**Module Coordinator** Prof. Dr. Ulrich Baumann, phone 470-3208, e-mail: ubaumann@uni-koeln.de

11	**Further Information** Focus of research: (B) Structural Biology, Biochemistry, 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* **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 also contains computer-based research/practicals as an important component. **Location:** The course will take place at the Institute of Biochemistry, Zülpicher Str. 47, 50674 Cologne. **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 **Introduction to the module**: May 19, 2025 at 10:00 a.m., Zülpicher Str. 47, Room 465 (further information/link will be sent to your Smail-Account) **Written examination:** July 18, 2025, second/supplementary examination August 29, 2025; the latter date may vary if students and module coordinator agree. More details will be given at the beginning of the module.