Module Name
Introduction to protein crystallography

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

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

1	**Course Types**	**Contact Time**	**Private Study**	**Group Size***
	a) Lecture	24 h	45 h	max. 16
	b) Practical/lab	154 h	108 h	max. 16
	c) Seminar	8 h	21 h	max. 16

2 Module Objectives and Skills to be Acquired

Students who successfully completed this module...

- are able to set up crystallization screens, analyse crystals by X-ray diffraction, and determine crystal structures by the application of the relevant computer programs
- have acquired a thorough knowledge of the principles of macromolecular crystallography and can use it to judge crystal structures generated by other scientists regarding their quality
- are familiar with different methods for 3D structure determination and can compare them with respect to their results and limits
- are able to set up crystallization screens, analyse crystals by X-ray diffraction, and determine crystal structures by the application of the relevant computer programs.
- can predict protein structure using state-of-the-art algorithms and judge their quality and usefulness
- are able to recognize different protein folds, analyze and visualize biological macromolecular 3D structures using molecular viewers and other programs
- can independently carry out small scientific projects related to the topic of the module
- have learned how to present research results in oral and written form and to critically discuss scientific publications related to the topic of the module on a professional level
- are able to transfer the acquired skills of this module to other fields of biochemistry and biology

3 Module Content

- Visualisation and analysis of protein structures
- Crystallographic foundations: crystal geometry, symmetries, theory and practice of X-ray diffraction
- Crystallization experiments on biological macromolecules
- Crystallographic data collection and analysis
- Approaches for solving the phase problem
- Structure building and refinement
- Validation and quality assessment
- Protein modelling
- Critical reading of publications in the field of Structural Biology
- Software used: ChimeraX, AlphaFold, Phenix, CCP4, Coot and other

4 Teaching Methods

Lectures; 4 week practical work [wet lab (30%), computer lab (60%) and guided excercises (10%)], 1 week project work ("Solve your *own* structure"); Seminar "Journal Club"; Guidance to independent research; Training on presentation techniques in oral and written form

5	**Prerequisites** Enrollment in the Master's degree course "Biological Sciences", in the Master's degree course "Biochemistry" or in the Master's degree course "Chemistry". For students from the Master's degree course "Chemistry" prior participation in an advanced Biochemistry module, including its practical lab part, during the Bachelor's degree course is required.
6	**Type of Examination** 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** Biochemical subject module in the master's degree course "Biochemistry" and in the master's degree course "Chemistry"
9	**Proportion of Final Grade** In the Master's degree course "Biological Sciences": 12 % of the overall grade (see also appendix of the examination regulations)
10	**Module Coordinator** Prof. Dr. Ulrich Baumann, phone 470-3208, e-mail: ubaumann@uni-koeln.de

11	**Further Information** **Participating faculty:** Prof. Dr. U. Baumann, Dr. J. Gebauer **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 • ChimeraX (https://www.rbvi.ucsf.edu/chimerax/) • Additional material and subject specific literature will be provided *ad hoc* via Ilias **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. Further information can be found online: https://px.uni-koeln.de/teaching/proteincrystallography **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 15, 2023 at 10:15 a.m., Zülpicher Str. 47, Room 465 (further information/link will be sent to your Smail-Account) **Written examination:** July 14, 2023, second/supplementary examination September 01, 2023; the latter date may vary if students and module coordinator agree. More details will be given at the beginning of the module.

* 4 students from the Master's degree course "Biological Sciences", 8 students from Master's degree course "Biochemistry and Molecular Medicine", and 4 from the Master's degree course "Chemistry".