Module Name Introduction to protein crystallography (Baumann)

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 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

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 (70 % of the total module mark) and an oral presentation of a self-chosen structural biology paper (30 % 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 Further information: https://px.uni-koeln.de/teaching/proteincrystallography 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* **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. Further information can be found online: https://px.uni-koeln.de/teaching/proteincrystallography **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) **Oral or 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.

* 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".