

BCH 6744- Fall Semester 2021: Molecular Structure Determination by X-ray Crystallography

Instructor: Dr. Robert McKenna (Lectures & Labs)

Credit: 1 or 2 hours

Course Description:

The objective of the course is to provide detailed theoretical and practical instructions on the methodology of X-ray crystallography, a biophysical technique at the forefront of research efforts aimed at structure-function elucidation of macromolecules. Students will learn the theory behind the technique of X-ray crystallography and will apply the knowledge obtained to the three-dimensional structure determination of a macromolecule (carbonic anhydrase). The laboratory class will provide practical experience in sample preparation, operation of the instrumentation, data acquisition, data analysis, phasing and refinement. The anticipation is that students will take both the theoretical and practical sections of the course for 2 credits, which will run concurrently. However, students may earn 1 credit by either attending the lectures on the theory of X-ray crystallography or the laboratory class. This hands-on approach will reinforce the applicability of this methodology in the analysis of the functional properties of a biological macromolecule.

Times and Places:

Lectures (L): Held Mondays (M), Wednesdays (W) and Fridays (F), 9th period (4:05 to 4:55 pm) in Communicore C2-33 (C2-033)

Laboratory practicals (P): Held Thursdays, 6th through 8th period (12:50 to 3:50 pm) in LG-171.

Prerequisites:

BCH 6740 or equivalent or consent of instructor.

Recommended Text:

Rhodes, G. 2000. Crystallography made crystal clear. Academic Press, Inc. USA.

Blow, D. 2002. Outline of Crystallography for Biologist, Oxford University Press.

Tests and Grading:

Lecture component will be graded based on a take home problems and a final take home exam. Laboratory component grade will be 30% homework and 70% completed lab. project report written in the form of crystal structure manuscript (Acta Cryst. D format).

Instructor Contacts:

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BCH 6744C: Course Schedule

Class	Date	Location	Time	TOPIC
L-1	8/23/21 Mon	C2-33	4:05-4:55	General Overview
L-2	8/25/21 Wed	C2-33	4:05-4:55	Sample preparation
L-3	8/27/21 Fri	C2-33	4:05-4:55	Crystallization
L-4	8/30/21 Mon	C2-33	4:05-4:55	Crystal preparation
L-5	9/01/21 Wed	C2-33	4:05-4:55	Diffraction theory: Braggs Law
P-1	9/02/21 Thr	LG-171	12:50 - 3:50	Crystallization of carbonic anhydrase
L-6	9/03/21 Fri	C2-33	4:05-4:55	Data collection/instrumentation
	9/06/21 Mon		Labor Day	No class
L-7	9/08/21 Wed	C2-33	4:05-4:55	Data collection theory
P-2	9/09/21 Thr	LG-171	12:50 - 3:50	Crystal preparation and data collection
L-8	9/10/21 Fri	C2-33	4:05-4:55	Space group determination: Symmetry
L-9	9/13/21 Mon	C2-33	4:05-4:55	Data processing and reduction
L-10	9/15/21 Wed	C2-33	4:05-4:55	Fourier transforms
P-3	9/16/21 Thr	LG-171	12:50 - 3:50	Data processing and reduction
L-11	9/17/21 Fri	C2-33	4:05-4:55	Phase determination: Heavy atom
L-12	9/20/21 Mon	C2-33	4:05-4:55	Phase determination: Molecular replacement
L-13	9/22/21 Wed	C2-33	4:05-4:55	Model building: Map interpretation
P-4	9/24/21 Thr	LG-171	12:50 - 3:50	Phasing and model building
L-14	9/24/21 Fri	C2-33	4:05-4:55	Model refinement, validation & interpretation
L-15	9/27/21 Mon	C2-33	4:05-4:55	Review
P-5	9/30/21 Thr	LG-171	12:50 - 3:50	Refinement /structure function analysis

10/01/21 Fri (10 am) - 10/04/21 Mon (5pm)

LG-179 FINAL EXAM (Take Home)

10/22/21 Fri (5pm)

LG-179 LAB REPORT DUE