

BCH 6744C: Molecular Structure Determination by X-ray Crystallography

Instructors:

Dr. Robert McKenna (Lectures) & Dr. Mavis Agbandje-McKenna (Labs).

Fall Semester 2007

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 (lysozyme). 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), 4th period (10:40 am to 11:30 am) in LG-110A (M) and LG-116 (W & F).

Laboratory practicals (P): Held Thursdays, 4th to 6th period (10:40 am to 1:30 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	8/24/07 Fri	LG-110A	10:40 - 11:30	General Overview
L-2	8/27/07 Mon	LG-110A	10:40 - 11:30	Sample preparation
L-3	8/29/07 Wed	LG-110A	10:40 - 11:30	Crystallization
P-1	8/30/07 Thur	LG-171	10:40 - 13:30	Crystallization of Lysozyme
L-4	8/31/07 Wed	LG-110A	10:40 - 11:30	Crystal preparation
	9/03/07 Mon		Labor Day	
L-5	9/05/07 Wed	LG-110A	10:40 - 11:30	Diffraction theory: Bragg's Law
P-2	9/06/07 Thur	LG-171	10:40 - 13:30	Crystal preparation and data collection
L-6	9/07/07 Fri	LG-110A	10:40 - 11:30	Data collection/instrumentation
L-7	9/10/07 Mon	LG-110A	10:40 - 11:30	Data collection theory
L-8	9/12/07 Wed	LG-110A	10:40 - 11:30	Space group determination: Symmetry
P-3	9/13/07 Thur	LG-171	10:40 - 13:30	Data processing and reduction
L-9	9/14/07 Fri	LG-110A	10:40 - 11:30	Data processing and reduction
L-10	9/17/07 Mon	LG-110A	10:40 - 11:30	Fourier transforms
L-11	9/19/07 Wed	LG-110A	10:40 - 11:30	Phase determination: Heavy atom & MAD
P-4	9/20/07 Thur	LG-171	10:40 - 13:30	Phasing and model building
L-12	9/21/07 Fri	LG-101A	10:40 - 11:30	Phase determination: Molecular replacement
L-13	9/24/07 Mon	LG-110A	10:40 - 11:30	Model building: Map interpretation
L-14	9/26/07 Wed	LG-110A	10:40 - 11:30	Model refinement
P-5	9/27/07 Thur	LG-171	10:40 - 13:30	Refinement and structure function analysis
L-15	9/28/07 Wed	LG-110A	10:40 - 11:30	Model validation & interpretation
	10/05/07 Fri (2pm) - 10/08/07 Mon (2pm)			LG-179 FINAL EXAM (Take Home)
	10/15/07 Mon (5pm)			LG-181 LAB REPORT DUE