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

Course Coordinator: Dr. Mavis Agbandje-McKenna

Instructors:

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

Fall Semester 2001

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.

Meeting Times and Places: Lectures (L): Held Mondays (M), Wednesdays (W) and Fridays (F), 4^{th} period (10:40 am to 11:30 am) in LG-110A (M) and LG-116 (W & F). Laboratory practicals (P): Held Thursdays, 4^{th} to 6^{th} 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. **And** current structural biology literature.

Tests and Grading: Lecture component will be graded based on a 2 hour final 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:	Dr. Mavis Agbandje-McKenna (MAM)	Dr. Robert McKenna (RM)
	Office: LG-179, 2-5694	Office: LG-181, 2-5696
	e-mail: mckenna@ufl.edu	e-mail: rmckenna@ufl.edu
Lab TAs:	David Duda	Rebecca Moose
	Lab: LG-171, 6-2001	Lab: LG-171, 6-2001
	e-mail: daveduda@ufl.edu	& ARB R3-183 2-3367
		e-mail: bmoose@ufl.edu

BCH 6744C: Course Schedule

Class	Date	Location	Time	TOPIC
L-1	8/22/01	LG-116	10:40 - 11:30	General Overview
L-2	8/24/01	LG-116	10:40 - 11:30	Sample preparation
L-3	8/27/01	LG-110A	10:40 - 11:30	Crystallization
L-4	8/29/01	LG-116	10:40 - 11:30	Crystal preparation
P-1	8/30/01	LG-171	10:40 - 13:30	Crystallization of Lysozyme
L-5	8/31/01	LG-116	10:40 - 11:30	Diffraction theory: Braggs Law
L-6	9/5/01	LG-116	10:40 - 11:30	Data Collection/instrumentation
P-2	9/6/01	LG-171	10:40 - 13:30	Crystal preparation and data collection
L-7	9/7/01	LG-116	10:40 - 11:30	Data Collection procedure
L-8	9/10/01	LG-110A	10:40 - 11:30	Space group determination: Crystal symmetry
L-9	9/12/01	LG-116	10:40 - 11:30	Data processing and reduction
P-3	9/13/01	LG-171	10:40 - 13:30	Data processing and reduction
L-10	9/14/01	LG-116	10:40 - 11:30	Fourier transforms
L-11	9/17/01	LG-110A	10:40 - 11:30	Phase determination: Heavy atom & MAD
L-12	9/19/01	LG-116	10:40 - 11:30	Phase determination: Molecular replacement
P-4	9/20/01	LG-171	10:40 - 13:30	Phasing, model building and refinement
L-13	9/21/01	LG-116	10:40 - 11:30	Model building: Electron density map interpretation
L-14	9/24/01	LG-110A	10:40 - 11:30	Model refinement
L-15	9/26/01	LG-116	10:40 - 11:30	Model validation and functional interpretation
P-5	9/27/01	LG-171	10:40 - 13:30	Structure function analysis
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	10/12/01	LG-181		LAB REPORT DUE