

## **BCH 6744- Fall Semester 2023: 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), 9<sup>th</sup> period (4:05 to 4:55 pm) in CG-041.

Laboratory practicals (P): Held Thursdays, 6<sup>th</sup> through 8<sup>th</sup> period (12:50 to 3:50 pm) in LG-150.

### **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:**

Dr. Robert McKenna

Office: LG-181

e-mail: [rmckenna@ufl.edu](mailto:rmckenna@ufl.edu)

### **TA:**

Mitch Gulkis

Lab: LG-150 e-mail: [mitchell.gulkis@ufl.edu](mailto:mitchell.gulkis@ufl.edu)

## BCH 6744C: Course Schedule

Class	Date	Location	Time	TOPIC
L-1	8/23/23 Wed	CG-041	4:05-4:55	General Overview
L-2	8/25/23 Fri	CG-041	4:05-4:55	Sample preparation
L-3	8/28/23 Mon	CG-041	4:05-4:55	Crystallization
L-4	8/30/23 Wed	CG-041	4:05-4:55	Crystal preparation
<b>P-1</b>	<b>8/31/23 Thr</b>	<b>LG-150</b>	<b>12:50 - 3:50</b>	<b>Crystallization of carbonic anhydrase</b>
L-5	9/01/23 Fri	CG-041	4:05-4:55	Diffraction theory: Braggs Law
	<b>9/05/23 Mon</b>		<b>Labor Day</b>	<b>No class</b>
L-6	9/06/23 Wed	CG-041	4:05-4:55	Data collection/instrumentation
<b>P-2</b>	<b>9/07/23 Thr</b>	<b>LG-150</b>	<b>12:50 - 3:50</b>	<b>Crystal preparation and data collection</b>
L-7	9/08/23 Fri	CG-041	4:05-4:55	Data collection theory
L-8	9/11/23 Mon	CG-041	4:05-4:55	Space group determination: Symmetry
L-9	9/13/23 Wed	CG-041	4:05-4:55	Data processing and reduction
<b>P-3</b>	<b>9/14/23 Thr</b>	<b>LG-150</b>	<b>12:50 - 3:50</b>	<b>Data processing and reduction</b>
L-10	9/15/23 Fri	CG-041	4:05-4:55	Fourier transforms
L-11	9/18/23 Mon	CG-041	4:05-4:55	Phase determination: Heavy atom
L-12	9/20/23 Wed	CG-041	4:05-4:55	Phase determination: Molecular replacement
<b>P-4</b>	<b>9/21/23 Thr</b>	<b>LG-150</b>	<b>12:50 - 3:50</b>	<b>Phasing and model building</b>
L-13	9/22/23 Fri	CG-041	4:05-4:55	Model building: Map interpretation
L-14	9/25/23 Mon	CG-041	4:05-4:55	Model refinement, validation & interpretation
L-15	9/27/23 Wed	CG-041	4:05-4:55	Review
<b>P-5</b>	<b>9/28/23 Thr</b>	<b>LG-171</b>	<b>12:50 - 3:50</b>	<b>Refinement /structure function analysis</b>

**9/29/23 Fri (10 am) - 10/02/23 Mon (5pm) LG-181 FINAL EXAM (Take Home)**

**10/20/23 Fri (5pm)**

**LG-181 LAB REPORT DUE**