

MACROMOLECULAR CRYSTALLOGRAPHY: METHODS AND APPLICATIONS

This is an introductory course on methods and applications of macromolecular structure determination using X-ray crystallography. The course will be broken up into three parts: 1) Principles of X-ray crystallography involving didactic lectures on the technique with weekly problem sets and a workshop; 2) Macromolecular structures by X-ray crystallography presented by selected faculty members; 3) Student "journal club" presentations on current high impact publications involving X-ray crystal structure determination.

Course Director

Ronen Marmorstein

Perelman School of Medicine, University of Pennsylvania

421 Curie Blvd.

BRB II/III, Room 454

Tel: (215) 898-7740

e-mail: marmor@upenn.edu

Office hours by appointment

Time and Place

Class will be on Tuesdays and Thursdays 10:30 A.M. - 12:00 P.M.

from Sept. 1 - Dec. 10 and held virtually at <https://upenn.zoom.us/j/91213280793>

(backup site: <https://bluejeans.com/5890790765>)

There will be no class on Nov. 26 for Thanksgiving

Required Text

Crystallography made crystal clear-third edition, Gail Rhodes, Academic Press

Course Outline

The Course will be broken up into three parts:

- (1) Principles of X-ray crystallography
- (2) Macromolecular structures by X-ray crystallography
- (3) Student presentations

Grading will be based on the following: There will be problem sets (10%) and a mid-term exam covering part 1 (30%), and a final exam covering parts 2 and 3 (30%). For part 3 of the course, students will also be required to make a 20-30 minute presentation on a manuscript describing a macromolecular structure of their choice (30%).

Tentative Schedule

Sep. 1, 3, 8, 10, 15, 17, 22, 24, 29; Oct. 1, 6, 8, 13, 15 (Midterm Exam)

Lecturer: Ronen Marmorstein

(1) Principles of X-ray crystallography. Topics will include:

- (i) Structural biology
- (ii) X-Ray diffraction.
- (iii) Preparation of crystals.
- (iv) Crystal symmetry, and space groups.
- (v) Data collection.
- (vi) The structure factor and Fourier synthesis.
- (vii) The phase problem (Multiple Isomorphous Replacement, Molecular Replacement, Anomalous Dispersion, Multiple Anomalous Dispersion)
- (viii) Electron density maps.
- (ix) Electron density modification
- (x) Crystallographic refinement and analysis.

* Oct 20, 22 and 27 - Crystallography workshop with Kushol Gupta and use of Pymol to visualize protein structures with Ronen Marmorstein

Oct. 29; Nov. 3, 5, 10, 12, 17

(2) Macromolecular structures will be presented by selected faculty members:

- Oct. 29: Greg Van Duyne
- Nov. 3: Kushol Gupta
- Nov. 5: Sriram Krishnaswamy
- Nov. 10: Ronen Marmorstein
- Nov. 12: Roberto Dominquez
- Nov. 17: Emmanuel Skordalakes

Nov. 19, 24; Dec. 1, 3, 7, 10

(3) Student Presentations:

Students will present a 20 min lecture on a manuscript describing a macromolecular structure of their choice. There will be 2 to 3 presentations per day depending on the number of students enrolled.

The Final Exam will be take-home and due on the Finals Day assigned to the course.