

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; 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

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Time and Place

Lectures will be on Tuesdays and Thursdays 10:15 A.M. - 11:45 P.M. from Sept. 2 - Dec. 2 in BRB 253

There will be no class on Sept. 23 (Rosh Hashanah), Oct. 2 (Yom Kippur), Oct. 9 (fall term break), Nov. 27 (Thanksgiving) and Dec. 4 (BBCB/BB Retreat)

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 give a 20-minute presentation on a manuscript describing a macromolecular structure of their choice (30%).

Tentative Schedule

Sept. 2, 4, 9, 11, 16, 18, 25, 30; Oct. 7, 14, 16, 21 (Midterm Exam)

Lecturer: Ronen Marmorstein

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

- (i) Why Use X-Rays in 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. 23, 28, 30; Nov. 4, 6

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

- Oct. 23: Greg Van Duyne
- Oct. 28: Ronen Marmorstein
- Oct. 30: Sriram Krishnaswamy
- Nov. 4: Roberto Dominguez
- Nov. 6: Kushol Gupta

Nov. 11, 13, 18, 20, 25; Dec. 2

Coordinator: Ronen Marmorstein

(3) Student Presentations:

Students will present a 30 min. lecture on a manuscript describing a macromolecular structure of their choice. There will be 1-2 presentations per day.

The Final Exam will be posted on the canvas site on the last day of class and will likely be take home. The exam will be due for upload on Dec. 16th at noon.

Office hours: by appointment

All course material will be uploaded on the Course Canvas site