

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 Aug. 30 - Dec. 8 in BRB 253 (unless otherwise indicated)

There will be no class on Sept. 27 (Rosh Hashanna), Oct. 6 (fall term break), Nov. 24 (Thanksgiving) and Dec. 1 (BMB 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

Aug. 30; Sept. 1, 6, 8, 13, 15, 20, 22, 29; Oct. 4, 11, 13, 18 (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. 20, 25, 27; Nov. 1, 3

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

- Oct. 20: Greg Van Duyne
- Oct. 25: David Christianson
- Oct. 27: Sriram Krishnaswamy
- Nov. 1: Roberto Dominquez
- Nov. 3: Ronen Marmorstein

Nov. 8, 10, 15, 17, 22, 29; Dec. 6, 8

Coordinator: Ronen Marmorstein

(3) Student Presentations:

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

The Final Exam will be posted on the canvas site on the last day of class and will be take home. The exam will be due for upload on Dec. XX (TBD) at noon.

Office hours: by appointment

All course material on Course Canvas site