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 Perelman School of Medicine, University of Pennsylvania 421 Curie Blvd. BRB II/III, Room 454 Tel: (215) 898-7740 e-mail: marmor@upenn.edu

Time and Place

Lectures will be on Tuesdays and Thursdays 10:30 A.M. - 12:00 P.M. from Sept. 3 - Dec. 3 in BRB 253 (unless otherwise indicated)

<u>There will be no class on Oct. 10 for fall term break, Dec. 5 for BMB Retreat and Nov.</u> <u>28 for Thanksgiving</u>

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 midterm 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

<u>Sep. 3, 5, 10, 12, 17, 19, 24, 26; Oct. 1, 3, 8*, 15, 17, 22 (Midterm Exam)</u> 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, Anamolous Dispersion, Multiple Anomalous Dispersion)
 - (viii) Electron density maps.
 - (ix) Electron density modification
 - (x) Crystallographic refinement and analysis.

* Crystallography demonstration with Kushol Gupta (meet in BRB 253 to go to G11 Blockley Hall)

Oct. 24, 29, 31; Nov. 5, 7

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

- Oct. 24: Roberto Dominquez
- Oct. 29: Sriram Krishnaswamy
- Oct. 31: Kushol Gupta
- Nov. 5: Emmanuel Skordalakes
- Nov. 7: Greg Van Duyne (Ronen Marmorstein will not attend this class)

Nov. 12, 14, 19, 21, 26; Dec. 3

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 to 3 presentations per day depending on the number of students enrolled.

The Final Exam will be held on the Finals Day assigned to the course.