

Protein Crystallography
JBB2025S
Departments of Biochemistry, Molecular Genetics and Medical Biophysics
January 2022

Instructors:

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Time: 10:00 am - 12:00 noon
Location: Medical Sciences Building, Rm 3290, unless otherwise instructed
Lecture Dates: Friday January 14, 2022 to Friday April 8, 2022

Course Evaluation:

Problem Set 1 (15%) - Re. Lectures 1-3 - due Friday Feb 11
Problem Set 2 (35%) - Re. Lectures 4-7 - due Friday Mar 11
Problem Set 3 (35%) - Re. Lectures 8-11 - due Friday Apr 8
Problem Set 4 (15%) - Re. Lectures 12-13 - due Friday Apr 22

Course Outline:

Lecture 1 - Lynne Howell - Jan 14
Lecture 2 - Lynne Howell - Jan 21
Lecture 3 - Lynne Howell - Jan 28

Rupp Chapters 5.1, 5.2, 5.4, 6, 9.1, (overview of 9.2 and 9.3)

- Crystals, lattices (real and reciprocal) and planes
- Diffraction basics: Scattering of X-rays, Ewald sphere, X-ray absorption

- Reconstruction of electron density: Fourier transforms, convolution and factors that affect electron density map calculation

Lecture 4 - Gil Privé - Feb 4

Lecture 5 - Gil Privé - Feb 11

Lecture 6 - Gil Privé - Feb 18

Lecture 7 - Gil Privé - Feb 25

Rupp Chapters 3, 4, 5.2, 5.3, 8, 9.2, 9.3 and part of 10.3

- Space groups and symmetry
- Crystallization
- Instrumentation and generation of X-rays
- Data collection and reduction

Lecture 8 - James Rini - Mar 4

Lecture 9 - James Rini - Mar 11

Lecture 10 - James Rini - Mar 18

Lecture 11 - James Rini - Mar 25

Rupp Chapters 9.4, 10 and 11

- Patterson and molecular replacement
- Heavy atom methods: MIR and MAD
- Phase improvement: symmetry averaging and solvent flattening

Lecture 12 - Trevor Moraes - Apr 1

Lecture 13 - Trevor Moraes - Apr 8

Rupp Chapters 12 and 13

- Model building
- Refinement
- Validation

Required Text Book:

1) *Biomolecular crystallography: principles, practice and applications to structural biology*. Rupp, B. New York: Garland Science, Taylor and Francis Group, 2010.

Highly Recommended Text Books:

1) International Tables for Crystallography (2012). Volume F, *Crystallography of Biological Macromolecules*. International Union of Crystallography 2012.

2) *Crystal Structure Analysis: a Primer*. Glusker, P, and Trueblood, K.N. Oxford University Press, New York, 1985

3) *Principles of Protein X-ray Crystallography*, Drenth, J., Springer-Verlag New York Inc., 2nd Edition, 1999.

Recommended Text Books:

1) *Crystallography Made Crystal Clear*. Rhodes, G. Academic Press, San Diego, 3rd Edition, 2006

2) *Crystallization of Nucleic Acids and Proteins: A practical Approach.*, Edited by A. Ducruix and R. Giege, 2nd Edition, 1999.

3) *Protein Crystallography: A Concise Guide*. E.E. Lattman and P.J. Loll, Johns Hopkins University Press (2008).

4) *Fundamentals of Crystallography*. Giacovazzo, C., Monaco, H.L. Artioli, G. Viterbo, D., Ferraris, G. Gilli, G., Zanotti, G, and Catti, M., Oxford University Press, Oxford, 2nd Edition, 2002.

5) *Introduction to Macromolecular Crystallography*, McPherson A., John Wiley and Sons, New York, 2002.

6) *Protein Crystallography*, Blundell, T.L, and Johnson, L.N., Academic Press, London, 1990.