STB 533. Crystallographic Methods of Structural Biology  
Course Syllabus and Class Schedule  
Fall Semester 2014. Class meetings 10:30-11:45 am Tuesdays and Fridays

The goal of the course is that students acquire sufficient knowledge and understanding of the basic principles of biomolecular crystal structure analysis that they will be able to comfortably, and with interest and insight, read and comprehend the articles in Volume F of the International Tables for Crystallography: Crystallography of Biological Macromolecules, and articles in the current and recent literature reporting research in structural molecular biology by diffraction methods.

Textbooks for the course are:

Baltimore, Maryland: Johns Hopkins University Press.


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<th>Dates</th>
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| 26, 29 Aug.      | Introduction  
Protein structural elements  
1° aa sequence; 2° α-helix, β strand, β sheet, loop;  
3° domain fold; 4° domain assembly.  
Overview of biomacromolecular crystallography  
Rupp, chs. 1-4 (Only §§ 1.1-1.5 and 3.2) | Blessing   |
| 2, 5 Sept. 9, 12 | Geometrical crystallography  
Laws of classical crystallography  
Lattices, point groups, space groups  
Crystal faces, lattice planes, and Miller indices  
The Bragg equation and the Ewald construction  
Reciprocal space and the reciprocal lattice  
Rupp, ch. 5 | Blessing   |
| 16, 19 Sept. 23, 26 | X-Ray diffraction physics  
X-Ray sources  
Wave nature of X-rays  
X-Ray scattering  
by an electron, an atom, a molecule  
by a lattice row, a lattice plane  
by a crystal – Laue diffraction / Bragg reflection  
The crystal structure factor  
Rupp, ch. 6 | Blessing   |
| 30 Sept, 3 Oct. 7, 10 | Statistics and probability in crystallography  
Descriptive statistics – error propagation  
Probability distributions – joint, marginal, and conditional  
Likelihood and Bayesian inference  
Rupp, ch. 7 | Blessing   |
<p>|                   | Mid-term exam                                                        |            |</p>
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| 14, 17 Oct. 21, (24) | **Diffraction measurements**  
Crystal classes and Laue groups  
Diffraction symmetry – Friedel and Bijvoet pairs  
Space group determination – Systematic extinctions  
Reading the *International Tables*  
Non-crystallographic symmetry | **Rupp, chs. 8, 6 (§6.5), and 5 (§5.2)** |
| 28, 31 Oct. 4, (7)  
(Fri., 7 Nov. BHT meeting) | **Diffraction measurements (cont’d)**  
Instrumentation – robotic sample handling, pixel detectors  
Data collection – local and remote control software  
Data processing – data reduction and error analysis | **Rupp, chs. 8 and 6 (§6.4 and §6.5)** |
| 11, 14 Nov. 18, 21 | **Structure determination – the phase problem**  
The “fundamental theorem” of structural crystallography  
\[ F_{hkl} = |F_{hkl}| e^{i\varphi_{hkl}} \frac{F}{F^{-1}} \rho(x,y,z) \]  
Fourier theory  
The Patterson function  
Patterson maps, Harker sections  
Molecular replacement methods | **Blessing** |
(Fri., 28 Nov. Thanksgiving recess) | **Structure modeling and refinement**  
SIR, MIR, SAD, SIR/SAD, MAD methods  
Stereochemical restraints  
NCS averaging and constraints  
Fourier methods  
Least-squares methods  
Maximum likelihood methods  
Energy minimization methods | **Blessing** |
| 9, 12 Dec. | **Structure refinement and validation**  
Precision indices  
Uncertainty estimates  
Ramachandran plots  
Richardson MolProbity analysis  
Real-space density residual | **Blessing** |
| 16 Dec. | Final exam |
Bibliography of Teaching and Learning Materials

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The following books and Internet sites provide very good teaching and learning materials for biocrystallography. Especially good websites, very well worth the time for extended and repeated visits, are those of Gervais Chapuis, Nicolas Schoeni, and Wes Hardecker (Lausanne); Martin Martínez Ripoll and Félix Hernández Cano (CSIC, Madrid); Gerard Kleywegt (Uppsala); Thomas Proffen (ORNL) and Reinhard Neder (Erlangen); Randy Read (Cambridge); Bernard Rupp (q.e.d. life sciences discoveries, inc.); Michael Sawya and Duilio Casico (UCLA); Bob Sweet (NSLS/BNL); and Joe Wedekind (U of R). The sites were accessible and functioning as of Sunday, 3rd August 2014.


http://escher.epfl.ch/eCrystallography/


http://cen.xraycrystals.org/


http://www.ccp4.ac.uk/html/pxmaths/index.html


http://www.sci.sdsu.edu/TFrey/Bio750/FourierTransforms.html  


Rod Nave (2002). *HyperPhysics and HyperMath*. Department of Physics and Astronomy, Georgia State University. [http://hyperphysics.phy-astr.gsu.edu/hbase/hph.html](http://hyperphysics.phy-astr.gsu.edu/hbase/hph.html) [http://hyperphysics.phy-astr.gsu.edu/hbase/hmat.html#hmath](http://hyperphysics.phy-astr.gsu.edu/hbase/hmat.html#hmath)


