MACROMOLECULAR CRYSTALLOGRAPHY
OCTOBER 14 - 27, 1997

INSTRUCTORS:

Furey, William, Ph.D., V.A. Medical Center, Pittsburgh, PA
Gilliland, Gary, Ph.D.,
McPherson, Alexander, Ph.D., University of California, Riverside, CA
Pflugrath, James, Ph.D., Molecular Structure Corporation, The Woodlands, TX

ASSISTANTS:

Vasquez, Gregory, National Institute of Standards & Technologies, Rockville, MD

Crystallography and X-ray diffraction yield a wealth of structural information unobtainable through other methods. This *intensive* laboratory/computational course focused on the major techniques used to determine the three-dimensional structures of macromolecules. It was designed for scientists with a working knowledge of protein structure and function, but who were new to macromolecular crystallography. Topics that were covered included crystallization (proteins, nucleic acids and complexes), crystal characterization, X-ray sources and optics, crystal freezing, data collection, data reduction, anomalous dispersion, multiple isomorphous replacement, phase determination, solvent flattening, molecular replacement and averaging, electron density interpretation, structure refinement, molecular graphics, molecular dynamics and multi-dimensional NMR. Participants learned through extensive hands-on experiments where they crystallized and determined a protein structure, along with lectures and informal discussions on the theory behind the techniques.

PARTICIPANTS (16):

Agianian, Bogos, B.S., Graduate Student, European Molecular Biology Laboratory, Heidelberg Germany

Bouvier, Marlene, Ph.D., Postdoctoral Fellow, University of Connecticut, Storrs, Connecticut

Downing, A. Kristina, Ph.D., Postdoctoral Fellow, University of Oxford, Oxford, United Kingdom

Eklof- Spink, Katy, B.A., Graduate Student, Stanford University, Stanford, California

Gaiser, Olaf, M.S., Graduate Student, Max Delbruck Center, Berlin, Germany

Gampe, Robert, M.S., Staff Scientist, Glaxo Wellcome, Research Triangle Park, North Carolina

Kappler, John, Ph.D., Investigator, Howard Hughes Medical Institute, Denver, Colorado

Li, Jia, B.S., Graduate Student, University of Virginia, Charlottesville, Virginia

Locher, Kaspar, M.S., Graduate Student, University of Basel, Basel, Switzerland

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McGrath, William, Ph.D., Postdoctoral Fellow, Brookhaven National Lab., Upton, New York

Mellman, David, B.S., Graduate Student, Vanderbilt University, Nashville, Tennessee

Nguyen, Duc, B.A., Graduate Student, Johns Hopkins University, Baltimore, Maryland

Nieves, Rene, B.S., Graduate Student, University of Puerto Rico, San Juan, Puerto Rico

Sertchook, Rotem, Ph.D., Graduate Student, Hebrew University, Jerusalem, Israel

Thoma, Nicolas, B.A., Graduate Student, University of Cambridge, Cambridge, United Kingdom

Wiencek, John, Ph.D., Associate Professor, University of Iowa, Iowa City, Iowa

SUMMARY: 6 Females; 10 Males

SEMINARS:

Brunger, Axel, Yale University, New Haven, Connecticut
Maximum Advances in Refinement: Torsion-Angle, Simulated-Annealing, Cross Validation,
Maximum Likelihood.

Clore, Marius, National Institutes of Health, Bethesda, Maryland
NMR Structure Determination of Proteins and Protein Complexes Beyond 20 kda

Davies, David, National Institute of Health, Bethesda, Maryland
Structure Determinations of Two Enzymes That Utilize Cofactors

Fitzgerald, Paula, Merck Research Laboratories, Rahway, New Jersey
Crystallographic Studies in Structure-Based Drug Design

Fleming, Pat, Yale University, New Haven, Connecticut
Xenon: Binding to proteins and use as a heavy atom derivative

Gilliland, Gary, National Institute of Standards & Technology, Gaithersburg, Maryland
Crystal structure of Recombinant Tetradeca-(3-Fluorotyrosyl)- Glutathione S-Transferase

Hendrickson, Wayne, Columbia University, New York, New York
Structural Biology of Immune Signaling Through CD4 and Lck

Joshua-Tor, Leemor, Cold Spring Harbor Laboratory, Cold Spring Harbor, New York
The C-terminus of Gal6/Bleomycin Hydrolase Acts as a Molecular Ruler for Proteolysis

Sussman, Joel, Brookhaven Nat'l Lab, Upton, NY/Weizmann Inst.of Science, Rehovot, Israel
Acetylcholinesterase in 3D: New Mysteries Revealed from the Crystal Structure

Sweet, Robert, Brookhaven National Laboratory, Upton, New York
Laue Diffraction and Other Metholds as a Tool for Study of Dynamic Effects in Protein
Crystals

Tronrud, Dale, University of Oregon, Eugene, Oregon
Strange Density

Xu, Ruiming, Cold Spring Harbor Laboratory, Cold Spring Harbor, New York
Crystal Structuare of the RNA-Binding Domain of Human hnRNP A1