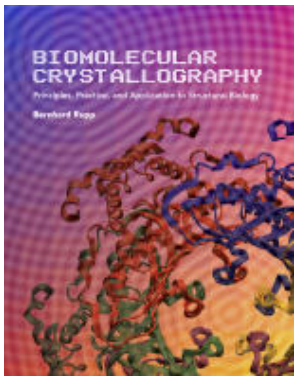
ONE-DAY
PRE-CONFERENCE COURSE
ON BIOMOLECULAR CRYSTALLOGRAPHY

Sponsored by the Brazilian Crystallographic Association - *ABCr*

Presented by: Dr. Bernhard Rupp, q.e.d. life science discoveries
Dr. Katherine Kantardjieff, California State University, Pomona

COURSE DESCRIPTION



The course is based on selected sections of the seminal textbook Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology. A twenty percent publisher's discount voucher is provided to workshop participants.

The course includes actual structure determination using multiple anomalous dispersion methods and molecular replacement, and selected stages of model building and refinement. Validation, analysis and interpretation of structures are treated with special emphasis on their use in in-silico ligand docking and virtual ligand screening.

Topics and Course Organization

9:00-10:30	**Introduction** Overview of Molecular Structure and Function The Role of Molecular Structure in Drug Discovery Basic Principles of Crystallography
	Q&A session 1 (15 min)
10:30-10:45	Coffee Break
10:45-12:00	**Protein Crystallization** Proteins for Crystallization Crystallization Techniques Crystallization Screening and Design Strategies Evaluation and Statistical Predictions Cryoprotection Crystal Harvesting
	Q&A session 2 (15 min)
12:00-13:00	Lunch
13:00-14:30	**From Data to Structure** Data Collection Principles Phasing Principles Example: Anomalous S-SAD phasing Phase Extension Model Building; Model Refinement Example: Molecular Replacement and Automated Rebuilding
	Q&A session 3 (15 min)
14:30-14:45	Coffee Break
14:45-16:00	**From Structure to Knowledge** The Nature of Crystallographic Models Evidence-based Validation of Protein Target Structures Pitfalls in Drug target and Ligand Structrues The Finer Art of Structure Refinement Fragment Analysis
16:00 - 17:00	***In silico* Ligand Docking** Methods for identifying ligand binding pockets Crystal and model structure preparation for docking Small-molecule docking methods Methods for considering receptor flexibility in ligand docking Combinatorial libraries Virtual ligand screening
17:00-17:30	Review and Wrap-up Discussions