



Primer on Protein X-ray Structure Determination

Protein crystallography is both an art and a science. Investigators planning their initial foray into this area should be aware of the obligatory steps in the process from isolating a protein to obtaining a structure. The KU **Protein Structure Laboratory** is here to help with any or all of these tasks. See www.medchem.ku.edu/COBRE/CoreLabs.htm.

Consultation and advice is also readily available at no charge. Contact Dr. Weijun Huang, Director, at 785-864-3772.

Necessary Steps	Personnel Involved
Isolate, purify and concentrate protein of interest for crystallization.	Totally up to personnel in PI's lab; PSL director is generally not involved in this step, although he can provide advice and guidance. The COBRE Core C (Protein Purification Group) is designed to help scale up expression and purification steps (www.medchem.ku.edu/COBRE)
Get crystals to grow (generally done in the PSL facilities). Isolate crystals and move them to harvesting buffer. Mount crystals and treat with cryoprotectant. Determine if crystals diffract well. Collect a complete data set from one or more good crystals.	Any or all of these tasks can be performed by PSL Staff, or by trained personnel from PI's lab. PSL Director of Staff will provide training to personnel from PI's lab if desired.
Solving the structure of the protein by molecular replacement when related structures are already known. Refine structure and prepare graphics and data files for deposition in the PDB.	One of the main functions of the PSL Director will be to perform this sophisticated service requiring considerable time, effort and expertise, and to help seriously interested students learn how to do this. Fees will vary according to complexity of the problem and the amount of effort required. Investigators should consider appointing the PSL director as a co-investigator on their grants.
For <i>de novo</i> structure determination, prepare at least two heavy-atom derivatives of the crystals, check their quality using local rotating anode machine, then go to Synchrotron lab and collect data.	PSL Director will advise personnel from PI's lab on preparation and initial evaluation of derivatives, and on making contact with synchrotron facility. If desired, the PSL Director may travel to the synchrotron for data collection.