Crystallography & Computational Biology Shared Resource

Todd Lowther, Biochemistry
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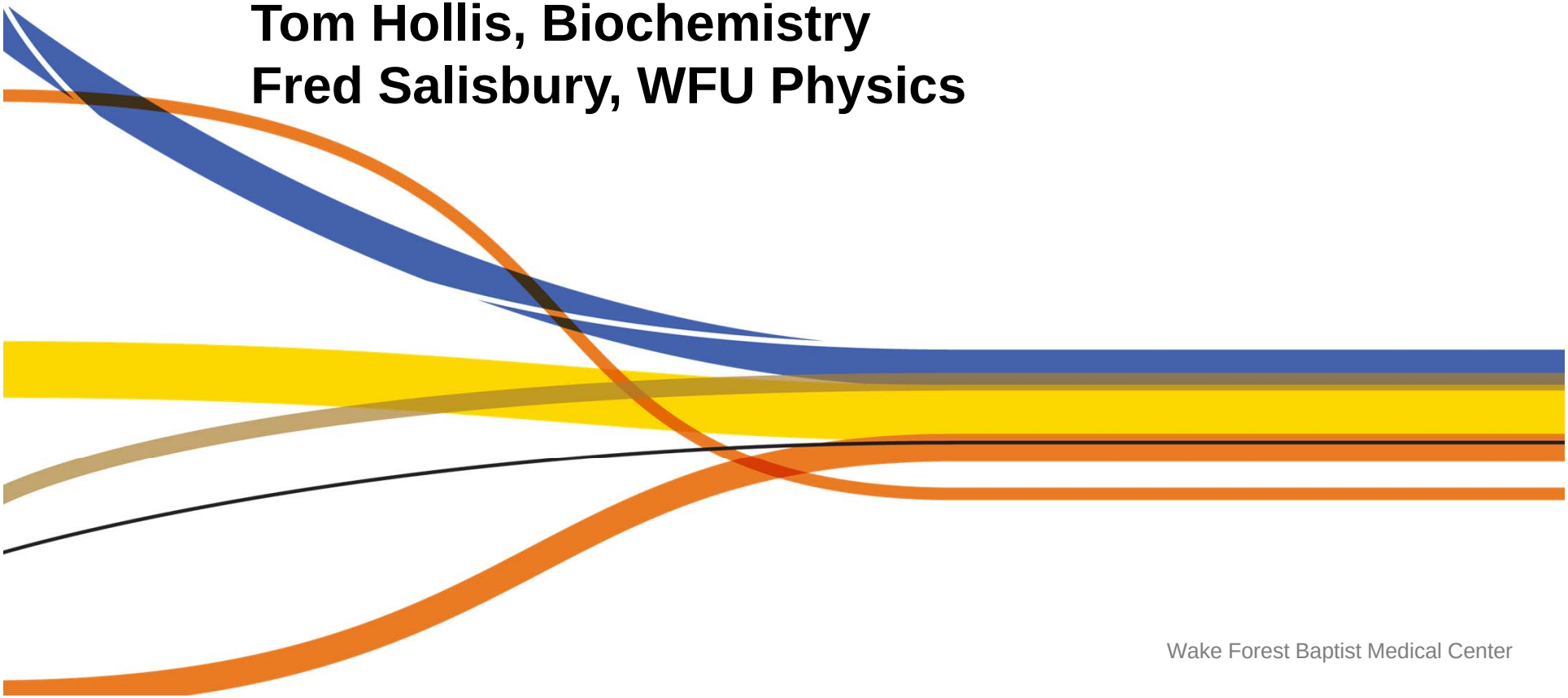
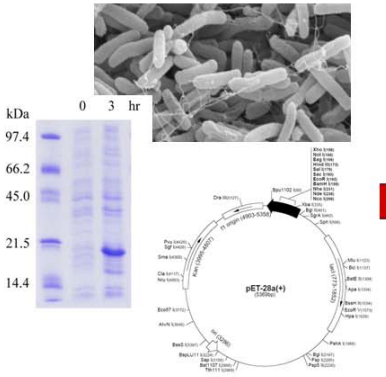


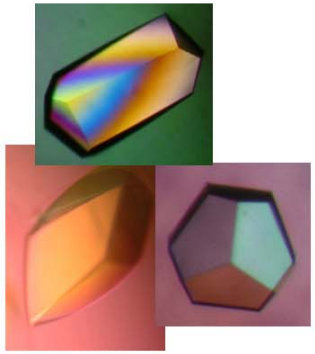
Scientific Value and Focus of Core

- Experimental and Computational Approaches to Understand Structure-Function– A Collaborative Model
  - Three-dimensional structure of proteins, DNA/RNA, their complexes, and ligand complexes, including cofactors, substrates, drug candidates
  - Cutting-edge modeling, simulation and docking methods for understanding ligand interactions, protein dynamics, and chemical reactivity
- Foci: Support ongoing and developmental projects- preliminary data
  - Consulting on all aspects of protein expression, purification, feasibility of structure determination, tractability and selection of computational approach
  - Identification of crystallization conditions and possible other existing structures; determination of the molecular structure and larger computational studies through collaboration

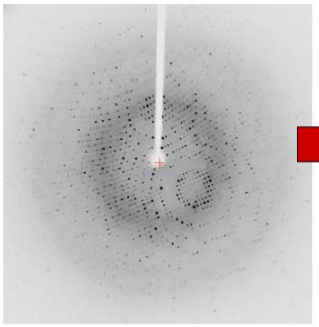
Services Available



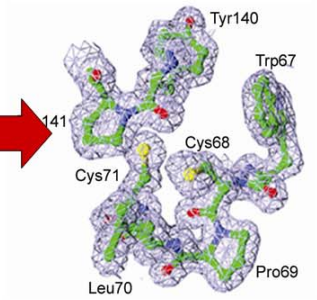
Recombinant Protein Expression and Purification



Crystallization Trials and Optimization



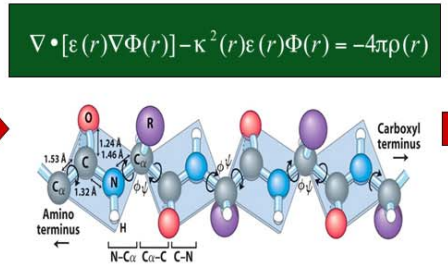
Collection of Diffraction Data



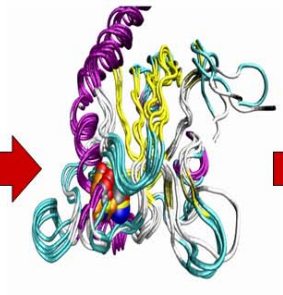
Electron Density Map Generation and Model Building

- Classical Molecular dynamics
- Quantum Mechanical calculations
- Virtual Screening
- Electrostatic Models

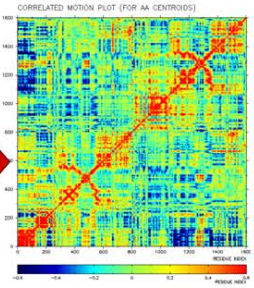
Consult and Determine Type and Scope of Calculations



Generate Appropriate Models



Trial Simulations



Full Simulation

Primary Shared Equipment

- X-ray Diffraction Facility
  - Rigaku Micromax 007 X-ray source with dual VariMax-HF Confocal Optic Systems coupled to Saturn92 CCD and RAXIS4+ detectors
  - Cryogenic data collection.
- Crystallization Facility
  - Gryphon 96 well crystallization robot (Art Robins Instruments), microscopes and crystallization cabinets.
- Computational facility
  - Several multi-processor graphics workstations with hardware stereo for model building and refinement.
  - Linux cluster with the appropriate software for computational calculations such as molecular dynamics, *in silico* drug docking and homology modeling
  - Intensive calculations and molecular dynamics simulations are also made possible by access to the DEAC computing cluster and GPU workstations.

Contact Information

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