**Center for Structural Biology Shared Resources**

**NMR**: Five Bruker spectrometers are housed in the Vanderbilt Biomolecular NMR Center; a dedicated NMR building located at the center of campus. Each of the Avance II 500, two 600, 800 and 900 MHz instruments are fully equipped with hardware for all modern multi-nuclear experiments including the capability for multi-channel pulsing with deuterium decoupling. Bruker cryoprobes are installed on all instruments. The utilization and support of these facilities is shared by the NMR research groups of Walter J. Chazin, Stephen Fesik, Chuck Sanders, Michael P. Stone, and any minor users. A total upgrade of all consoles and cryoprobes has just been completed, funded from shared instrumentation grants from NIH and NSF in combination with a substantial institutional investment.

**Crystallization**: A high-throughput protein crystallization facility is available, under the direction of Professor Tina Iverson. The facility has four integrated components: 1. a Hamilton Star-Let liquid handler; 2. a Mosquito nano-liter drop setter; 3. a Xantus Cubic Lipid handling robot; 4. a Formulatrix imager with UV fluorescence detector. These robots are located on the 4th floor of the Robinson Research Building in a 400 ft2 temperature-controlled room, currently maintained at 20 °C. Bar-coding coordinates the information transfer between robotic instruments, which be operated remotely through the network. The automated crystallization facility has improved the efficiency of making crystallization screens, increased the speed of initial crystallization trials, decreased the amount of sample need for crystallization, decreased the amount of time required to analyze the crystals, and decreased the rate of false positives. Training on the instruments maintained within the robotic facility is through one on one consultations.

**X-ray Crystallography**: A Bruker Microstar high-brilliance rotating anode X-ray generator is available, equipped with Montel multilayer confocal optics and two Proteum PT-135 CCD area detectors with kappa goniometers. Both detectors include low temperature devices. The facility maintains all software necessary for data reduction, phasing, model refinement and structure analysis. The cost of operations is supported by a flexible system of user fees. In addition, Vanderbilt owns a 1/2 share of the Life Sciences Collaborative Access Team (LS-CAT) beamline, which provides our institution with over 40 days of synchrotron experiments per year.

**Biophysical Instrumentation:** The CSB instrumentation core facility maintains a variety of instruments for studying the conformation and stability of macromolecules and for measuring the affinity and thermodynamics of biomolecular interactions. The instruments include a Jasco J-810 circular dichroism spectropolarimeter, a Horiba Jobin Yvon Fluoromax-3 fluorometer, a MicroCal VP-DSC differential scanning calorimeter and a MicroCal VP-ITC isothermal titration calorimeter.  The facility is supported by user fees and provides instrument training and access as well as assistance with data collection, analysis and troubleshooting.

**Small Angle X-ray and Neutron Scattering (SAXS, SANS):** SAXS experiments are performed using the SIBYLS beamline (<http://www.sibyls.org/>) of the Advanced Light Source at Lawrence Berkeley National Laboratory. Data collection is performed either by our group members or by staff at the beamline. Our group processes and analyzes all of the data, with assistance as needed from Drs. Susan Tsutakawa and Michal Hammel. SANS experiments are performed using the Bio-SANS instrument of the CG-3 beamline at the High Flux Isotope Reactor (HIFR) at Oak Ridge National Laboratory. Data collection is performed by our group members with the support and assistance of the staff of the Center for Structural Molecular Biology. We collaborate with Dr. William T. Heller for acquisition, processing and secondary analysis of SANS data.

**Computational Structural Biology**: High performance and throughput computing are handled by three primary systems. The Advanced Computing Center for Research and Education (ACCRE) maintains a 3000 processor-core compute cluster with ~2GB of RAM per processor. The CSB faculty have continuous access to 135 CPUs at ACCRE. The facility is operated by ACCRE staff and is supported through user fees. The CSB maintains additional high performance computing resources: 1) An SGI Altix system with 32 Intel Itanium2 CPUs and 64GB of RAM; and 2) A 31-node cluster with 912GB of RAM and 272 Intel Nehalem processor-cores interconnected with a 40 Gbit Infiniband fabric. These systems are all interconnected to a 25TB high-performance gigabit Ethernet network-attached storage system, which facilitates data sharing between all the above computing resources and local workstations. Desktop workstations and CSB computational facilities are maintained by the CSB Computing Core, which is responsible for supporting all local computing resources. This group keeps the central computers and network updated, trouble-shoots, coordinates for outside repair and service contracts, does regular data backups and maintains shared software and databases, remote access into the network, color and black-and-white laser printers, and a data management system for short-term and archival file storage. The CSB Computing Core is supported through a system of user fees. Payments are also made via an annual laboratory fee to maintain a membership with the SBGrid consortium. SBGrid provides access to a comprehensive suite of up-to-date and optimized structural biology software packages, which are maintained on all local systems by staff in the CSB Computing Core.