The GM/CA@APS Structural Biology Facility Upgrade Plan and APS-Upgrade

Dr. Robert F Fischetti[1], Dr. Nagarajan Venugopalan[1], Dr. Michael Becker[1], Stephen Corcoran[1], Dale Ferguson[1], Mark Hilgart[1], Dr. David J Kissick[1], Dr. Oleg Makarov[1], Dr. Craig M Ogata[1], Dr. Sergey Stepanov[1], Dr. Qingping Xu[1], Dr. Shenglan Xu[1], Professor Janet L Smith[1]

[1]*Argonne National Laboratory/APS*

rfischetti@anl.gov

The National Institute of General Medical Sciences and National Cancer Institute Structural Biology Facility at the Advanced Photon Source (GM/CA@APS) operates a national user facility for structural biology with synchrotron beamlines specializing in intense, tunable micro-beams for crystallography. The facility includes canted-undulator beamlines, 23ID-B, and 23ID-D, that provide stable, intense X-ray beams of user-selectable size down to 5- micron, an intuitive user interface for experiment control, and an automated data processing pipeline. The beamlines have high-capacity automounters and PAD detectors (Dectris), allowing rapid data collection. GM/CA users have been very productive, resulting in almost 2000 publications and over 3350 protein data bank deposits. Our micro- crystallography developments supported the research of Brian Kobilka, who was awarded the 2012 Nobel Prize in Chemistry for studies of G-protein-coupled receptors (GPCRs).

We plan to upgrade the beamlines during the APS dark period to exploit the high brightness of the APS-U. New state-of-the-art focusing optics and endstation instrumentations will be installed. The focusing optics will be replaced with EEM-polished mirrors (JTEC) in mechanical benders (AXILON) and compound refractive lenses (CRLs) (RXOPTICS, AXILON). The mirrors could focus the full beam down to 5 microns with an intensity of over 5×10^{13} photons/sec, and with the CRL transfocator, the beam could be focused to sub-micron dimensions with an intensity greater than 1×10^{13} photons/sec at 12 keV. The new optics will provide extremely intense, clean, stable, and rapidly adjustable beam sizes between 1-30 microns. The monochromator on 23-ID-D will be modified to increase thermal and mechanical stability and raise the maximum energy to 35 keV to exploit the high intensity of the APS-U at high energy. Each endstation will be replaced, and one high-stability table will support the CRL translocator and sample environment. The new goniometer will allow data collection on crystals as small as one micron and provide rapid scanning of random or periodic fixed target samples. A Dectris Eiger2 16M CdTe detector will allow high-speed, high-efficiency X-ray detection on 23-ID-D. The new pyBluIce GUI and beamline control software will enable sophisticated data collection routines such as 3D- rastering and helical data collection, fully automated (unattended) data collection, and routine serial crystallography data collection from fixed target and injector-based sample delivery systems. Here we will present the new designs and game-changing opportunities for structural biology research enabled by these small, ultra-intense, high-energy beams.

GM/CA@APS has been funded by the National Cancer Institute (ACB-12002) and the National Institute of General Medical Sciences (AGM-12006, P30GM138396). The Eiger 16M detector was funded by an NIH-Office of Research Infrastructure Programs, High-End Instrumentation Grant (1S10OD012289-01A1).This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.