

even from the outside of beamlines over HTTPS protocol.

Keywords: automated data collection, robots, macromolecular synchrotron X-ray crystallography

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### A proposed suite of macromolecular crystallography facilities for NSLS-II

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A new, highly-optimized 3rd-generation synchrotron radiation (SR) source, the National Synchrotron Light Source -II (NSLS-II), is being planned as a replacement of the existing 2nd-generation SR source NSLS at Brookhaven National Laboratory. When operational, NSLS-II will deliver unprecedented brightness in the soft and hard x-ray spectral regions, e.g. at 8 keV about 10 times that of the brightest SR sources now available. NSLS hosts a strong macromolecular crystallography (MX) program, nearly 40% of its user community. At NSLS-II, MX is expected to be closely associated with other life sciences programs including small angle x-ray scattering, x-ray absorption spectroscopy, x-ray footprinting, and nanoscale imaging. We are preparing plans for a set of MX beamlines that would view canted, tunable undulator radiation sources in multiple straight sections of the storage ring, which would work independently. The experimental apparatus would include diffractometers to handle crystals of microns dimension or smaller, fast-framing active-pixel detectors, automated sample exchange and cryogenic apparatus, VUV/visible spectroscopy, and fluidic-based sample handling systems. These bright sources will extend MX into unexplored realms of sample size, perfection, and state of complexity and environment. Research and development in all of these areas are proposed, including methods for overcoming the effects of radiation damage, in order to exploit the properties of these sources. In addition to these undulator-based beamlines, it is also proposed to implement a set of MX beamlines viewing three-pole wiggler radiation sources, somewhat brighter than current NSLS bending magnet radiation sources. This work is supported by the US Dept. of Energy and the US National Institutes of Health.

Keywords: synchrotron radiation crystallography, synchrotron radiation optics, synchrotron radiation sources

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### A new macromolecular crystallography beamline for softer X-ray at the Photon Factory

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The use of softer X-ray for phase determination in macromolecular crystallography has gained quite some popularity, owing to the interest in utilizing weak anomalous signals provided by light atoms such as sulfur and phosphorus present in native protein and nucleic acid molecules. The method is quite useful especially for the range of macromolecules which are difficult to prepare heavy atom derivatives. The Photon Factory has started to develop a new macromolecular crystallography beamline for softer X-ray at BL-1A of the 2.5 GeV ring, funded by the national project 'Targeted Proteins Research Program'. The beamline is designed to deliver an intense softer X-ray beam at around 4 keV using the first harmonics of a short gap undulator to enhance the weak anomalous signal from light atoms. The optics and the diffractometer are optimized for the softer X-ray beam. The expected beam intensity at around 4 keV is more than  $10^{11}$  photons/sec on the area of 10 square microns at the sample position. The beamline can also cover the energy range of 12-13 keV with the 3rd harmonics, which enables Se- or Hg-MAD data collection from very small crystals with the intense 10 micron beam. The beamline development is particularly dedicated to the crystallographic study of integral membrane proteins and macromolecular complexes, systems of enormous biological significance which are currently difficult to be measured due to crystallization problems. The construction of the beamline is scheduled in the summer of 2009, followed by six months of commissioning. The beamline will be opened to the members of the national project in 2010.

Keywords: biological macromolecular crystallography, protein crystallography with synchrotron, synchrotron X-ray instrumentation

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### AR-NE3A, a new pharmaceutical beamline for macromolecular crystallography at the Photon Factory

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In recent years, advancements in high-throughput techniques for macromolecular crystallography have heightened the importance of structure-based drug design (SBDD) and demand for synchrotron use by pharmaceutical researchers has increased. In order to meet this demand, we are constructing a new high-throughput macromolecular crystallography beamline AR-NE3A, dedicated to SBDD. This is funded in partnership with Astellas Pharma Inc. The light source is an in-vacuum undulator in the PF-AR 6.5GeV ring, providing a high flux X-ray beam. The optics consist of three main components, a collimating mirror, double crystal monochromator with liquid nitrogen cooling system, and a toroidal double-focusing mirror. Ray-tracing simulations suggest that new AR-NE3A affords higher X-ray beam flux at the sample position than existing high-throughput beamlines at the Photon Factory, AR-NW12A and BL-5A. In the experimental hutch, there will be a high precision diffractometer, a fast-readout and high-gain CCD detector and a sample exchange robot which can handle more than two hundred cryo-cooled samples in a Dewar. In order to realize high-throughput data collection required for pharmaceutical researches, we are developing a fully-

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