



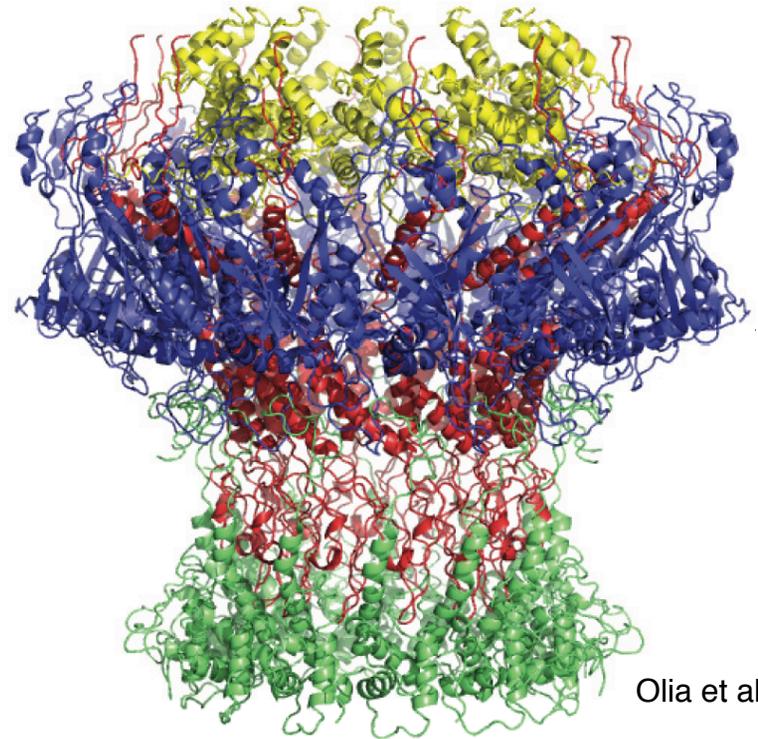
NIGMS East Coast Structural Biology Research Facility

<http://protein.nsls.bnl.gov>

Science Advisory Committee meeting

10 February 2012

Vivian Stojanoff
for the X6A team



Olia et al



Our Mission

Provide first class resources to the biological- biochemical-, and biophysics- communities to explore all aspects of structural biology. It is the goal of this facility to provide assistance to expert and non-expert crystallographers.

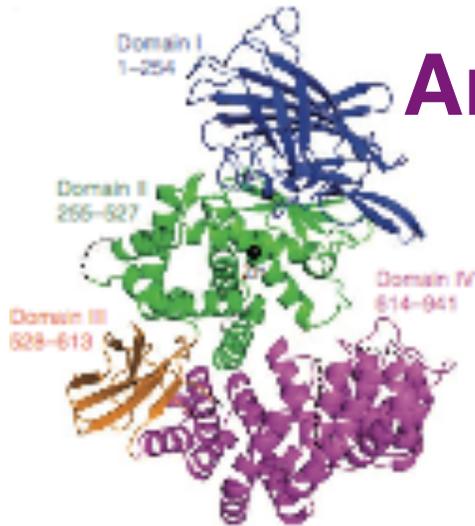
This goal includes:

- Beam line access to a structural biology community at large.
- Fast access to beam time for the user community.
- Crystal screening and high-throughput data collection.
- Assistance and training for academic and professional users.

NIGMS metrics review requirement

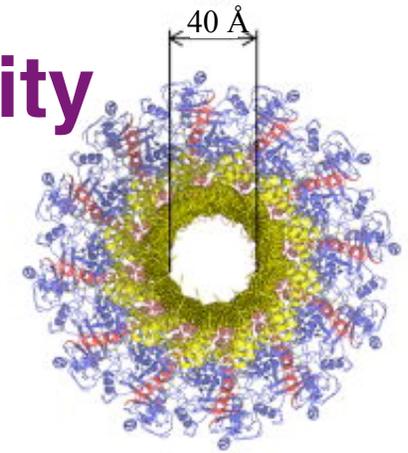
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- Scientific Productivity
 - user number
 - quality of science
 - comparison with similar beam lines
 - User satisfaction
 - Beamline performance
 - Technical and infrastructure development
 - quality
 - importance
 - relevance to user program
 - Resource allocation
 - Interaction with other programs at the NSLS
 - Future plan

An engaged user community



L Stern Lab, UMASS
Structural Basis For Antigenic Peptide
Precursor Processing by ERAP1,
Nat. Struct. Mol. Biol.

Davies's team Queen's
University
Anchored Clathrate Waters
Bind Antifreeze Proteins to Ice
PNAS



Cingolani's Lab, Thomas Jefferson
3D structure of a viral genome-
delivery portal vertex
Nat. Struct. Biol.



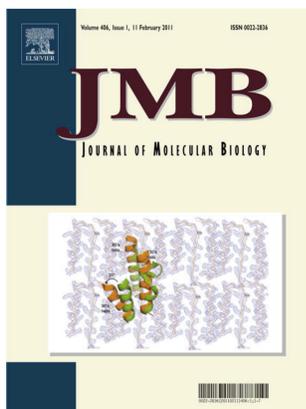
Hardy's Group, UMASS
Substrate-Induced Conformational Changes Occur in Caspase-6
J. Mol. Biol.



Marmorstein's team, Wistar
MYST protein acetyltransferase activity
requires active site lysine autoacetylation
EMBO J.

A vibrant user community

53 Publications in 2011 with 9 in premier journals.



<IMPACT>= 5.2



Imperiali	Nat.Chem.Biol. 7: 81-91
Cingolani	Nat. Struct. Mol. Biol. 18:597-603
Stern ¹	Nat.Struct. Mol. Biol. 18:604-13
Cingolani	Nat. Struct. Mol. Biol. 18:701-7
Skordalakes	Curr. Opin. Struct. Biol. 21:92-100
Davies ¹	Proc.Natl.Acad.Sci.USA 108: 7363-7367
Berg	Proc.Natl.Acad.Sci.USA 108: 10121-10126
Nimigean	Proc.Natl.Acad.Sci.USA 108: 5272-5277
Marmorstein	EMBO J. 31:58-70
Hardy ¹	J Mol Biol. 406: 75-91
Stewart ²	ACS Catal. , 1,989-993

¹The X6A Workbench ²ProteinXpress

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Outline

- Background
- Resources
- Staffing
- User Program
- Productivity
- Education and outreach
- Synergy
- Summary



Background

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The 1999 NIGMS Initiative at the NSLS

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Bending magnet source recommended by NIGMS

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- 2000 procurement slits, mirror, detector
- 2001 construction and installation, monochromator NSLS design
- 2001, two FTE's hired for operation support
- X6A program includes support for four FTE's
- 2002 operation start
- 2003 \$1,200K supplement for detector upgrade
- 2008 End-station upgrade (November, 2008)
- 2009 End-station commissioned (March 2009)

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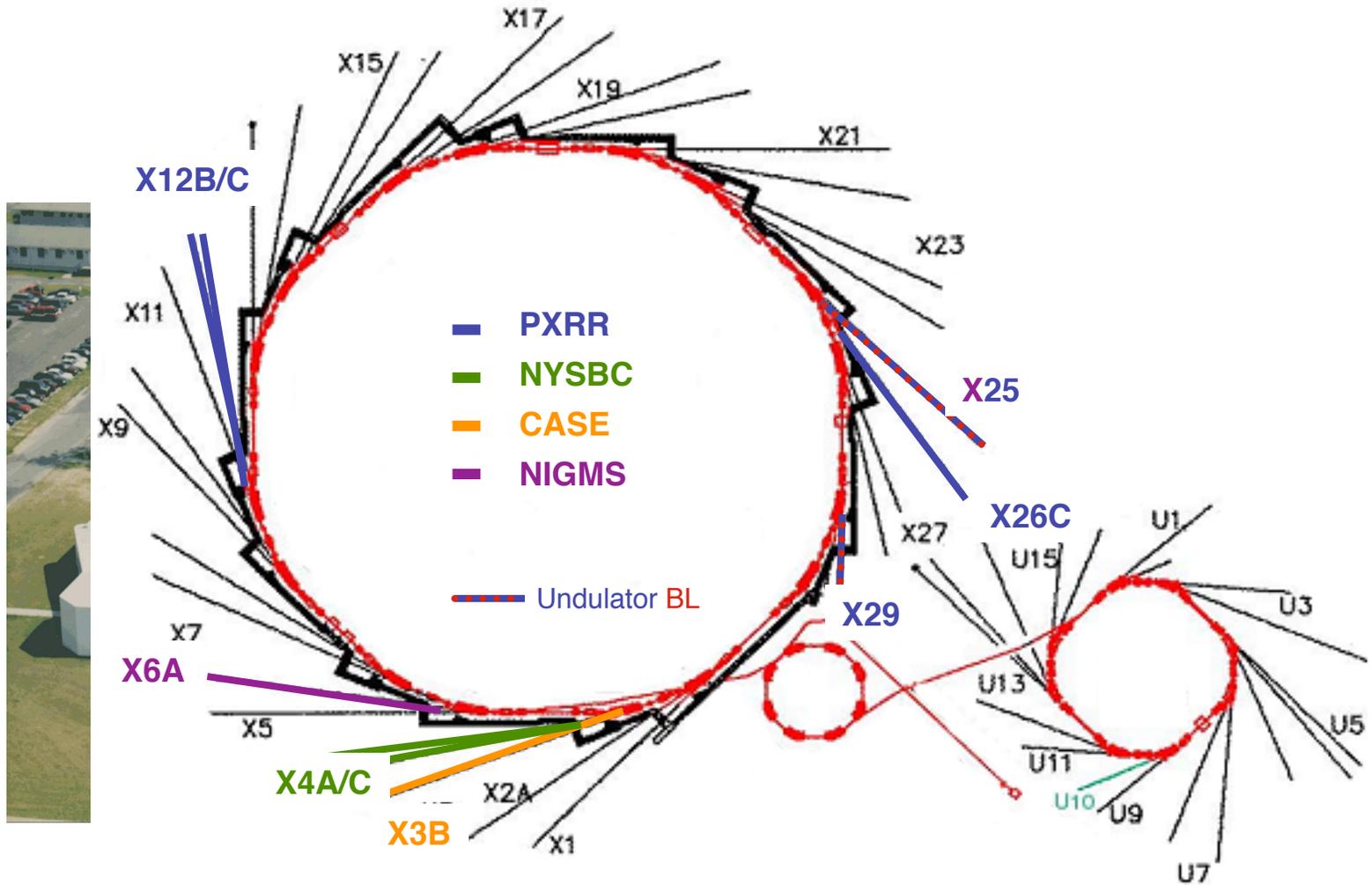
MX at the NSLS

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Resources

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The X6A Experimental Environment

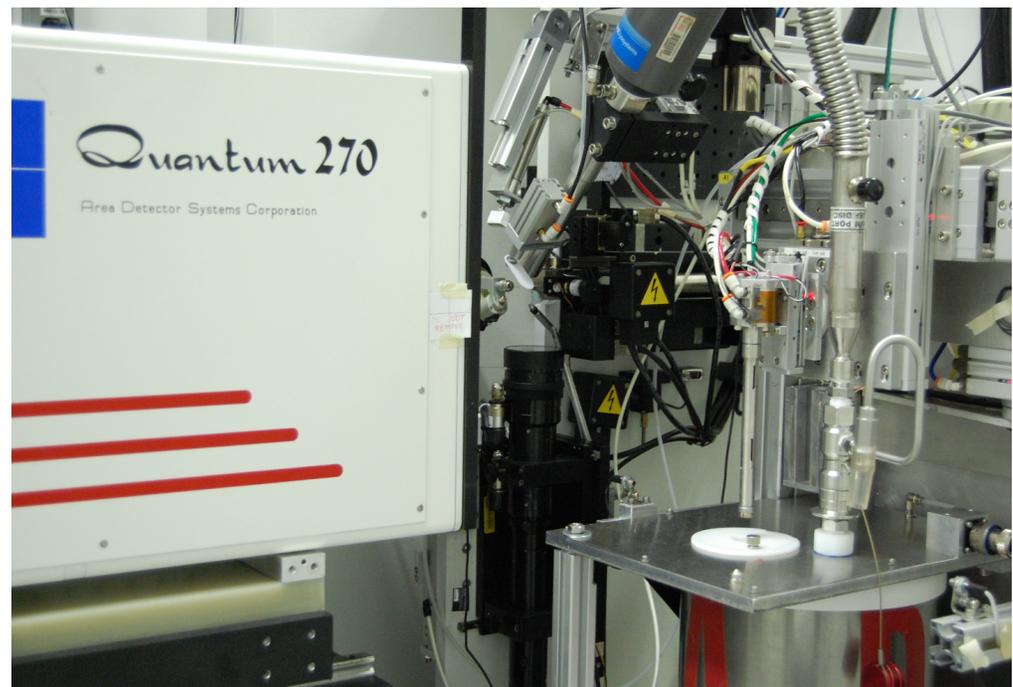
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- *Standard optical design: current operation mode 7 to 16 keV;*
- *Single axis diffractometer (Crystal Logic);*
- *ADSC Q270 CCD detector*
- *ALS automated sample changer;*
- *Oxford cryosystem sample cooling system*
- *Control and Processing workstations with parallel CPUs*
- *RAID based storage system*

Small upgrades were carried out to improve efficiency and friendliness of the data collection process.



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The X6A Web and Data Base Environment

The screenshot shows the X6A web portal. At the top, a purple banner reads "Welcome To X6A Beamline". Below this is a "Main Page" section featuring a 3D molecular model of a protein structure. The left sidebar contains several navigation menus: "X6A Home" (News, PDB deposits, X6A Publications, Collaboration Policy, X6A People), "User Corner" (User Login, X6A Schedule, Safety Approval Form, Dry Shipper Shipments, Smooth Arrival, Smooth Departure), "Beam Line Facilities" (Optics, End Station, Automounter, Crystallization Lab), "User Guide" (Use Lab Facilities, Preparation, Run Experiment: Manual, Run Experiment: Automounter, Data Analysis, Data Back Up, FAQ), and "X6A Team" (X6A SAC Login, SAC Members Only). The main content area has three columns: "MISSION" (describing the NIGMS East Coast structural biology facility), "ACKNOWLEDGEMENTS" (listing funding from NIGMS and Brookhaven National Laboratory), and "News and Events" (announcing the next beamtime on February 16, 2007, and a new website launch). The footer includes logos for NIGMS, NSLS, and Brookhaven National Laboratory, along with a search bar.

Media Wiki

- Improve communication

User and Experimental Control Databases

- Communication between databases

User Database

- Improve User Access
- Improve Beam Line Management
- Real time Statistical Analysis of beam time usage



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Staff

Organizational Chart



Qun Shen *1
Photon Science Division

Scientific Advisory
Committee

Mario Amzel
John Hopkins
chair

Hao Wu
Weil Medical

Craig Ogata
GM/CA CAT

Vivian Stojanoff
Project Director

Jean Jakoncic
Associate Scientist

Kun Qian
IT Associate

Edwin Lazo
Science Associate

Lisa Miller *1
Photon Science Associate
Life Science Div Head

Marc Allaire *2
Associate Scientist

Scientific, Technical,
ES&H, Administrative *1
Support as required

*1 PS Directorate scientific staff

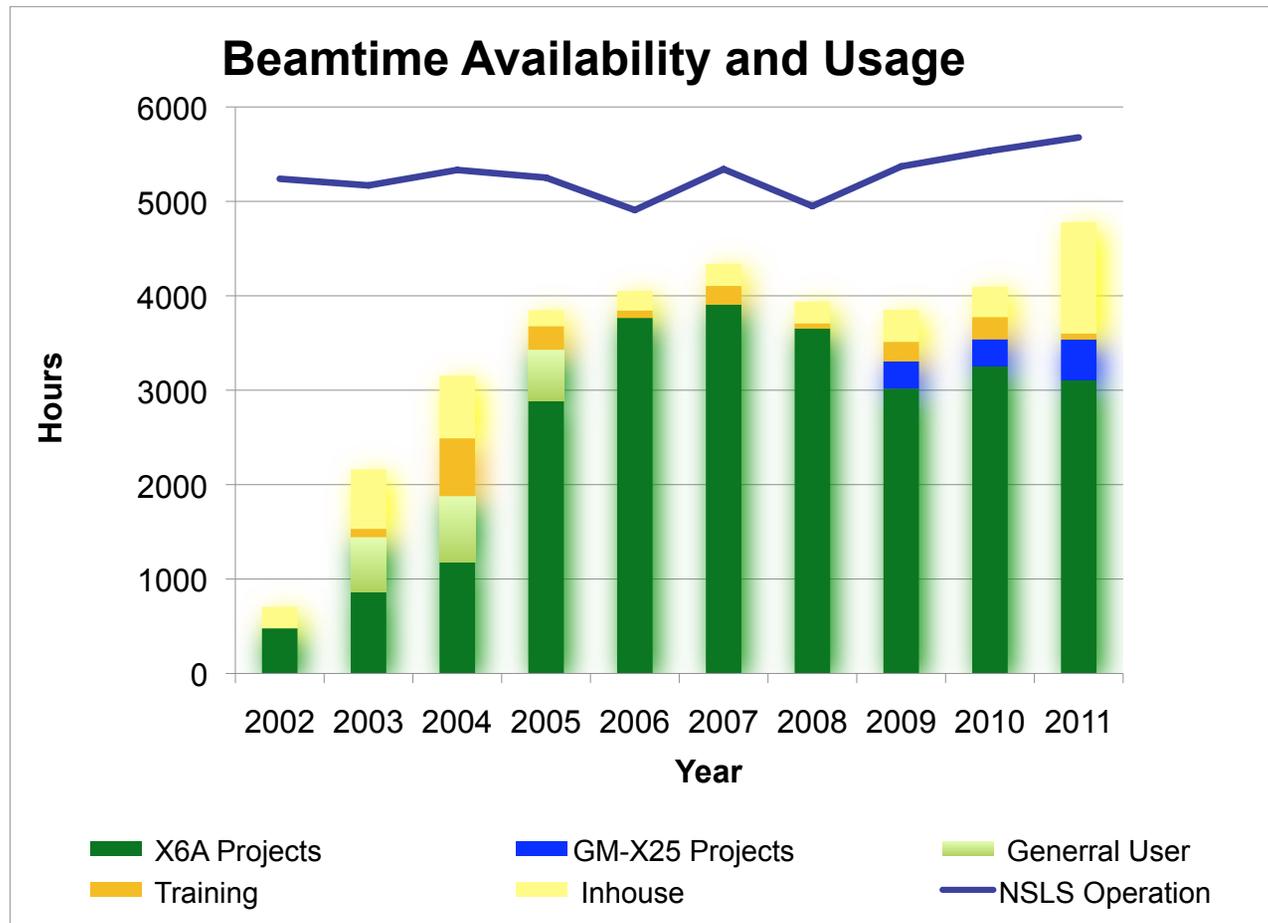
Science Advisory Committee Meeting

*2 1/4 FTE



Beam time usage

Available beam time



Approximately 75% of the NSLS user available beam time at the Facility was dedicated towards external research and collaborations.

Beam time Utilization

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X6A Program 2011*

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- X6A user projects 55%
- Available 12%
- X6A beam line 33%
 - ✓ X6A commissioning 11%
 - ✧ Instrumentation upgrade
 - ✧ Instrumentation failure (alignment, automounter)
 - ✓ X6A inhouse projects 21%
 - ✧ Scientific staff research and external collaborations
 - ✧ Student training and mentoring

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*percentages are calculated relative to NSLS total available time for operation

User beam time usage 2011

Total # images	469152
Total # images screened	28885
Total # data sets*	1126
Total # crystals screened and collected	7634
Automated Sample Changer	
Total # images screened	6157
Total # data sets*	98
Total # crystals screened and collected	2435
usage	34d 16h

*data set 40 or more images

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User Program

Self scheduling

The self scheduling calendar continues to be a preferred feature amongst users. Since February 2011 approximately 1/2 of the GM-25 scheduled user time was requested through this feature.

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Welcome To X6A Beamline

Schedule -> X6A Schedule

My Account

- Edit User Profile
- Change Password
- Build Collaborator List
- LOG OUT
- Account Status

Manage Projects

- Create new proposals
- Create new proposals based on existing projects
- Edit proposals
- View projects
- Assign project members
- Find review results

X6A Schedule

- View X6A Schedules
- Create X6A schedules
- Edit X6A schedules
- Adjust Schedule Projects
- Cancel X6A schedules

GM-X25 Beamtime

- GM-X25 Schedule
- GM-X25 Beamtime request
- Edit GM-X25 Beamtime request
- Cancel GM-X25 Beamtime request

View GM-X25 Schedule

December 2011

Sun	Mon	Tue	Wed	Thu	Fri	Sat
			1 NSLS Commissioning [From: 00:00:00 Till: 11:59:59]	2 NSLS Studies [From: 12:00:00 Till: 23:59:59]	3 Available [From: 00:00:00 Till: 18:59:59]	x6a180; x6a209 [From: 18:59:59 Till: 18:59:59]
4 USER Available	5 USER Available [From: 18:59:59 Till: 18:59:59]	6 x6a274 [From: 06:59:59 Till: 06:59:59]	7 x6a85 [From: 06:59:59 Till: 06:59:59]	8 x6a85 [From: 06:59:59 Till: 06:59:59]	9 USER Available [From: 07:00:00 Till: 13:59:59]	10 USER Available
11 USER Available	12 USER Available [From: 11:59:59 Till: 11:59:59]	13 NSLS Studies [From: 19:59:59 Till: 19:59:59]	14 Available [From: 00:00:00 Till: 00:00:00]	15 Available	16 Available	17 Available

X6A Schedule Form

Fields marked with * are required.

Schedule available Beam Time

Projects : INH2

Begin Date : 1 January 2009

Shift Begin Time : 0:00:00

End Date : 1 January 2009

Shift END Time : 0:00:00

Visit X6A Beamline : YES NO

Schedule Reset

LEGEND

- Available
- Maintenance
- InHouse
- Projects
- Studies
- Conditioning
- Training
- Commissioning
- Template
- Shutdown
- Holiday
- UnAvailable

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On site users

Most of the X6A projects are carried out by users who visit the facility

- Number of visiting individuals is decreasing
- Average experiments are 1.5 days
- Most leave with scaled data, some with electron density maps

Automounter demand continues to increase steadily with several groups owning their own set of pucks

- 34.70 days scheduled
- 2435 samples were screened
- 98 data sets collected

SCREENING!

Off-site users

User group need to have visited at least once.

ProteinXpress*

Your protein structure one shipment away

- User leaves behind or MAIL their samples;
- Receive image files and scaled data.

RemotAccess

- User controls the end-station and data reduction from home Institution;
- Increased interest.

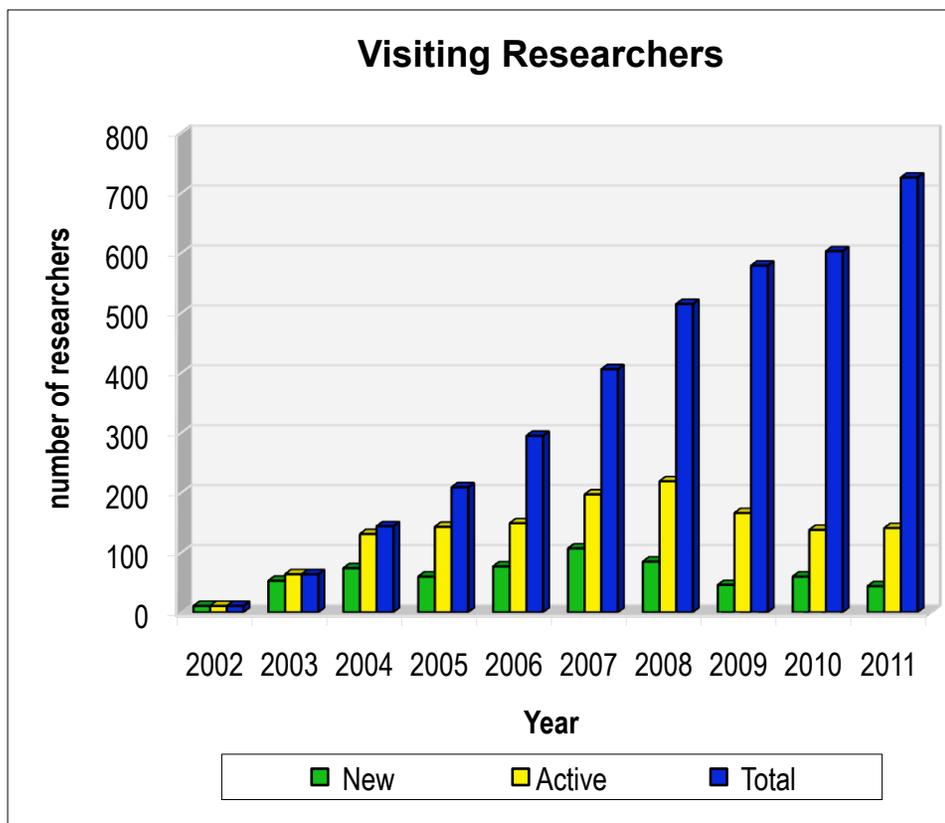
* Is the preferred mode by off-site users

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BLOSA (Beam Line Operation and Safety Awareness) trained users*



BLOSA training is valid for two years.

**New Users*: are experimenters who got trained in a specific year and were never BLOSA trained in previous years.

**Valid Users*: are experimenters who keep a valid BLOSA Training Status in a specific year.

**Total Trained Users*: are experimenters who trained in that year or before (accumulated number). Numbers include new and returning users.

*Source NSLS PASS System December 2011

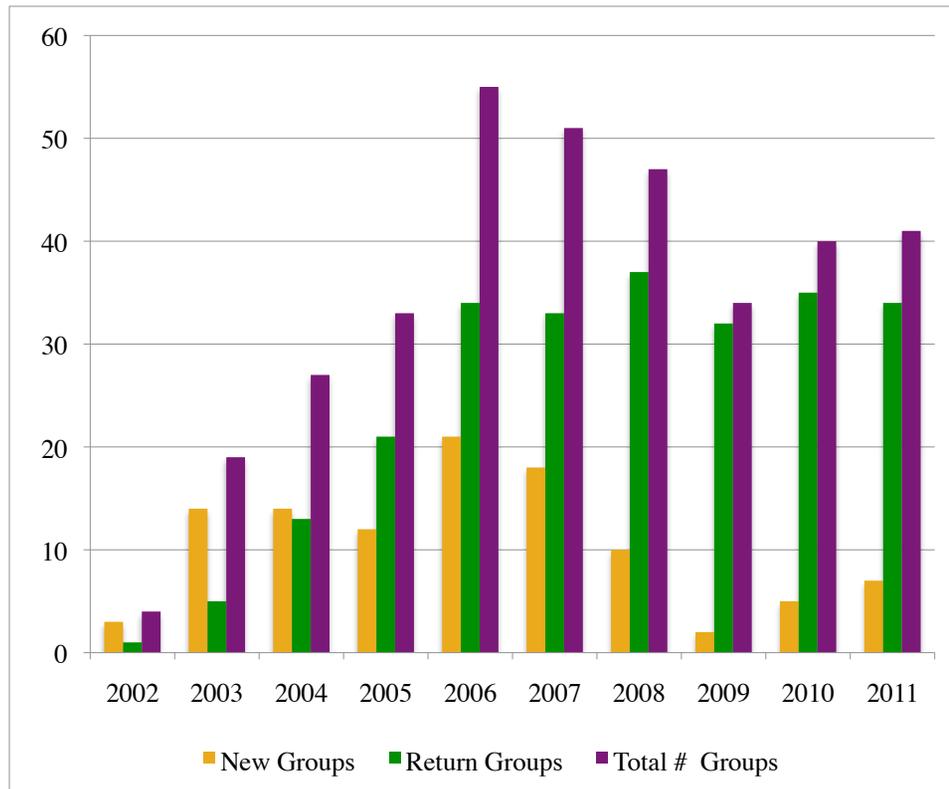
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Consolidation of the user community*



New groups: scheduled their projects only once in 2011.

Return groups: scheduled their projects at least 2x in 2011.

*Source X6A Survey December 2010

The number of user groups returning to the beam line is approximately constant with a 5% fluctuation over the past years. The number of new user groups has increased yearly over the last years.

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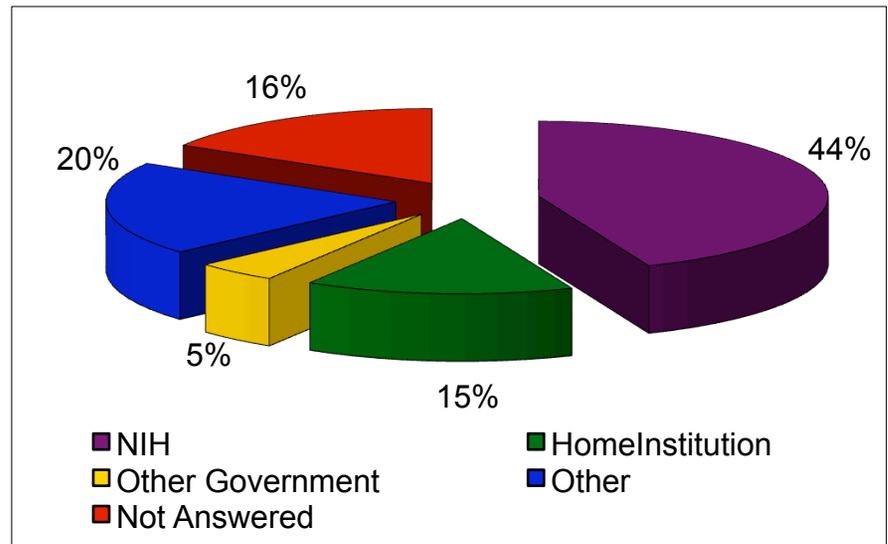
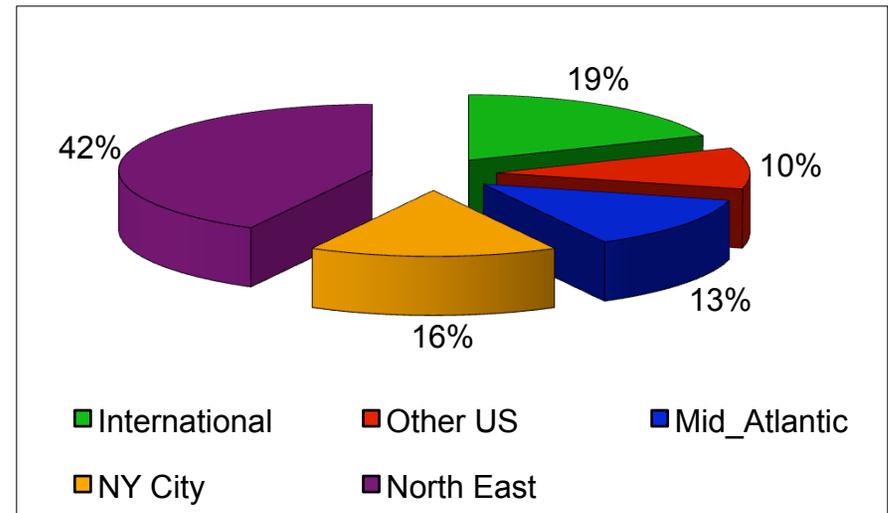
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User demographics and funding*

- Primary usage by academic institutions located in the Northeast;
- Registered researchers are mostly expert crystallographers but less than 54% provide this information. Most non-expert crystallographers do not register on the X6A webpages.
- Funding for projects developed at X6A is provided by NIH institutes, with start up funds accounting for 15% of the projects.

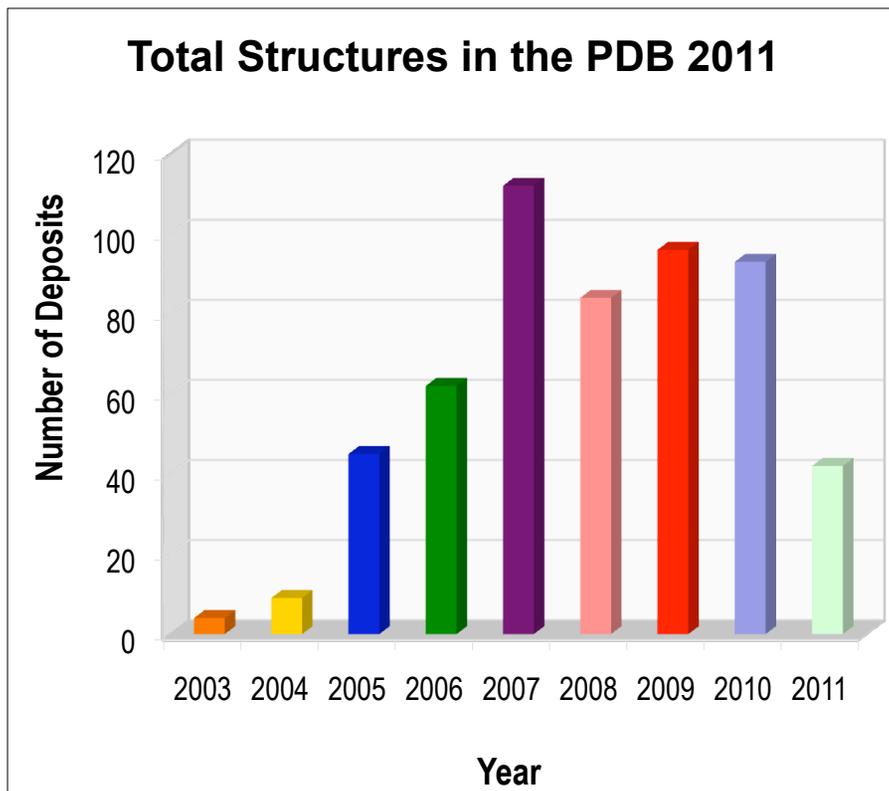
*X6A survey Dec2011



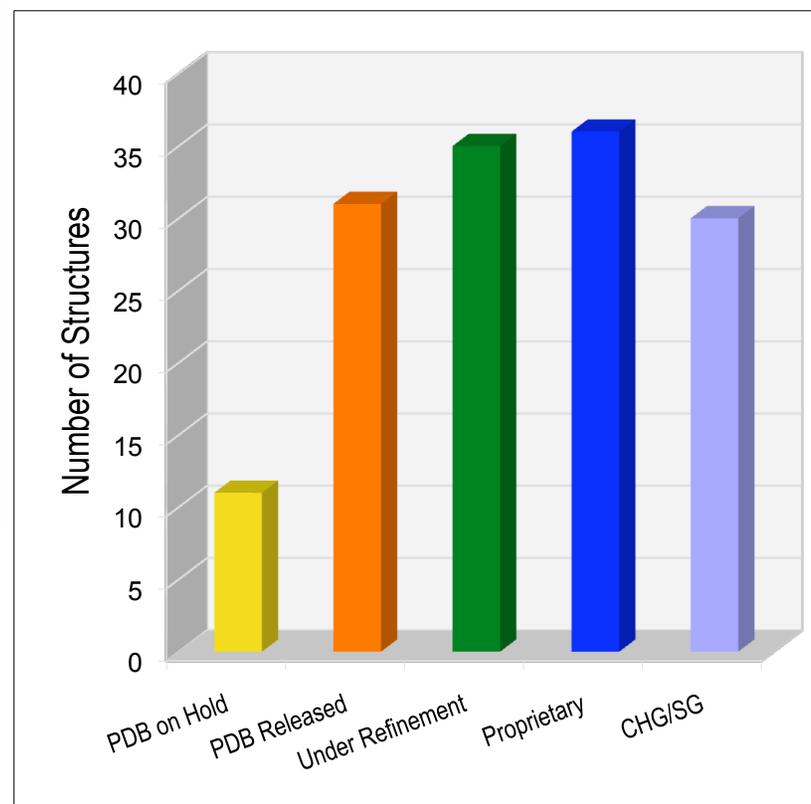


Impact

Protein Data Bank Deposits*



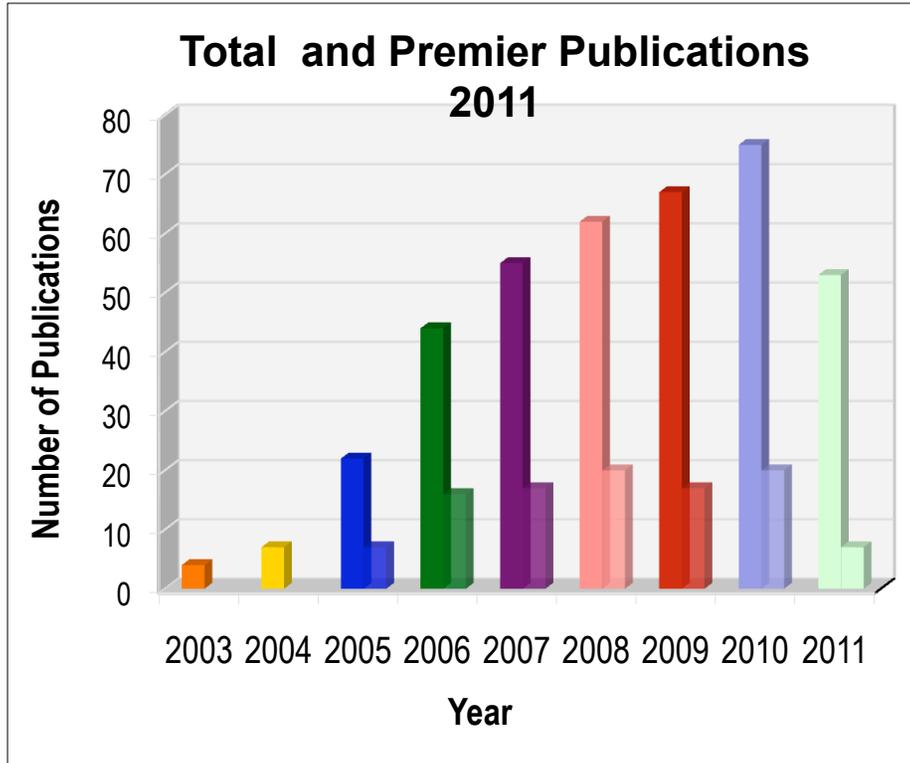
Number of deposits (released and on hold) decreased but overall number of structures increased.



The number of structures deposited in the PDB is not complete. Each year a few new releases are captured for past years as far as 5 years back.

*Source X6A Survey December 2011

Publications*



Publications*	
Total	High Impact**
389	106
2011	
53	9

*Source X6A Survey December 2011

** Journals with an impact of 6.0 or greater. Source JCR 2007

In spite of a thorough survey the total number of publications in a given year are not completely captured. An increase in the number of publications is frequently observed in later years.

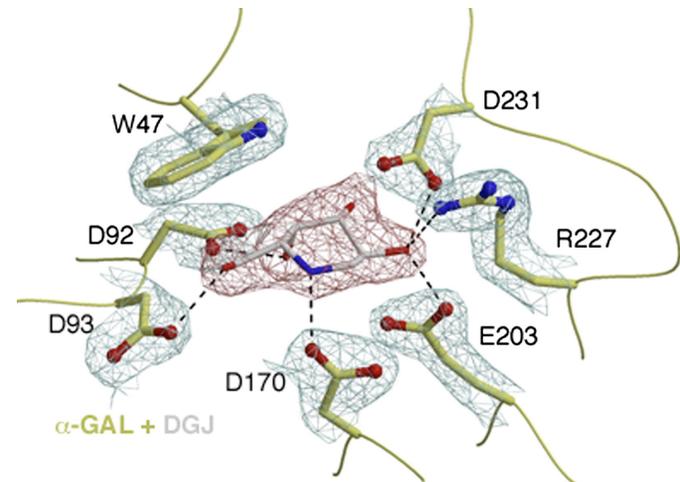
Publications 2011 - Highlights

In 2011 our user community published 53 papers, 9 in premier journals with impact factor over 6 and 18 in journals with impact factor between 5-6.

<Impact> = 5.2

Projects developed by the user community

- appeared in editorials
- subject broad impact media
- Journal covers



Chem. & Biol. Garman Group

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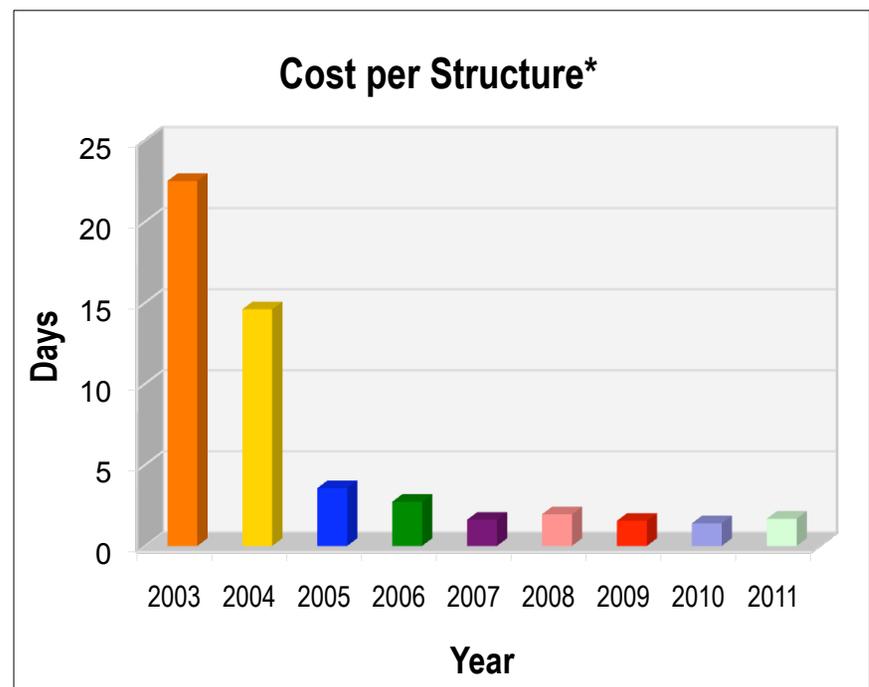
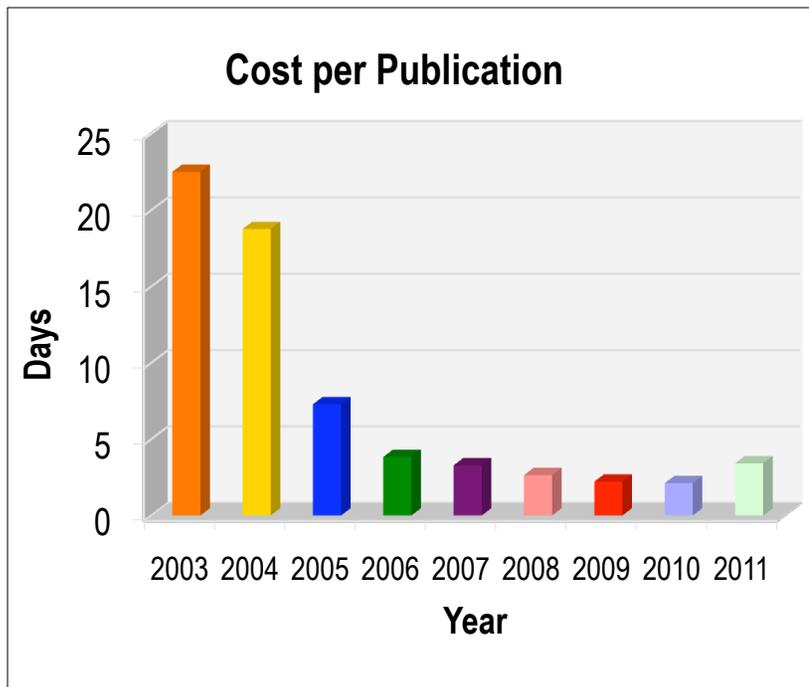
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Other impact factors*

It is common to refer to the cost per structure, per paper.....



* Includes proprietary and SG structures

The cost per structure as a function of scheduled user hours decreased if proprietary and SG data are taken into account

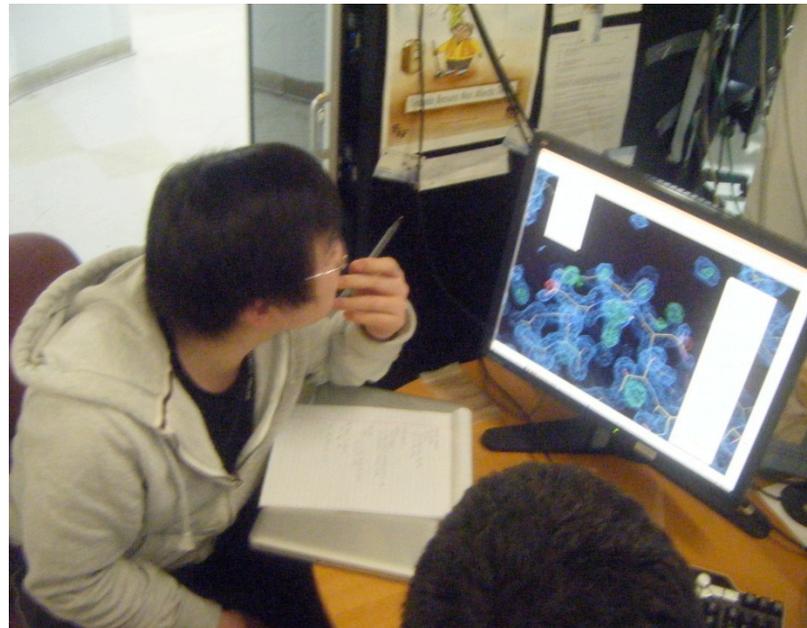


Education and Outreach

Education and outreach

X6A team members and interns participate in courses and workshops. This is an important activity to attract new users.

- Workbench
- Crystallization workshop
- DOE summer internship program
- NSLS Summer Sunday
- CCNY Summer Program
- Graduate Course



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Synergy

Synergy

The X6A team continues to make the facility available to user groups from other communities and promotes complementary methods between its user community. In specific:

❖ X4 PRT

- User beam time re-allocation
- Technical and scientific approaches to crystallography
- Educational outreach (X6A Workbench)

❖ Complementary methods

- SAXS
- EXAFS, XANES, ...

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Outlook

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Outlook

- Organization of a workshop to survey the community needs at the NSLSII.
- Proposal of a high energy beam line for macromolecular crystallography was submitted and presented.
- We expect to continue beam line operations until Feb/14.



Summary

- FOCUS on the USER.
- Junior Faculty User base.
- USER RESEARCH program ALIGNED with NIGMS Road Map
- One of the most productive beam lines at the NSLS.
- Continued upgrade of instrumentation assures optimal beam time usage.

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