NIGMS East Coast Structural Biology Research Facility

http://protein.nsls.bnl.gov

Science Advisory Committee meeting

15 March 2010

Vivian Stojanoff
for the X6A team

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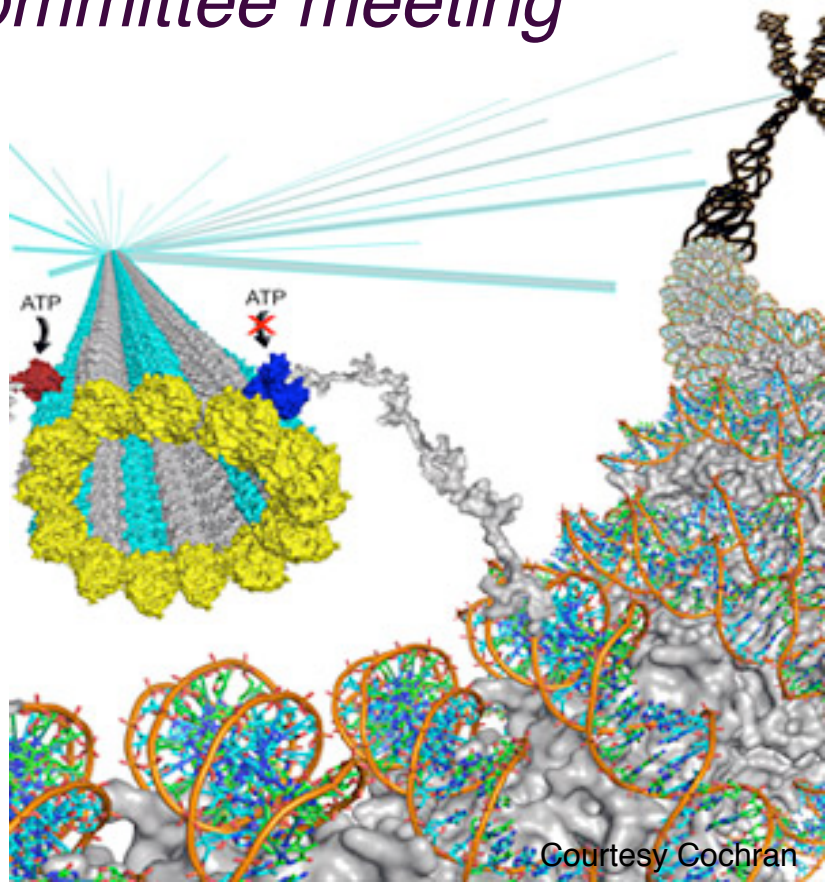

Courtesy Cochran

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.

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SAC Meeting February 2009 - Summary

The high degree of utilization of X6A relies heavily on the ease of requesting and scheduling beam time.

Proposed hardware and software improvements:

- Sample illumination
- Sensors for improved remote access smart magnets (for automounter operation)
- Beam stop (SSRL like) dose limited experiments
- Beam position monitor
- Improved He flight path for improved signal
- KB mirrors for improved intensity
- Access to insertion devices is awarded same metrics are applied and clear guidelines be established

X6A NSLS NIGMS

Report from the Synchrotron Advisory Board to the NIH NIGMS Council on the Effectiveness of the Staff Initiated Grant Supplements to Increase Access of NIGMS Grantees to Synchrotron X-ray Facilities.

Future support should be reduced with the anticipated closing of this beamline

Positive:

The committee acknowledged the useful niche role occupied by X6A and were pleased with the overall performance of staff and the facility.

- Infrastructure
  - auto-mounter
  - BluIce interface
- Staffing
  - 4 Full Time Equivalent (FTE)
- Productivity
  - some excellent science
  - publication exceeded 50 in 2008
- User
  - access: self-scheduling
  - demographics: ½ supported by NIH

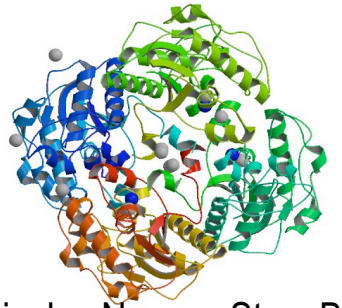
Negative:

Significant concern was expressed for the future of the facility. Overall the committee feeling was that, while the personnel associated with this beamline had made the best of a less than optimal facility.

- Infrastructure
  - Bending magnet source
  - Detector replacement in case of failure
  - Remote access

X6A NSLS NIGMS

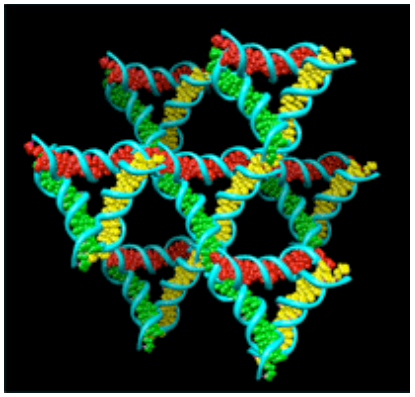
A dynamic user community



Nicolas Nassar, StonyBrook,
Characterization of 2H-Phosphatase

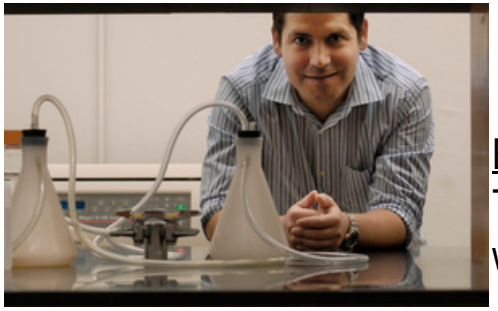
Rebecca Page Group
Brown University
Plos Pathog., 5: e1000706

Patrick Loll Group, Drexel
'Non-trivial' Crystallization Reveals
Antibiotic's Molecular Mode of Action



Seeman, Lab, NYU
Nature, 458, 367-370

Bert van den Berg Lab,
University of Massachusetts
Nature, 458, 367-370



Emmanuel Skordalakes, Wistar
Telomerase structure paves the
way for new cancer therapies

Andre Hoelz, Caltech; former member Blobel Lab
Proc Natl Acad Sci USA, **106**, 3089-3094

Jon Kull Group, Dartmouth College
Cell 136,110-122

2009 publications in premier journals

In 2009 our user community was very productive with 58 publications, 17 in premier journals.

Nature, **458**, 367-370 (van den Berg)
Nature, **460**, 1040-1043 (Miller)
Nature, **461**, 74-77 (Seeman)
Nature, **461**, 621-626 (Nathan)
Cell **136**,110-122 (Kull)
Cell **138**, 514-524 (Schlessinger)
Science, **324**, 657-659 (Xiong)
Nat. Chem. Biol., **5**, 407-413 (Amzel)
Nat. Chem. Biol., **5**, 827-834 (Crane)
Proc Natl Acad Sci USA, **106**, 3089-3094 (Hoelz)
Proc Natl Acad Sci USA, **106**, 4864-4869 (Stebbins)
Proc Natl Acad Sci USA, **106**, 13242-13247 (Wah)
Proc Natl Acad Sci USA, **106**, 13759-13764 (Loll)
Proc Natl Acad Sci USA, **106**, 16996-17001 (Amzel)
Proc. Natl. Acad. Sci. USA, **106**, 17693-17698 (Hoelz)
J. Am. Chem. Soc., **131**, 8848-8854 (Berghuis)
Embo Rep., 5, 722-728 (Nikolov)

<IMPACT>= 7.96

Outline

- Background
- Resources
- Current status of developments
- Staffing
- User Program
- Productivity
- Education and outreach
- Synergy
- Summary

Background

The 1999 NIGMS Initiative at the NSLS

Bending magnet source recommended by NIGMS

- 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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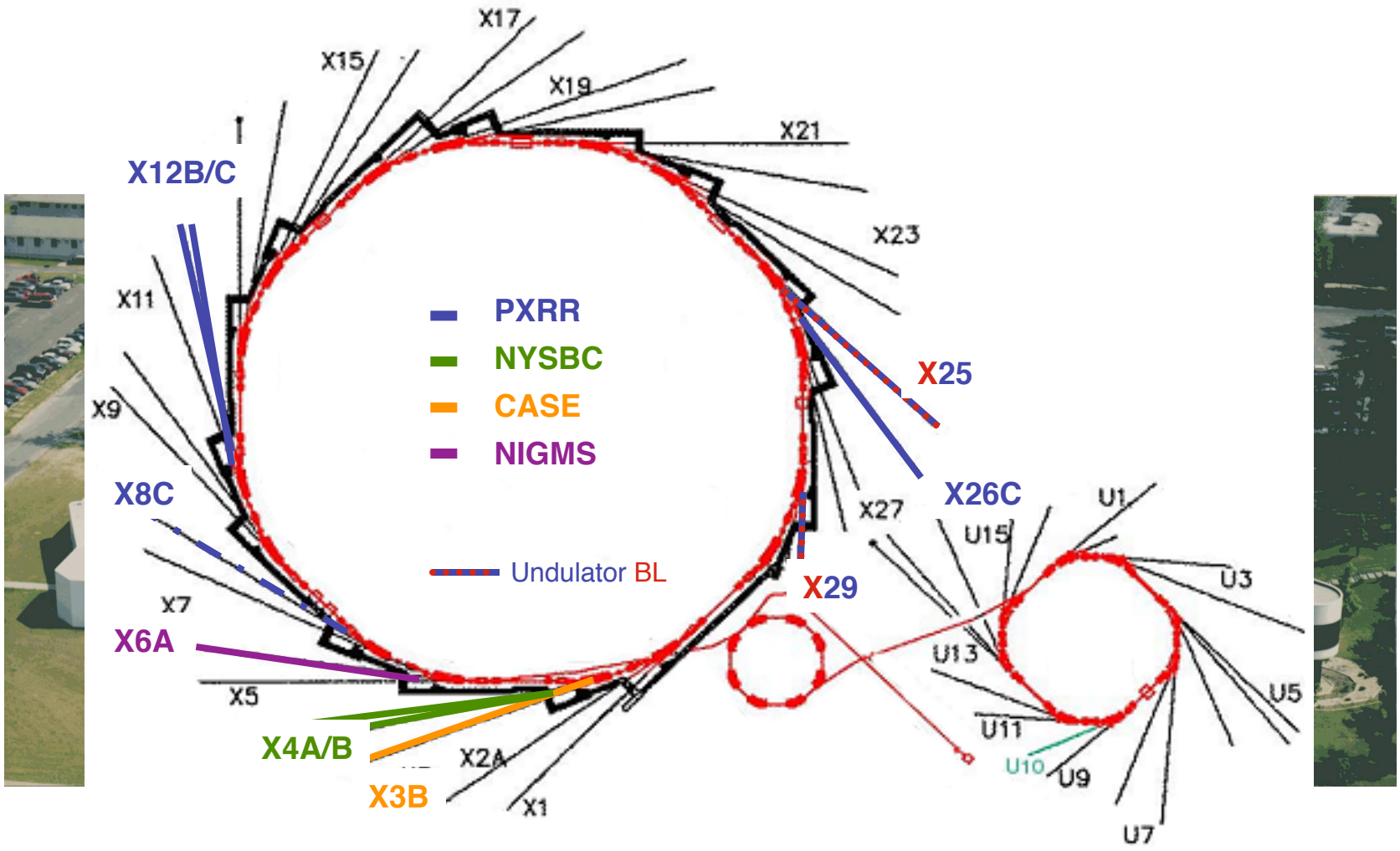
MX at the NSLS



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Resources

Optics

Standard optics design: current operation mode 7 to 16 KeV

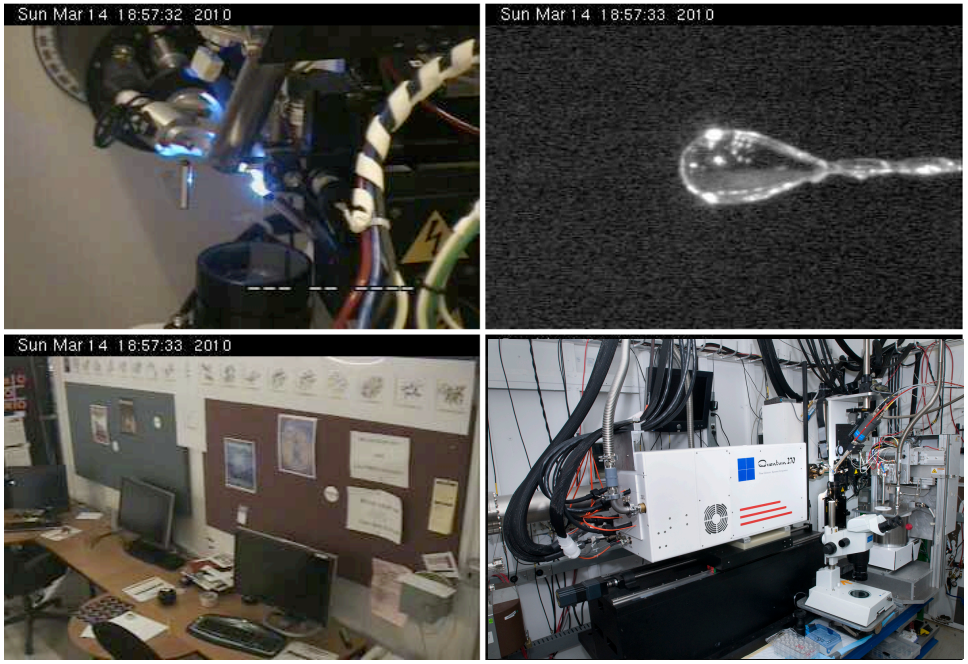
Optical element				
	crystal channel cut	*energy range*	*band pass*	*Total Flux*
monochromator	Si(111)	6 -23 KeV	1.9×10^{-4}	1.2×10^{12} ph/s
	coating	figure	magnification	acceptance
mirror	Rh	Thoroidal	1:1	3mrad

* I=260 mA, 10KeV

Have not yet explored the lower (6-7 KeV) and higher (16 – 19 KeV) end of energy range

Experimental Environment

In the Q270 first year of operation it became clear that the storage capability needs to be upgraded



	Configuration after the 2008 upgrade
Data collection Beamline control	4 x 2.2 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10
Data processing Storage	4 x 2.8 GHz CPUs 4 Gb RAM GiBit Network 1 TB RAID 10
	4 x 3 GHz CPUs 4 Gb RAM GiBit Network 3.6 TB RAID 10
Storage	Inhouse Storage GiBit Network 1.8 TB RAID 1

The X6A Web and Data Base Environment

Media Wiki

- Improve communication

User and Experimental Control Databases

- Communication between databases

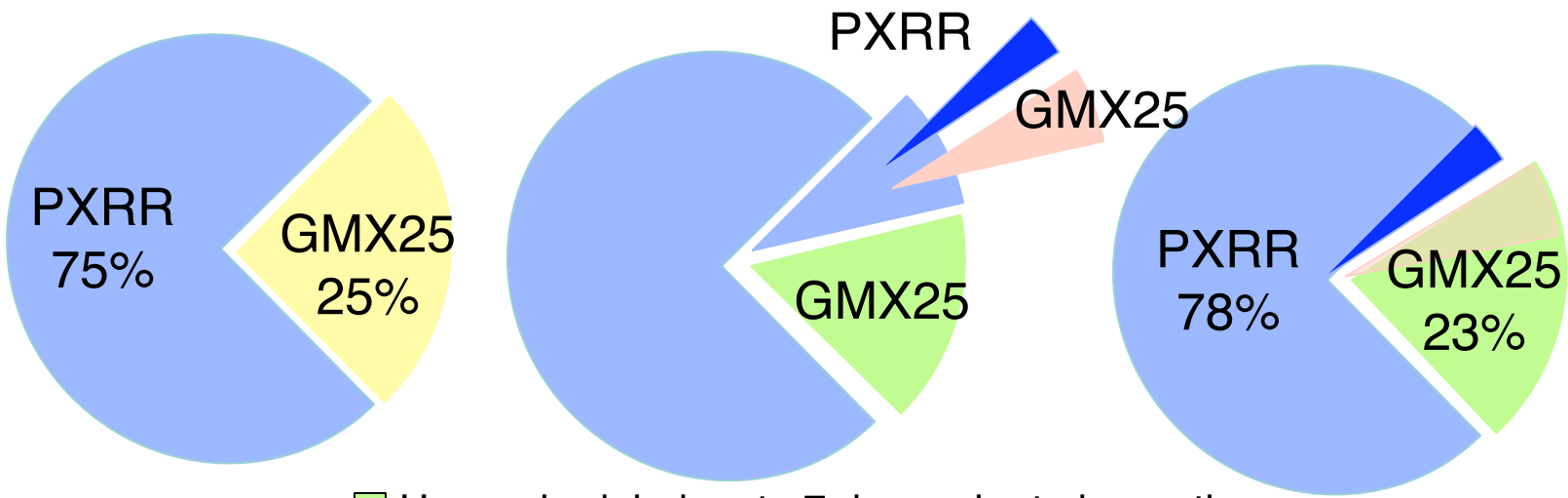
User Database

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

GMX25

A formal mode of application for beam time on the PXRR operated X25 Facility beam line is being pursued.

A self-scheduling calendar like the X6A self-scheduling calendar was developed by Kun Qian. 25% of NSLS User beam time would be set aside for the X6A User Community.



Status update – X6A environment

The high degree of utilization of X6A relies heavily on the ease of requesting and scheduling beam time.

Proposed hardware and software improvements:

- Sample illumination visualization (KQ)
  - Installed and commissioned
- Sensors for improved remote access smart magnets (for automounter operation)
  - use laser sensors instead (KQ)
- Beam stop (SSRL like) dose limited experiments (JD)
  - interlocked beam stop under design (JJ, CO)
- Beam position monitor (CO, JJ, VS)
  - installed and commissioned, needs to be integrated in either into EPICS or DCS (KQ, JJ)

Status update – X6A environment (cont)

The high degree of utilization of X6A relies heavily on the ease of requesting and scheduling beam time.

Proposed hardware and software improvements:

- Improved He flight path for improved signal (JJ)
- Focusing Optics
  - KB mirrors > viability studies, ray tracing (VS, JJ, KQ)
  - Kinoform lenses > preliminary experiments (KEL, KQ,JJ,VS)
- DCS robustness (KQ, JJ)
- Autocentering (KQ, JJ, AJ)
- Access to insertion devices same metrics are applied and clear guidelines be established
  - A self scheduling calendar was developed and has been presented to the PXRR; discussions are under way (MA)

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X6A

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Staff

Organizational Chart

Chi-Chang Kao *1
NSLS Chair

Lisa Miller *1
Life Science Div Head

Scientific Advisory Committee

Mario Amzel
John Hopkins
chair

Hao Wu
Weil Medical

Craig Ogata
GM/CA CAT

Vivian Stojanoff
Project Director

Jean Jakoncic
Assistant Scientist

Kun Qian
IT Associate

TBD
Assistant Scientist

Marc Allaire *2
Associate Scientist

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

*1 NSLS scientific staff

*2 as of June 1st 1/4 FTE

X6A

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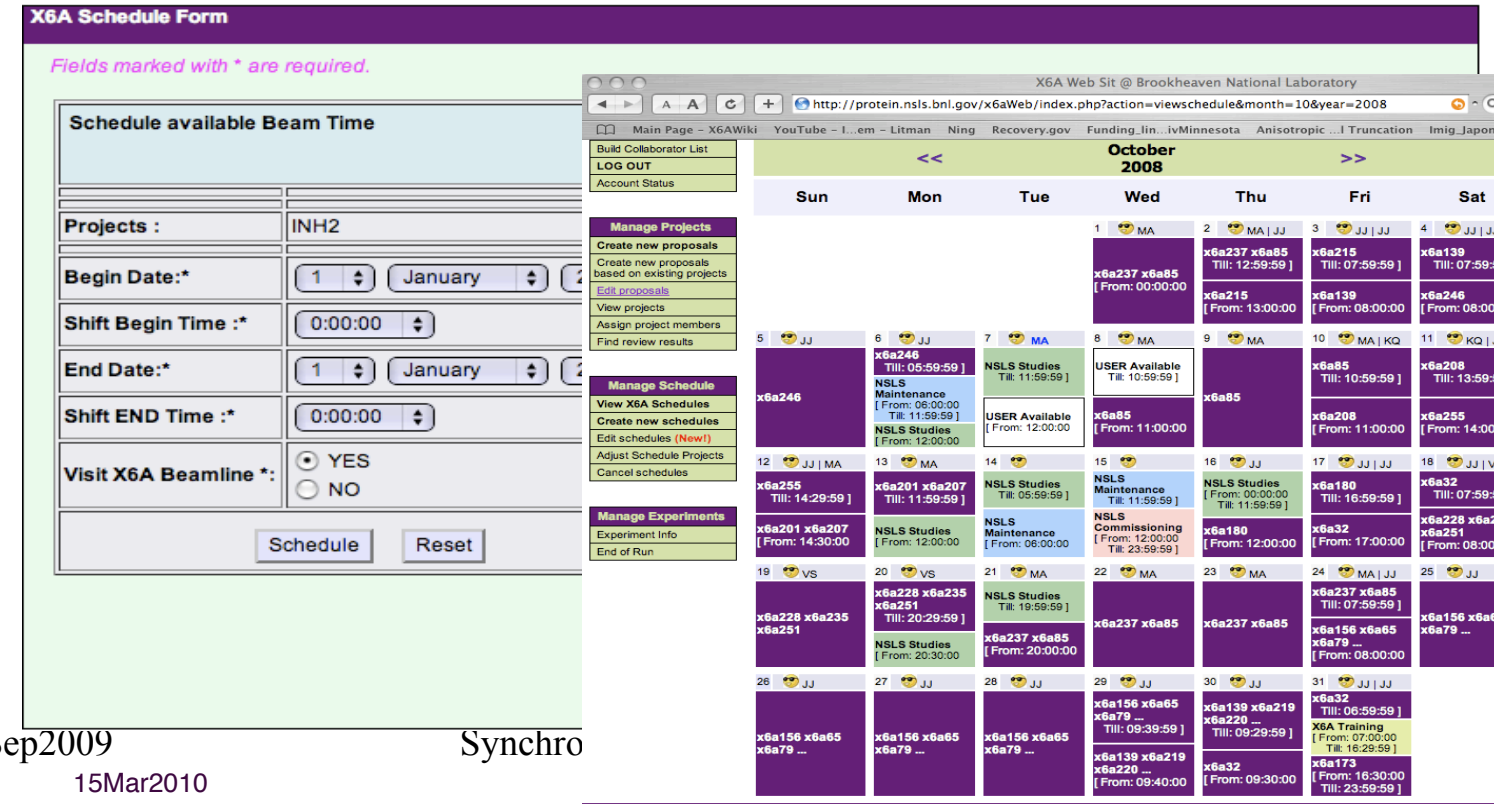
User Program

…"in many instances we choose X6A over other beamlines because of the great help and support we obtain"

Self scheduling

Powered by Media Wiki the X6A web and data base environment is unique amongst MX beam lines world wide for providing users with the ability to schedule their own beam time.



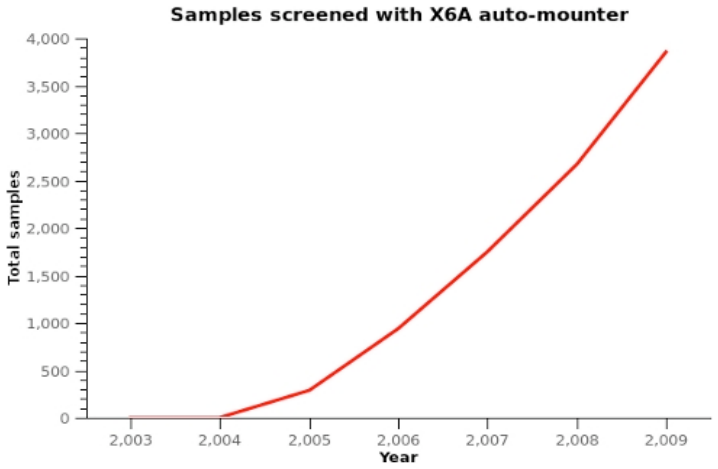
On site users

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

- Groups are in average composed of 2-3 individuals
- Average experiments are 1.5 days
- Most leave with an electron density map

Automounter demand is increasing significantly

- 28 days
- 1380 samples were screened
- 87 data sets collected



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Off-site users

User group need to have visited at least once .

ProteinXpress
Your protein structure one shipment away

Staff demanding

- Users leave behind or MAIL their samples
- Receive image files and scaled data
- Receive an electron density map

Remote Users

Still requires significan staff involvement

- User controls the end-station and data reduction from home Institution. limited staff assistance (access through NoMachine)

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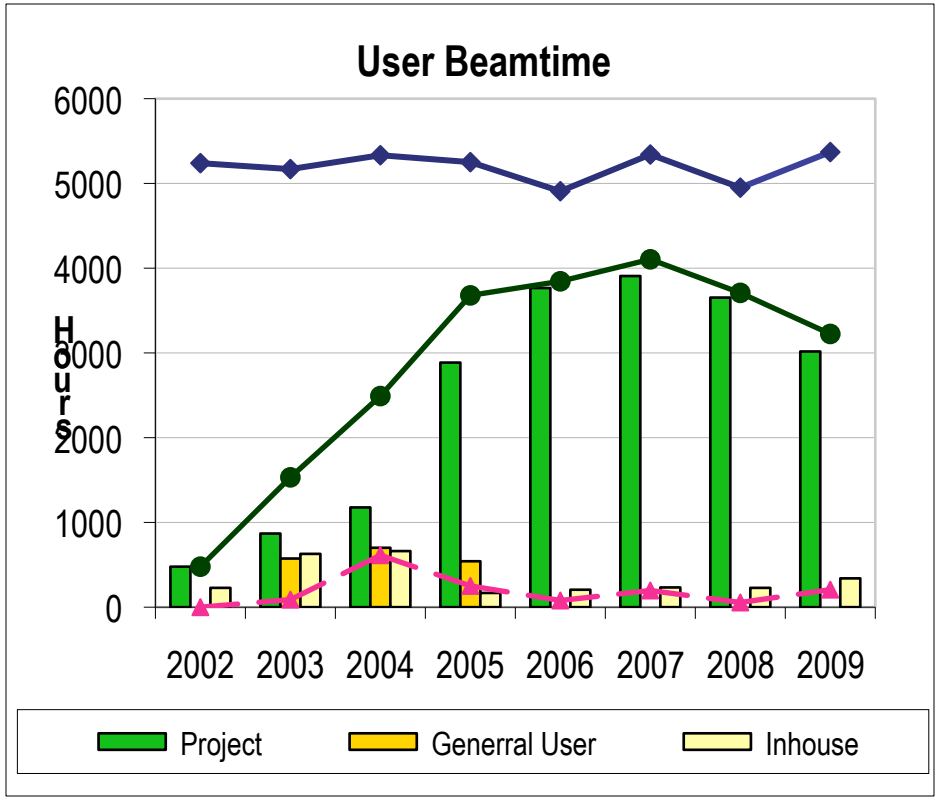
Available beam time



X6A Program 2009

- X6A user projects 60%
- X6A beam line 24%
  - ✓X6A commissioning 74%
  - ✓X6A inhouse projects 26%
- Available 16%

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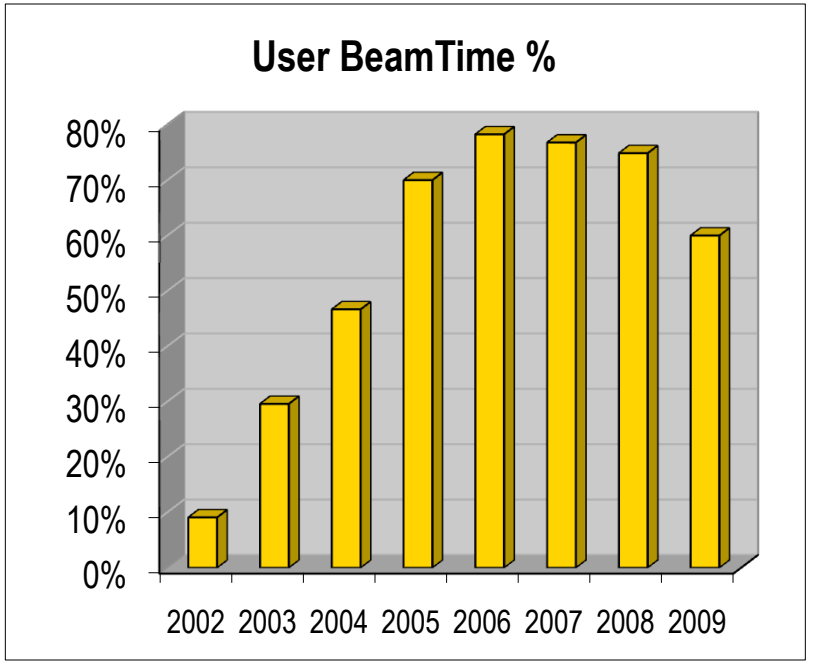
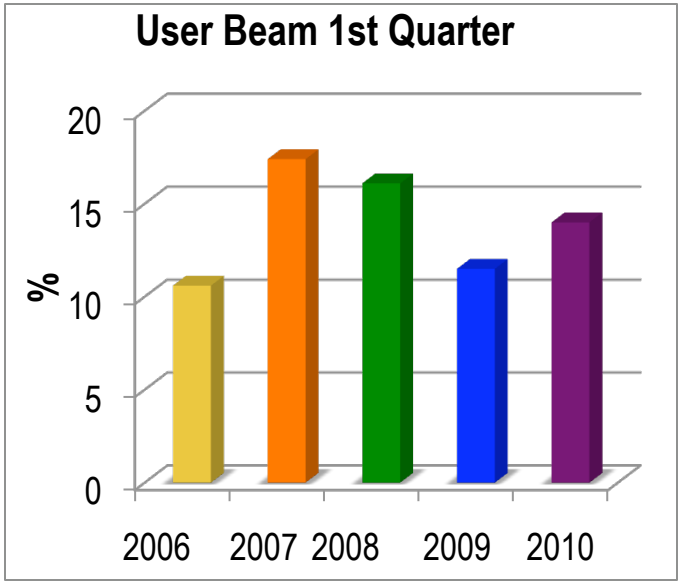
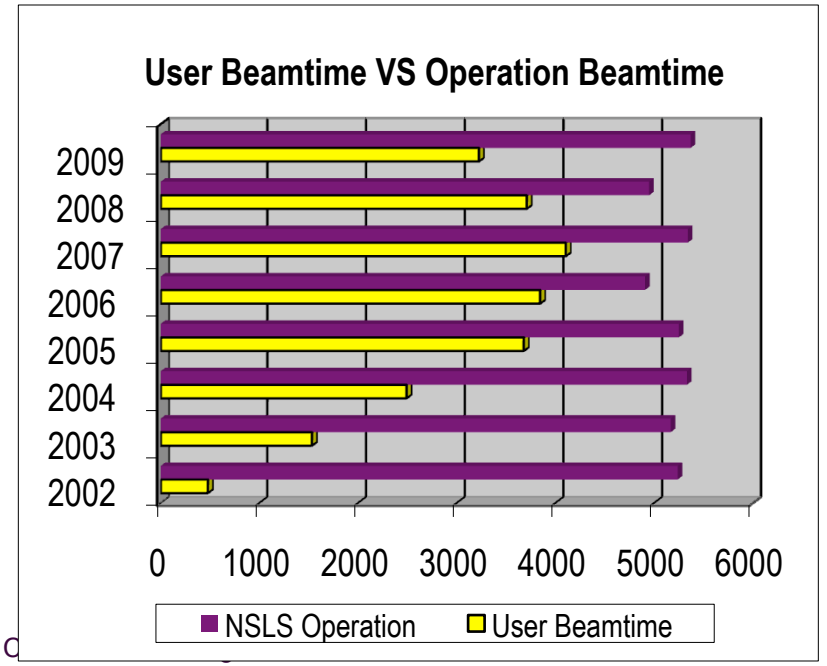
Available beam time

X6A Program – 2009

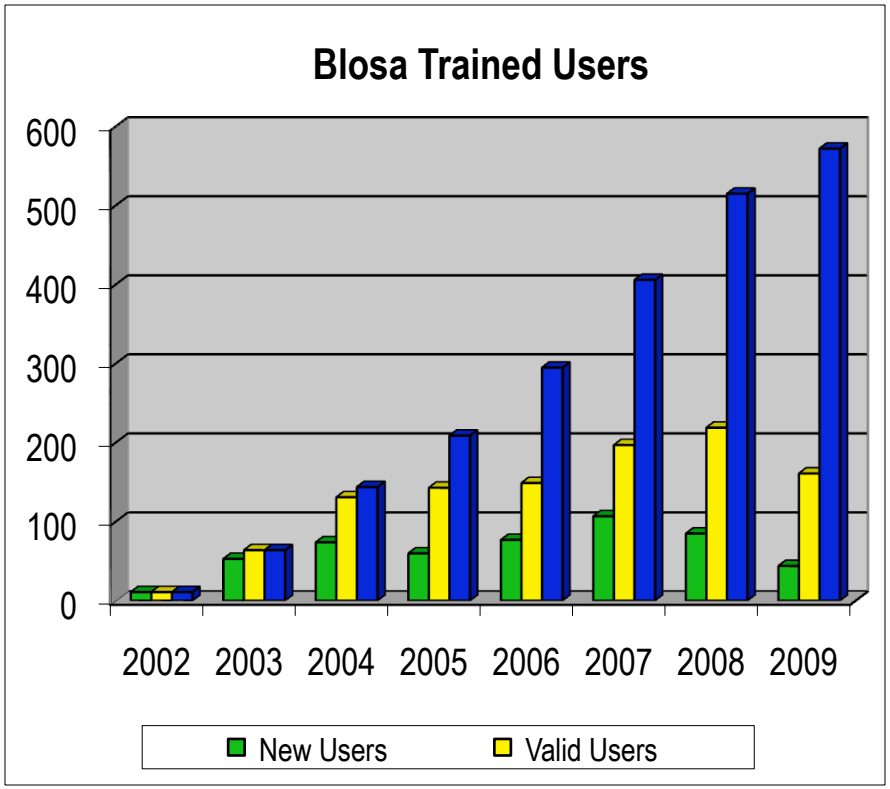
- New hardware, Q270, allows about 1/3 time saving
- Significant cancelations 1st quarter







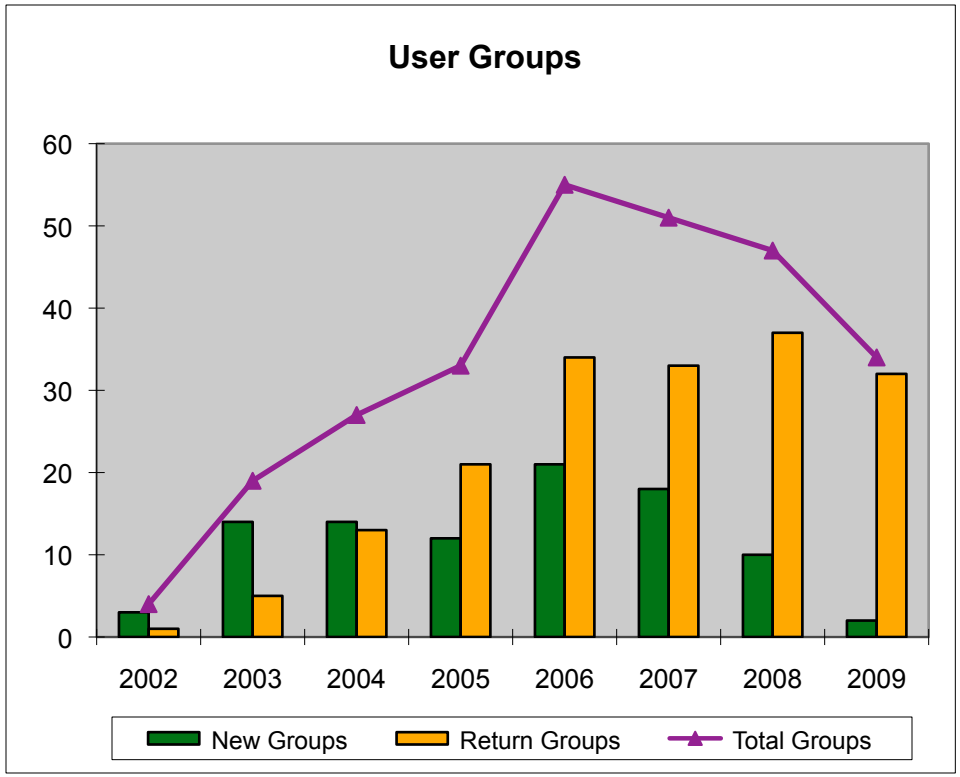
BLOSA (Beam Line Operation and Safety Awareness) trained users



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.

Consolidation of the user community*



*Source X6A Survey December 2009

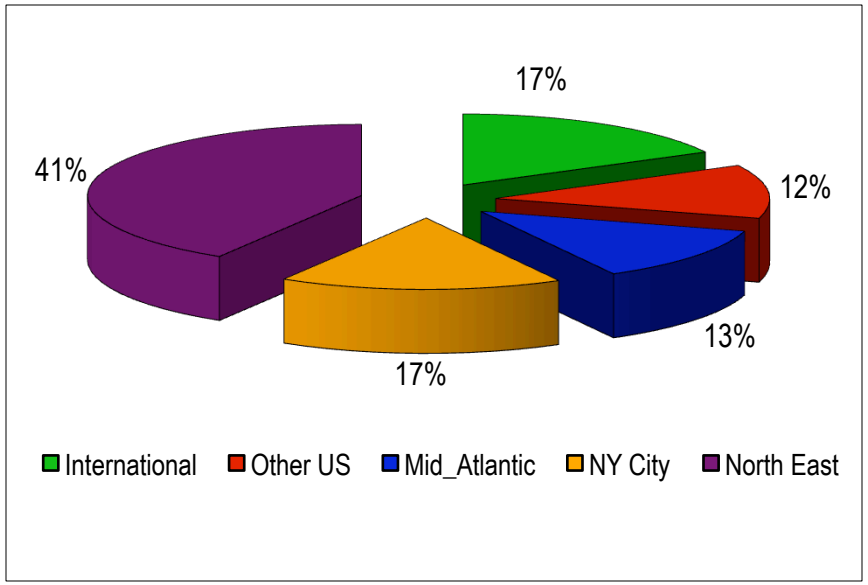
New groups: scheduled their projects only once in 2009.

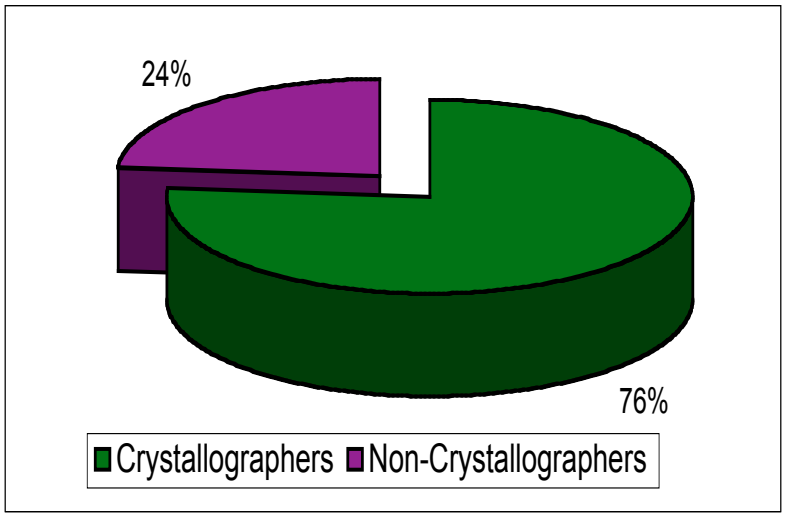
Return groups: scheduled their projects at least 2x in 2009.

The number of user groups returning to the beam line leveled off with ~32 groups scheduling at least twice their projects in 2009.

User demographics*

The number of user groups from academic institutions located in the MidAtlantic states and abroad visiting the beam line increased by ~ 5%.

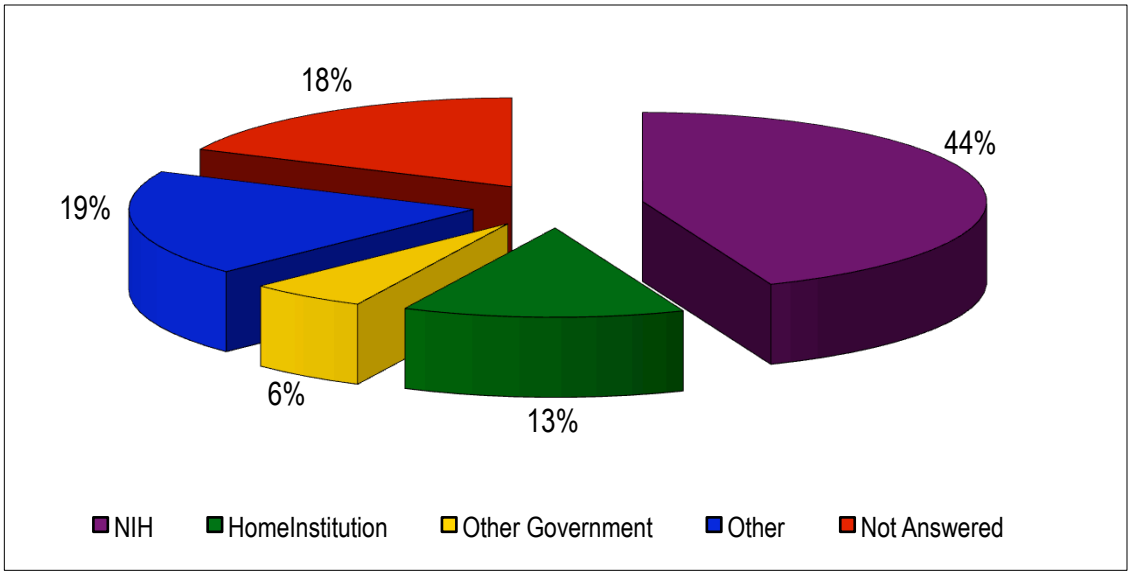




The number of non-expert users fluctuates. Less then 54% of the users provide this information when registering as X6A member.

*X6A survey Dec2009

User Funding Sources*

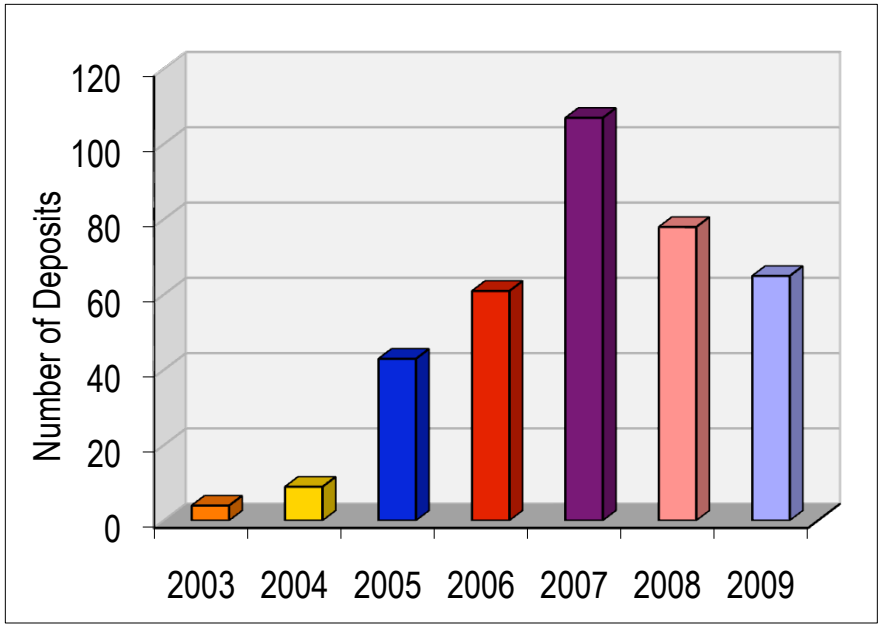


Over the last three years the number of groups supported by the NIH and by home institutions fluctuated +/- 1%.

*Data X6A survey Dec2009

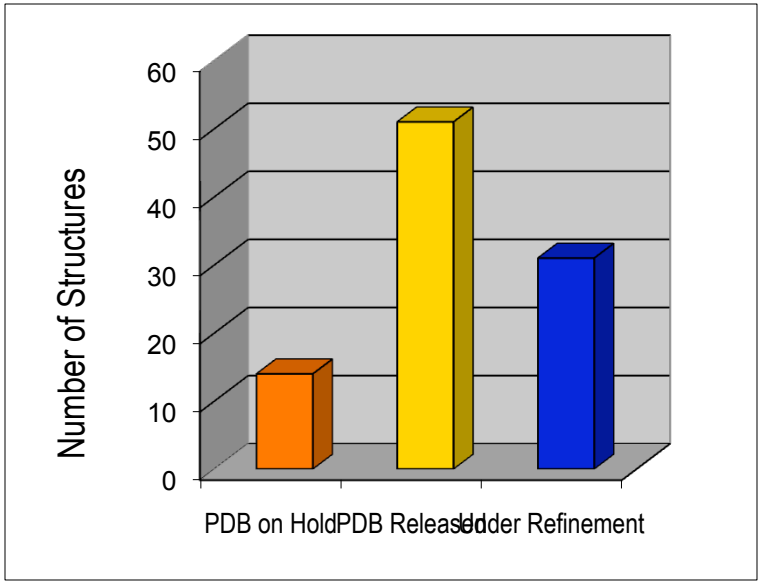
Impact

Protein Data Bank Deposits*



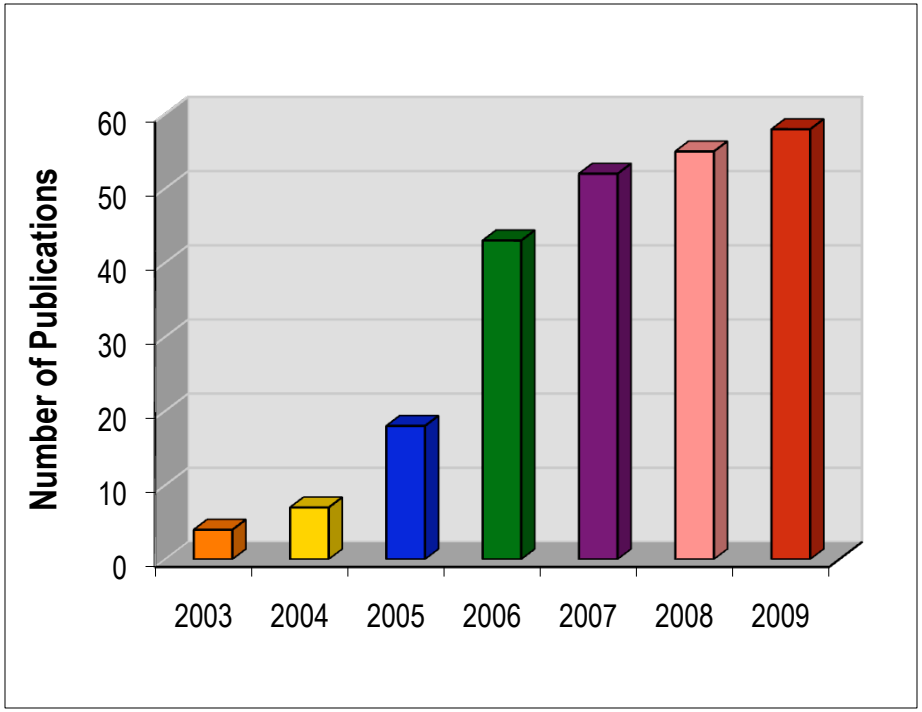
Number of deposits (released and on hold) is leveling off at about 60 per year.

The number of structures deposited in the PDB is not complete. For example for 2007 only 61 structures were reported in the Survey.



*Source X6A Survey December 2009

Publications*



Publications*	
Total	High Impact**
239	92
2009	
60	17

*Source X6A Survey December 2009

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

In spite off a thorough survey the total number of publications in a given year are not completely captured. An overall increase in publication numbers was observed for the last three years. As expected for a maturing beam line the number of publications/year seems to be leveling at about 53 pub/year.

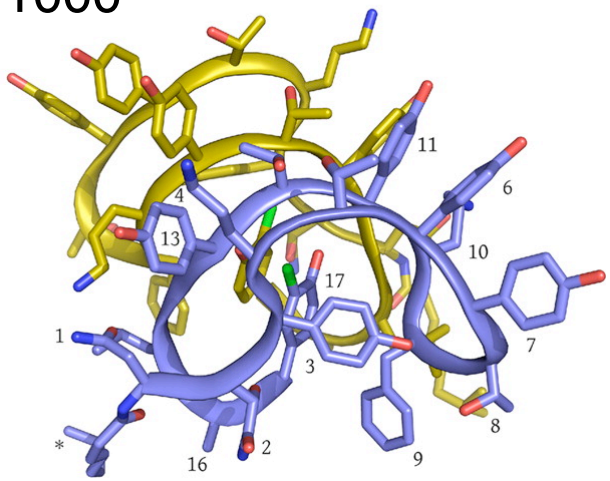
Publications 2009 - Highlights

In 2009 our user community was very productive with 60 publications, 17 in premier journals. The average impact factor is:

<Impact> = 8.25

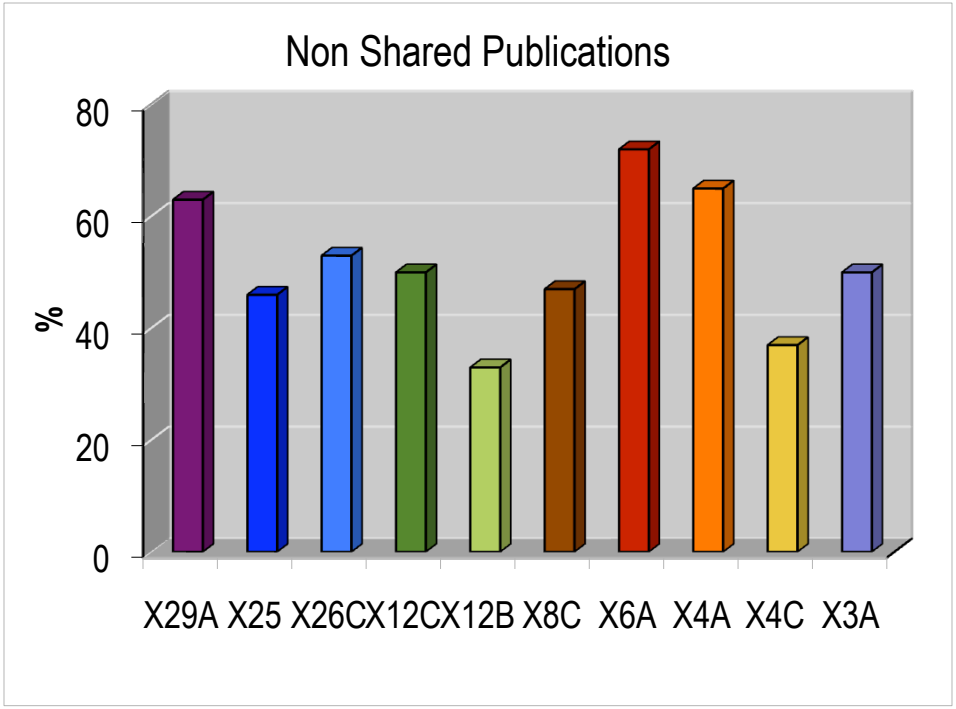
Projects developed by the user community

- were recommended by Faculty of 1000
- appeared in editorials
- subject broad impact media



Proc Natl Acad Sci USA, 106, 13759-13764 (Loll)

Publications shared with other NSLS BL*



Publications shared with NSLS insertion devices:

X29 - 10%

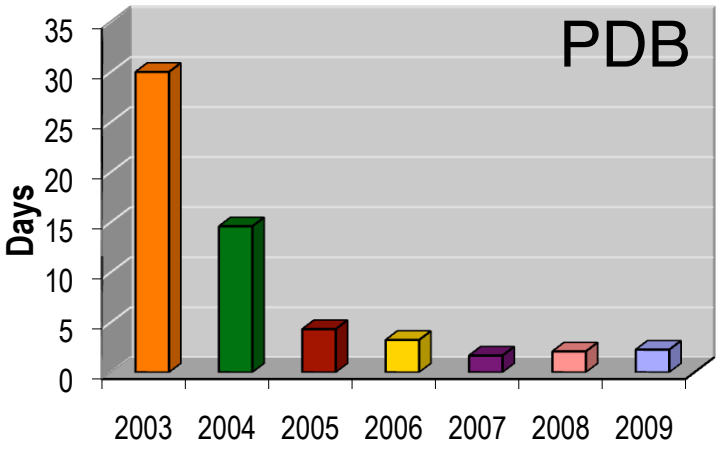
X25 - 6.6%

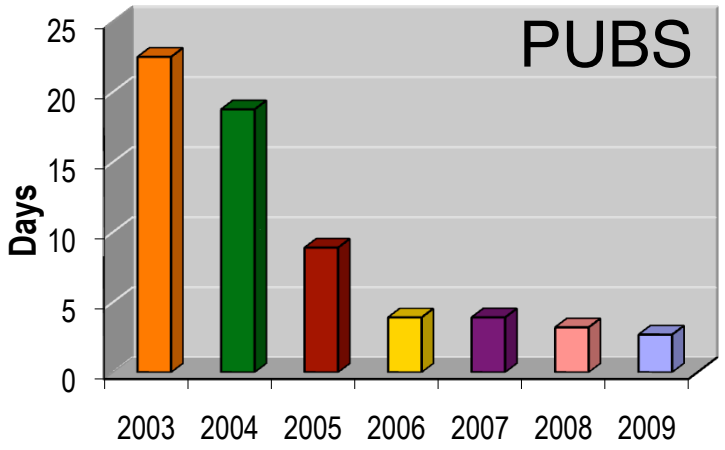
Compared to other user communities at the NSLS the X6A community is very active and loyal. According to the NSLS publication survey only ~ 28% of the X6A publications were shared with other Facilities.

*Source NSLS website 2009

Other impact factors*

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

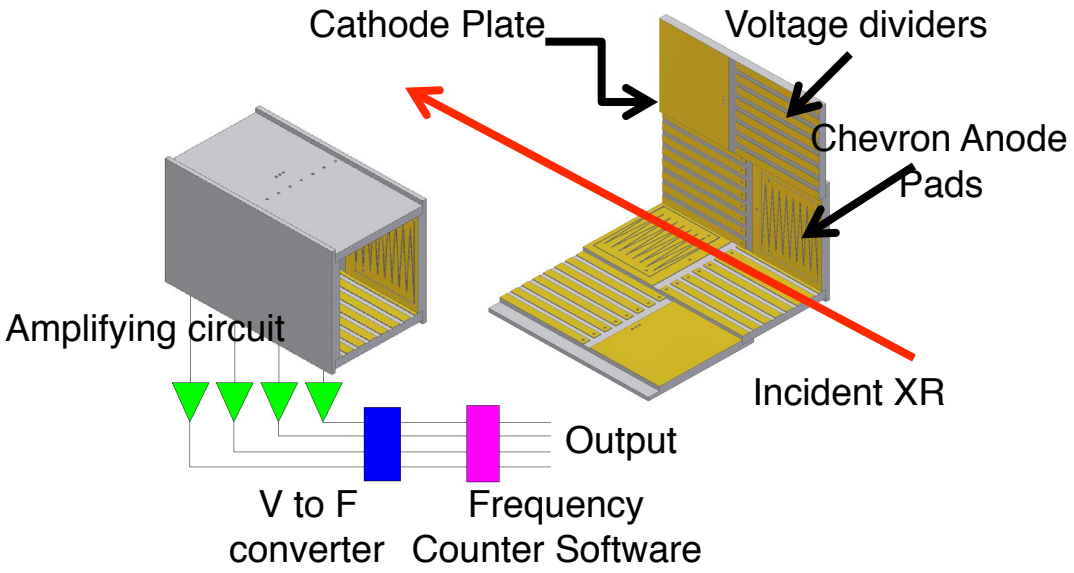


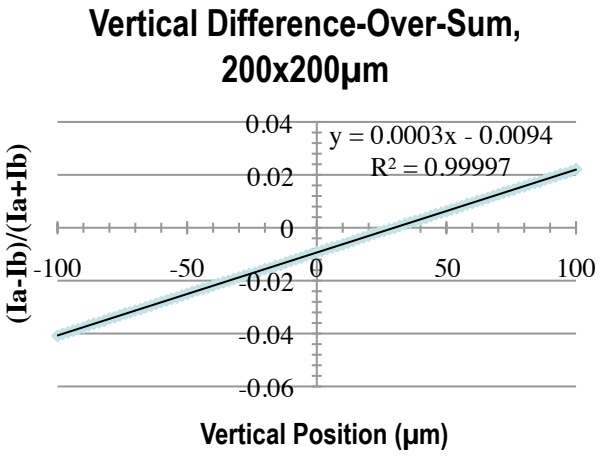


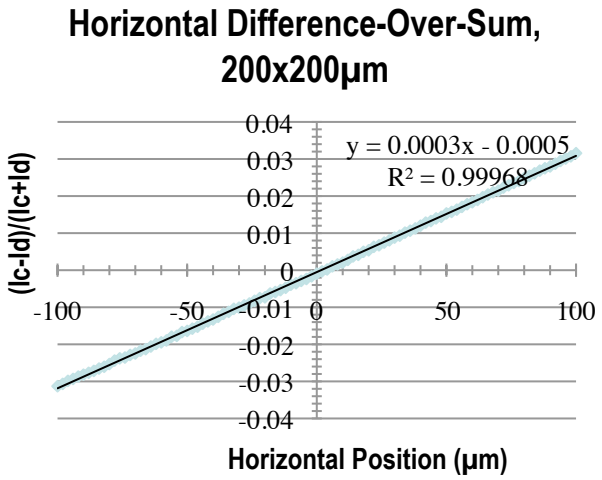
The cost per paper per structure as a function of scheduled user hours leveled off.

Education and outreach

Supported by Laboratory (BNL) programs summer interns have contributed significantly to the development of the beam line instrumentation and research program.







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Education and outreach

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

- Workbench
- 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)
- PXRR
  - Hardware support; the Q210 was lent to the PXRR while the Q315 on X25 was being upgraded

Summary

- FOCUS on the USER.
- Young 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.

"aaahhhh...personal attention! I love it!"

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