

MBB KI

PSF Xray Newsletter 3

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The ambition of this newsletter is to create a simple summary of current actions and issues taking place at PSF Xray instead of sending out several emails.

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Merging BioStructX-2939 and BioStruct-4452

The research groups listed in Table 1 have created a joint BioStructX proposal. Previously these research groups divided themselves between two BioStructX proposals named 2939 and 4452. Since the majority are using joint BAG applications at Diamond and Bessy, having two BioStructX proposals was confusing to these facilities and both synchrotrons requested that we merge our two BioStructX proposals into a single one. In the past BioStructX-2939 had 30 MX-shifts and BioStructX-4452 had 60 MX-shifts of beamtime per year and we will now apply for 90 MX-shifts of beamtime and a few SAXS-shifts from Dec 15 2013.

<u>University</u>	<u>Department</u>	<u>Division</u>	<u>Principal Investigators</u>
Karolinska Institutet	Biosciences and Nutrition	Center for Biosciences	Luca Jovine
Karolinska Institutet	Cell and Molecular Biology	RNA Structural Biology group	Martin Hällberg
Karolinska Institutet	Medical Biochemistry and Biophysics	Biophysics	Herwig Schuler
Karolinska Institutet	Medical Biochemistry and Biophysics	Biophysics	Pär Nordlund
Karolinska Institutet	Medical Biochemistry and Biophysics	Chemistry II	Agnes Rinaldo-Matthis
Karolinska Institutet	Medical Biochemistry and Biophysics	Molecular Structural Biology	Bernhard Lohkamp
Karolinska Institutet	Medical Biochemistry and Biophysics	Molecular Structural Biology	Gunter Schneider
Karolinska Institutet	Medical Biochemistry and Biophysics	Molecular Structural Biology	Jodie Guy
Karolinska Institutet	Medical Biochemistry and Biophysics	Molecular Structural Biology	Robert Schnell
Karolinska Institutet	Medical Biochemistry and Biophysics	Molecular Structural Biology	Ylva Lindqvist
Karolinska Institutet	Medical Biochemistry and Biophysics	Protein Science Facility	Helena Berglund
Karolinska Institutet	SciLifeLab	Structural and Biophysical Immunology	Adnane Achour
Karolinska Institutet	SciLifeLab	Taipale group	Jussi Taipale
Karolinska Institutet	Tumor and Cell Biology	Tumor and Cell Biology	Lars-Gunnar Larsson
Linköping University	Physics, Biology and Chemistry	Molecular Biotechnology	Maria Sunnerhagen
Royal Institute of Technology	Biotechnology	Industrial biotechnology	Christina Divne
Stockholm University	Biochemistry and Biophysics	Högbom group	Martin Högbom
Stockholm University	Biochemistry and Biophysics	Stenmark group	Pål Stenmark
Stockholm University	Biochemistry and Biophysics	Drew group	David Drew
Uppsala University	Chemistry	Dobritzsch group	Doreen Dobritzsch

Table 1. Members of BioStructX-2939 and 4452 now writing a joint BioStructX proposal

BioStructX claiming guide online

What can be claimed and claiming procedures varies a lot between different light sources and therefore a [BioStructX claiming guide](#) have been constructed. Please contribute to this guide by sharing your claiming experiences with PSF.

Remote data collection at Diamond - how does it work?

Remote data collection at Diamond I03 was performed on Dec 9 by Damian Niegowski from MBB, Chemistry II however after a few hours there was a connection issue due to firewall problems at Diamond and Damian did not finish his three pucks of crystals!

Previous experiences of remote data collection at Diamond have sometimes been run at PSF (I02, Oct 06) and outside PSF (I04-1, Oct 17 and I02, Oct 23) and of these occasions only the Oct 06 remote event was run without any issues. The remote data collection on Oct 06 was performed by the research groups most often visiting Diamond and maybe this contributed to the absence of problems on Oct 06. Our five hour remote visits will hopefully be combined into longer visits during 2014 as requested 25 Oct 2013 and our current beamtime schedule is available at <http://psf.ki.se/Xray/BeamtimeSchedule.html>.

Interestingly the recent improvement in network speed performance at MBB did not have any impact on the “alertness” of the GDA interface when running remote at Diamond at Dec 9 i.e. it was still a bit slow in its response to actions taken by experimentalists using GDA. From colleagues comment remote data collection works better at ESRF and this might be due to being more familiar with ESRF but likely also less connection issues with ESRF compared to Diamond.



Figure 1. Diamond device for network monitoring

Diamond are aware of that GDA is not as alert as it should and previously thought the problem was at our end and gave us the pictured device to monitor our network performance. The PSF remote data collection computer was moved outside the PSF firewall early 2013 to abolish any impact on the PSF firewall on remote data collection at Diamond. The device was recently moved outside the PSF firewall as well since moving computer outside the PSF firewall only marginally improved GDA performance.

Two displays connected to remote data collection computer at PSF



Figure 1. New 24'' display (left) added to previous 23'' display (right) for remote data collection

Prior to login one need to move cursor to the right for entering the left display to the left however after login the two displays work as a single display. The remote data collection computer runs Fedora18 and is neither connected to the PSF Linux setup nor behind the PSF firewall and dedicated to remote data collection only.

Bessy and Diamond beamtime applications granted

At BESSY we applied for 12 shifts on 1 Sep 2013 and were awarded 12 shifts to be spent in six months starting Jan 2014. At DIAMOND we applied for 24 shifts divided as 9 shifts at I24 (microfocus beamline) shifts and 15 shifts at I02, I03 and I04 (MAD beamlines) on 1 Oct 2013 and were granted 22 shifts divided as 4 shifts at I24 and 18 shifts at I02, I03, I04 and I04-1 where I04-1 is a fixed wavelength beamline (0,9163Å) ideal for SAD phasing from many heavy atom compounds (<http://diamond.ac.uk/mx-home/I04-1.html>) to be used from April 2014. Compare Diamond beamlines here at <http://diamond.ac.uk/mx-home/I04-1/Resources.html>. We will not use five hour remote data collection at Diamond from April 2014.

Crystal Screen HT demand shaking prior to Phoenix liquid transfer

On a user training session 17 Dec 2013 it was discovered that when dispensing well solution using Crystal Screen HT with Phoenix robot a few conditions where splashed into drop wells and in between. The splash failure can be easily abolished by shaking "Crystal Screen HT" using the PSF plate shaker at 600 rpm for 10 minutes before setting up the crystallization experiment.

The following wells of crystal screen HT where splashed:

A8 (8) - containing 30% (v/v) iso-propanol

B7 (19) - containing 30% (v/v) iso-propoanol

F5 (65) - containing 35% (v/v) tert-butanol

H5 (88) - containing 25% (v/v) tert-butanol

The Crystal Screen HT splash phenomena was recorded in the logbook and repeated on 19 Jan 2013 and 6 Jan 2014 by others. Interestingly condition A12 from Crystal Screen HT also contain 30% iso-propoanol but were not splashed. Tert-butanol is not present in common screens (JCSG, PACT, MemGold) while iso-propanol is present in JCSG+ however at lower concentrations (10-14% v/v). Tert-butanol conditions 23 and 24 in Classics are identical to Crystal Screen HT condition 65 and 88 however Classics and ClassicsLite are not used much at PSF.

Hanging drop plates added to RockImager

Madhuranayaki Thulasingam from Chemistry II wanted to run Hanging drop plates at the Mosquito robot. The hanging drop base plate from TTP Labtech (<http://psf.ki.se/Xray/ConsumablesTable.html>) is called 4150-05700 and could be filled with 90uL of well solution and was already defined in Tecan, Phoenix and Mosquito however not in the 4C and 20C imagers. The 1-drop experiment is imaged without issues while the 3-drop experiment needs further trimming to be imaged perfectly. The Mosquito robot adds liquid to a tape called 4150-05600 from TTP Labtech that contain glue for fixation to the base plate and therefore drop positions can vary slightly like when doing manual 24-well hanging drop plates. The imager are using the "drop location" option for imaging however additional trimming is required to capture all drops of a 96-well 3 drop hanging drop experiment run in the Mosquito. The hanging drop experiment has never been particularly popular at PSF since tape with small droplets need to be cut during crystal mounting from these plates.

Phoenix computer maintenance performed and planned

The Phoenix computer is frequently frozen however this is simply due to too little RAM memory. Chad Tunell added more RAM memory to the Phoenix computer. Ideally we should mirror the Phoenix computer hard drive since the software installation at our Phoenix computer is unique with respect to the added NaOH wash station by Andy Wong from SGC Toronto.