PSF Xray Newsletter 2

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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.

Contents

PSF Xray homepage updates

PSF software settings online

To simplify upgrading for PSF Xray software users press "PSF Software settings - 11 Nov 2013" and exchange *PSFuser* for your own username and store this file as .user_settings in your home directory.

PSF Xray User Meeting protocols online

Our common decisions stored in PSF Xray user meeting protocols have been placed online at PSF Xray User meeting protocols.

PSF Xray risk assessments online

To make PSF Xray risk assessments more available to its users we decided to place them online at PSF Xray Risk Assesments. Documents and instructions from chemical sanitization training Jan 18 2013 are also available there. PSF want to thank its users for participating in risk assessment and next risk assessment and chemical sanitization training in English will occur during 2014.

NSC Startup info online

Protein crystallography software is frequently updated at NSC and therefore the "NSC User Guide" is already outdated. Please click "NSC startup info - 28 Nov 2013" to get the latest NSC settings and instructions.

PSF iRODS application granted

Our first iRODS 10TB application has been granted and iRODS have been updated into version 3.3 at PSF. For increased security Yubikeys have been sent to us that generate one-time passwords when connected to a local computer usb port and user presses a Yubikey button (http://www.yubico.com/about/intro/). Data has been transferred from PSF to our new iRODS zone and Diamond need to upgrade iRODS from 3.1 into 3.3 to enable Yubikey usage. Please contact Martin Moche if you want to join PSF iRODS project.

Figure 1. Yubikey button highlighted

First experience of Phenix MR Rosetta at NSC

The first runs of phenix 1.8.4 with MR Rosetta version 3.4 was performed at NSC recently. Starting from a 2.2Å dataset, a sequence file and a search model,"phenix MR rosetta" solved the MR problem but also rebuilt the search model to the extent that only side chain flipping and disordered loop building remained (Table 1).

The final dimeric model, not yet deposited in PDB, has 146 and 135 residues in chain A and B respectively and has been compared to the dimeric search model and the models generated after Phenix MR rosetta and PHASER – arpWarp (Table 1). The current final model and is quite non-symmetric and comparing chain A and B using SSM in COOT results in 130 aligned residues with an rmsd of 2.2 and a sequence identity of 84 % for the aligned residues. The non-symmetry of the dimer caused some human headache during original model building however are now confirmed by Phenix MR rosetta autobuilding. The arpWarp model chain A has an "out of register" error as compared to the final model that is easily identified in the electron density maps and therefore a bad score (62%) for Sequence ID in Table 1.

	Final model chain A - 146 aa			Final model chain B - 135 aa		
	# aligned aa	rmsd (A)	Sequence ID (%)	# aligned aa	rmsd (A)	Sequence ID (%)
search model chain A - 140 aa	129	2.21	91.5	135	0.96	96.3
search model chain B - 134 aa	123	2.07	91.1	128	1.72	95.3
arpWarp model chain A - 147 aa	142	0.39	62	128	2.08	41.4
arpWarp model chain B - 134 aa	127	2.04	83.5	134	0.15	100
phenix MR rosetta chain A - 129 aa	125	2.07	84.8	129	0.12	100
phenix MR rosetta chain B - 137 aa	136	0.23	100	121	2.2	75.2

Table 1. Chain-wise comparison of search model, arpWarp model and Phenix MR rosetta models against the final model of a quite non-symmetric dimer using SSM alignment option in COOT. Chains of the search model dimer are more similar to chain B than chain A of the final model.

The job was running on a single NSC node with 16 processors for less than 10 hours. No supercomputer adaptions are yet done to the phenix code, however the sbatch scheduling of phenix jobs at NSC was used that are advantageous when long time jobs are to be submitted at NSC (maximum time 168 hours) or when you want to run several jobs at the time varying parameters. Protein crystallography software is frequently updated at NSC so please click "NSC startup info - 28 Nov 2013" to get the latest NSC settings and instructions.

Tecan software settings improved

People using the Tecan frequently experience that tip1 dispensing row1 in the back of the robot is failing in liquid detection. We exchanged tip-adapter and IC-circuit for tip1 two years ago however the issue did not disappear completely. A recent review of Tecan liquid classes settings showed that 50% PEG 10K and a few other PEG liquid classes had suboptimal settings such as Liquid conductivity "good" instead of "bad" and On detection error "user prompt" instead of "go to z-max".

The following settings should be selected for 50% PEG 10K and other PEGs (ELN: EXP-13-BG0449).

- Liquid conductivity: bad (Figure 1)
- On detection error: "go to z-max" (Figure 2 and 3)

The majority of the RockMaker ingredients belong to the "water" liquid class where

- Liquid conductivity: good
- On detection error: "user prompt"

is correctly selected.

Maybe "go to z-max" could be selected for "water" liquid class as well? with the following consequences:

- positive: no stops when running Tecan
- negative: Tecan might aspirate air when "go to z-max" is selected and vial is empty