

Agenda PSF MX User Meeting on ZOOM 2022-06-22

Time and Place: 4 pm Wednesday 22 June 2022 <https://ki-se.zoom.us/j/2552303941>

Participants: Martin Moche and Emma Rose-Scaletti

§1 INFO: Next PSF MX User Meeting

In late August, or early September 2022 to be announced

§2 INFO: Diamond and MAX IV

We have been awarded 112 BioMAX shifts for the upcoming two-year period ending in Aug 2024. One weekend 16-hour visit consumes 4 shifts (weekday 24-hour BAG visit consumes 6 shifts) so this is enough for 2-years of monthly BioMAX visits using a majority of weekend beamtime.

Please complement BioMAX by shipping crystals to Diamond Light Source following guidelines in:

- [MX Responsive Beamtime Guide](#)
- [Operations Calendar 2022](#)

§4 DECISION: Assign experimentalists

Light source	Beamline	Date	Duration	Start	Experimentalists
MAX IV	BioMAX	2022-07-02	16	09:00	Martin 2-3 pucks

Table 1. More beamtime at <http://ki.se/en/mbb/psf-mx>.

§5 INFO: PSF MX updates

Protein Science Facility staff are engaged in an “Integrated Structural Biology” course organized by InfraLife. A general introduction to PRESTO on Aug 22 and a study visit to Protein Science Facility on Aug 31 is planned for course participants - <https://media.infralife.se/2022/05/InfraLife-Course-Flyer-2022-8.pdf>

The Cambridge Structural Database is now part of PRESTO and therefore ligand libraries can be generated from the command-line in a convenient manner without use of external servers. Currently available only at NSC Tetralith but installs are ongoing at LUNARC Aurora as well. To make dictionaries from smiles string (cyclic-AMP example below) and visualize in mogul do:

```
$ module load BUSTER/20220608-2-PRESTO
$ grade2 'C1C2C(C(C(O2)N3C=NC4=C(N=CN=C43)N)O)OP(=O)(O1)O'
$ mogul LIG.xyz.pdb
```

§6 INFO: PSF in iLab - https://karolinska.corefacilities.org/service_center/show_external/3663

- ✓ Please register your research group, students, postdocs and project numbers in iLab.
- ✓ Visit <https://staff.ki.se/the-cfm-project-and-ilab> for guidance
- ✓ Ask cfm-support@ki.se for help

Almost all PSF users now enrolled!