The year 2020 of remote operation at P11

Current and future trends in Macromolecular Crystallography experiments:

Focus on Automation, high data rate analysis and User Interfaces

18.03.21

Guillaume Pompidor

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

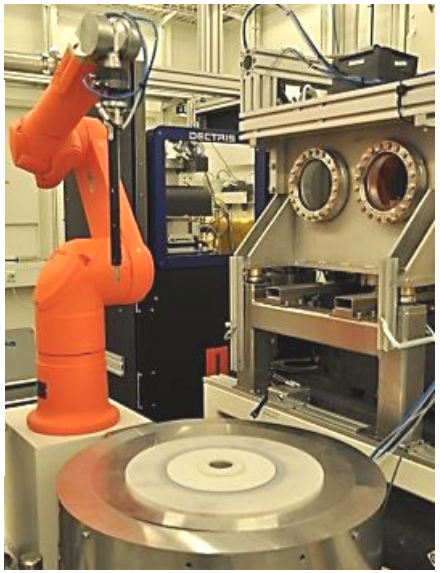
Outline

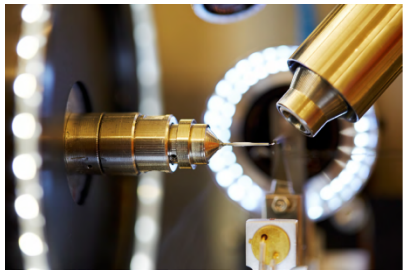
- The P11 beamline at PETRA III
- User Interface
- Remote data collection
- The 2020 year

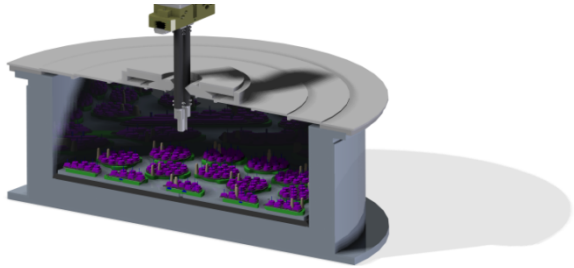
P11 – High Throughput MX beamline at PETRA III

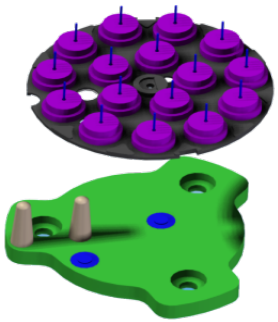
1) Crystallography experiment

- In user operation since 2013
- Broad energy range: 5.5 - 28 keV
- High-speed sample changer with capacity (23 unipcuks = 364 samples)
- Various focusing options (beamsize from 4 x 9 to 200 x 200 um)
- Pilatus 6M, Eiger2 16M (permanent)
- XRF for experimental phasing (SAD/ MAD) and element analysis
- Serial crystallography



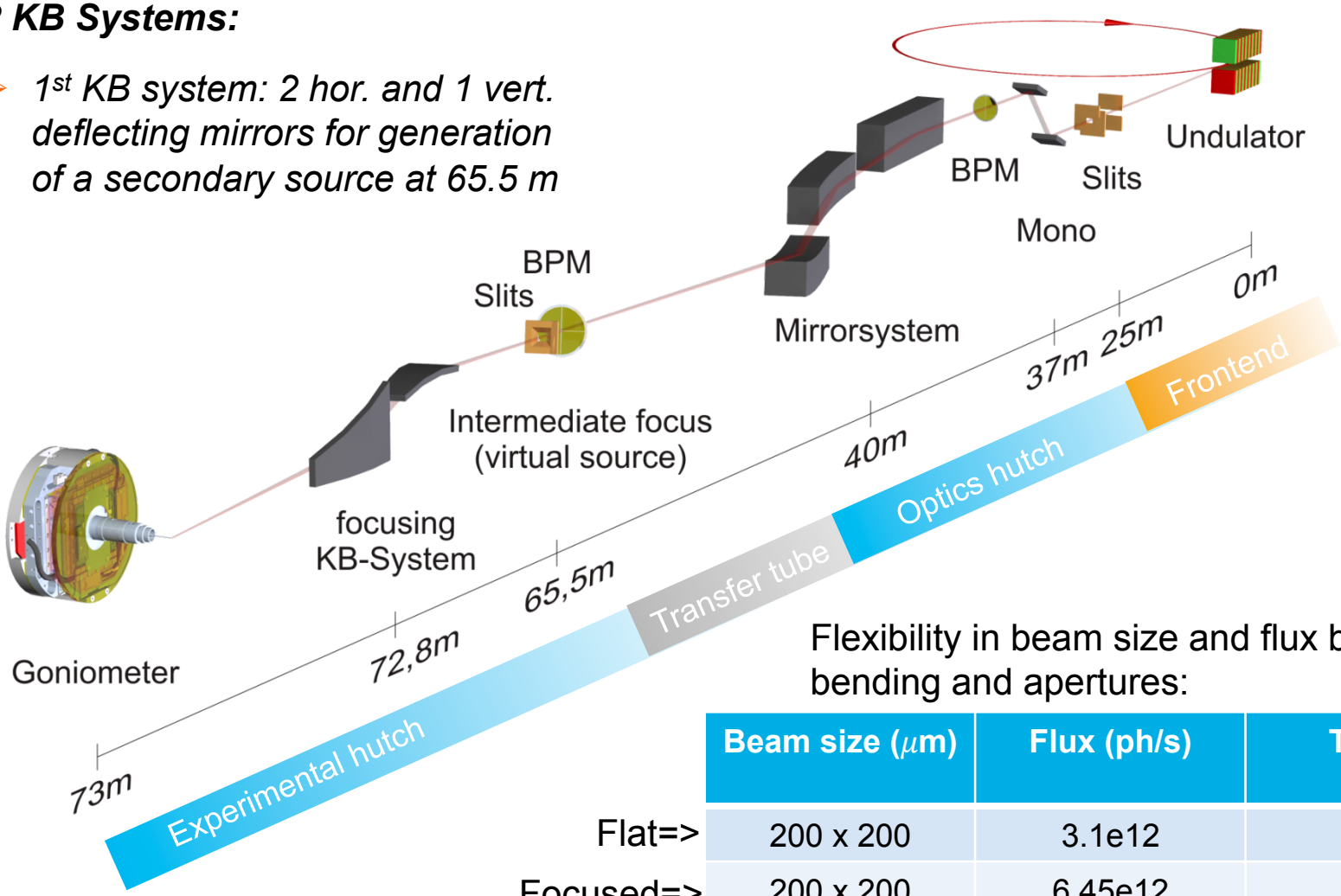






2 KB Systems:

- *1st KB system: 2 hor. and 1 vert. deflecting mirrors for generation of a secondary source at 65.5 m*

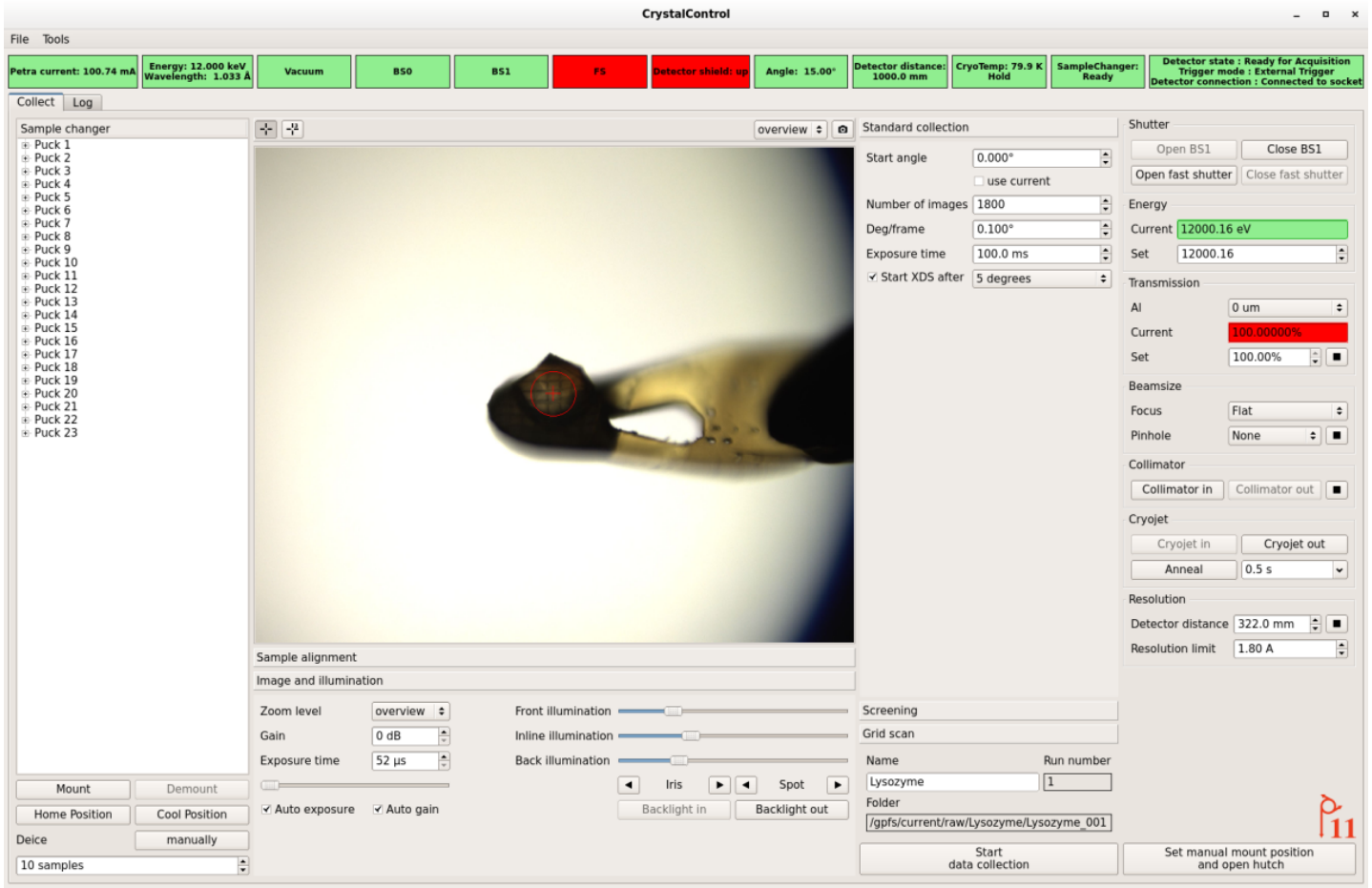


Flexibility in beam size and flux by mirror bending and apertures:

	Beam size (μm)	Flux (ph/s)	T_{xtal} (s)
Flat=>	200 x 200	3.1e12	800
Focused=>	200 x 200	6,45e12	360
	100 x 100	1e13	40
	50 x 50	1e13	10
	20 x 20	1e13	1,6
	4 x 9	1e13	0,17

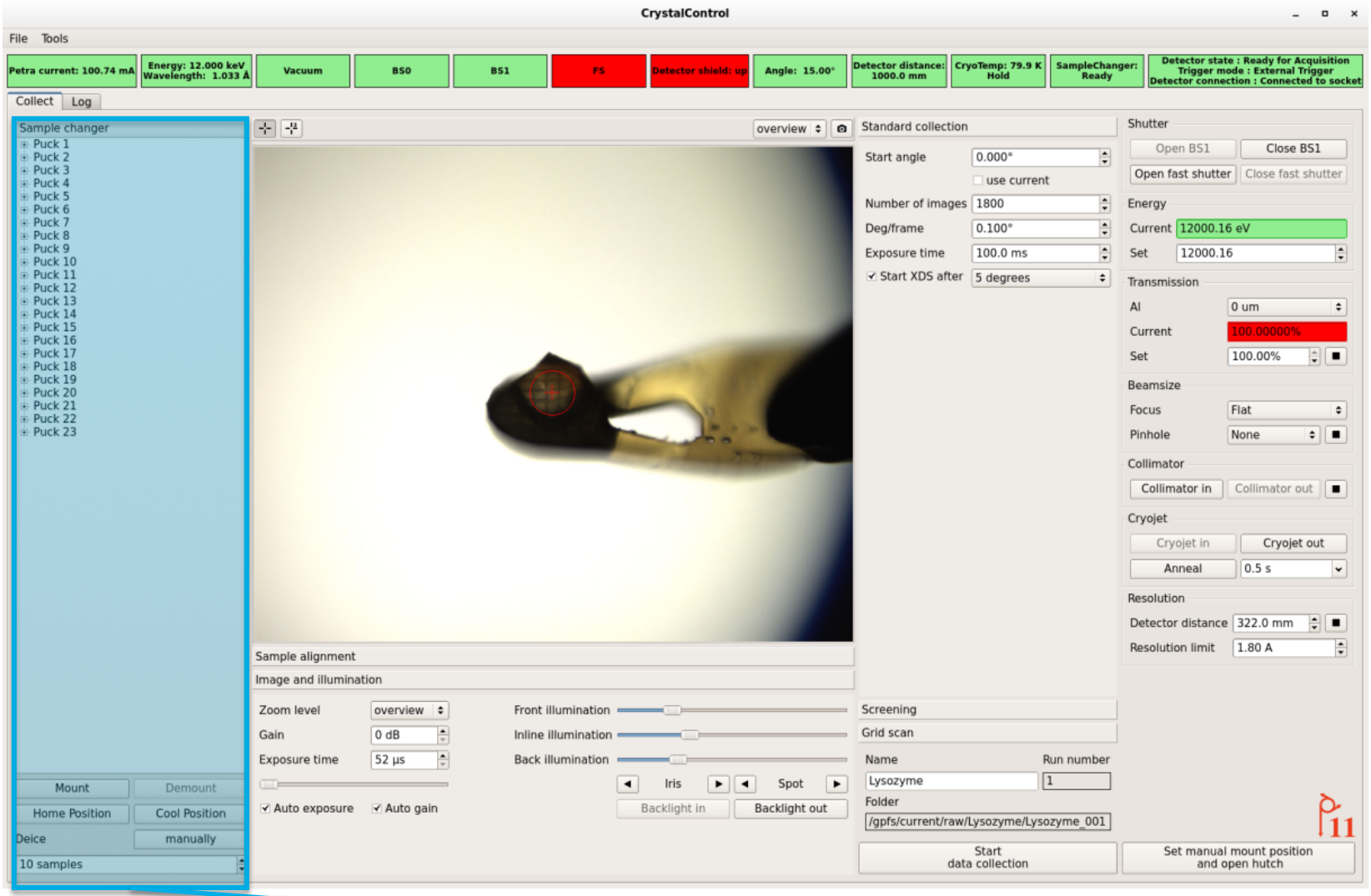
CrystalControl

- Inhouse-developed Python-based GUI for standard MX applications including SAD/MAD phasing



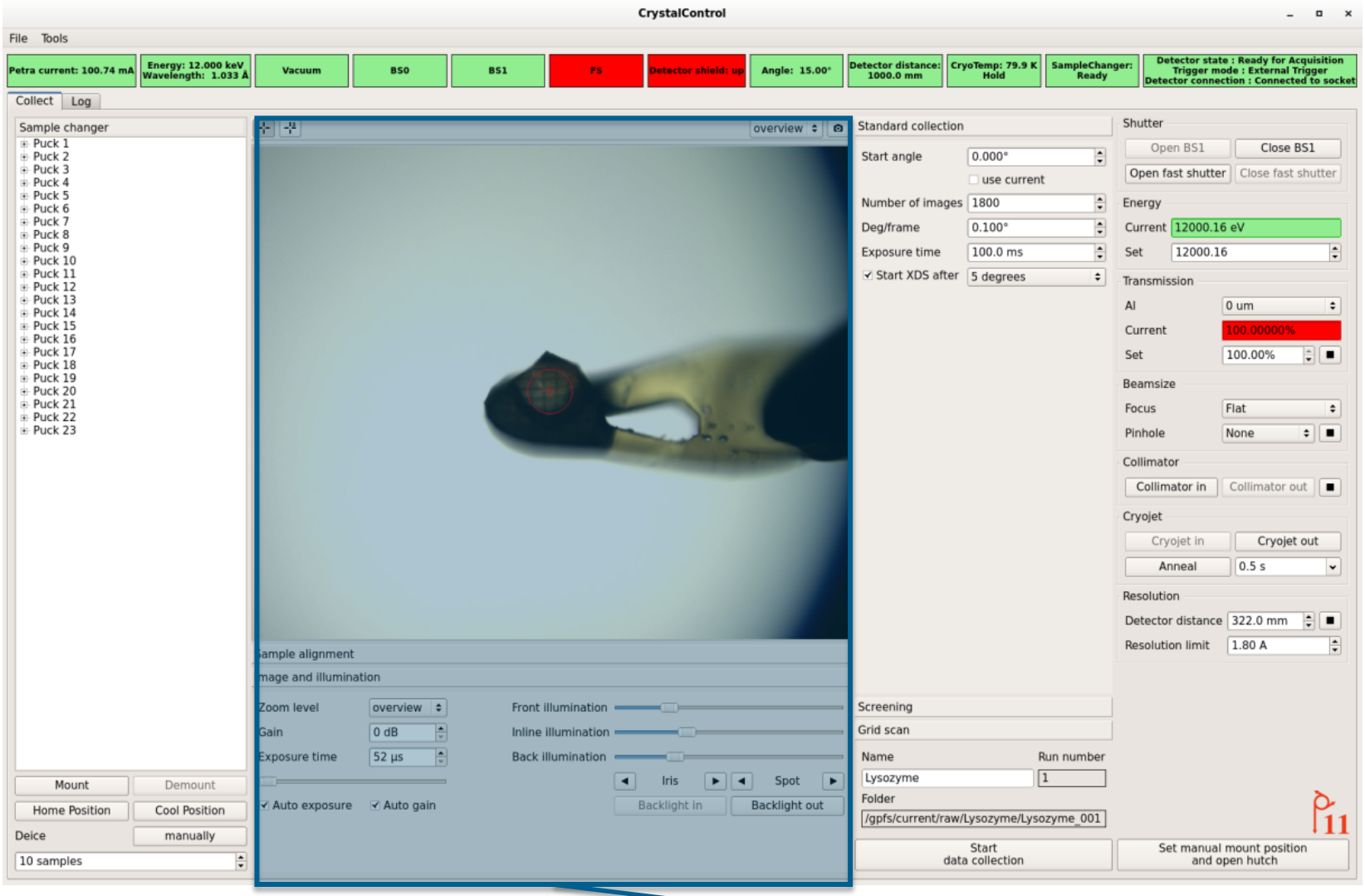
- Expert mode for beamline support (apertures, rotation axis, beam position...)

CrystalControl



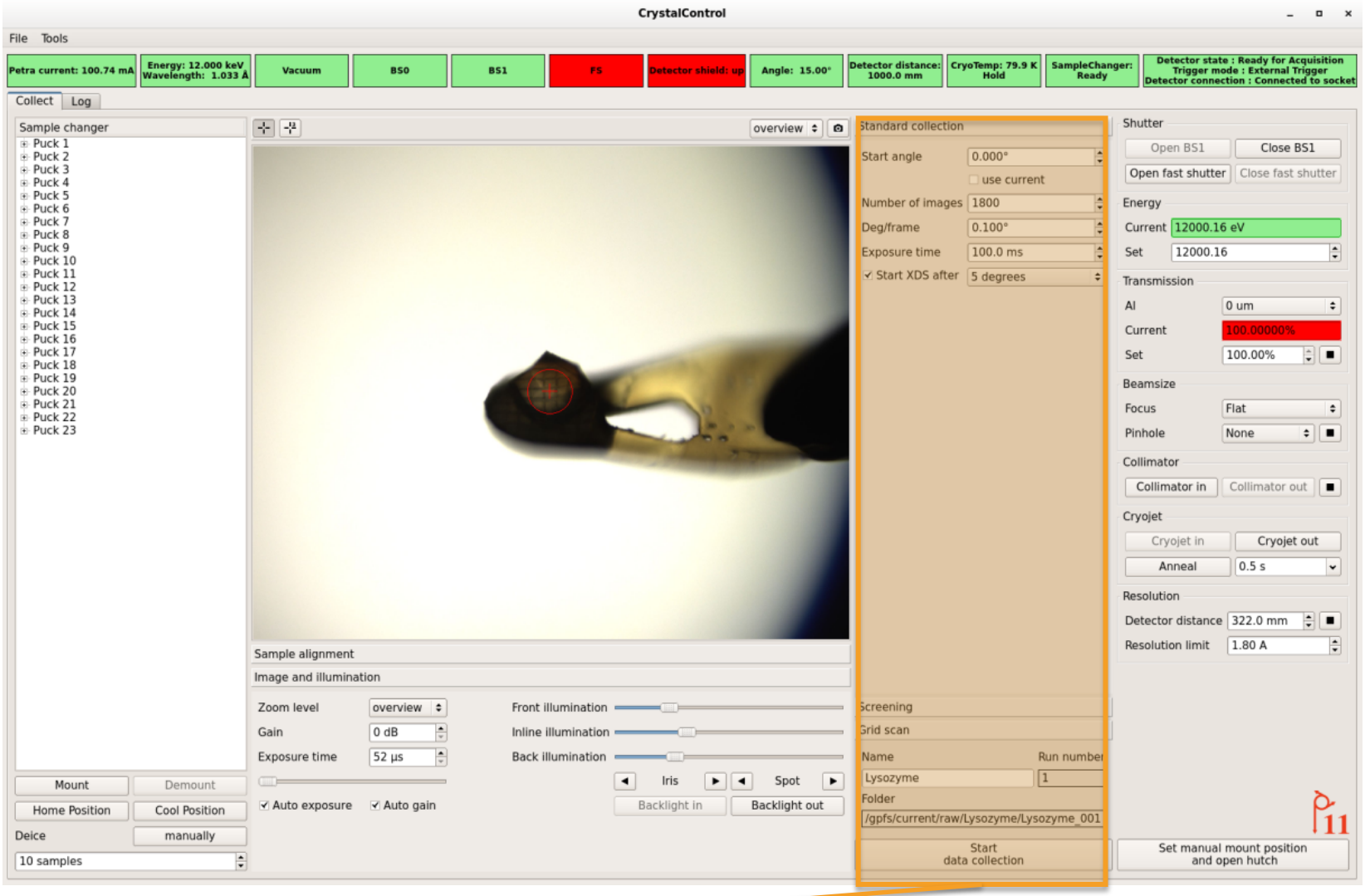
Sample changer : Puck and sample selection

CrystalControl



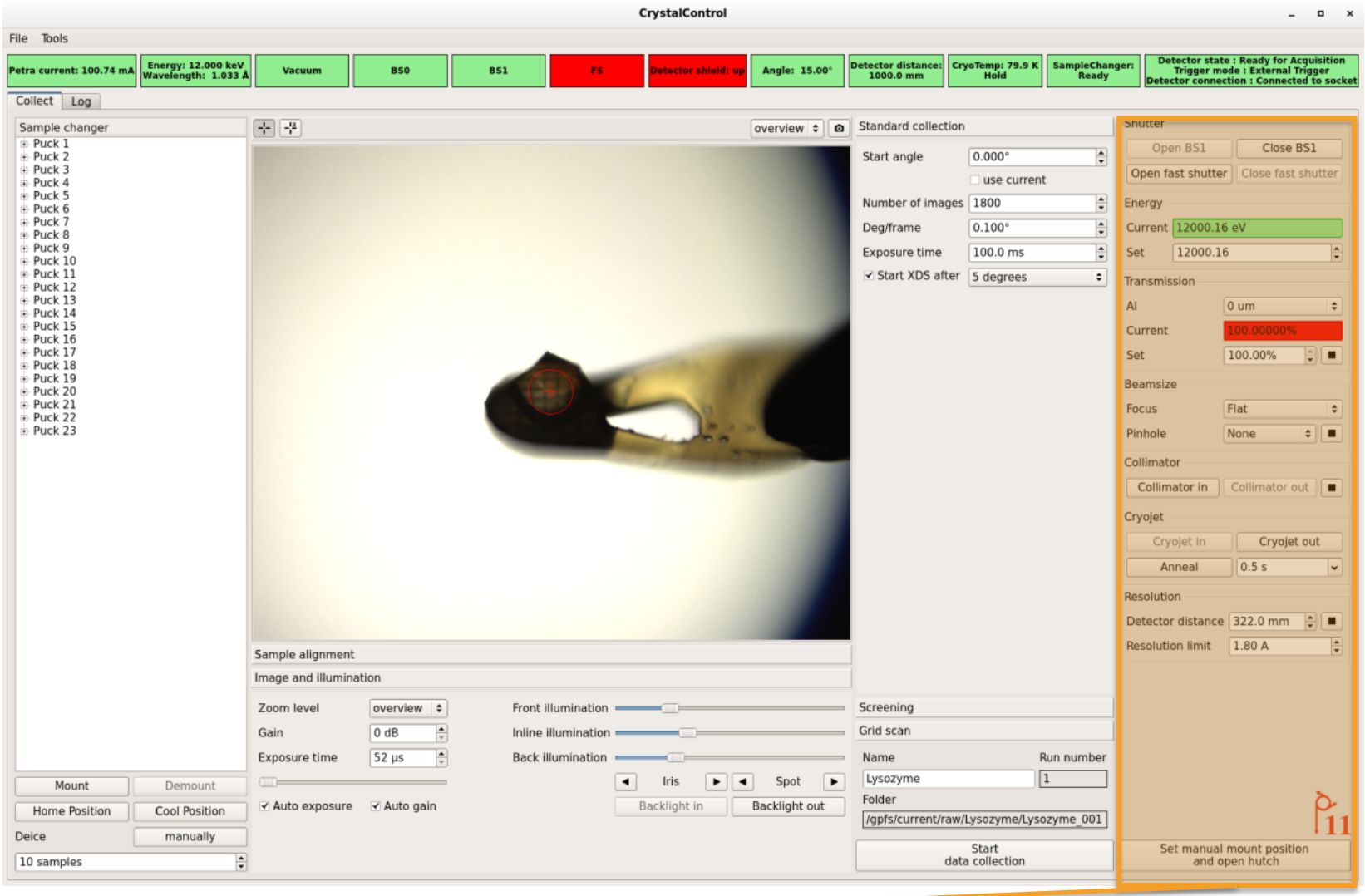
Crystal View: zoom selection and 3 clicks centering

CrystalControl



Data collection: Number of frames, exposure time, angular step

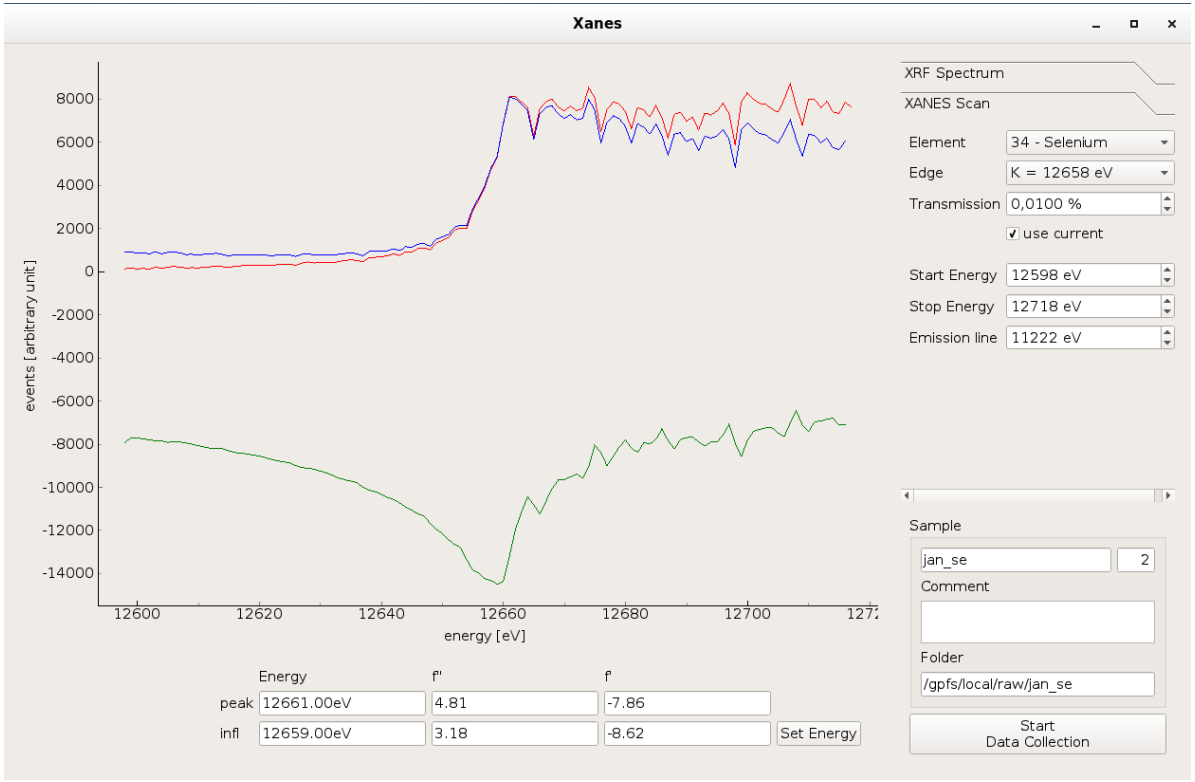
CrystalControl



Data collection: Energy, Focus selection, Pinholes, transmission, resolution (det. distance)

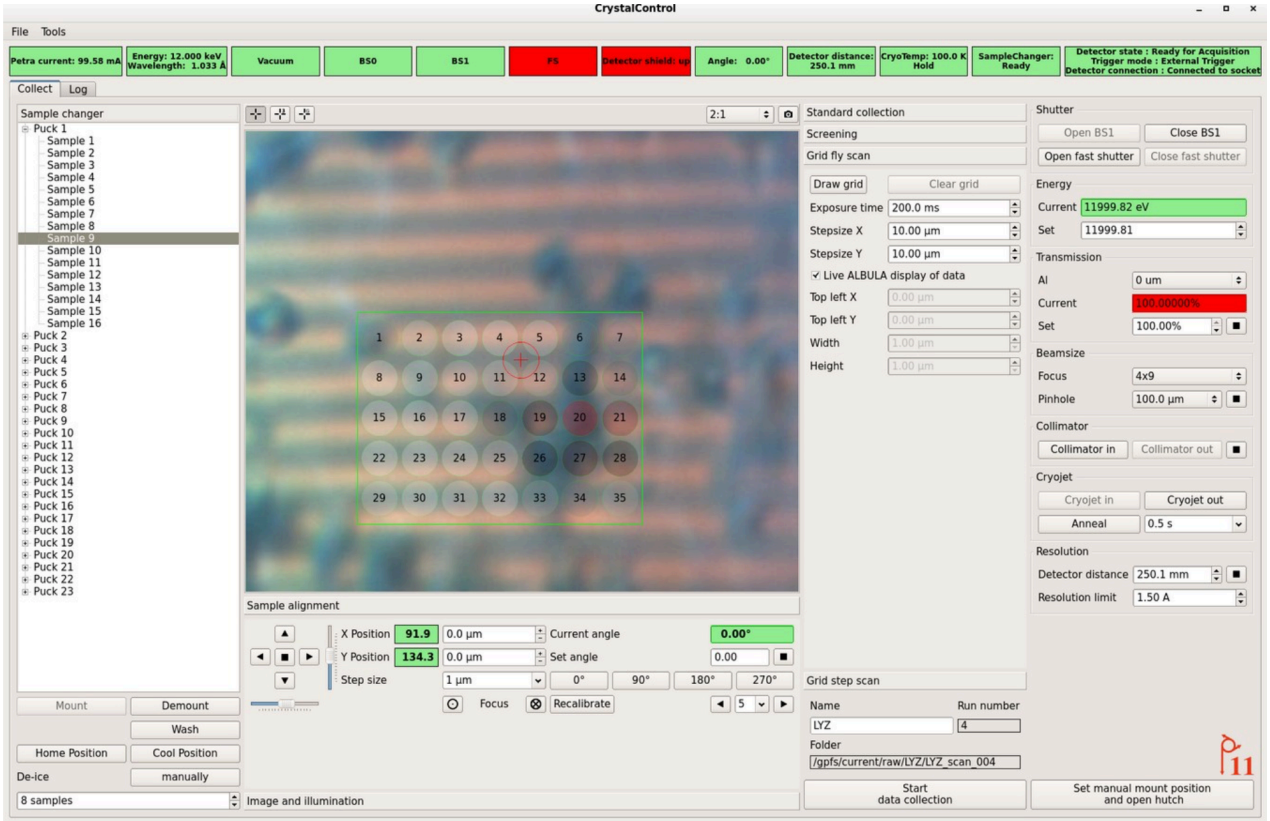
CrystalControl

- SAD/MAD phasing



CrystalControl

- ISMO scantool: GUI for fixed-target SSX, data collection with (rotation wedges) and without ϕ rotation (still images)



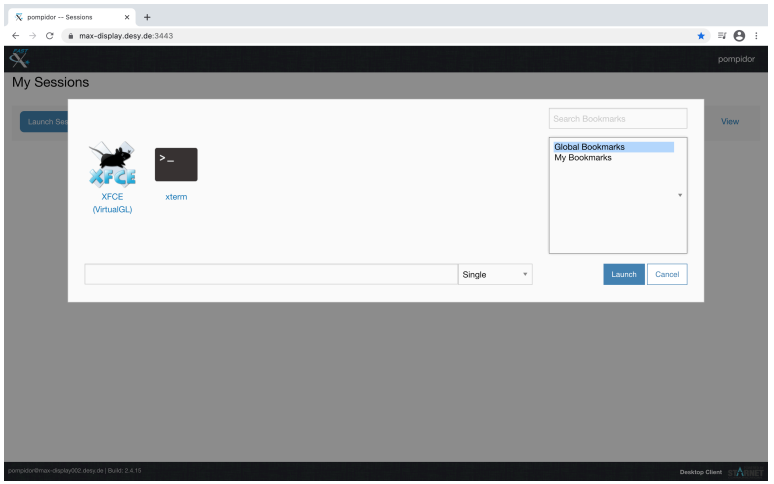
- Heat map overlayed on the sample view

Implementation of remote data collection

- Beamline control by one user only
- Access to needed functionalities only
- Monitoring of user actions
- Possibility to take back the control at any time for the local contacts
- No need of special hardware, software or OS dependencies for the user community
- Authentication against personalized account
- Remote access dependent on valid safety training

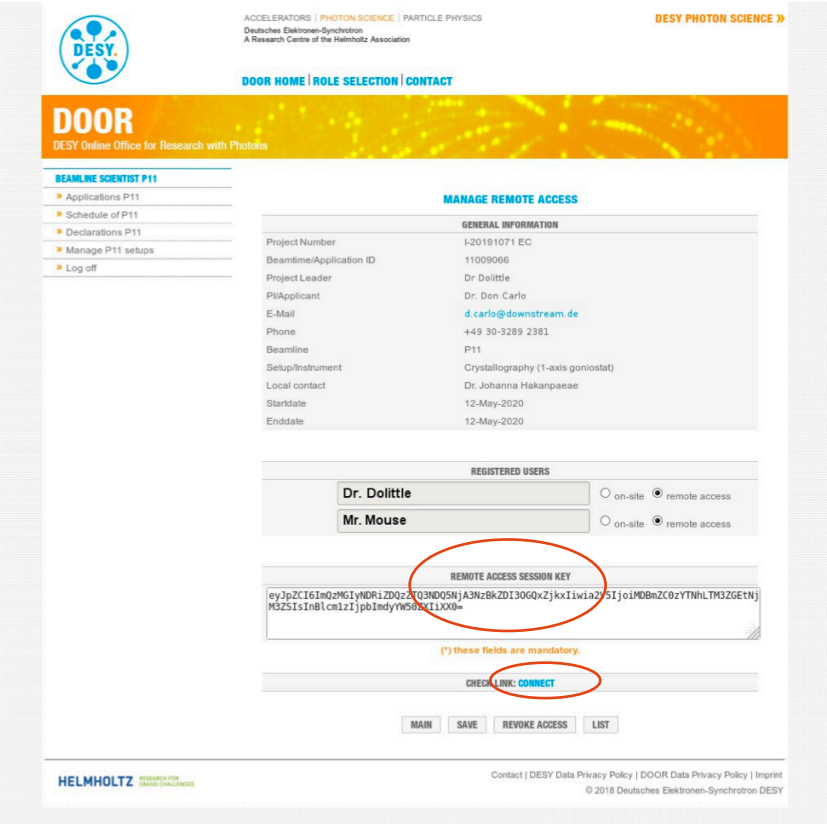
Technical Implementation (Spring 2020)

- **FastX**
- Commercial software for Linux remote desktop
- X server from a web browser
- Similar to Maxwell Cluster (computing at DESY)
- Sessions between several users with only one controlling
- Running on a dedicated host

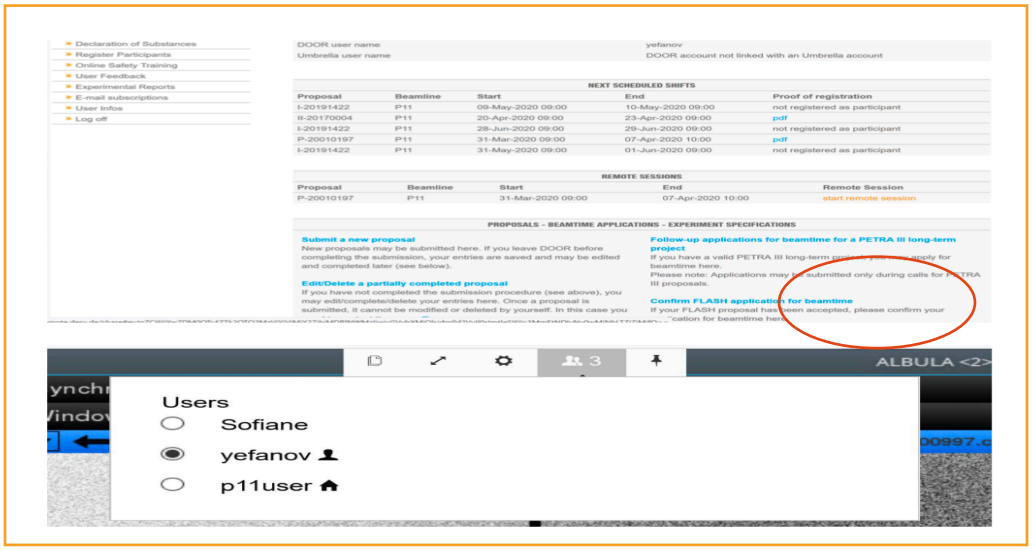


Remote identification via user database: Door

Staff view

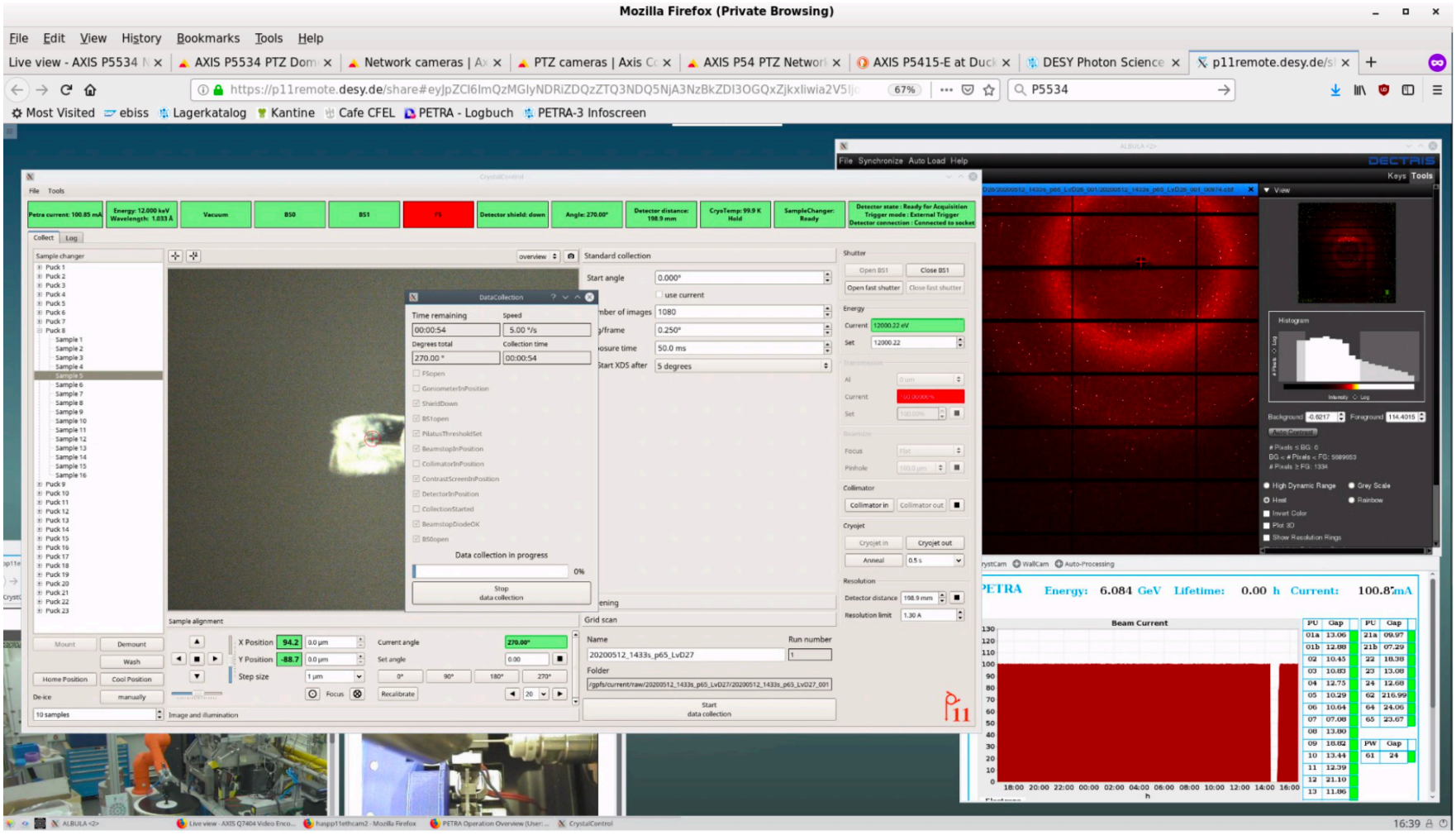


User view



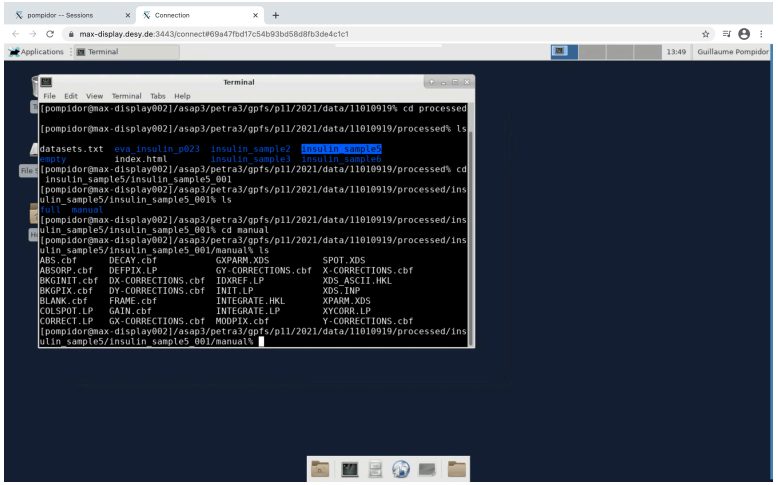
- Selection of ‘remote’, ‘onsite’ or ‘data-access’ during user registration
- Automated e-mail notification once the remote is open
- All participants can log-in at the same time from different locations, one has control over the experiment, can be swapped independently among the users
- Detailed instructions on our public webpage for shipment, remote session and data processing
- Support via zoom
- Successful operation also with users who were never onsite; connection stabile and shipments running e.g. to China and India

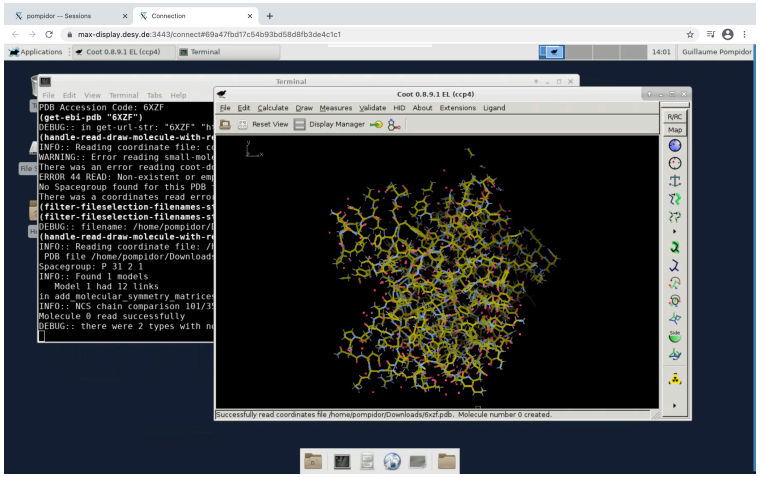
Remote data collection



Remote data processing on Maxwell Cluster

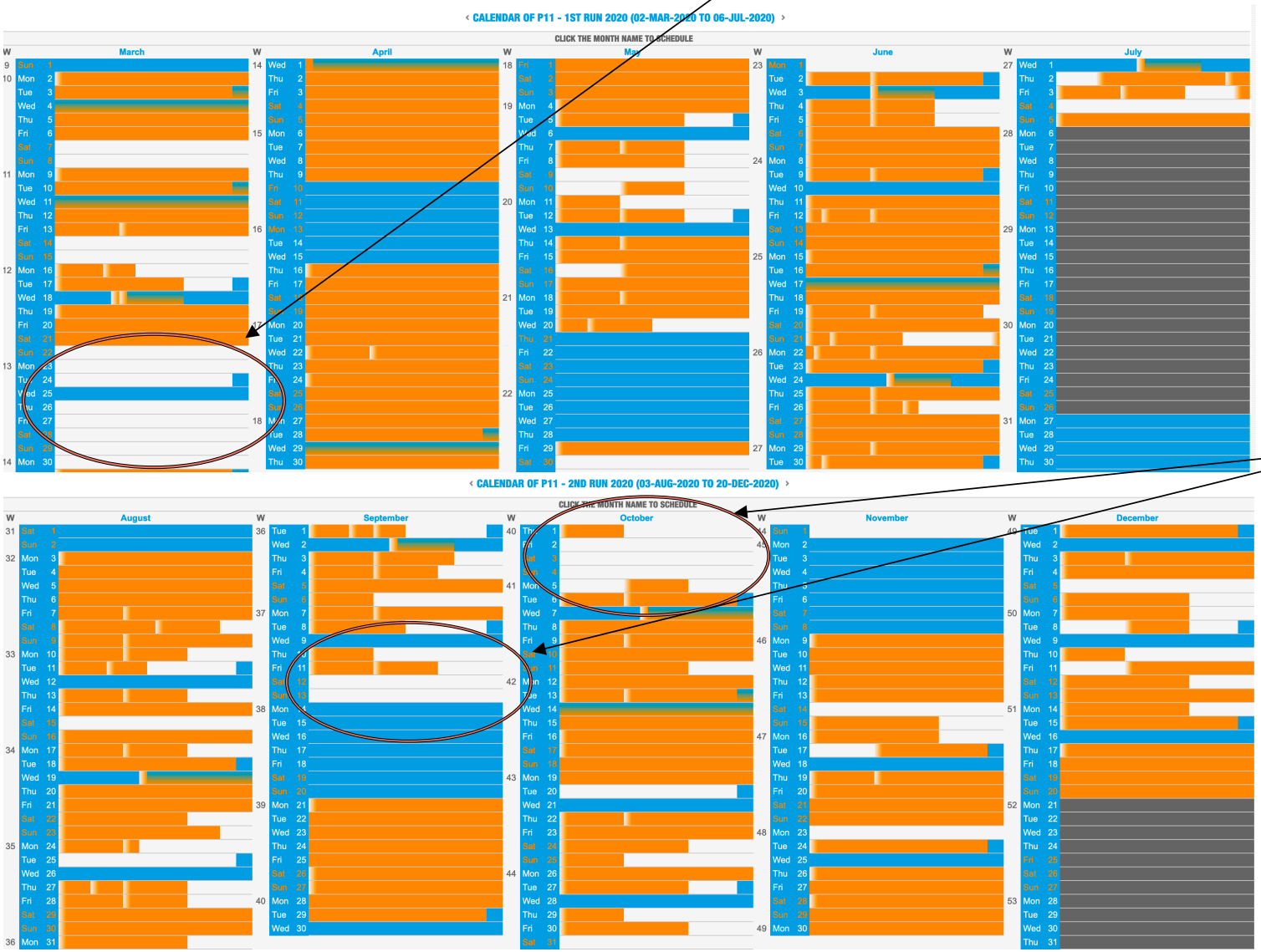
- Computing cluster for DESY
- Access via scientific account
- Backup (or via Gamma portal)
- Data processing
  - Albula, adxv
  - XDS, imosflm
  - ccp4, Phenix
  - Coot, Chimera





2020 at P11

Machine down due to the lock-down!



Gripper repairs

Pandemic vs user operations 2020

Suspended user operations mid-March - April 2020: only Fast-track open

Masks & distancing: May-October 2020

Enhanced remote at P11 since October 2020
Covid-tests since November 2020

IMPORTANT INFORMATION ON COVID-19

FOR WORKERS AND USERS AT P11 BEAMLINE

Dear User/DESY worker,

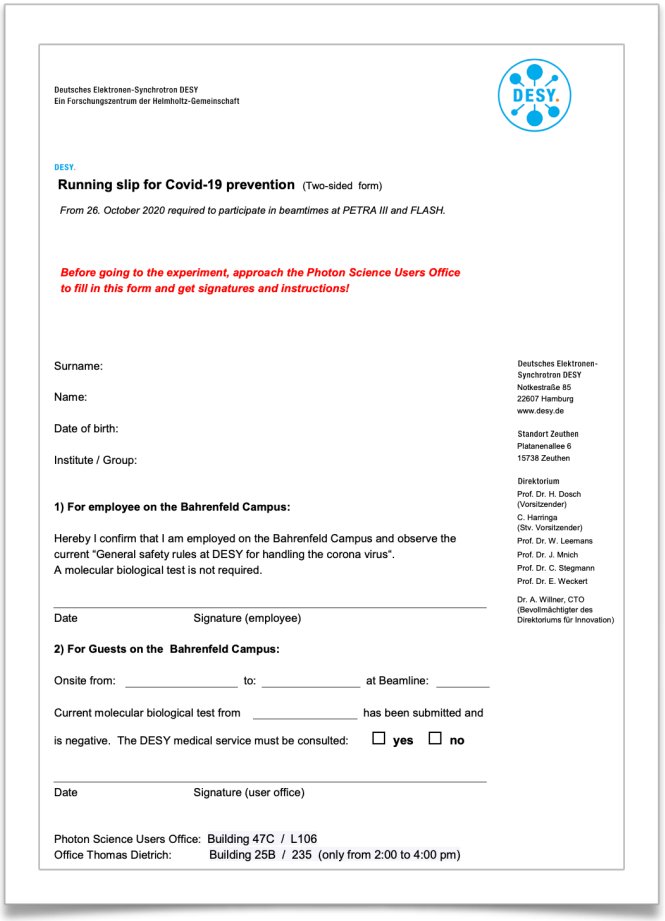
Due to the current COVID-19 restrictions, the following **safety procedures are mandatory for experiments and technical work** at P11 Beamline/DESY Campus:

1. The **maximum** number of **participants coming at DESY campus** per experiment is **3 persons.**
2. The **maximum** number of **participants on-site at the beamline** (control hutch and experimental hutch) is **2 persons**, preferably **only 1 if possible**.
3. Two persons in a **ventilated room** can work **without masks** only if they keep a **steady distance of 2 meters**.
4. If 2 persons must work in a **non-ventilated room for less than 15 minutes** at a distance **below 2 meters**, a **simple mouth/nose protection** must be worn (so-called surgical masks). Self-sewn masks are also permitted.
5. If 2 persons must work in **a non-ventilated room for more than 15 minutes** at a distance **below 2 meters**, **FFP3 masks must be worn**, and provisionally also FFP2 masks.
6. **Gloves** should be always used if possible.
7. Please **disinfect your hands** and any shared equipment (keyboards etc) after use.

In case of doubts, please ask a P11 Team member.

Thank you for your collaboration,

Your P11 Team



Deutsches Elektronen-Synchrotron DESY
Ein Forschungszentrum der Helmholtz-Gemeinschaft

DESY.

Running slip for Covid-19 prevention (Two-sided form)

From 26. October 2020 required to participate in beamtimes at PETRA III and FLASH.

Before going to the experiment, approach the Photon Science Users Office to fill in this form and get signatures and instructions!

Surname:

Name:

Date of birth:

Institute / Group:

1) For employee on the Bahrenfeld Campus:

Hereby I confirm that I am employed on the Bahrenfeld Campus and observe the current "General safety rules at DESY for handling the corona virus".
A molecular biological test is not required.

Date Signature (employee)

2) For Guests on the Bahrenfeld Campus:

Onsite from: _____ to: _____ at Beamline: _____

Current molecular biological test from _____ has been submitted and

is negative. The DESY medical service must be consulted: ☐ **yes** ☐ **no**

Date Signature (user office)

Photon Science Users Office: Building 47C / L106
Office Thomas Dietrich: Building 25B / 235 (only from 2:00 to 4:00 pm)

Deutsches Elektronen-Synchrotron DESY
Notkestraße 85
22607 Hamburg
www.desy.de

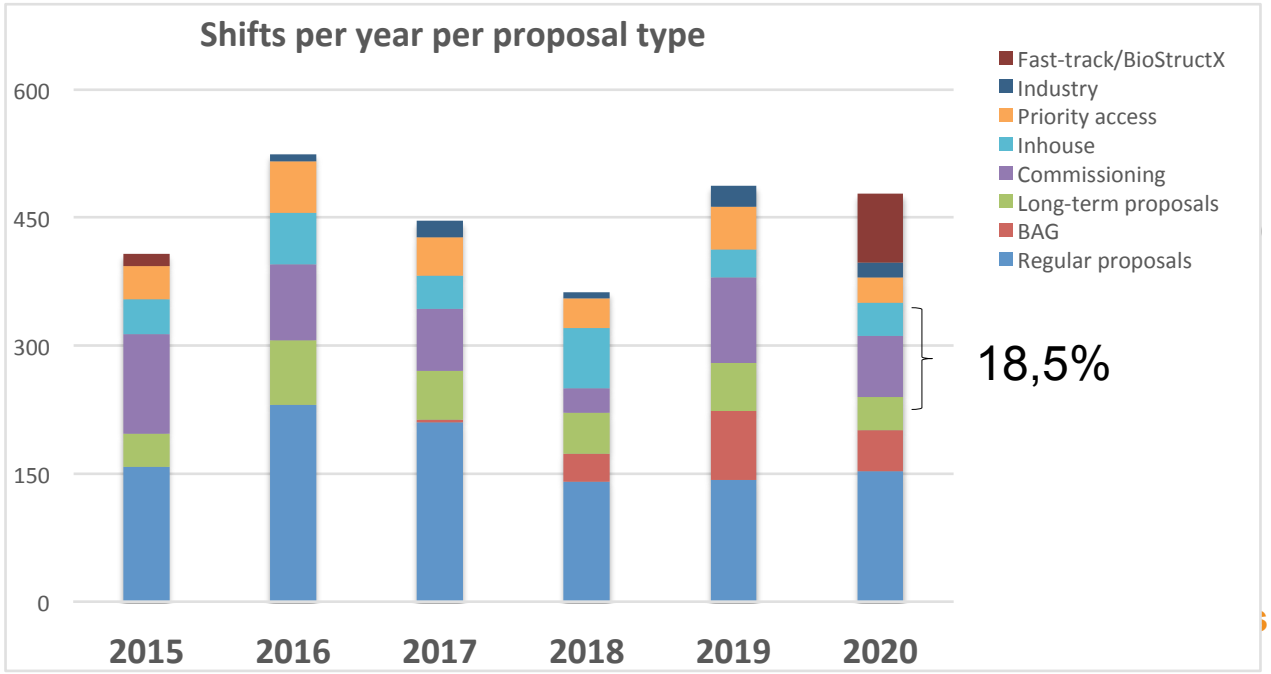
Standort Zeuthen
Platanenallee 6
15738 Zeuthen

Direktorium
Prof. Dr. H. Dosch (Vorsitzender)
C. Harringa (Stv. Vorsitzender)
Prof. Dr. W. Leemans
Prof. Dr. J. Mnich
Prof. Dr. C. Stegmann
Prof. Dr. E. Weckert

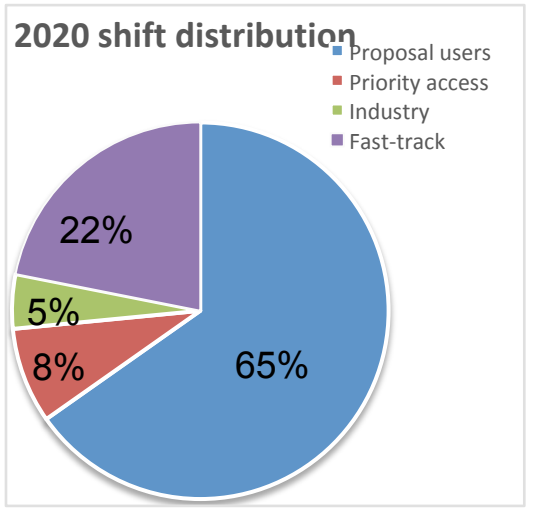
Dr. A. Willner, CTO (Bevollmächtigter des Direktoriums für Innovation)

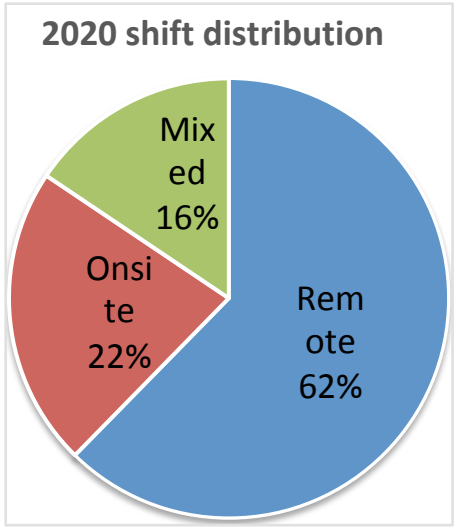
User statistics

All shifts



Excluding inhouse/ commissioning

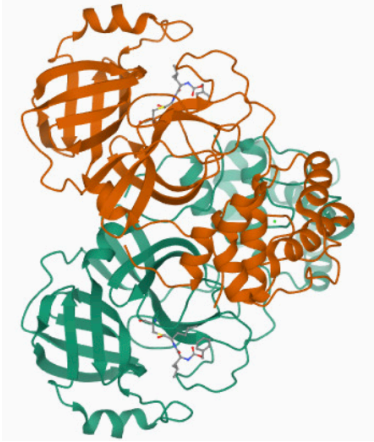




Numbers extracted from shifts actually carried out
Inhouse and commissioning are by P11 staff only
Serial Synchrotron Crystallography with tape-drive 24 shifts, with chips 18 shifts
Some empty days due to repairs and short-notice cancellation
11 shifts given out from INH for ‘friendly users’ i.e. users with no valid proposal => need for rolling access scheme

SARS-CoV2 -related research arising from P11

Also outside of the fast-track procedure



37 structures deposited from P11 (Main Protease)

- 30 from the fast-track screening campaign by Alke Meents
- 3 through other fast-track projects
- 2 through priority access
- 2 through regular proposals

Publications:

“Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved α-ketoamide inhibitor” (Zhang et al., 2020, Science, 368, 409-412)

“Catalytic cleavage of HEAT and subsequent covalent binding of the tetralone moiety by the SARS-CoV-2 main protease” (Günther et al., 2020)

“SARS-CoV-2 MPro inhibitors and activity base probes for patient-sample imaging” (Rut et al., Nat. Chem. Biol., 2020)

“Repurposing the HCV NS3–4A protease drug boceprevir as COVID-19 therapeutics“ (Oerlemans et al., RSC Medicinal Chemistry 2021)

Thank you

Johanna Hakanpää

Sofiane Saouane

Eva Crosas

Spyros Chatziefthymiou

Jan Meyer

Bernhard Kistner

Jakob Urbschat

Jan-Peter Kurz