



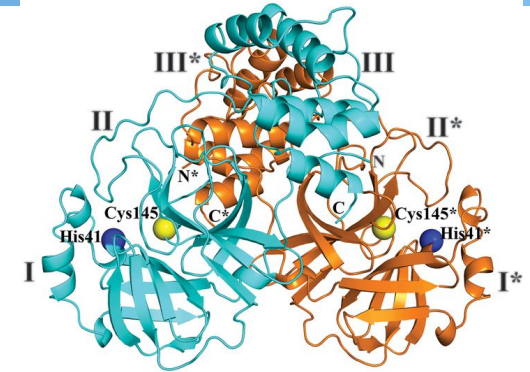
Status of MXCuBE Beamline Control at BESSY II

Michael Hellmig,
on behalf of the HZB-MX group

MXCuBE/ISPyB Joint Meeting, 29.06.-30.06.2020,
Virtual Meeting, organized by ALBA (Barcelona)

- **Structure of the CoV2 main protease**

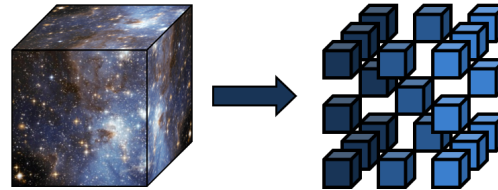
- Solved by Hilgenfeld lab (University Lübeck) at BESSY II MX beamlines
- Essential enzyme for the virus, potential drug target



Zhang et al., Science, 2020

- **Crystallographic Fragment Screening at BESSY II**

- F2X-Entry Screen representing chemical space of fragments (96 compounds)

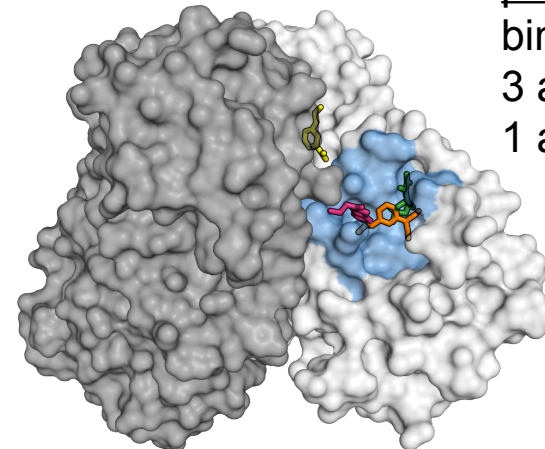


Wollenhaupt and Metz et al., Structure, accepted

- **Drug Design against CoV2 protease initiated**

- Collaboration: BESSY MX / Uni Lübeck / DESY
- F2X-Entry Screen vs CoV2 main protease

preliminary results:
binders identified:
3 at **active site**
1 at dimer interface



Wollenhaupt et al., unpublished

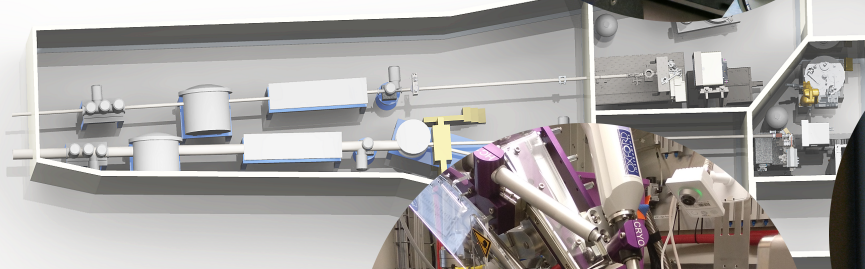
MX experimental floor at BESSY II

BL 14.1 MAD

- MD2 with MK3
- **Pilatus3 6M 25 Hz**
- CATS: 90 SPINE samples
- MXCuBE 2.2 Qt4

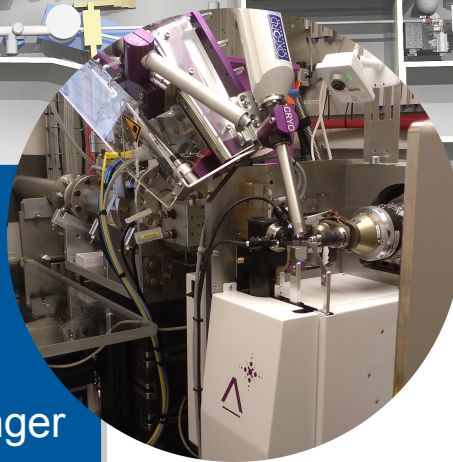


- standard user operation schedule:
24/5 (Tuesday to Saturday)



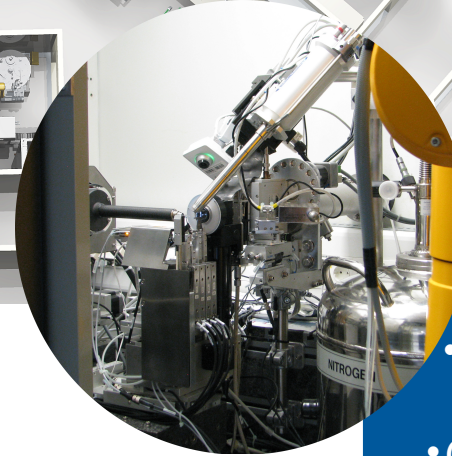
BL 14.3 13.8 keV

- MD2S with MK3
- **Pilatus2 6M 12 Hz**
- HClab & REX nozzle changer
- MXCuBE 2.2 Qt4



BL 14.2 MAD

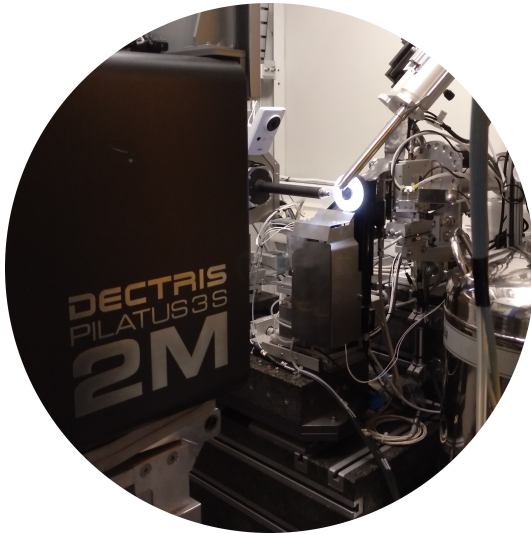
- **Nanodiff goniometer**
- Pilatus3 2M
- GROB: 294 SPINE & Unipuck samples
- MXCuBE 2.2 Qt4





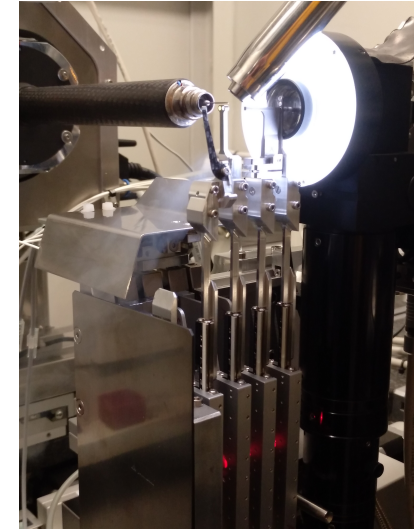
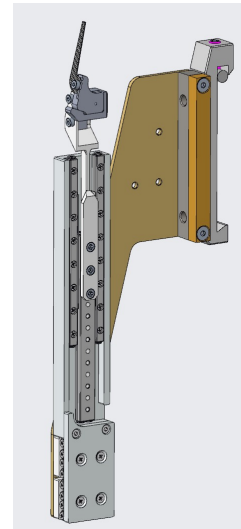
BL 14.1 MAD

- Pilatus3S 6M
 - installed February 2020
 - first user experiments March 2020
- PPU-XL under commissioning
 - more reliable data acquisition & faster data processing
 - full control-system integration in summer shutdown
- Irelec CATS upgrade
 - rebuild to Uni-puck sample standard
 - ~50% more capacity
 - scheduled for summer shutdown



BL 14.2 MAD

- new Smaract beam-shaping devices for the Nanodiff diffractometer
 - longer travel range, faster operation
 - more reliable, better protection against contamination with LN2
 - sample exchange time ~ 1 minute



- GROB sample changer
 - continuously migrate from SPINE to Uni-puck standard

- installation finished December 2019
- user operation January 2020
- DESY Smaract MCS2 Tango DS



BL 14.3 13.8 keV

- Pilatus2 6M 12 Hz
 - re-use old BL14.1 detector
- installation in progress
 - delayed due to Corona shutdown
- mechanical adaptations currently in progress
- control-system integration in summer shutdown
- re-opening planned for winter semester

MXCuBE: status and future plans

- current status:
 - MXCuBE 2.2 Qt4 running on all three HZB-MX beamlines

- current issues:

- resources mostly spend on new hardware, testing, maintenance, training
- commissioning time at the beamline strongly limited
- MXCuBE control computer at the beamline
 - Debian 7, **32-bit**

No progress in first semester 2020!

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- summer-shutdown plans:

- modernization of MXCuBE control computer
- Debian 9/10, 64-bit

- **new (Docker-based?) installation of MXCuBE3 and ISPyB**

- HardwareRepository → branch 3.x
- initial testing of MXCuBE3 with mockup hardware objects already started

- MXCuBE2 version available as backup solution

No progress in first semester 2020!

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Jan Wollenhaupt



The MXCuBE collaboration



Industrial partners:



Thank you for your attention.

Questions?