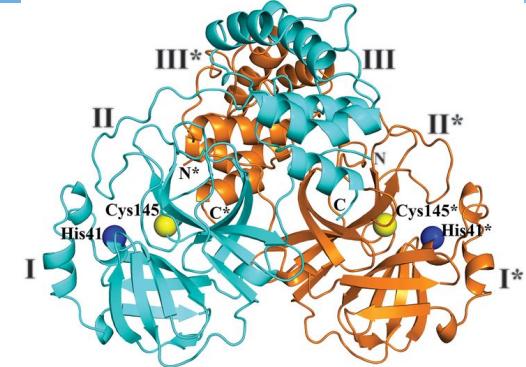


Status of MXCuBE Beamline Control at BESSY II

Michael Hellmig,
on behalf of the HZB-MX group

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

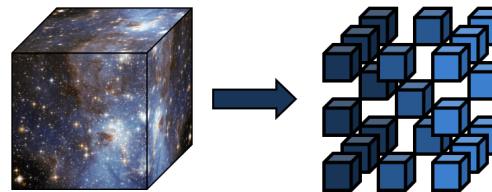
- **Structure of the CoV2 main protease**
 - Solved by Hilgenfeld lab (University Lübeck) at BESSY II MX beamlines
 - Essential enzyme for the virus, potential drug target



Zhang et al., Science, 2020

- **Crystallographic Fragment Screening at BESSY II**

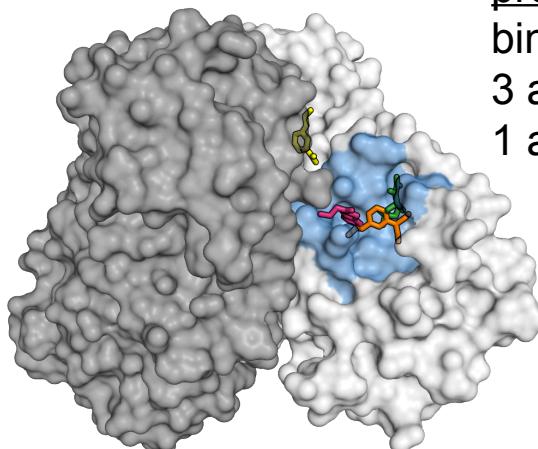
- F2X-Entry Screen representing chemical space of fragments (96 compounds)



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

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





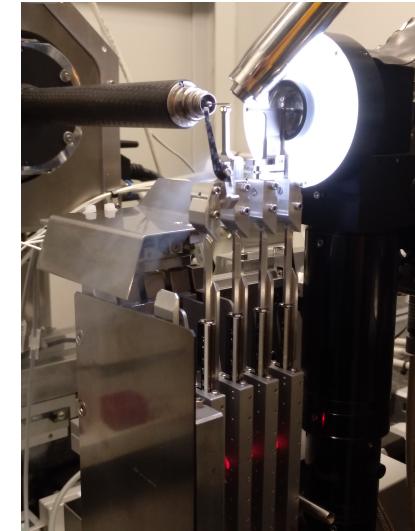
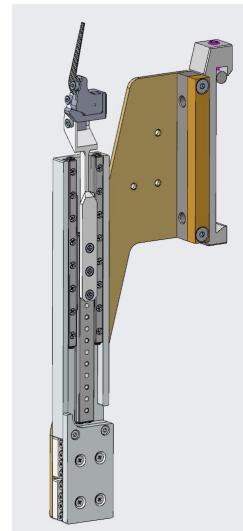
BL 14.1 MAD

- 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

- current status:

- MXCuBE 2.2 Qt4 running on all three HZB-MX beamlines

- current issues:

- resources mostly spent on maintenance, testing, ...
- configuration time at the beamline strongly limited
- old MXCuBE control computer at the beamline
 - Debian 7, **32-bit**

No progress in first semester 2020!

MXCuBE: status and future plans

- current status:

- MXCuBE 2.2 Qt4 running on all three HZB-MX beamlines

- current issues:

- resources mostly spent on maintenance, testing, ...
- configuration time at the beamline strongly limited
- MXCuBE control computer at the beamline
 - Debian 7, **32-bit**

- 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!

Acknowledgements

BESSY-MX team

Manfred Weiss

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Christine Gless

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Uwe Mueller

Michael Steffien

Helena Taberman

Jan Wollenhaupt



The MXCuBE collaboration



Industrial partners:

NatX-ray

IRELEC

DECTRIS®

ARINAX
Advanced Research Instrumentation for Neutrons & X-rays

Thank you for your attention.

Questions?