

HEC20 – Program

Thursday, September 28th, 2017

12:00 – 16:00 Arrival & registration

16:00 – 16:10 **Marcin Nowotny and Matthias Bochtler (IIMCB, Poland)** – Welcome & opening remarks

Session I – Chair: Marcin Nowotny

16:10 – 16:30 **Michael Kugler (ASCR, Czech Republic)** – Carboranes and metallacarboranes as highly selective inhibitors of cancer specific Carbonic Anhydrase IX

16:30 – 16:50 **Nina Schwemmlein (HZI, Germany)** – Insights into diffocins – crystal structure of a phage-tail-like protein from Clostridium difficile

16:50 – 17:00 **Christin Reuter (Jena Bioscience)** – *Frag Xtal Screen* for direct crystallographic fragment screening

17:00 – 17:20 **Sascha Walzer (FAU, Germany)** – Characterizing herpesviral nuclear egress complexes

17:20 – 17:40 Coffee break

Session II – Chair: Sutapa Chakrabarti

17:40 – 18:00 **Julian Pfahler (Uni Bayreuth, Germany)** – Crystal structure of a PARP-1 complex with an isoform specific inhibitor

18:00 – 18:10 **Marcus Winter (Rigaku Oxford Diffraction)** – Advances in X-ray crystallography

18:10 – 18:30 **Zora Nováková (IBT CAS, Czech Republic)** – Sulfonamides and phosphoramidates as inhibitors of bimetallic peptidases: structural characterization

18:30 – 18:50 **Ronja Janke (FU Berlin, Germany)** – Insights into the catalytic mechanism of CotB2

18:50 – 19:00 **Kevin Denkmann (Dunn Labortechnik)** – “Four Corner Grid” and “Wobble Concentration Grid”

19:00 – 20:00 Dinner

HEC Lecture – Chair: Matthias Bochtler

20:00 – 21:00 **Tim Clausen (IMP Vienna, Austria)** – The phospho-kiss of death: Revealing a specific phosphor-signal that serves as degradation tag

21:00 – late Discussion & Bar

Friday, September 29th, 2017

Session III – Chair: Jan Dohnalek

08:30 – 08:50 **Dominic Pühringer (Uni Vienna, Austria)** – Structural and functional characterization of phosphoglucomutase 5

08:50 – 09:10 **Giridhar Shivalingaiah (MUI, Austria)** – t.b.a.

09:10 – 09:30 **Martin Bommer (MDC Germany)** – Interaction of NKX2.1 with DNA

09:30 – 09:40 **James M. B. Gordon (Molecular Dimensions)** – Improving Crystals by Collaboration - Innovation from Molecular Dimensions

09:40 – 10:00 **Anna Piasecka (IIMCB, IBB PAS, Poland)** – Structural characterization of Anbu, a novel proteasome-like protein that does not form rings

10:00 – 10:20 **Yvette Roske (FMP, Germany)** – Structural rearrangements of TasA in *B. subtilis* biofilm formation

10:20 – 10:30 **Patrick Shaw Stewart (Douglas Instruments Ltd.)** – Microseed matrix-screening (rMMS): introduction, theory, practice and a new technique for membrane protein crystallization in LCP

10:30 – 10:55 Coffee break

10:55 – 11:00 HEC20-photo

Session IV – Chair: Wulf Blankenfeldt

11:00 – 11:20 **Karolina Górecka (IIMCB, Poland)** – RuvC resolvase: from structure to mechanism of action

11:20 – 11:40 **Vidhyadhar Nandana (FU Berlin, Germany)** – Structural and biochemical analysis of UPF1-assisted histone mRNA decay.

11:40 – 11:50 **Hans van Beek (Formulatrix Inc.)** – Sensitive detection of RNA microcrystals using SONICC imaging

11:50 – 12:10 **Agnieszka Pietrzyk-Brzezińska (Lodz Tech Uni, Poland)** – *Escherichia coli* HrpB – a DExH-box helicase

12:10 – 12:30 **Sebastian Glatt (MPI, Uni Cracow, Poland)** – tRNA modifications protect the proteome

12:30 – 12:50 **Barbora Kascakova (Uni České Budějovice, Czech Republic)** – Molecular-Biological and Structural Studies of Avian Reovirus Protein σ NS

12:50 – 13:00 **Vernon Smith (Bruker AXS GmbH)** - Automating the D8 VENTURE to improve the productivity of home-lab crystallography

13:00 – 14:00 Lunch

14:00 – 18:00 Social event

Session V – Chair: Kristina Djinovic-Carugo

18:00 – 18:20 **Julia Kratky (Uni Leipzig, Germany)** – Structural studies on the substrate and cofactor binding mode of FAD-dependent monooxygenases

18:20 – 18:40 **Maria Rutkiewicz-Krotewicz (Uni Lodz, Poland)** – Structural insights into the mechanism of β -D-galactosidase with transglycosylation activity

18:40 – 18:50 **Andreas Förster (DECTRIS Ltd.)** – Gentle data collection at laboratory X-ray sources

18:50 – 19:10 **Terezia Kovalová (VSCHT, Czech Republic)** – Novel quaternary structure of glycosidase from family GH 29 and its relation to function

19:10 – 19:30 **Tobias Bock (MDC, Germany)** – Futurama meets structural biology – mechanism of an unusual myxobacterial decarboxylase in alternative isovaleryl CoA biosynthesis

19:30 – 19:40 **Wim Voorhout (Thermo Fisher Scientific)** – Cryo-electron microscopy: An indispensable solution for Structural Biology

20:15 – late Gala Dinner & Dance

Saturday, September 30th, 2017

Session VI – Chair: Sebastian Glatt

08:30 – 08:50 **Birthe Steigemann (Uni Halle, Germany)** – Structure determination of DltD from *Streptococcus pneumoniae*

08:50 – 09:10 **Jana Škerlová (ASCR, Czech Republic)** – Crystal structure of native β -N-acetylhexosaminidase from *Aspergillus oryzae*: substrate specificity, stability, and regulation by propeptide

09:10 – 09:30 **Joanna Śliwiak (IBC PAS, Poland)** – Melatonin binding by plant PR-10 proteins

09:30– 09:50 **Artur Biela (MCB, Poland)** – Unusual/impossible geometry of protein cages

09:50– 10:00 **Ralf Siebrecht (ARINAX)** – Modern Sample Visualization in MX-Crystallography

10:00 – 10:30 Coffee break

Session VII – Chair: Milton T. Stubbs

- 10:30 – 10:50 **Dariusz Brzezinski (Poznan Tech Uni, Poland)** – Using Machine Learning to Automate Ligand Recognition in Electron Density
- 10:50 – 11:10 **Karine Röwer (HZB, Germany)** – The HZB Fragment-Screening (FS) Manager
- 11:10 – 11:30 **Christian Feiler (HZB, Germany)** – Facilities for Macromolecular Crystallography at the Helmholtz-Zentrum Berlin
- 11:30 – 11:40 Announcement of HEC21
- 11:40 – 11:50 **Matthias Bochtler & Marcin Nowotny (IIMCB, Poland)** – HEC-prize and concluding remarks
- 12:00 – 13:00 Lunch & departure