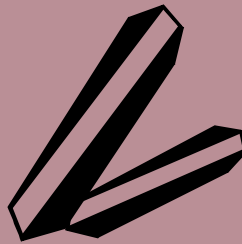


Programme

HEC²⁵

Salem, Germany, 2023



21st-23rd September 2023

Day 1: Thursday, 21st September 2023

from 11:00 registration

14:45-15:00 Welcome and opening remarks (Michael Lammers)

15:00-15:15 Presentation of the new HEC-groups
1. **Ingrid Span**, FAU Erlangen-Nürnberg
2. **Johanna Hakanpää**, PETRA III, DESY/Hamburg

Session 1: Structure-function analyses in bacterial and viral infection
chairs: Miriam Linnert, Norbert Sträter

15:15-15:30 **Frank Lennarz** /Berlin [Manfred Weiss group]
Title: "Fragment screening against SARS CoV 2 proteins Nsp1 and Nsp3b"

15:30-15:45 **Xinyuanyuan Sun** /Lübeck [Barbora Kašćáková group]
Title: "The SARS-Cov-2 main protease as a target for antivirals: Crystal structures, new inhibitors, and mutants"

15:45-16:00 **Ole Schmöker** /Greifswald [Michael Lammers group]
Title: "Elucidating the role of CE-clan protease-related bacterial virulence factors with DUB/Act activity in bacterial infection"

16:00-16:15 **Michael Krummhaar** /Potsdam [Christian Roth group]
Title: "Structural and functional insight into Glycocin-glycosyltransferases"

16:15-17:00 Coffee break and industrial exhibition

Session 1 (*continued*)

17:00-17:15 **Dominik Rafalski** /Warsaw [Matthias Bochtler group]
Title: "Structural characterisation of CRISPR-associated Rossmann Fold (CARF) family members: Csx15 and Csx20"

17:15-17:30 **Stephanie Himpich** /Berlin [Markus Wahl group]
Title: "Structural and functional analysis of a putative phage defense system in enterohemorrhagic *E. coli*"

17:30-17:35 *flash talk:* **Lea Jänisch** /Berlin [Manfred Weiss group]
Title: "Fragment Screening to tackle bacterial biofilm defense: TasA Inhibitor development guided by crystallography"

17:35-17:40 *flash talk:* **Laila Benz** /Berlin [Manfred Weiss group]
Title: "Towards new SARS-CoV-2 inhibitors through crystallographic compound screening"

Session 2: Inhibitor development and disease
chairs: Markus Wahl, Manfred Weiss

17:40-17:45 *flash talk:* **Paulina Borysiuk** /Poznań [Krzysztof Brzeziński group]
Title: "Structure based design of KDM4 proteins inhibitors for cancer therapy"

17:45-18:00 **Yvonne Scarmacia** /Wien [Kristina Djinović group]
Title: "Uncovering Fatigue Endurance in Alpha-actinin-3 Deficient Runners/population: The Structural and Biochemical Analysis of Calcineurin:FATZ-1 interaction"

18:00-18:15 **Anna Koutská** /České Budějovice [Ivana Smatanová group]
Title: "Investigating the effect of neurodevelopmental disorder missense variants on cognitive function"

18:15-18:30 **Lucia Motlová** /Vestec [Cyril Bařínka group]
Title: "Oxadiazole-based inhibitors of histone deacetylase 6 are hydrolyzed upon enzyme engagement"

18:30-18:35 *flash talk:* **Adela Fejfarová** /Prague [Pavlna Řezáčová group]
Title: "Structural and biophysical characterization of cancer-related enzyme Carbonic Anhydrase IX"

18:35-18:40 *flash talk:* **Jialing Song** /Hamburg [Johanna Hakanpää group]
Title: "Structural biology of Zonulin in Celiac Disease"

18:40 Dinner and get together

20:00 HEC committee meeting

Day 2: Friday, 22nd September 2023

Session 3: Nucleic acids and nucleotide-modifying enzymes

chairs: Cyril Bařinka, Sebastian Glatt

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| 9:00-9:15 | Martyna Mateja-Pluta /Poznań [Rypniewski Group] Title: "Stabilization of RNA structures using small molecules for crystallographic research" |
| 9:15-9:30 | Gopika Sasikumar /Berlin [Markus Wahl group] Title: "Large-scale conformational changes in a spliceosomal RNA helicase induced by allosteric inhibitors" |
| 9:30-9:45 | Stefan Djukic /Prague [Pavlina Řezáčová group] Title: "Structural studies of purine nucleoside phosphorylase inhibitors" |
| 9:45-10:00 | Marta Walczak /Krakow [Sebastian Glatt group] Title: "Structural and functional characterization of the human tRNA thiolation cascade" |
| 10:00-10:15 | Yvette Roske /Berlin [Oliver Daumke group] Title: "Structural analysis of PLD3 reveals insights into the 5' exonuclease-mediated nucleic acid degradation" |
| 10:15-10:20 | <i>flash talk:</i> Martyna Graczyk /Poznań [Miroslaw Gilski group] Title: "Solving and refining the crystal structure of m6A-modified RNA, ups and downs" |

10:20-11:00 Coffee break and industrial exhibition

Session 4: Structures of macromolecular complexes and mechanisms

chairs: Pavlina Řezáčová, Milton T. Stubbs

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| 11:00-11:15 | Jules Van Der Walt /Wien [Kristina Djinović group] Title: "An integrative approach to structurally and biophysically characterise the human Alpha-actinin 2: ZASP sarcomeric complex" |
| 11:15-11:30 | Shuangshuang Dong /Braunschweig [Wulf Blankenfeldt group] Title: "Unravelling molecular mechanisms involved in the action of cytotoxic necrotizing factor(CNF)" |
| 11:30-11:45 | Paweł Kochanowski /Krakow [Przemysław Grudnik group] Title: "Structural and functional characterization of the DHS-ERK2 complex" |
| 11:45-12:00 | Jana Nedvěďová /Vestec [Cyril Bařinka group] Title: "Characterization of TTL11 as a Tubulin Polyglutamylase" |
| 12:00-12:15 | Manal Ebrahim /Berlin [Patrick Scheerer group] Title: "Structural insights into a red-light photoreceptor" |
| 12:15-12:20 | <i>flash talk:</i> Piotr Wilk /Krakow [Przemysław Grudnik group] Title: "Targeting human DHS through crystallographic fragment screening" |
| 12:20-12:25 | <i>flash talk:</i> Evangelia Nathanail /Berlin [Oliver Daumke group] Title: "Regulating mitochondrial form: Structure-to-function studies of MICOS" |

12:25-13:30 Lunch

13:30-15:30 Free time

15:30-16:30 Coffee and industrial exhibition

Day 2: Friday, 22nd September 2023 (continued)

Session 5: Sponsors

chairs: Ivana Smatanová, Christian Roth

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| 16:30-16:40 | Dr. Vernon Smith/Dr. Anna Luebben, Bruker Title: „Tools for best in-house data collection“ |
| 16:40-16:50 | Dr. Kateryna Slipeniuk, Rigaku Europe Title: “Rigaku's Advances in X-ray and Electron Crystallography“ |
| 16:50-17:00 | Dr. Ignazio Garaguso, Beckmann Coulter Life Sciences Title: “Analytical Ultracentrifugation for thermodynamic characterisation of biological macromolecules“ |
| 17:00-17:10 | Dr. Maren Thomsen, Proteros Biostructures GmbH Title: “Alternative career paths to academia - Proteros Biostructures GmbH” |
| 17:10-17:20 | Dr. Karin Kühnel, Structure, Cell Press Title: “A short introduction to Structure and Cell Press“ |

Session 6: HEC25 Lecture

chair : Michael Lammers

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| 17:20-17:30 | Introduction and welcome of Fred Wittinghofer (MPI of Molecular Physiology/Dortmund) |
| 17:30-18:30 | HEC25 Lecture: Fred Wittinghofer (MPI of Molecular Physiology/Dortmund) Title: “Nature uses Phosphates” |
| 18:30 | Conference Dinner, get together and bar |

Day 3: Saturday, 23rd September 2023

Session 7: Structure-function analyses of bacterial enzymes and catalytic mechanisms

chairs: Wulf Blankenfeldt, Przemyslaw Grudnik

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| 9:00-9:15 | Kasia Woźniak /Poznań [Krzysztof Brzeziński group] Title: "Crystallographic study of methylenetetrahydrofolate reductase from <i>Pseudomonas aeruginosa</i> " |
| 9:15-9:30 | Ingrid Span /Erlangen-Nürnberg Title: "Structural insights into catalysis of the [FeFe] hydrogenase from <i>Desulfovibrio desulfuricans</i> " |
| 9:30-9:45 | Leonie Graf /Greifswald [Michael Lammers group] Title: "Structural and functional studies on prokaryotic classical deacetylases" |
| 9:45-10:00 | Honorata Czapińska /Warsaw [Matthias Bochtler group] Title: "N ϵ -rule for serine catalytic triads" |

Session 8: Structure determination, methods and mechanisms

chairs: Kristina Djinović, Yves Muller

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| 10:00-10:15 | Johanna Hakanpää /Hamburg Title: "Beamline P11 at DESY DESY MX @ PETRA IV" |
| 10:15-10:20 | <i>flash talk</i> : Marianne Mühlbacher /Leipzig [Norbert Sträter group] Title: "Conformational switch of the venus flytrap domain of the calcium sensing receptor" |
| 10:20-10:25 | <i>flash talk</i> : Chun-Chiao Yang /Leipzig [Norbert Sträter group] Title: "Crystallographic fragment screening using amino acid derivatives" |
| 10:25-11:00 | Coffee break |
| 11:00-11:15 | Announcement of HEC26 by Sebastian Glatt /Krakow |
| 11:15-11:30 | HEC25 prizes (sponsored by: <i>Structure/Cell Press, IUCr Journals, GBM</i>) |
| 11:30 | Closing remarks and end of conference/packed lunch upon departure |