# Conference Schedule

European Rosetta Con
Ljubljana, 2025

| | Monday 20th | Tuesday 21st | Wednesday 22nd |
|---|---|---|---|
| 08:15 | **Registration** | | |
| 08:20 | | | |
| 08:25 | | | |
| 08:30 | | **Registration** | **Registration** |
| 08:35 | | | |
| 08:40 | | | |
| 08:45 | | | |
| 08:50 | | | |
| 08:55 | | | |
| 09:00 | Welcome | **Roman Jerala** (Sythetic biology)<br>chair: Dominik Gront | **Tanja Kortemme** (Multistate proteins)<br>chair: Enrique Marcos |
| 09:05 | | | |
| 09:10 | **Birte Höcker** (Molecular machines)<br>chair: Ajasja Lubetic | | |
| 09:15 | | | |
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| 09:45 | | Ben Hardy<br>Design and Engineering of Artificial Membrane Cytochromes for Synthetic Bioenergetics | Adam Broerman<br>Design of facilitated dissociation enables timing of cytokine signaling |
| 09:50 | | | |
| 09:55 | Liza Ulčakar | | |
| 10:00 | De novo designed random walker | Miguel Atienza Juanatey<br>Towards meta-stable de novo protein assemblies | Eva Rajh<br>Toehold mediated strand displacement as a tool for kinetic control of protein dissociation |
| 10:05 | | | |
| 10:10 | Alena Khmelinskaia | | |
| 10:15 | From Nature to the drawing board: design of dynamic protein assemblies | Alexandra Dashevsky<br>Unexpected modes of cooperativity in the enzyme glutathione reductase | Marian Novotny<br>Bound or not bound - annotating conformational state of protein structure models |
| 10:20 | | | |
| 10:25 | Anna Backeberg | | Lorenzo Scutteri<br>De Novo Design Of Light-Regulated Dynamic Proteins Using Deep Learning |
| 10:30 | De novo design of multiple-geometry forming protein scaffolds | Florian Pretorious (DNA and heterodimers) | |
| 10:35 | | | |
| 10:40 | Federico Alberto Olivieri | | |
| 10:45 | Prosculpt: An Open-Source Pipeline for Accessible Protein Design | | Kathryn Shelley (Light switches) |
| 10:50 | | | |
| 10:55 | Michael Adrian Jendrusch | Leoni Abendstein<br>Designing for exclusivity: Can we engineer orthogonal heterodimers de novo using sequence-based design approaches? | |
| 11:00 | Efficient and Versatile Protein Structure Generation with SALAD | | |
| 11:05 | | | |
| 11:10 | Coffee break<br>Sponsored by Fidabio | Coffee break<br>Sponsored by Novartis | Coffee break |
| 11:15 | | | |
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| 11:40 | Gustav Oberdorfer (Enzyme design)<br>chair: Paola Panizza | Jeff Gray (Antibodies)<br>chair: Georg Kuenze | Amelie Stein (PPI prediction & binders)<br>chair: Alena Khmelinskaia |
| 11:45 | | | |
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| 12:00 | | | |
| 12:05 | Sajith Kolathuparambil | Pedro Moreira<br>Computational design of monobody binders to target viral epitopes | Gustavo Avelar Molina<br>Versatile In-Vitro Validation of AI-Designed Protein Binders |
| 12:10 | Computational design of new proteases | | |
| 12:15 | | | |
| 12:20 | Rajarshi SinhaRoy | Tomer Cohen<br>Epitope-specific antibody design using diffusion models on the latent space of ESM embeddings | Enrique Marcos<br>De novo design principles for stabilizing β-sheet frameworks to enable novel binding functions |
| 12:25 | pHoptNN: Predicting Enzyme pH-Optima from Structure Using Equivariant Graph Neural Networks | | |
| 12:30 | | | |
| 12:35 | Salomé Guilbert | Klara Kropivsek<br>Multi-Objective Active Learning for Nanobody Development | Simon Kohl<br>Generating All-Atom De Novo Protein Binder Designs with High Lab Success Rates |
| 12:40 | Binding affinities and computational optimisation of fluoroacetate dehalogenase to break carbon-fluorine bonds in "forever chemicals" | | |
| 12:45 | | | |
| 12:50 | Georg Kuenze | Natalia Rincon<br>Evaluating The Biological Realism Of Iglm-Generated Antibody Sequences | Xinchen Lyu<br>De novo design of mini-protein binders broadly neutralizing Clostridioides difficile toxin B variants |
| 12:55 | Computational design of high-efficiency PET-degrading enzymes with Rosetta and structure-guided fragment recombination | | |
| 13:00 | | | |
| 13:05 | Natasha Poppy Murphy | Tadej Medved<br>Analysis of Pareto optimality at the antibody-antigen interface | Kasper H Björnsson<br>A strategy for the de novo design of highly polyspecific proteins targeting coral snake three-finger toxins |
| 13:10 | Engineering and application of a thermostable MHETase for PET de-polymerization | | |
| 13:15 | | | |
| 13:20 | Group photo | Lunch | Lunch |
| 13:25 | | | |
| 13:30 | Lunch | | |
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|---|---|---|---|
| 14:20 | Jens Meiler (AI & small molecule design)<br>chair: Marian Novotny | Patrick Bryant (Non-canonicals & AI)<br>chair: Florian Praetorius | Moritz Ertelt<br>Practically useful computational liability analysis for protein-based binders |
| 14:25 | | | |
| 14:30 | | | |
| 14:35 | | | Chentong Wang<br>Generative Design of Functional Proteins by Fusing Sequence and Structural Modalitie |
| 14:40 | | | |
| 14:45 | Johnny Alexander Jimenez Siegert<br>Scalable and Energy-Efficient Ultra-Large Library Screening on a SpiNNaker2 Neuromorphic Chip | Alex Li<br>All-atom protein design via SE(3) flow-matching with ProteinZen | |
| 14:50 | | | Rita Melo<br>Targeting the RANK-TRAF6 Axis: A Molecular Approach |
| 14:55 | | | |
| 15:00 | Andrea Hunklinger<br>Explainable AI Insights for Biologically Informed Training, Evaluation, and Interpretation of Protein Language Models | Tereza Neuwirthova<br>Prediction of Amino Acid Dispensability in Model Organisms | |
| 15:05 | | | Yang Yang<br>AI protein design at ACE2 binding interface |
| 15:10 | | | |
| 15:15 | Henry Dieckhaus<br>Building hydrogen bond networks in silico with HBDesigner | Tadeas Kalvoda<br>Amino Acid Alphabet (R)Evolution: Changing the Molecular Basis of Life | |
| 15:20 | | | |
| 15:25 | | | Anastassia Vorobieva (Membrane proteins)<br>chair: Adam Broerman |
| 15:30 | Ana Paola Panizza Scasso<br>Leveraging Computational tools for Cost-Effective Enzyme Design in Uruguay, South America. | Tal Levin<br>Combinatorial assembly and design of novel enzyme specificities | |
| 15:35 | | | |
| 15:40 | | | |
| 15:45 | Bijoy Desai<br>The Open Datasets Initiative and Protein Engineering Tournament | Qihao Zhang<br>Heme3D: A Heme Location Prediction Tool with 3dCNN/Docking Procedure | Alvaro Martin<br>Expression of a de novo fluorescence-activating transmembrane β-barrel in mitochondrial membranes |
| 15:50 | | | |
| 15:55 | | | |
| 16:00 | Coffee break<br>Sponsored by Fidabio | Coffee break<br>Sponsored by Novartis | Closing |
| 16:05 | | | |
| 16:10 | | | |
| 16:15 | | | Coffee break |
| 16:20 | | | |
| 16:25 | | | |
| 16:30 | Flash talks 1<br><br>(Odd poster numbers) | Flash talks 2<br><br>(Even poster numbers) | **Industry career panel**<br><br>Julian Englert<br>Marina Klemenčič<br>Franziska Geiger<br>Daniella Pretorius<br>George Sutherland<br>Adam Kral<br>Anna Macintyre |
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| 17:00 | | | |
| 17:05 | | | |
| 17:10 | | | |
| 17:15 | Poster session 1<br><br>(Odd poster numbers)<br>(With beer, wine or drinks) | Poster session 2<br><br>(Even poster numbers)<br>(With beer, wine or drinks)<br>(Light snack -- pizza and štruklji) | |
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| 19:00 | | | |
| | PI meeting<br>19:30-20:00 | | |
| | Gala dinner<br>20:00-22:00 | David Baker<br>(remote lecture streamed in Grand hall)<br>20:00-21:00 | |