

## Program

Thursday 22 <sup>th</sup> June 2023	
Time	
12:00 – 13:45	<b>Registration</b>
13:45 – 13:55	Opening Remarks: <b>András Perczel</b> (ELTE, Budapest, Hungary)
13:55 – 14:00	Welcome: <b>Anastassis Perrakis</b> (iNEXT-Discovery coordinator)
	<b>X-ray and cryo-EM approaches</b> Chair: Anastassis Perrakis
14:00 – 14:30	<b>L1. Tobias Krojer:</b> Towards comprehensive analysis of large crystallographic fragment screening campaigns
14:30 – 15:00	<b>L2. Darren Fearon:</b> Accelerating structure-enabled drug discovery with high-throughput crystallographic fragment screening
15:00 – 15:30	<b>L3. Jonathan Grimes:</b> How does flu virus replicate
15:30 – 16:00	<b>L4. Bruno Klaholz:</b> High-resolution cryo-EM analysis of macromolecular complexes: when chemistry and biology meet.
16:00 – 16:30	<b>Coffee Break</b>
	<b>Integrating Europe</b> Chair: Dóra Karancsiné Menyhárd
16:30 – 16:45	<b>L5. Corinna Brockhaus:</b> The role of Instruct-ERIC in Europe
16:45 – 17:30	<b>Poster pitches from young scientists</b>
17:30 – 20:00	<b>Young section - Posters and Welcome reception</b>

Time	<b>Poster pitches from young scientists</b> Chair: Dóra Karancsiné Menyhárd
16:45 – 16:50	<b><i>Fruzsina Bencs (P4)</i></b> Molecular interactions underlying amyloid formation and stability.
16:50 – 16:55	<b><i>Zsolt Dürvanger (P5)</i></b> Structures of calmodulin-melittin complexes show multiple binding modes lacking classical anchoring interactions.
16:55 – 17:00	<b><i>Humberto Fernandes (P6)</i></b> CryoET analysis of rod outer segments: is PDE6 the molecular driver of the light-induced photoreceptor morphological changes?
17:00 – 17:05	<b><i>Ádám Kelemen (P10)</i></b> Mapping of the reaction route of amide cis-trans interconversion.
17:05 – 17:10	<b><i>Dániel Kovács (P13)</i></b> How much do we know about the secondary structural propensities of IDPs? What does the random coil chemical shift prediction show and what is hidden?
17:10 - 17.15	<b><i>Zsuzsanna Tardi (P25)</i></b> Electrophysiological and structural characterization of a recently discovered scorpion toxin with significant pharmacological activity.
17:15 – 17:20	<b><i>Tamara Teski (P26)</i></b> Structural and dynamic determinants of site-selectivity in human ileal bile acid-binding protein.
17:20 – 17:25	<b><i>Zoé Tóth (P28)</i></b> Investigation of proteinaceous inhibition of M. tuberculosis dUTPase.
17:25 – 17:30	<b><i>Soma Varga (P30)</i></b> Structural characterization of the postsynaptic Drebrin protein.
17:30 – 20:00	<b><i>Young section - Posters and Welcome reception</i></b>

## Friday 23<sup>th</sup> June 2023

Time	
	<b>Studying amyloids by structural biology approaches</b> Chair: András Perczel
09:00 – 09:30	<b>L6. Chao Qi:</b> Cryo-EM structures of tau filaments from human brain
09:30 – 10:00	<b>L7. Roland Riek:</b> Phase Transition from Liquid to Solid (amyloids): from the origin to the end of life ssNMR and amyloid
10:00 – 10:30	<b>L8. Matthias Schmidt:</b> Common structural features of wild type and variant ATTR amyloid fibrils extracted from different patients
10:30 – 11:00	<b>L9. Philipp Neudecker:</b> solid state NMR with respect to amyloids
11:00 – 11:30	<b>Coffee Break</b>
	<b>Towards Structural Cell Biology</b> Chair: Andrea Bodor
11:30 – 12:00	<b>L10. Harald Schwalbe:</b> RNA structural biology by NMR spectroscopy
12:00 – 12:30	<b>L11. Philipp Selenko:</b> In-Cell NMR as a tool in Cellular Structural Biology
12:30 – 13:00	<b>L12. Maria Harkiolaki:</b> Correlative imaging using soft X-ray tomography to investigate cell structure and function
13:00 – 14:00	<b>Buffet Lunch</b>
	<b>Computational approaches for experimental data</b> Chair: Kevin Gardner
14:00 – 14:30	<b>L13. Peter Güntert:</b> Accelerating protein chemical shift assignment by deep learning for visual spectra analysis, structure and shift prediction
14:30 – 15:00	<b>L14. Dóra Karancsiné Menyhárd:</b> The inner dealings of a tetrameric serine protease: calculations based on cryo-EM structures
15:00 – 15:30	<b>L15. Jose Maria Carazo:</b> Novel tools to analyze macromolecular heterogeneity and increase resolution by cryo-EM
15:30 – 16:00	<b>Coffee Break</b>
	<b>Computational learning methods for structural biology and beyond</b> Chair: Rolf Boelens
16:00 – 16:30	<b>L16. Robbie Joosten:</b> AlphaFill: Enriching AlphaFold models with co-factors, small molecules and metal ions
16:30 – 17:00	<b>L17. Danny Sahtoe:</b> Computational design of de novo protein-protein interactions
17:00 – 17:30	<b>L18. Jonas Teuwen:</b> Deep learning for image reconstruction
19:00 – 22:00	<b>Conference Dinner</b>

## Saturday 24<sup>th</sup> June 2023

Time	
	<b>Structural Biology</b> Chair: Magali Mathieu
09:00 – 09:30	<b>L19. Márton Gadanez + Zsolt Fazekas:</b> Structure determination of the magnesium ion free and bound KRas G12C+GDP complex using NMR data driven molecular dynamics simulations
09:30 – 10:00	<b>L20. Vineeta Kaushik:</b> Structural elucidation of Retinol binding protein 3: One step closer to unfolding the effect of ligands on the conformation of the protein
10:00 – 10:30	<b>L21. Kinga Nyíri:</b> Antirepressor specificity is shaped by highly efficient dimerization of the repressors in regulation of staphylococcal pathogenicity islands
10:30 – 11:00	<b>L22. Viktor Viglasky:</b> Non-canonical structural motifs of nucleic acids
11:00 – 11:30	<b>Coffee Break</b>
11:30 – 12:00	<b>L23. Andreas Schlundt:</b> Using integrated structural biology to determine the specificity in RNA-protein interactions
12:00 – 12:30	<b>L24. José A. Brito:</b> Structural and functional insights into hydrogen sulfide homeostasis in pathogenic bacteria
12:30 – 13:00	<b>L25. Francois-Xavier Theillet:</b> In-cell structural biology using NMR: overview and latest developments to depict IDPs at 310K
13:00 – 14:30	<b>Buffet Lunch</b>
	<b>Departure</b>

## Poster presentations

### **P1. Stabilization of proteins with cyclodextrins**

*György Tibor Balogh, István Puskás, Zoltán Fülöp, Levente Szőcs, Lajos Szente*

### **P2. AlphaFold2 and NMR structures of antifungal disulfide proteins**

*Gai Jiawei, András Czajlik, Gyula Batta*

### **P3. Get Funding to access Instruct-ERIC Structural Biology services via ISIDORe, canSERV, and Euro4Access**

*Corinna Brockhaus, Pauline Audergon, Claudia Alen Amaro, Natalie Haley, Harald Schwalbe*

### **P4. Molecular interactions underlying amyloid formation and stability**

*Fruzsina Bencs, Viktor Farkas, Loránd Románszki, András Perczel*

### **P5. How Euro-BioImaging can support your research with access to the best imaging tools**

*Johanna Bischof*

### **P6. Discrimination of anomeric chimera oligopeptides using cIM-MS and NMR**

*Kim Hoang Yen Duong, Gitta Schlosser, Dániel Horváth, Viktória Goldschmidt Gőz, András Perczel*

### **P7. Structures of calmodulin-melittin complexes show multiple binding modes lacking classical anchoring interactions**

*Zsolt Dürvanger, Tünde Juhász, Károly Liliom, Veronika Harmat*

### **P8. CryoEM analysis of rod outer segments: is PDE6 the molecular driver of the light-induced photoreceptor morphological changes?**

*Vineeta Kaushik, Luca Gessa, Sławomir Tomczewski, Sathi Goswami, Łukasz Olejnik, Nelam Kumar, Humberto Fernandes*

### **P9. Polymorphic amyloid nanostructures of hormone peptides involved in glucose homeostasis: Designed for reversible amyloid formation**

*Dániel Horváth, Zsolt Dürvanger, Dóra K. Menyhárd, Máté Sulyok-Eiler, Fruzsina Bencs, Gergő Gyulai, Péter Horváth, Nóra Taricska, András Perczel*

### **P10. Mapping of the reaction route of amide *cis-trans* interconversion**

*Ádám András Kelemen, Dániel Horváth, András Perczel, Imre Jákli*

### **P11. SAXS Mail in on B21**

*Nikul Khunti, Nathan Cowieson, Katsuaki Inoue, Jodie Lavender, Robert P. Rambo, Diamond*

### **P12. Cryo-EM structure of acylpeptide hydrolase: substrate selection by a multi state serine-protease triad and inhibition by Meropenem**

*Anna J. Kiss-Szemán, Luca Takács, Zoltán Orgován, Pál Stráner, Imre Jákli, Naoki Hosogi, Simonas Masiulis, Gitta Schlosser, Veronika Harmat, Dóra K. Menyhárd, András Perczel*

**P13. How much do we know about the secondary structural propensities of IDPs?  
What does the random coil chemical shift prediction show and what is hidden?**

*Dániel Kovács, Andrea Bodor*

**P14. Structural elucidation of Retinol binding protein 3: One step closer to unfolding  
the effect of ligands on the conformation of the protein**

*Vineeta Kaushik, Luca Gessa, Nelam Kumar, Humberto Fernandes*

**P15. Basic residues are associated to functional phosphorylation sites in the Unique  
domain of c-Src**

*Andras Lang, Alejandro Fernández, Francisco Cárdenas, Margarida Gairí, Miquel Pons*

**P16. A novel Semaphorin-5A fold variation enables bifunctional glycosaminoglycan  
specificity and regulates signalling strength.**

*Gergely N. Nagy, Xiao-Feng Zhao, Richard Karlsson, Karen Wang, Ramona Duman, Karl Harlos, Kamel El Omari, Armin Wagner, Henrik Clausen, Rebecca L. Miller, Roman J. Giger, E. Yvonne Jones*

**P17. A new spider peptide that affects the Kv1.5 voltage-gated potassium channel,  
making it a potential antiarrhythmic agent**

*Jesús Borrego, Ádám Fehér, Ágota Csóti, Diana Alvarado, Samuel Cardoso-Arenas, Ligia-Luz Corrales-García, Herlinda Clement, Iván Arenas, Pavel Andrei Montero-Dominguez, Timoteo Olamendi-Portugal, Fernando Zamudio, György Panyi, Zoltán Varga, Gerardo Corzo, Ferenc Papp*

**P18. Initial insight into the proline-rich region of the postsynaptic Shank3 protein**

*Bálint Péterfia, Soma Varga, Zsuzsanna Stráner, Fanni Farkas, Brigitta Maruzs, Anna Sánta, Zoltán Gáspári*

**P19. Mechanism of asparagine deamidation – tunneling in tetrapeptides?**

*Fruzsina Pilhál, Imre Jákli, Ernő Keszel, András Láng, András Perczel*

**P20. At the mitochondrial level we are electric living beings.**

**How properties of electron and proton help the reaction rate in mitochondria?**

*András Róka*

**P21. Proline *cis/trans* isomerization in intrinsically disordered proteins and peptides**

*Fanni Sebák, Nándor Papp, János Szolomájer, Gábor K. Tóth, Andrea Bodor*

**P22. Analysis of intertwined side chains of amyloidogenic oligopeptide crystals:  
revisiting of amyloid interface descriptors**

*Máté Sulyok-Eiler, Veronika Harmat, Perczel András*

**P23. Protein diffusion under denaturing conditions and in crowded environments**

*Csenge Lilla Szabó, Fanni Sebák, Andrea Bodor*

**P24. Molecular pathomechanisms in lipoamide dehydrogenase deficiency**

*Eszter Szabó, Attila Ambrus*

**P25. Electrophysiological and structural characterization of a recently discovered scorpion toxin with significant pharmacological activity**

*Zsuzsanna Tardi, Tamás Milán Nagy, Muhammad Umair Naseem, Katalin E. Kövér, György Panyi, István Timári*

**P26. Structural and dynamic determinants of site-selectivity in human ileal bile acid-binding protein**

*Tamara Teski, Gergő Horváth, Orsolya Tőke*

**P27. Investigating carbohydrate-galectin interactions with advanced multinuclear NMR and computational methods**

*István Timári, László Bence Farkas, Álex Kálmán Balogh, Fanni Hőgye, Jesús Jiménez-Barbero, Helen Blanchard, Krisztina Fehér, Tünde Zita Illyés, László Szilágyi, Katalin E. Kövér*

**P28. Investigation of proteinaceous inhibition of *M. tuberculosis* dUTPase**

*Zoé Tóth, Ibolya Leveles, Veronika Harmat, Olivér Ozohanics, Kinga Nyíri, Beáta G. Vértessy, András Benedek*

**P29. Lipid binding by the human Caskin1 SH3 domain suggests a novel regulatory mechanism**

*Orsolya Tőke, Kitti Koprivanacz, Károly Liliom, László Buday*

**P30. Structural characterization of the postsynaptic Drebrin protein**

*Soma Varga, Bálint Ferenc Péterfia, Zoltán Gáspári, Perttu Permi*