3D-BioInfo | ISCB 3D-SIG | ELIXIR Czech Republic

Community Meeting in Structural Bioinformatics

15–17 November 2023 in Prague, Czech Republic

REGISTER

All times are CET

Wednesday 15th November – *Elixir CZ*

Elixir CZ	*Chair: Jiří Damborský* Masaryk University, Czech Republic	
09.00 – 09.15	Welcome.	Jiří Vondrášek IOCB Prague, Czech Republic
09.15 – 09.35	A PDB-wide assignment of apo & holo relationships based on individual protein-ligand interactions	Marián Novotný Charles University, Czech Republic
09.35 – 09.55	Binding residue prediction with protein language models: Does the structure matter?	David Hoksza Charles University, Czech Republic
09.55 – 10.15	New ways of protein family visualization in AlphaFold era	Radka Svobodová CEITEC and NCBR, Masaryk University Brno, Czech Republic
10.15 - 10.45	**Coffee**	
Elixir CZ	*Chair: Radka Svobodová* U CEITEC and NCBR, Masaryk University Brno, Czech Republic	
10.45 – 11.05	Dynamics from Alphafold - Elastic network approach	Vojtěch Spiwok University of Chemistry and Technology, Prague, Czech Republic
11.05– 11.25	FireProt and FireProt-ASR – Web Tools for Computational Protein Stabilisation	David Bednář Masaryk University, Czech Republic St. Anne´s Univ Hospital, Brno, Czech Republic
11.25 – 11.45	Annotation, validation, refinement, and modeling of nucleic acid structures.	Jiří Černý Insitute of Biotechnology of the Czech Academy of Sciences, Czech Republic
11.45 – 12.00	Are kuravirus capsid diameters quantized? The first all-atom genome tracing method for double-stranded DNA viruses.	Samuel Coulbourn Flores Swedish University of Agricultural sciences, Stockholm, Sweden
12.00 – 13.00	**Lunch and get together of the Czech and Interantional sections**	

Wednesday programme continues with Activity 1 on next page

- Please email Katharina Heil if you have any questions: katharina.heil@elixir-europe.org
- https://elixir-europe.org/communities/3d-bioinfo

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Wednesday 15th November – *Elixir 3D-BioInfo / ISCB 3D-SIG / Elixir CZ*

13.00 – 13.10	**Welcome and organizational notes** *Chair: Bohdan Schneider* Institute of Biotechnology of the Czech Academy of Sciences, Czech Republic	
13.10 – 13.20	Introduction to 3D-BioInfo	Christine Orengo University College London, UK
13.20 – 13.30	ELIXIR welcome	ELIXIR Rep I
	Activity 1 To develop the infrastructure for FAIR structural and functional annotations	
	Chair: Sameer Velankar European Bioinformatics Institute, UK	
13.30 – 13.45	Welcome. PDBe-KB in 2023: New data pipelines and improved functionality.	Mihaly Varadi EMBL-EBI,UK
13.45 – 14.15	Computational Enzymology in 3D: Modules and Mechanisms.	Janet Thornton EMBL-EBI, UK
14.15 – 14.30	The Evolution of Local Energetic Frustration in Protein Families and Superfamilies.	R. Gonzalo Parra Barcelona Supercomputer Centre, Spain
14.30 – 14.45	Finding structure specific entity types in literature.	Melanie Vollmar EMBL-EBI, UK
14.45 - 15.00	FiTMuSiC: Leveraging structural and (co)evolutionary data for protein fitness prediction.	Matsvei Tsishyn Université Libre de Bruxelles, Belgium
15.00 - 15.15	The MOKCa database 2023	Frances Pearl University of Sussex, UK
15.15 - 15.30	Developing Training Materials for Structural Biology.	Paulyna Magana EMBL-EBI, UK
15.30 – 16.00	**Coffee Break**	

Wednesday programme continues with Activity 2 on next page

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Activity 2
To create open resources for sharing, integrating and benchmarking software tools for modelling the proteome in 3D

Chair: Shoshana Wodak VIB, Belgium

16.00 – 16.30	An atlas of protein homo-oligomerization across domains of life.	Hugo Schweke Weizmann Institute, Israel
16.30 – 17.00	Datasets and models for modeling of antibody-antigen complexes	Dina Schneidman Hebrew University of Jerusalem, Israel
17.00 – 17.15	Discriminating physiological from non-physiological interfaces in structures of protein complexes: a community-wide study.	Emmanuel Levy Weizmann Institute, Israel
17.15 – 17.30	Explaining Conformational Diversity in Protein Families through Molecular Motions.	Elodie Laine Sorbonne Université, France
17.30 – 17.45	Systematic identification and characterisation of domain movements in proteins from low-dimensional representations of conformational ensembles.	Sergei Grudinin LJK CNRS, Grenoble, France;
17.45 – 18.00	FAIR workflow to chart and characterize the conformational landscape of native proteins. A combined work of ELIXIR 3D-BioInfo structural community and the BioExcel Centre of Excellence for Computational Biomolecular Research.	Adam Hospital Gasch IRB Barcelona, Spain
18.00 – 21.00	**Dinner on site and poster session**	

End of Wednesday programme

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Thursday 16th November – *Elixir 3D-BioInfo / ISCB 3D-SIG / Elixir CZ*

Chair: Christine Orengo University College London, UK

09.00 – 09.30	ELIXIR program 2024-2028	Elixir Rep 2 Elixir

Activity 4
To develop tools to Describe, Analyse, Annotate, and Predict Nucleic Acid Structures

Chair: Bohdan Schneider Institute of Biotechnology of the Czech Academy of Sciences, Czech Republic

09.30 – 10.00	RNA-Puzzles : Blind Assessments of (Semi)-Automatic 3D RNA Modeling.	Eric Westhof Institut de biologie moléculaire et cellulaire du CNRS, Strasbourg, France
10.00 – 10.30	Rfam, RNA 3D structures, and issues facing RNA 3D structure prediction.	Blake Sweeny EMBL-EBI, UK
10.30 – 10.45	Unraveling the RNA web: detecting and deciphering entanglements in 3D structures.	Marta Szachniuk Poznan University of Technology; Institute of Bioorganic Chemistry PAS, Poland
10.45 –11.00	Posttranscriptional Modifications in RNA Experimental 3D Structures: Occurrences and Effect on Interbase Hydrogen Bonding.	Romina Oliva Department of Sciences and Technologies, University Parthenope of Naples, Italy
11.00 – 11.15	RNAdvisor: Evaluation of RNA 3D structures with metrics and energies.	Clément Bernard IBISC, France
11.15 – 11.30	Prediction of secondary structure for long non-coding RNAs using a recursive cutting method based on deep learning.	Loïc Omnes Université Paris-Saclay, Univ. Evry, France
11.30 –12.00	**Coffee Break**	

Additional talks from Activities 2 & 5

Chairs: Bohdan Schneider & Lynne Regan

12.00 – 12.30	Protein Quaternary Structures in Solution are a Mixture of Multiple forms.	Gideon Schreiber Weizmann Institute, Israel
12.30 – 13.00	Structural plasticity in the loop region of engineered lipocalins with novel ligand specificities – Anticalins.	Arne Skerra Technical University of Munich, Germany
13.00 – 14.00	**Lunch**	

Thursday programme continues with Activity 5 on next page

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Activity 5
To establish a Biostudies database of protein engineering results

Chair: Lynne Regan University of Edinburgh, UK

14.00 – 14.30	Novel Strategies and Web-based Tools for Protein Engineering.	Jiri Damborsky Masaryk University and ICRC-FNUSA, Czech Republic
14.30 – 15.00	Novel immunotherapeutic drugs through computational protein design.	Clara Tabea Schoeder Leipzig University, Faculty of Medicine, Germany
15.00 – 15.15	Using molecular dynamics (MD) calculations for the characterization of structural transitions.	Outi Tuulikki Lampela Biocenter Oulu, University Of Oulu, Finland
15.15 – 15.30	From AlphaFold to PyMOL: enabling seamless access to Structural Bioinformatics Tools.	Serena Rosignoli Sapienza University, Rome, Italy
15.30 – 16.00	**Coffee Break**	
16.00 – 16.15	Design of novel peptides targeted to human primary amine oxidase.	Marion Alix Åbo Akademi university, Finland
16.15 – 16.30	Assessing the performance of protein regression models.	Wouter Boomsma University of Copenhagen, Denmark
16.30 – 16.45	Prediction of bacterial interactomes based on genome-wide coevolutionary networks: an updated implementation of the ContextMirror approach.	Miguel Fernandez Barcelona Supercomputing Center, Spain
16.45 – 18.00	Elixir Platform Discussions.	Sameer Velankar Shoshana Wodak Vincent Zoete Bohdan Schneider Lynne Regan

End of Thursday programme

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Activity 3
To help develop models for protein-ligand interactions

Chair: Vincent Zoete SIB Swiss Institute of Bioinformatics, Switzerland

09.00 – 09.15	Introduction and status of the ligand-protein activity.	Vincent Zoete SIB Swiss Institute of Bioinformatics, Switzerland
09.15 – 09.45	AlphaFill: enriching AlphaFold models with ligands and cofactors.	Robbie Joosten Netherlands Cancer institute, Amsterdam, NL
09.45 - 10.15	A Bottom-Up Approach to Screening Massive Virtual Collections.	Xavier Barril Barcelona University, Spain
10.15 – 10.30	SiteMine: large scale binding site similarity searching in protein databases.	Thorben Reim Center for Bioinformatics, Universität Hamburg, Germany
10.30 – 10.45	Automated benchmarking of protein-ligand complex prediction.	Janani Durairaj Biozentrum, University of Basel, Switzerland; SIB Swiss Institute of Bioinformatics
10.45 – 11.00	Jumpcount: Exact confidence intervals for free energy difference estimations.	Jan Beránek Department of Biochemistry and Microbiology, University of Chemistry and Technology, Prague, Czech Republic
11.00 – 11.30	**Coffee Break**	

Final Session

Chair: Bohdan Schneider Institute of Biotechnology of the Czech Academy of Sciences, Czech Republic

11.30 - 12.30	Keynote.	Michael Sternberg Imperial College, London, UK
12.30 - 13.00	Discussion and Concluding Remarks.	Mihaly Varadi Gerardo Tauriello Shoshana Wodak Vincent Zoete Bohdan Schneider Lynne Regan
13.00 – 14.00	**Lunch**	

End of Conference

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