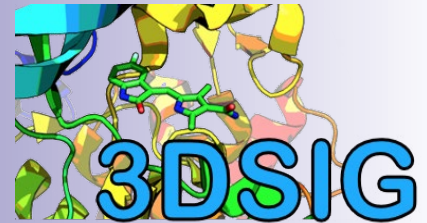


3D-BioInfo | ISCB 3D-SIG | ELIXIR Czech Republic

Community Meeting in Structural Bioinformatics

15–17 November 2023 in Prague, Czech Republic



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 p. 177	Marián Novotný Charles University, Czech Republic
09.35 – 09.55	Binding residue prediction with protein language models: Does the structure matter? p. 178	David Hoksza Charles University, Czech Republic
09.55 – 10.15	New ways of protein family visualization in AlphaFold era p. 178	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 p. 179	Vojtěch Spiwok University of Chemistry and Technology, Prague, Czech Republic
11.05– 11.25	FireProt and FireProt-ASR – Web Tools for Computational Protein Stabilisation p. 179	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. p. 180	Jiří Černý Institute 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. p. 180	Samuel Coulbourn Flores Swedish University of Agricultural sciences, Stockholm, Sweden
12.00 – 13.00	Lunch and get together of the Czech and Interantional sections	

Please email Katharina Heil if you have any questions: katharina.heil@elixir-europe.org

<https://elixir-europe.org/communities/3d-bioinfo>



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	PDBe-KB in 2023: New data pipelines and improved functionality. p. 181	Mihaly Varadi EMBL-EBI, UK
13.45 – 14.15	Computational Enzymology in 3D: Modules and Mechanisms. p. 182	Janet Thornton EMBL-EBI, UK
14.15 – 14.30	The Evolution of Local Energetic Frustration in Protein Families and Superfamilies. p. 182	R. Gonzalo Parra Barcelona Supercomputer Centre, Spain
14.30 – 14.45	Finding structure specific entity types in literature. p. 183	Melanie Vollmar EMBL-EBI, UK
14.45 - 15.00	FITMuSiC: Leveraging structural and (co)evolutionary data for protein fitness prediction. p. 183	Matsvei Tshishyn Université Libre de Bruxelles, Belgium
15.00 - 15.15	The MOKCa database 2023 p. 185	Frances Pearl University of Sussex, UK
15.15 - 15.30	Developing Training Materials for Structural Biology. p. 185	Paulyna Magana EMBL-EBI, UK
15.30 – 16.00	Coffee Break	

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. p. 186	Hugo Schweke Weizmann Institute, Israel
16.30 – 17.00	Datasets and models for modeling of antibody-antigen complexes p. 186	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. p. 187	Emmanuel Levy Weizmann Institute, Israel
17.15 – 17.30	Explaining Conformational Diversity in Protein Families through Molecular Motions. p. 188	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. p. 188	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. p. 189	Adam Hospital Gasch IRB Barcelona, Spain
18.00 – 21.00	Dinner on site and poster session	

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. p. 190	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. p. 190	Blake Sweeny EMBL-EBI, UK
10.30 – 10.45	Unraveling the RNA web: detecting and deciphering entanglements in 3D structures. p. 191	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. p. 192	Romina Oliva Department of Sciences and Technologies, University Parthenope of Naples, Italy
11.00 – 11.15	RNAadvisor: Evaluation of RNA 3D structures with metrics and energies. p. 193	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. p. 194	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. p. 196	Gideon Schreiber Weizmann Institute, Israel
12.30 – 13.00	Structural plasticity in the loop region of engineered lipocalins with novel ligand specificities – Anticalins. p. 196	Arne Skerra Technical University of Munich, Germany
13.00 – 14.00	Lunch	

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