ELIXIR 3D-BioInfo Community in Structural Bioinformatics, AGM

24–26 November 2020

REGISTER

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Tuesday 24th November

Activity 1 — Infrastructure for FAIR structural and functional annotations

Coordinator: Sameer Velankar

1.00 – 1.15	Updates on PDBe-KB	Mihaly Varadi EMBL-EBI, UK
1.15 – 1.35	3D-Beacons use cases and prototype	Ian Sillitoe University College London, UK
1.35 – 1.55	Survey on visualisation	Wim Vranken Vrije Universiteit Brussel, Belgium Jim Proctor University of Dundee, UK
1.55 – 2.05	Coffee break	
Discussion: 3D-Beacons and model quality		***Moderator*** Christine Orengo University College London, UK
2.05 – 2.15	Model quality estimates for 3D-Beacons	Gerardo Tauriello Swiss Institute of Bioinformatics, Switzerland
2.15 – 2.25	Model uncertainty: identification, quantification and interpretation	Daniel Saltzberg University of California, San Francisco, USA
2.25 – 2.35	ModFOLD: global and local quality estimates for 3D protein models	Liam McGuffin University of Reading, UK
2.35 – 2.45	How failed homology modelling lead to the identification of a novel fold in CPA/AT transporters by ab-initio structure prediction	Arne Elofsson Stockholm University, Sweden
3.00 – 4.00	**POSTERS**	

Tuesday programme continues with Activity 5 on next page

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

3D Bio Info

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Activity 5 — 3D-BioInfo Protein Engineering Session for AGM Nov 24th

Coordinator: Lynne Regan

4.00 – 4.05	Introduction to the new Protein Engineering section of 3D-BioInfo. Scope and plans for the future	Lynne Regan University of Edinburgh, UK

Four short presentations on examples of protein engineering and design:

4.05 – 4.17	Computational design of enzyme repertoires	Rosalie Lipsh Weizmann Institute, Israel
4.17 – 4.29	Fragment based protein design guided by evolutionary relationships	Noelia Ferruz Universität Bayreuth, Germany
4.29 – 4.41	Modular Protein Design from structural databases	Fabio Parmeggiani University of Bristol, UK
4.41 – 4.53	The road to extreme stabilisation of a computationally redesigned thioredoxin fold	Kristoffer Johansson University of Copenhagen, Denmark

The importance of databases and how they can be used:

4.53 – 5.07	Use of quality assessments for assessing homology models and protein design.	Arne Eloffson University of Stockholm, Sweden
5.07 – 5.25	The Biostudies Protein Engineering and Design database	Ugis Sarkar EBI, Hinxton, UK
5.25 – 5.37	Using physical features of protein cores to distinguish real proteins from decoys	Alex Grigas Yale University, USA
5.37 – 5.49	The Biostudies Protein Engineering and Design Database: A community resource for data-driven design	Chris Wood University of Edinburgh, UK
5.49 – 6.00	'Open mike' for comments and discussion	***Moderators:*** Lynne Regan University of Edinburgh, UK Amelie Stein University of Copenhagen, Denmark

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Wednesday 25th November

Activity 2 — Open resources for sharing integrating and benchmarking software tools for modelling the proteome in 3D

Coordinator: Shoshana Wodak

1:00 – 1.05	Introduction: Activity 2 implementation study, current status.	Shoshana Wodak VIB-VUB Center for Structural Biology, Brussels, Belgium
Session 1: The benchmark datasets		
1:05 – 1.25	Update on PDB-wide Clustering of protein-protein interfaces and protein assemblies	Qifang Xu Roland Dunbrack Fox Chase Cancer Center, USA
1:25 – 1.35	The current version of the benchmark dataset of homodimers: salient features	Emmanuel Levy Weizmann Inst. Israel
1:35 – 1.40	Break	
Session 2: The benchmarked tools and analysis method. Tools		
1:40 – 1.50	Using ISPRED4 predicted interfaces to distinguish from non-physiological complexes	Pier Luigi Martelli University of Bologna, Italy
1:50 – 2.00	The pyDock interface scoring functions	Juan Fernandez-Recio EXBSC Life Sciences, Barcelona, Spain
2.00 – 2.10	A novel scoring pipeline integrating CONSRANK with clustering and interface analysis	Romina Oliva University "Parthenope" of Naples, Italy
Analysis		
2.10 – 2.25	Comparing interface models: a multivariate data analysis perspective	Frederic Cazals Frederic Cazals, INRIA, France
2.25 – 3.00	General discussion	***Moderators:*** Emmanuel Levy & Frederic Cazals
3.00 – 4.00	**POSTERS**	

Activity 3 — Protein-ligand interactions

Coordinator: Vincent Zoete

4.00 – 4.10	Objectives of Activity 3, and current status	Vincent Zoete University of Lausanne, Switzerland
4.10 – 4.25	ProteinsPlus: Web-Based Molecular Design from Protein Structure Analytics to Protein-Ligand Docking	Katrin Stierand University of Hamburg, Germany
4.25 – 4.50	Automating benchmarks with the Continuous Automated Model EvaluatiOn (CAMEO)	Xavier Robin SIB Swiss Inst of Bioinformatics, University of Basel, Switzerland
4.50 – 5.10	TBA	Robbie Joosten Netherlands Cancer Institute, Dept of Biochemistry, Amsterdam, Netherlands
5.10 – 5.15	Break	
5.15 – 5.30	Challenges in the development and validation of protein-ligand scoring functions using structural and affinity databases	Maria Kadukova University Grenoble Alpes, CNRS, Inria, Grenoble, France
5.30 – 5.45	Identifying crystal lattices suitable for fragment screening to identify and develop protein-protein inhibitors	Joseph Ng Randall Centre for Cell and Molecular Biophysics, King's College London, UK
5.45 – 6.00	Discussing status of the project and next steps	All

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Thursday 26th November

Activity 4 — Nucleic Acid Activity breakout session

Coordinator: Bohdan Schneider

1.00 – 1.15	Overview of RNA quality criteria	**Eric Westhof** BMC/CNRS, Strasbourg, France
1.15 – 1.25	RNA-Puzzles – the evaluation and automation of RNA 3D structure prediction	**Zhichao Miao** EBI, Hinxton, UK
1.25 – 1.40	BGSU RNA 3D structure annotation pipeline and its applications	**Craig L. Zirbel** Bowling Green State University, USA
	Nucleic Acid Knowledge Base	**Cathy Lawson** Rutgers University, USA
1.40 – 1.55	Tools for RNA secondary structure analysis	Marco Pietrosanto, Andrea Guarracino, Gabriele Ausiello, **Manuela Helmer Citterich** Universita' di Roma Tor Vergata, Rome, Italy
1.55 – 2.05	Reliability of RNA – small molecule complex data in the PDB	Filip Stefaniak, **Janusz M. Bujnicki** International Institute of Molecular and Cell Biology, Warsaw, Poland
2.05 – 2.15	mqapRNA: a method for model quality assessment for RNA 3D models	Marcin Magnus, Albert Bogdanowicz, **Janusz M. Bujnicki** International Institute of Molecular and Cell Biology, Warsaw, Poland
2.15 – 2.25	RNAtive: a tool for reference-free evaluation and ranking of RNA 3D structures	**Maciej Antczak**, Tomasz Zok, Marcin Zablocki, Marta Szachniuk Institute of Bioorganic Chemistry, Polish Acad. Sci.,Poznan, Poland
2.25 – 2.35	RNANet: An automatically built dual-source dataset integrating homologous sequences and RNA struc-tures	Louis Becquey, Eric Angel, **Fariza Tahi** BISC, Université Evry, Université Paris-Saclay, France
2.35 – 2.40	Nucleic Acid Valence Geometry Working Group – a progress report	**Bohdan Schneider** Institute of Biotechnology, Czech Acad. Sci., CZ
2.40 – 2.50	RestraintLibE: nucleic acids restraints that evolve with minimum supervision	**D. Brzezinski**, M. Kowiel, M. Jaskolski Institute of Bioorganic Chemistry, Polish Acad. Sci.,Poznan, Poland
2.50 – 3.00	Discussion: Possibility to form an RNA quality 3D taskforce?	***Moderator:*** **Bohdan Schneider**
3.00 – 3.30	Discussion: Possible collaborations with the Intrinsically Disordered Proteins and Proteomics Communities	Wim Vranken, Brussels University, Belgium Lennart Martens University of Gent, Belgium
3.30 – 4.30	Feedback and discussion Activities 1,2,3	
4.30 – 5.00	Break	
5.00 – 6.00	Feedback and discussion Activities 4,5 and final wrap-up	