

Synergic Entanglements Between Structural Biology & Machine Learning: Looking into the Future

Day 1 : Wednesday 13th May

Opening session

13.40 - 13.50 **Welcome Address on behalf of the Host Institution Representative of the University of Malta**

13.50 - 14.00 **Annalisa Pastore (KCL, UK), Gian Gaetano Tartaglia (IIT, IT), Silvia Onesti (Elettra, IT)** *Conference vision: the horizons of AI in Structural Biology*

Session 1: Structure prediction, classification and inference

14.00 - 14.30 **Christine Orengo (UCL, UK)** *Deep Learning approaches revolutionize protein knowledge*

14.30 - 15.00 **Cedric Notredame (CGR Barcelona, ES)** *Building multiple sequence alignments and phylogenies on LLM embeddings: opportunities and challenges*

15.00 - 15.30 **Paolo De Los Rios (EPFL, CH)** *Statistical physics of protein folding and interactions*

15.30 - 16.00 **Coffee break**

Session 2: AI in drug design

16.00 - 16.30 **J.P. Ebejer (UM, MT)** *Learning Molecular Interactions: AI Methods for Predicting and Interpreting Protein-Ligand Binding*

16.30 - 17.00 **Shane Gonen (Irvine, US)** *Inhibition of voltage-gated sodium channels by animal toxins*

Day 2 : Thursday 14th May

Session 3: AI prediction in Cryo-EM pipelines

9.00 - 9.30 **Jianyi Yang (Shandong, CN)** *Structure prediction meets Cryo-EM: CRYOATOM for atomic model building*

9.30 - 10.00 **Marta Carroni (SciLifeLab, SE)** *Bioinformatics of Cryo-EM data analysis: getting the most out of molecules' images and combining them with prediction methods.*

10.00 - 10.30 **Luigi De Colibus (CNR-IOM, IT)** *Frozen titans: structural Insights into a Jumbo Virus enabled by AI-assisted Cryo-EM modelling*

10.30 - 11.00 **Coffee break**

Session 4: Protein aggregation, assemblies and disease

11.00 - 11.30 **Selected talks from participants**

11.30 - 12.00 **Michele Vendruscolo (Cambridge, UK)** *Drug design for undruggable targets using AI*

12.00 - 12.30 **Sandra Macedo-Ribeiro (i3S, PT)** *Protein self-assembly and amyloid structures*

12.30 - 14.00 **Lunch**

Session 5: Nucleic acid structure and function

- 14.00 - 14.30 **Marco Marcia (Uppsala, SE)** *Cryo-EM molecular movies of dynamic large non-coding RNAs guide AI-driven RNA structure prediction*
- 14.30 - 15.00 **Gian Gaetano Tartaglia (IIT, IT)** *Modelling protein–RNA networks and phase separation*
- 15.00 - 15.30 **Irene Farabella (IIT, IT)** *Nanoscale investigation of 3D genome structures*
- 15.30 - 16.00 **Coffee break**

Session 5: Structure and dynamics

- 16.00 - 16.30 **Alfredo De Biasio (KAUST, SA)**: *Visualizing enzymatic motion: Cryo-EM variability analysis and the future of dynamics structural biology*
- 16.30 - 17.00 **Francesco Gervasio (Geneve, CH)** *Dynamics and protein simulations to experiments*
- 17.00 - 17.30 **Selected talks from participants**

Day 3: Friday 15th May

Session 6: A changing landscape in structural biology: the impact of AI in emerging countries

- 9.00 - 9.30 **Trevor Sewell (UCT, ZA)** *How artificial intelligence is changing the structural landscape in Africa*
- 9.30 - 10.00 **Richard Garratt (USP, BR)** *Molecular recognition by septins: Monomers, dimers, oligomers, filaments and bundles*
- 10.00 - 10.30 **EMBO GLOBAL INVESTIGATOR LECTURE Aravind Penmatsa (IIS Bangalore, IN)**: *Membrane Protein Transporters*
- 10.30 - 11.00 **Coffee break**
- 11.00 - 11.30 **Serdal Kirmizialtin (NYU Abu Dhabi, UAE)**: *Exploring RNA Conformational Ensembles: Integrating SAXS-Guided Molecular Dynamics with Explainable AI*
- 11.30 - 12.00 **Selected talks from participants**
- 12:00 - 13:00 **Panel discussion** (Michele Vendruscolo, Christine Orengo, Michele Parrinello, Marta Carroni, Richard Garratt, Trevor Sewell, Aravind Penmatsa, Jiangi Yang, Alfredo De Biasio)
- 13:00 - 14.00 **Lunch**
- 14.00 - 14.30 **Franca Fraternali (UCL, UK)**: *Decoding Immunity: Structural and Dynamical Insights Driving Antibody Innovation*
- 14.30 - 15.30 **Plenary Lecture: Michele Parrinello (IIT, IT)** *The seeds of the future are in the present*
- 15.30 - 16.15 **Closing remarks: Andrew Harrison (CERIC-ERIC)**
- 16.15 - 16.45 **Farewell Coffee**