

# 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*

14:00 - 14.30 **Andrew Harrison (CERIC)**  
*The Central European Research Infrastructure Consortium - CERIC - and the Life Sciences*

### Session 1: Structure prediction, classification and inference

14.30 - 15.00 **Christine Orengo (UCL, UK)** *Deep Learning approaches revolutionize protein knowledge*

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

15.30 - 16.00 **Jens Kleinjung (UCL, UK)** *AllohubPy: Decoding Allosteric Signal Transmission from Molecular Dynamics*

16:00 - 16.30 **Coffee break**

### Session 2: AI in drug design & protein interactions

16.30 – 17:00 **Jean Paul Ebejer (UM, MT)** *Learning Molecular Interactions: AI Methods for Predicting and Interpreting Protein-Ligand Binding*

17.00 – 17:15 **Pasquale Miglionico (SNS Pisa, IT)** *Predicting and Engineering GPCR-G Protein Coupling Specificity with AlphaFold*

17.15 – 17:30 **Francesca Cuturello (Area Science Park, IT)** *Decoding the Grammar of Protein–Protein Interaction Interfaces with Multimodal Representation Modeling*

17:30 – 19:00 **Welcome drinks & tapas**

## 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 (Elettra, 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 **Michele Vendruscolo (Cambridge, UK)** *Drug design for undruggable targets using AI*
- 11.30 - 12.00 **Sandra Macedo-Ribeiro (i3S, PT)** *Protein self-assembly and amyloid structures*
- 12:00-12:15 **Maria Baczynska (Kings College, UK)** *Structural studies into the N-terminal domain of the biofilm forming *L. pneumophila* collagen- like protein*
- 12:00-12:15 **Elias Fernandez (University of Tennessee, US)** *On the interactions with distal 5'-flanking DNA and the control of transcription by nuclear hormone receptors*
- 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 6: 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*

### Conference dinner

## Day 3: Friday 15th May

### Session 7: A changing landscape in structural biology: the impact of AI in emerging countries

- 9.00 - 9.30 **FRONTIERS Lecture**  
**Trevor Sewell (UCT, ZA)** *How artificial intelligence is changing the structural landscape in Africa*
- 9.30 - 10.00 **FRONTIERS Lecture**  
**Richard Garratt (USP, BR)** *Molecular recognition by septins: Monomers, dimers, oligomers, filaments and bundles*
- 10.00 - 10.30 **EMBO GLOBAL INVESTIGATOR LECTURE**  
**Vinothkumar Kutti Rangunath (IIS Bangalore, IN):** *Macromolecular structures and dynamics*
- 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 - 12.15 **Flash presentations from submitted Abstracts**
- 12:15 - 13:00 **Panel discussion** (Michele Vendruscolo, Christine Orengo, Michele Parrinello, Marta Carroni, Richard Garratt, Trevor Sewell, Vinothkumar Kutti Rangunath, Jiangi Yang, Alfredo De Biasio)
- 13:00 - 14.00 **Lunch**

### Session 8: Future perspectives in science and medicine

- 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 - 16.00 **Closing remarks: Carlo Rizzuto (CERIC-ERIC) & organizers**
- 16.00 - 16.30 **Coffee & goodbye**