

Computational Analysis and Deep Data Mining of Cryo-Electron Microscopy Structural Data



Challenges

Single-particle cryo-electron microscopy (cryo-EM) has become one of the leading technologies for determining the three-dimensional structures of biological macromolecules. Rapid advances in microscopes, detectors, image processing and specimen preparation have transformed structural biology, yet significant scientific and technical challenges remain:

- Understanding the physical and practical limits governing attainable resolution.
- Extending cryo-EM to smaller and more heterogeneous molecular complexes.
- Quantifying how molecular weight, radiation damage and specimen quality influence structure determination.
- Extracting biological insight from rapidly expanding collections of experimentally determined cryo-EM structures.
- Guiding future developments in instrumentation, methodology and specimen preparation using quantitative evidence.

Technology

Dr. Ardan Patwardhan's current research focuses on analysis and deep data mining of structural data derived from cryo-electron microscopy. The group's work combines quantitative analysis of experimentally determined cryo-EM structures to investigate the current capabilities, limitations and future opportunities for single-particle cryo-EM. Core technology areas include:

- Large-scale analysis of structural data deposited in the Electron Microscopy Data Bank (EMDB), the Electron Microscopy Public Image Archive (EMPIAR) and the Protein Data Bank (PDB).
- Quantitative analysis of relationships between molecular weight, attainable resolution and experimental data requirements.
- Evaluation of theoretical and practical limits imposed by radiation damage, signal-to-noise ratio, molecular flexibility and specimen preparation.
- Identification of technological opportunities to extend the application of single-particle cryo-EM to smaller molecular targets and improve specimen preparation, instrumentation and methodology:
- Computational analyses that identify opportunities for future developments in cryo-electron microscopy technologies and methodologies.

Dr. Patwardhan previously led the development of EMDB and EMPIAR the Electron Microscopy Public Image Archive (EMPIAR). His current research focuses on computational analysis and deep data mining of cryo-electron microscopy structural data.

Internal EMBLEM Reference

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Key Inventors

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Applications

- Analysis of cryo-electron microscopy structural datasets
- Quantitative assessment of cryo-EM performance
- Structural biology and macromolecular structure determination
- Evaluation of cryo-EM methodologies
- Identification of opportunities to extend single-particle cryo-EM
- Computational analysis supporting technology development

Resources

- EMBL-EBI Cellular Structure & 3D Bioimaging team
- Electron Microscopy Data Bank (EMDB)
- Protein Data Bank (PDB)
- Large-scale cryo-electron microscopy structural datasets used for quantitative analysis

Seeking

- Collaborations
- Commercial partners
- Sponsored research
- Joint technology development

Benefits

- Provides quantitative insight into the current capabilities and limitations of single-particle cryo-EM
- Uses large-scale structural datasets to identify opportunities for extending the application of single-particle cryo-EM and to help guide future technology development.
- Identifies opportunities for extending cryo-EM to increasingly challenging biological targets
- Supports the development of improved experimental methodologies
- Broad applicability across structural biology and cryo-electron microscopy research

Keywords

Cryo-electron microscopy
Single-particle cryo-EM
Structural biology
Structural data analysis
Deep data mining
Computational biology
Electron Microscopy Data Bank (EMDB)
Protein Data Bank (PDB)
Technology development

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Commercial Opportunity

- Pharmaceutical and biotechnology organisations applying cryo-electron microscopy in structural biology and drug discovery.
- Cryo-EM technology developers seeking quantitative assessment of experimental performance.
- Structural biology facilities developing improved cryo-EM workflows.
- Computational structural biology and bioinformatics organisations analysing large-scale cryo-EM datasets.

Further Reading

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Intellectual Property

- Know-how

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