

Molecular Modelling Workshops

Molecular Modelling Workshops

NTHRYS BIOTECH LABS provides a diverse array of workshops in the realm of Molecular Modelling. Explore our comprehensive offerings below

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Explore Cutting-Edge Molecular Modelling: Start Your Journey Here!

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1. Workshop in Introduction to Molecular Modelling

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Fundamentals of Molecular Modelling

Hands-on workshop covering the basic concepts of molecular modelling.

Protocols for building molecular structures, understanding force fields, and setting up simulations.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Molecular Dynamics Simulations

Practical session on setting up and running molecular dynamics simulations.

Protocols for simulating molecular behavior over time and analyzing trajectory data.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Energy Minimization and Optimization

Hands-on training on energy minimization techniques.

Protocols for optimizing molecular structures to find the lowest energy conformations using various algorithms.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Visualization of Molecular Models

Practical session on visualizing molecular structures.

Protocols for using molecular graphics software to render 3D models and analyze molecular interactions.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

2. Workshop in Advanced Molecular Modelling Techniques

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.
Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Quantum Mechanics in Molecular Modelling

Hands-on workshop on quantum mechanical calculations in molecular modelling.
Protocols for applying quantum chemistry techniques to small molecules and reaction mechanisms.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Hybrid QM/MM Simulations

Practical session on hybrid quantum mechanics/molecular mechanics (QM/MM) approaches.
Protocols for simulating complex systems that combine quantum and classical mechanics.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Free Energy Calculations in Molecular Modelling

Hands-on training on free energy calculations.
Protocols for estimating binding free energies and analyzing molecular interactions using advanced simulation techniques.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Coarse-Grained Modelling

Practical session on coarse-grained modelling techniques.
Protocols for simplifying large molecular systems to study their behavior over longer timescales.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.
Dialogue on overcoming challenges in adopting new technologies in similar sectors.
Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

3. Workshop in Protein Modelling and Docking

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.
Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Homology Modelling of Proteins

Hands-on workshop on building protein models through homology modelling.
Protocols for generating 3D models of proteins based on homologous templates

using software like MODELLER.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Protein-Ligand Docking Techniques

Practical session on molecular docking of ligands to protein targets.
Protocols for using docking software like AutoDock and analyzing binding poses and affinities.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Virtual Screening of Small Molecules

Hands-on training on virtual screening techniques.
Protocols for performing high-throughput virtual screening of compound libraries to identify potential drug candidates.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Protein-Protein Docking and Complex Modelling

Practical session on modelling protein-protein interactions.
Protocols for docking proteins together and analyzing protein complexes using molecular modelling software.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.
Dialogue on overcoming challenges in adopting new technologies in similar sectors.
Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

4. Workshop in Molecular Modelling in Drug Design

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Structure-Based Drug Design

Hands-on workshop on structure-based drug design techniques.

Protocols for designing small molecule inhibitors by leveraging the 3D structures of target proteins.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Ligand-Based Drug Design Approaches

Practical session on ligand-based drug design.

Protocols for developing pharmacophores and QSAR models to guide the design of new compounds.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Fragment-Based Drug Discovery

Hands-on training on fragment-based drug discovery techniques.

Protocols for screening and growing small molecular fragments to optimize drug binding.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: ADMET Modelling in Drug Development

Practical session on ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) modelling.

Protocols for predicting drug pharmacokinetics and toxicity using computational methods.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

5. Workshop in Molecular Modelling of Membranes and Lipids

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Modelling Lipid Bilayers and Membranes

Hands-on workshop on molecular modelling of lipid bilayers.

Protocols for building and simulating membrane models and understanding their interactions with proteins and small molecules.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Simulating Membrane-Protein Interactions

Practical session on membrane-protein interactions.

Protocols for simulating how membrane proteins interact with lipid bilayers and other membrane components.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Molecular Modelling of Ion Channels

Hands-on training on modelling ion channels.

Protocols for simulating ion transport through membrane channels and studying

their conformational changes.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Modelling Drug Interactions with Membranes

Practical session on drug-membrane interactions.

Protocols for simulating the interaction of drugs with lipid bilayers to study permeability and drug transport.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

6. Workshop in Molecular Modelling of Nucleic Acids

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Modelling DNA and RNA Structures

Hands-on workshop on modelling nucleic acid structures.

Protocols for building 3D models of DNA and RNA and simulating their behavior using molecular modelling tools.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Protein-Nucleic Acid Docking

Practical session on docking proteins with nucleic acids.

Protocols for studying how proteins bind to DNA or RNA using molecular docking techniques.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Molecular Dynamics of Nucleic Acids

Hands-on training on molecular dynamics simulations of nucleic acids.

Protocols for simulating the dynamics of DNA and RNA in different environments.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: RNA Structure Prediction and Modelling

Practical session on RNA structure prediction.

Protocols for predicting RNA secondary and tertiary structures and simulating their folding pathways.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

7. Workshop in Molecular Modelling of Enzymes

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Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Enzyme Mechanism Modelling

Hands-on workshop on modelling enzyme mechanisms.

Protocols for simulating enzyme-catalyzed reactions and studying transition states

and intermediates.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Modelling Enzyme-Substrate Complexes

Practical session on modelling enzyme-substrate interactions.

Protocols for building enzyme-substrate complexes and simulating their binding and reaction pathways.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Computational Enzyme Design

Hands-on training on designing enzymes in silico.

Protocols for using computational tools to engineer enzymes with new or improved catalytic properties.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Predicting Enzyme Kinetics Using Molecular Modelling

Practical session on predicting enzyme kinetics.

Protocols for using molecular modelling to calculate kinetic parameters like K_m , V_{max} , and catalytic efficiency.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

8. Workshop in Molecular Modelling for Materials Science

+

Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Modelling Polymers and Nanomaterials

Hands-on workshop on molecular modelling of polymers and nanomaterials. Protocols for building and simulating polymer structures and nanoparticles in different environments.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Molecular Modelling of Crystals and Solid-State Materials

Practical session on modelling crystalline materials.

Protocols for studying the properties and behaviors of solid-state materials at the

molecular level.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Modelling Molecular Interactions in Materials

Hands-on training on studying molecular interactions in materials.

Protocols for simulating van der Waals forces, hydrogen bonding, and electrostatic interactions in materials science.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Predicting Material Properties Using Molecular Modelling

Practical session on predicting material properties.

Protocols for using molecular modelling to calculate mechanical, thermal, and electronic properties of materials.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

9. Workshop in Molecular Modelling for Biomaterials and Tissue Engineering

+

Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Modelling Biomaterials for Tissue Scaffolds

Hands-on workshop on molecular modelling of biomaterials.

Protocols for designing and simulating tissue scaffold materials at the molecular level.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Simulating Biodegradation of Biomaterials

Practical session on modelling the biodegradation of biomaterials.

Protocols for simulating the degradation processes of biodegradable polymers and tissues.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Molecular Modelling of

Biointerfaces

Hands-on training on studying biointerfaces.

Protocols for simulating the interactions between biomaterials and biological molecules, such as proteins and cells.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Predicting Mechanical Properties of Biomaterials

Practical session on predicting the mechanical properties of biomaterials.

Protocols for using molecular modelling to calculate the tensile strength, elasticity, and durability of biomaterials.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

10. Workshop in Emerging Trends in Molecular Modelling

+

Date: Pre Selected Date

Fee: Rs 6000/-

Duration: One Day

Mode: Offline and Virtual

Location for Offline: NBL Cherlapalli IDA Branch

Facilitator(s): NTHRYS TEAM

8:00 AM - 8:30 AM: Registration and Welcome Coffee

Participants arrive, register, and network over coffee.

8:30 AM - 8:45 AM: Opening Remarks

Welcome by the host.

Brief overview of today's focus.

8:45 AM - 10:15 AM: Session 1: Machine Learning in Molecular Modelling

Hands-on workshop on integrating machine learning with molecular modelling. Protocols for applying AI to predict molecular behaviors, optimize simulations, and accelerate drug discovery.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Molecular Modelling for Synthetic Biology

Practical session on modelling synthetic biological systems. Protocols for simulating the design and function of synthetic genes, proteins, and metabolic pathways.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Modelling for Nanomedicine Applications

Hands-on training on molecular modelling for nanomedicine. Protocols for simulating nanoparticle-based drug delivery systems and nanocarriers for therapeutic use.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Multiscale Modelling of Complex Biological Systems

Practical session on multiscale modelling.

Protocols for integrating molecular modelling with larger-scale biological systems, bridging the gap between molecular, cellular, and tissue-level simulations.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes

Note: NTHRYS Management reserves the right to modify the workshop module at any time without prior notice. Registered or enrolled candidates will receive the module that is current on the day of enrollment.

NTHRYS Workshops Department

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Molecular Modelling Workshops Application Process

1. Select a workshop from the list.
2. Contact via whatsapp on the number present above to request fee details and dates suitable for joining. Alternatively, you can send an email to workshops (a t) nthrys [d 0 t] com.
3. Our Workshop department will contact you promptly to provide further assistance.