

Molecular Modeling Internship

Advanced Focussed Areas for Interns in Molecular Modeling Internships

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• Fundamentals of Molecular Modeling

- Introduction to Molecular Modeling
- Quantum Mechanics and Molecular Mechanics
- o Force Fields and Potential Energy Surfaces
- Molecular Dynamics Simulations
- Monte Carlo Simulations
- Computational Chemistry Methods
- Applications of Molecular Modeling in Research
- Ethics and Safety in Computational Research
- Future Directions in Molecular Modeling

• Techniques and Algorithms in Molecular Modeling

- Structure Prediction and Homology Modeling
- Docking Studies and Virtual Screening
- Quantum Mechanical Methods and Density Functional Theory (DFT)
- Molecular Dynamics and Enhanced Sampling Techniques
- Free Energy Calculations and Binding Affinity Predictions
- Machine Learning in Molecular Modeling
- Visualization and Analysis Tools
- Case Studies in Computational Methods
- Future Trends in Molecular Modeling Techniques
- Integrating Experimental and Computational Data

• Applications in Drug Design and Discovery

- Structure-Based Drug Design
- Ligand-Based Drug Design
- Pharmacophore Modeling and Screening
- ADMET Prediction and Toxicity Assessment
- Case Studies in Drug Discovery
- Clinical Applications of Computational Chemistry
- Future Trends in Drug Design
- Challenges in Translational Research

- Regulatory Aspects of Drug Development
- Ethical Considerations in Drug Design

• Materials Science and Nanotechnology

- Modeling of Nanomaterials and Nanostructures
- Polymer Modeling and Simulation
- Crystallography and Solid-State Modeling
- Surface and Interface Properties
- Mechanical Properties and Durability
- Electronic Properties and Device Simulation
- o Case Studies in Materials Science
- Future Trends in Computational Materials
- Environmental Impact and Sustainability
- Future Directions in Nanotechnology

• Future Directions and Emerging Trends

- Innovations in Molecular Modeling and Simulation
- o Role of Computational Chemistry in Precision Medicine
- o Emerging Applications in Biomedical Research
- o Global Trends in Computational Research
- o Future of Molecular Modeling in Industry and Academia
- Ethics and Regulation in Computational Research
- o Future Research Priorities in Molecular Modeling
- Impact of Molecular Modeling on Society
- Public Engagement and Education in Computational Sciences
- o Integration of Molecular Modeling with AI and Data Science

Contact Via Whatsapp on +91-7993084748 for Fee Details

Apply

Internship Fee Structures					
Duration	Academic Mode	Technical Mode	Research Mode		
5 Days	Rs 3750	Rs 6000	Rs 9000		
10 Days	Rs 4500	Rs 6750	Rs 9750		
15 Days	Rs 4950	Rs 7200	Rs 12000		
20 Days	Rs 6750	Rs 9000	Rs 15000		
30 Days	Rs 7500	Rs 10500	Rs 19500		

45 Days	Rs 9000	Rs 12000	Rs 22500
2 Months	Rs 10500	Rs 13500	Rs 27000
3 Months	Rs 12000	Rs 22500	Rs 34500
4 Months	Rs 18000	Rs 28500	Rs 42000
5 Months	Rs 22500	Rs 31500	Rs 49500
6 Months	Rs 27000	Rs 36000	Rs 54000
7 Months	Rs 28500	Rs 40500	Rs 64500
8 Months	Rs 31500	Rs 45000	Rs 72000
9 Months	Rs 36000	Rs 52500	Rs 82500
10 Months	Rs 43500	Rs 60000	Rs 97500
11 Months	Rs 48000	Rs 67500	Rs 112500
1 Year	Rs 57000	Rs 75000	Rs 142500

18% additional GST on all fee structures.

Installment options are available for all durations.

NTHRYS Students



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Deliverables	Academic Mode	Technical Mode	Research Mode
Certification		Z	✓
Hands-On Practical Exposure	Z	Z	✓
Thesis	✓	×	V
PowerPoint Assistance	Z	Z	✓
Protocol Repetitions	×	Z	V
Publication Coauthorships	×	×	3 Months Duration onwards
References	×	✓	✓
Recommendations	×	×	V
Experience Letters	×	×	6 Months Duration Onwards
Placement Assistance	×	×	6 Months Duration Onwards
Placement Guarantee	×	×	1 Year Duration

Offline Locations

Hyderabad
Cherlapalli IDA, 500051 Chennai

Jalahalli, Bahubali Nagar

Aroma Gardens, Beside Townhall Metro

Address will be updated in few days

Contact Us for further queries

Offline Timetable

3 - 5 Hours per day \mid 4 Days Practicals / week \mid 1 Day Reporting

Weekly Schedule

Tuesday to Friday: Practical Sessions

Saturday: Documentation Day

Sunday & Monday: Weekend Holidays

Lab Working Hours

9:30 AM to 5:30 PM

Students/Scholars are assigned **3 to 5 hours/day** based on their protocols.

Online Mode Workflow

2 to 4 hours per day as per discussed with NTHRYS Management before booking the slot.

All activities (Online / Virtual and Offline) are managed through the **NTHRYS Project Dashboard System** — a web portal designed exclusively to facilitate, guide, and track your progress throughout each phase.

Phase 1: Topic / Title Finalization

Guided assistance in selecting and refining your research topic or project title within the dashboard interface.

Phase 2: Research Methodology Finalization

Step-by-step guidance in defining objectives, research questions, and methodology using interactive templates and mentor feedback on the dashboard.

Phase 3: Software, Tools, and Statistical Approaches

Installation assistance, tool demonstrations, and access to recommended software provided via the dashboard with mentor instructions and documentation.

Phase 4: Task Execution

Students/scholars execute research tasks on their own systems while mentors monitor and guide progress through the dashboard system.

Phase 5: Results Analysis

Data analysis, results review, and interactive discussions are facilitated through dedicated dashboard modules ensuring research integrity.

Phase 6: Documentation

Proper documentation of results, methodology, and conclusions using dashboard templates, ensuring consistency and completeness.

No Video Calls, No Theory Classes: All learning is task-based, with hands-on execution by students/scholars under the guidance of mentors using the **NTHRYS Project Dashboard System**.

Click Here to know schedule, offline locations, calendar, modes of operation etc.,

Important Note

- Note 1: Candidates may select any one of the focused areas listed for their internship.
- Note 2: Fundamental concepts are provided as guidance for candidates who require them; however, candidates may choose to bypass these sections if desired.
- Note 3: All candidates will gain practical, hands-on experience with every step outlined in the provided methodology.
- Note 4: Comprehensive placement assistance and career guidance will be available to all candidates during and after the internship.
- Note 5: We understand that many students may lack basic practical exposure due to shortcomings in their college education. This is not the fault of the students but rather a failure of the institutions and their staff. At NTHRYS, our staff excel at training every student from the ground up, ensuring they gain the necessary skills and experience.