Computational Chemistry Internship

Unpublished Futuristic Focussed Areas in Computational Chemistry

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- **Quantum-Inspired Molecular Design**
  - Quantum algorithms for predicting molecular stability
  - Qubit-based mapping of chemical interactions
  - Quantum neural networks for energy minimization
  - Simulating chemical reactivity using quantum emulators
  - Quantum tunneling effects in enzymatic catalysis
  - Quantum computing applications in reaction kinetics
  - Hybrid quantum-classical simulations for protein folding
  - Quantum-enhanced retrosynthesis prediction
  - Quantum cryptography for molecular data security
  - Optimization of basis sets for quantum accuracy
- **AI-Powered Predictive Cheminformatics**
  - Generative models for novel compound prediction
  - AI in reaction mechanism discovery
  - Neural networks for binding affinity prediction
  - Reinforcement learning in synthetic chemistry planning
  - Explainable AI models in molecular activity profiling
  - AI-enhanced ligand docking simulations
  - Predictive toxicology using deep learning
  - AutoML for structure-activity relationship modeling
  - Big data analytics for metabolomics pathways
  - AI-based formulation of pharmaceutical compounds
- **Cloud-Integrated Molecular Simulations**
  - Deploying molecular dynamics on cloud GPUs
  - Edge computing in real-time reaction simulations
  - IoT-enabled simulation pipelines
  - Cloud-based parallelization of Monte Carlo simulations
  - Data fusion from multiple simulation platforms
  - Blockchain-secured simulation data tracking
  - Decentralized model training for reaction libraries

    - Cloud-native visualization of molecular events
    - Hybrid computing architectures in chemical dynamics
    - Cloud orchestration for AI-driven chemical discovery
- **Green and Sustainable Computational Chemistry**
    - Eco-molecular modeling for green solvent design
    - Simulating bio-based degradable polymers
    - Predictive modeling of eco-toxicological pathways
    - AI for energy-efficient reaction mechanism prediction
    - Computational optimization of catalytic converters
    - Life cycle modeling of chemical products
    - Atom economy simulations for greener synthesis
    - Carbon footprint analysis using molecular data
    - AI for designing biodegradable surfactants
    - Virtual screening for sustainable nanomaterials
- **High-Throughput Virtual Experimentation**
    - AI-curated high-throughput compound libraries
    - Cloud-based HTS pipelines for lead discovery
    - GPU-accelerated virtual reaction screening
    - Integrating robotics with in silico modeling
    - Parallel computation for synthetic route analysis
    - Machine-learned feedback loops in HTS
    - Automation of reaction feasibility simulations
    - Predicting multi-target effects in combinatorial libraries
    - Deep learning for cross-target pharmacokinetics
    - HTS benchmarking using quantum-inspired solvers

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	✓	✓	✓
Hands-On Practical Exposure	✓	✓	✓
Thesis	✓	✘	✓
PowerPoint Assistance	✓	✓	✓
Protocol Repetitions	✘	✓	✓
Publication Coauthorships	✘	✘	3 Months Duration onwards
References	✘	✓	✓
Recommendations	✘	✘	✓
Experience Letters	✘	✘	6 Months Duration Onwards
Placement Assistance	✘	✘	6 Months Duration Onwards
Placement Guarantee	✘	✘	1 Year Duration

Offline Locations

Hyderabad

Cherlapalli IDA, 500051 Chennai

Parrys Corner, 600001 Bangalore

Jalahalli, Bahubali Nagar Kochi

Aroma Gardens, Beside Townhall Metro Visakhapatnam

Address will be updated in few days Bhubaneswar

Address will be updated in few days Kolkata

Address will be updated in few days Patna

Address will be updated in few days Lucknow

Address will be updated in few days Chandigarh

Address will be updated in few days Jaipur

Address will be updated in few days Ahmedabad

Address will be updated in few days Indore

Address will be updated in few days Dallas

825 Watters Creek Blvd, Allen

Contact Us for further queries

Offline Timetable

3 - 5 Hours per day | 4 Days Practicals / week | 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.**