# Molecular Modelling Research Outsourcing Services

Our molecular modelling research outsourcing services simulate and visualize biomolecular structures and interactions to support rational drug design and protein engineering projects.

## Our Molecular Modelling Research Capabilities

Our computational chemists and bioinformaticians use advanced software tools and high-performance computing clusters to predict, analyze, and optimize molecular interactions and properties.

## Types of Molecular Modelling Research We Handle

- Homology Modelling
- Molecular Docking Studies
- Ligand-Protein Interaction Analysis
- Pharmacophore Modelling
- Quantitative Structure-Activity Relationship (QSAR) Analysis
- Virtual Screening of Compound Libraries
- Free Energy Calculations
- Molecular Dynamics Simulation
- Binding Site Prediction
- Protein-Ligand Binding Affinity Estimation
- Protein-Protein Interaction Modelling
- Enzyme Mechanism Simulation
- Protein Mutagenesis Modelling
- Structure-Based Drug Design
- Ligand-Based Drug Design
- ADMET Property Prediction
- Lead Compound Optimization
- Fragment-Based Drug Discovery
- Conformational Analysis
- Energy Minimization and Optimization
- Hydrogen Bond and Electrostatic Analysis
- Solvation and Desolvation Studies
- Coarse-Grained Modelling
- Replica Exchange Simulations

- 3D-QSAR and Comparative Molecular Field Analysis (CoMFA)
- Ligand Efficiency and Drug Likeness Analysis
- In Silico Toxicity Prediction
- Regulatory-Compliant Modelling Reports
- Publication-Ready Modelling Data
- Custom Molecular Modelling Projects

## Key Research Outsourcing Services Offered

- Target Protein Structure Retrieval and Preparation
- Ligand Library Preparation
- Molecular Docking Protocol Setup
- Binding Pocket Analysis
- Interaction Energy Calculation
- Pharmacophore Hypothesis Generation
- QSAR Model Development and Validation
- Virtual Screening of Large Databases
- Molecular Dynamics Simulation Execution
- Free Energy Perturbation and MM-PBSA Analysis
- Conformational Sampling and Analysis
- Lead Compound Prioritization
- ADMET Profiling and Toxicity Prediction
- Comparative Modelling and Homology Building
- Protein-Ligand Interaction Visualization
- Bioinformatics Pipeline Setup
- Data Analysis and Report Generation
- Regulatory-Compliant Documentation
- Confidential Data Handling and NDA
- Interim Reports and Stakeholder Updates
- Publication-Ready Figures and Manuscripts
- Stakeholder Presentation Support
- Workshops and Training in Molecular Modelling
- Post-Project Technical Consulting
- IP Filing and Patent Drafting Support
- Grant Proposal and Manuscript Assistance
- Sample Archiving and Secure Backup
- Cross-Lab Validation and Collaboration
- Compliance with GLP, GCP, ISO Standards
- Long-Term Modelling Research Partnerships

## Why Choose Us for Molecular Modelling Research Outsourcing?

Our specialists deliver high-precision computational data to guide drug discovery, lead optimization, and biomolecular interaction studies efficiently.

## Industries & Sectors We Serve

- Pharmaceutical and Biotech R&D
- Academic Drug Discovery Labs
- Structural Biology and Protein Engineering Units
- Regulatory and Toxicology Research Agencies
- Clinical Research Organizations (CROs)
- Bioinformatics and Computational Chemistry Firms

## Customized Molecular Modelling Solutions

We design docking studies, QSAR models, and dynamic simulations aligned with your therapeutic targets, lead compounds, and regulatory requirements.

## Quality Assurance & Regulatory Compliance

Our modelling workflows comply with GLP, GCP, ISO, and international drug development standards, ensuring validated, reproducible, and audit-ready outputs.

## Case Studies & Client Success Stories

Explore how our molecular modelling outsourcing has supported hit identification, lead optimization, and novel mechanism elucidation in drug discovery. References available on request.

## How It Works: Our Research Outsourcing Process

1. **Requirement Gathering:** Define targets, ligands, and modelling objectives.
2. **Proposal & Quotation:** Provide a clear plan, timeline, and cost estimate.
3. **Execution:** Perform docking, simulations, and energy calculations.
4. **Data Reporting:** Deliver interaction maps, scores, and compliance-ready reports.
5. **Post-Project Support:** Offer follow-up consulting, manuscript help, and IP assistance.

## Frequently Asked Questions (FAQs)

**Q:** Do you perform protein-ligand binding affinity estimation?
**A:** Yes — we estimate binding energies using MM-PBSA, FEP, and other validated methods.

**Q:** Can you assist with lead compound optimization?
**A:** Absolutely — we provide QSAR modelling and pharmacophore refinement services.

**Q:** How secure is my compound library and model data?
**A:** Strict NDAs, encrypted servers, and compliance with data security protocols ensure total confidentiality.

# Get Started / Request a Quote

Contact us today to discuss your molecular modelling project and receive a custom plan, timeline, and cost estimate aligned with your discovery goals.

# Contact Us

Email: research-outsourcing@nthrys.com
Phone: +91-8977624748