



Cheminformatics Research Outsourcing Services

Our cheminformatics research outsourcing services offer computational pipelines for chemical data analysis, property prediction, and smart compound selection for drug discovery, agrochemicals, and materials research.

Our Cheminformatics Research Capabilities

Our expert computational chemists leverage high-end software tools and custom scripts to handle complex chemical datasets, predict molecular properties, and design robust virtual libraries under strict QA/QC.

Types of Cheminformatics Research We Handle

- Chemical Data Curation and Standardization
- 2D and 3D Structure Generation
- Molecular Descriptor Calculation
- Fingerprint Generation and Similarity Search
- QSAR/QSPR Model Development
- Property Prediction Models (LogP, solubility)
- Virtual Compound Library Generation
- Fragment-Based Drug Design
- Substructure Searching and Filtering
- Pharmacophore Modeling and Screening
- Structure Clustering and Diversity Analysis
- ADMET Property Prediction
- Lead-Likeness and Drug-Likeness Assessment
- De Novo Compound Design
- Data Mining of Chemical Databases
- Integration with High-Throughput Screening
- Cross-Target Binding Prediction
- Machine Learning for Cheminformatics
- Big Data Analytics for Chemical Datasets
- Custom Algorithm Development
- InChI and SMILES Conversion
- Chemical Space Visualization
- Scaffold Hopping Analysis

- Property-Based Compound Filtering
- Regulatory-Compliant Reports
- Data Security and Backup Solutions
- Custom Cheminformatics Pipelines
- Integration with Bioinformatics Data
- Automated Workflow Scripting
- Long-Term Computational Support

Key Research Outsourcing Services Offered

- Chemical Structure Standardization
- Descriptor and Fingerprint Generation
- Similarity and Diversity Analysis
- QSAR/QSPR Model Building
- Virtual Screening of Compound Libraries
- Pharmacophore Hypothesis Development
- Property Prediction (ADMET, LogP)
- Lead and Drug-Likeness Scoring
- Substructure and Scaffold Analysis
- Machine Learning Model Development
- Database Mining and Management
- De Novo Molecule Generation
- Fragment-Based Library Design
- Visualization Dashboards for Chemical Space
- Custom Scripting and Automation Tools
- API Development for Cheminformatics Tools
- Big Data Analysis Pipelines
- Publication-Ready Figures and Tables
- Confidential Data Handling with NDA
- Secure Cloud Data Storage
- Compliance with Industry Standards
- Progress Reports and Data Snapshots
- Detailed SOPs and User Guides
- Integration with LIMS/ELN Systems
- Regulatory Documentation Preparation
- Custom Algorithm Development
- Training Workshops for Client Teams
- Post-Project Consulting and Updates
- Custom Dashboard and Report Generation
- Long-Term Partnership for Data Mining

Why Choose Us for Cheminformatics Research Outsourcing?

Our cheminformatics teams blend computational power, chemical expertise, and secure data systems to deliver actionable insights for smarter compound prioritization and faster innovation

cycles.

Industries & Sectors We Serve

- Pharmaceutical and Biotech Firms
- Agrochemical and Pesticide Companies
- Specialty Chemical Manufacturers
- Academic Computational Chemistry Labs
- Contract Research Organizations (CROs)
- Regulatory and IP Consulting Agencies

Customized Cheminformatics Solutions

We build tailored cheminformatics pipelines, predictive models, and visualization dashboards adapted to your R&D objectives and regulatory requirements.

Quality Assurance & Regulatory Compliance

Our processes align with industry best practices and follow robust QA/QC, ensuring validated, reproducible computational results with audit trails.

Case Studies & Client Success Stories

See how our cheminformatics support has enabled discovery teams to narrow candidate lists, improve property predictions, and speed up lead optimization. References available on request.

How It Works: Our Research Outsourcing Process

1. **Requirement Gathering:** Define project goals, compound classes, and output needs.
2. **Proposal & Quotation:** Provide detailed workflow plan, cost estimate, and timeline.
3. **Execution and Modeling:** Perform data curation, model building, and validation.
4. **Data Reporting:** Deliver complete reports, visualizations, and raw data exports.
5. **Post-Project Support:** Offer consulting for integration, IP support, and next steps.

Frequently Asked Questions (FAQs)

Q: Do you handle proprietary and large libraries securely?

A: Yes — NDAs, encryption, and strict data protocols protect your chemical IP and datasets.

Q: Can you customize your pipelines for our internal databases?

A: Absolutely — we adapt pipelines to fit your in-house data structures and formats.

Q: How fast can I get a custom QSAR model?

A: Timelines depend on complexity but typical delivery ranges from 2–6 weeks.

Get Started / Request a Quote

Contact us today to discuss your cheminformatics research and receive a detailed plan and competitive quote tailored to your discovery pipeline.

Contact Us

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