Cheminformatics Internship Topics

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50	40	Internships
Active Categories	Focused Areas	Internships

Cheminformatics Internship Categories

AI Generative Molecular Design Research https://internships.nthrys.com/cheminformatics/ai-generative-molecular-design-research	**Machine Learning QSAR/QSPR Research** https://internships.nthrys.com/cheminformatics/machine-learning-qsar-qspr-research
AI Virtual Compound Library Design Research https://internships.nthrys.com/cheminformatics/ai-virtual-compound-library-design-research	**AI Chemical Graph Neural Network Research** https://internships.nthrys.com/cheminformatics/ai-chemical-graph-neural-network-research
AI Bioactivity Prediction Research https://internships.nthrys.com/cheminformatics/ai-bioactivity-prediction-research	**AI Chemical Retrosynthesis Informatics Research** https://internships.nthrys.com/cheminformatics/ai-chemical-retrosynthesis-informatics
AI Polypharmacology Cheminformatics Research https://internships.nthrys.com/cheminformatics/ai-polypharmacology-cheminformatics-research	**AI Drug-Likeness Filtering Research** https://internships.nthrys.com/cheminformatics/ai-drug-likeness-filtering-research
AI Scaffold Analysis & Hopping Research https://internships.nthrys.com/cheminformatics/ai-scaffold-analysis-hopping-research	**AI Metabolite-Drug Interaction Research** https://internships.nthrys.com/cheminformatics/ai-metabolite-drug-interaction-research
Molecular Fingerprint Development and Optimization https://internships.nthrys.com/cheminformatics/molecular-fingerprint-development-optimization	**Chemical Space Exploration Mapping** https://internships.nthrys.com/cheminformatics/chemical-space-exploration-mapping
Protein-Ligand Docking Scoring Function Research https://internships.nthrys.com/cheminformatics/protein-ligand-docking-scoring-function	**Fragment-Based Drug Discovery Informatics** https://internships.nthrys.com/cheminformatics/fragment-based-drug-discovery-informatics
Chemical Compound Database Curation https://internships.nthrys.com/cheminformatics/chemical-compound-database-curation	**Natural Product Cheminformatics Analysis** https://internships.nthrys.com/cheminformatics/natural-product-cheminformatics-analysis
Chemotoxicology Predictive Modeling Research https://internships.nthrys.com/cheminformatics/chemotoxicology-predictive-modeling-research	**De Novo Drug Design Algorithm Development** https://internships.nthrys.com/cheminformatics/de-novo-drug-design-algorithm-development
Chemical Patent Analysis and Mining https://internships.nthrys.com/cheminformatics/chemical-patent-analysis-mining	**Cheminformatics Pipeline Automation Development** https://internships.nthrys.com/cheminformatics/cheminformatics-pipeline-automation-development
Molecular Diversity Assessment Algorithms https://internships.nthrys.com/cheminformatics/molecular-diversity-assessment-algorithms	**Chemical Structure Standardization Methods** https://internships.nthrys.com/cheminformatics/chemical-structure-standardization-methods
Enzyme Substrate Specificity Prediction https://internships.nthrys.com/cheminformatics/enzyme-substrate-specificity-prediction	**Chemical Ontology and Knowledge Graph Construction** https://internships.nthrys.com/cheminformatics/chemical-ontology-knowledge-graph-construction
Solubility and ADME Property Prediction Research https://internships.nthrys.com/cheminformatics/solubility-adme-property-prediction-research	**Chemical Reaction Type Classification Learning** https://internships.nthrys.com/cheminformatics/chemical-reaction-type-classification-learning
Multi-Target Activity Prediction Cheminformatics https://internships.nthrys.com/cheminformatics/multi-target-activity-prediction-cheminformatics	**Chemical Similarity and Clustering Methods** https://internships.nthrys.com/cheminformatics/chemical-similarity-clustering-methods
Molecular Descriptor Development and Selection https://internships.nthrys.com/cheminformatics/molecular-descriptor-development-selection	**Lead Compound Optimization Strategy Research** https://internships.nthrys.com/cheminformatics/lead-compound-optimization-strategy-research
Bioisostere Database and Prediction Systems https://internships.nthrys.com/cheminformatics/bioisostere-database-prediction-systems	**Off-Target Toxicity Prediction Modeling** https://internships.nthrys.com/cheminformatics/off-target-toxicity-prediction-modeling
Chemical Data Integration and Harmonization https://internships.nthrys.com/cheminformatics/chemical-data-integration-harmonization	**High-Throughput Screening Data Analysis** https://internships.nthrys.com/cheminformatics/high-throughput-screening-data-analysis
Chemical Prioritization and Ranking Systems https://internships.nthrys.com/cheminformatics/chemical-prioritization-ranking-systems	**Molecular Dynamics Trajectory Analysis Research** https://internships.nthrys.com/cheminformatics/molecular-dynamics-trajectory-analysis-research

Chemical Intuition and Rule-Based Systems https://internships.nthrys.com/cheminformatics/chemical-intuition-rule-based-systems	**Compound Library Design and Optimization** https://internships.nthrys.com/cheminformatics/compound-library-design-optimization
Drug-Disease Association Network Analysis https://internships.nthrys.com/cheminformatics/drug-disease-association-network-analysis	**Chemical Affordability and Synthetic Accessibility Assessment** https://internships.nthrys.com/cheminformatics/chemical-affordability-synthetic-accessibility-assessment
Pharmacophore Modeling and Pattern Recognition https://internships.nthrys.com/cheminformatics/pharmacophore-modeling-pattern-recognition	**Chemical Structure Novelty Assessment Methods** https://internships.nthrys.com/cheminformatics/chemical-structure-novelty-assessment-methods
Metabolism-Based Drug-Drug Interaction Prediction https://internships.nthrys.com/cheminformatics/metabolism-based-drug-drug-interaction-prediction	**Cheminformatics for Immunotherapy Research** https://internships.nthrys.com/cheminformatics/cheminformatics-immunotherapy-research
Chemical Combinatorial Space Sampling Research https://internships.nthrys.com/cheminformatics/chemical-combinatorial-space-sampling-research	**Peptide and Protein Sequence Cheminformatics** https://internships.nthrys.com/cheminformatics/peptide-protein-sequence-cheminformatics
Chemical Fingerprint Comparison and Benchmarking https://internships.nthrys.com/cheminformatics/chemical-fingerprint-comparison-benchmarking	**Machine Learning Model Interpretability in Chemistry** https://internships.nthrys.com/cheminformatics/machine-learning-model-interpretability-chemistry
Chemical Batch Effect Detection and Correction https://internships.nthrys.com/cheminformatics/chemical-batch-effect-detection-correction	**Emerging Contaminant Prediction and Detection** https://internships.nthrys.com/cheminformatics/emerging-contaminant-prediction-detection

Cheminformatics Internship Topics and Focused Areas

AI Generative Molecular Design Research

- Generative Models for Drug-like Molecule Synthesis
- Molecular Property Prediction using Deep Learning
- De Novo Drug Discovery with Reinforcement Learning
- Molecular Scaffold Optimization and Library Design
- Explainable AI for Structure-Activity Relationship Modeling

Machine Learning QSAR/QSPR Research

- Molecular Descriptor Engineering for QSAR Model Development
- Machine Learning Algorithm Optimization for QSPR Predictions
- Dataset Curation and Validation for Cheminformatics Modeling
- Model Interpretation and Explainability in Chemical Property Prediction
- Transfer Learning and Deep Learning for Chemical Space Exploration

AI Virtual Compound Library Design Research

- Molecular Generation Models for Drug Discovery
- Virtual Screening and Molecular Docking Workflows
- Chemical Space Exploration and QSAR Modeling
- Synthetic Accessibility Assessment and Retrosynthesis Planning
- Cheminformatics Database Development and Curation

AI Chemical Graph Neural Network Research

- Molecular Property Prediction using Graph Neural Networks
- Drug Discovery Pipeline Optimization with GNNs
- Chemical Reaction Outcome Prediction

- Molecular Graph Generation and De Novo Drug Design
- Attention Mechanisms in Chemical Graph Networks

Molecular Fingerprint Development and Optimization

- Fingerprint Algorithm Comparison and Benchmarking
- Machine Learning-Based Fingerprint Feature Selection
- Custom Fingerprint Design for Drug-Like Molecules
- Fingerprint-Based Molecular Diversity Analysis
- Deep Learning Models for Fingerprint Generation and Optimization

Molecular Descriptor Development and Selection

- Quantitative Structure-Activity Relationship (QSAR) Descriptor Engineering
- Machine Learning-Based Molecular Descriptor Selection and Feature Reduction
- 3D Molecular Descriptor Generation and Conformational Analysis
- Cheminformatics Descriptor Benchmark Development and Validation
- Custom Descriptor Implementation and Chemical Space Characterization

Lead Compound Optimization Strategy Research

- Structure-Activity Relationship (SAR) Analysis and Machine Learning Modeling
- Molecular Descriptor Generation and Feature Engineering for Lead Optimization
- Virtual Screening and Docking-Based Lead Prioritization
- ADME Property Prediction and Drug-Likeness Assessment
- Scaffold Hopping and Chemical Space Exploration for Novel Lead Generation

Metabolism-Based Drug-Drug Interaction Prediction

- Cytochrome P450 Enzyme Inhibition Modeling
- Metabolic Pathway Analysis and Substrate Classification
- Machine Learning Models for DDI Prediction
- Pharmacophore Development for Metabolic Enzyme Binding
- DDI Database Curation and Structure-Activity Relationship Mining