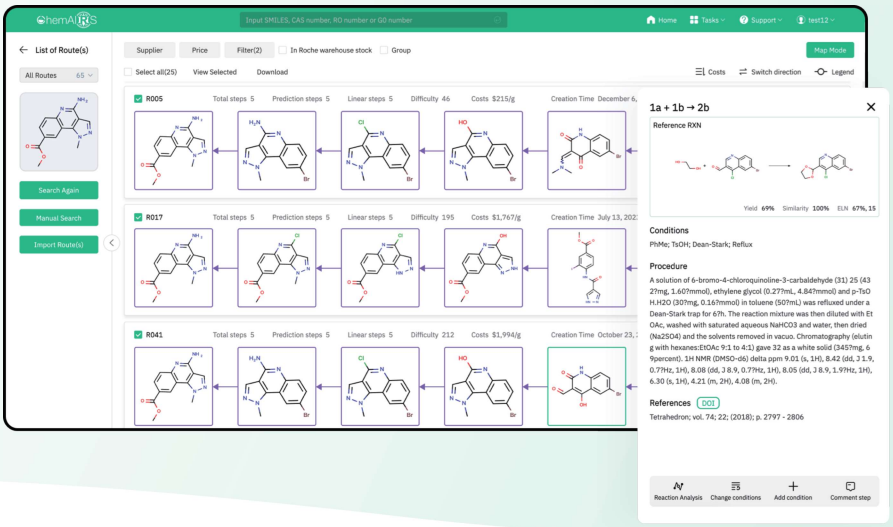
Chemical AI

ChemAIRS

THE MOST ADVANCED RETROSYNTHETIC PLANNING TOOL IN THE INDUSTRY

Based on chemical big data mining and deep learning algorithms, ChemAIRS can design multiple synthetic routes for a target molecule within a few minutes, fully considering factors including reaction feasibility, functional group compatibility, chiral synthesis strategies, and many more key factors in synthesis, providing chemists diverse viable synthetic ideas.



OUR AI-EMPOWERED CHEMISTRY EXPERTISE

Retrosynthetic Analysis

- Diverse and creative route design
- Equivalent to 10 years of medicinal chemist experience
- Real-time costs, yield, and condition prediction

Process Chemistry

- Recommend process routes and real-time cost accounting
- Filtering solvents, reagents, hazardous and precious metals
- Optimize both safety and cost-efficiency in synthesis

Forward Synthesis

- Generates virtual libraries based on core structures
- Centered around synthesis routes and accessible raw materials
- Evaluates reactivity, stability, protecting group, ring number, etc.

Synthesizability Assessment

- Addresses feasible routes and raw material availability
- High-throughput assessment for large real and virtual libraries
- Enhances practicality of synthesis routes

Impurity Prediction

- Predicts possible impurities in chemical reactions
- Offers >10 predictions and analysis based on MW
- Accounts for reagents, catalysts, and practical reaction factors

Advanced UI and Integratability

- Fully integrable with internal ELN system and BB libraries
- Customizable via local deployments and cloud with AES-256 encryption
- Learnings retained locally to improve long-term productivity

Contact us

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ChemAIRS

OUTPERFORMS COMPETING CASP TOOLS BY BLIND, HEAD-TO-HEAD COMPARISON

Challenge

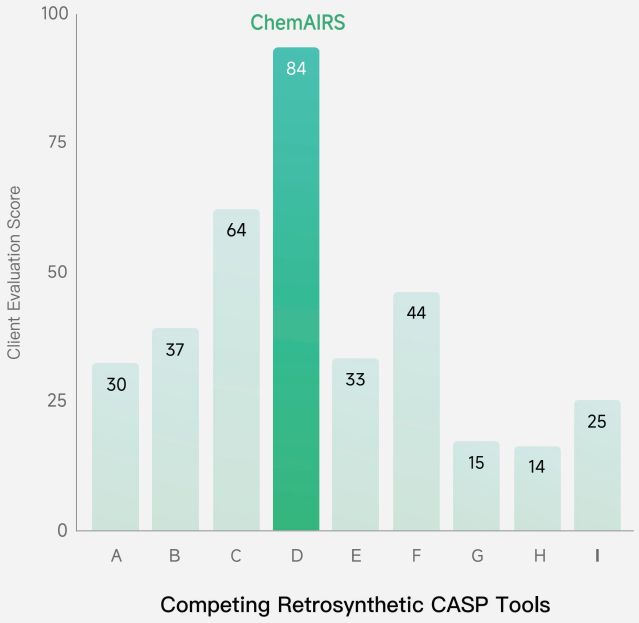
A top-tier CRO blind tested 9 competing retrosynthetic algorithms to propose synthetic routes for 60 structurally diverse, difficult target molecules.

Evaluation

An expert team of decades' experience in synthesis evaluated the diversity and feasibility of ideas beyond existing human options.

Outcome

ChemAIRS outperformed all other competing rule and/or data-based algorithms. The client further evaluated and incorporated ChemAIRS in its chemistry synthesis workflow.



HOW YOUR PROJECTS BENEFIT FROM ChemAIRS

Expand Synthesis Strategies

Finds new synthesis ideas and strategies, offers multi-dimensional condition filtering, optimizes existing synthesis routes, lowers synthesis costs, and improves research efficiency.

Secure Local Deployment

Supports local deployment to ensure data security. Integrates with corporate ELN data for local reuse, further reducing synthesis steps and risks.

Save Time in Route Generation

Quickly generates synthesis routes, reducing trial-and-error costs and enhancing research and development efficiency.

ABOUT CHEMICAL.AI

Founded in 2018, Chemical.AI leverages proprietary algorithms, comprehensive chemical data, and cutting-edge robotic lab automation to enhance chemical synthesis efficiency. With offices in Shanghai, Wuhan, Singapore, Boston, and Toronto, Chemical.AI has a team of 150 multidisciplinary experts skilled in retrosynthetic planning, automation, and lab digitalization, coupled with a rich database of chemical information and algorithms to pave the way in delivering advanced solutions across diverse sectors such as pharmaceuticals, biomedicine, chemical engineering, and new materials.

15+ years of research in chemistry synthesis

150+ multidisciplinary experts in chemistry, algorithm, and automation

60% hold a PhD or Master's degree

100+ pharma, biotech, and CROs

40+ local deployments of Chemical.AI tools

100,000+ online users registered for ChemAIRS

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