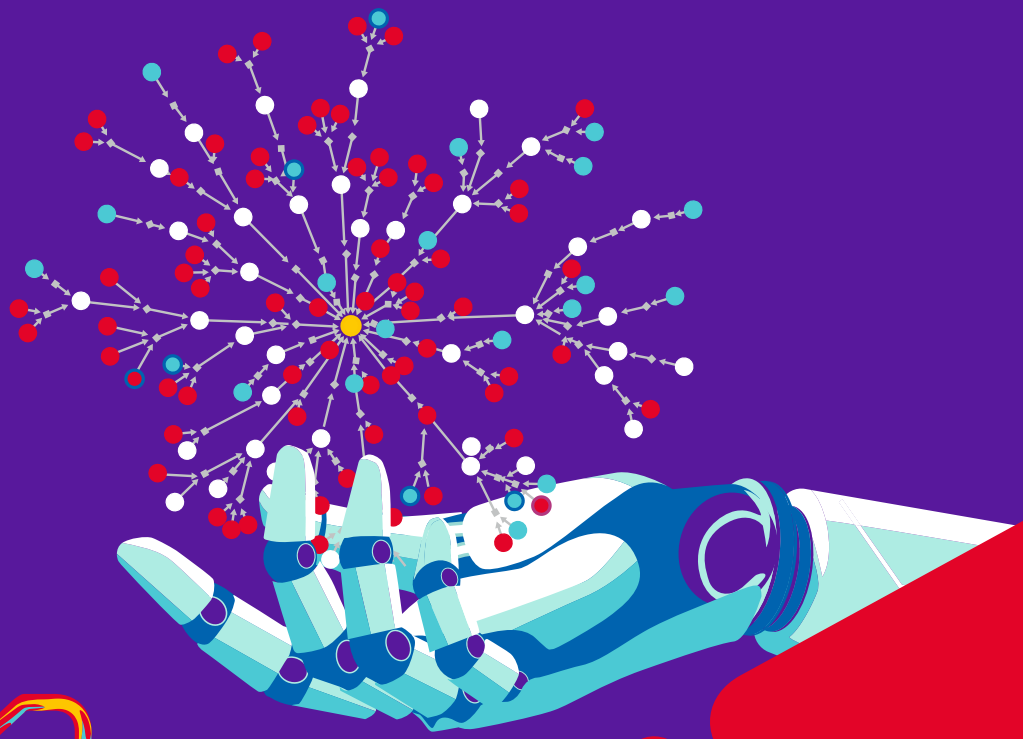
MERCK

SYNTHIA© Retrosynthesis Software

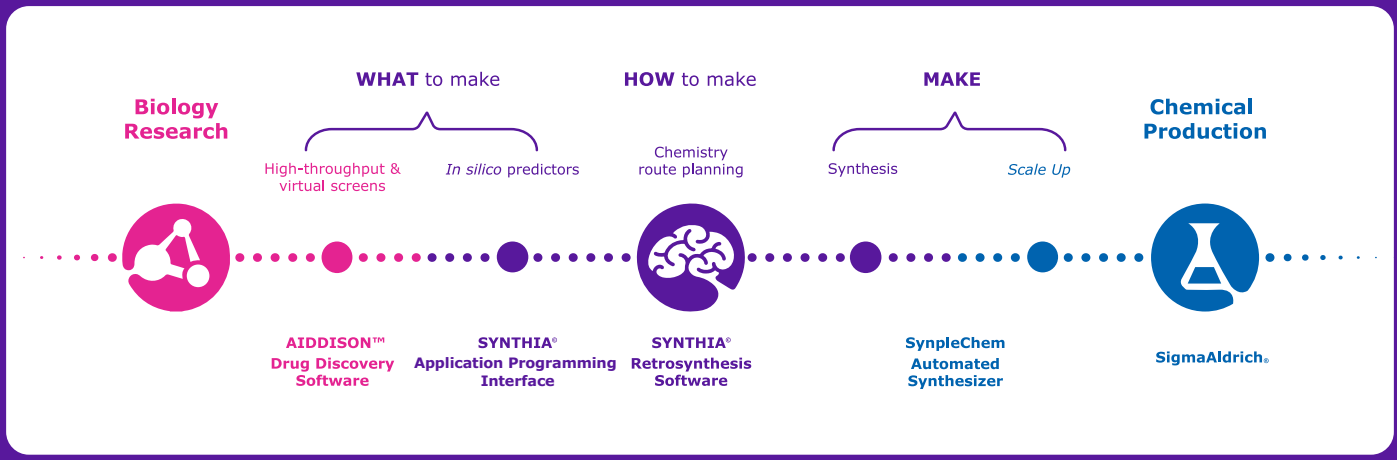
Discovery at your fingertips

Expert-coded by chemists and engineered by computer scientists, SYNTHIA© allows scientists to quickly discover novel pathways for new and published target molecules.



Accelerate Your Pathway Design

Chemistry R&D Process

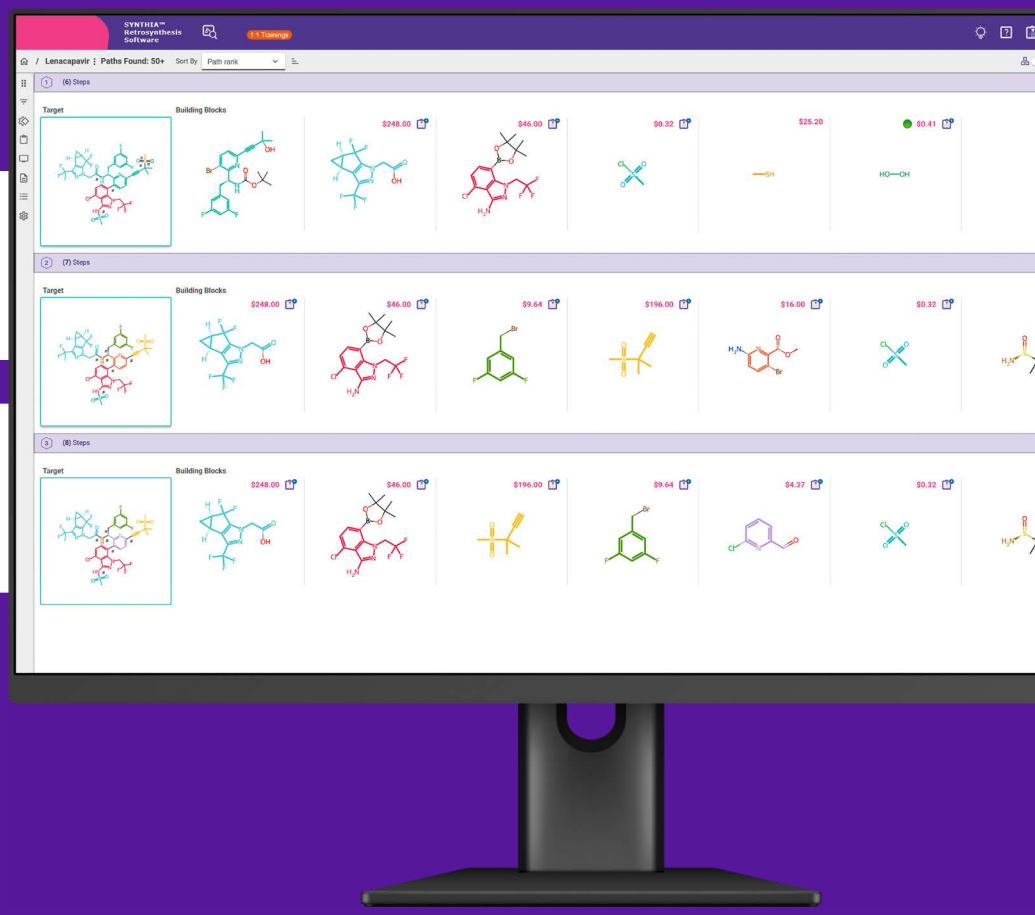


Quickly go from imagining what's possible to testing what's probable. Integrated into your daily work routine, our software unlocks its full potential by enhancing the speed, safety, and cost efficiency of your work.

Developed over a 21 year period, this SaaS based software platform develops synthetic routes using expert-coded rules based on proven chemical transformations. With a catalog of over 12 million commercially available starting materials and building blocks, SYNTHIA© provides access to a broad portfolio of available chemistry.

ISO 27001 CERTIFIED by schellman

Rated Platinum 2025 by cybervadis



Benefits

SIMPLIFY ROUTE DESIGN
Quickly and efficiently scan hundreds of pathways to help you identify the best option according to your needs.

SAVE TIME AND REDUCE COSTS
Explore the most cost-effective routes to your target molecules with state of the art visualization and filtering options.

MEET PROJECT DEMANDS
Easily customize search parameters to eliminate or promote reactions, reagents or classes of molecules.

GENERATE NEW IDEAS AND IP
Explore unique and innovative syntheses that may be unknown for building your desired molecule.

QUICKLY BUILD A SHOPPING LIST
Easily generate a list of commercially available starting materials for your synthesis.

SUPPORT GREEN CHEMISTRY
Customize search parameters to avoid hazardous reagents and find greener alternatives.

The Workflow

1

Input your Target Molecule

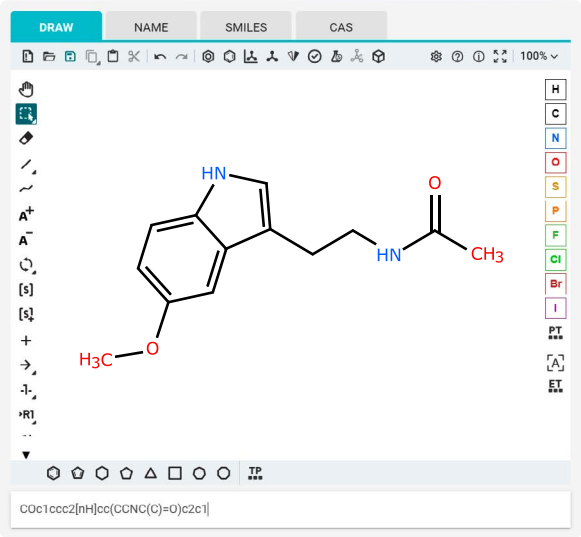
Run Analyses for Known or Unknown Compounds

Draw or paste your target molecule in the editor, or search for a known compound in our database.

- Define stereochemistry
- Define bonds to make or preserve through the synthesis

Select Analysis Type:

- Automatic
- Step-by-Step
- Similiar molecules
- Shared Path Library



2

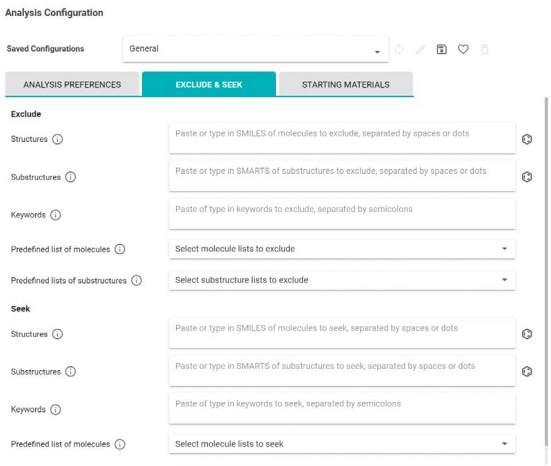
Customize your Analysis

Increase efficiency and reduce risk

Quickly find routes that start with commercially available starting materials or your proprietary inventory compounds.

Define search criteria:

- Use preset parameters or customize them to your needs
- Include preferred reactions
- Exclude unwanted reactions or reagents
- Define starting materials
- Set price limit for commercial compounds
- Integrate in-house inventory



3

4

pathway to innovation

View up to 50 synthetic pathways and use filters based on:

- Number of steps
- Similarity of pathways
- Cost of starting materials
- Unwanted or desired reactions or molecules

View results in a single map or as individual reaction schemes, including:

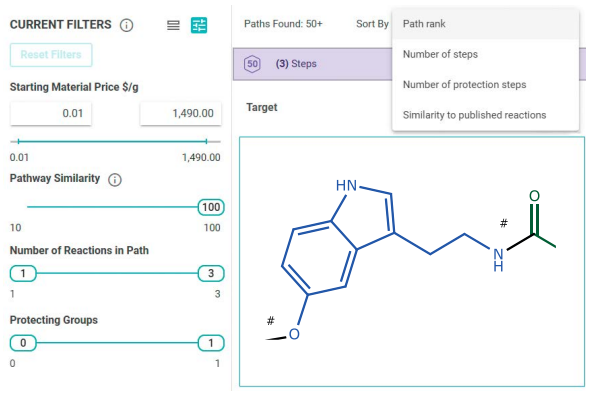
- Typical reaction conditions
- Illustrative Publications
- Protecting group requirements
- Possible side products

Exclude reactions that are undesirable due to:

- Specialized equipment or technical needs (ozone, gaseous reagents, moisture-sensitive materials)
- “Exotic” or complex chemistry

Collaborate with colleagues:

- Share analyses directly with team members
- Export results by downloading pathways as PDF, RDF, SVG
- Copy reactions and structures



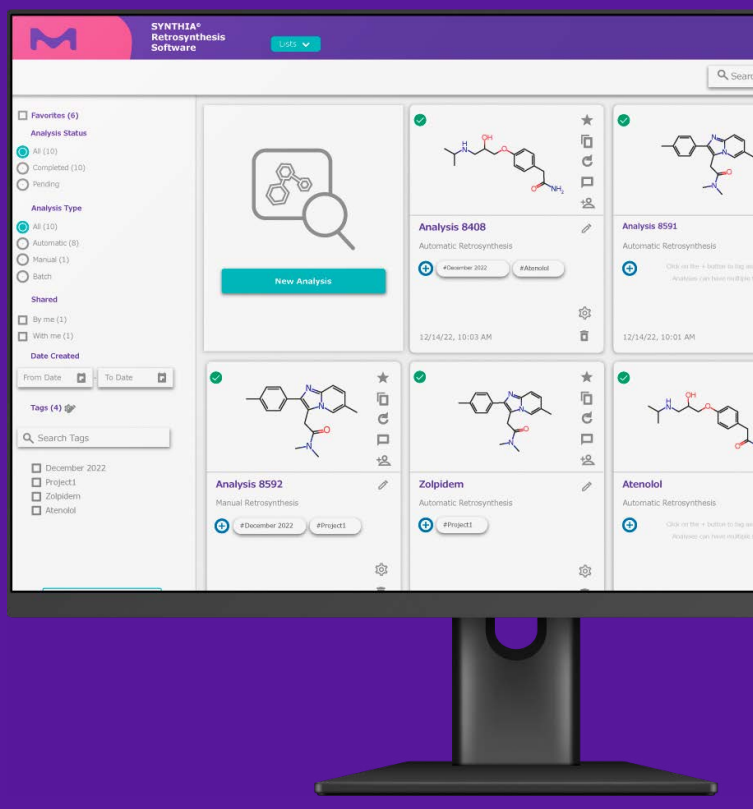
start your synthesis

With a catalog of over 12 million commercially available starting materials or building blocks, SYNTHIA© provides access to a broad portfolio of available chemistry.

proven results

In laboratory validation, SYNTHIA© Retrosynthesis Software found robust and reliable pathways that reduce synthetic steps, increase yields, and decrease costs for both known and novel targets.

Read More
www.synthiaonline.com/publications



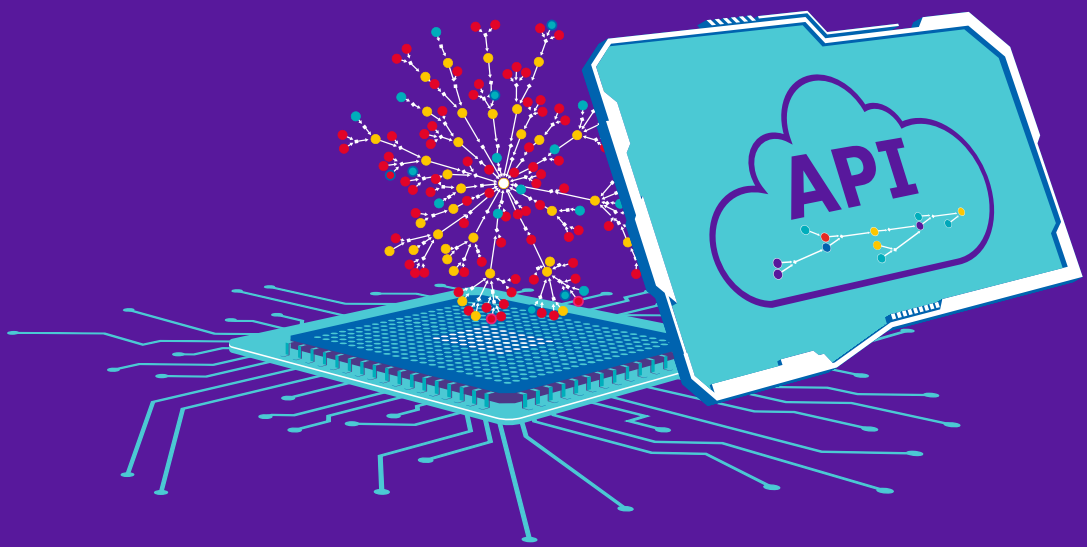
Application Programming Interface

Connect SYNTHIA© with your preferred cheminformatics software for high-throughput pathway design & molecular synthesis assessment.

Two Types of SYNTHIA© API

SYNTHIA©	Output	Speed	Basis
Full Retro API	Reaction SMILES and names, references, prices and CAS numbers of starting materials, pathway scores	50 molecules per hour	Entire SYNTHIA© engine
Synthetic Accessibility Score (SAS) API	SAS (0 to 10)	Up to 100,000 molecules per hour	AI model trained on SYNTHIA© expert-coded rules

Our Application Programming Interface (API) allows you to incorporate SYNTHIA© Retrosynthesis Software with your preferred cheminformatics tools to streamline retrosynthetic analysis for promising leads and assess synthetic accessibility scores (SAS) of thousands of virtual molecules in minutes.



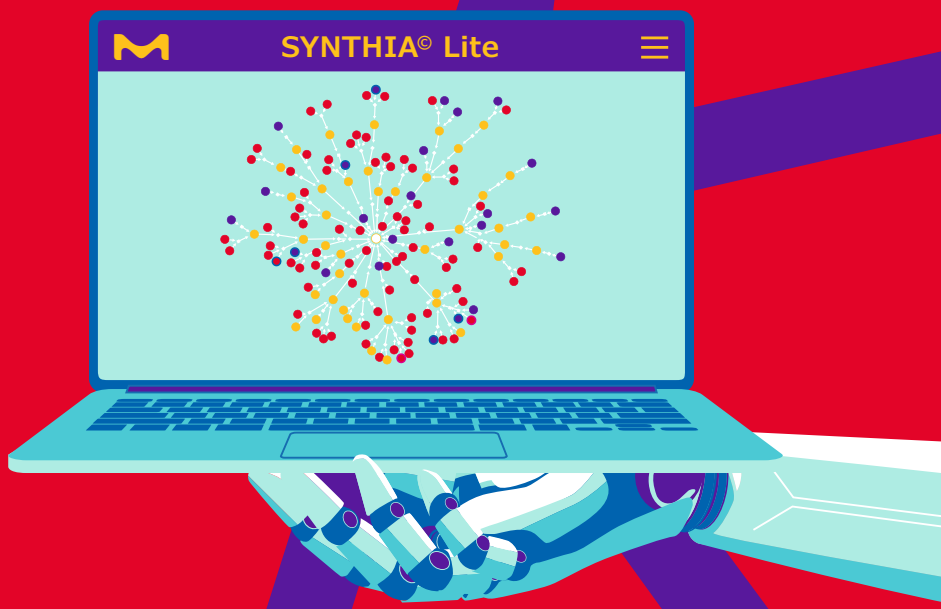
Discover More
www.synthiaonline.com/api

Free Trial

Experience our powerful SYNTHIA© retrosynthesis software with a free individual trial

Three Options of SYNTHIA© Retrosynthesis Software

Free Limited Trial	Premium	Enterprise
1 month Limited Free Trail for up to 5 unique target molecules	Retrosynthesis for 10 / 50 or unlimited unique target molecules in 3 months	Site licensing options available
Unlimited re-runs with a variety of SYNTHIA© Lite options	Unlimited re-runs with a variety of SYNTHIA© Lite options	Collaborate and share results with colleagues
Upgrade options after free trial		Batch analysis, custom inventory
		Single Sign-on (SSO)



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Sigma-Aldrich®

Lab & Production Materials

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