MilliporeSigma

Discovery at your fingertips

Accelerate synthesis design with **SYNTHIA™ Retrosynthesis Software**

OVERVIEW

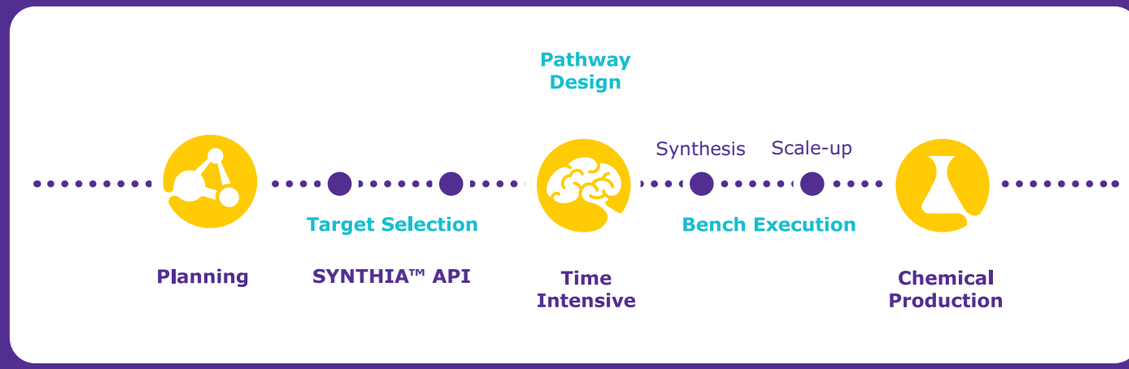
MilliporeSigma is the U.S. and Canada Life Science business of Merck KGaA, Darmstadt, Germany.

Sigma-Aldrich®

Lab & Production Materials

SYNTHIA™

Retrosynthesis Software that augments your expertise

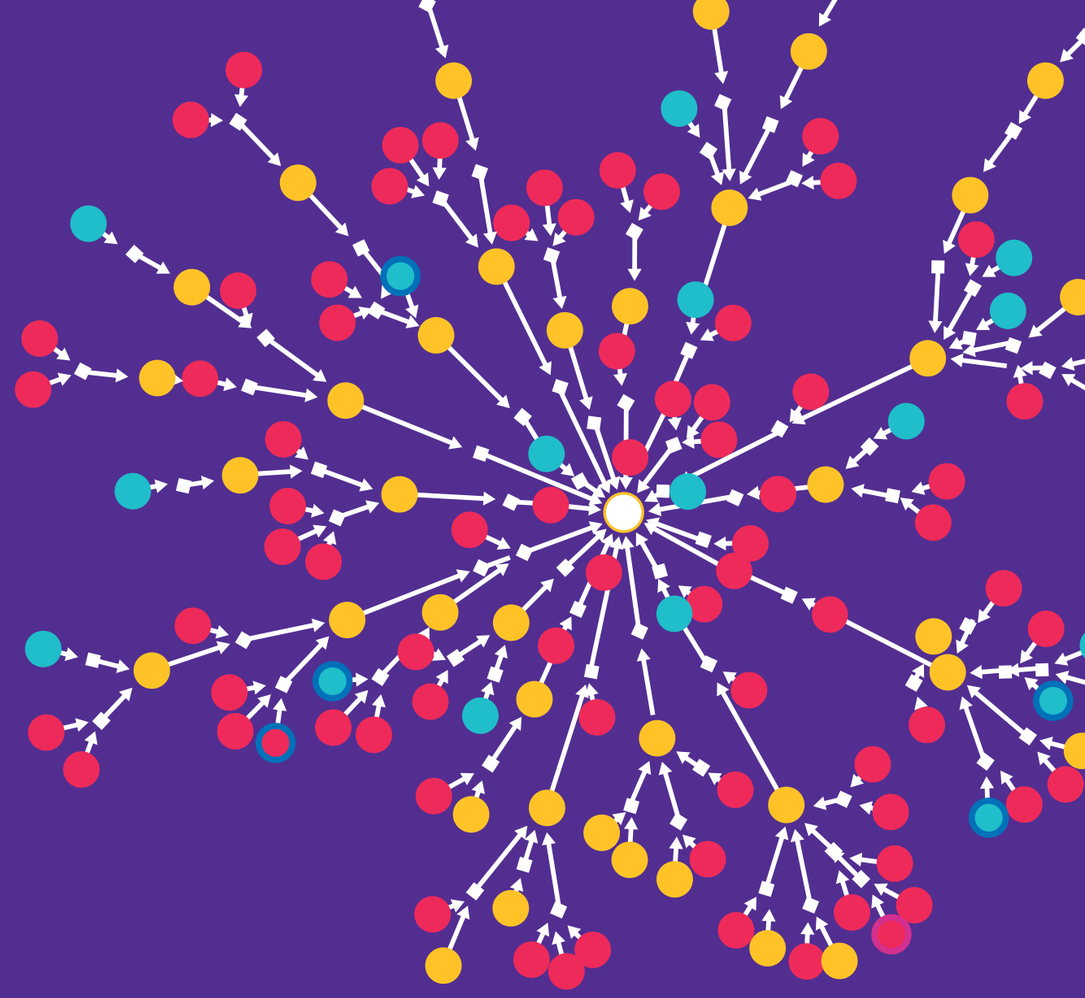


Chemical synthesis is not just tricky – it's risky.

From supply chain shortages to regulatory restrictions to safety considerations – reducing risk is a top priority.

SYNTHIA™ Retrosynthesis Software reduces risk by identifying multiple, shorter, more robust pathways, which saves time and reduces costs.

Using expert-coded rules and advanced algorithms powered by AI developed over 15 years, this decision support tool has become the strategic partner of organic chemists in laboratories across pharma, biotechnology, chemical industry and academia.



SYNTHIA™ Retrosynthesis Software provides an unbiased, objective, computer-aided approach to route planning

- **Simplify your discovery of robust pathways**
- **Generate novel ideas and IP**
- **Reduce risk in your synthesis planning**

Quickly go from imagining what's possible to testing what's probable

1 2 3

Input your Target Molecule

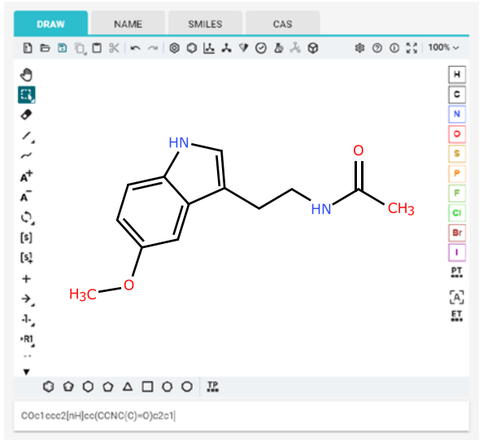
Database Includes Known and Unknown Compounds

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

- Define stereochemistry
- Designate bonds to either make or break

Select Search Mode

- Automatic
- Step-by-Step
- Similiar molecules



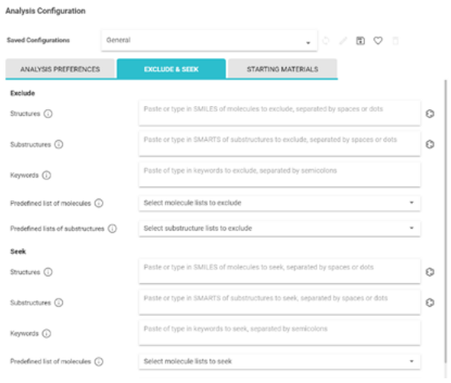
Customize your search

Increase efficiency and reduce risk

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

Define search criteria based on project needs:

- Use preset or customized search parameters
- Favor pathways using preferred reactions
- Define starting materials or intermediates
- Hide or avoid specific reactions and reagents
- Use in-house inventory and set price limits for commercial compounds



Pioneer your pathway

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

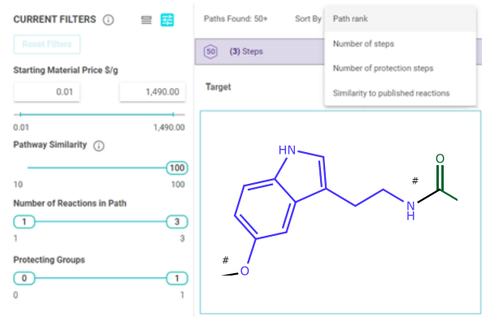
- Number of steps
- Similarity of pathways
- Cost of starting materials
- Exclude or limit to specific reactions or molecules

View results in a single map or as individual pathways with reaction including:

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

Share, save and export results:

- Download pathways as PDF, RDF, SVG
- Copy reactions and structures
- Share search results with colleagues directly through the platform
- Order starting materials and reagents from direct links to **SigmaAldrich.com**

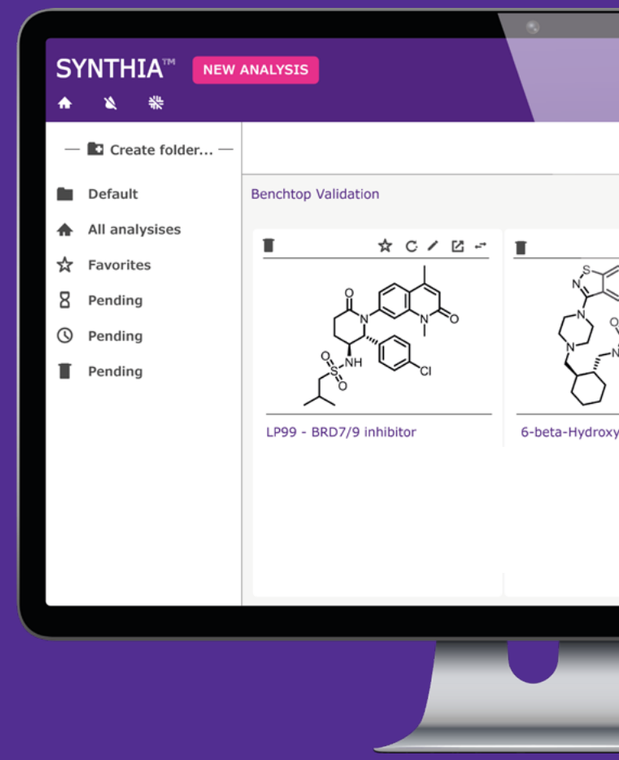


Proven Results

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.

Benefits

- Overall yield increased by 500%
- Significant cost savings anticipated in production batch
- By-passed patented route
- New Product added to catalog
- 50% cost savings
- Overall yield improved from 1% to 60%



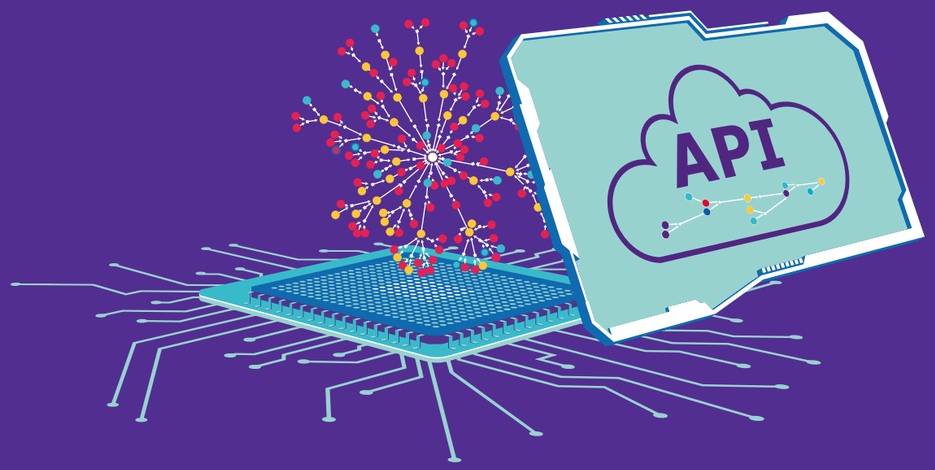
SYNTHIA™ API

Connect SYNTHIA™ with your preferred cheminformatics software for high-throughput pathway design & molecular synthesis feasibility

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	20 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

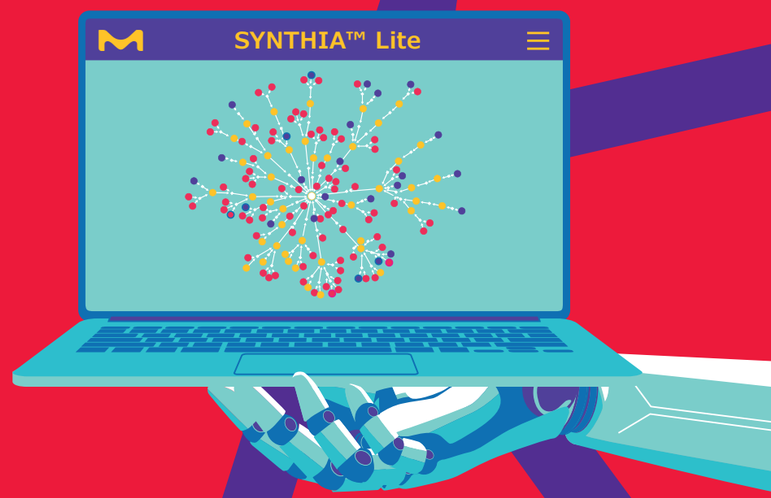
SYNTHIA™ Lite

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)

In laboratory validation, SYNTHIA™ Lite retrosynthesis software found robust and reliable pathways that reduce synthetic steps, increase yields, and decrease costs for both known and novel targets.



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