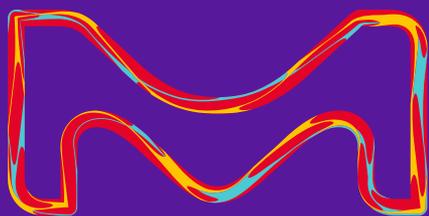
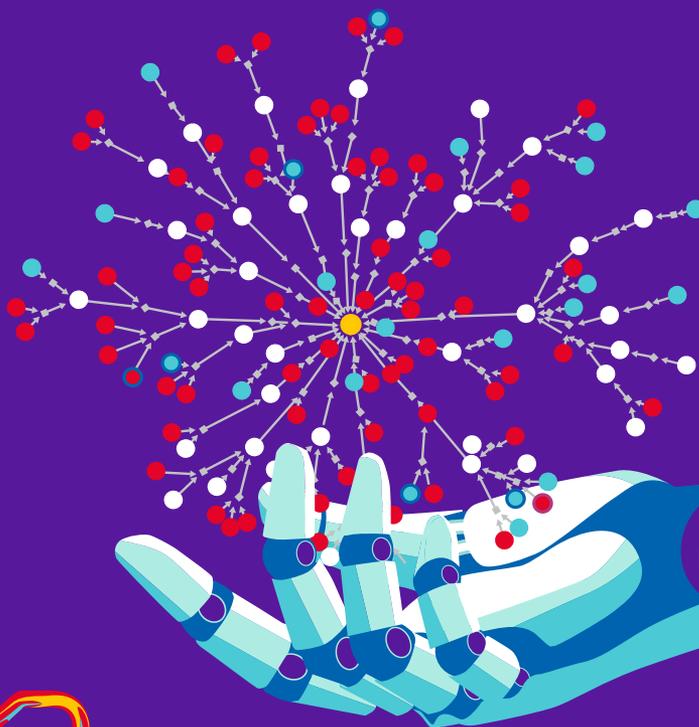


**MERCK**

SYNTHIA<sup>®</sup> Retrosynthesis Software

# Discovery at YOUR Fingertips

Expert-coded by chemists and engineered by computer scientists, SYNTHIA<sup>®</sup> allows scientists to quickly discover novel pathways for new and published target molecules.

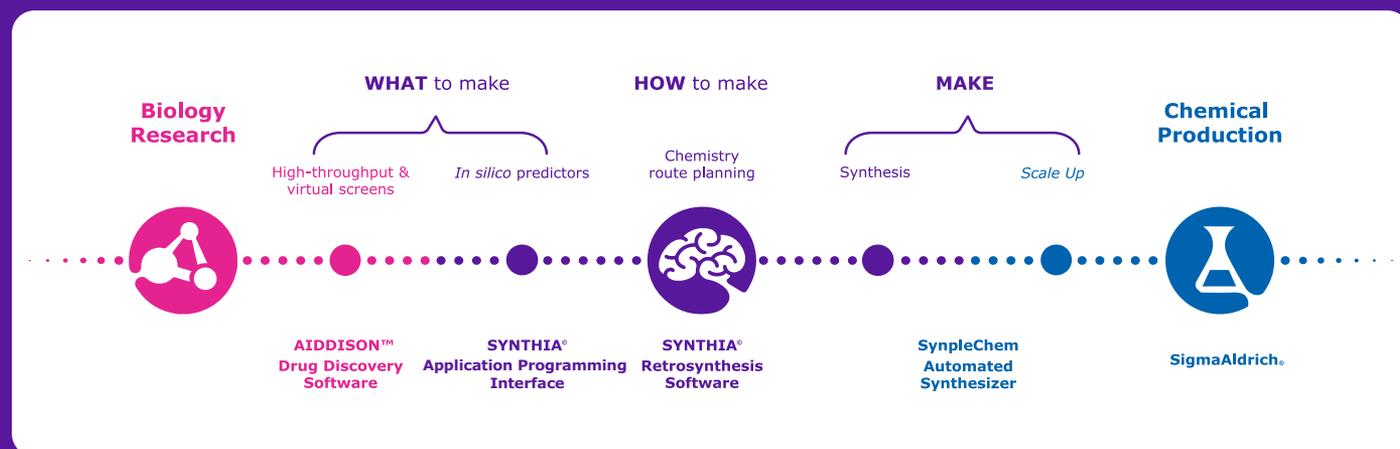


The Life Science  
business of Merck  
operates as  
MilliporeSigma in the  
U.S. and Canada.

**Sigma-Aldrich<sup>®</sup>**  
Lab & Production Materials

# Accelerate Your Pathway Design

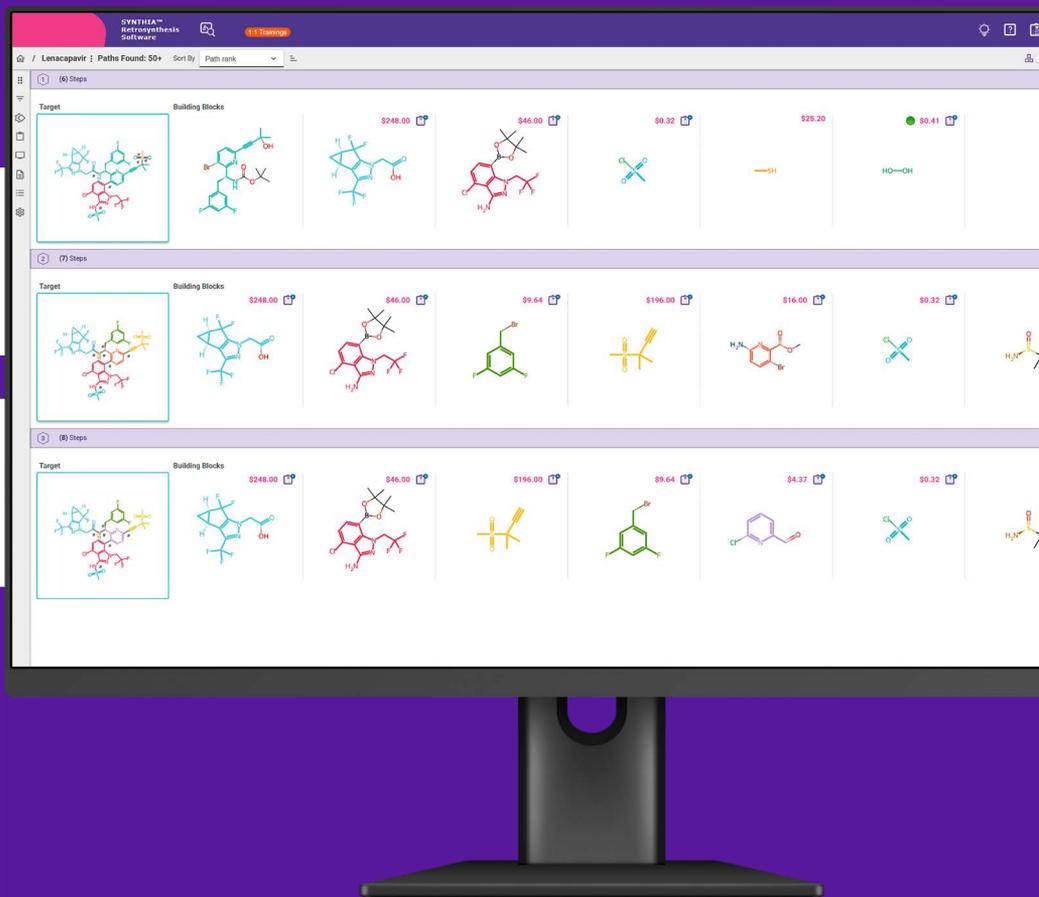
## Chemistry R&D Process



**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<sup>®</sup> provides access to a broad portfolio of available chemistry.



## 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

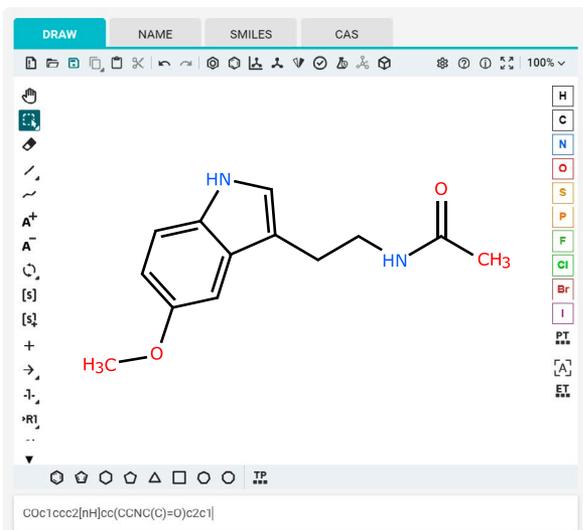
### Run Analyses for Known or Unknown Compounds

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

#### Analysis Configuration

Saved Configurations: General

#### ANALYSIS PREFERENCES EXCLUDE & SEEK STARTING MATERIALS

<b>Exclude</b>	
Structures	Paste or type in SMILES of molecules to exclude, separated by spaces or dots
Substructures	Paste or type in SMARTS of substructures to exclude, separated by spaces or dots
Keywords	Paste or type in keywords to exclude, separated by semicolons
Predefined list of molecules	Select molecule lists to exclude
Predefined lists of substructures	Select substructure lists to exclude
<b>Seek</b>	
Structures	Paste or type in SMILES of molecules to seek, separated by spaces or dots
Substructures	Paste or type in SMARTS of substructures to seek, separated by spaces or dots
Keywords	Paste or type in keywords to seek, separated by semicolons
Predefined list of molecules	Select molecule lists to seek

3



## 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

CURRENT FILTERS ⊙ ≡ ⚙️ Paths Found: 50+ Sort By Path rank  
 Reset Filters ⊙ 50 (3) Steps Number of steps  
 Starting Material Price \$/g 0.01 1,490.00 Number of protection steps  
 0.01 1,490.00 Similarity to published reactions  
 Pathway Similarity ⊙ Target  
 10 100  
 Number of Reactions in Path 1 3  
 1 3  
 Protecting Groups 0 1  
 0 1

COC1=CC=C2C(=C1)C(=CN2)CCCN(C)C(=O)C

4



## 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](http://www.synthiaonline.com/publications)

SYNTHIA® Retrosynthesis Software ⚙️ ⌵ 🔍 Search

Favorites (6)  
 Analysis Status  
 All (10)  
 Completed (10)  
 Pending  
 Analysis Type  
 All (10)  
 Automatic (8)  
 Manual (1)  
 Batch  
 Shared  
 By me (1)  
 With me (1)  
 Date Created  
 From Date 📅 To Date 📅  
 Tags (4) 🏷️  
 December 2022  
 Project1  
 Zolpidem  
 Atenolol

Analysis 8408  
 Automatic Retrosynthesis  
 #December 2022 #Atenolol  
 12/14/22, 10:03 AM

Analysis 8591  
 Automatic Retrosynthesis  
 12/14/22, 10:03 AM

Analysis 8592  
 Manual Retrosynthesis  
 #December 2022 #Project1

Zolpidem  
 Automatic Retrosynthesis  
 #Project1

Atenolol  
 Automatic Retrosynthesis

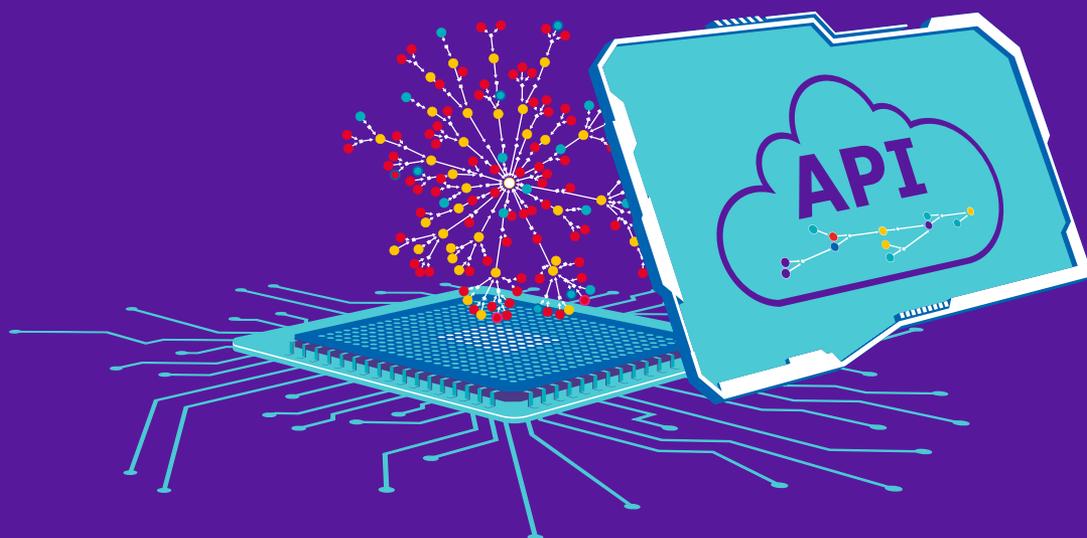
# Application Programming Interface

Connect SYNTHIA<sup>®</sup> with your preferred cheminformatics software for high-throughput pathway design & molecular synthesis assessment.

## Two Types of SYNTHIA<sup>®</sup> API

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

Our Application Programming Interface (API) allows you to incorporate SYNTHIA<sup>®</sup> 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.



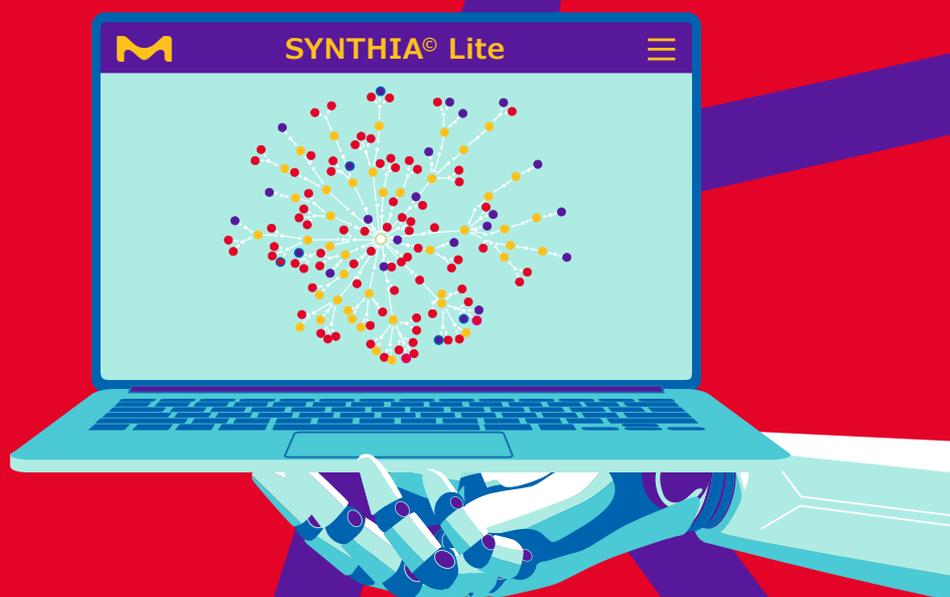
Discover More  
[www.synthiaonline.com/api](http://www.synthiaonline.com/api)

# Free Trial

Experience our powerful SYNTHIA<sup>®</sup> retrosynthesis software with a free individual trial

## Three Options of SYNTHIA<sup>®</sup> 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 <sup>®</sup> Lite options	Unlimited re-runs with a variety of SYNTHIA <sup>®</sup> Lite options	Collaborate and share results with colleagues
Upgrade options after free trial		Batch analysis, custom inventory Single Sign-on (SSO)



Register with your business email address.

[Lite.SynthiaOnline.com](http://Lite.SynthiaOnline.com)

# Sigma-Aldrich®

Lab & Production Materials

Merck KGaA  
Frankfurter Strasse 250  
64293 Darmstadt, Germany

**Synthiaonline.com**

© 2025 Merck KGaA, Darmstadt, Germany and/or its affiliates. All Rights Reserved.  
Merck, the Vibrant M, Sigma-Aldrich, and Synthia are trademarks of Merck KGaA, Darmstadt,  
Germany or its affiliates. All other trademarks are the property of their respective owners.  
Detailed information on trademarks is available via publicly accessible resources.

MK\_BR13149EN Ver. 6.0 06/2025