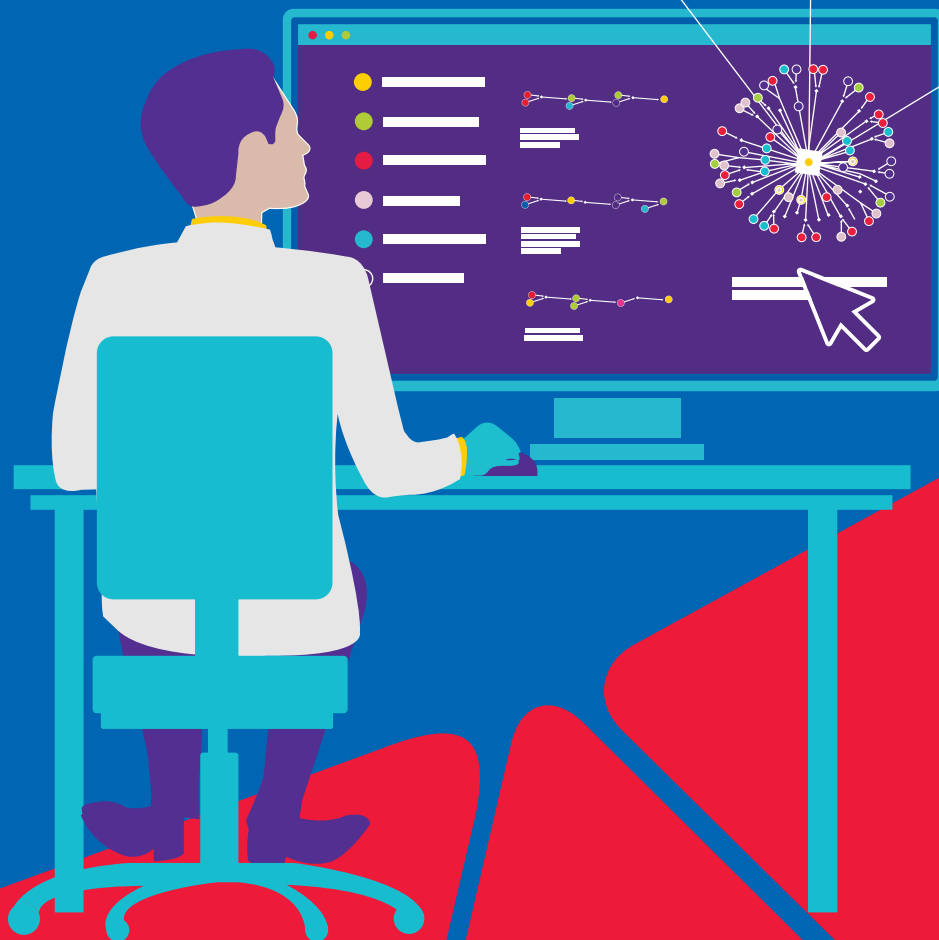
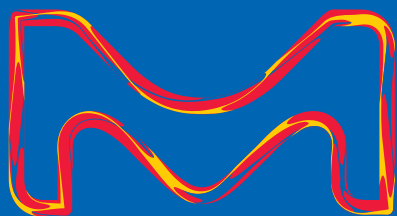


Millipore
SIGMA

SYNTHIA™

Retrosynthesis Software

Pioneer Your Pathway



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

Sigma-Aldrich®
Lab & Production Materials

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

1



select a search Mode

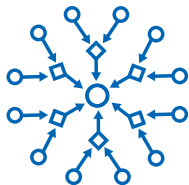
Automatic Retrosynthesis

Design customized pathways according to your preferences starting from commercially available starting materials, building blocks or synthons



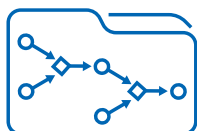
Manual Retrosynthesis

Take a hands-on approach and navigate potential reactions one step at a time



Automatic Batch Analysis

Upload multiple molecules to analyze with the same search criteria



2

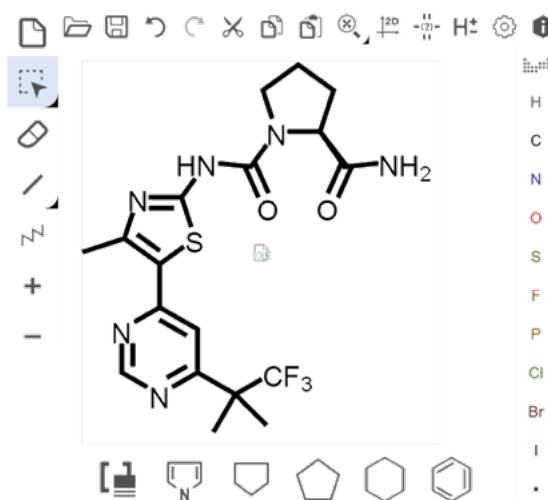


Identify a Target Molecule

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



4

3



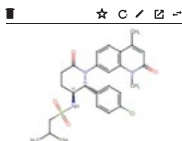
customize your search

Increase efficiency and reduce risk

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

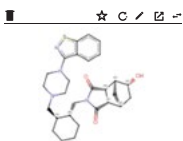
Define search criteria based on project needs:

- 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



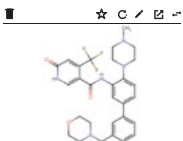
LP99 - BRD7/9 inhibitor

- Overall yield increased by 500%
- Significant cost savings anticipated in production batch



6-beta-Hydroxylurasidone

- By-passed patented route
- New Product added to catalog



WDR5-MLL1 interaction Antagonist

- 50% cost savings
- Overall yield improved from 1% to 60%



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.

The screenshot displays the SYNTHIA™ software interface. The top navigation bar includes 'NEW ANALYSIS' and 'SUPPORT'. A sidebar on the left lists analysis categories: 'Default', 'All analyses', 'Favorites', and three 'Pending' items. The main content area, titled 'Benchtop Validation', features three panels, each with a chemical structure and associated results:

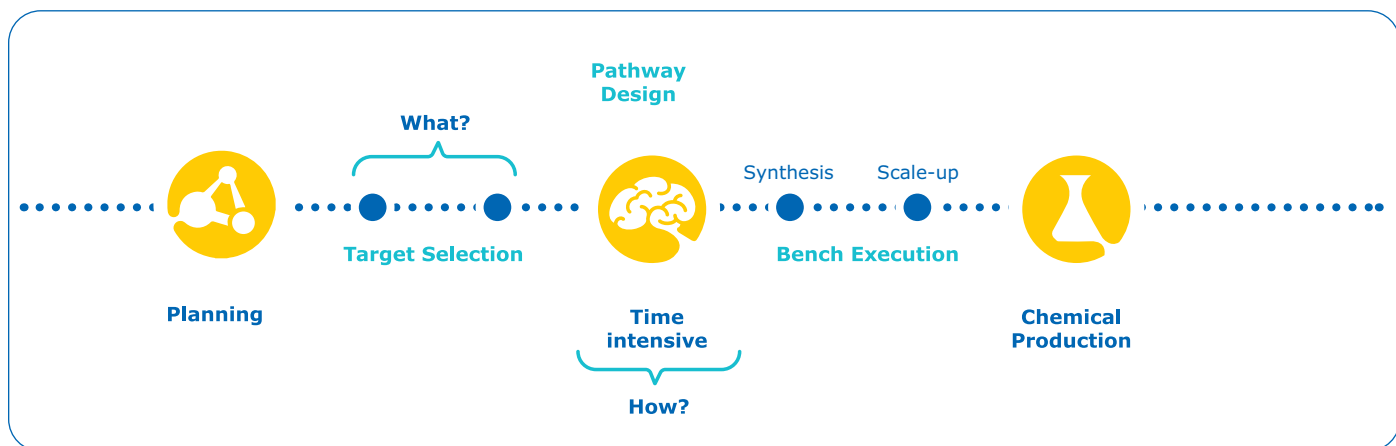
- LP99 - BRD7/9 inhibitor**
 - Overall yield increased by 500%
 - Significant cost savings anticipated in production batch
- 6-beta-Hydroxylurasidone**
 - By-passed patented route
 - New Product added to catalog
- WDR5-MLL1 interaction Antagonist**
 - 50% cost savings
 - Overall yield improved from 1% to 60%

Experience how **SYNTHIA™ Retrosynthesis Software** can enhance your expertise to quickly go from imagining what's possible to testing what's probable. Are you ready to join the retrosynthesis revolution?

Contact us to learn more:
SigmaAldrich.com/SYNTHIA

SYNTHIA™

Retrosynthesis software that augments your expertise

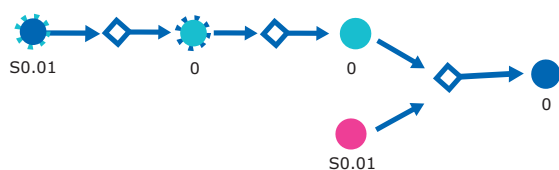


Chemical synthesis is not just tricky – it's risky.

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 hand-coded rules and powerful 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™ 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

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