MERCK

SYNTHIA™

Retrosynthesis Software

Coded by chemists for chemists.

The life science business of Merck operates as MilliporeSigma in the U.S. and Canada.

Sigma-Aldrich®

Lab & Production Materials

SYNTHIA™

Retrosynthesis software that augments your expertise

One of the most significant challenges in organic chemistry is finding viable synthetic pathways by painstakingly navigating the complex matrix of retrosynthetic possibilities while simultaneously accounting for what has been done, what could be done, and what starting materials are available.

Engineered by organic chemists and computer scientists over the course of 15 years, SYNTHIA™ harnesses the potential of advanced, highly nuanced algorithms powered by an ever-growing database of more than 100,000 hand-coded reaction rules.

SYNTHIA™ is easily customized to find the most relevant pathways for known and novel molecules based on your search criteria.

For each step, SYNTHIA™ takes the entire molecule into account going beyond local interactions to factor in potential conflict and selectivity issues, while providing stereoselective and regioselective reactions.

SYNTHIA™ explores novel and known solutions, eliminates nonviable options and presents the user with the most promising pathways to explore.

- **Simplify your discovery of novel pathways**
- **Save time and reduce costs**
- **Generate new ideas and intellectual property**
- **Design pathways that lead back to commercial starting materials**

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

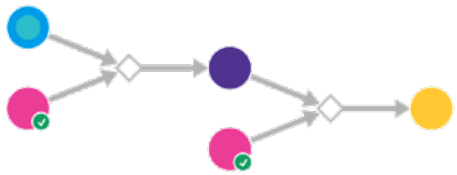
1

2

Select the Type of Analysis

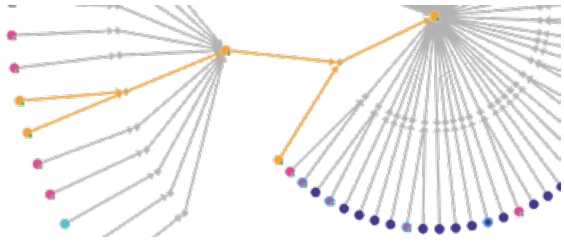
- **Automatic Retrosynthesis**

Design full retrosynthetic pathways customized according to your preferences



- **Manual Retrosynthesis**

Take a hands-on approach and navigate step-by-step working iteratively backward until you reach viable starting materials

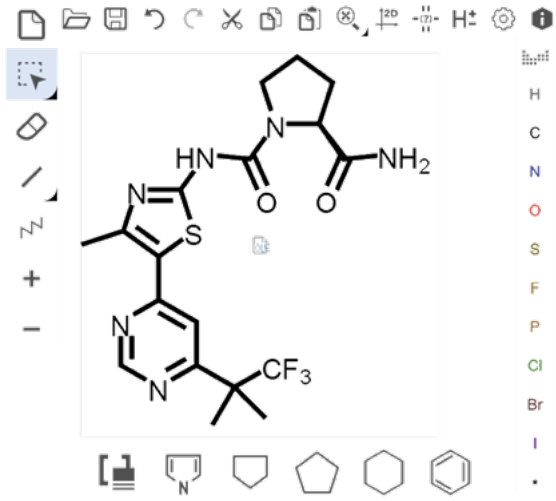


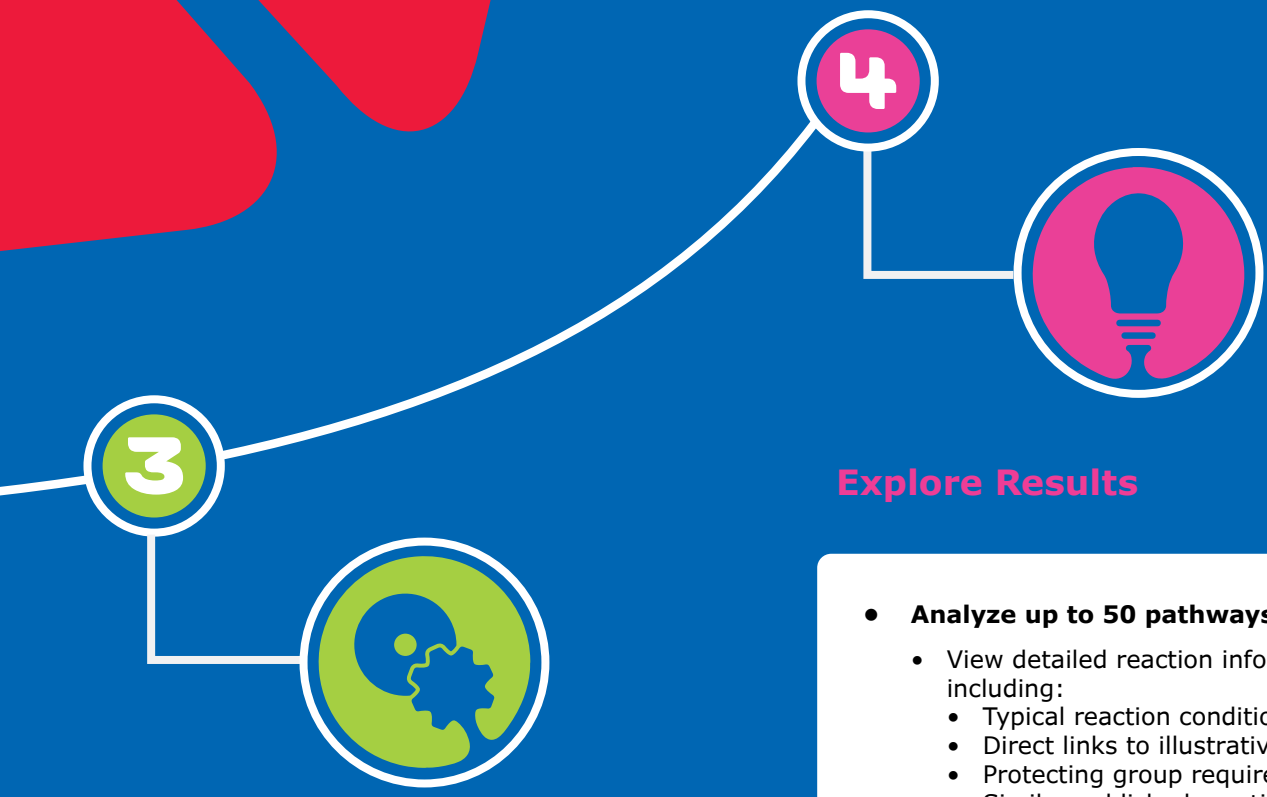
Choose a Target Molecule

- **Select from Known and Unknown Compounds**

Use SYNTHIA™ to find complete pathways to known or novel target molecules

- Draw a novel structure
- Search the SYNTHIA™ database





Customize Search Parameters

1. **Choose your starting materials**
   - Select from different compound databases:
     - 4 million commercial building blocks
     - 10 million published molecules
     - Your custom inventory
   - Set price threshold for commercial compounds
2. **Rank your pathways**
   - Choose criteria to prioritize routes:
     - Number of steps
     - Cost of starting materials
     - Protecting group preferences
3. **Fine-tune your results**
   - Eliminate undesirable pathways containing:
     - Specific starting materials or intermediates
     - Reagents or reaction classes
     - Lists of molecules or substructures

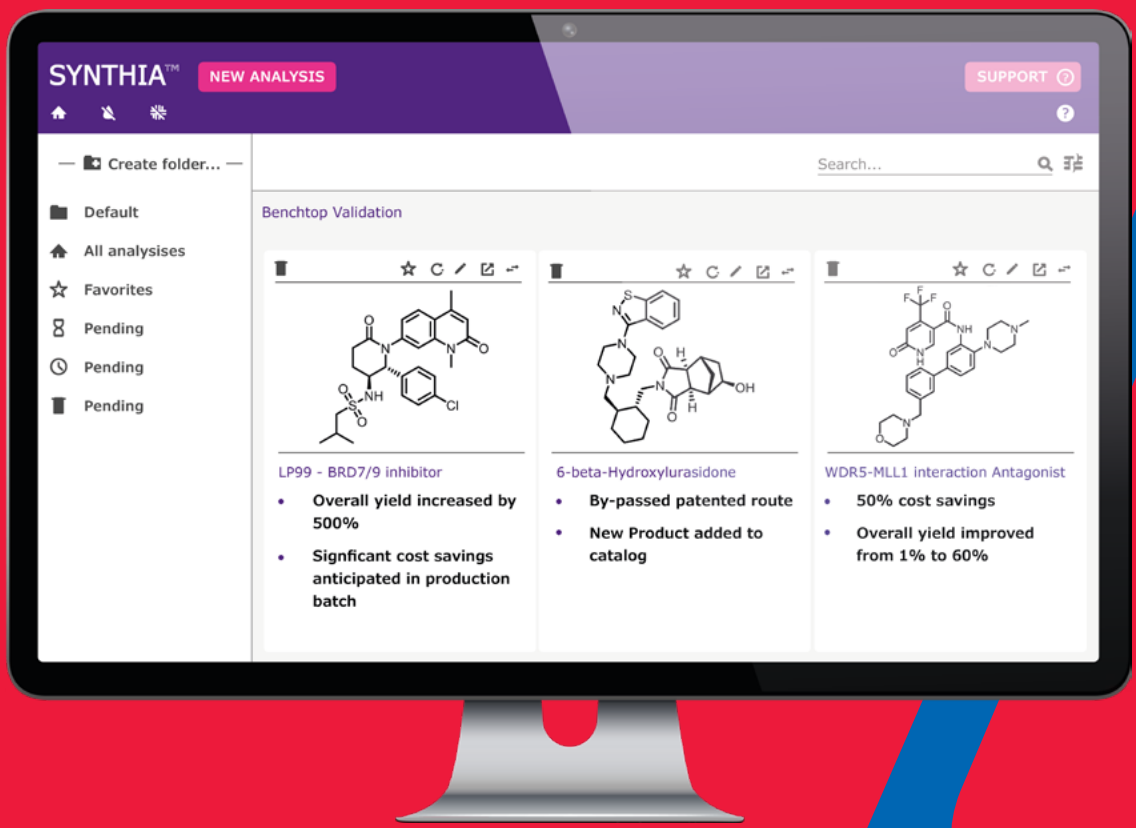
START YOUR SEARCH

Explore Results

- **Analyze up to 50 pathways**
  - View detailed reaction information including:
    - Typical reaction conditions
    - Direct links to illustrative references
    - Protecting group requirements
    - Similar published reactions
    - Possible side products
- **Filter routes based on:**
  - Number of steps
  - Similarity of reactions
  - Protecting groups
- **Analyze all results on one graph**
  - Find pathways with common intermediates and starting materials
  - Sort Reactions based on:
    - Reaction type
    - Stereogenic reactions
    - Ring forming reactions
- **Save pathways as PDF**
- **Copy reactions to paste in structure editor**
- **Order building blocks directly from sigmaaldrich.com to get your synthesis started**

Proven & Published

In the first successful laboratory validation of a retrosynthetic design software, SYNTHIA™ found robust and reliable pathways that reduced synthetic steps, increased yields, and decreased costs for both known and novel targets.



Experience how SYNTHIA™ can augment your expertise to quickly go from imagining what's possible to testing what's probable. Ready to join the Future of Retro?

Contact us today:
www.sigmaaldrich.com/SYNTHIA

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