MERCK

SYNTHIA™ Retrosynthesis Software

Discover greener pathways

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

The path to a greener future

Designing an efficient process for synthesizing a target compound with minimal environmental impact presents numerous challenges. Our powerful retrosynthesis software, SYNTHIA™, can greatly facilitate prediction of more sustainable synthetic routes, starting from commercially available raw materials.

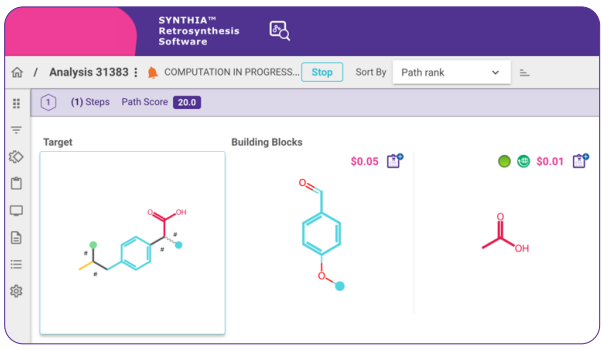
Learn how our advanced algorithms help you optimize pathway design based on price, step count, and atom economy, leading to more efficient, economical, and ecological routes.

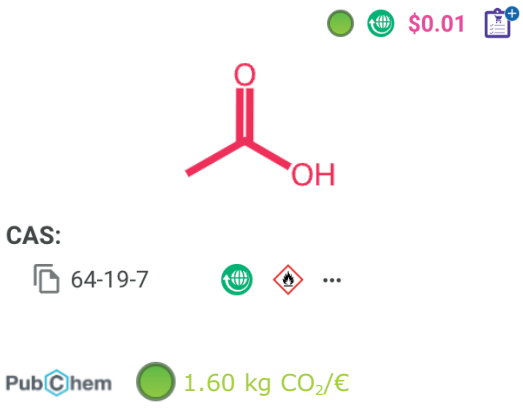
Sustainability Information on Building Blocks

Building blocks that support Green Chemistry are clearly labeled in pathways.

Greener Alternative Product
High standards, environmental goals, and ecosystem partnerships.

EPA Safer Chemical Ingredients List
Includes chemicals evaluated through the Safer Choice Program





Spend-based emission factor
Reported in kg CO_2/EUR and according to the Environmentally Extended Input-Output (EEIO) model.

For more information,please visit:
WWW.SYNTHIAONLINE.COM

Building block details with one click:

- Link to PubChem
- Chemical Hazard Symbols
- Greener Alternative Product Symbol
- EPA Safer Chemical Ingredients Labels
- Spend-based emission factor in $kgCO_2$ eq/EUR

Greener Alternative Products

This symbol indicates that the compound is part of our Greener Alternative Product portfolio and belongs to one of the 4 categories shown below.

4 Categories of Greener Alternative Products

Re-Engineered Products
are developed by our scientists to significantly reduce environmental impact

12 Principles Aligned Products
follow at least one of the 12 Principles of Green Chemistry

Enabling Products
help make greener alternatives possible through new technologies

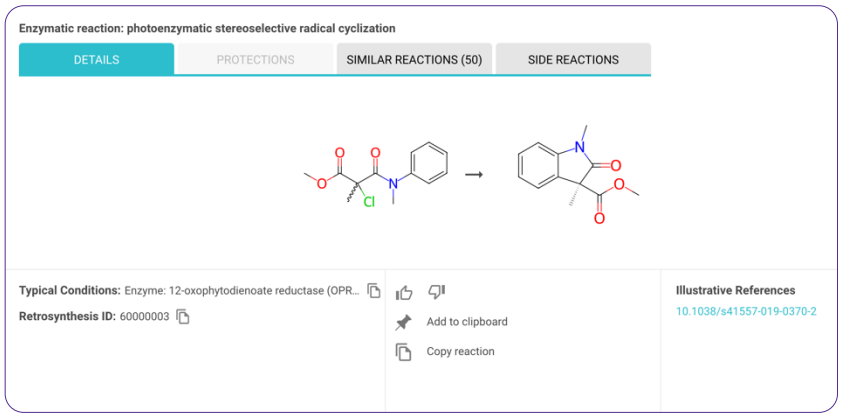
Design for Sustainability (DfS) Developed Products
demonstrate significant sustainability improvements

Enzymatic Reactions

Enzymatic reactions are found in our expert-coded "Enzymatic Transformations" database. Reaction information includes reported conditions and enzyme details along with reference links.

Benefit

Another benefit is reaction conditions for enzymatic transformations are often greener themselves - not using harsh chemical reagents or solvents required in other processes.



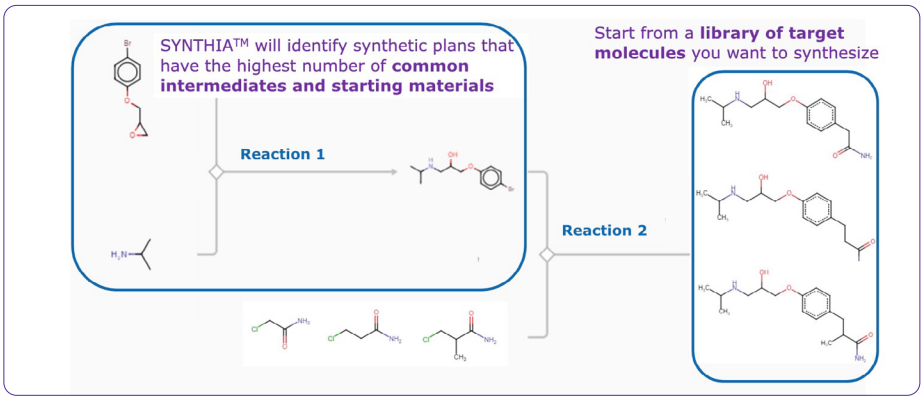
Shared Path Library

Shared Path Library in SYNTHIA™ allows you to plan a synthetic pathway for an entire library of target molecules simultaneously via multi-target analysis.

Simply upload a library of target molecules you want to synthesize, and SYNTHIA™ will identify and prioritize synthetic routes that have the highest number of common intermediates and starting materials.

- **Multi-target analysis** for efficient, autonomous retrosynthetic analysis of entire target library
- **Prioritization of routes** with shared synthetic steps

This functionality enables quick prediction of the optimal strategy for synthesizing an entire library of target molecules using shared synthetic steps.

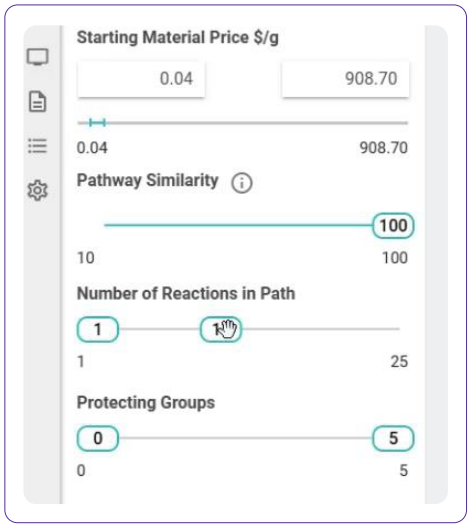


Customize for Sustainable Pathways

Requirements for synthesis projects can differ greatly. That's why SYNTHIA™ offers numerous customization options for adjusting results according to your project's needs. This is especially important in the context of sustainable chemistry.

SYNTHIA™ offers limitless options for customization:

- Avoid using gaseous reagents/reactants
- Eliminate metal catalysis
- Limit the number of synthesis steps
- Minimize the cost of starting materials
- Specify protecting group requirements
- Define bond disconnections
- Exclude toxic or hazardous molecules
- Select catalyst/reagents type
- Promote or exclude specific chemistry reaction classes, such as enzyme-catalyzed reactions
- Choose starting materials: commercial, known, or internal inventory



YOUR BENEFITS

- Reduce risk of overlooking a more sustainable pathway
- Limit use of hazardous reactants/reagents
- Save time finding the best synthetic route, including for target molecule libraries
- Find pathways that meet your synthetic needs
- Quickly filter molecule sets based on synthesizability, or connect with other tools using SYNTHIA™ API

12 principles of Green Chemistry

Waste Prevention

It is better to prevent waste than to treat or clean up waste after it has been created.

Atom Economy

Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

Less Hazardous Chemical Synthesis

Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

Designing Safer Chemicals

Chemical products should be designed to affect their desired function while minimizing their toxicity.

Safer Solvents and Auxiliaries

The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used.

Design for Energy Efficiency

Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be conducted at ambient temperature and pressure.

Use of Renewable Feedstocks

A raw material or feedstock should be renewable rather than depleting whenever technically and economically practicable.

Reduce Derivatives

Unnecessary derivatization (use of blocking groups, protection/ deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste.

Catalysis

Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

Design for Degradation

Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.

Real-time Analysis for Pollution Prevention

Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.

Inherently Safer Chemistry for Accident Prevention

Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions, and fires.

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