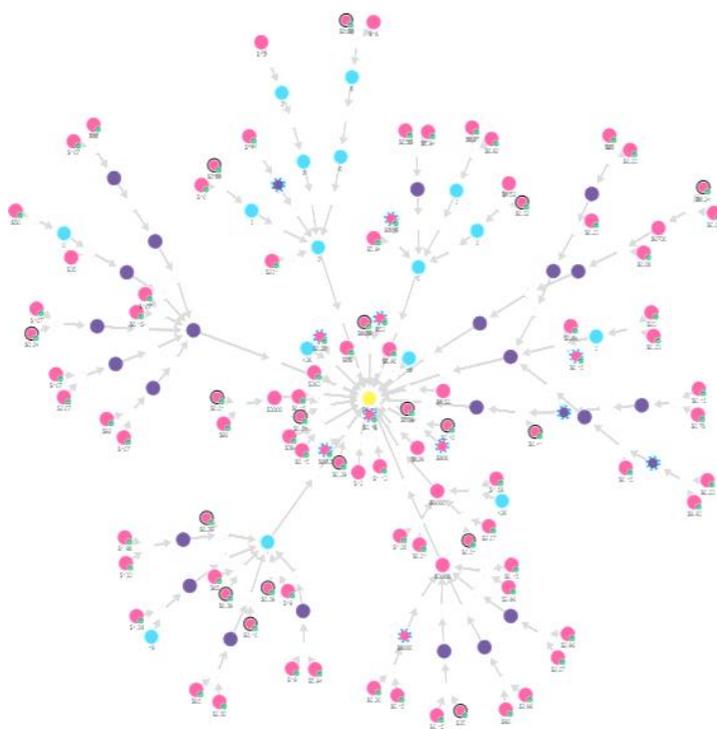


SYNTHIA™

Retrosynthesis Software



Quick-Start Guide

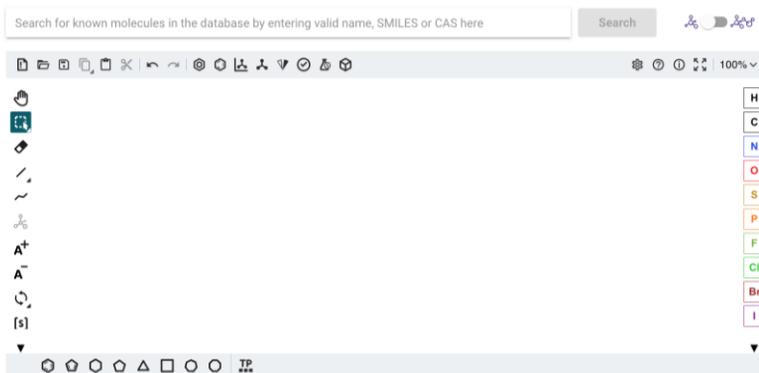


SYNTHIA™ Retrosynthesis Software

Quick-start guide: New Analysis

1

Select New Analysis



2

Input your target

- Draw or paste a SMILES in the sketcher
- Search for a known molecule by name or CAS
- Upload or drag and drop a molecule file (mol or sdf)

Upload File

OR

Drag and Drop a molecule file here

3

Choose Analysis Type

Retrosynthesis

Automatic



General



Shared Path Library

Step-by-step

Similarity Search

Similar molecules

Start

Single Target Multiple Targets

- **Automatic:** Up to 50 pathways for each target from commercial starting materials or
- **Shared Path Library:** Up to 3 convergent routes to make library of targets from commercial starting materials
- **Step-by-step:** All reactions to make target, one step at a time



SYNTHIA™ Retrosynthesis Software

quick-start guide: customize

4

Customize Search

For Automatic or Shared Path Retrosynthesis click the **DROP-DOWN** and choose a **CONFIGURATION**

				
General	Medium	S-M	\$\$	
Complex Molecules	Long	M-L	\$\$\$	
Common Chemistry	Medium	S-M	\$\$\$	
Quick Analysis	Short	S-M	\$\$\$\$	

Exclude & Seek Structures/Sub-Structures/Keywords/Lists:

1. Click  to Edit Configurations
2. Choose the **EXCLUDE & SEEK** Tab
3. Paste a SMILES or DRAW () using the **Structure Editor** to exclude/seek a starting material, intermediate, or sub-structure.
4. Use **Keywords** to exclude/seek a **catalyst, reagent, solvent, or reaction type**.
5. Exclude/Seek predefined **Lists of Molecules**

Create or Edit Molecule Lists

ANALYSIS PREFERENCES | **EXCLUDE & SEEK** | STARTING MATERIALS

Exclude

Structures

Substructures

Keywords

Predefined list of molecules

Predefined lists of substructures

Seek

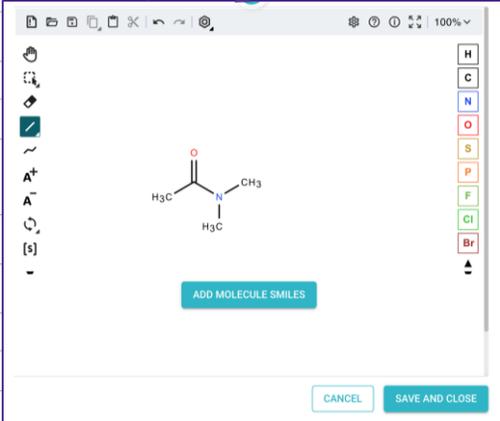
Structures

Substructures

Keywords

Predefined list of molecules

Predefined lists of substructures



Click **Done** after Configuration is Complete then

Start Analysis



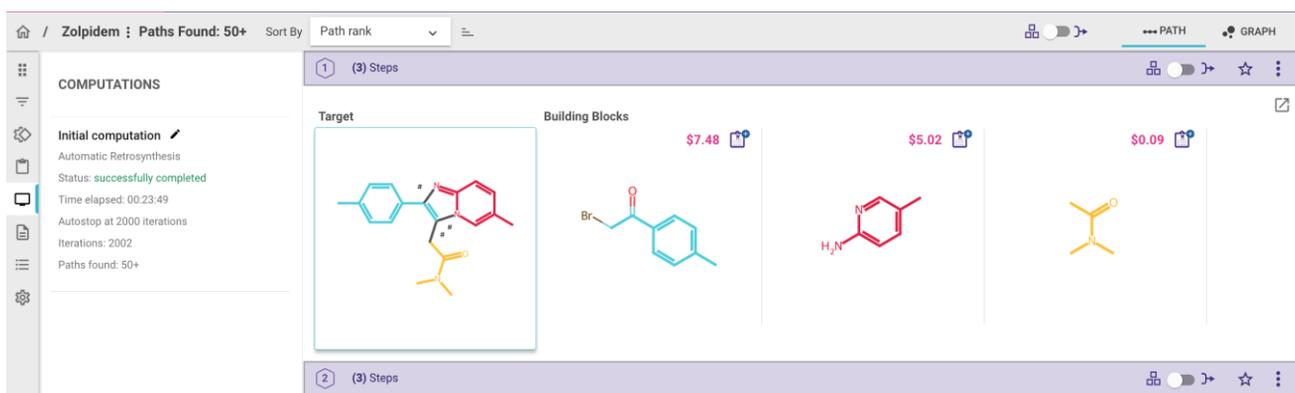
SYNTHIA™ Retrosynthesis Software

Quick-start Guide: RESULTS

5

View Initial Results

Once the **computations**  are complete, the status will change to **'Successfully Completed'** and default to the **Building Blocks View** sorted by **Path Rank**.



COMPUTATIONS

Initial computation 

Automatic Retrosynthesis

Status: **successfully completed**

Time elapsed: 00:23:49

Autostop at 2000 iterations

Iterations: 2002

Paths found: 50+

Target

Building Blocks

\$7.48 

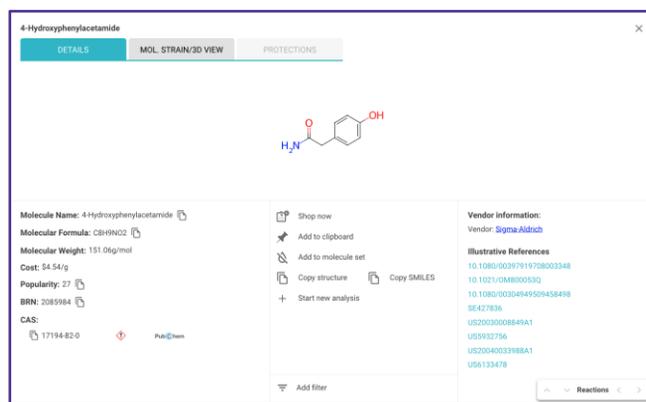
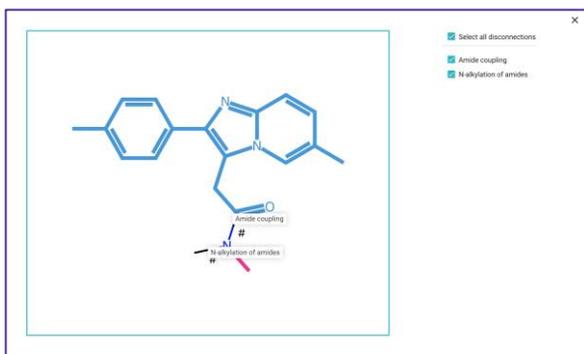
\$5.02 

\$0.09 

6

View Results:
Building Block View

Click on Target to see disconnection summary. Click on any building block to view **Molecule Details** including **chemical hazard information**, **PubChem link**, and **Illustrative references**



4-Hydroxyphenylacetamide

DETAILS MOL STRAIN/3D VIEW PROTECTIONS

Molecule Name: 4-Hydroxyphenylacetamide 

Molecular Formula: C₈H₉NO₂ 

Molecular Weight: 151.06g/mol

Cost: \$4.54/lb 

Popularity: 27 

BRN: 2085984 

CAS:
17194-82-0 

PubChem 

Shop now 

Add to clipboard 

Add to molecule set 

Copy structure 

Copy SMILES 

Start new analysis 

Vendor information:
Vendor: [Sigma-Aldrich](#)

Illustrative References
[10.1080/0097919708003348](#)
[10.1021/OM800053Q](#)
[10.1080/00304949509458498](#)
[SC47636](#)
[UC2002000849A1](#)
[US9322756](#)
[US2004063988A1](#)
[US6133478](#)

Add filter 

Reactions 



SYNTHIA™ Retrosynthesis Software

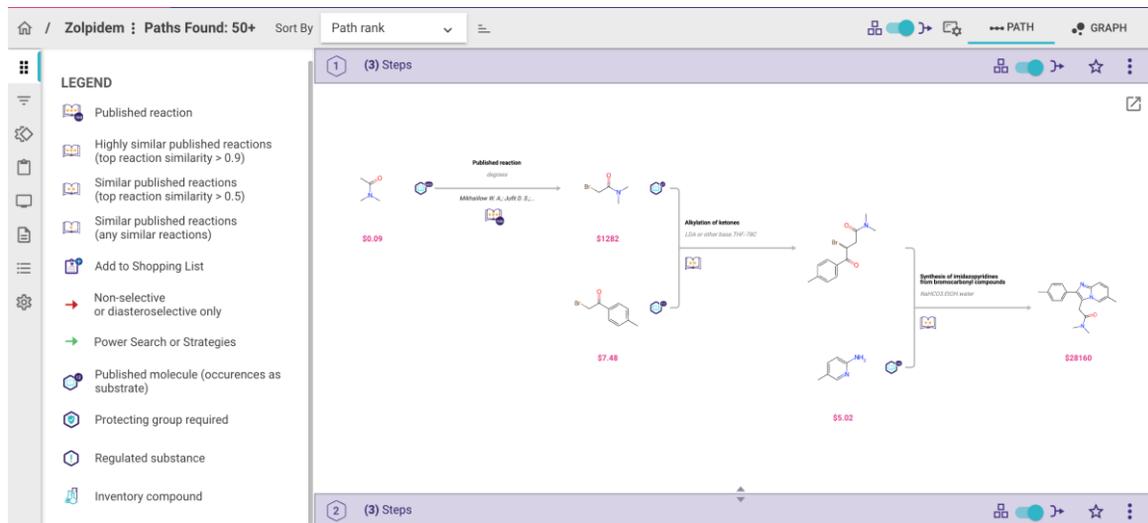
QUICK-START GUIDE: REFINE PATH VIEW

7

Results: Pathway View

Toggle entire results or individual pathways to see **Pathway View**   

Click on  to see symbols **Legend**.



Sort and View Results: Single Path View

Choose option to Sort by:

- Path rank
- Number of steps
- Number of protection steps
- Similarity to published reactions

Click any molecule or reaction to view corresponding **Molecule Details** or **Reaction Details**.

Click on  to view **Similar published reactions**.

Click on  (top right of pathway box) to open **Full Screen Pathway**



SYNTHIA™ Retrosynthesis Software

quick-start guide: MOLECULE REPORT

10

View Molecule Report:
Graph View

The screenshot displays the SYNTHIA software interface. On the left, the 'MOLECULE REPORT' panel shows 'Results contain 42 unique molecules'. Three molecules are listed: Dimethylamine (3 results), 2-Amino-5-picoline (2 results), and p-Tolualdehyde (2 results). The main area shows a retrosynthetic graph for Zolpidem, with a central node and multiple branches leading to various precursors. The graph is labeled 'Filtered results: 9'. The interface includes a top navigation bar with 'PATH' and 'GRAPH' tabs, and a right-side toolbar with 'Force', 'Dagre', and 'Polar' options.

1. Click  to view the **Molecule Report**
2. Select a molecule to highlight in the graph.
3. Click  then select:
 1.  **More Information** – for a detailed look at the molecule
 2.  **Shop now** – to see pricing & availability
 3.  **Copy Structure** – to copy for use in the drawing tool or other application
 4. **+ Start New Analysis** – to view retrosynthesis of the selected molecule
 5.  **Add Filter – Exclude / Limit To** – to further refine the answer set & view a filtered pathway graph.



SYNTHIA™ Retrosynthesis Software

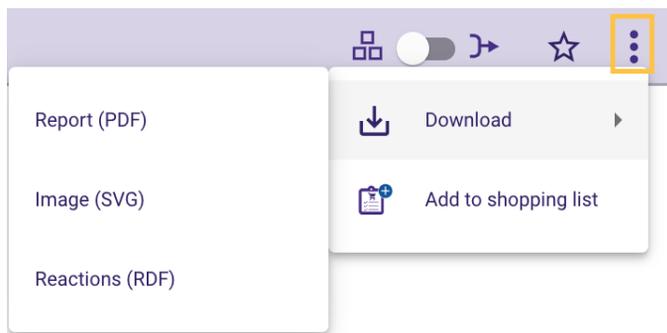
quick-start guide: EXPORT



Export Pathway Results

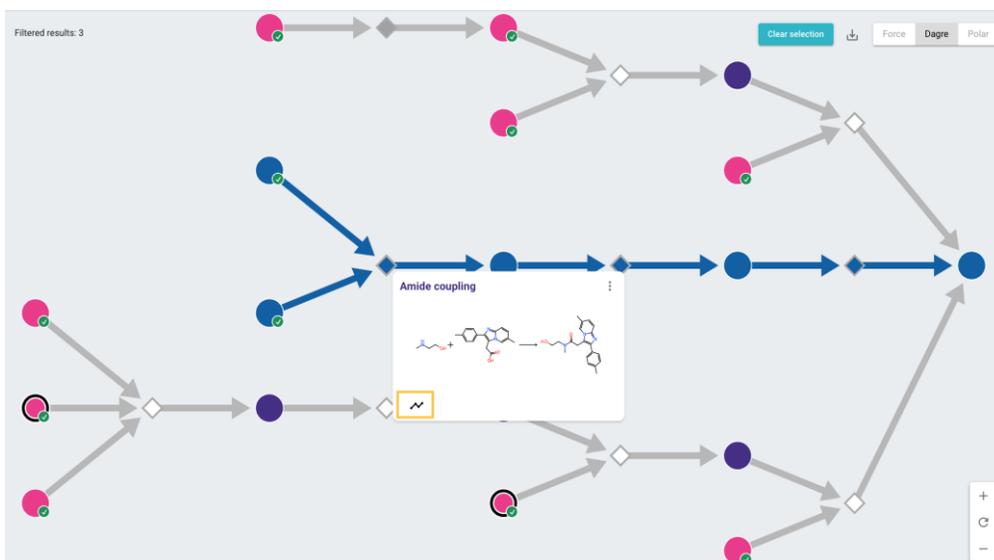
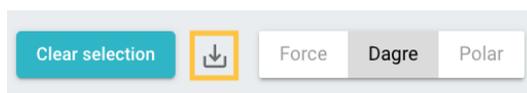
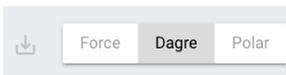
Export Single Pathway(s)

1. Click the desired analysis tile
2. Review & select the desired pathway(s)
3. Click
4. Choose **Download**
5. Select Export type:
 1. **PDF** – Document file
 2. **SVG** – Image file
 3. **RDF** – Reaction data file



Export Pathways in Graph View

1. Click on GRAPH to view reaction nodes
2. Choose **Dagre** to view pathways as a tree
3. Select the desired pathway(s) by clicking the reaction node furthest from the target
4. Click on the **Pathway** icon at the lower left of the window for selected reaction
5. Click
6. Export selected pathway as a **PDF** document



SYNTHIA™ Retrosynthesis Software

quick-start guide: SHOPPING LIST



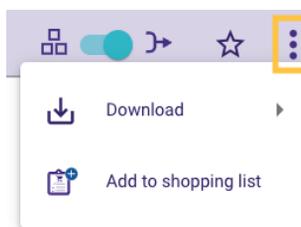
Shopping List

1. Link SYNTHIA™ to E-Commerce Account (first time only)

Click on  and follow prompts to login to Sigma-Aldrich E-commerce Account

2. Add to Shopping List from Pathway

1. Click the desired analysis tile
2. Review & select the desired pathway(s)
3. Click 
4. Choose  **Add to shopping list** to open Price and Availability window
5. Click  to see product options for desired compound
6. Click **Expand** to see price and availability details
7. Click + to add Quantity and then choose **Add to List**
8. Repeat for all desired compounds



Showing 5 results for "127-19-6, 1603-41-4" within Products

Product No.	Brand	Description	Pricing	
17308	Sigma-Aldrich	suitable for peptide synthesis, ≥99.8% (GC)	Hide ^	
SKU	Pack Size	Availability	Price	Quantity
17308-2.5L	2.5 L	Estimated to ship on 9/18/23, 8:00 PM	\$223	- +
17308-1L	1 L	Available to ship on 6/15/23, 8:00 PM	\$110	- 1 +
				Add To List
271012	Sigma-Aldrich	anhydrous, 99.8%	Expand v	

3. Export Shopping List

1. Click 
2. Check box for **Select All**
3. Choose  **Export** to download as .csv file
4. Choose **Buy Online** to open shopping list in **E-Commerce site**

YOUR LIST (2)

Select All Export Remove

 **391956-900ML**
Dimethylamine solution
2.0 M in THF
Qty: 1 Remove

 **ARK2190-1L**
N,N-Dimethylacetamide
Qty: 1 Remove

Buy Online

SYNTHIA™ Retrosynthesis Software

QUICK-START GUIDE: SHARING



Organize & Share Results

Organize Pathway Results on Homepage using Tags

1. Click to add a **Tag** to a search tile
2. Type the name of the Tag to create a new Tag or Choose an existing Tag
3. Click You may add multiple tags to a single search.
4. Click
5. Use **Filters** on left side to limit results list to corresponding tag

Shared

By me

With me

Date Created

From Date - To Date

Tags (8)

Demo Batch

April Batch

Project A

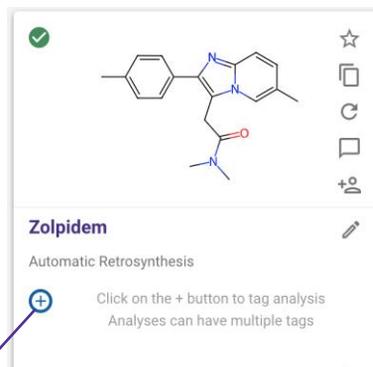
Search Tutorials

Todays search

Training 1

Training 2

Training Examples



Tags for Zolpidem

Add a single tag and press Enter or click on Add button

#Project A

Share Pathway Results



1. Click on the share icon on the search results tile and type the email of the person you want to share the result with. SYNTHIA™ will show the name(s) of any matching users.
2. Click the **Share** button to send the pathway to colleague.
3. Use the **Filters** on left side of homepage to see searches that have been shared with me or by me

