



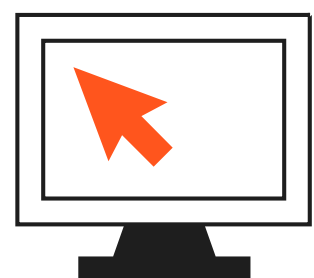
# Reference guide



Advancing human progress together

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This document contains interactive elements. Use the table of contents on this page and the arrows on each page to navigate through the sections.



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5

Bioactivities

# Welcome to Reaxys



# Welcome to Reaxys

Chemistry data and AI to accelerate R&D

Reaxys is a comprehensive chemical database and chemistry search engine that combines a billion chemistry data points across substances, reactions, documents, patents and bioactivity.

**Discover chemistry, plan synthesis routes and validate evidence across sectors, including:**

- **Industry:** pharmaceutical, biotech, CRO and CDMO, chemicals and materials, energy, engineering and technology.
- **Academic and government:** universities, government, institutes and labs.

## Enterprise-grade privacy and security

Everything you do in Reaxys is [private](#), [secure](#) and encrypted. Your prompts are never stored or used to train any large language models.

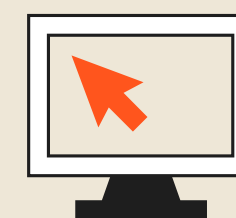
Learn more about [how Elsevier ensures privacy and security every step of the way](#).



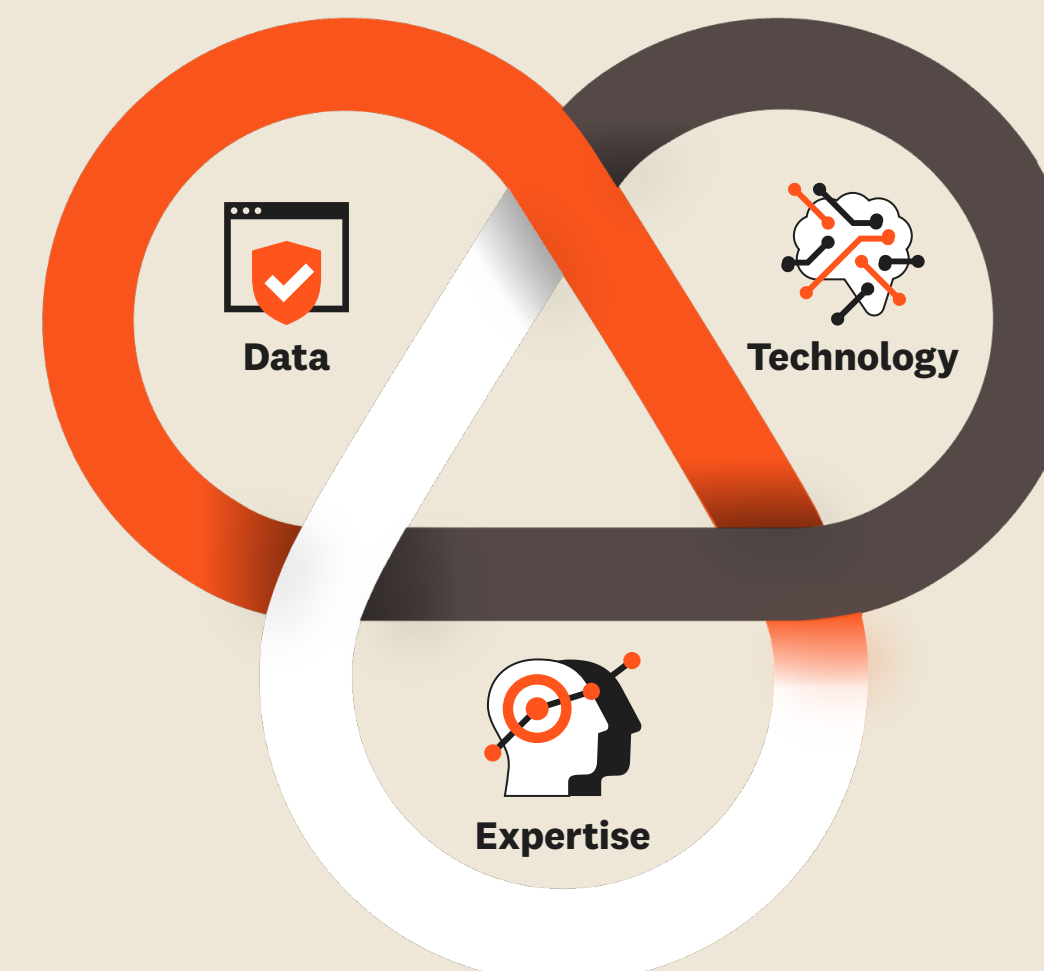
## Stay updated with Reaxys latest developments

[Release Notes](#)

[2026 Roadmaps](#)



## Trusted data, technology and expertise to support chemistry research



**Get started today**  
Register | Sign in



# Homepage tour

Start your search, find key data and accelerate discovery

- A.** Quick Search: Find substances, reactions and documents using keywords, structures or natural language.
- B.** AI-powered natural language search: Enter a question in everyday language. AI summaries appear on the results page with cited references.
- C.** Structure Search: Draw molecules (Marvin JS, ChemDraw JS).
- D.** Query Builder: Build advanced searches using structured fields, Boolean logic, Search operators, bioactivity, spectra and patent querylets.
- E.** Results: Review, filter by reaction type, bioactivity, patents and export for analysis.
- F.** Retrosynthesis: Plan synthesis routes with AI.
- G.** History/Alerts: Save searches, research and set alerts.
- H.** Content Overview: Sign in to see the latest content numbers.



Sign in or log in to save searches and set alerts.  
[Learn more about access.](#)

The screenshot shows the Reaxys homepage interface. At the top, the Reaxys logo is on the left, and navigation links for Quick search, Query builder, Results, Retrosynthesis, and History/Alerts (G) are on the right. Below the navigation bar, the main heading is "Explore Chemistry with Reaxys" followed by a subtext "Discover substances, reactions, documents and bioactivity data with our powerful integrated databases". The central section is titled "Discover the most relevant insights with keywords, everyday language and AI summaries." and contains a search bar (A2) with the placeholder text "Substance Molecular Formula, e.g. Pt(PPh3)3". To the right of the search bar is a callout letter B. Below the search bar is a section for "Draw Structure / Reaction" (C) and a "Search" button (H). At the bottom, there is a content overview section (H) showing statistics: 352M Substances, 71M Reactions, 123M Documents, 48M Patents, and 50M Bioactivities. A disclaimer at the bottom states: "Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial."



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# Core features



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## Quick search

## Select your input method

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# Quick search: *select an input — or combine them*

Type text AND draw a structure/reaction to refine the same search

## Natural language query

Search Reaxys [Learn how it works](#) [New](#) [Import](#)

What are the key challenges in Mn based catalysts for VOCs removal? [×](#)

AI-powered natural language search and summaries **in Quick Search.**

NLQ understanding plus keyword logic retrieves and ranks Documents. Eligible searches generate a cited summary from titles and abstracts of up to 20 top-ranked documents.

### What you get

- Ranked Document results
- Cited summary
- In-line citations → reference preview → abstract/full text

### Use when

- Scope a topic fast
- Triage evidence before deep reading
- Build a cited starting set

### Verify

- Open in-line citations → reference preview → abstract/full text
- Filter after verification (filters change the document set and can hide the summary)

### Note

Summaries appear only for eligible Quick Search Document searches, not for structure or mixed queries, or Query Builder searches

## Indexed keyword search

Search Reaxys [Learn how it works](#) [New](#) [Import](#)

oxe [×](#)

**Chemical Names**

oxepan-2-one  
oxetan-3-on

**High-precision search using indexed fields and extracted entities** Keyword logic matches terms across indexed metadata and extracted chemistry. Results return as structured sets (Documents, Substances, Reactions, Commercial Substances), with links to related Target & Bioactivity evidence where available.

### What you get

- Structured result sets by query type
- Filters (Limit To / Exclude) and sorting
- Linked records and evidence objects

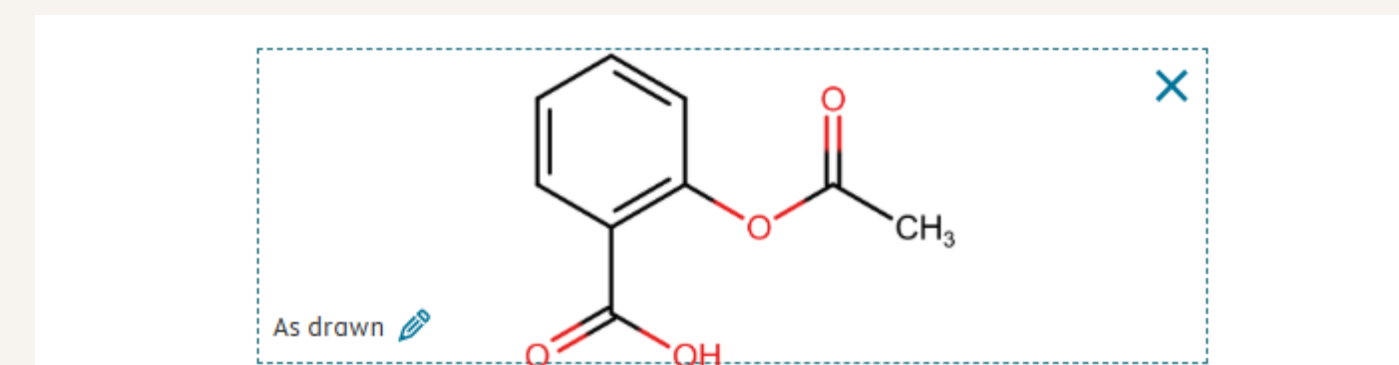
### Use when

- Searching for exact terms and known entities
- Identifier-heavy queries (names, patent and CAS numbers)
- Controlled recall and reproducible retrieval

### Verify

- Use filters, then open linked records and sources
- Use Edit in Query Builder for explicit field logic

## Draw structure/reaction



### Chemistry-native retrieval using structure and reaction input

Marvin JS or ChemDraw JS tool to draw structure or reaction. Reaxys matches by exact, substructure, or similarity and links hits to reactions, documents (including patents) or Target & Bioactivity evidence where available, and commercial availability.

### What you get

- Substances and Reactions result sets linked to evidence
- Pivot links to Documents (including Patents), Target & Bioactivity evidence, and commercial availability
- Filters and sorting to shortlist candidates

### Use when

- Analog and scaffold exploration
- Reaction pattern and condition scouting
- Make-or-buy decisions using availability signals

### Verify

- Open linked reaction steps/conditions and source records
- Validate similarity hits against properties and evidence



## Quick search

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# Overview

Start a Reaxys search from one entry point.

Quick Search is the fastest way to start a Reaxys query. Choose a query type, then run a text or structure search to get ranked results you can refine and export.

## Workflow

- A.** Select Quick Search from the top menu.
- B.** Import saved queries: Reload saved searches.
- C.** Enter NL query, keywords (e.g. CAS and patent number)
- D.** Structure-based search: Use Draw to sketch or paste chemical structures or reactions. Reaxys supports Marvin JS and ChemDraw
- E.** Run your search. Quick search supports substances, reactions, and document search. Eligible document searches may show a cited summary when enabled.



**Article:**  
[Learn more about search](#)



**Power user tip:** Combine a text term with a structure, then filter by solvent or yield to converge fast. This reduces noise and improves the set you export for analysis too.

The screenshot shows the Reaxys Quick Search interface. At the top, the Reaxys logo and navigation menu are visible. The main heading is "Explore Chemistry with Reaxys". Below this, a search bar is labeled "Search for 'Ot'". A search input field contains the text "Ot". Below the input field, there is a button labeled "Search". The interface also displays statistics: 352M Substances, 71M Reactions, 123M Documents, 48M Patents, and 50M Bioactivities. A disclaimer at the bottom states: "Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial."

Annotations on the screenshot:

- A:** Points to the "Quick search" link in the top navigation menu.
- B:** Points to the "Import" button next to the search input field.
- C:** Points to the search input field containing the text "Ot".
- D:** Points to the "Draw Structure / Reaction" button.
- E:** Points to the "Search" button.



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# AI enhanced document discoverability and summaries

Get a cited literature summary for eligible document searches

Hybrid retrieval (semantic + keyword) ranks the most relevant papers/patents. A structured summary is generated from titles + abstracts of up to 20 top results with traceable citations.

## Workflow

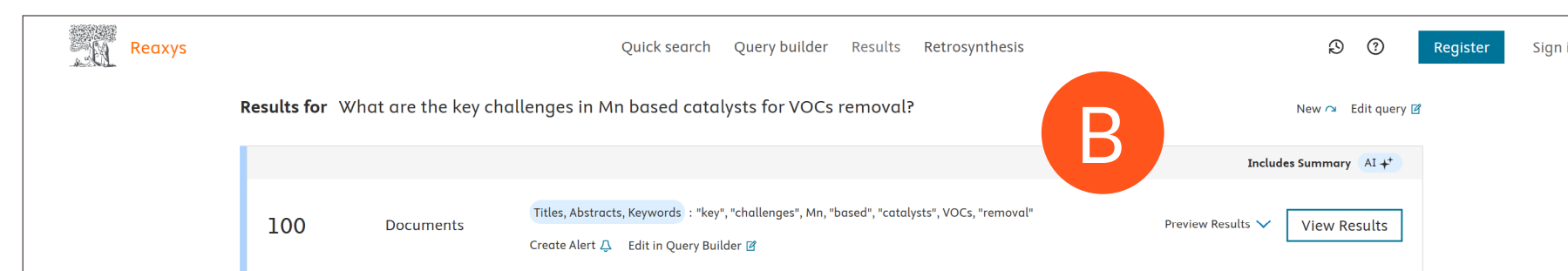
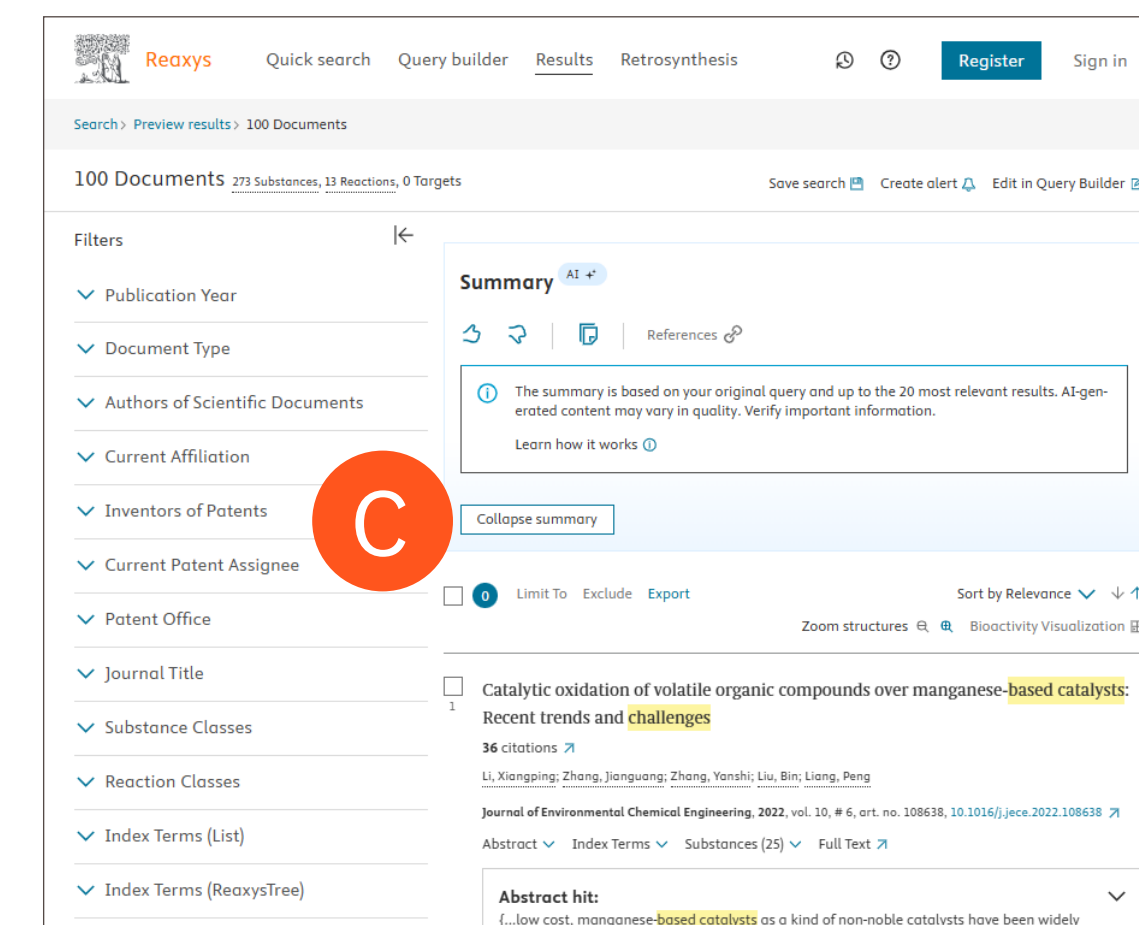
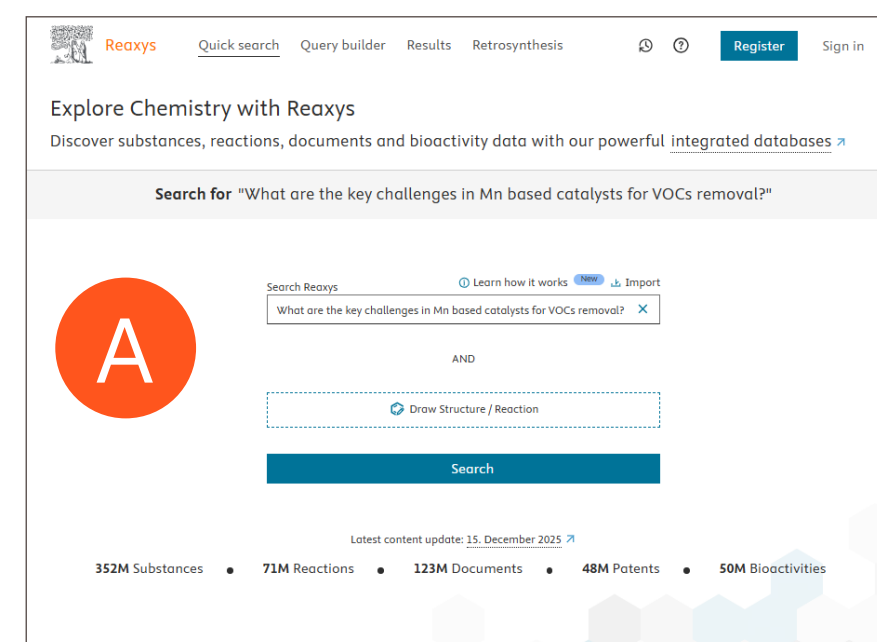
- Type a natural-language question (or keywords) to start a Document search in Quick Search.
- On the results preview page, choose the result set marked “Includes Summary (AI+)” and click View Results → AI Summary
- Verify (traceability to source): Read the Summary, then click numbered citations → open Reference Preview → jump to Document details / Abstract / Full text for validation → Export

### Note:

Applying filters changes the Document set and can hide the summary. Return to the original unfiltered results to restore it.



**Power user tip:** Start with everyday language to scope a topic then tighten with keywords for precision. Verify statements by opening cited documents in a Results list view. All user interactions are private, with no data used to train external model



Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



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# Structure editors

Draw or paste structures to power structure-based searching

Structure editors let you draw, paste, or generate a molecule or reaction for structure-based searching. Transfer the structure into a query to retrieve matched substances or reactions for review and export.

## Workflow

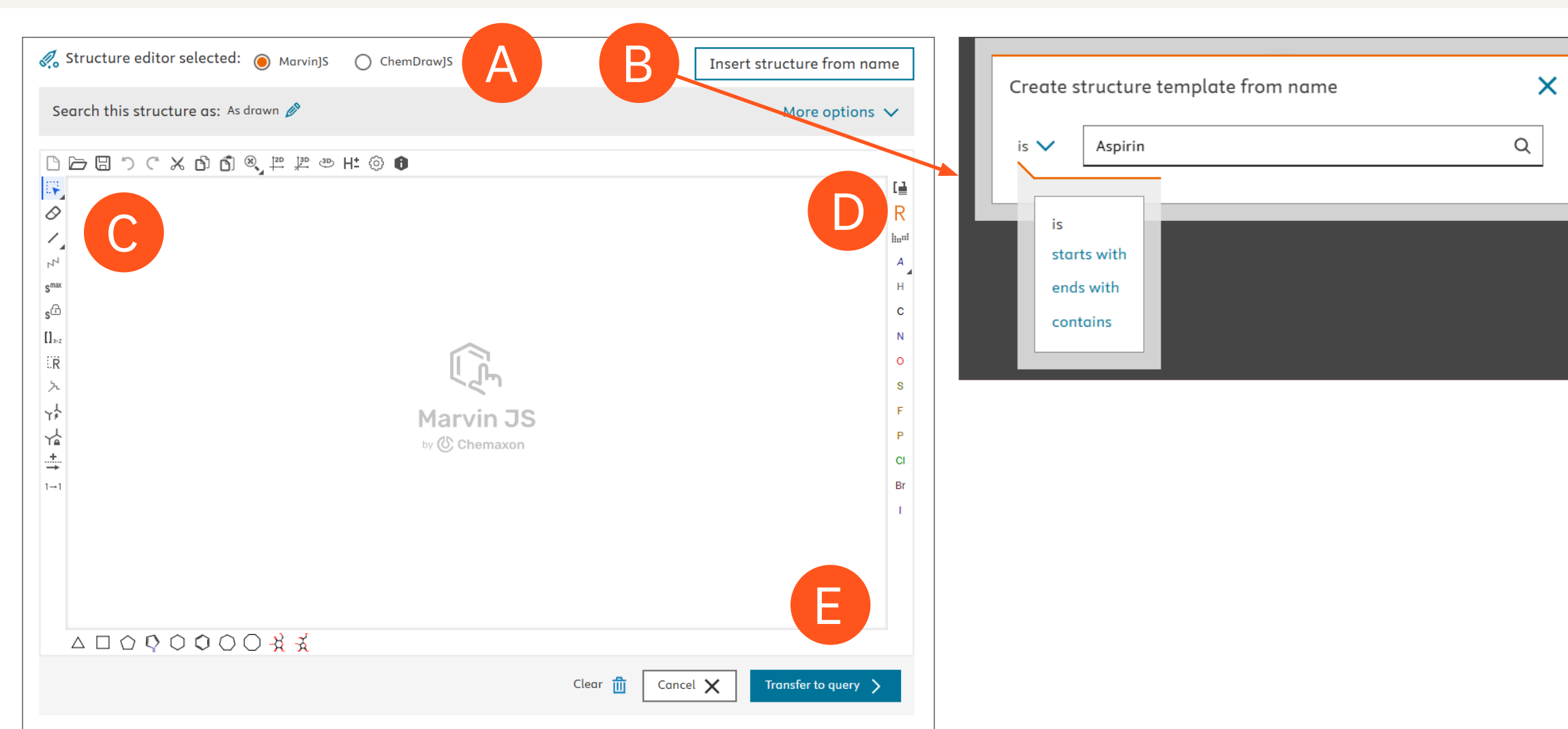
- A.** Choose a structure editor: Select MarvinJS or ChemDrawJS (default: MarvinJS recommended).
- B.** Insert structure from name: Enter a chemical name, CAS-RN, InChIKey or SMILES to auto-generate a structure (see F).
- C.** Draw your structure: Use the drawing tools to create or modify your structure or reaction.
- D.** Apply search modifications: Expand searches by selecting tautomers, stereo configurations, isotopes or radicals.
- E.** Transfer to query: Click Transfer to Query to add the structure to your search and refine your parameters.
- F.** Create structure from name: Use structure templates to generate exact or partial matches.



**Power user tip:** Generate a structure from name or identifier, then review it before Transfer to Query.



**Article:**  
[How to create a Structure Drawing in Reaxys](#)



Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



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## Triage result categories and top hits before deep filtering

## Workflow

- 

[illegible]

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# Results: Overview

Refine, inspect and export an evidence ready results set

The Results page is where you refine and inspect hits with filters, sorting, and row options. Open linked substances, reactions, targets, and documents, then export a clean set.

## Workflow

- A.

Results context: See the result set and counts for the current category and database

B.

Filters panel: Refine results using filters. Use Limit To or Exclude to include or remove matching results.

C.

Structure thumbnail: Preview the structure for each hit in the results list.

D.

Change database scope: use the dropdown to switch better Reaxys and other data bases.
- E.

Results tools: Use in-page tools such as search within results, grid view, or Bioactivity Visualization when available.

F.

Sort menu: Sort results using category-specific criteria.

G.

Row options menu: Open item-level actions such as Find Similar, Copy structure to query, Copy SMILES, Use as filter, or Open in database.

H.

Linked data shortcuts: Jump from a result to linked data such as preparations, reactions, targets, or documents.



**Power user tip:** Start broad, then narrow. Use Limit To to focus on the most relevant hits and Exclude to remove unwanted classes. Open linked reactions, targets, or documents to validate the evidence before exporting.

Reaxys

Quick search   Query builder   Results   Retrosynthesis

Register   Sign in

Search > Preview results > 393 Substances

Reaxys - 393   Commercial Substances - 81   PubChem - 6,063

393 Substances   out of 14,699 Documents, containing 50,085 Reactions, 119 Targets

Filters

By Structure

Measurement pX

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Available Data

Document Type

Publication Year

Current Patent Assignee

LogP

H Bond Donors

H Bond Acceptors

Rotatable Bonds

TPSA

Limit to

Exclude

Clear

D

A

B

C

G

Indole

C8H7N   117.15   107693   120-72-9

Identification   Bioactivity (All)   Spectra - 453

Druglikeness   Physical Data - 607   Other Data - 440

acetic acid

CC(=O)O   117.07   13192702   Retrieve CAS RN

Identification   Druglikeness

3H-Indole

C8H7N   117.15   107688   271-36-1

Identification   Physical Data - 5   Spectra - 11

Druglikeness   Other Data - 9

Indole propionic acid

CC(=O)OCC1=CC=CC=C1   191.23   13283301   Retrieve CAS RN

Identification   Druglikeness

Indole anion

C8H6N-   116.142   1563368   22774-73-8

F

Sort by No of References

Zoom structures   Grid   Bioactivity Visualization

E

H

Preparations - 731 >

Reactions - 49,260 >

Targets - 113 >

Documents - 47,552 >

Preparations - 1 >

Reactions - 1 >

Documents - 6,324 >

Preparations - 24 >

Reactions - 92 >

Documents - 982 >

Reactions - 1 >

Documents - 207 >

Feedback

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.

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# Results: *Filter options 1*

Narrow results with fields that match each result type

Filters adapt to each result type so you can narrow with the fields that matter. Substances focus on properties, Commercial Substances on supplier data, and Reactions on conditions and experimental details.

## Workflow

- A.** Substance results: Filter by structure, molecular weight, pH, availability, publication year and patent assignee.
- B.** Commercial substance results: Filter by supplier, stock, price, purity, location and package size.
- C.** Reaction: Filter by conditions, reagents, catalysts, and solvents; toggle single-step reactions or experimental procedures.
- D.** Target results: Filter by target attributes such as species, target type, measurement and parameters.
- E.** Document results: Filter by publication year and document type, and refine by bibliographic, patent and chemistry fields such as patent office, index terms and substance classes.



**Power user tip:** Start with Limit To and Exclude, then add one high-impact chemistry filter.

The illustration shows five panels of filter options, each with a red circle letter label (A-E) at the top. Each panel contains a list of filter categories with expandable arrows. At the bottom of each panel are buttons for 'Limit to', 'Exclude', and 'Clear'.

- Panel A (Substance results):** By Structure, Measurement pH, Targets, Parameters, Substance Classes, Molecular Weight, Number of Fragments, Availability, Available Data, Document Type, Publication Year, Current Patent Assignee, LogP, H Bond Donors, H Bond Acceptors, Rotatable Bonds, TPSA.
- Panel B (Commercial substance results):** Molecular Weight, Number of Fragments, Availability, Commercial Suppliers, Supplier Preferences, Supplier Geolocation, Usage Classification, Package Size, Currency, Price, Purity, Stock Availability, Shipping Time, Shipment Country.
- Panel C (Reaction):** By Structure, Yield, Reagent/Catalyst, Solvent, Catalyst Classes, Solvent Classes, Product Availability, Reactant Availability, Reaction Classes, Document Type, Publication Year. Includes checkboxes for 'Single step reactions only' and 'Experimental procedure only'.
- Panel D (Target results):** Targets, Target Species, Target Type, Measurement pH, Parameters, Substance action on target, Document Type, Publication Year, Current Patent Assignee.
- Panel E (Document results):** Publication Year, Document Type, Authors of Scientific Document, Current Affiliation, Inventors of Patents, Current Patent Assignee, Patent Office, Journal Title, Substance Classes, Reaction Classes, Index Terms (List), Index Terms (ReaxysTree). Includes a checkbox for 'Manually curated content only'.

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



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## Results: *Bioactivity visualization*

Compare bioactivity across substances and targets in one view. Visualize bioactivity profiles to assess structure–activity relationships (SAR), potency and target selectivity. The matrix displays normalized **pX values** across substances and targets.

Use Export, Settings, Navigator, and Legend to adjust the view and extract pX data for analysis and reporting.

## Workflow

- A.** Use Export, Settings, Navigator, and Legend to configure the view and export pX values.
  - B.** Use the Navigator panel to move across large matrices.
  - C.** Hover over substances or targets to view structures and identifiers.
  - D.** Select a cell to open detailed bioactivity evidence and linked sources.
  - E.** Use column options to sort by activity and limit or exclude columns.
- **Article:**  
[What is a Bioactivity visualization map?](#)

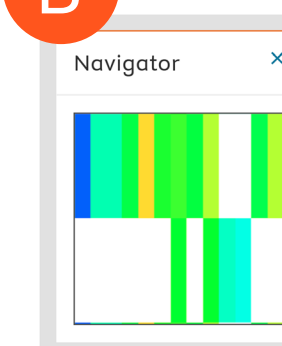
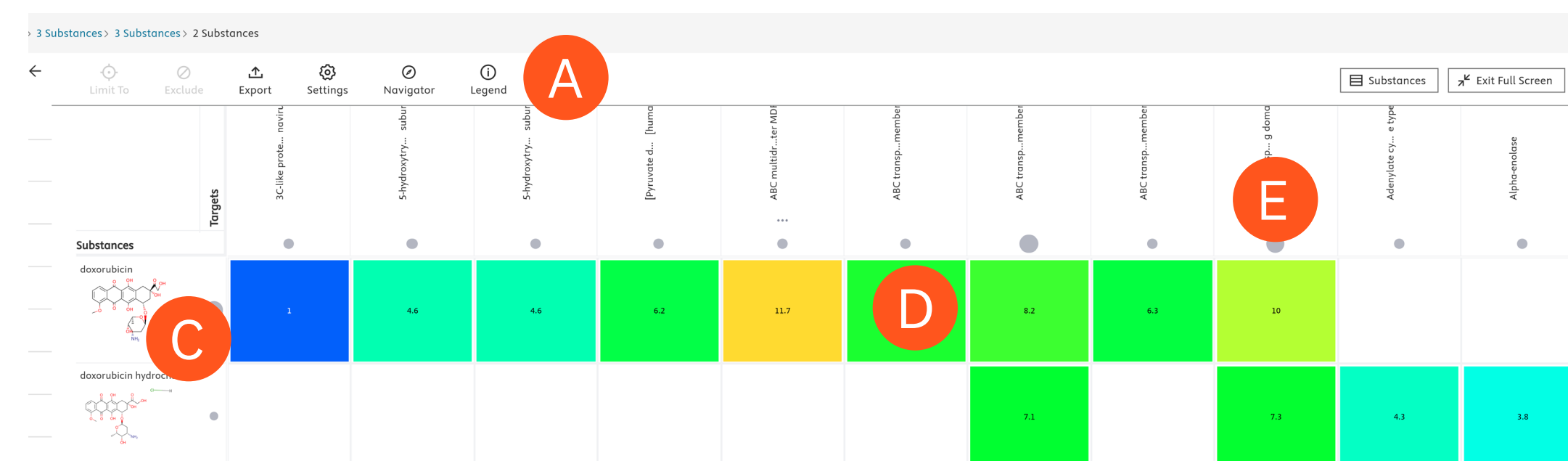


## Article:

## What is a Bioactivity visualization map?



**Power user tip:** Use Bioactivity Visualization to spot SAR inflection points, where small structure changes drive large potency shifts.



*Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.*



| Quick search             |          |                                                     |                   |                   |                          |                          |
|--------------------------|----------|-----------------------------------------------------|-------------------|-------------------|--------------------------|--------------------------|
| Select your input method | Overview | AI enhanced documents discoverability and summaries | Structure editors | Results           | Export and query history | Create and manage alerts |
|                          |          |                                                     |                   | Personal settings |                          |                          |

# Export and query history

Download results and reuse searches without rebuilding

## Workflow: Export

- A. Open export window from Results: access export options.
- B. Select format: Choose the file format (see G)
- C. Define range: Export all results, selected results or a custom selection.
- D. Choose data to export: Select all data, ID-only, hit-only or specific fields.
- E. Additional options: Include structures or descriptions to enrich reports.
- F. Initiate export: Click Export to start or cancel anytime.

## Workflow: Query history

- G. History tab: Click History to access both recent and saved searches.
- H. Recent queries: Displays queries and actions from your current session.
- I. Saved queries: Shows queries saved from earlier sessions (see inset E).
- J. Edit and reuse: Click Edit Query, Save, Alert or View to modify or reuse recent searches.
- K. Saved query options: Edit, rename or delete queries from the Saved list.



**Power user tip:** Keep key queries saved for fast recall to reduce repetition and improve research efficiency.

Export substances Reaxys

Choose a format: PDF/Print

Range: All results - 105

Export: 

All available data

Identification data only

Hit data only

Choose specific data

Additional options: 

Include structures

Include a description in the document

Disclaimer: please refer to our Terms and Conditions before downloading data.

Export >

Export substances Reaxys

Choose a format: PDF/Print

Range:

Export: 

PDF/Print

XML

Microsoft Word

Microsoft Excel

Tab-delimited text

Electronic Lab Notebook

RD File

SD/Molfile

Smiles

Additional options: 

Include a description in the document

Disclaimer: please refer to our Terms and Conditions before downloading data.

Reaxys

History

Recent

Saved

105 Substances

4 TgItems

1104 TgItems

47 TgItems

82 TgItems

Today 15:12

Today 15:12

Today 15:00

Today 15:00

Today 15:00

Context Switch from 4 Targets

Quick Search: "ger"

Context Switch from 82 Targets

Context Switch from 94 Targets

Edit Query

Save

Alert

View

Edit Query

Save

Alert

View

Edit Query

Save

Alert

View

History

Recent

Saved

Reaxys

32087 Reactions

Feb 19 2026

001

Query Builder: in reactions - Other Condi

Edit Query

Delete

Rename

Alert

View

100 Citations

Feb 17 2026

test\_summary\_Save\_search

Quick Search: "What are the key challenges in Mn based catalysts for VOCs removal?"

Edit Query

Delete

Rename

Alert

View

100 Citations

Feb 17 2026

fromresultsave

Edit Query

Delete

Rename

Alert

View

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# Create and manage alerts

Monitor saved queries and get notified when new matches appear

## Workflow: Create alerts

- A.** Click Create Alert from Results Preview or History.
- B.** Enter an alert name to organize topics (e.g., molecule, competitor, project).
- C.** Add recipients: Your email is auto-added; add others if needed.
- D.** Set frequency/timing: Choose weekly, bi-weekly, monthly or after database updates
- E.** Set trigger conditions: Trigger alerts on document updates or first appearance. (Optional: exclude alerts with zero results).
- F.** Customize alert content: Select data source (e.g., Reaxys) and what to include (Title, Abstract, Hit details). For advanced alerts, use Query Builder first.
- G.** Activate alert: Click Create to finalize and receive notifications

## Workflow: Manage alerts

- H.** Click Alerts on the main navigation to view and manage your saved alerts.
- I.** Alerts appear from the newest to the oldest with details on query type (Substances, Reactions, Targets, Documents, Commercial Substances), creation date, database and alert name
- J.** Previous results: Use results from the dropdown menu to view earlier iterations of an alert – useful for spotting what’s new.
- K.** Edit settings such as name and frequency. To change the query, modify it in Query Builder and create a new alert.

Create Alert

Query: Quick Search: "gpcr"

Alert name: 

Name

 GPCR

Send alerts to: 

C

Frequency: 

Every week

 on: 

Wednesday

D

Send alert: 

Upon first appearance in the database

E

☐ Do not send alerts with zero results

ADVANCED ALERT CONTENT: ⓘ

From databases: ☒ Reaxys 

F

Include in email: ☐ Title and bibliographic information ☒ Abstract ☐ Full abstract ☒ Partial abstract ☐ Hit details (keywords, substances, reactions or targets)

Email alerts will produce an email with a maximum of 99 records. ⓘ 

G

Cancel

Create

Power user tip:

Set alert frequency based on research needs – weekly for updates and monthly for trends.

Power user tip:

Monitor competitors by setting an alert using Current Patent Assignee.

Quick search

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Retrosynthesis

History

Alerts 

H

Alerts

Targets

GPCR - In Reaxys

Since Apr 9, 2025

Quick Search: "gpcr"

Results from: No alert results

Edit Delete

Documents

steroid - In Reaxys

Since Apr 9, 2025

Document Basic Index : "anabolic agents"; "anabolic agents"; "anabolic ...

Results from: Apr 4, 2025

Show details Edit Delete

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.

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|                          |          |                                                     |                   |         |                          | Personal settings        |

# Personal settings

Tailor Reaxys defaults for search, retrosynthesis, and results display

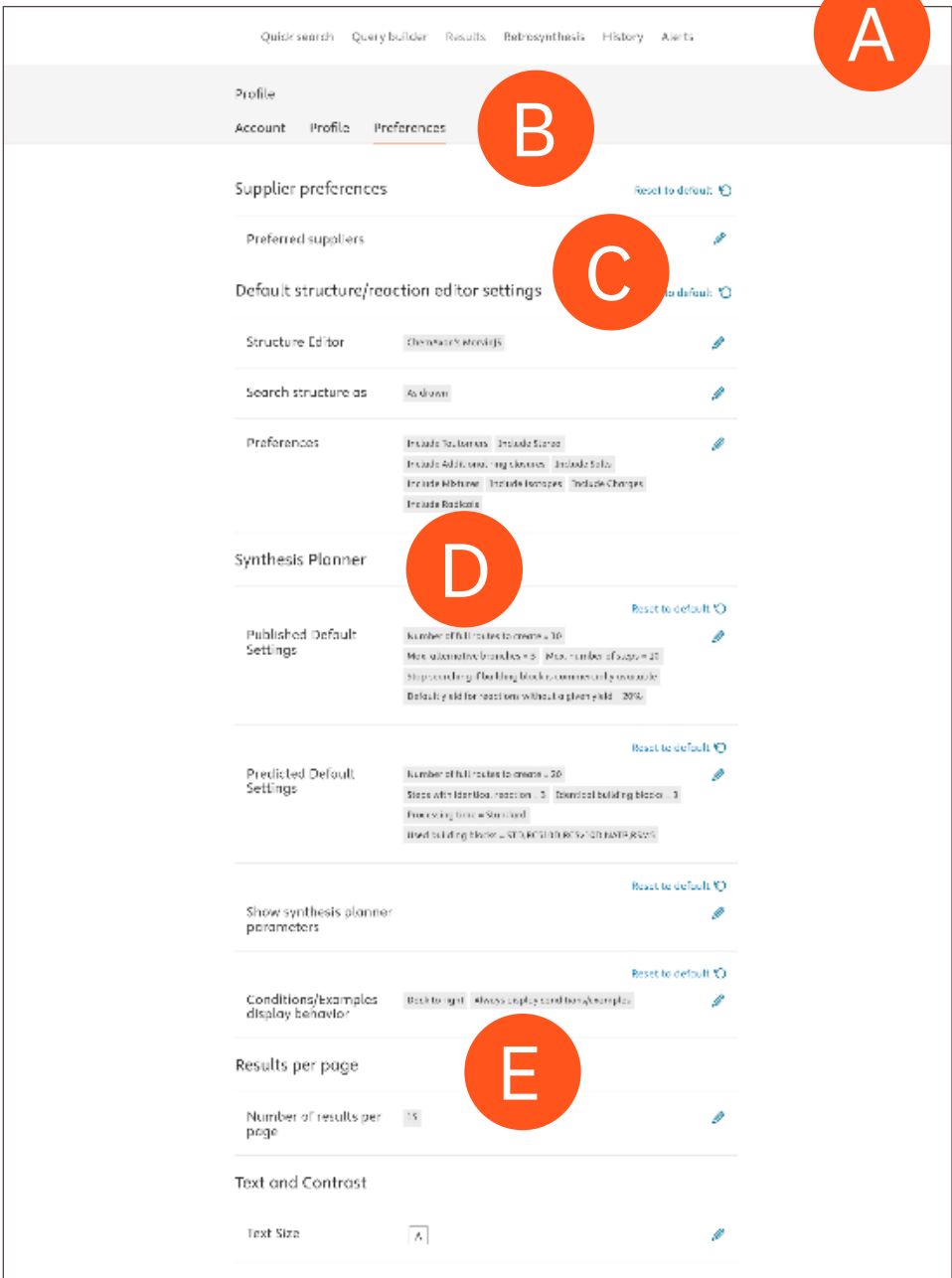
**Micro paragraph:** Personal settings tailor Reaxys defaults for how you search, plan routes, and view results. Set your structure editor, Autoplan limits, and results display so sessions stay consistent.

## Workflow

- A. Sign in by clicking your name or the person icon, then select Profile.
- B. Click Account to edit username, email and password. Access Preferences to adjust query settings
- C. In the Structure Editor, select MarvinJS or ChemDrawJS as your preferred editor, and modify settings (e.g., include/exclude tautomers, salts).
- D. Among the settings for Autoplan, choose how many plans are auto-generated and the maximum number of steps
- E. Choose the number of results per page.



**Power user tip:** Set your preferred structure editor and tautomer settings once, then keep them consistent across projects so comparisons and exports align.



Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



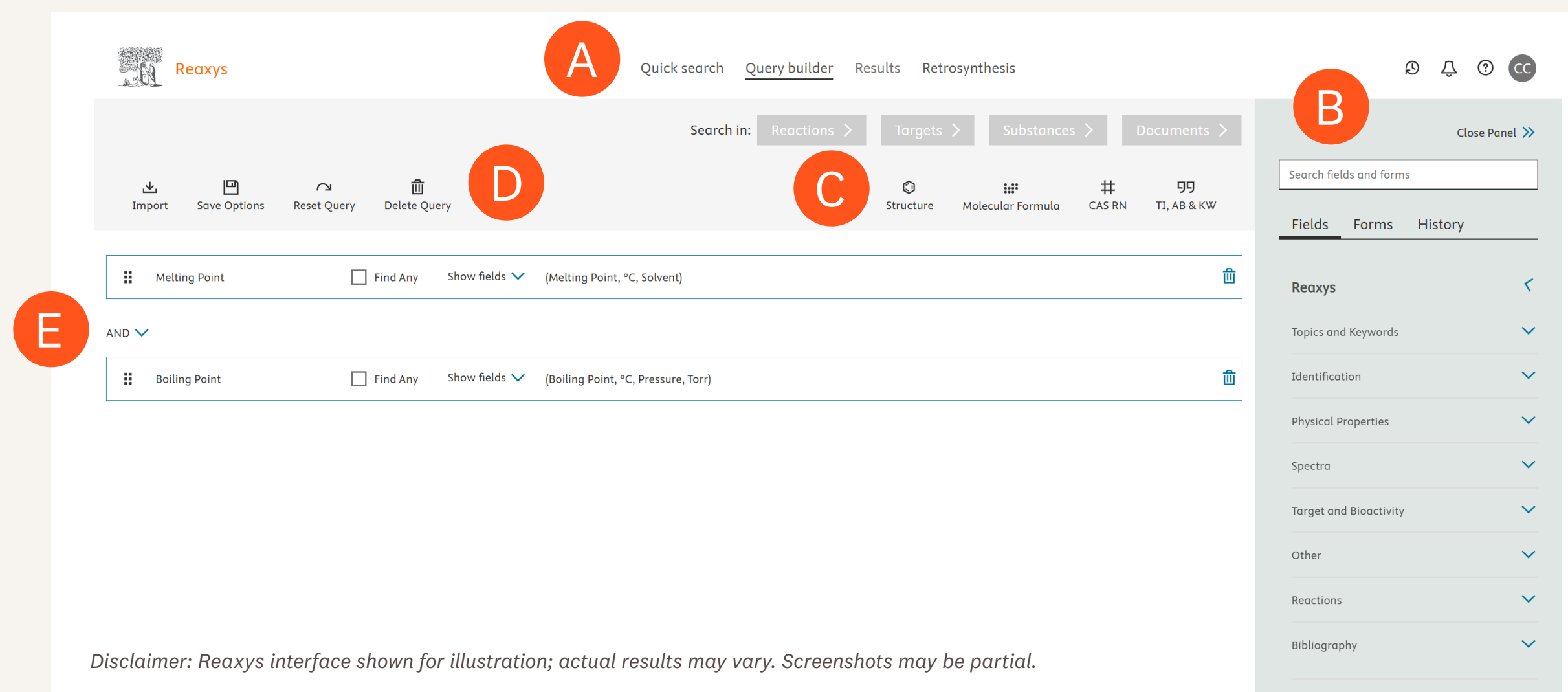
# Overview

Build precise multi parameter queries with fielded filters and Boolean logic

Query Builder builds precise multi parameter searches with drag and drop fields and Boolean logic. Combine chemistry, bioactivity, and patent fields to target the records you need and reuse the query.

## Workflow

- A.** Open Query Builder: Launch from the top navigation or use Edit Query to customize your search.
- B.** Add fields with drag-and-drop: Combine chemical, biological and patent fields (e.g., Melting Point, CAS Numbers, Patent Assignee).
- C.** Combine science and IP data: Find high-potency compounds with known synthesis routes, not patented by competitors.
- D.** Save, reuse and set alerts: Save queries for later use and set alerts for new data (substances, reactions, patents).
- E.** Boolean logic and other operators: Use AND, OR, NOT, in addition to proximity, text, and comparison operators to broaden, narrow, or qualify your query - perfect for refining SAR or patent filters.



**Power user tip:** Combine Current Patent Assignee, Bioactivity and Synthesis fields to accelerate discovery of high-potency, synthesizable compounds not claimed in patents to help you unlock novel, innovation-ready opportunities.



**Power user tip:** Combine Current Patent Assignee with Bioactivity and Synthesis fields to find potent, synthesizable hits and screen ownership early.



# Analyze patent ownership

Analyze patent ownership across linked results from a single assignee view

Query Builder can map patent ownership across linked substances, reactions, and documents. Select an assignee and result type, then filter and review patent families to spot trends and gaps.

## Workflow

- A. Launch Query Builder from the main navigation.

B. Select current patent assignee, original assignee or ultimate owner (under Bibliography) to focus on ownership data across substances, reactions and documents.

C. Enter a company or institution name: Use contains for flexible search. Type the full or partial name (e.g., Pfizer) to return a wide match.

D. Choose result types: Select Substances, Reactions, Targets or Documents to explore data linked to the selected assignee.

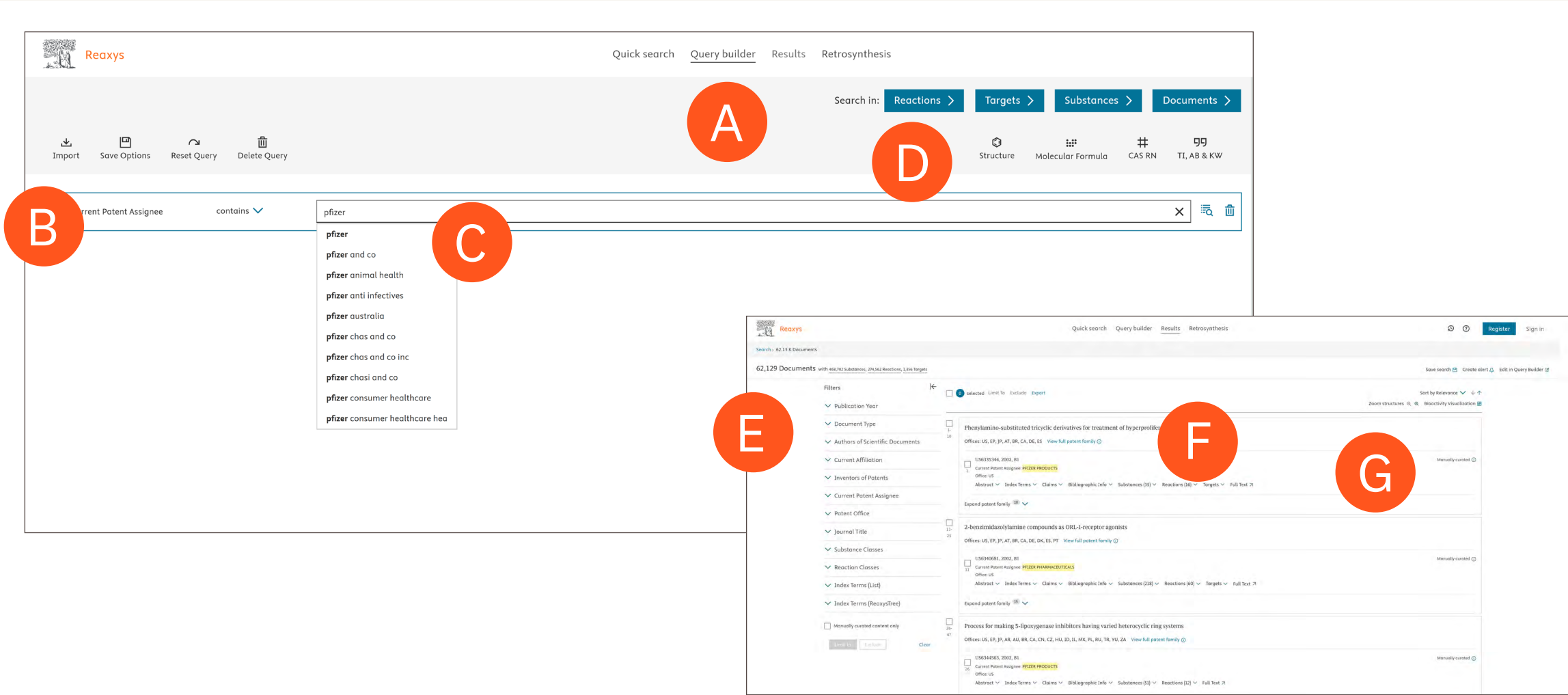
E. Filter and analyze results: Use Results filters to refine by target, structure, property, or document type and identify ownership trends.

F. View the list of patent families: Click to check the patent entire family cluster.

G. Data manually curated or automated: See if data is curated manually or automatically generated.



**Article:**  
[Query builder articles](#)



Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



**Power user tip:** Use Results filters to analyze ownership trends across linked substances, reactions and targets – ideal for whitespace analysis or portfolio benchmarking

# Published and predicted

Find literature-based synthesis routes with step details and cited sources

Published Retrosynthesis finds literature-based routes linked to Reaxys reaction evidence. Draw a substance and run Synthesize to compare step by step pathways, conditions, and cited sources.

## Workflow

- Go to the Retrosynthesis page and draw a compound or import your compound of interest.
- Define search parameters for published synthesis routes. Available to all users with a Reaxys account.
- If your institution has access to the Predictive Retrosynthesis module, you'll also see the option to select Predicted routes.
- Click synthesize: Run the query to generate available retrosynthetic pathways based on your structure.
- A Retrosynthesis Project is Added to Your Projects Page: Sign-in required to save, revisit or track retrosynthesis workflows over time.
- Analyze synthesis route: Review full reaction steps, intermediates and experimental conditions in a structured, interactive view.



**Power user tip:** Use Published routes for validated, literature-based synthesis pathways. Facing synthesis bottlenecks? Try Predicted routes (subscription required) to explore novel, machine-suggested alternatives.

The top screenshot shows the 'Structure editor' with a chemical structure and the 'Parameters' panel. The 'Parameters' panel includes options for 'Predicted' (checked), 'Length and depth of routes' (set to 20), 'Diversity of routes' (set to 3), 'Processing time' (set to Standard), and 'Select Building Block Libraries' (checked for Commercial Substances in 10 days (RCS10D), Commercial Substances >10 days (RCS>10D), and Commercial Substances <\$10/g (RCS\$10)).

The bottom screenshot shows the 'Projects' table with two projects listed:

|                          | Date        | Project name     | No. of routes                 |
|--------------------------|-------------|------------------|-------------------------------|
| <input type="checkbox"/> | 09 Apr 2025 | Project #2765077 | Predicted: 10<br>Published: 8 |
| <input type="checkbox"/> | 17 Sep 2024 | Project #2271749 | Predicted: 10<br>Published: 8 |

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



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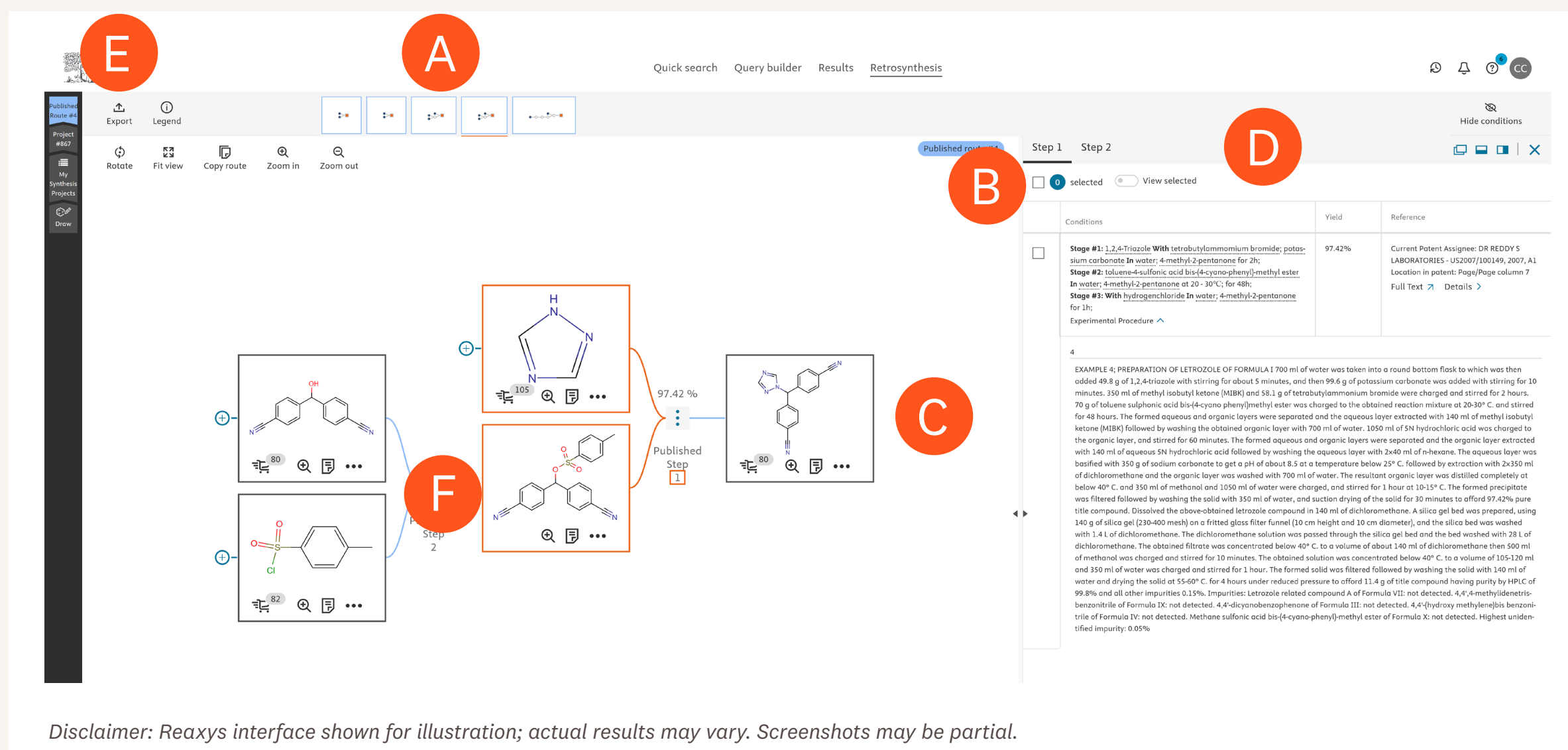
## Analyze results

## Compare routes, inspect steps, and expand pathways in Tree View

Analyze results compares alternative routes and surfaces step level details. Toggle route and step views, inspect conditions, and insert multi step schemes in Tree View to expand routes faster.

## Workflow

- A.** Toggle between published and predicted synthesis routes: Use the navigation buttons to switch between alternative synthesis plans
- B.** Review experimental conditions for each step: View reaction yields, temperatures, solvents and literature references for each step.
- C.** Access experimental procedures: When available, open full-text procedures to replicate or assess reactions
- D.** Switch layout or use the Fit View: Toggle between vertical/horizontal layout and zoom to fit complex pathways more easily.
- E.** Export synthesis routes: Download structure diagrams and experimental data, or export directly to ChemDraw for lab planning or collaboration.
- F.** View/Insert multi-step schemes directly in Tree View to expand routes faster.



Learn more:

## Pending.AI Reaxys Predictive Retrosynthesis

## Predictive Retrosynthesis Guide – Iktos

Contact us: to enroll in the Reaxys Predictive Retrosynthesis subscription.



**Power user tip:** Insert a reaction step to refine and adapt a route to your specific synthesis goals.



# Core content



# Core content

Explore validated chemistry and bioactivity evidence linked to source literature and patents

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <div><b>Substances</b></div> <div>352M</div> <div><b>Validated substance records across organic, inorganic and organometallic chemistry</b></div> <div><b>How it works</b><br/>Substances are captured in structured fields (names, identifiers, structure, properties) and cross-linked to reactions, documents, patents and bioactivity evidence.</div> <div><b>What you get</b><ul style="list-style-type: none"><li>Structures plus identifiers and synonyms</li><li>Property fields across chemical, physical, spectral and environmental data</li><li>Links to reactions, documents, patents, bioactivities and commercial availability</li></ul></div> <div><b>Verify</b><br/>Open the linked source document or patent behind each extracted data point.</div> <div><b>Note</b><br/>Reaxys contains about 500 million experimental properties in around 500 property search and display fields.</div> | <div><b>Reactions</b></div> <div>71M</div> <div><b>Curated experimental reactions with conditions and supporting evidence</b></div> <div><b>How it works</b><br/>Reaction steps are captured as structured transformations and linked back to the underlying journal or patent source.</div> <div><b>What you get</b><ul style="list-style-type: none"><li>Reaction conditions and yields (where available)</li><li>Procedures and supporting references for step-by-step review</li><li>Links to substances, documents, patents and commercial availability</li></ul></div> <div><b>Verify</b><br/>Open the cited source to inspect scope, limitations and experimental context.</div> | <div><b>Documents</b></div> <div>123M</div> <div><b>Literature and patent documents that connect narrative evidence to extracted chemistry entities</b></div> <div><b>How it works</b><br/>Documents are indexed and linked to extracted substances, reactions and bioactivity, so you can pivot from reading to evidence objects without re-running searches.</div> <div><b>What you get</b><ul style="list-style-type: none"><li>Document records with bibliographic fields</li><li>Links to extracted substances, reactions and bioactivity evidence</li><li>Updated weekly; publication-to-ingestion timing varies by source and content type</li></ul></div> <div><b>Verify</b><br/>Open the document record and follow links to the underlying evidence objects and source text</div> <div><b>Note</b><br/>Some records appear within two weeks of publication; others complete within two months depending on source and content type.</div> | <div><b>Patents</b></div> <div>48M</div> <div><b>Chemistry-rich patent coverage across global authorities, structured for search and linking</b></div> <div><b>How it works</b><br/>Patent records are indexed with key bibliographic fields and connected entities to support ownership and competitive analysis.</div> <div><b>What you get</b><ul style="list-style-type: none"><li>Chemistry-rich patent records for R&amp;D and IP analysis across industries./105 patent offices; title/abstract/claims translated to English.</li><li>Bibliographic and classification fields to support competitive and IP analysis.</li><li>Links from patents to extracted substances, reactions and bioactivity evidence</li></ul></div> <div><b>Verify</b><br/>Review patent family context and open the original patent source when needed.</div> | <div><b>Bioactivities</b></div> <div>50M</div> <div><b>Curated bioactivity and target evidence to support SAR and selectivity decisions</b></div> <div><b>How it works</b><br/>Bioactivity measurements and targets are integrated and linked to substances and source documents and patents for traceable SAR analysis.</div> <div><b>What you get</b><ul style="list-style-type: none"><li>Bioactivity measurements mapped to targets and substances</li><li>Linked evidence to documents and patents for verification</li><li>SAR workflows supported by structured fields</li></ul></div> <div><b>Verify</b><br/>Open the linked source to confirm assay context, endpoint type and limitations.</div> |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

Commercial availability is a sourcing layer linked to substances and retrosynthesis, using supplier data integrated into Reaxys workflows.

Reaxys content is curated by expert chemists, updated weekly, and traceable to source publications and patents.

Content current as of March 2026. Reaxys content is continuously updated; please log in to access the most recent data.



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|            |           |           |         |               |
|------------|-----------|-----------|---------|---------------|
| Substances | Reactions | Documents | Patents | Bioactivities |
|------------|-----------|-----------|---------|---------------|

# Substances

Design molecules from curated substance records and linked evidence

Substances results show curated compound records with key properties and links. Start from a name or structure, filter, open linked reactions or documents, and export a focused set.

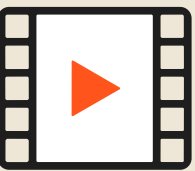
## Workflow

- A. Start with chemical structure or name input.
- B. Filter by physicochemical properties (e.g., logP, MW, solubility)
- C. Toggle supplier availability for sourcing: view commercial availability linked to substance records.
- D. Explore linked reactions, targets and literature.
- E. Export or reuse the curated dataset.
- F. Analyze synthesis route: Review full reaction steps, intermediates and experimental conditions in a structured, interactive view.



**Power user tip:** Sort by similarity to find close analogs, then filter by key properties and availability to shortlist feasible candidates faster.

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



How to [search for substances](#) by name?  
Watch 2m Video

How to quickly [obtain a commercial substance](#)?

How to set your [supplier preferences](#) workflow?

How to [avoid structural motifs](#) with known safety issues

## Plan synthesis routes from experimentally reported reaction evidence

## Workflow

- 
- Power user tip:** Quickly identify the most viable synthetic pathways using conditions reported in the literature — not just predictions.

*Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.*



# Documents

Find documents (including peer reviewed articles and patents) across disciplines with exact compound or reaction mention not just keywords.

## Workflow

- A.** Run a structure, substance, keyword or NLQ search
- B.** View documents result and read the AI summary if available with link to used references
- C.** Filter by: journal type, patent office, and more.
- D.** Access highlighted chemical context in full-text, abstracts, claims, and index terms
- E.** Trace back to extracted substances, reactions and bioactivity

**Note:** Documents include journals and patents.



**Power user tip:** Ask questions in plain language, read the summary for orientation, then verify key claims by opening the cited documents in Reference preview and the abstract or full text.

The screenshot illustrates the Reaxys interface for searching scientific documents. The interface is divided into several sections:

- Header (A):** Includes the Reaxys logo, navigation links (Quick search, Query builder, Results, Retrosynthesis), and user options (Register, Sign in).
- Search Bar (B):** Located at the top, it contains the search query and filters.
- Filters (C):** A sidebar on the left with various filters such as Publication Year, Document Type, Authors of Scientific Documents, Current Affiliation, Inventors of Patents, Current Patent Assignee, Patent Office, Journal Title, Substance Classes, Reaction Classes, Index Terms (List), and Index Terms (ReaxysTree).
- Search Results (D):** A list of documents. The first result is highlighted, showing its title, abstract, index terms, and substances.
- Substances (E):** A section within the highlighted result showing chemical structures and their corresponding Reaxys IDs.

The highlighted result (D) is titled "Recent Developments and Implementations of Conductive Polymer-Based Flexible Devices in Sensing Applications". Its abstract discusses the use of conductive polymers in nanocomposites for electromagnetic interference shielding. The index terms include "conductive polymers", "Nanocomposites", "Electromagnetic interference shielding", "Energy storage", and "Sensors...". The substances section displays three chemical structures: a simple ring (Reaxys ID 71), a complex polymer network (Reaxys ID 45), and a long-chain molecule (Reaxys ID 55).



# Patents

Track novelty and ownership with patent linked chemistry evidence

Patents results connect patent documents to mapped chemistry so you can track novelty and ownership. Filter by patent office and export a focused set for review or reporting.

## Workflow

- Enter compound or keyword.
- Filter by patent office (e.g., EPO, USPTO)
- View mapped reactions or targets.
- Export into patent report.



**Power user tip:** Mine patent databases to surface compounds and reactions, identify therapeutic claims, and compare protected synthetic routes across jurisdictions.



How to obtain SAR data for compounds in a patent? Watch 2m [video](#)



**Article:** What is the patent coverage in Reaxys? See quick [article](#)

The screenshot displays the Reaxys Patents search results page. At the top, the Reaxys logo and navigation links (Quick search, Query Builder, Results, Retrosynthesis) are visible. A search bar contains the text "232 Documents with 13,849 Substances, 19,151 Reactions, 18 Targets". Below the search bar, a list of filters is shown on the left, including Publication Year, Document Type (with a checkbox for "patent"), Authors of Scientific Documents, Current Affiliation, Inventors of Patents, Current Patent Assignee, and Patent Office (with checkboxes for wo, cn, us, ep, tw, kr). The main results area on the right shows a list of patent entries, each with a title, publication number, current patent assignee, and office. The first entry is "MACROCYCLIC INHIBITORS OF THE PD-1/PD-L1 AND CD80(B7-1)/PD-L1 PROTEIN/PROTEIN INTERACTIONS" (WO/2014/151634, 2014, A1) by Bristol Myers Squibb. The second entry is "Macrocytic inhibitors of the PD-1/PD-L1 and CD80(B7-1)/PD-L1 protein/protein interactions" (US9308236, 2016, B2) by Bristol Myers Squibb. The third entry is "Cyclic Peptidomimetic Compounds as Immunomodulators" (US2015/73042, 2015, A1) by Aurigene Oncology. The fourth entry is "Human monoclonal antibodies to programmed death ligand 1 (PD-L1)" (US9102725, 2015, B2) by E R Squibb Sons. Each entry has a "Manually curated" label and a "View full patent family" link. A "Feedback" button is located at the bottom right.

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.



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# Bioactivities

Profile targets and activity outcomes to guide SAR and MoA work

Bioactivities results link compounds to targets and assay outcomes to support SAR and MoA work. Filter by endpoint and target attributes, then export tables for analysis or submission.

## Workflow

- A. Run structure or compound name input.
- B. Filter by bioactivity outcome (e.g., IC50, Ki, EC50).
- C. Toggle filters for target type, target class or species.
- D. Navigate to linked targets, compounds and documents.
- E. Export bioactivity tables for SAR, validation or submission.



**Power user tip:** Explore how compounds act on biological targets – and identify therapeutic potential, safety flags or optimization paths using trusted, experimentally validated bioactivity data.



Watch Target & Bioactivity expert tips playlist

Reaxys

Quick searchQuery builderResultsRetrosynthesis

RegisterSign in

Search > Preview results > 4.47 K Substances > 1.01 K Targets

1,008 Targets out of 66,502 Documents, 4,475 Substances, 1,393 Reactions

Save searchCreate alertEdit in Query Builder

Filters

Targets

Target Species

Target Type

Measurement pX

Parameters

Substance action on target

Document Type

0 selectedLimit ToExcludeExport

Sort bySort alphabetically A-Z

Zoom structuresBioactivity Visualization

ic501,214

qualitative359

inhibition percentage239

percentage of cells in s phase196

percentage of cells in g2/m phase186

percentage of early apoptotic cells178

inhibition rate178

Filter by value

View more

1

Single protein

1-phosphatidylinositol-3-kinase (human, Wild)

Synonyms: 1-phosphatidylinositol-3-kinase

Mutant/chimera Details: Wild

Show target details

2

Single protein

1-phosphatidylinositol-3-kinase (Wild)

Synonyms: 1-phosphatidylinositol 3-kinase, 1-phosphatidylinositol-3-kinase, 1-phosphatidylinositol-3-kinase activity, pi3k

Mutant/chimera Details: Wild

Show target details

3

Single protein

17-beta-hydroxysteroid dehydrogenase type 1 (human, Wild)

Synonyms: 17-beta-hsd 1, 17-beta-hydroxysteroid dehydrogenase type 1, 20 alpha-hydroxysteroid dehydrogenase, 20-alpha-hsd, e17ksr, e2dh, edh17b1, edh17b2, edhb17, estradiol 17-beta-dehydrogenase 1, hsd17b1, placental 17-beta-hydroxysteroid dehydrogenase, sdr28c1, short chain dehydrogenase/reductase family 28c member 1

Mutant/chimera Details: Wild

Show target details

Substances - 24 >

Documents - 1 >

Most active substance:

IC50=0.09µM

Substances - 21 >

Documents - 3 >

Most active substance:

Substances - 10 >

Documents - 1 >

Most active substance:

Feedback

Disclaimer: Reaxys interface shown for illustration; actual results may vary. Screenshots may be partial.

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# What users say

*“Reaxys gives us the ability to query and download structures, link them to bioactivity data, and explore structure-activity relationships... Reaxys gives us confidence we won’t miss critical insights.”*

**Dr Christine Richardson**

Principal Scientist, Sygnature Discovery

*“Every chemist should try Reaxys! It’s so simple and intuitive to use. The return of information is so fast; it’s guaranteed to save ... time.”*

**Fabrizio Fabris**

Associate Professor, Dept of Molecular Sciences and Nanosystems at  
Università Ca’Foscari Venezia

*“Reaxys automates bringing data together so our scientists can focus on analysis and making more confident decisions.”*

**Colin Sambrook Smith**

Director of Computational Sciences and Informatics at Sygnature  
Discovery

*“Reaxys helps students to learn how to apply chemical reaction data.”*

**Prof. Keiji Hirose**

Associate Professor at Osaka University

*“Reaxys provides our researchers with rich data and comprehensive perspectives for problem solving, and thus ensures that our synthetic work is based on better solutions.”*

**Rujian Ma**

Vice President of Chemistry at WuXi AppTec

*“Reaxys is, in my opinion, the most complete database that allows a researcher to access the vast corpus of chemistry knowledge quickly and accurately.”*

**Gustavo Pablo Romanelli, Dr.**

GISOE Group Leader at Universidad Nacional de La Plata

**Get started today**

[Register](#) | [Sign in](#)



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