



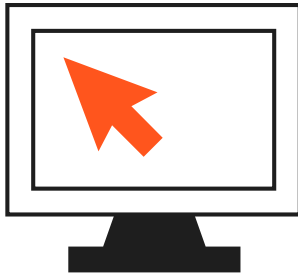
Reference guide



Advancing human progress together

Table of Contents

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



**Welcome
to Reaxys**

**Reaxys core
features**

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**Reaxys resources
and support**

Welcome to Reaxys

Welcome to Reaxys

Accelerate R&D with AI-driven chemistry, unmatched data and advanced tools.

Reaxys empowers faster innovation by combining over a billion chemistry data points with AI. Quickly explore patents, substances, bioactivities and retrosynthesis to drive discoveries in drug development, chemical R&D and academia.

Unlock faster discoveries and actionable insights across industries, including:

- **Industry:** Pharmaceutical, CROs, CDMOs, Chemical and Materials Science, Agrochemicals, Consultancy, IT, Software, Banking and Finance, Manufacturing, among others.
- **Academic and Government:** Leading universities, government, research labs and more.

Trusted data, technology and expertise to support chemistry research



Data



Technology



Expertise



Sign in or log in

Sign in or log in to gain access to the most comprehensive datasets and advanced AI-powered tools.

How to register

- Click Sign In and then Register. Fill out your details.
- Agree to the Terms and click Register.
- To register with Institution [Registration ID](#), visit the Registration ID site, enter your details to link account.

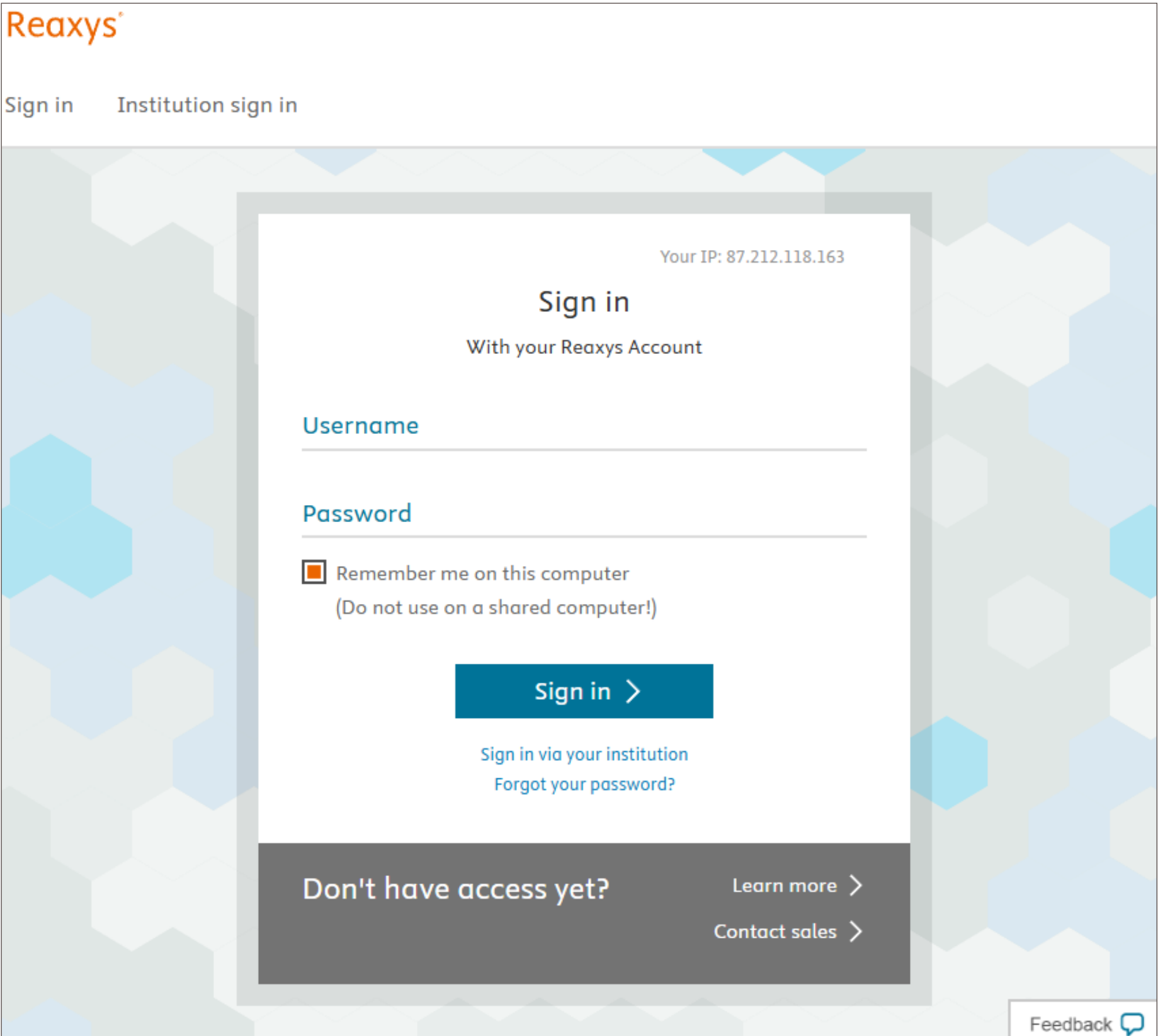


Pro tip: [Sign in or log in](#) to save searches and set alerts.

[Learn more about access.](#)

Registered users can:

- Save searches and set alerts to stay updated on research developments.
- Export results for integration into reports or slides.
- Extend session time to 6h (vs. 30m guests).
- Click the Click the help icon inside [Reaxys.com](#) Resource Center to access Knowledge, Learning, and Support.

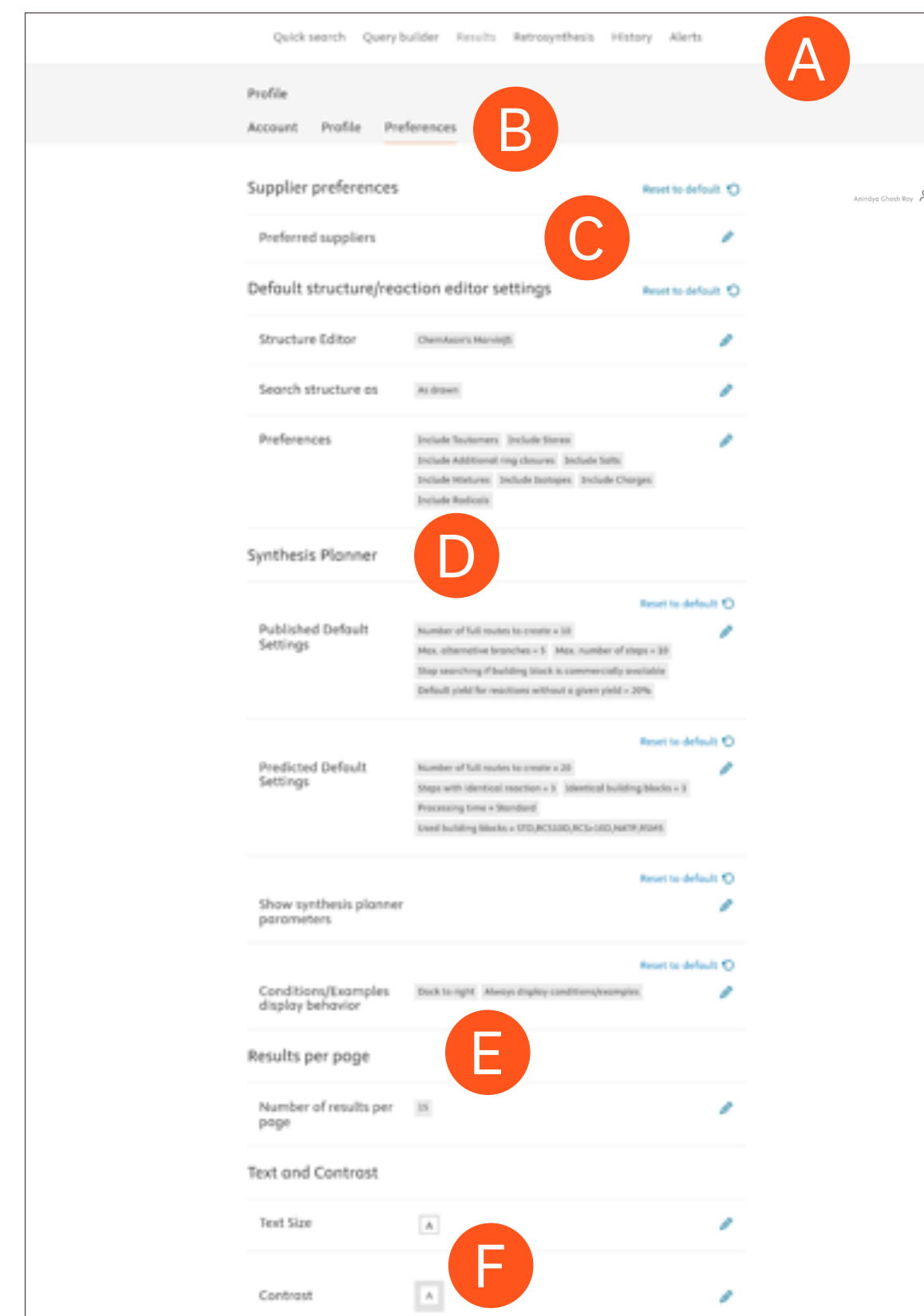


Personal settings

Tailor Reaxys to your scientific workflow. Sign in to customize Reaxys settings, including structure editors, automation, result display and accessibility options.

- 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.
- F.** Adjust text size, contrast and text color for better accessibility.



Pro tip: Optimize Reaxys for your workflow – adjust settings for structure editors, automation steps, and display preferences for enhanced efficiency.



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Homepage tour

Start your search, find key data and accelerate discovery.

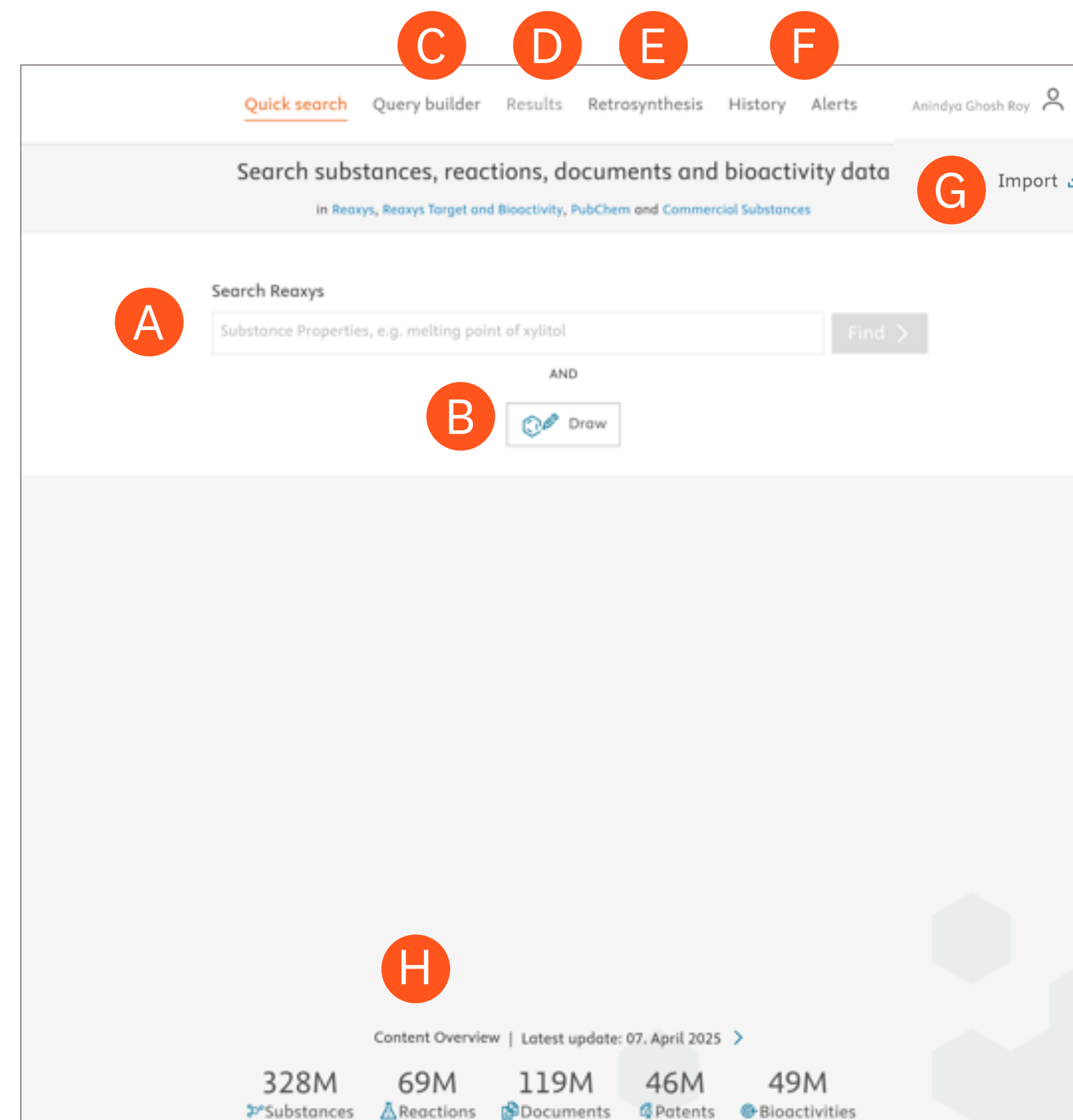
- A. Quick Search:** Find substances, reactions, patents and documents.
- B. Structure Search:** Draw molecules (Marvin JS, ChemDraw JS).
- C. Query Builder:** Build searches with fields, Boolean logic, bioactivity, spectra and patent querylets.

- D. Results:** Review, filter by reaction type, bioactivity, patents and export for analysis.
- E. Retrosynthesis:** Plan synthesis routes with AI.
- F. History/Alerts:** Save searches, research and set alerts.
- G. Import/Integrate Data:** Upload queries or datasets.
- H. Content Overview:** See the latest content numbers.



Pro tip: AI [Predictive Retrosynthesis](#) delivers faster, smarter synthesis routes to help you cut time, reduce costs and accelerate research.

[Contact us](#) to upgrade.

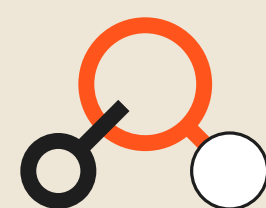


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Reaxys core features

Reaxys core features

Advance discovery, plan synthesis and make confident decisions across industries.



Quick Search

Instantly find substances, reactions, documents, patents and bioactivities.

- Explore experimental data
- Draw molecules
- Filter results

Access validated data for quick insights, enabling fast exploration.



Results

Leverage curated, context-rich data for trusted R&D decisions.

- Analyze experimental data
- Compare structures
- Export and share insights

Analyze SAR, yield, and compound data to inform synthesis routes.



Query Builder

Build precise, multi-dimensional queries for enhanced discovery.

- Combine fields
- Apply filters
- Query properties

Conduct multi-parameter searches for effective design and analysis.



Retrosynthesis

Plan AI-powered and published synthesis routes to accelerate outcomes.

- Plan synthesis
- AI-powered routes
- Reaction pathways

Boost route design with AI-enhanced pathways for efficient synthesis planning.



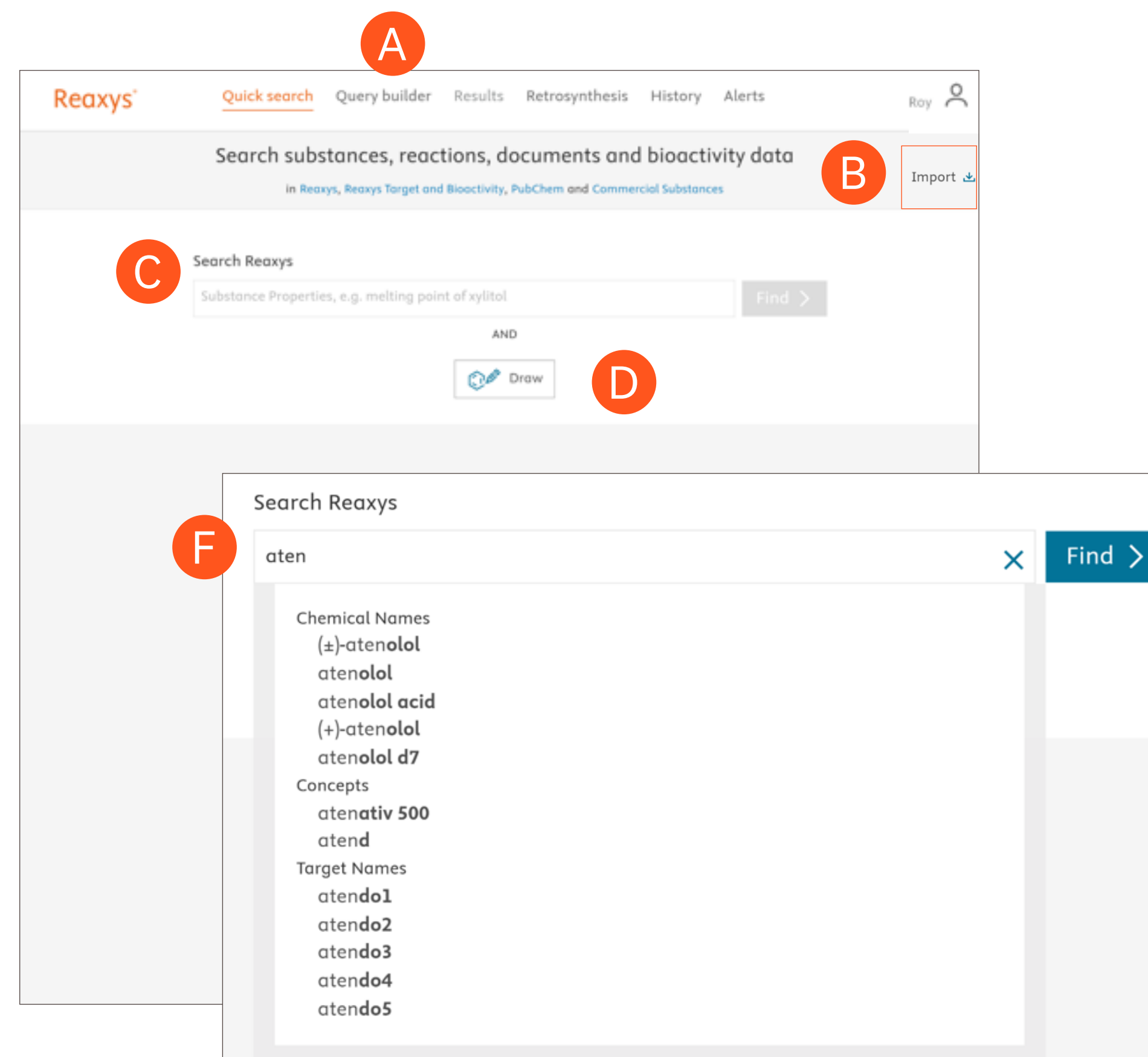
Pro tip: Sign in or sign up to stay updated with the latest [Reaxys releases](#).



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Quick Search

- A. Navigate to Quick Search:** One click from top menu.
- B. Import saved queries:** Reload saved searches.
- C. Enter search terms:** Search by chemical name, reaction, target, patent assignee or author. Auto Suggest recommends terms and synonyms (see F).
- D. Structure-based search:** Use the Draw function to sketch or paste chemical structures. Reaxys supports Marvin JS and ChemDraw JS for intuitive, web-based structure input.
- E. Run your search:** Click Find to retrieve and rank results. Results Preview displays key hits.
- F. Auto-suggest assistance:** AI-powered autosuggestions help you complete search terms, like author names, chemical synonyms and targets, speeding up precise query building.



Pro tip: Combine chemical names and structures to enhance search precision.

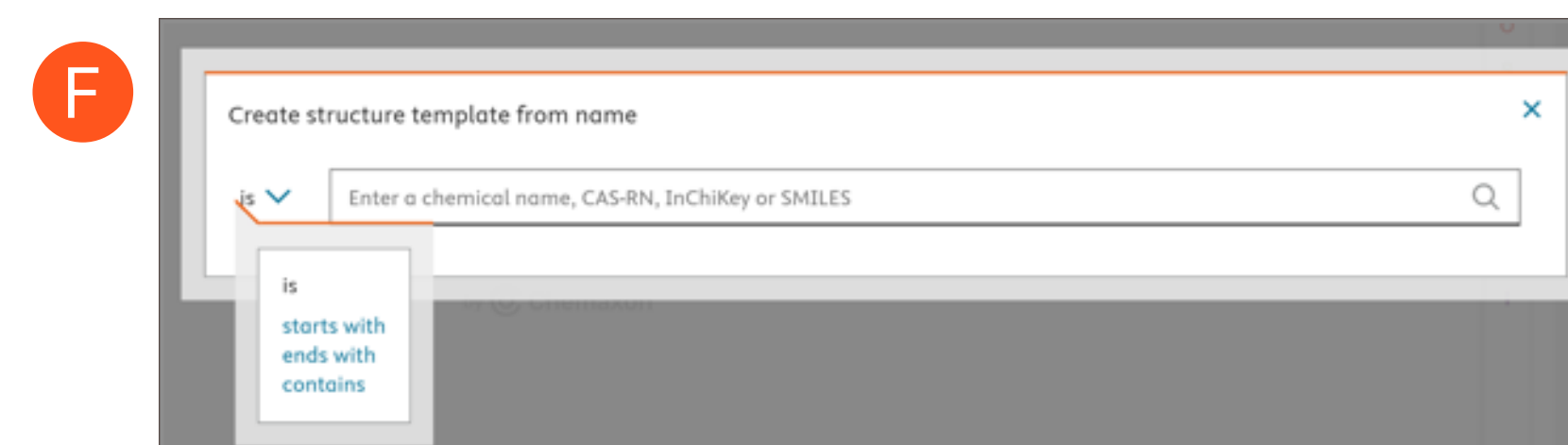
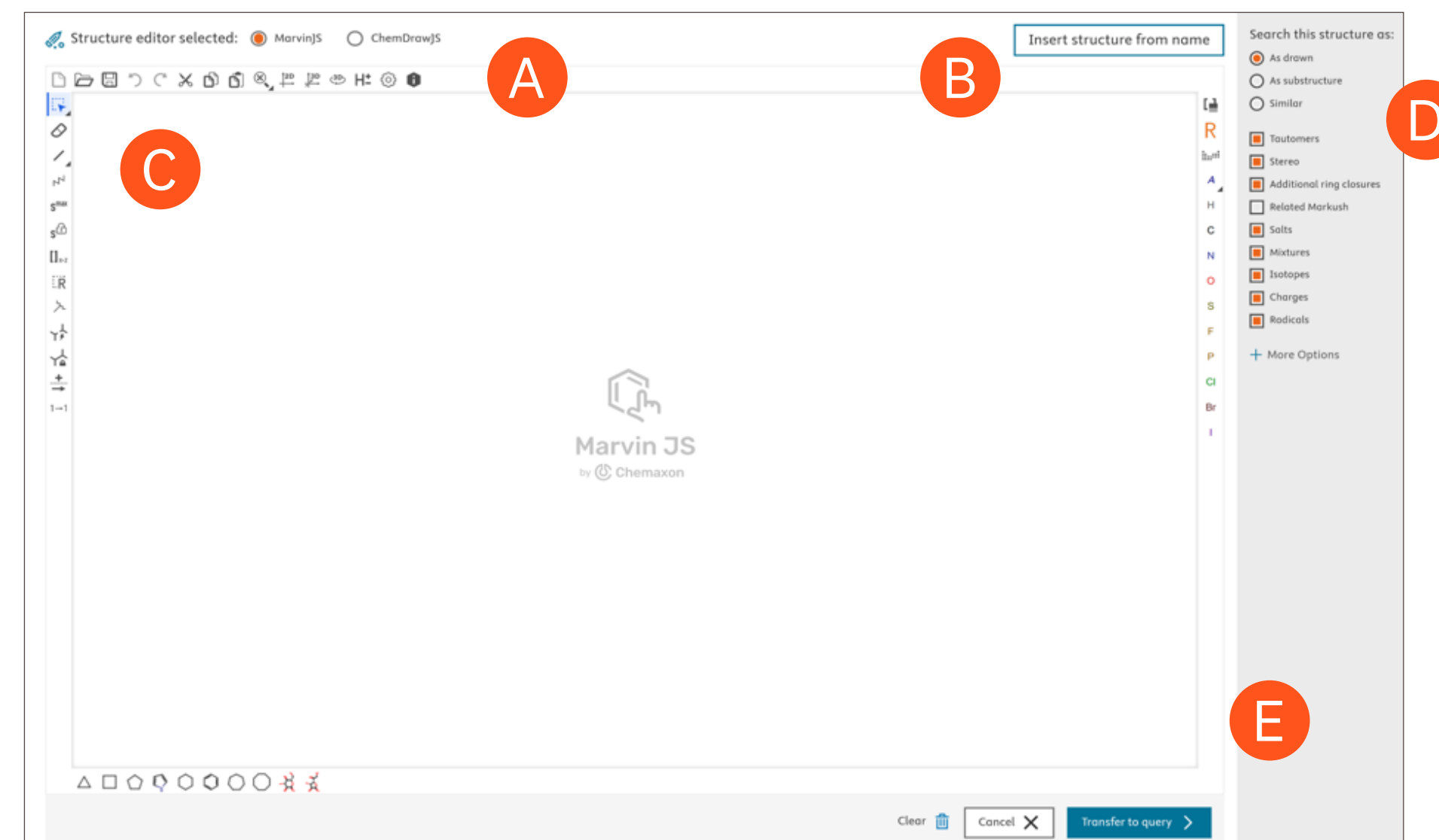
Article: [Learn more about search.](#)



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Quick Search: Structure editors

- 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.



Pro tip: Use Boolean operators (AND, OR, NOT) for complex searches.

[How to create a Structure Drawing in Reaxys.](#)



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Results: Preview

- A. **Search term display:** See your original query – keywords, structure, and filters.

B. **Start new or edit search:** Click New for a fresh search or Edit to modify.

C. **Data overview:** Categorize results across substances, reactions, documents, targets, or suppliers.

D. **Preview key results:** View the top three entries for any data type.

E. **Access full results:** Click View Results for complete results for filtering and further analysis.

F. **Inset:** Preview top hits, and see key properties and structures.
- Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Results for "her2" AND

New Edit

2

Targets

Structure: as drawn

Target(s): her2

Edit in Query Builder

Create Alert

Preview Results

View Results

1

Substances

Structure: as drawn

Target(s): her2

Edit in Query Builder

Create Alert

Preview Results

View Results

11

Documents

Structure: as drawn

Titles, Abstracts, Keywords: "her2"

Preview Results

View Results

149

Reactions

Structure: as drawn

Preview Results

View Results

44,116

Substances

Structure: as drawn

Target(s): her2

Edit in Query Builder

Create Alert

Preview Results

View Results

6

Documents

Structure: as drawn

Titles, Abstracts, Keywords: "her2"

Preview Results

View Results

174,964

Reactions

Structure: as drawn

Preview Results

View Results

2

Suppliers

Structure: as drawn

Preview Results

View Results

44,116

Substances

Target(s): her2

Edit in Query Builder

Create Alert

Preview Results

View Results

Top 3 results

cis-Octadecenoic acid

C17H33CH2CH(CH2)7COOH

282.467 1726542 112-80-1

Identification

Physical Data - 791

Preparations - 158

Druglikeness

Spectra - 206

Reactions - 4,419

Bioactivity (Hit Data)

Other Data - 1,426

Targets - 275

Bioactivity (All)

Documents - 70,708

quercetol

[H]O2C6H2C6H2O(O)(OH)3

302.24 317313 117-39-5

Identification

Physical Data - 1,268

Preparations - 208

Druglikeness

Spectra - 1,936

Reactions - 1,634

Bioactivity (Hit Data)

Other Data - 5,219

Targets - 1,596

Bioactivity (All)

Documents - 67,513

doxorubicin

C27H29NO11

543.527 1445814 2321492-8

Identification

Physical Data - 247

Preparations - 92

Druglikeness

Spectra - 356

Reactions - 514

Bioactivity (Hit Data)

Other Data - 8,932

Targets - 773

Bioactivity (All)

Documents - 59,823
-
- Pro tip:** Use the **Edit in Query Builder** feature to refine your search and highlight key taxonomies for more targeted and accurate results.
- Back to table of contents
- 12

Results:

- A. Navigate categories:** Switch between results types.
- B. Apply filters:** Refine searches using multiple filters like Limit or Exclude.
- C. Export data:** Open the Export dialog for dataset extraction.
- D. Change database scope:** Use the dropdown to switch between Reaxys and other databases.



Pro tip: Use filters strategically to refine results faster. Apply exclusions or limits by reaction type, yield, solvent or even **ultimate patent owner** to surface only the most relevant findings.

Use structure-based tools to identify key properties and synthesis viability before proceeding with lab testing.

- E. Sort results:** Sort results by relevant criteria using *category-specific* options.
- F. Dynamic results filtering:** Each results category has unique options.
- G. Commercial substance availability:** Use the shopping cart icon to check substance availability across suppliers (see inset J).
- H. Structure-based analysis:** Refine synthesis plans and structure details based on drug-likeness properties and real spectra information.
- I. Explore document links:** Access key data excerpts and related result sets.
- J. Inset:** Displays commercial availability across suppliers.
- K. Structure-based analysis:** Options for structure-based refinements and database exploration.

The screenshot displays the Reaxys search results page for 'Atenolol'. The interface is divided into several sections: a left sidebar for filters, a main results table, and a right sidebar for document links. Annotations A-K highlight key features: A (Database scope), B (Filters), C (Export), D (Database dropdown), E (Sort), F (Dynamic filtering), G (Commercial availability), H (Structure-based analysis), I (Document links), J (Commercial availability inset), and K (Structure-based analysis options).

Results: Filter options 1

- 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.

A

Filters

Limit to > Exclude >

By Structure

Draw

Measurement pH

Targets

Substance Classes

Molecular Weight

Filter by value

View more

Reaxys - 158

Commercial Substances - 12

PubChem - 99

0 selected

Limit To

Exclude

Export

Preparations

Search

Sort by No of References

Grid

Bioactivity Visualization

[S]-Atenolol

C₁₄H₁₉N₂O₃

266.34

4234251

93379-545

Identification

Bioactivity [All]

Spectra - 24

Druglikeness

Physical Data - 32

Other Data - 3

[S]-Atenolol

C₁₄H₁₉N₂O₃

266.34

4234250

56715-130

Identification

Bioactivity [All]

Spectra - 13

Druglikeness

Physical Data - 29

Other Data - 5

B

Filters

Limit to > Exclude >

By Structure

Draw

Molecular Weight

Number of Fragments

Availability

Commercial Suppliers

Supplier Preferences

Supplier Geolocation

Usage Classification

Package Size

Price

Purity

Stock Availability

Filter by value

View more

12 Substances

0 selected

Limit To

Exclude

Export

Sort by Commercial Substance ID

Grid

Atenolol

C₁₄H₁₉N₂O₃

266.34

6616

29122-68-7

Identification

Commercial Suppliers - 82

Shipping time: Up to 5 days

Best price: 9 USD/g

Largest available package size: Greater than 10 kg

C

Filters

Limit to > Exclude >

By Structure

Draw

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability

Filter by value

View more

Reaxys - 110

Commercial Substances - 12

PubChem - 99

0 selected

Limit To

Exclude

Export

Hide Conditions

Search

Sort by No of References

Grid

Reaction ID: 5156274

Conditions

Find Similar

Reaction ID: 5156274

With Sulfated tungstate at 70°C; for 0.333333h; Green chemistry;

Experimental Procedure

Stage #1: (S)-1-[(4-carbamoylmethyl)phenoxyl]-2,3-epoxypropane; isopropylamine In N,N-dimethyl-formamide at 60°C; for 12h; Sealed tube;

Stage #2: With water In N,N-dimethyl-formamide at 60°C; for 12h; Solvent; Temperature; Sealed tube; regioselective reaction;

In methanol for 2h; Heating; Yield given;

In methanol at 20°C; for 20h;

82.5%

Lizén, Joseph R.; Mauro-Letts, Gustavo

[Synthesis, 2017, vol. 49, # 6, art. no. 55-2016-M0590-OP, p. 1231 - 1242]

Full Text

Cited 16 times

Details

Abstract

Domle, Subhash V.; Poth, Prashant N.; Salunkhe, Atankrao M.

[Synthetic Communications, 1999, vol. 29, # 10, p. 1639 - 1644]

Full Text

Cited 13 times

Details

Abstract

Akinniyi, Joseph; Perkins, Adrian W.; Storey, Jonathan W.

[Organic Process Research and Development, 1998, vol. 2, # 4, p. 274 - 276]

Full Text

Cited 43 times

Details

Abstract



Pro tip: Sustainability Filters –
Identify **Green Chemistry**
reactions and materials to support
sustainable research.

Results: Filter options 1 (continued)

- D. Target results:** Filter by species, target type, biological parameters and action on target
- E. Document results:** Filter by index terms, patent office and document type. Toggle curated datasets for validated literature.

D

Filters

Limit to > Exclude >

221 Targets out of 79 Documents, 170 Substances, 110 Reactions

Target Species

human 147

rat 128

guinea pig 18

leopard 18

cryptococcus neoformans 11

paraphymonas gingivalis 10

leishmania braziliensis 10

Filter by value View more

Target Type

wild 754

mutated 22

chimera 1

Measurement pK

Ki (inhibition constant) 118

IC50 110

Kcat 95

Qualitative 90

Kcat/Km 80

Inhibition percentage 77

pop (p-h) 54

Filter by value View more

Substance action on target

Document Type

Single protein

2-Oxaldehyde Dehydrogenase (sheep, Wild)

Synonyms: 2-oxaldehyde dehydrogenase

Mutant/chimera Details: Wild

Show target details >

Single protein

5-hydroxytryptamine receptor 1A (rat, Wild)

Synonyms: 5-HT1A, 5-HT1A, 5-hydroxytryptamine receptor 1a, 5HT1a, htr1a, ser

Mutant/chimera Details: Wild

Uniprot: p19327

Show target details >

Single protein

5-hydroxytryptamine receptor 1B (rat, Wild)

Synonyms: 5-HT1b, 5-HT1b, 5-hydroxytryptamine receptor 1b, 5HT1b, htr1b, ser

Mutant/chimera Details: Wild

Uniprot: p78564

E

Filters

Limit to > Exclude >

79 Documents with 170 Substances, 110 Reactions, 221 Targets

Publication Year

Document Type

article 46

patent 11

Authors of Scientific Documents

Current Affiliation

Inventors of Patents

Current Patent Assignee

Patent Office

us 9

wo 1

jp 1

ep 1

de 1

View more

Journal Title

Substance Classes

Reaction Classes

Index Terms (list)

chemical 34

reaction 33

chromatography 33

spectrum 29

kinetics 29

toxicol 28

1

ALKANOLAMINE DERIVATIVES FOR TREATING HYPERTENSION

Current Patent Assignee: ZENECA - US394032, 1976, A

Patent Family Members: IL33911 DO; BE746107 A; IE34003 L; NL7002414 A; DE2007751 A1; ...

Abstract > Claims > Bibliographic Info > Substances > Reactions > Targets > Full Text >

Hit Substances >

2

Enteric coated mixture of 4-[2-hydroxy-3-isopropylamino-propoxy] indole and sodium lauryl sulphate

Current Patent Assignee: BP CHEMICALS - US4291016, 1981, A

Patent Family Members: PT66850 A; IL52587 DO; DK325877 A; BE857122 A; IE45534 L; ...

Abstract > Claims > Bibliographic Info > Substances > Reactions > Full Text >

Hit Substances >

3

Process for preparing novel N-(acyloxy-alkoxy)carbonyl derivatives useful as bioreversible prodrug moieties for primary and secondary amine functions in drugs

Current Patent Assignee: MERCK - US4916230, 1990, A

Patent Family Members: EP167451 A2; JP5611/8747 A; EP167451 A3; US4916230 A; EP167451 B1; ...

Abstract > Claims > Bibliographic Info > Substances > Reactions > Full Text >

Hit Substances >

4

Process for producing optically active atenolol and intermediate thereof

Current Patent Assignee: DAISO - US5130482, 1992, A

Patent Family Members: CA2032098 A1; CA2157938 A1; EP435068 A2; JP4032/7753 A; EP435068 A3; ...

Abstract > Claims > Bibliographic Info > Substances > Reactions > Full Text >

Hit Substances >

5

NOVEL DIASTERIOMERIC SALTS OF ATENOLOL AND THEIR USE IN THE PRODUCTION OF OPTICALLY ACTIVE ATENOLOL

WO2006/46252, 2006, A2

Current Patent Assignee: IPCA LABORATORIES

Office: WO View full patent family >

Abstract > Index Terms > Claims > Bibliographic Info > Substances > Reactions > Full Text >

Hit Substances >

6

No title

Current Patent Assignee: IMPERIAL CHEMICAL INDUSTRIES - DE2007751, 1970, A1[Chem.Abstr., 1970, vol. 73, # 120118]

Patent Family Members: IL33911 DO; BE746107 A; IE34003 L; NL7002414 A; DE2007751 A1; ...

Substances - 6 >

Documents - 1 >

Most active substance:

CC(C)(O)CO

Pro tip: Sustainability Filters – Identify **Green Chemistry** reactions and materials to support **sustainable research**.

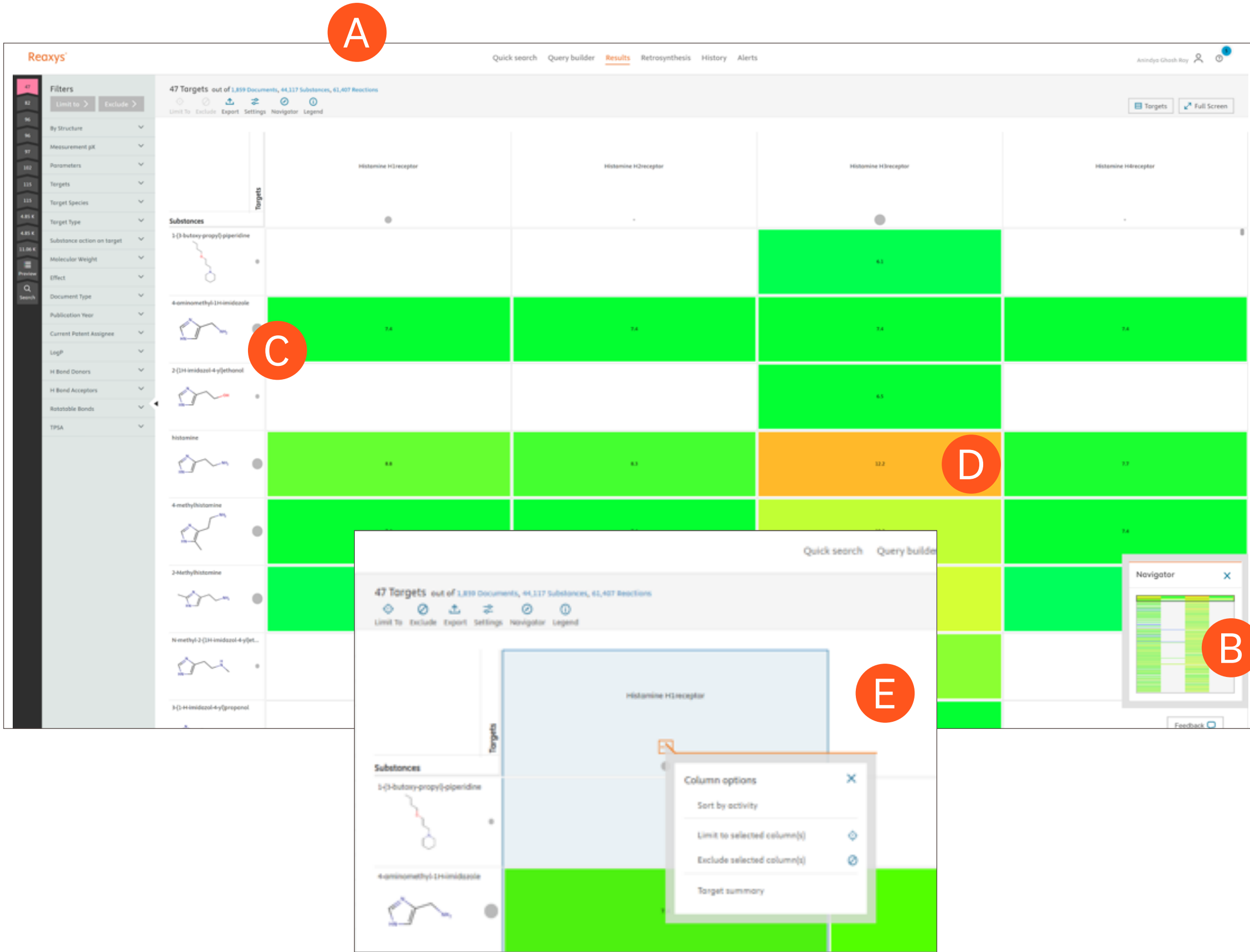
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Results: Bioactivity Visualization

Visualize bioactivity profiles using the **Bioactivity Visualization feature** to assess Structure-Activity Relationships (SAR), compound potency and target selectivity. Powered by normalized **pX values**, the interactive matrix displays bioactivity strength across substances and targets. Use Export, Settings, Navigator and Legend to customize your view and extract data. Export pX values for analysis, sharing or reporting – especially useful for comparing across targets or identifying SAR trends.

- A.** Use Export, Settings, Navigator and Legend to customize your view and extract data. Export pX values for analysis, sharing or reporting – especially useful for comparing across targets or identifying SAR trends.
- B.** Use the Navigator panel (bottom right) to jump to regions of interest in large matrices.
- C.** Hover over substance or target names to reveal structures, synonyms and identifiers.
- D.** Click any cell to unlock detailed bioactivity insightspotency, drug-likeness, target validation and linked literature.
- E.** Customize your visualization map by excluding columns and rows.



Pro tip: Use the *Bioactivity Visualization* to spot SAR inflection points – where small structure changes lead to major shifts in potency.

Learn more: [What is a Bioactivity visualization map?](#)

Results: Create an alert

- A

A. Open alert window: Click Create Alert from *Results Preview* or *History*.

B

B. Define alert name: Enter a name to organize topics (e.g., molecule, competitor, project).

C

C. Add recipients: Your email is auto-added; add others if needed.

D

D. Set frequency/timing: Choose weekly, bi-weekly, monthly or after database updates.

E

E. Set trigger conditions: Trigger alerts on document updates or first appearance. (Optional: exclude alerts with zero results).

F

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

G. Activate alert: Click Create to finalize and receive notifications.



Pro tip: Monitor your competitors – set an alert by **patent assignee** to track new filings from key players in your space.

Create Alert

Query:

Quick Search: "gpcr"

Alert name:

Name

GPCR

Send alerts to:

a.ghoshroy@elsevier.com

X

Frequency:

Every week

▼

on:

Wednesday

▼

Send alert:

Upon first appearance in the database

▼

☐ Do not send alerts with zero results

i

ADVANCED ALERT CONTENT: i

From databases:

☒ Reaxys

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. i

Cancel >

Create >

Results: Manage alerts

- A. Alerts tab:** Click Alerts on the main navigation to view and manage your saved alerts.
- B. Alerts list overview:** 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.
- C. Previous results:** Use results from the dropdown menu to view earlier iterations of an alert – useful for spotting what’s new.
- D. Edit or delete alerts:** Click Edit to update alert frequency or name (query and email settings cannot be changed). Use Delete to permanently remove an alert.

The screenshot shows the 'Alerts' tab in the Reaxys interface. At the top, a navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts' (highlighted with callout A). Below the navigation bar, the 'Alerts' section displays a list of alerts. The first alert, labeled with callout B, is for 'Targets' with the query 'GPCR - in Reaxys' and 'Quick Search: "gpcr"'. It shows 'Results from: No alert results' and has 'Edit' and 'Delete' buttons. The second alert, labeled with callout C, is for 'Documents' with the query 'steroid - in Reaxys' and 'Document Basic Index : "anabolic agents"; "anabolic agents"; "anabolic ...'. It shows 'Results from: Apr 4, 2025' with '2 hits' and a 'Show details' link. Both alerts have 'Edit' and 'Delete' buttons, with the 'Delete' button for the second alert labeled with callout D. A blue arrow button is also present next to the 'Show details' link for the second alert.



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



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Results: Export

- A. **Open export window:** Click Export from the Results page to access export options.

B. **Select format:** Choose the file format (see G), including PDF, Word, Excel, SDfile and others.


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.

G. **Export formats (inset):** Export all results, selected results or a custom selection.



Pro tip: Use **Excel** or **SDfile** formats for modeling and analysis. Reaxys exports up to **500 records per batch** – only the first 500 will be included if more are selected.

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 >

PDF/Print

PDF/Print

XML

Microsoft Word

Microsoft Excel

Tab-delimited text

Electronic Lab Notebook

RD File

SD/Molfile

Smiles

Results: Query history

- A. **History tab:** Click History to access both recent and saved searches.

B. **Recent queries:** Displays queries and actions from your current session.

C. **Saved queries:** Shows queries saved from earlier sessions (see inset E).

D. **Edit and reuse:** Click Edit Query, Save, Alert or View to modify or reuse saved searches.

E. **Saved query options:** Edit, rename or delete queries from the Saved list.

Reaxys

Quick searchQuery builderResultsRetrosynthesisHistoryAlerts

Antindya Ghosh Ray

History

RecentSaved

Reaxys

105 Substances	Today 15:20	Context Switch from: 4 Targets	Edit Query	Save	View	
4 Tgitems	Today 15:12	Filtered by: manually selected items	Edit Query	Save	View	
11064 Tgitems	Today 15:11	Quick Search: "gpcr"	Edit Query	Save	Alert	View
47 Tgitems	Today 15:01	Context Switch from: 82 Targets	Edit Query	Save	View	
82 Tgitems	Today 15:00	Context Switch from: 96 Targets	Edit Query	Save	View	
96 Tgitems	Today 14:59	Context Switch from: 96 Targets	Edit Query	Save	View	
96 Tgitems	Today 14:59	Context Switch from: 97 Targets	Edit Query	Save	View	
97 Tgitems	Today 14:57	Context Switch from: 102 Targets	Edit Query	Save	View	
102 Tgitems	Today 14:56	Context Switch from: 115 Targets	Edit Query	Save	View	
115 Tgitems	Today 14:56	Context Switch from: 115 Targets	Edit Query	Save	View	

History

RecentSaved

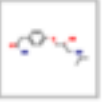
Reaxys

124 Substances

Feb 18 2021

atenolol

Quick Search: "Atenolol" AND



Edit Query

Delete

Rename

Alert

View

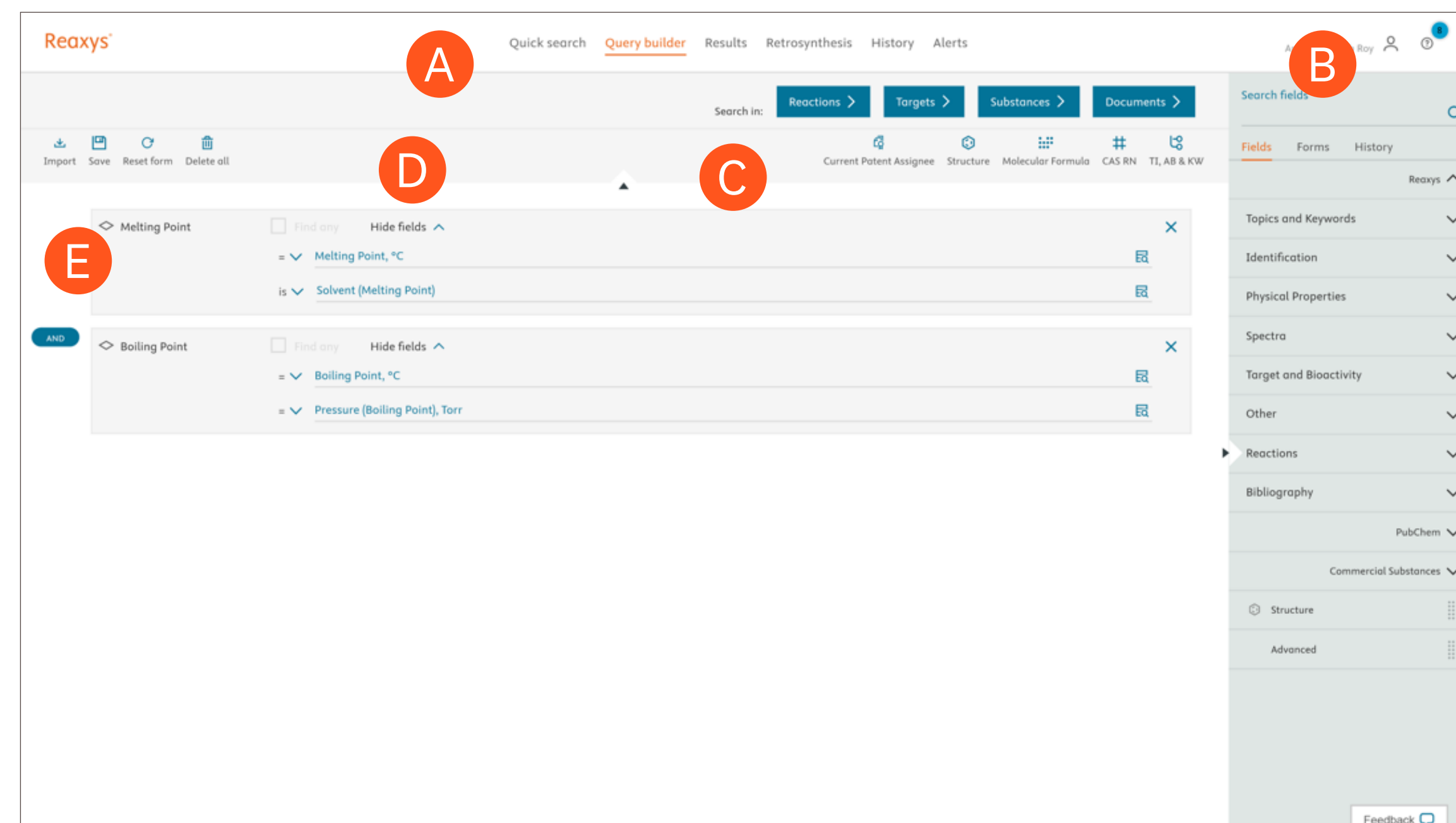


Pro tip: Keep key queries saved for *fast recall* to reduce repetition and improve research efficiency.

Query Builder

- 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:** Use AND, OR and NOT to expand or narrow your query – perfect for refining SAR or patent filters.



Pro tip: Combine *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.




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Query Builder results: Analyze patent ownership

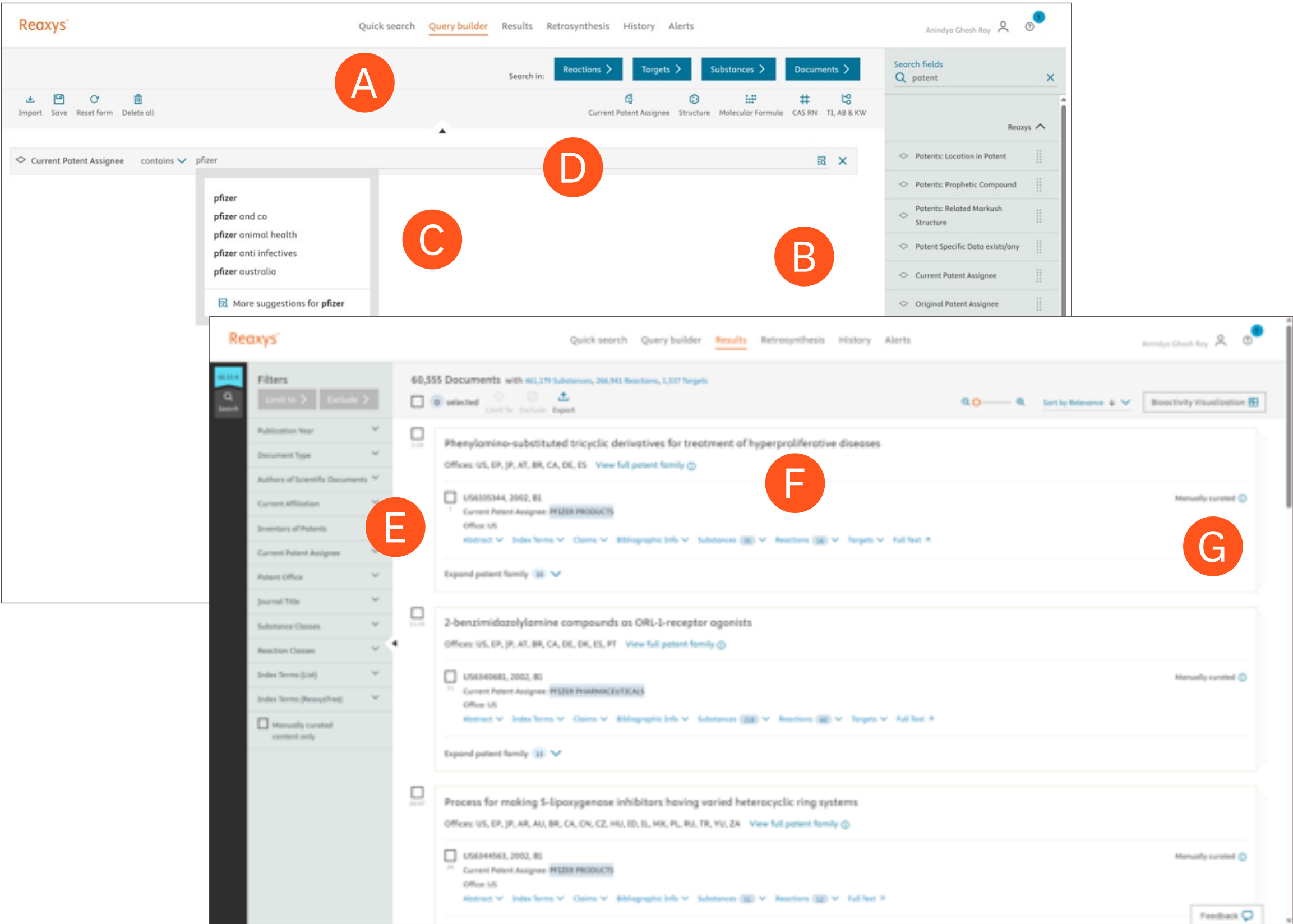
- A. Launch Query Builder** from the main navigation.
- B. Select current patent assignee, original assignee or ultimate owner** (under Bibliography) to focus on ownership data across substances, reactions and documents.
- C. Enter a company or institution name:** Use contains for flexible search. Type 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 the Results page to filter by target, structure or property and identify patent-linked compounds, reactions and 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.



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

Learn more: [Query builder articles](#).



Retrosynthesis: Published

Set up a Retrosynthesis Query

- A. Go to the Retrosynthesis page and draw a compound:** Launch the structure editor to sketch or import your compound of interest.
- B. Define search parameters for published synthesis routes.** Available to all users with a Reaxys account. If your institution has access to the Predictive Retrosynthesis (AI) module, you'll also see the option to select Predicted routes.

- C. Click *synthesize*:** Run the query to generate available retrosynthetic pathways based on your structure.
- D. A Retrosynthesis Project is Added to Your Projects Page:** Sign-in required to save, revisit or track retrosynthesis workflows over time.
- E. Analyze synthesis route:** Review full reaction steps, intermediates and experimental conditions in a structured, interactive view.

The screenshot displays the Reaxys Retrosynthesis interface. At the top, there's a navigation bar with 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. Below this, a chemical structure of a complex molecule is shown in the center. To the right, a 'Parameters' panel allows users to define search criteria: 'Length and depth of routes' (Full routes: 20, Last step only), 'Diversity of routes' (Allow, identical reaction steps per project, identical building blocks per project), 'Processing time' (Standard, Extended), and 'Select Building Block Libraries' (Standard Lab Chemicals (STL), Commercial Substances in 10 days (RCS100), Commercial Substances >10 days (RCS>100), Commercial Substances <510g (RCS510), Natural Products (NATP), Reaxys Starting Materials Occur 3 (RSM3), Reaxys Starting Materials Occur 4 (RSM4), Reaxys Starting Materials Occur 5 (RSM5)).

Below the main interface, a 'Synthesis Projects' table is shown, listing projects with columns for 'No.', 'Date', 'Project name', and 'No. of routes'. The table contains two entries: Project #2765077 (09 Apr 2025) and Project #2271749 (17 Sep 2024). Each entry has a 'Delete' button and a 'View' button. A 'Draw new structure' button is also present.

Red circles with letters A through E are overlaid on the interface to indicate key steps: A points to the 'Retrosynthesis' tab, B points to the 'Parameters' panel, C points to the 'View' button in the project table, D points to the 'Draw new structure' button, and E points to the 'View' button in the project table.



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



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Retrosynthesis: Analyze results

A. Toggle between synthesis routes and reaction steps: Use the navigation buttons to switch between alternative synthesis plans and step-by-step pathways.

B. Review experimental conditions: 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.

Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Anindya Ghosh Roy

Published Route #2

Export Legend

My Synthesis Projects

Draw

Rotate Fit view Copy route

Published route #2

Step 1 Step 2

0 selected View selected

Conditions	Yield	Reference
Stage #1: $C_{15}H_{13}NO_{11}$ With sodium hydroxide In aq. phosphate buffer; water at 37°C; for 1h; pH=8 - 10; Darkness; Stage #2: In aq. phosphate buffer at 25°C; for 5h; pH=6.5; Temperature; pH-value; Time; Darkness; Experimental Procedure	77 %Spectr.	Current Patent Assignee: RESEARCH FOUNDATION OF STATE UNIVERSITY OF NEW YORK MISC - US2021/128592, 2021, A1 Location in patent: Paragraph 0165; 0267-0269; 0274-0277; 0352; 0354-0356 Full Text Details

2 HPLC Assay of Dox Release from DMA Prodrugs 2/4/6 at Different pH Values.

Release of Dox from Dox-DMA 2a/b, Dox-DMA-Glu 4a/b and Dox-DMA-Cys 6a/b were studied at different pH and temperature (25° C. or 37° C.) through monitoring by HPLC condition C (mobile phase at pH 8-9). Various DMA prodrugs of Dox were converted from their corresponding DMI pre-prodrugs (see general procedure of DMI to DMA conversion section above for more details on DMA solution preparations). The pH of the DMA prodrug solution was adjusted to different pH values in the range of pH 7.4-6.0. Then the solution was allowed to sit at rt (25° C.) or placed in an incubator at 37° C. in the dark for up to a few days (the pH did not change significantly during this time). Release of Dox, consumption of DMA prodrug (s.m.) and formation of DMI byproduct were monitored using HPLC condition C (pH 8-9, 480 nm, 5 nmol of s.m. per HPLC run). Representative HPLC traces are shown in ESI FIGS. 524-529 (see these figures and their captions for more detailed information). Areas under the peaks were integrated using the HPLC program LabSolutions Lite to give the percentages reported in FIGS. 24-28.

Feedback



Pro tip: Use *Toggle* and *Fit View* to rapidly compare alternative synthesis routes and evaluate feasibility, yield and conditions for optimal pathway selection.



Back to table of contents

Predictive Retrosynthesis: Synthesis plan

- A. Open the Retrosynthesis** page and draw your compound. Use the structure editor to sketch or import a compound of interest.
- B. Select Predicted Synthesis Route:** Only visible if your institution has access to the *Predictive Retrosynthesis* module.
- C. Adjust parameters:** Customize diversity, speed and building blocks to guide AI output.
- D. Click Synthesize:** Generate AI-predicted synthetic routes based on internal algorithms and published knowledge.
- E. Review in Projects Page:** Compare AI routes with published routes (if available) and refine as needed. Sign-in required to save or revisit.



Pro tip: Use AI-predicted routes when published options hit bottlenecks. Quickly uncover patent-free or novel synthetic routes tailored to your criteria.

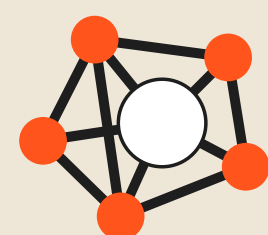
[Contact us](#) to enroll in the Reaxys Predictive Retrosynthesis subscription.

Learn more: [\[Pending AI Guide\]](#)
[\[Iktos Guide\]](#).

Reaxys core content

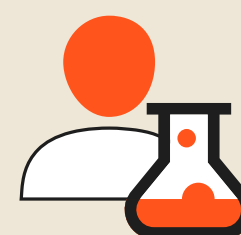
Reaxys core content

Explore the most comprehensive validated chemistry and bioactivity insights.



Substances

Explore hundreds of millions of experimentally validated compounds – with full physicochemical data, commercial availability and supplier sourcing.



Reactions

Access one of the world's largest collections of synthetic reactions – with detailed conditions, catalysts, yields and predictive route planning.



Documents

Search across thousands of journals and reference sources – connecting literature to chemical structures, reactions and bioactivities.



Patents

Mine chemistry-rich patents from global authorities – structured by chemical entities and searchable by reactions, targets and claims.



Pro tip: Sign in or sign up to see the latest [Reaxys content](#) updated numbers.



Bioactivities

Discover tens of millions of curated bioactivity datapoints – mapped to targets, SAR, MoA and therapeutic outcomes.

Substances

Design new molecules with experimentally validated substances.

A. Start with chemical structure or name input.

B. Filter by physicochemical properties (e.g., logP, MW, solubility).

C. Toggle supplier availability for sourcing:

Explore commercial availability across hundreds of global suppliers – directly linked to Reaxys substance records.

D. Explore linked reactions, targets and literature.

E. Export or reuse the curated dataset.



Pro tip: Use Reaxys to find, validate and source compounds – instantly.

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.

The screenshot displays the Reaxys search results page for 'doxorubicin'. The interface is annotated with letters A through E:

- A:** Points to the 'Filters' sidebar on the left, which includes options like 'Limit to', 'Exclude', 'By Structure', 'Measurement pX', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', and 'Number of Fragments'.
- B:** Points to the 'Molecular Weight' filter section in the sidebar.
- C:** Points to the top navigation bar, which includes 'Search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'.
- D:** Points to the 'Results' tab in the top navigation bar.
- E:** Points to the 'Export' button in the top right of the results area.

The main results area shows two entries for doxorubicin and doxorubicin hydrochloride, each with a chemical structure, molecular formula, and various data links (Identification, Bioactivity, Spectra, etc.).




Back to table of contents

Reactions

Plan optimized synthesis routes using experimentally validated reaction.

- A. Draw or import a target molecule.
- B. Open the reactions tab to explore all viable synthetic transformations.
- C. Filter by reagents, catalysts, solvent, yield and temperature.
- D. Rank by reaction yield or experimental conditions.
- E. Export the route or validate with predictive AI tools, grounded in real lab-reported data.



Pro tip: Quickly identify the most viable synthetic pathways using conditions reported in the literature – not just predictions.

Reaxys

Anindya Ghosh Roy

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

1.34 K

4.35 K


Preview

Filters

Limit to >

Exclude >

By Structure



As drawn

Measurement pX

Targets

Parameters

Substance Classes

Reaxys - 4,348

Commercial Substances - 13

PubChem - 417

4,348 Substances

65,577 Documents

1,342 Reactions

961 Targets

Limit To

Exclude

Export

Preparations

No of References

Grid

Bioactivity Visualization

doxorubicin

C₂₇H₂₉NO₁₁

543.527

1445814

23214-92-8

1.34 K

4.35 K

Preview

Search

Filters

Limit to >

Exclude >

By Structure

Yield

Reagent/Catalyst

Solvent

Catalyst Classes

Solvent Classes

Product Availability

Reactant Availability

Reaction Classes

Reaxys - 1,342

Commercial Substances - 13

PubChem - 417

1,342 Reactions

65,577 Documents

4,348 Substances

961 Targets

Limit To

Exclude

Export

Hide Conditions

Reaxys Ranking



26

119

6 Conditions

Find Similar

Reaction ID: 32866602

Yield

Reference

With N-ethyl-N,N-diisopropylamine In N,N-dimethyl-formamide

100%

Current Patent Assignee: TVA ABC - WO/2016/1048-2016

Sort search results

Reaxys Ranking

No of References

Reactant Availability

Product Availability

MW of product

Yield

Publication Year

Documents

Find literature across disciplines with exact compound or reaction mention – not just keywords.

A. Run a structure, substance or keyword search.

B. View documents result.

C. Filter by source type (e.g., journal vs. patent).

D. Access highlighted chemical context in the full-text.

E. Trace back to linked substances, reactions and bioactivity.

F. Export and reuse filtered references for reporting, compliance or formulation insights.

The image displays three overlapping screenshots of the Reaxys web application, illustrating various search and document management features. The top-left screenshot shows the search bar with the text "doxorubicin" and a red circle 'A' highlighting the search input field. The top-right screenshot shows the search results for "doxorubicin", displaying 4,348 substances and 355,378 documents, with a red circle 'B' highlighting the results list. The bottom screenshot shows a detailed view of a patent document titled "METHODS AND COMPOSITIONS FOR SENSITIZING CANCER CELLS TO DRUG-INDUCED APOPTOSIS", with red circles 'C', 'D', 'E', and 'F' highlighting the filters, chemical structure, document details, and the claims section respectively.



Pro tip: Link documents directly to compounds and reactions and skip generic keyword mining to access real experimental insights, faster.




Back to table of contents

Patents

Discover novel compounds, reactions or targets disclosed in global patents.

- A. Enter compound or keyword.
- B. Filter by jurisdiction (e.g., EPO, USPTO).
- C. View mapped reactions or targets.
- D. Export into patent report.



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

Reaxys

Anindya Ghosh Roy

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Search for pd1

Import

Search Reaxys

pd1

Find

AND

Draw

329M

Substances

Remote access

Terms and Conditions

615

42.63 K

57.98 K

Preview

Search

Filters

Limit to

Exclude

Publication Year

Document Type

Authors of Scientific Documents

Current Affiliation

Inventors of Patents

Current Patent Assignee

Patent Office

Journal Title

Substance Classes

Reaction Classes

615 Documents

173,876 Substances

Reactions, 701 Targets

Limit To

Exclude

Export

Relevance

Bioactivity Visualization

Programmed cell death protein receptor-1 targeted molecular probe and preparation

CN112028916, 2020, A

Current Patent Assignee: JIANGSU INSTITUTE OF NUCLEAR MEDICINE

Office: CN

View full patent family

Abstract hit:

{...programmed cell death protein receptor-1 targeted molecular probe and a preparation method and application...}

Claims hit:

{...programmed cell death protein receptor-1, characterized in that it has the structure...}

Index Terms hit:

{...Programmed cell death 1 ligand 1, Programmed cell death protein 1...}

COMPOUNDS AS PD1/PD-L1 INHIBITORS AND METHODS THEREOF

Feedback

Bioactivities

Profile molecular targets and bioactivity outcomes to guide SAR, MoA and pharmacology insights.

- 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. Run your search Click Find to retrieve and rank results. Results Preview displays key hits. AI-powered autosuggestions help you complete search terms, like author names, chemical synonyms and targets, speeding up precise query building.

Reaxys

Anindya Ghosh Roy

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Search for pd1

Import

A

Search Reaxys

pd1

Find

AND

Draw

Reaxys

Anindya Ghosh Roy

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Filters

Limit to

Exclude

Targets

Target Species

Target Type

Measurement pK

Parameters

IC50

Inhibition rate

EC50

IC50 (tumor growth inhibition rate)

Tumor volume decrease

Increase rate

tested

32 Targets

335 Documents, 15,345 Substances, 34,135 Reactions

0

Limit to

Exclude

Export

Sort alphabetically A-Z

Bioactivity Visualization

1

Single protein

Arogenate dehydratase 3, chloroplastic (Wild)

Synonyms: odt3, arogenate dehydratase 3, chloroplastic, atpdt1, pd1, pdt1, prephenate dehydratase 1

Mutant/chimera Details: Wild

Show target details

2

Protein complex - 2

Hemagglutinin [Influenza B virus] (Chin

Synonyms: hemagglutinin

Reaxys

Anindya Ghosh Roy

Quick search

Query builder

Results

Retrosynthesis

History

Alerts

Filters

Limit to

Exclude

Targets

Target Species

Target Type

Measurement pK

Parameters

Substance action on target

Document Type

Publication Year

Current Patent Assignee

14 Targets

220 Documents, 13,604 Substances, 26,210 Reactions

0

Limit to

Exclude

Export

Sort alphabetically A-Z

Bioactivity Visualization

1

Single protein

Programmed cell death protein 1 (Wild)

Synonyms: cd279, hpd-1, mpd-1, pd1, pdcd1, programmed cell death protein 1, protein pd-1

Mutant/chimera Details: Wild

Show target details

Substances - 4318

Documents - 94

Most active substance:

IC50=0.032nM

2

Protein complex - 2

Programmed cell death protein 1 (Wild)

Synonyms: cd279, hpd-1, mpd-1, pd1, pdcd1, programmed cell

Most active substance:

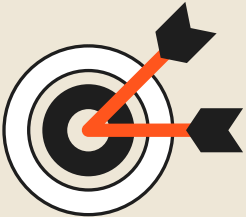
Feedback

Pro tip: Watch Target & Bioactivity expert tips.

Reaxys resources and support


Reaxys resources and support

Learn, build knowledge, gain insights, stay updated on product advancements and connect with peers through community events.




Learning

Watch tutorials, register for courses and webinars and access how-to guides.



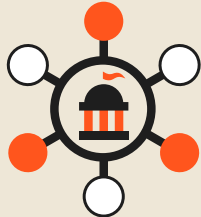
Knowledge

Fast-track your knowledge with scientific articles, webinars, videos and tips from experts.




Product

Read reference documentation for API, browse solutions and manuals, see the latest releases and contact support.



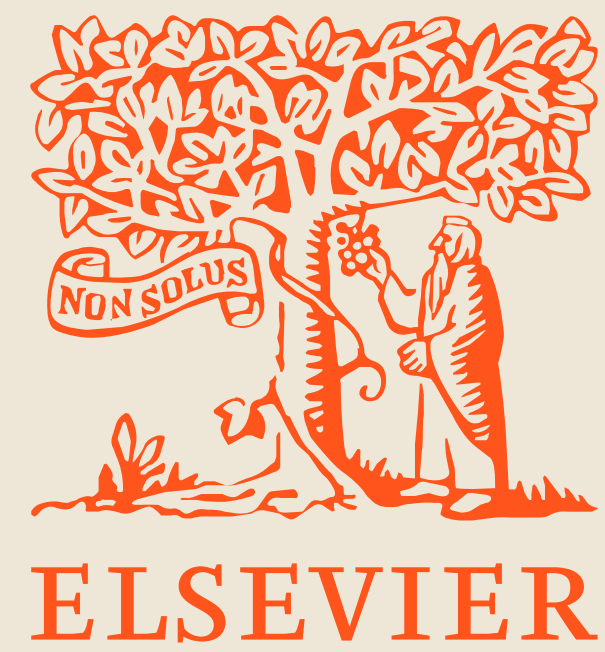
Community

Learn how real customers use Reaxys for their business. Participate in Reaxys events and connect with your peers.



Need more help?

See [Reaxys Resources](#) or [Contact us](#).



Advancing human progress together