



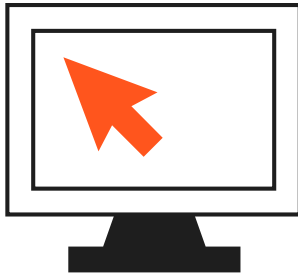
Reference guide



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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Welcome to Reaxys

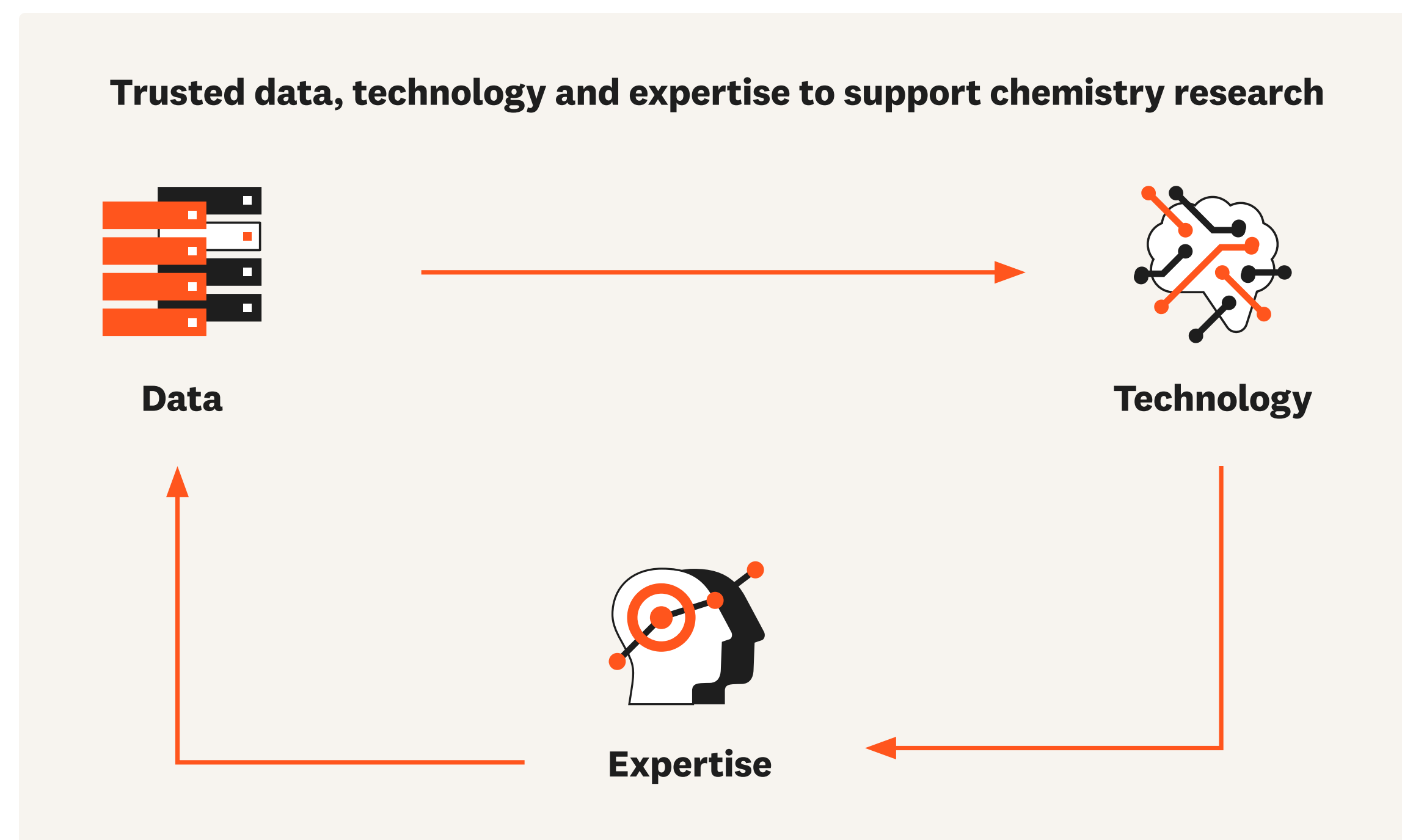
Welcome to Reaxys

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.



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.

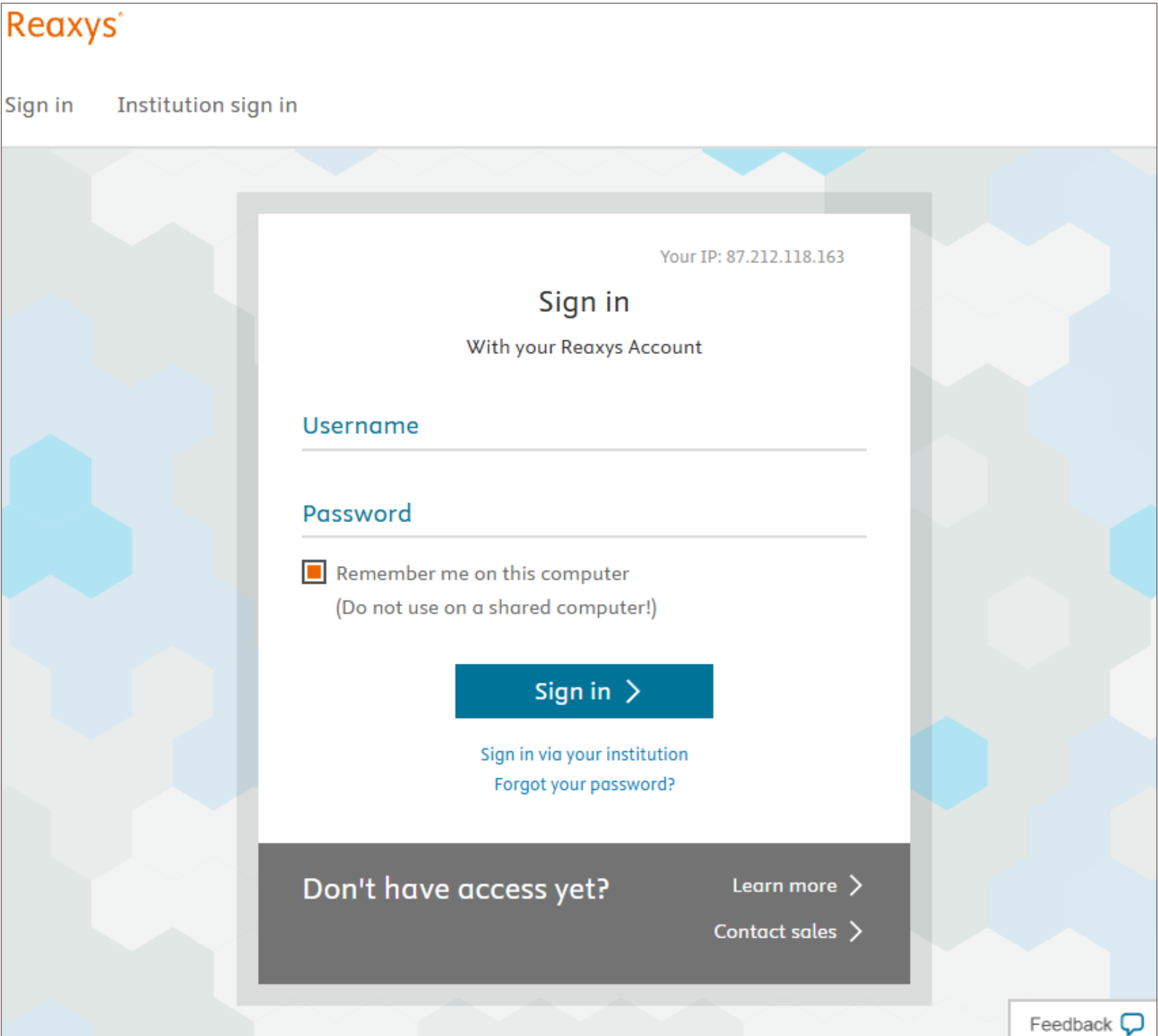


Pro tip: [Sign in or log in](#) to save searches and set alerts.

[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.

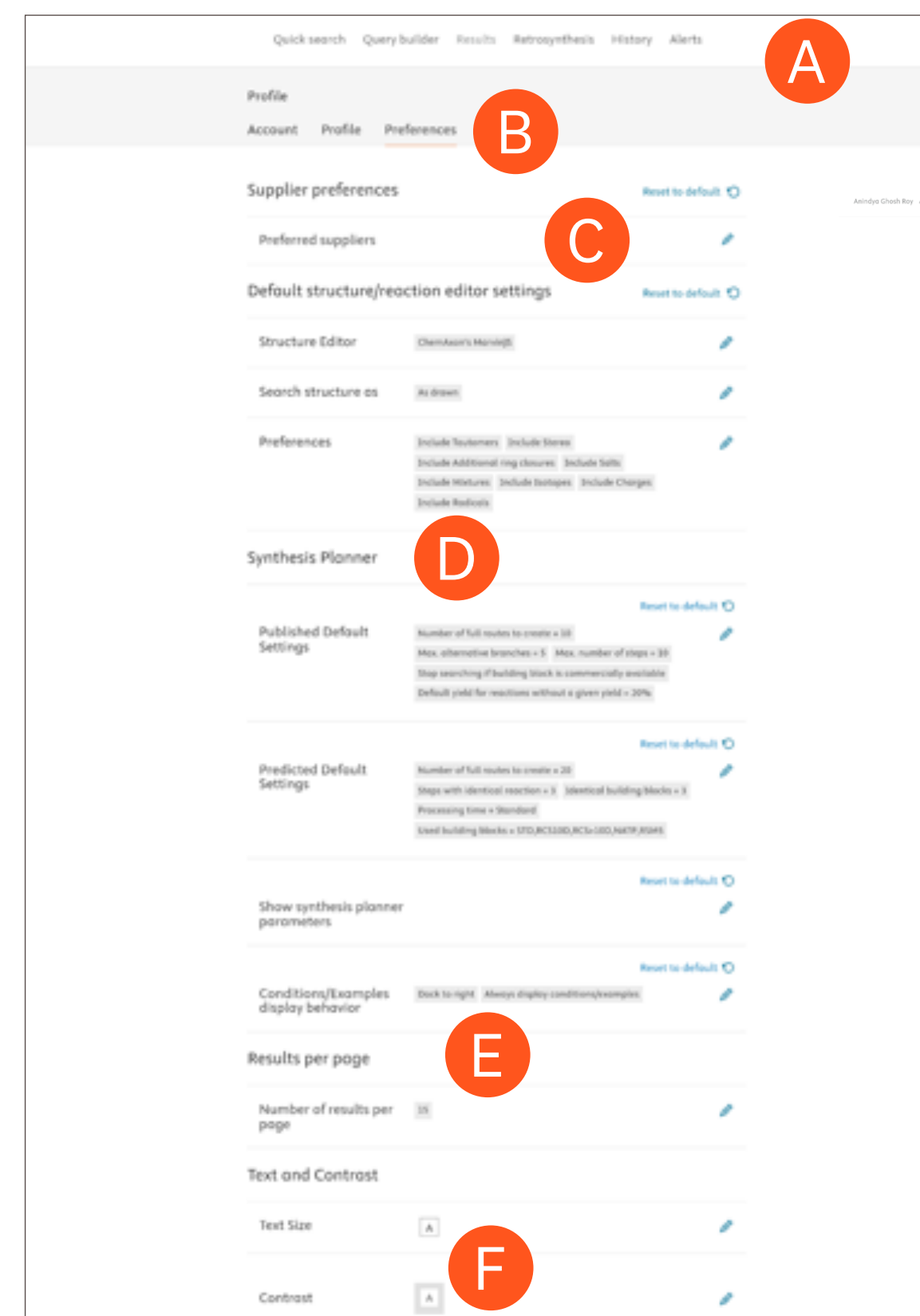


Personal settings

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.

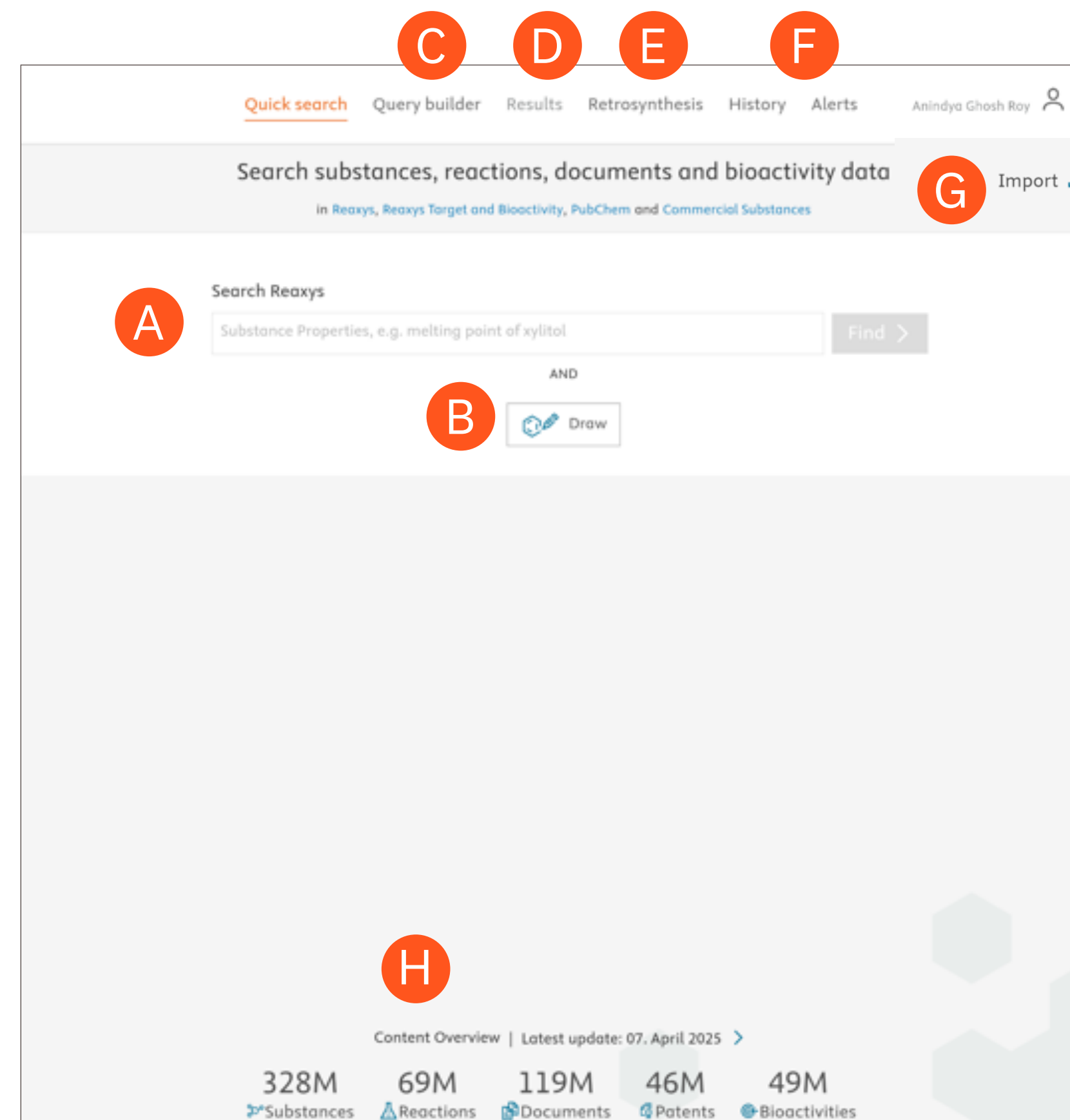
- A. Quick Search:** Find substances, reactions, patents and documents.
- B. Structure Search:** Draw molecules (Marvin JS, ChemDraw JS).
- C. Query Builder:** Build searches with fields, Boolean logic, bioactivity, spectra and patent querylets.

- 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.

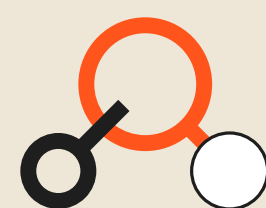


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Reaxys core features

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

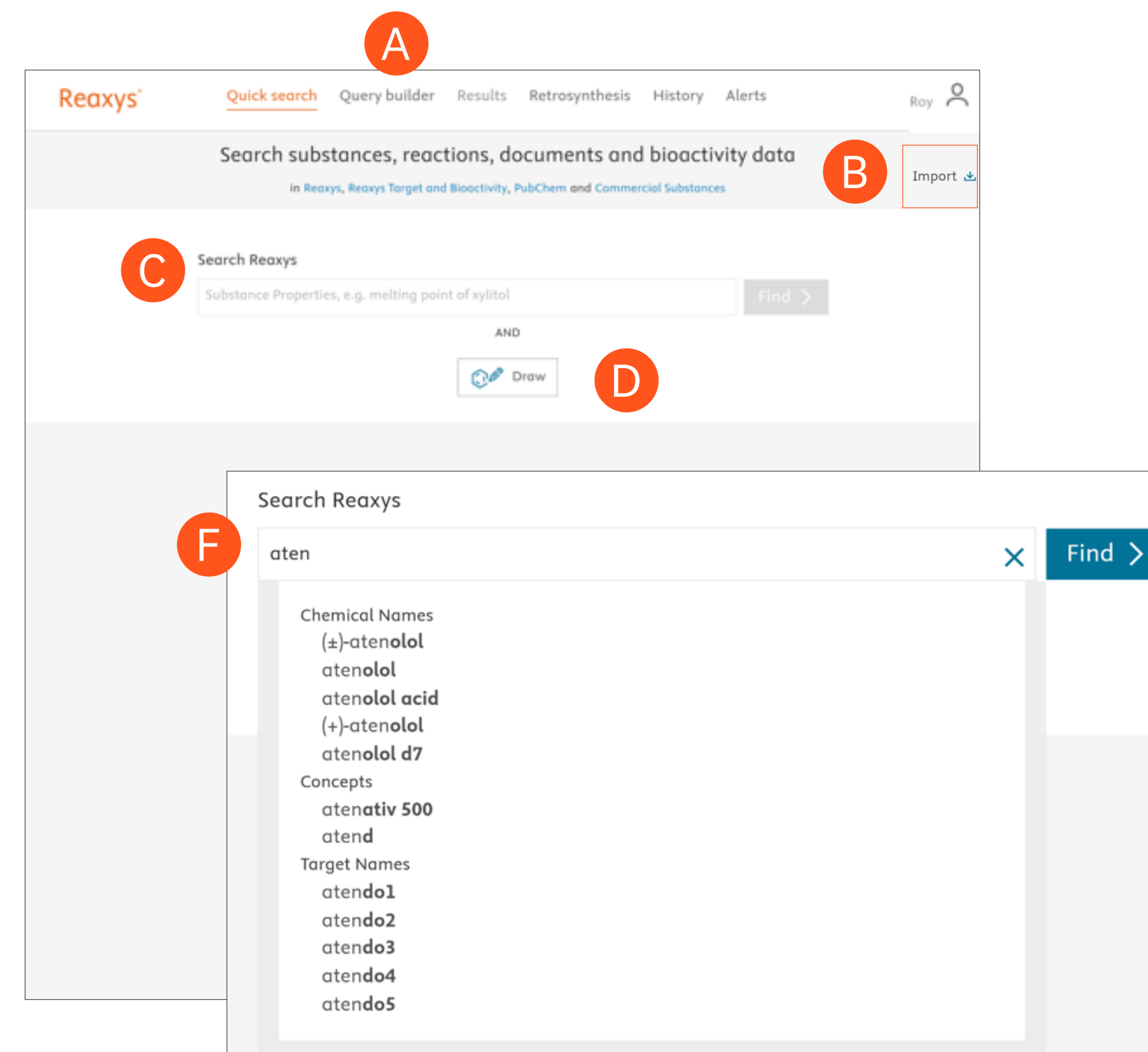
Boost route design with AI-enhanced pathways for efficient synthesis planning.



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

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.

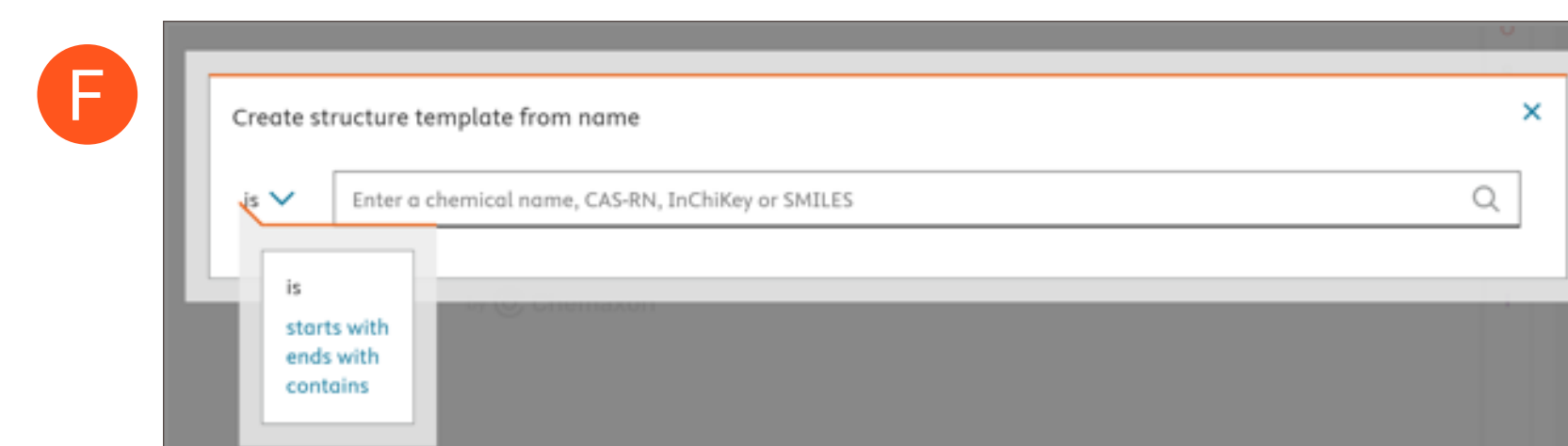
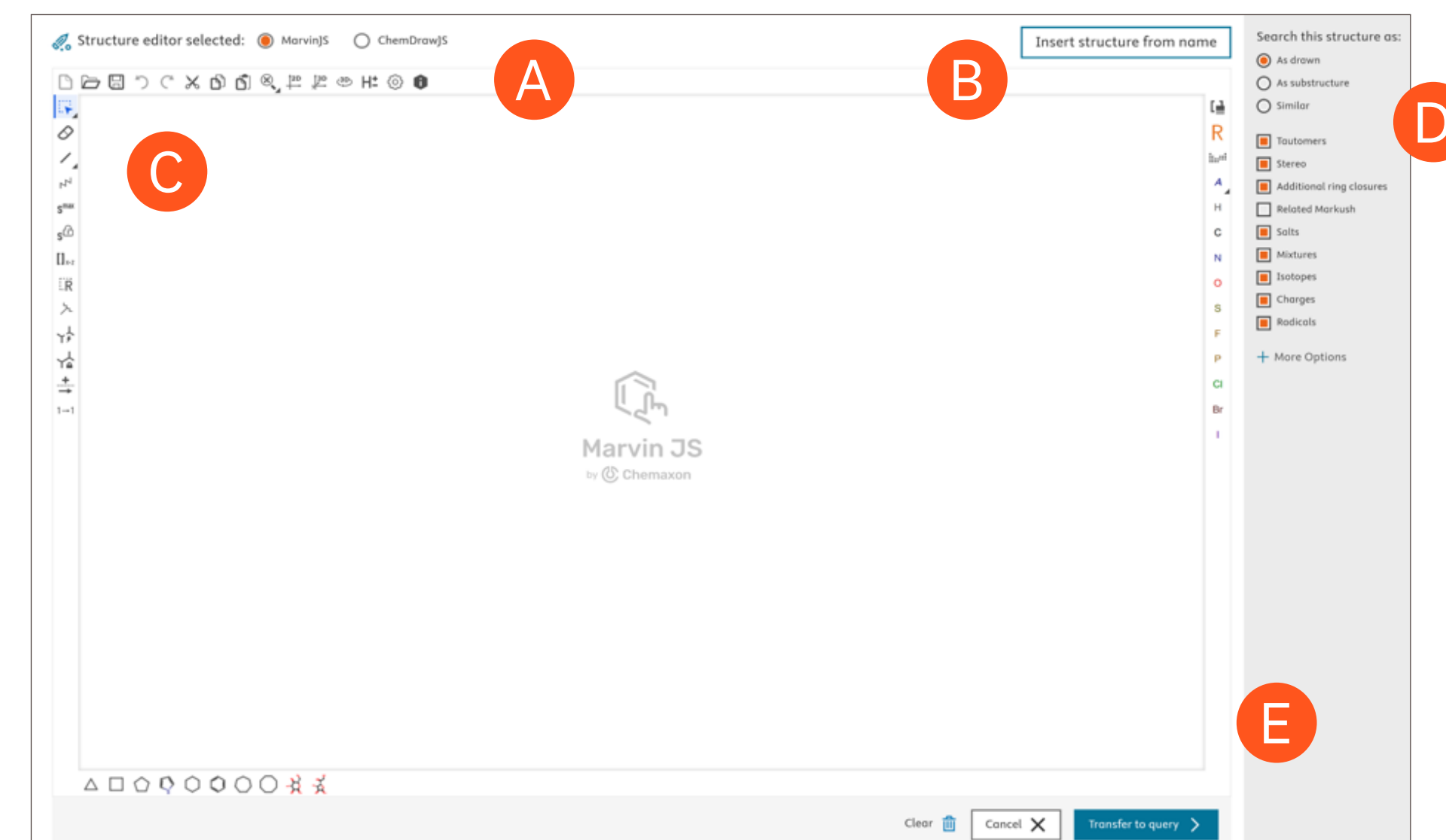
Article: [Learn more about search.](#)



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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.

The screenshot displays the Reaxys search results interface for the query "her2" AND [structure]. The interface is divided into several sections:

- Search Term Display (A):** The top navigation bar shows the search query "her2" AND [structure].
- Start new or edit search (B):** The top right corner contains buttons for "New" and "Edit".
- Data Overview (C):** The left sidebar shows a categorized list of results: 2 Targets, 1 Substances, 11 Documents, 149 Reactions, 44,116 Suppliers, 6 Other, 174,964 Documents, and 2 Suppliers.
- Preview key results (D):** The main content area displays the top three results for each category: Targets, Substances, and Documents. Each result entry includes a colored icon, a count, the category name, and a "View Results" button.
- Access full results (E):** The "View Results" buttons provide access to the complete results for each category.
- Inset (F):** An inset window shows the "Top 3 results" for the "Substances" category, listing "cis-Octadecenoic acid", "quercetol", and "daxorubicin" with their chemical structures and key properties.



Pro tip: Use the **Edit in Query Builder** feature to refine your search and highlight key taxonomies for more targeted and accurate results.



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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.

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

selected

Limit To

Exclude

Export

Preparations

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

[+]-[R]-atenolol

C14H19N2O3

266.34

4234250

56715-130

Identification

Bioactivity [All]

Spectra - 13

Druglikeness

Physical Data - 29

Other Data - 5

110 Reactions out of 79 Documents, containing 176 Substances, 221 Targets

selected

Limit To

Exclude

Export

Hide Conditions

Conditions

Find Similar

Reaction ID: S156274

With Sulfated tungstate at 70°C; for 0.33333h; Green chemistry; Experimental Procedure

Stage #1: (S)-1-[p-(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; Experimental Procedure

In methanol for 2h; Heating; Yield given;

In methanol at 20°C; for 20h;

82.5%

Lizén, Joseph R.; Mauro-Letts, Gustavo [Synthesis, 2012, vol. 49, # 6, art. no. 55-2016-M0090-OP, p. 1231 - 1242] Full Text Cited 16 times Details Abstract

Dominic, Subhash V.; Pothl, Prashant N.; Subramanian, Anandkiran 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

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

Commercial Suppliers

Product

Purity

Package size & price

Availability

Hangzhou APIChem Technology Co., Ltd. [29122-68-7 AC-8245] 100 g upon inquiry Last updated: 2025-03-14

Hangzhou APIChem Technology Co., Ltd. [29122-68-7 AC-8245] 25 g upon inquiry Last updated: 2025-03-14

Hangzhou APIChem Technology Co., Ltd. [29122-68-7 AC-8245] 5 g upon inquiry Last updated: 2025-03-14

GLSyntech, LLC USA [29122-68-7 C-6444-2] 98% upon inquiry upon inquiry Stock availability: in stock Shipping Time Up to 10 days Last updated: 2025-03-12

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

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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

selected

Limit To

Exclude

Export

Sort by Sort alphabetically A-Z

Bioactivity Visualization

Target Species

human 147

rat 128

guinea pig 18

leopard 18

cryptococcus neoformans 11

paraphimomas gingivitis 10

Reveria bidensis 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

papp (s-1) 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

selected

Limit To

Exclude

Export

Sort by Relevance

Bioactivity Visualization

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

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

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

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

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

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

No title

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

Patent Family Members: IT 33911 DO; BE746107 A; IF 46081 I; NL 7002414 A; DE2007751 A1; ...

Manually curated

Feedback

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

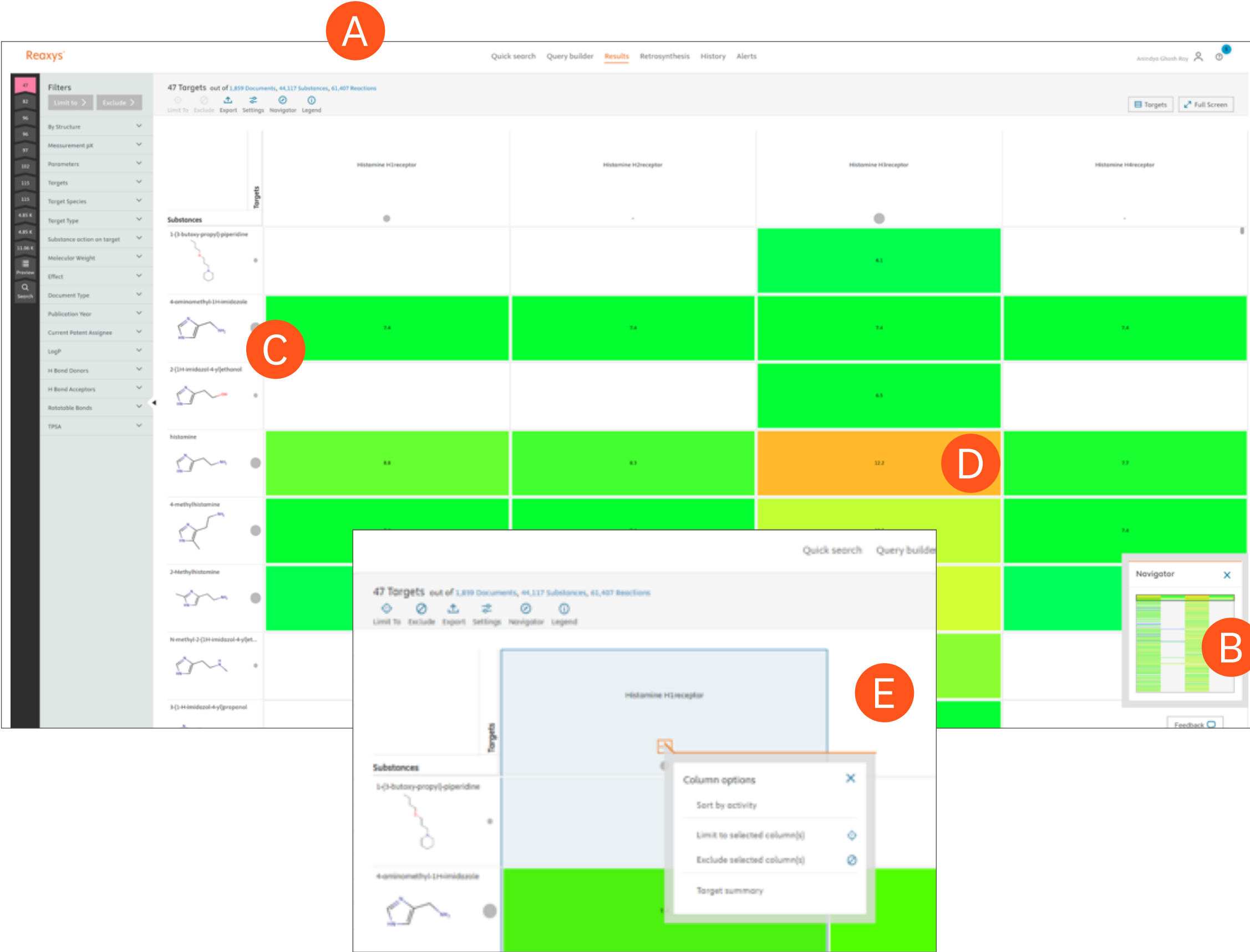
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Results: Bioactivity Visualization

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. Open alert window:** Click Create Alert from *Results Preview* or *History*.
- B. Define alert name:** Enter a 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.



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

The screenshot shows the 'Create Alert' dialog box with the following fields and options:

- Query:** Quick Search: "gpcr"
- Alert name:** GPCR
- Send alerts to:** a.ghoshroy@elsevier.com
- Frequency:** Every week, on: Wednesday
- Send alert:** Upon first appearance in the database
- ☐ Do not send alerts with zero results
- ADVANCED ALERT CONTENT:**
 - From databases:** ☒ Reaxys
 - Include in email:**
 - ☐ Title and bibliographic information
 - ☒ Abstract
 - ☐ Full abstract
 - ☒ Partial abstract
 - ☒ Hit details (keywords, substances, reactions or targets)

At the bottom, there is a note: "Email alerts will produce an email with a maximum of 99 records." and two buttons: "Cancel" and "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, 'Targets', is titled 'GPCR - in Reaxys' and 'Quick Search: "gpcr"', with a creation date of 'Since Apr 9, 2025'. It shows 'Results from: No alert results' and has 'Edit' and 'Delete' buttons (callout B). The second alert, 'Documents', is titled 'steroid - in Reaxys' and 'Document Basic Index : "anabolic agents"; "anabolic agents"; "anabolic ..."', also with a creation date of 'Since Apr 9, 2025'. It shows 'Results from: Apr 4, 2025' with '2 hits' and a 'Show details' link (callout C). Both alerts have 'Edit' and 'Delete' buttons (callout D).



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

i

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

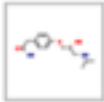
Reaxys

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.

The screenshot displays the Reaxys Query Builder interface. At the top, the 'Query builder' tab is selected in the navigation bar (callout A). Below the navigation bar, a search bar and several filter buttons (Reactions, Targets, Substances, Documents) are visible (callout C). On the left, a sidebar contains icons for Import, Save, Reset form, and Delete all (callout D). The main area shows two query conditions: 'Melting Point' and 'Boiling Point', each with a 'Find any' checkbox and a 'Hide fields' dropdown (callout E). The 'Boiling Point' condition is expanded, showing sub-conditions like 'Boiling Point, °C' and 'Pressure (Boiling Point), Torr'. On the right, a sidebar lists various search fields such as Topics and Keywords, Identification, Physical Properties, Spectra, Target and Bioactivity, Other, Reactions, Bibliography, PubChem, Commercial Substances, Structure, and Advanced (callout B). A 'Feedback' button is located at the bottom right of the sidebar.



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.

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](#).
- Reaxys

Quick search Query builder Results Retrosynthesis History Alerts

Anindya Ghosh Ray

Search in: Reactions Targets Substances Documents

Import Save Reset form Delete all

Current Patent Assignee Structure Molecular Formula CAS RN TL AB & KW

Search fields patent

Current Patent Assignee contains pfizer

pfizer
pfizer and co
pfizer animal health
pfizer anti-infectives
pfizer australia
More suggestions for pfizer

60,555 Documents with 461,179 Substances, 268,341 Reactions, 1,107 Targets

selected

Sort by Relevance

Bioreactivity Visualization

Phenylamino-substituted tricyclic derivatives for treatment of hyperproliferative diseases

Offices: US, EP, JP, AT, BR, CA, DE, ES View full patent family

US6390344, 2002, B1

Current Patent Assignee: PFIZER PRODUCTS

Office: US

Abstract Index Terms Claims Bibliographic Info Substances Reactions Targets Full Text

Expand patent family

Manually curated

2-benzimidazolylamine compounds as OIR-1-receptor agonists

Offices: US, EP, JP, AT, BR, CA, DE, DK, ES, PT View full patent family

US6340681, 2002, B0

Current Patent Assignee: PFIZER PHARMACEUTICALS

Office: US

Abstract Index Terms Claims Bibliographic Info Substances Reactions Targets Full Text

Expand patent family

Manually curated

Process for making 5-lipoxygenase inhibitors having varied heterocyclic ring systems

Offices: US, EP, JP, AR, AU, BR, CA, CN, CZ, HK, ID, IL, MX, PL, RU, TR, YU, ZA View full patent family

US6344563, 2002, B0

Current Patent Assignee: PFIZER PRODUCTS

Office: US

Abstract Index Terms Claims Bibliographic Info Substances Reactions Targets Full Text

Expand patent family

Manually curated

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 'Structure editor' is active, showing a chemical structure of a complex molecule. To the right of the editor is a 'Parameters' panel with various settings: 'Predicted' (checked), 'Length and depth of routes' (Full routes: 20, Last step only), 'Diversity of routes' (Allow, identical reaction steps per project: 3, identical building blocks per project: 3), '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 <500g (RCS500), Natural Products (NATP), Reaxys Starting Materials Occur 3 (RSM3), Reaxys Starting Materials Occur 4 (RSM4), Reaxys Starting Materials Occur 5 (RSM5)).

Below the main editor is a 'Synthesis Projects' table with columns: 'No.', 'Date', 'Project name', and 'No. of routes'. It lists two projects: 'Project #2765077' (09 Apr 2025) and 'Project #2271749' (17 Sep 2024). Each project has a 'Delete' button and a 'View' button. To the right of the table is a 'Feedback' section with 'Predicted' and 'Published' buttons, each with a 'View' button and a 'Feedback' button.



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.



Back to table of contents

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 Project #2765077 My Synthesis Projects Draw

Export Legend 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. S24-S29 (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.

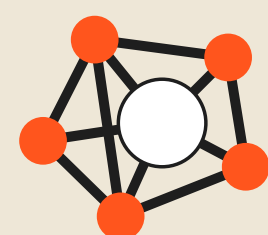
[Contact us](#) to enroll in the Reaxys Predictive Retrosynthesis subscription.

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

Reaxys core content

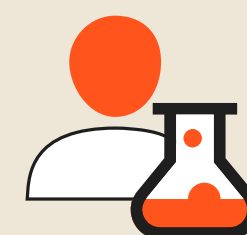
Reaxys core content

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 divided into several sections:

- Filters (A):** A sidebar on the left containing various filter categories such as 'By Structure', 'Measurement pX', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', and 'Number of Fragments'.
- Search Bar (C):** Located at the top, it includes the 'Reaxys' logo and a search input field.
- Results Summary (D):** A horizontal bar at the top of the main content area showing the number of results found (4,348 Substances) and the number of documents (65,577 Documents).
- Chemical Structure (E):** A large chemical structure of doxorubicin is displayed in the center, with a molecular weight of 543.527 and a molecular formula of C₂₇H₂₉NO₁₁.
- Data Links:** To the right of the structure, there are links to various data sources: 'Identification', 'Bioactivity (All)', 'Spectra - 356', 'Preparations - 92', 'Reactions - 514', 'Targets - 773', and 'Documents - 59,847'.
- Additional Results:** Below the main structure, there is a section for 'doxorubicin hydrochloride' with its own chemical structure and associated data links.

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

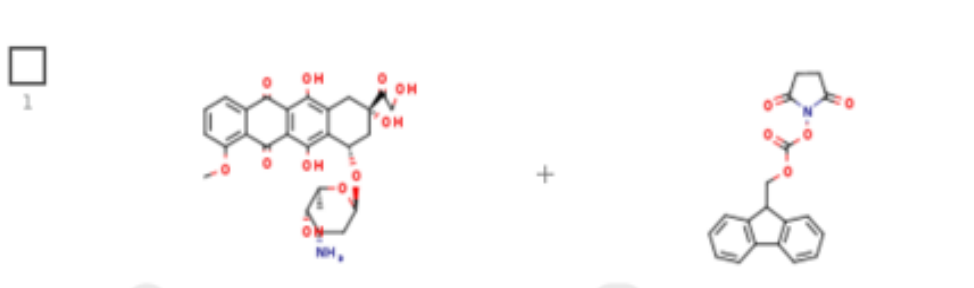
Limit To

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 collage illustrates the Reaxys interface for document search and analysis. It shows the search bar (A), the search results page (B), the filters sidebar (C), and the detailed view of a patent document (E) with a 'Claims hit' section (D) containing chemical structures and text. A 'Feedback' button is visible in the bottom-right corner of the patent view.



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

Index Terms

Claims

Bibliographic Info

Substances

Reactions

Full Text

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

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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

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

Limit to

Exclude

Targets

Target Species

Target Type

Measurement pK

Parameters

ic50

inhibition rate

ec50

tgi (tumor growth inhibition rate)

tumor volume decrease

increase rate

tested

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

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

Limit to

Exclude

Targets

Target Species

Target Type

Measurement pK

Parameters

Substance action on target

Document Type

Publication Year

Current Patent Assignee

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

2

Protein complex - 2

Programmed cell death protein 1 (Wild)

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

Most active substance:

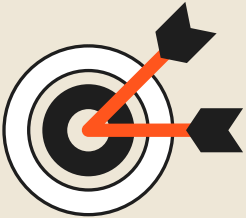
IC50=0.032nM

Pro tip: Watch Target & Bioactivity expert tips.

Reaxys resources and support

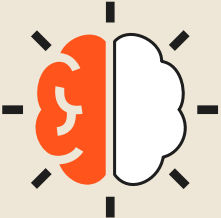
Reaxys resources and support

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.



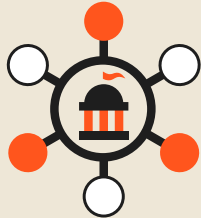
Knowledge

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.



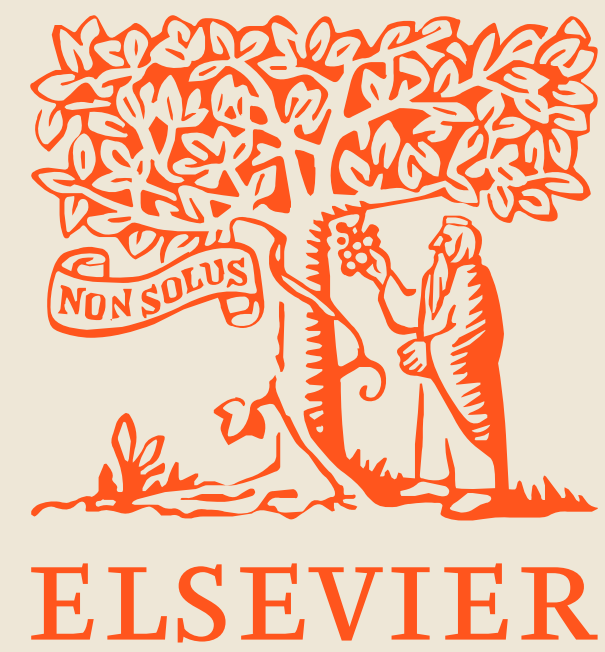
Community

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