Reaxys

Reference guide

ELSEVIER

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

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

Sign in or log in

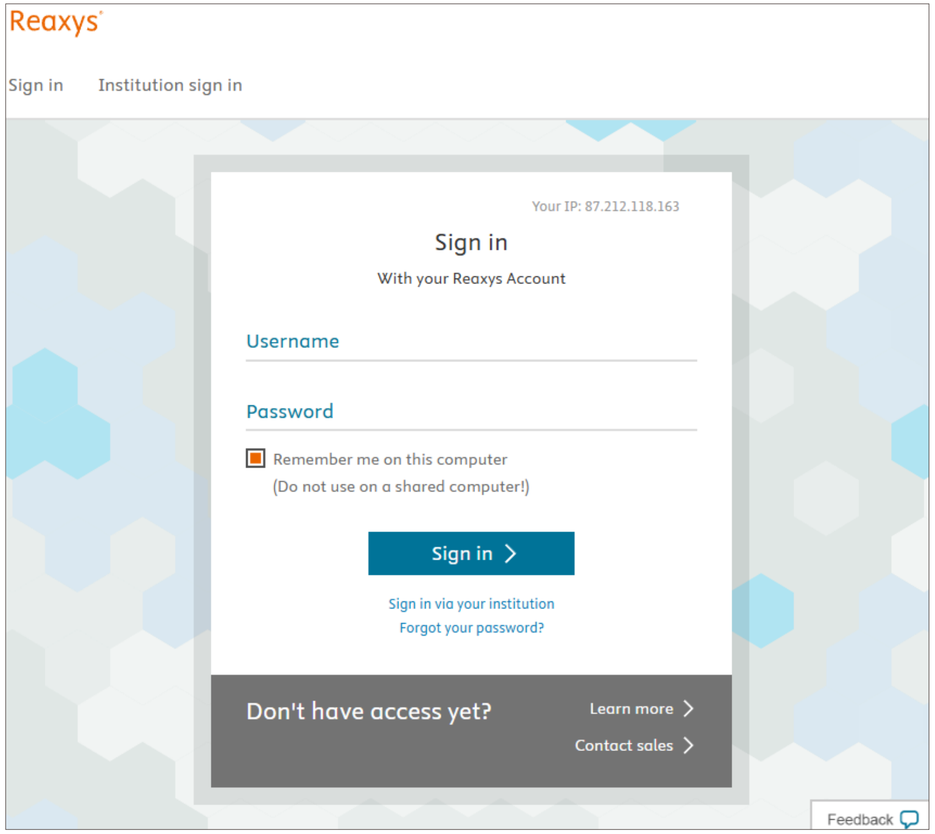
Sign in or log in to gain access to the most comprehensive datasets and advanced AI-powered tools.

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.

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.



Pro tip: Sign in or log in to save searches and set alerts.

Learn more about access.

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.

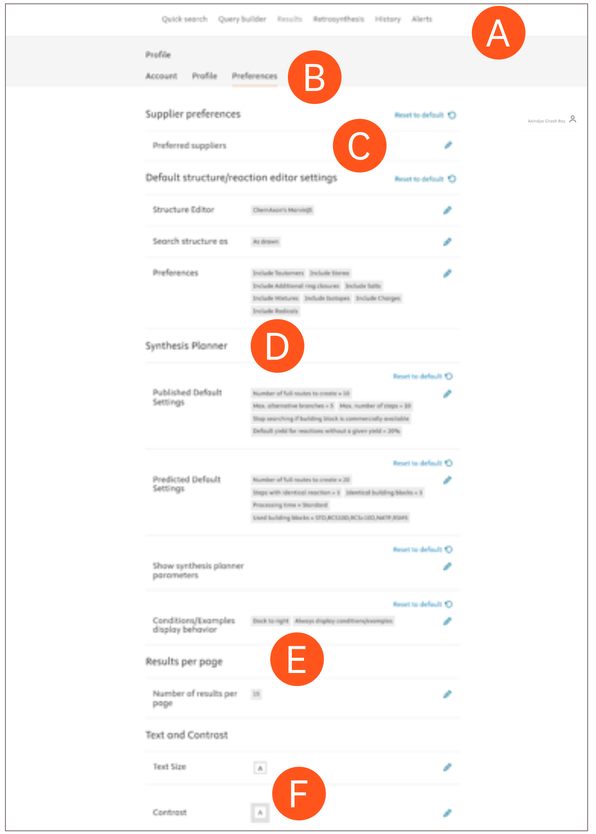
B. Click Account to edit username, email and password. Access Preferences to adjust query settings.

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.

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.

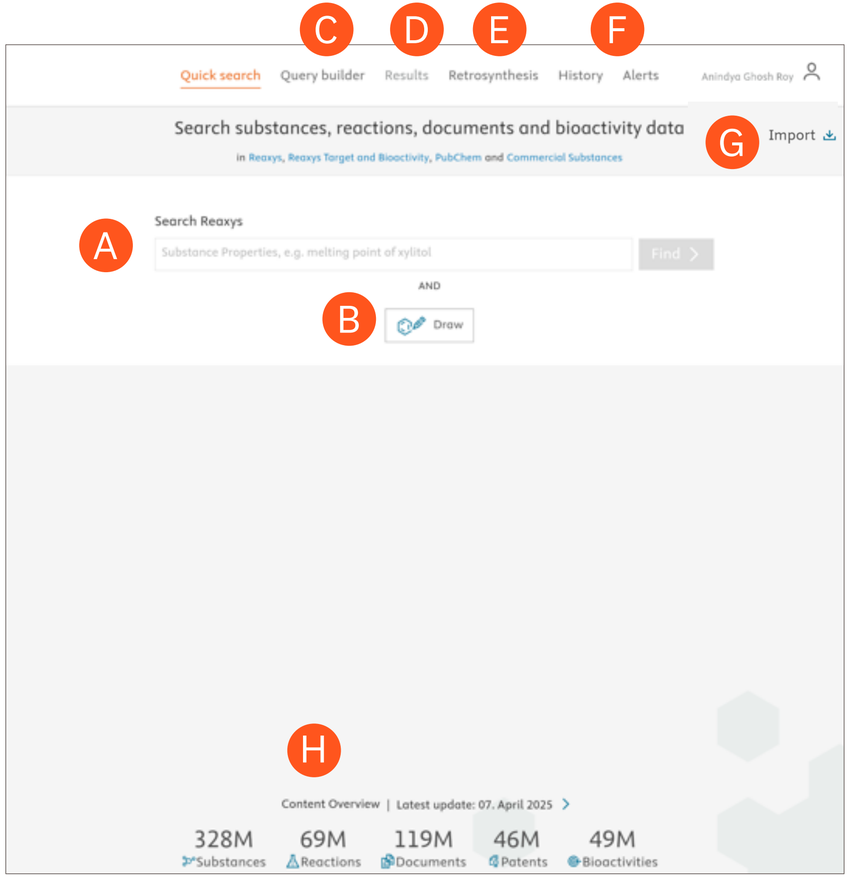
D. Results: Review, filter by reaction type, bioactivity, patents and export for analysis.

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.

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.

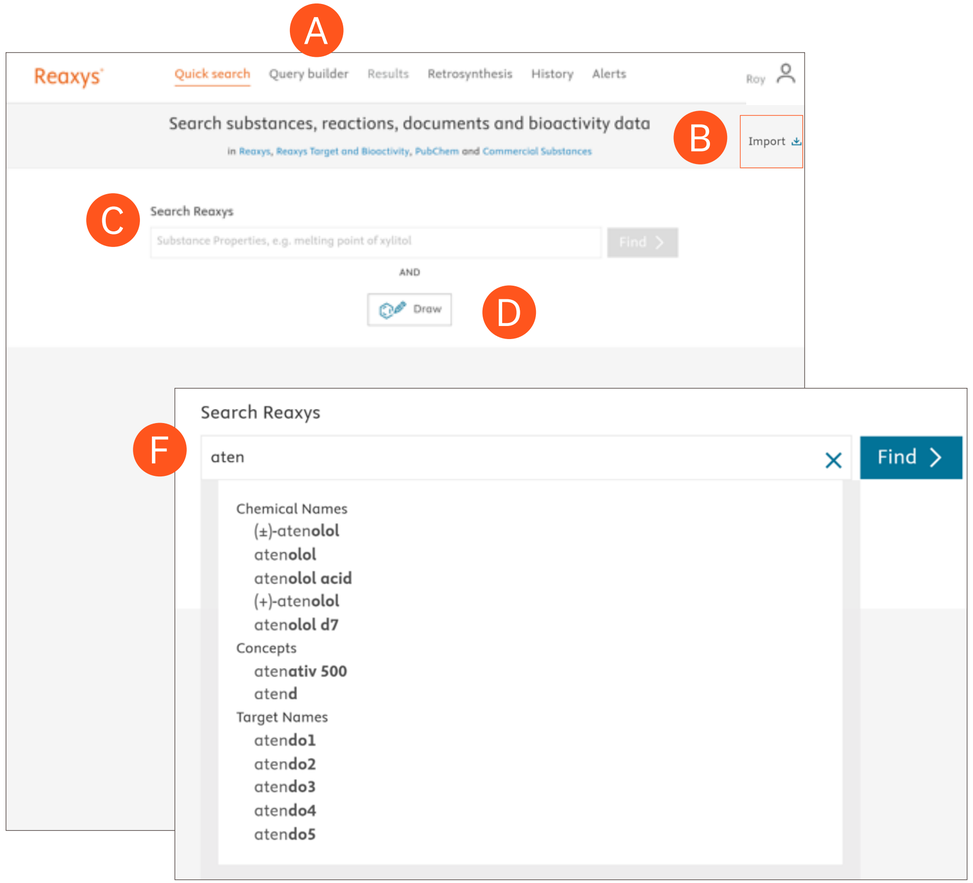
B. Import saved queries: Reload saved searches.

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.

Quick Search: Structure editors

A. Choose a structure editor: Select MarvinJS or ChemDrawJS (default: MarvinJS recommended).

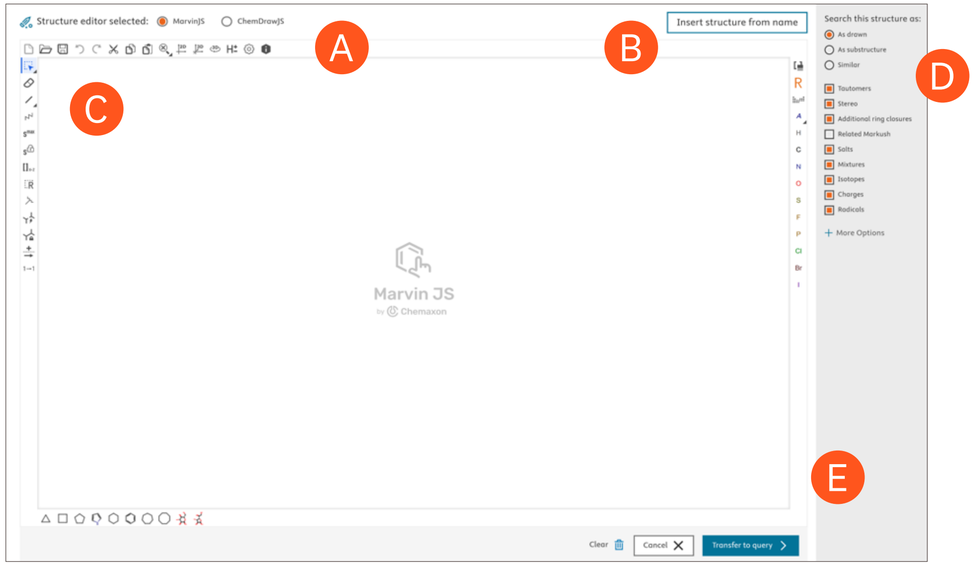
B. Insert structure from name: Enter a chemical name, CAS-RN, InChIKey or SMILES to auto-generate a structure (see F).

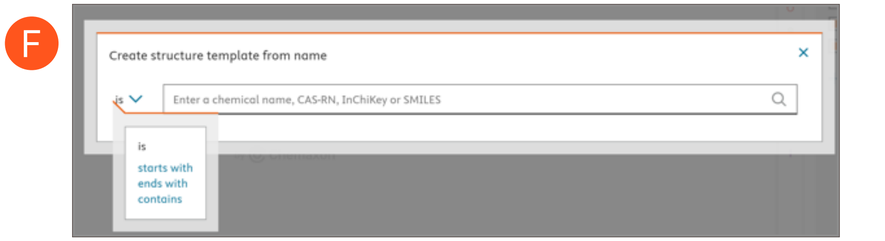
C. Draw your structure: Use the drawing tools to create or modify your structure or reaction.

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.

Results: Preview

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

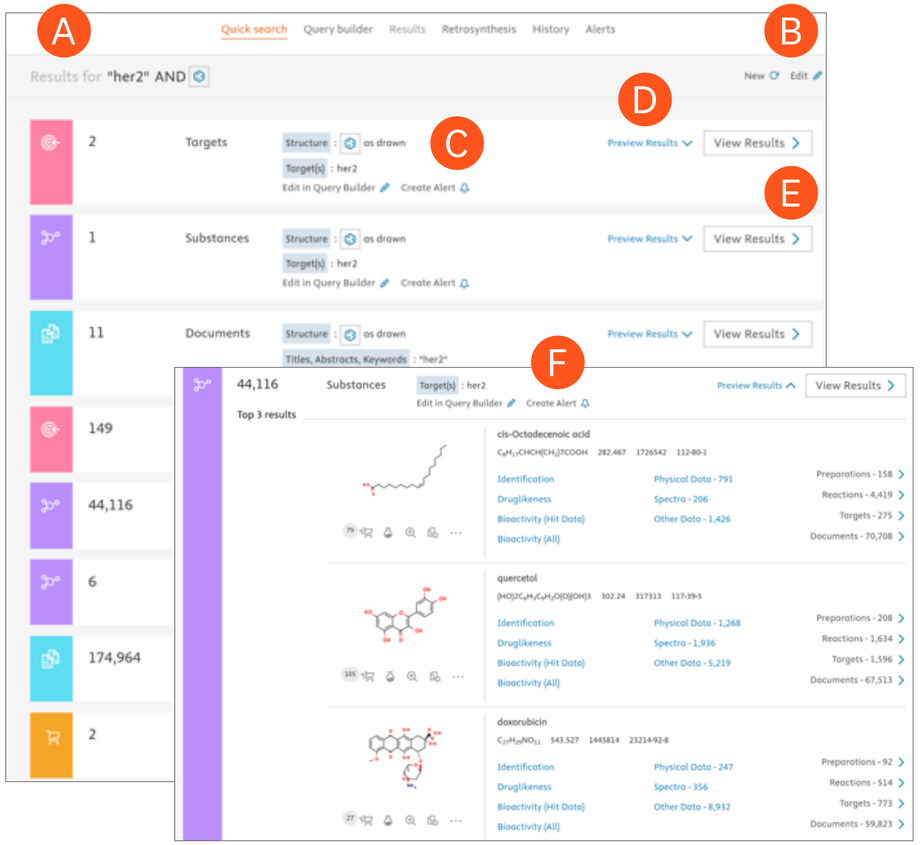
B. Start new or edit search: Click New for a fresh search or Edit to modify.

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.



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

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.

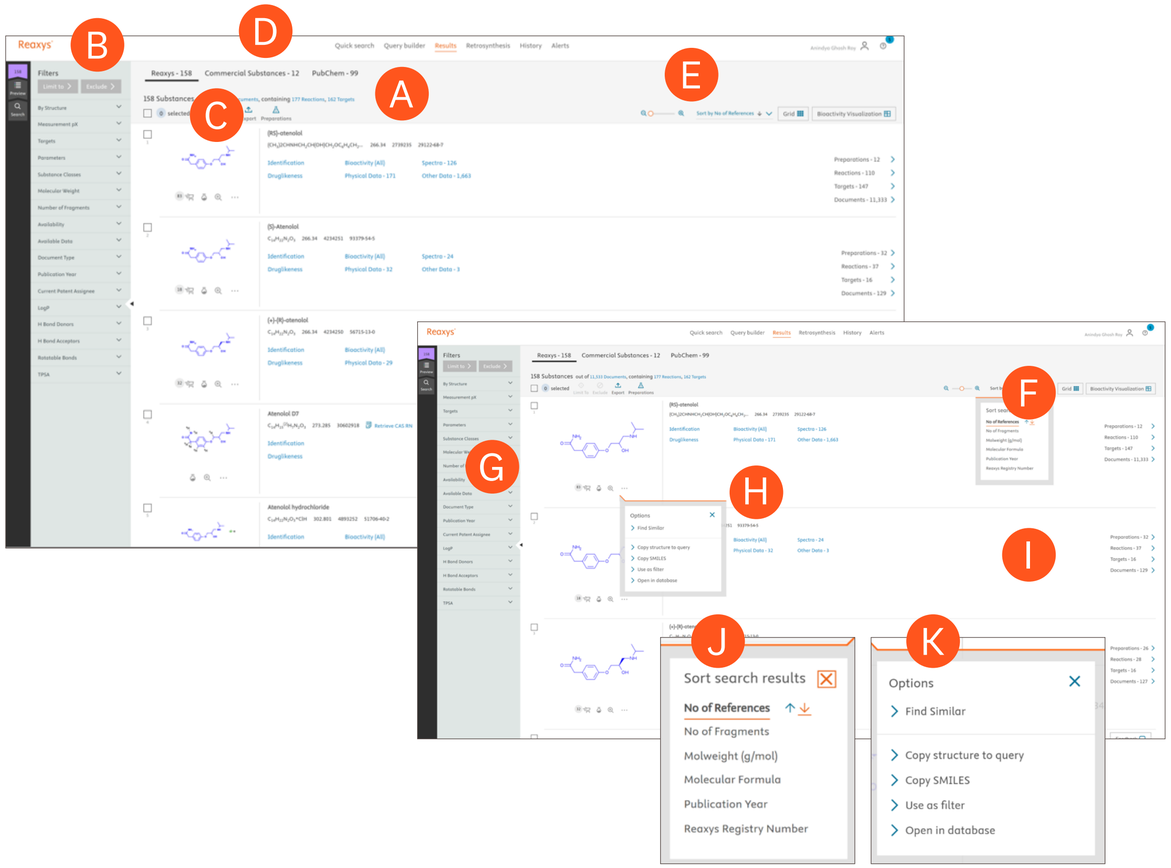
G. Commercial substance availability: Use the shopping cart icon to check substance availability across suppliers (see inset J).

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.

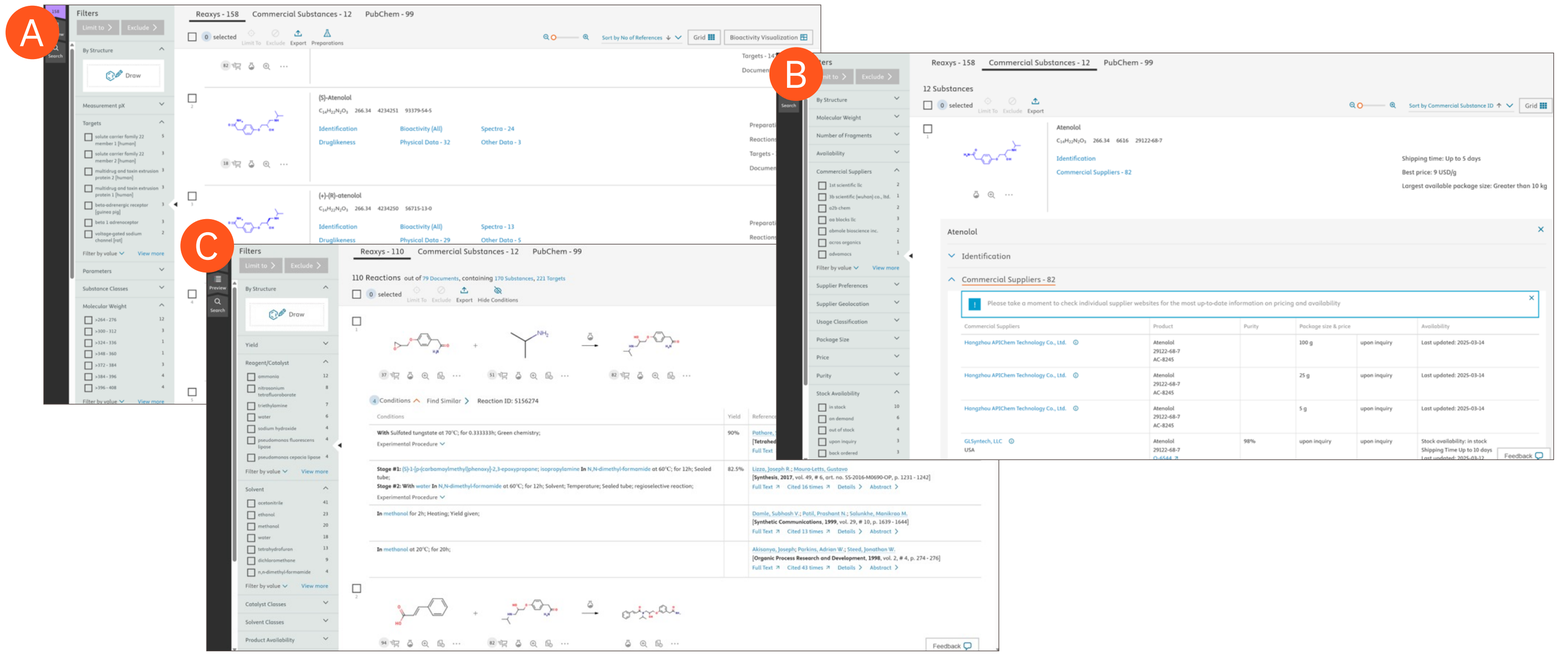


Results: Filter options 1

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.

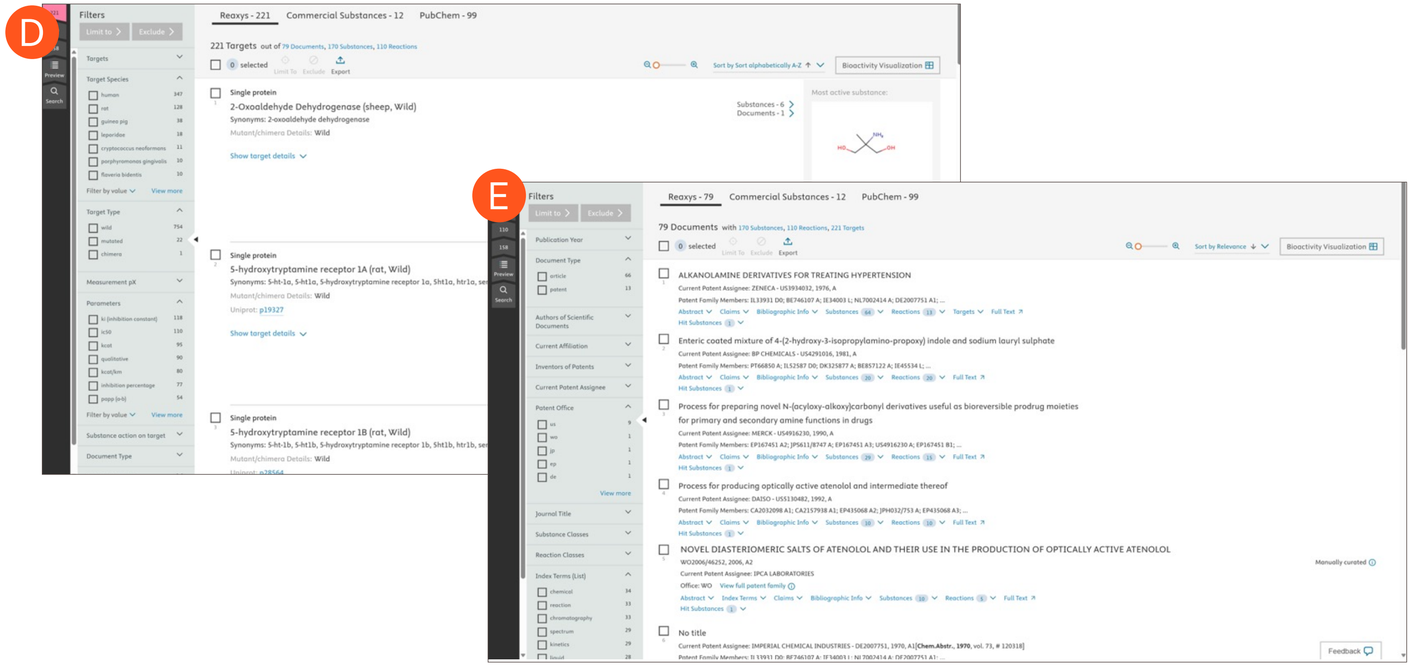


Pro tip: Sustainability Filters – Identify **Green Chemistry** reactions and materials to support **sustainable research**.

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.



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

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.

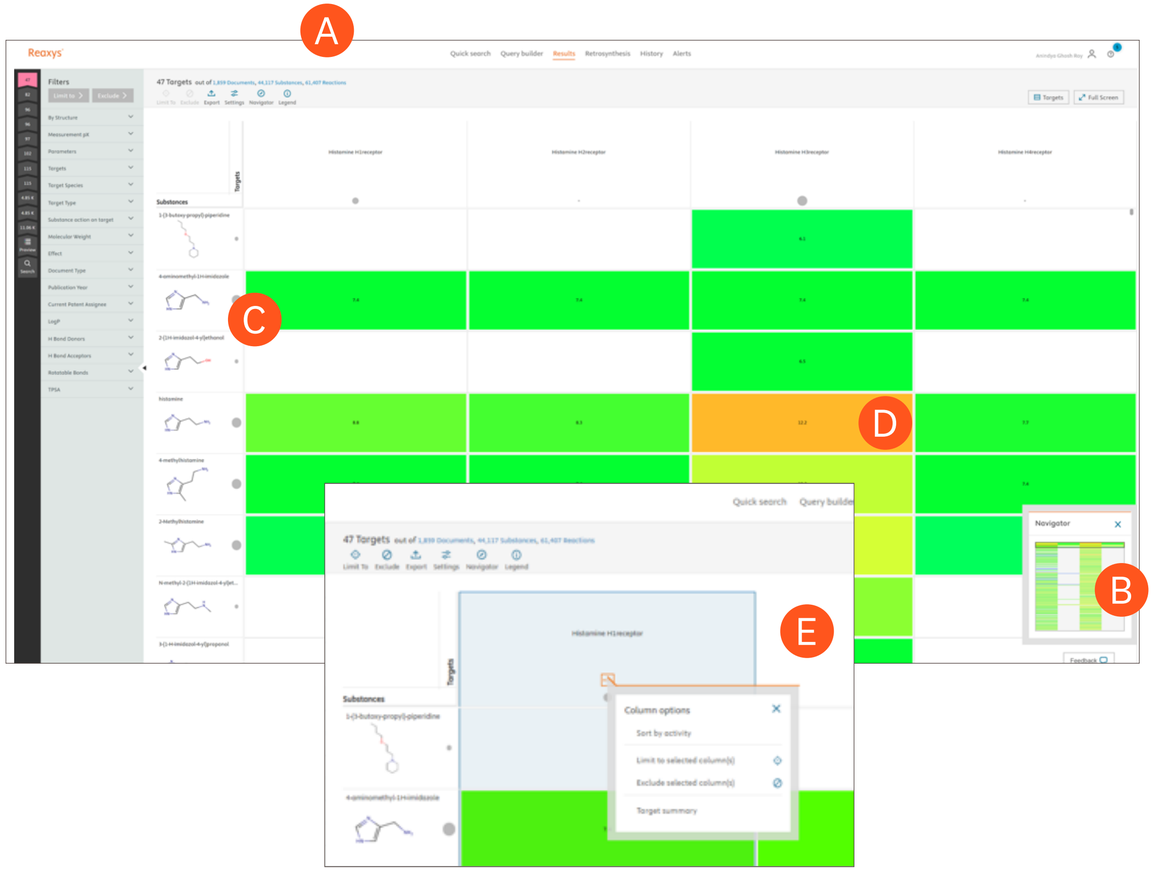
A. Use Export, Settings, Navigator and Legend to customize your view and extract data. Export pX values for analysis, sharing or reporting – especially useful for comparing across targets or identifying SAR trends.

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).

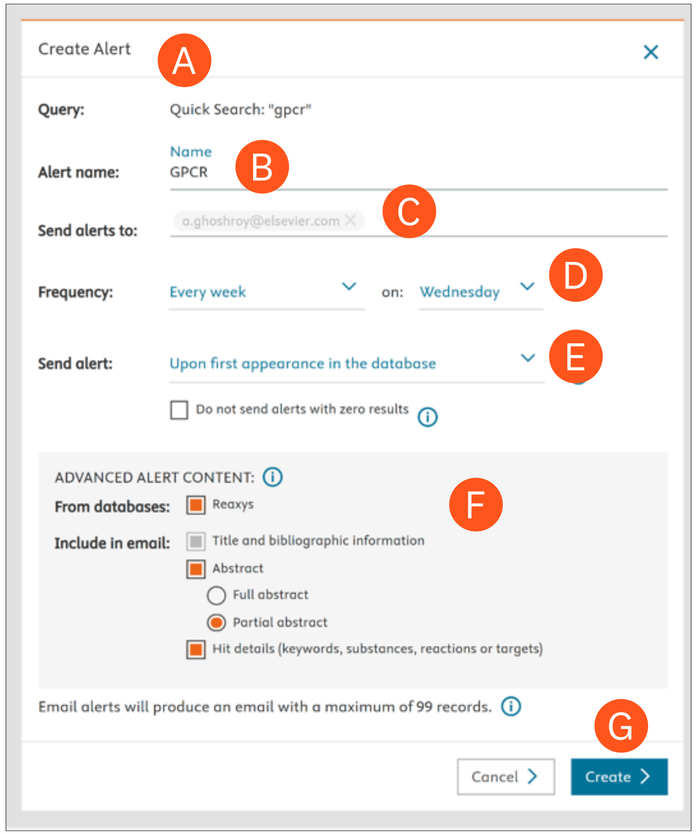
C. Add recipients: Your email is auto-added; add others if needed.

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.

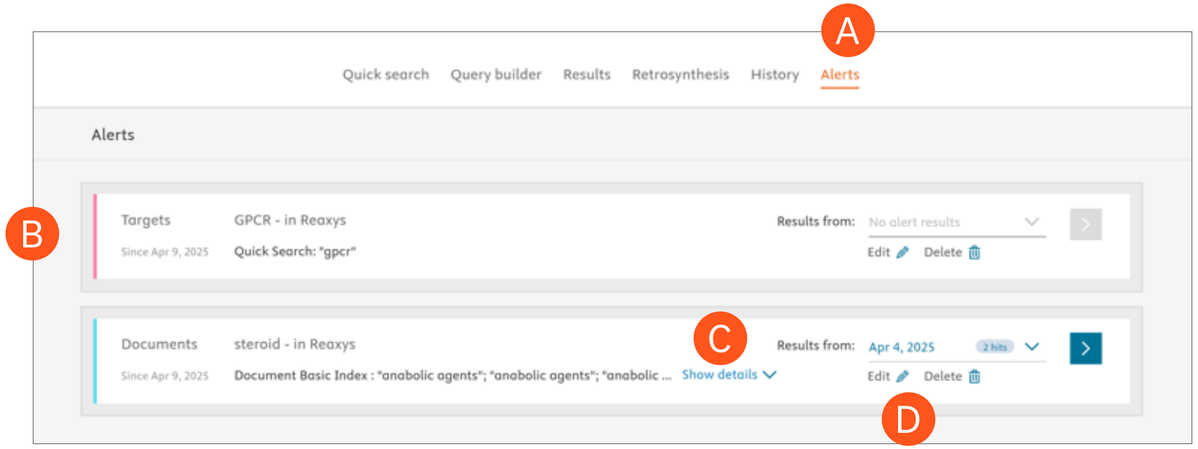
Results: Manage alerts

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.



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

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.

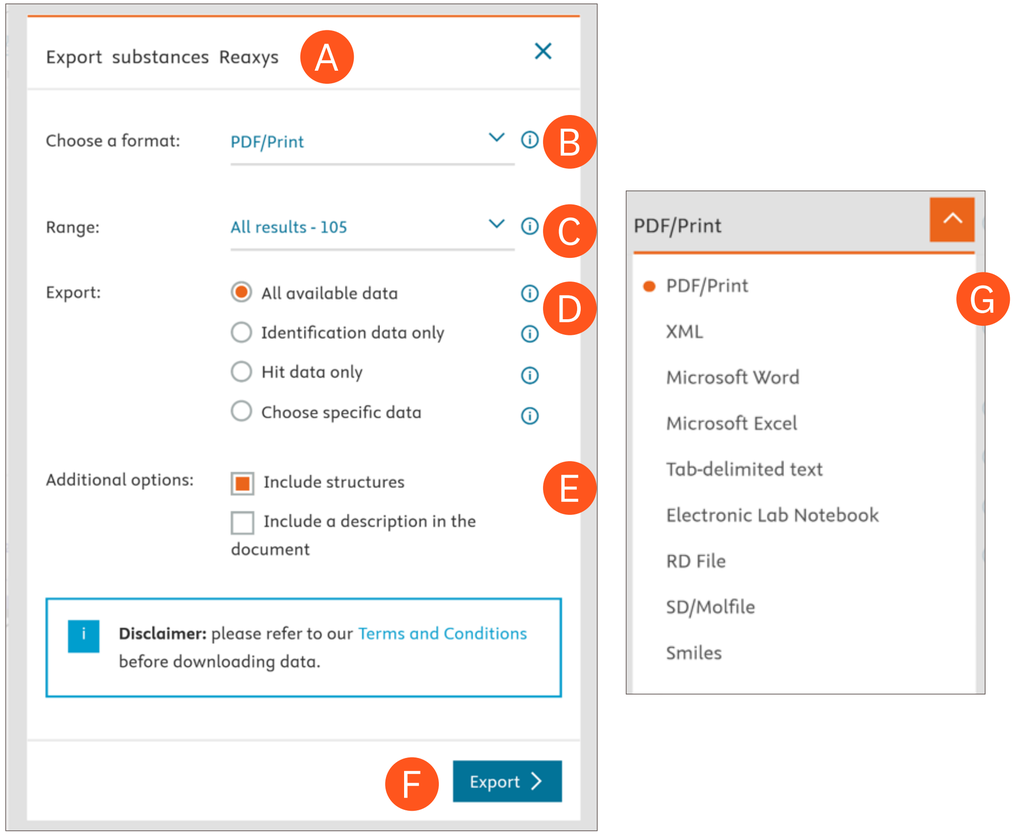
C. Define range: Export all results, selected results or a custom selection.

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.

Results: Query history

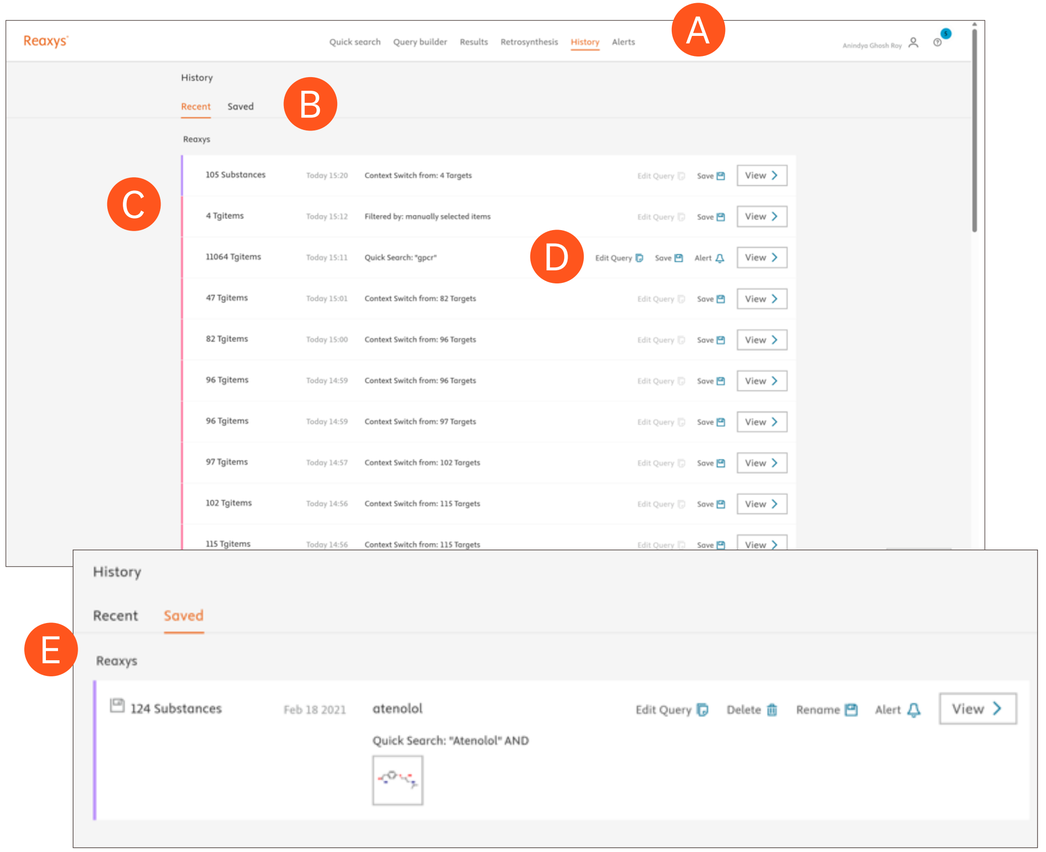
A. History tab: Click History to access both recent and saved searches.

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.



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

Query Builder

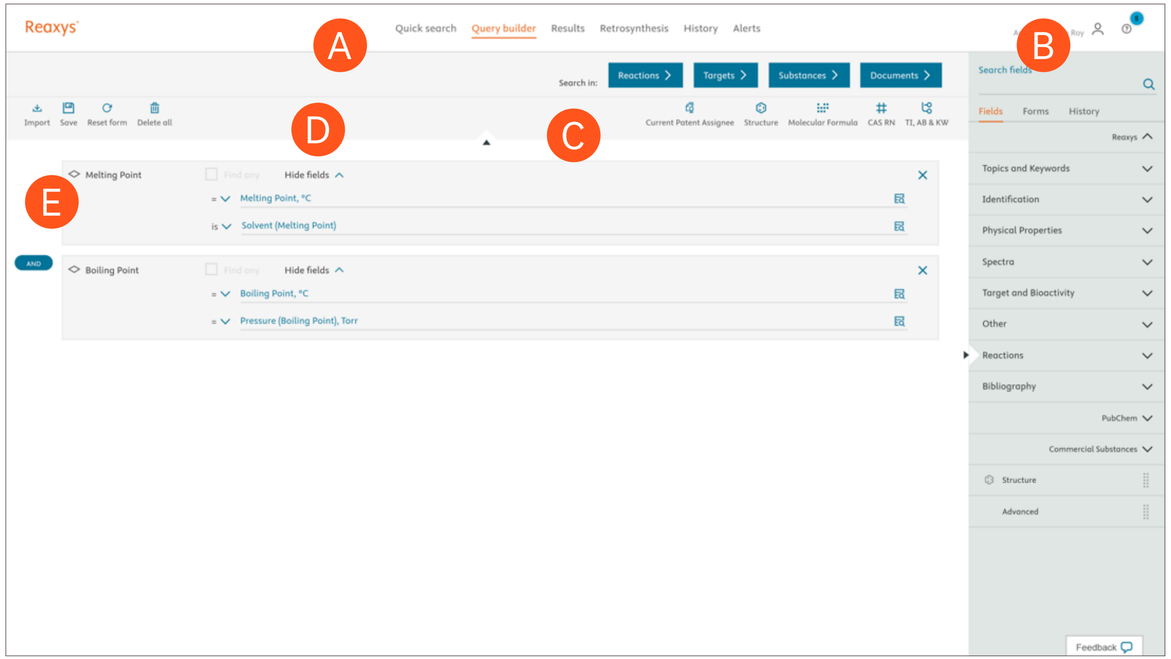
A. Open Query Builder: Launch from the top navigation or use Edit Query to customize your search.

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.

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.

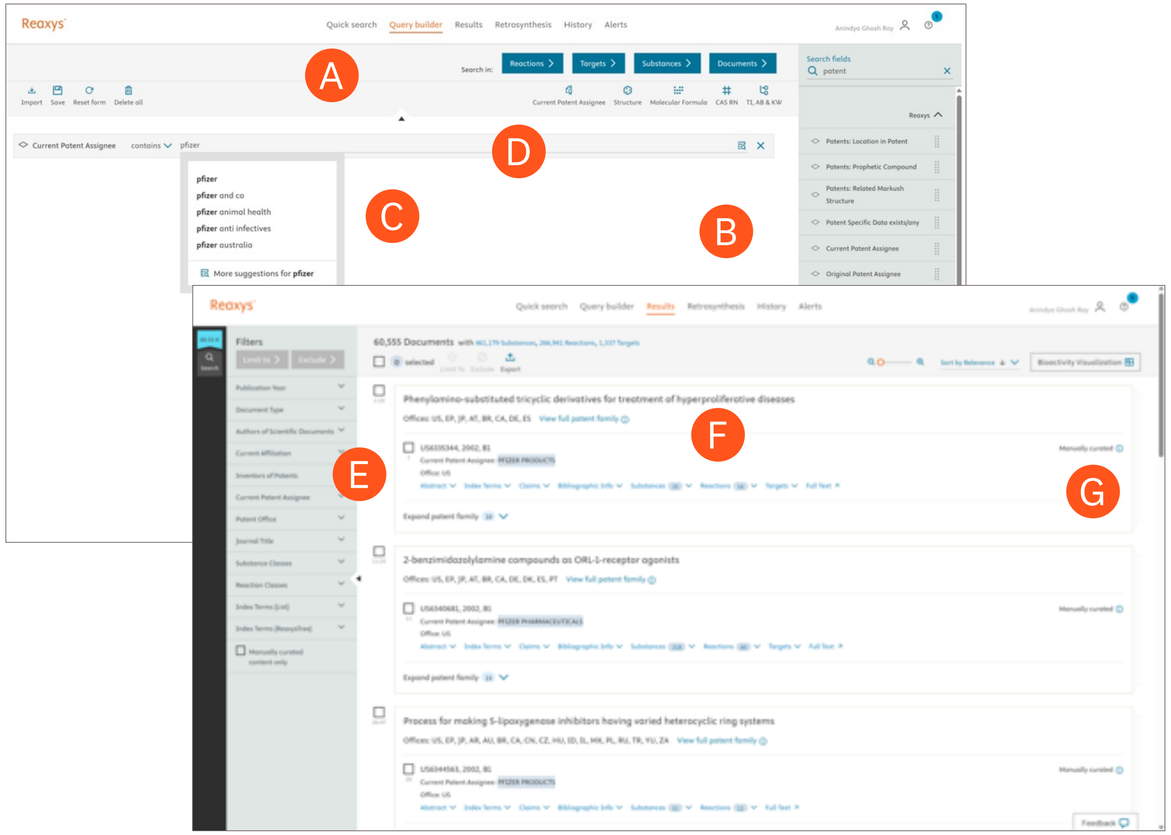
C. Enter a company or institution name: Use contains for flexible search. Type the full or partial name (e.g., Pfizer) to return a wide match.

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

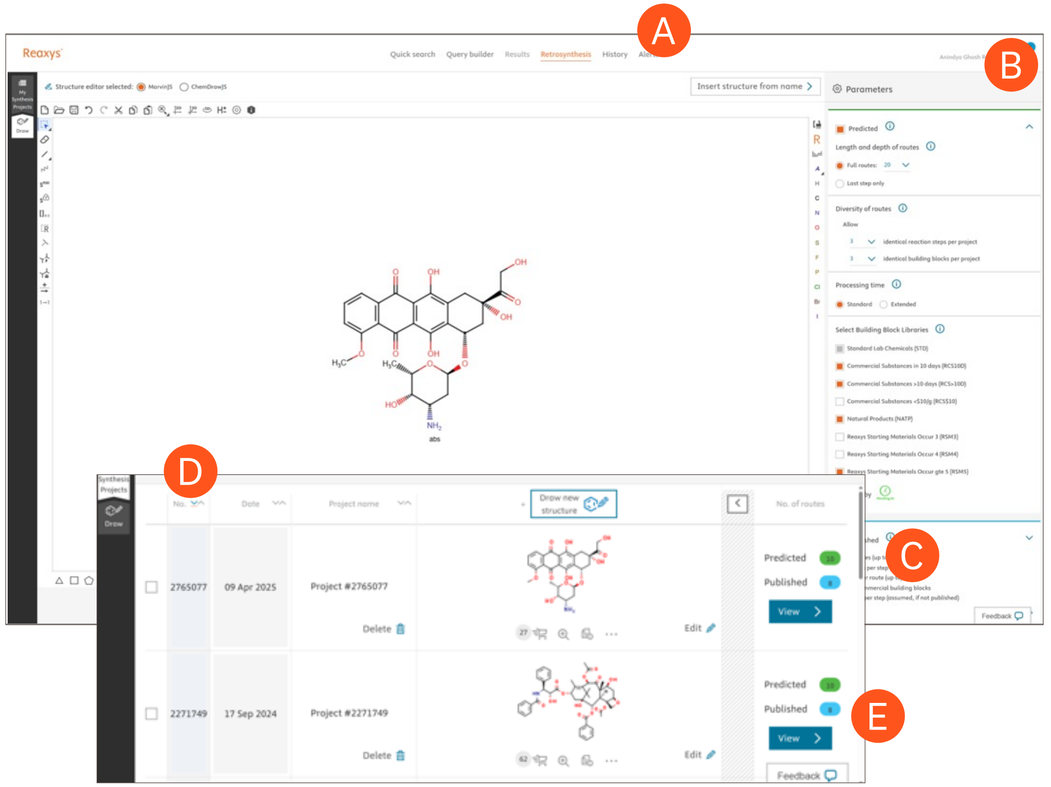
A. Go to the Retrosynthesis page and draw a compound: Launch the structure editor to sketch or import your compound of interest.

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.



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.

Retrosynthesis: Analyze results

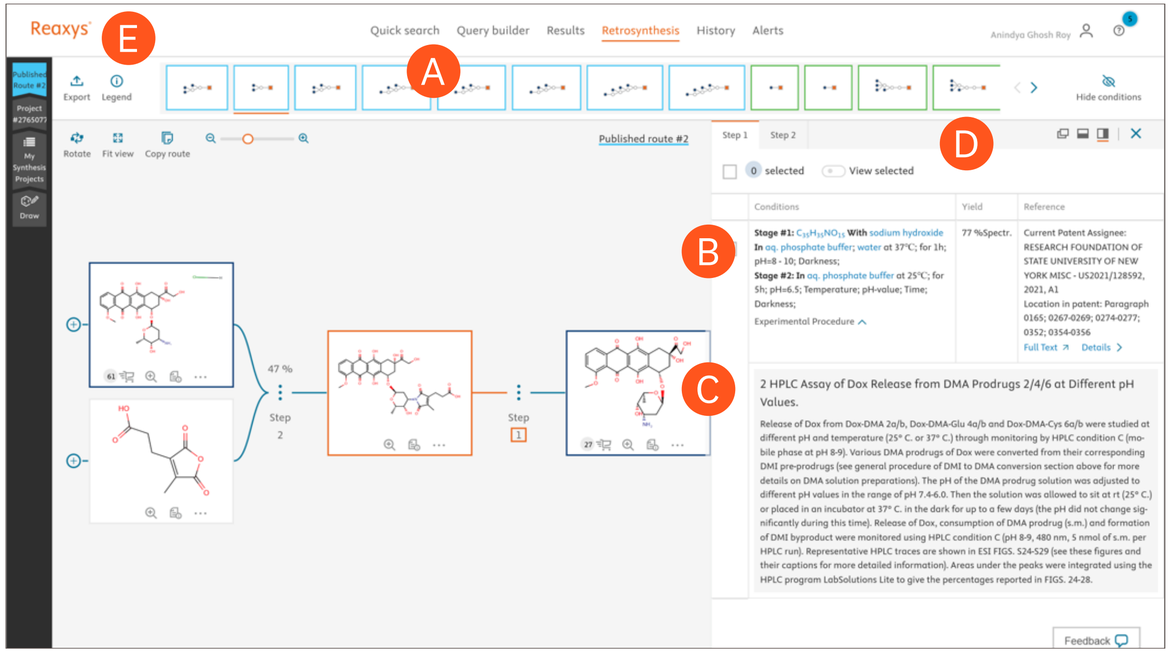
A. Toggle between synthesis routes and reaction steps: Use the navigation buttons to switch between alternative synthesis plans and step-by-step pathways.

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.



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

Predictive Retrosynthesis: Synthesis plan

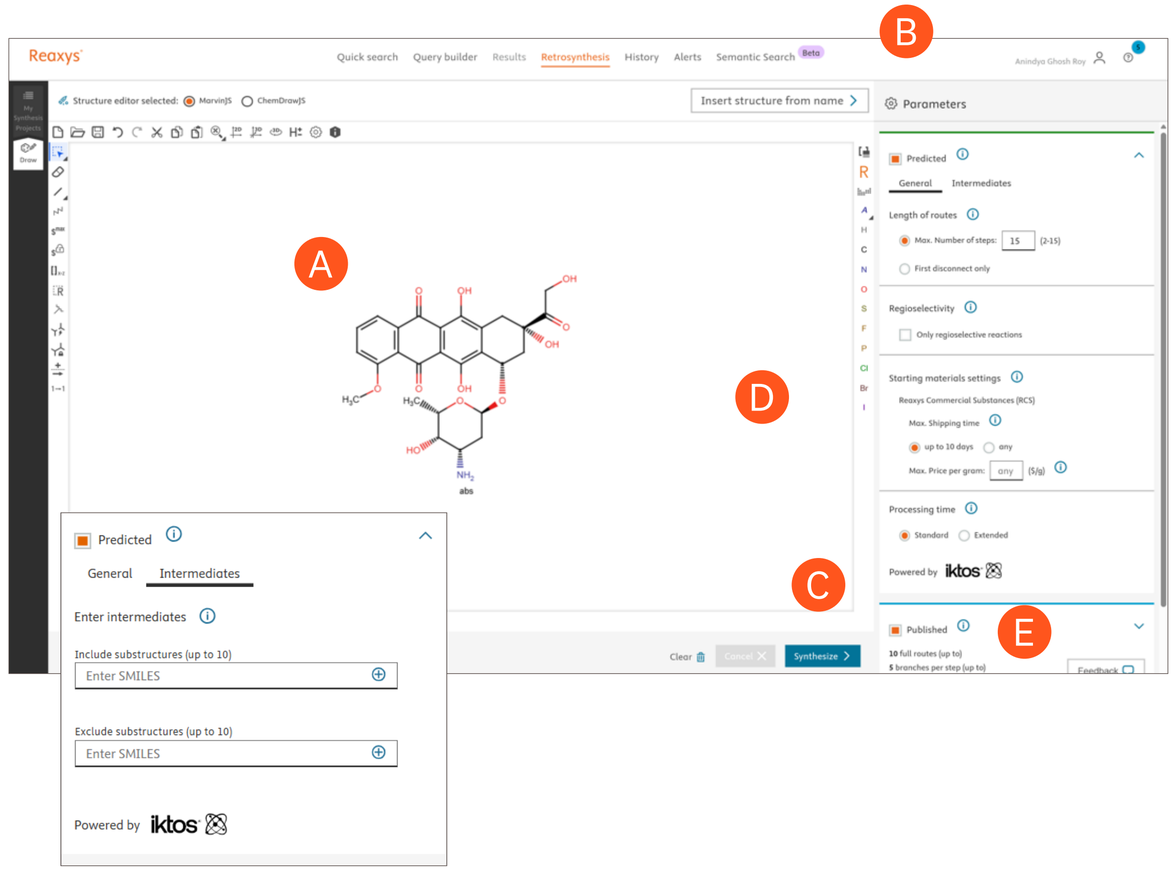
A. Open the Retrosynthesis page and draw your compound. Use the structure editor to sketch or import a compound of interest.

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.

Bioactivities

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

Pro tip: Sign in or sign up to see the latest Reaxys content updated numbers.

Substances

Design new molecules with experimentally validated substances.

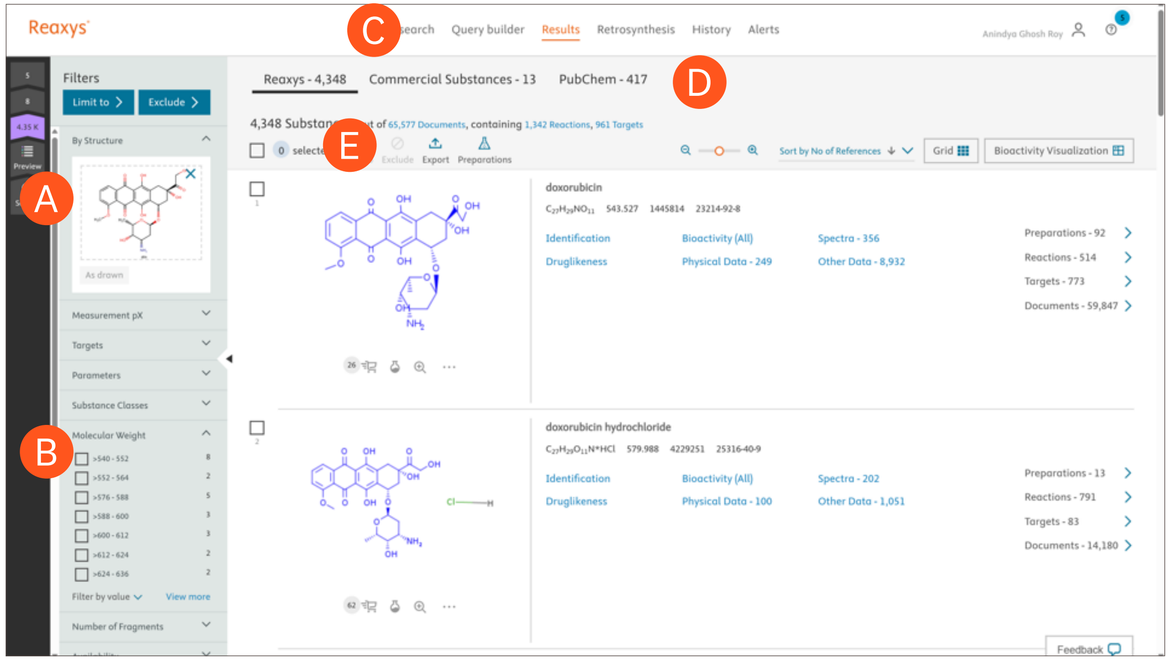
A. Start with chemical structure or name input.

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.

Reactions

Plan optimized synthesis routes using experimentally validated reaction.

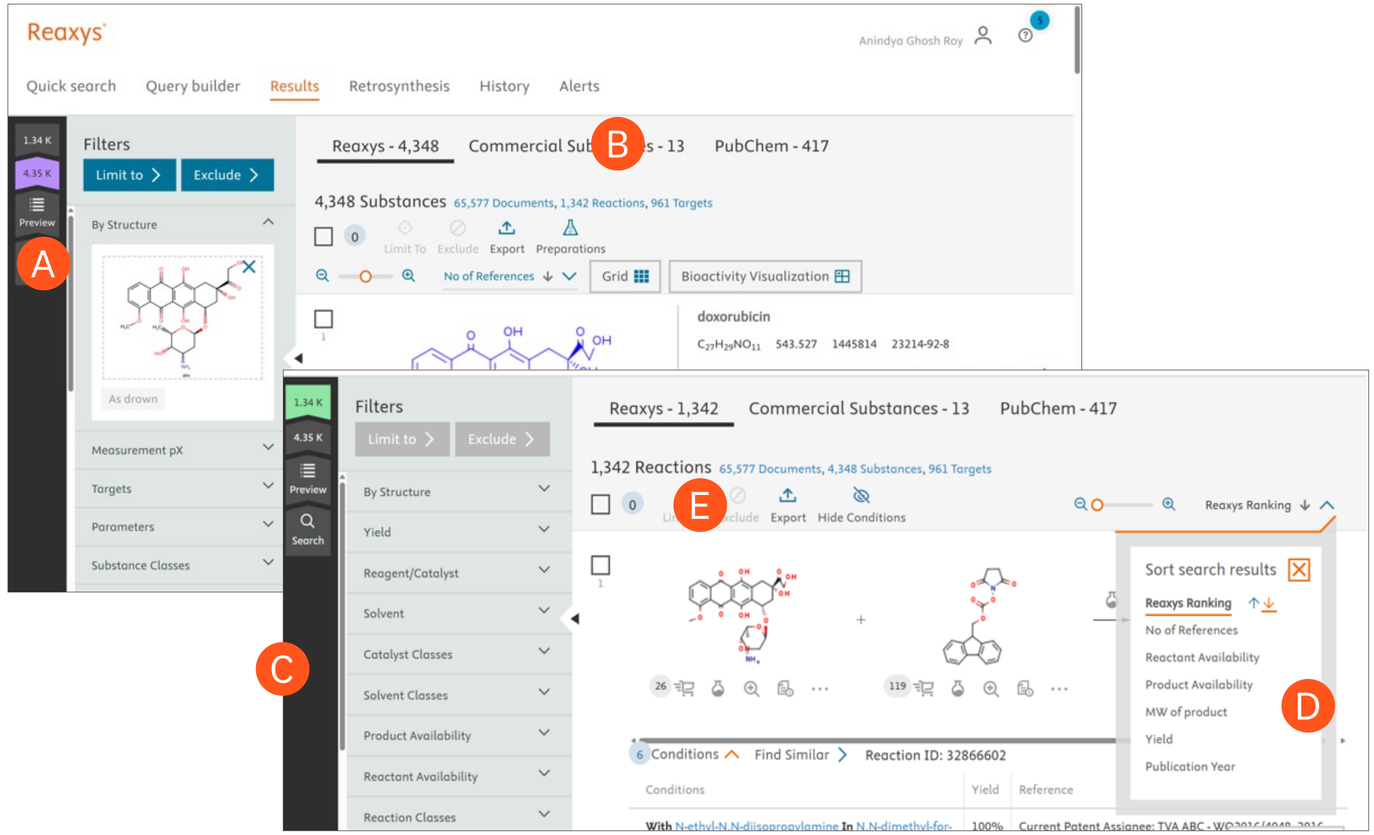
A. Draw or import a target molecule.

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.

Documents

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

A. Run a structure, substance or keyword search.

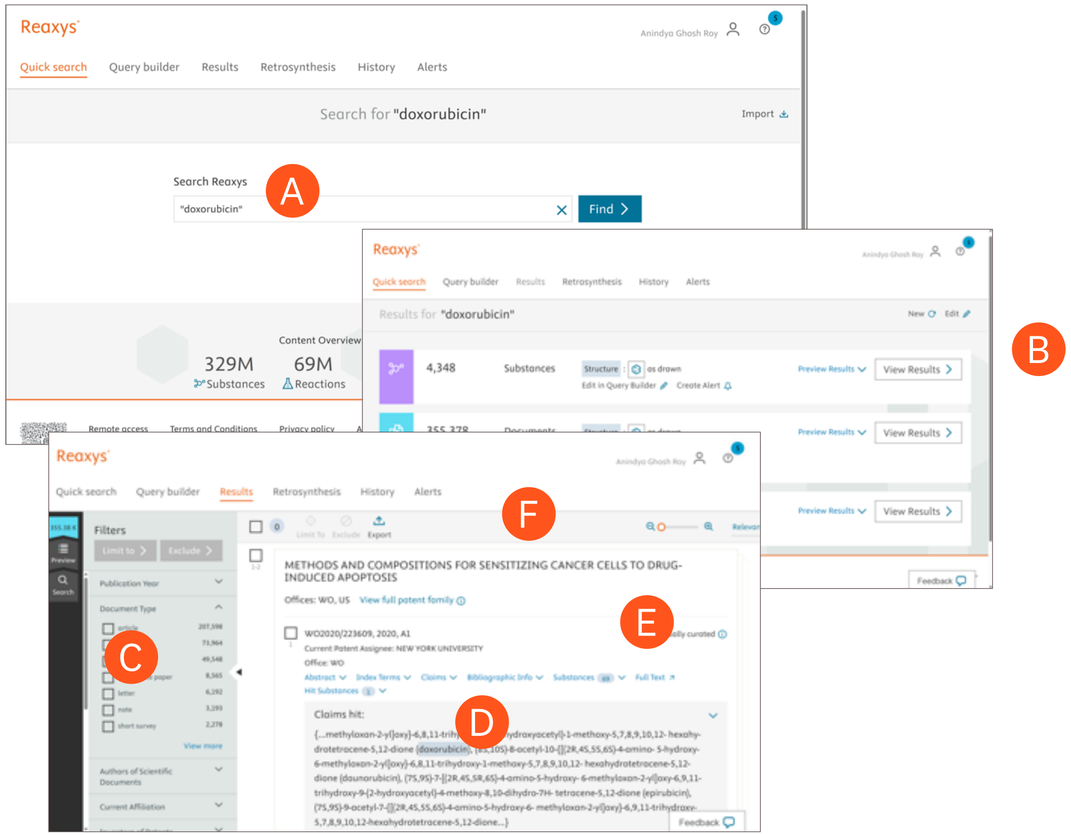
B. View documents result.

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.



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

Patents

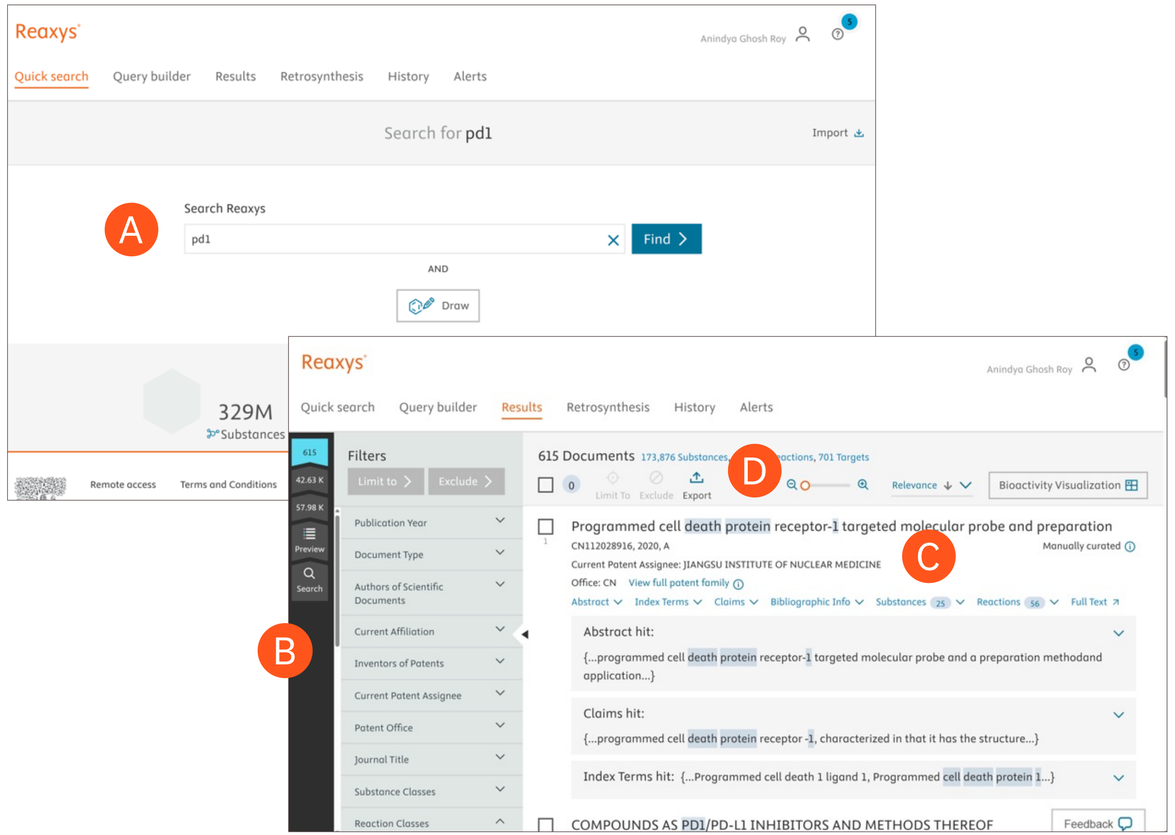
Discover novel compounds, reactions or targets disclosed in global patents.

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.

Bioactivities

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

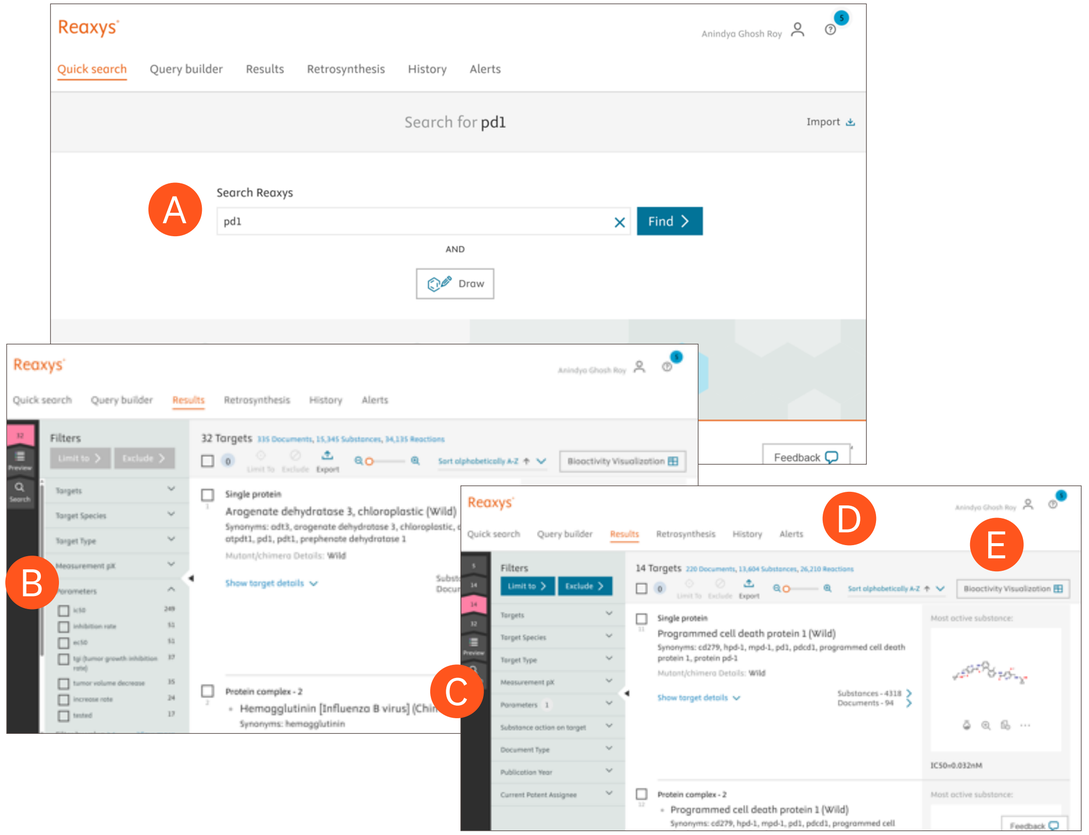
A. Run structure or compound name input.

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.



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

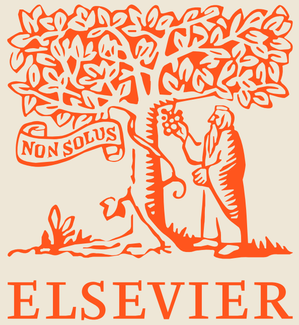
Read reference documentation for API, browse solutions and manuals, see the latest releases and contact support.

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