



Reaxys



May 2025



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0. Welcome to Reaxys

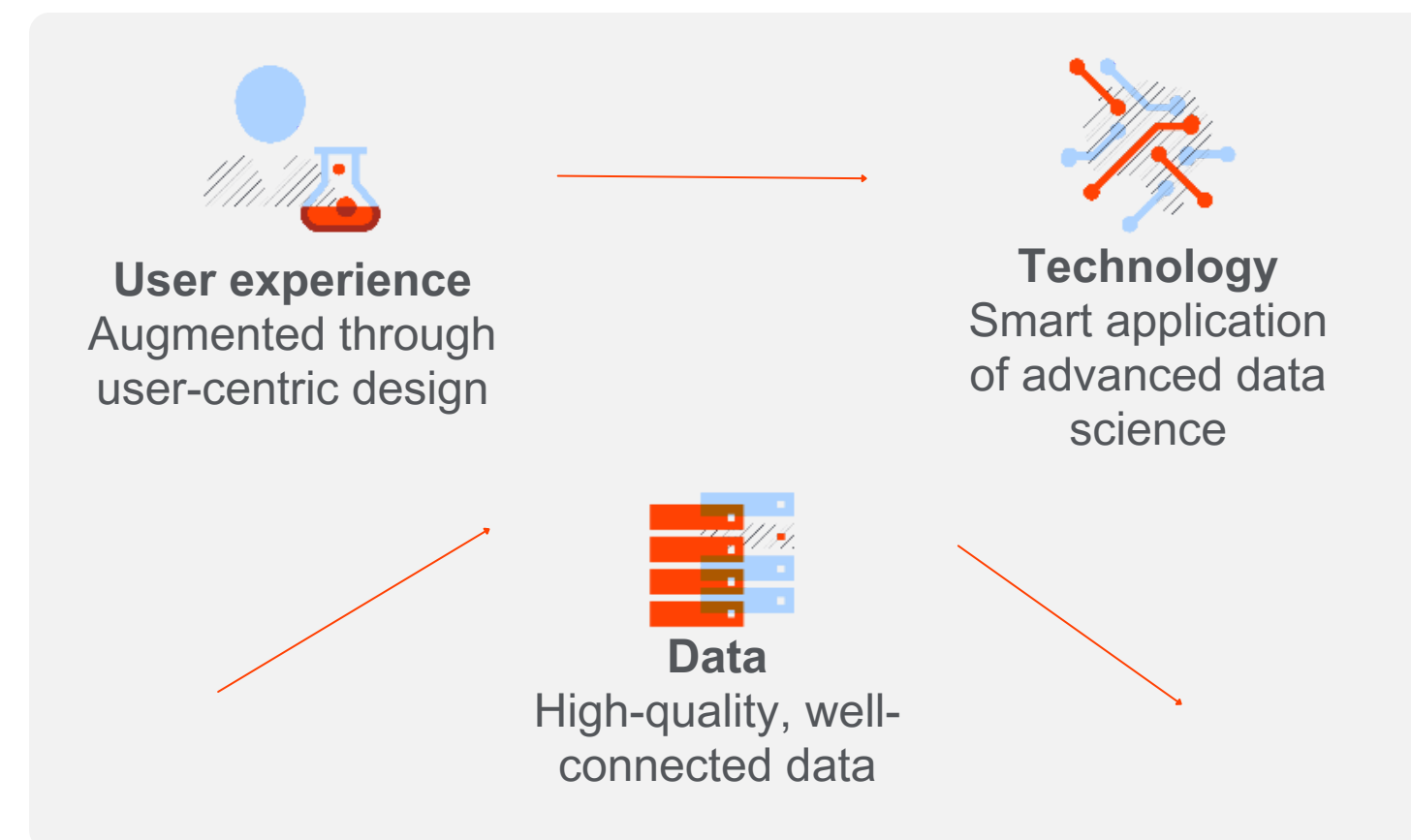
Welcome to Reaxys

Accelerate R&D with AI-driven chemistry, trusted data and intelligent tools.

Reaxys helps scientists and innovators accelerate discovery by combining over a billion chemistry data points with advanced AI. Quickly explore substances, reactions, bioactivity insights, patents, and retrosynthesis to drive faster decision-making across drug discovery, chemical R&D, and academia.

Unlock faster insights and impact across sectors:

- **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 register



1. Sign in or log in

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

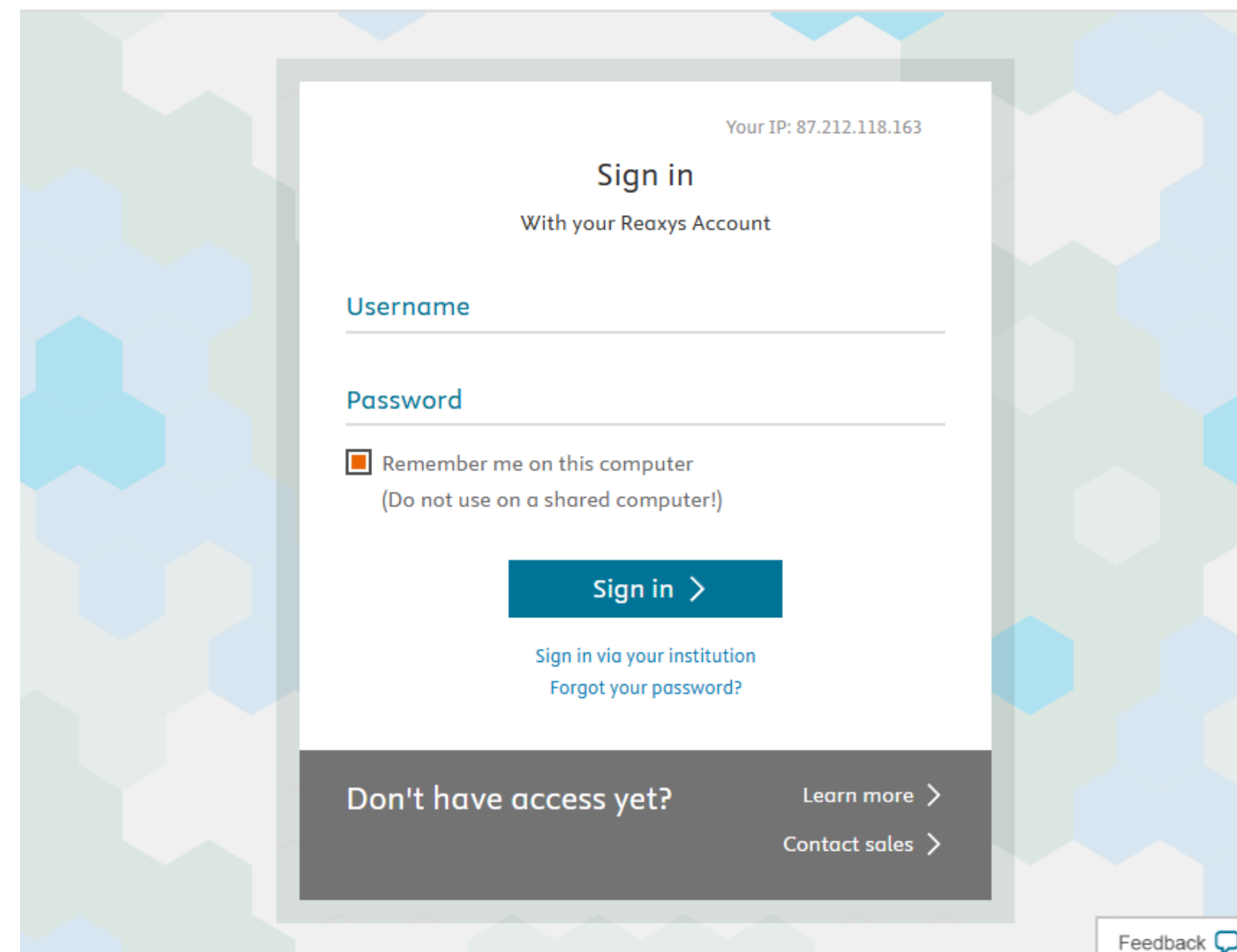
- Click Sign In and then Register. Fill out your details.
- Agree to the Terms and click Register.
- To register with Institution Registration ID, visit the [Registration ID site](#), enter your details to link account.

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 help icon inside [Reaxys.com](#) to access Resource Center for Knowledge, Learning, and Support.


Reaxys[®]

Sign in Institution sign in



The image shows the Reaxys sign-in page. At the top, it says 'Reaxys' and has links for 'Sign in' and 'Institution sign in'. Below this, it displays 'Your IP: 87.212.118.163'. The main heading is 'Sign in' with the subtext 'With your Reaxys Account'. There are input fields for 'Username' and 'Password'. Below these is a checkbox labeled 'Remember me on this computer' with a warning '(Do not use on a shared computer!)'. A large blue button says 'Sign in >'. Below the button are links for 'Sign in via your institution' and 'Forgot your password?'. At the bottom, there is a dark grey box with the text 'Don't have access yet?' and links for 'Learn more >' and 'Contact sales >'. A 'Feedback' icon is in the bottom right corner.

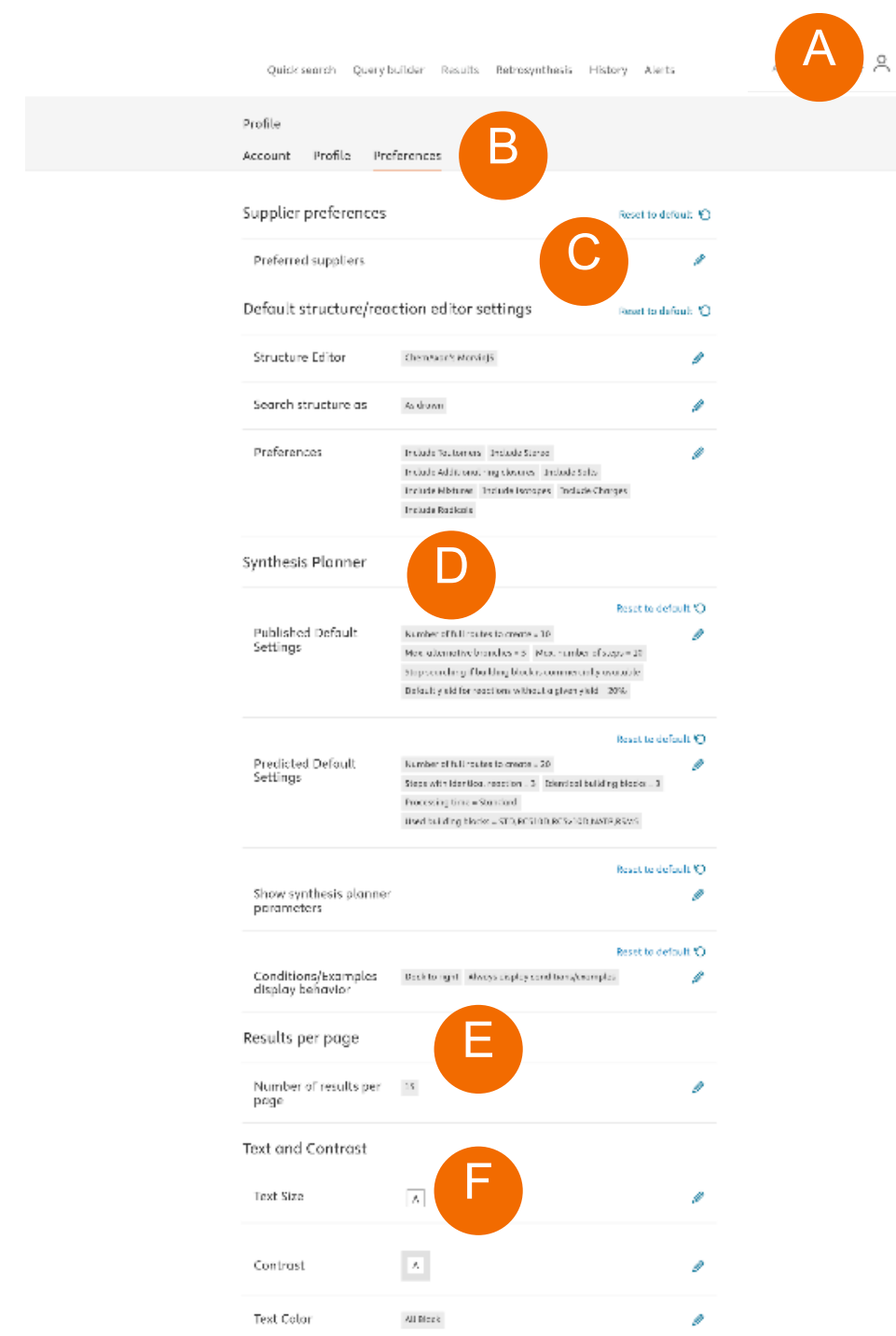
 **Pro Tip:** [Sign in or log in](#) to save searches and set alerts.


 [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.

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



 **Pro Tip:** Enable MarvinJS and set default structure filters (e.g., include tautomers, exclude salts) to streamline substructure searches and avoid irrelevant hits during synthesis planning.



2. Homepage tour

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. Upload queries or datasets to import or integrate data
- h. View latest statistics in Reaxys content overview

The screenshot shows the Reaxys homepage with several annotations:

- A**: Search Reaxys input field with the placeholder text "Substance Properties, e.g. melting point of xylitol".
- B**: Draw button with a chemical structure icon.
- C**: Reaxys logo.
- D**: Quick search link.
- E**: Query builder link.
- F**: Results link.
- G**: Import button with a download icon.
- H**: Content Overview section showing statistics: 328M Substances, 69M Reactions, 119M Documents, 46M Patents, and 49M Bioactivities. It also includes a "Latest update: 07. April 2025" link.

Other visible elements include the Elsevier logo in the top right, a user profile for "Anindya Ghosh Roy", and a navigation bar with links to Retrosynthesis, History, and Alerts.

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

 [Contact us](#) to upgrade.



3. Reaxys core features

Reaxys core features

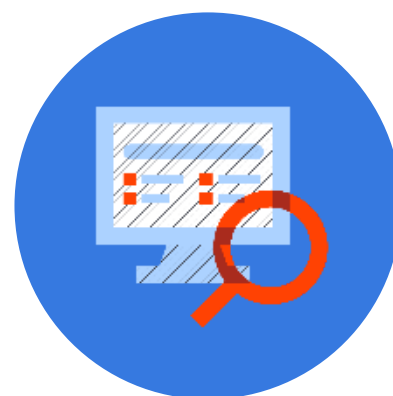
Advance discovery, plan synthesis and make confident decisions across industries.



1. Quick Search

Instantly explore validated chemistry data for substances, reactions, patents, and bioactivities.

- Search experimental data
- Draw molecules
- Apply filters



2. Results

Leverage curated, context-rich results to support trusted R&D decisions.

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



3. Query Builder

Build multi-parameter searches with precision using filters, fields, and properties.

- Combine query fields
- Apply advanced filters
- Search by properties



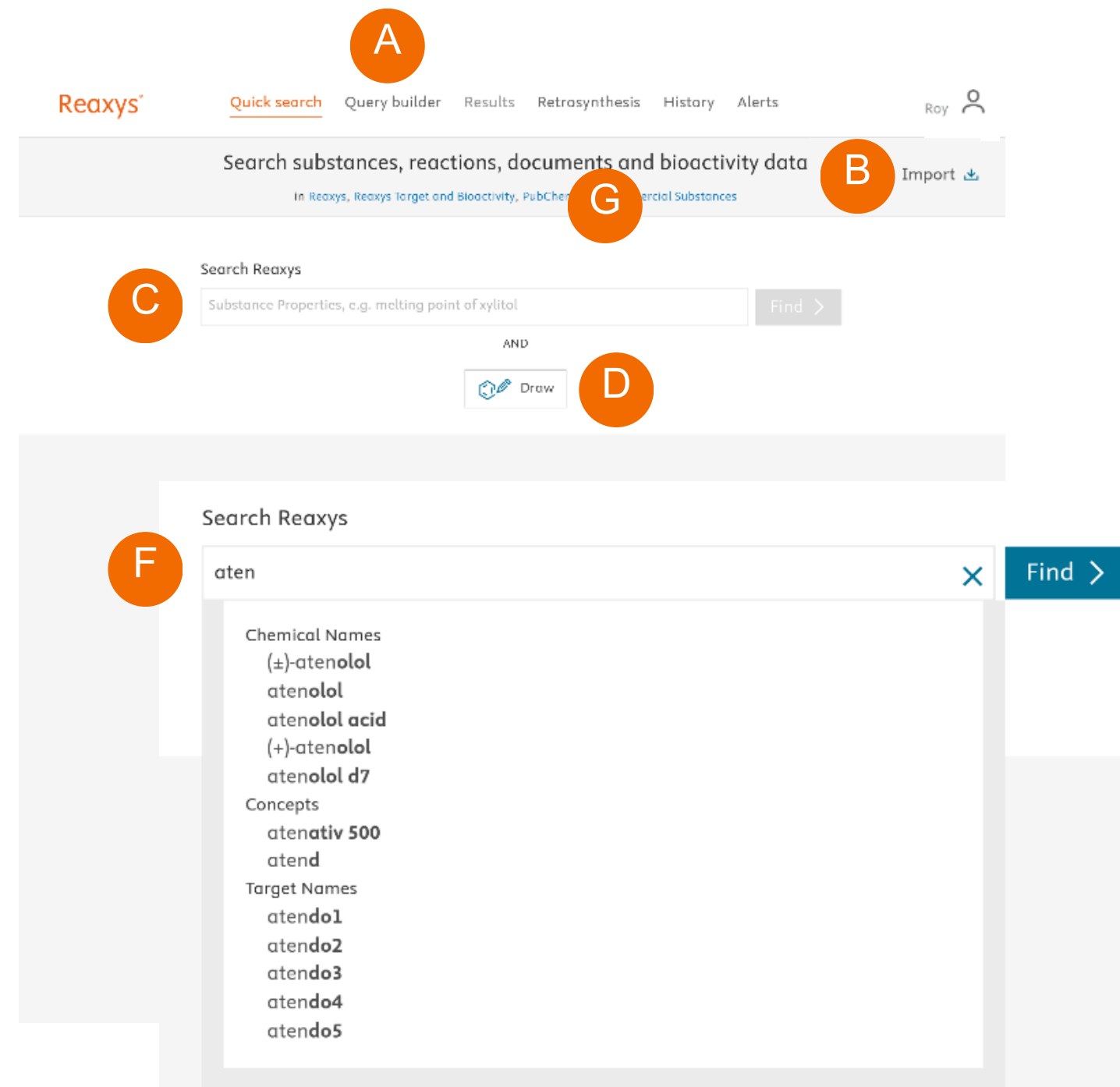
4. Retrosynthesis

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

- Generate synthesis plans
- Explore AI-powered alternatives
- Compare reaction options

Quick Search

- Navigate to Quick Search: Click from top menu
- Import saved queries: Reload saved searches
- Enter search terms (chemical name, reaction, target, patent assignee, or author). *Auto-suggest* recommends synonyms (see F).
- Use the structure editor to sketch or paste chemical structures. Supports MarvinJS and ChemDraw JS.
- Click *Find* to run your search and preview ranked results.
- Use auto-suggest to complete terms like author names, synonyms, or targets — speeding up precise query building.



The screenshot shows the Reaxys Quick Search interface. Annotations are as follows:

- A**: Reaxys logo
- B**: Search bar with text "Search substances, reactions, documents and bioactivity data"
- C**: Search input field containing "Substance Properties, e.g. melting point of xylitol"
- D**: "Draw" button with a chemical structure icon
- E**: "Find" button
- F**: Auto-suggest dropdown menu for the search term "aten", showing categories like Chemical Names, Concepts, and Target Names.
- G**: "Import" button

The auto-suggest dropdown (F) lists the following suggestions:

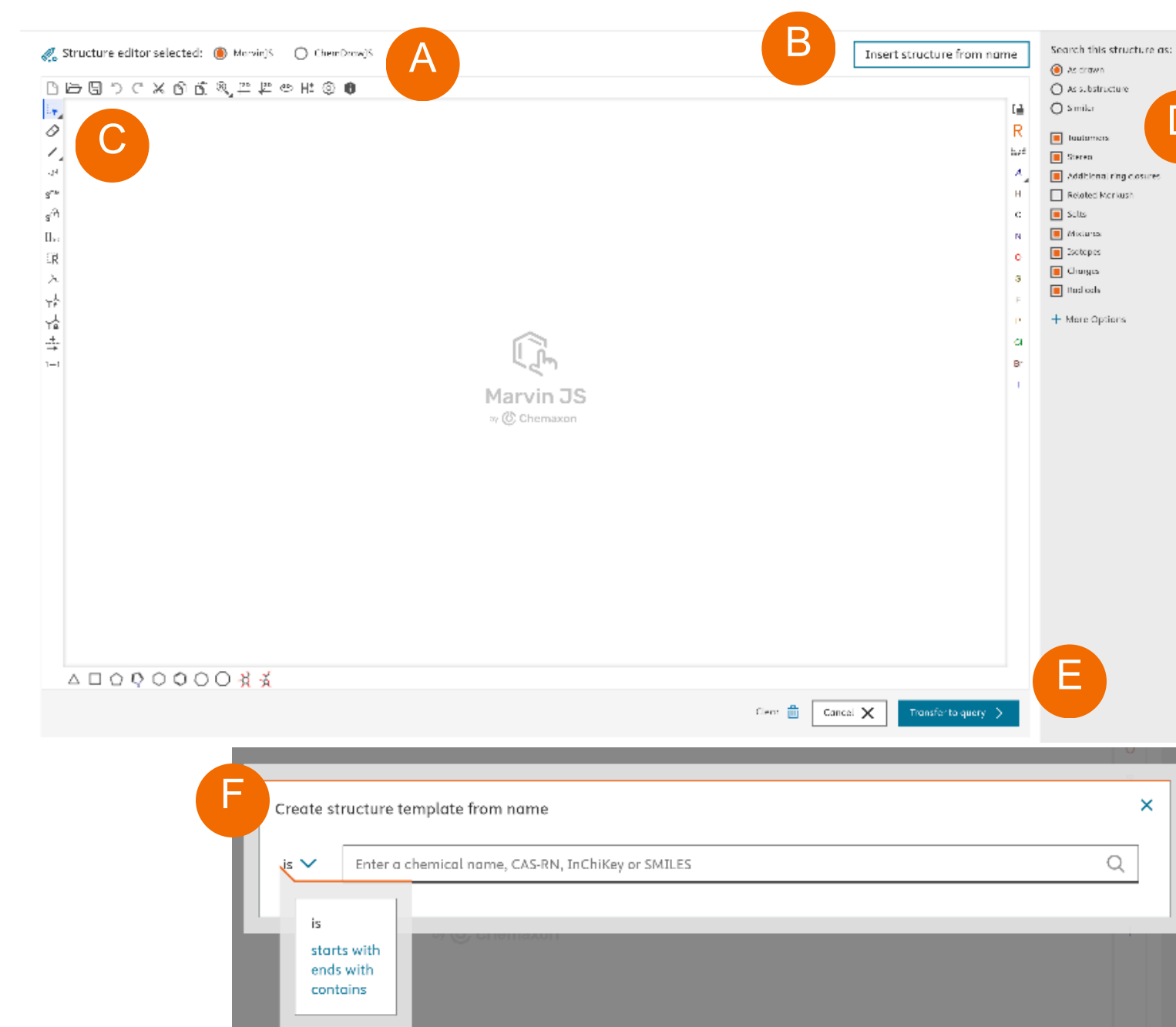
- Chemical Names
 - (±)-atenolol
 - atenolol
 - atenolol acid
 - (+)-atenolol
 - atenolol d7
- Concepts
 - atenativ 500
 - atend
- Target Names
 - atendo1
 - atendo2
 - atendo3
 - atendo4
 - atendo5


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

 Article: [Learn more about search](#)

Quick Search: Structure editors

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



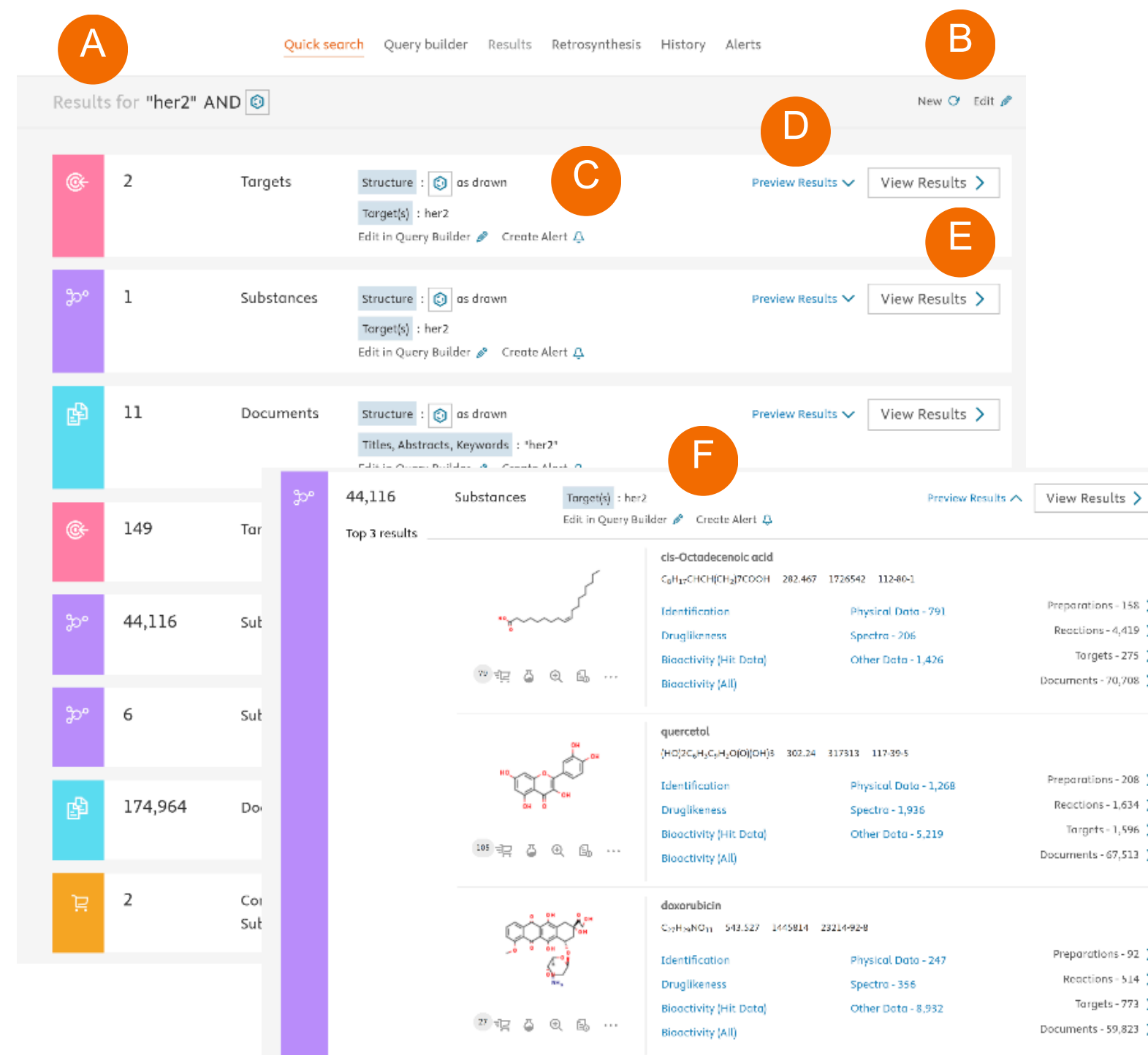
 **Pro Tip:** Use Boolean operators (AND, OR, NOT) for complex searches.

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

 Learn more: [Structure drawing workflow](#)

Results: Preview

- Search term display: See your original query — keywords, structure, and filters
- Start new or edit search: Click New for a fresh search or Edit to modify
- Data overview: Categorize results across substances, reactions, documents, targets, or suppliers
- Preview key results: View the top three entries for any data type
- Access full results: Click View Results for complete results for filtering and further analysis
- Inset: Preview top hits, and see key properties and structures



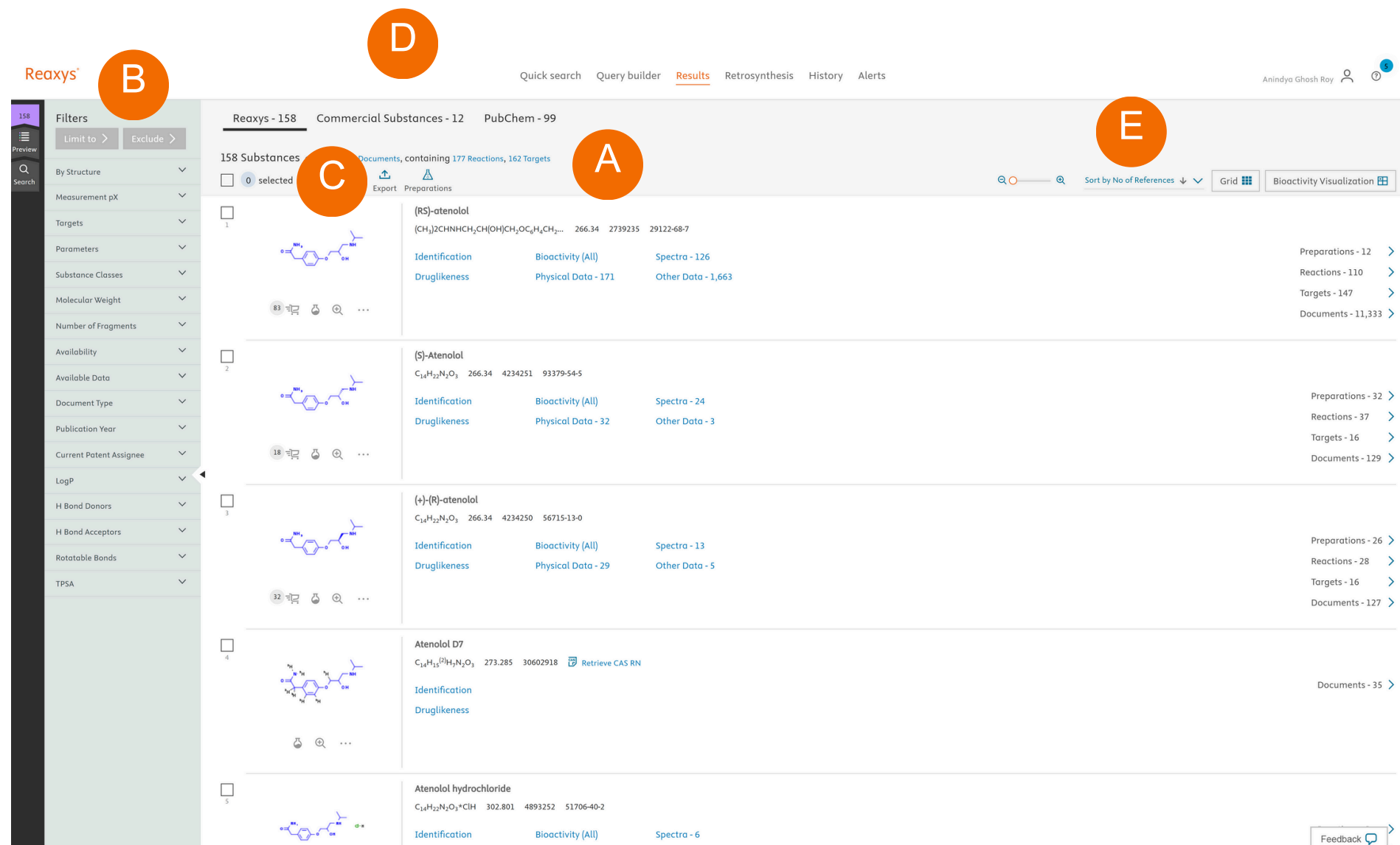
The screenshot shows the search results page for the query "her2" AND [structure]. The interface includes a top navigation bar with links for Quick search, Query builder, Results, Retrosynthesis, History, and Alerts. The main content area displays a list of results categorized by type: Targets (2), Substances (1), Documents (11), and a detailed view for Substances (44,116). The detailed view shows the top 3 results for Substances, including chemical structures and key properties for cis-Octadecenoic acid, quercetin, and doxorubicin. Annotations A-F highlight specific features: A points to the search term display, B points to the New/Edit buttons, C points to the structure and target filters, D points to the Preview Results button, E points to the View Results button, and F points to the detailed result view.



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

Results

- Navigate categories: Switch between results types
- Apply filters: Refine searches using multiple filters like Limit or Exclude
- Export data: Open the Export dialog for dataset extraction
- Change database scope: Use the dropdown to switch between Reaxys and other databases
- Sort results: Sort results by relevant criteria using *category-specific options*



The screenshot shows the Reaxys search results page for a query. The interface includes a left sidebar with filters (B), a top navigation bar with database tabs (D), a search bar and sorting options (E), and a main results table (A). The results table lists chemical compounds with their structures, names, and various data links.

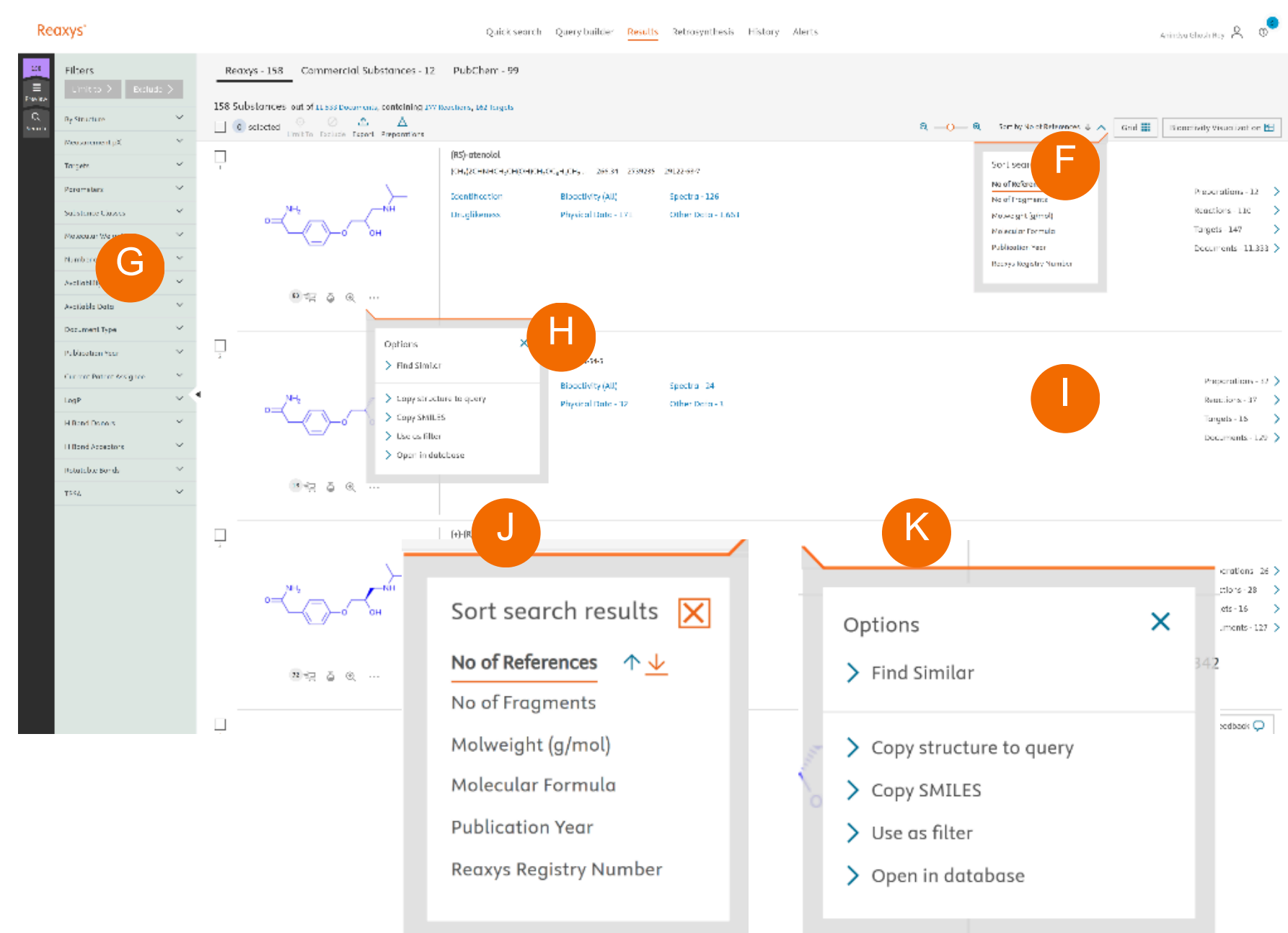
Compound	Chemical Formula	Identification	Bioactivity (All)	Spectra	Other Data	Preparations	Reactions	Targets	Documents
(R)-atenolol	<chem>C14H22N2O3</chem>	266.34	4234251	93379-54-5		12	110	147	11,333
(S)-Atenolol	<chem>C14H22N2O3</chem>	266.34	4234251	93379-54-5		32	37	16	129
(+)-[R]-atenolol	<chem>C14H22N2O3</chem>	266.34	4234250	56715-13-0		26	28	16	127
Atenolol D7	<chem>C14H13D7N2O3</chem>	273.285	30602918		Retrieve CAS RN				35
Atenolol hydrochloride	<chem>C14H22N2O3.ClH</chem>	302.801	4893252	51706-40-2					



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.

Results

- a. Dynamic results filtering: Each results category has unique options
- b. Commercial substance availability: Use the shopping cart icon to check substance availability across suppliers (see inset J)
- c. Structure-based analysis: Refine synthesis plans and structure details based on drug-likeness properties and real spectra information
- d. Explore document links: Access key data excerpts and related result sets
- e. Inset: Displays commercial availability across suppliers
- f. Structure-based analysis: Options for structure-based refinements and database exploration



The screenshot displays the Reaxys search results page for the query "(R,S)-atenolol". The main results area shows 158 substances, with 12 commercial substances and 99 publications. The results are organized into a table with columns for chemical structure, name, and various properties. Several inset windows are overlaid on the main results area, each labeled with a letter in an orange circle:

- G**: A sidebar menu showing various filters and options.
- H**: A context menu for a specific result, showing options like "Find Similar", "Copy structure to query", "Copy SMILES", "Use as filter", and "Open in database".
- I**: A context menu for a specific result, showing options like "Find Similar", "Copy structure to query", "Copy SMILES", "Use as filter", and "Open in database".
- J**: A context menu for a specific result, showing options like "Find Similar", "Copy structure to query", "Copy SMILES", "Use as filter", and "Open in database".
- K**: A context menu for a specific result, showing options like "Find Similar", "Copy structure to query", "Copy SMILES", "Use as filter", and "Open in database".
- F**: A context menu for a specific result, showing options like "Find Similar", "Copy structure to query", "Copy SMILES", "Use as filter", and "Open in database".



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

Results: Filter options

- Substance results: Filter by structure, molecular weight, pH, availability, publication year and patent assignee
- Commercial substance results: Filter by supplier, stock, price, purity, location and package size
- 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.

A

Filters: Reaxys - 158 Commercial Substances - 12 PubChem - 99

By Structure

Measurement pH

Toxigenicity

Reactions

Substance Class

Molecular Weight

Availability

Commercial Suppliers

Supplier

Stock Availability

Price

Package Size

Location

Publication Year

Patent Assignee

Filter by value

B

12 Substances

Atenolol

Commercial Suppliers - 82

Atenolol

Commercial Supplier

Product

Purity

Package size & price

Availability

Stock Availability

Price

Package Size

Location

Publication Year

Patent Assignee

Filter by value

C

110 Reactions out of 78

Conditions

With 1,1-dichloroethane

Experimental Procedures

Stage #1: 1,1-dichloroethane/2,3-dichloropropane/isopropanol in N,N -dimethylformamide at 60 °C for 22 h; cooled tube

Stage #2: With water in N,N -dimethylformamide at 60 °C for 12 h; solvent temperature cooled tube; regenerative reaction

In methanol, 2 h; Heating: Yes given

In methanol, at 20 °C for 20 h

Full Text

Cited 28 times

Details

Abstract

Ueda, Joseph R.; Moriguchi, Shunzo

Synthesis, 2017, vol. 45, # 6, art. no. 5645650420, p. 1711 - 1742

Full Text

Cited 16 times

Details

Abstract

Domé, Subash V.; Pelt, Paschot H.; Raj, Nikh. Manikav.

Synthetic Communications, 2009, vol. 39, # 10, p. 1619 - 1640

Full Text

Cited 13 times

Details

Abstract

Alkany, Joseph; Baskin, Adnan W.; Seid, Jonathan W.

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

Full Text

Cited 13 times

Details

Abstract

- Filters**

Limit To > Exclude >

Target Species

 - ☐ human 117
 - ☐ rat 128
 - ☐ guinea pig 10
 - ☐ lapidus 28
 - ☐ erythrocyte membranes 11
 - ☐ parathyroid glands 10
 - ☐ flower buds 10

Filter by value > View more

Target Type

 - ☐ wild 146
 - ☐ mutant 22
 - ☐ chimera 1

Measurement pH

 - ☐ inhibition constant 118
 - ☐ n50 210
 - ☐ kcat 95
 - ☐ quantiles 40
 - ☐ kmcat 10
 - ☐ inhibition percentage 37
 - ☐ papp100 14

Filter by value > View more

Substance action on target

Document Type

Publication Year

Reaxys - 221 Commercial Substances - 12 PubChem - 99

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

☐ 0 selected Limit To Exclude Export

Single protein

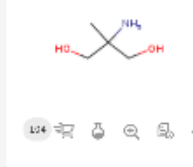
2-Oxaldehyde Dehydrogenase (sheep, Wild)

Synonyms: 2-oxaldehyde dehydrogenase
(Mutant/Chimera Details: Wild)

Show target details >

Substances - 6 Documents - 1

Most active substance:



Km (Michaelis constant)=4.2 mM

Single protein

5-hydroxytryptamine receptor 1A (rat, Wild)

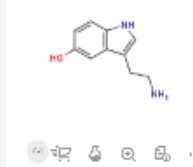
Synonyms: 5-HT-1A, 5-HT1A, 5-Hydroxytryptamine receptor 1A, 5-HT1A, htr1a, serotonin receptor 1A
(Mutant/Chimera Details: Wild)

UniProt: [P19377](#)

Show target details >

Substances - 232 Documents - 5

Most active substance:



Ki (inhibition constant)=0.01 nM

Filters

Limit To > Exclude >

Publication Year

Document Type

 - ☐ article 44
 - ☐ patent 13

Authors of Scientific Documents

Current Affiliation

Inventors of Patents

Current Patent Assignee

Patent Office

 - ☐ us 3
 - ☐ eu 1
 - ☐ jp 1
 - ☐ ep 1
 - ☐ cn 1

View more

Journal Title

Substance Classes

Reaction Classes

Index Terms (List)

 - ☐ chemical 34
 - ☐ reaction 33
 - ☐ chemical property 38
 - ☐ structure 21
 - ☐ disease 39

Reaxys - 79 Commercial Substances - 12 PubChem - 99

79 Documents with 170 Substances, 110 Reactions, 221 Targets

☐ 0 selected Limit To Exclude Export

ALKANOLAMINE DERIVATIVES FOR TREATING HYPERTENSION

Current Patent Assigned: ZENECA - US5994032, 1975, A

Patent Family Members: IL35951.0, BE746107 A, DE400514, NL7002434 A, DE2027751 A2, ...

Abstract > Claims > Bibliographic Info > Substances (24) > Reactions (22) > Full Text 7

Hit Substances (1)

Enteric coated mixture of 4-(2-Hydroxy-3-isopropylamino-propoxy) indole and sodium lauryl sulfate

Current Patent Assigned: EP-CHENOGLAS - US4281016, 1981, A

Patent Family Members: FR68594, IL52587 D0, DE325877 A, BE887221 A, DE453414, ...

Abstract > Claims > Bibliographic Info > Substances (21) > Reactions (20) > Full Text 7

Hit Substances (1)

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

Current Patent Assigned: MERCK - US4946230, 1990, A

Patent Family Members: EP170491, AT129211, DE476767 A2, EP16751 A2, US4946230 A, EP170491 B1, ...

Abstract > Claims > Bibliographic Info > Substances (22) > Reactions (32) > Full Text 7

Hit Substances (1)

Process for producing optically active atonalol and intermediate thereof

Current Patent Assigned: DAISO - US5206482, 1992, A

Patent Family Members: CA2013968 A1, CA2119308 A1, EP19568 A2, EP4001191 A, EP412068 A1, ...

Abstract > Claims > Bibliographic Info > Substances (32) > Reactions (30) > Full Text 7

Hit Substances (1)

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

WO9306462B2, 1993, A2

Current Patent Assigned: NUCLABORSA DRUGS


Office WO - View full patent family

Abstract > Index Terms > Claims > Bibliographic Info > Substances (10) > Reactions (5) > Full Text 1

Hit Substances (1)

No title

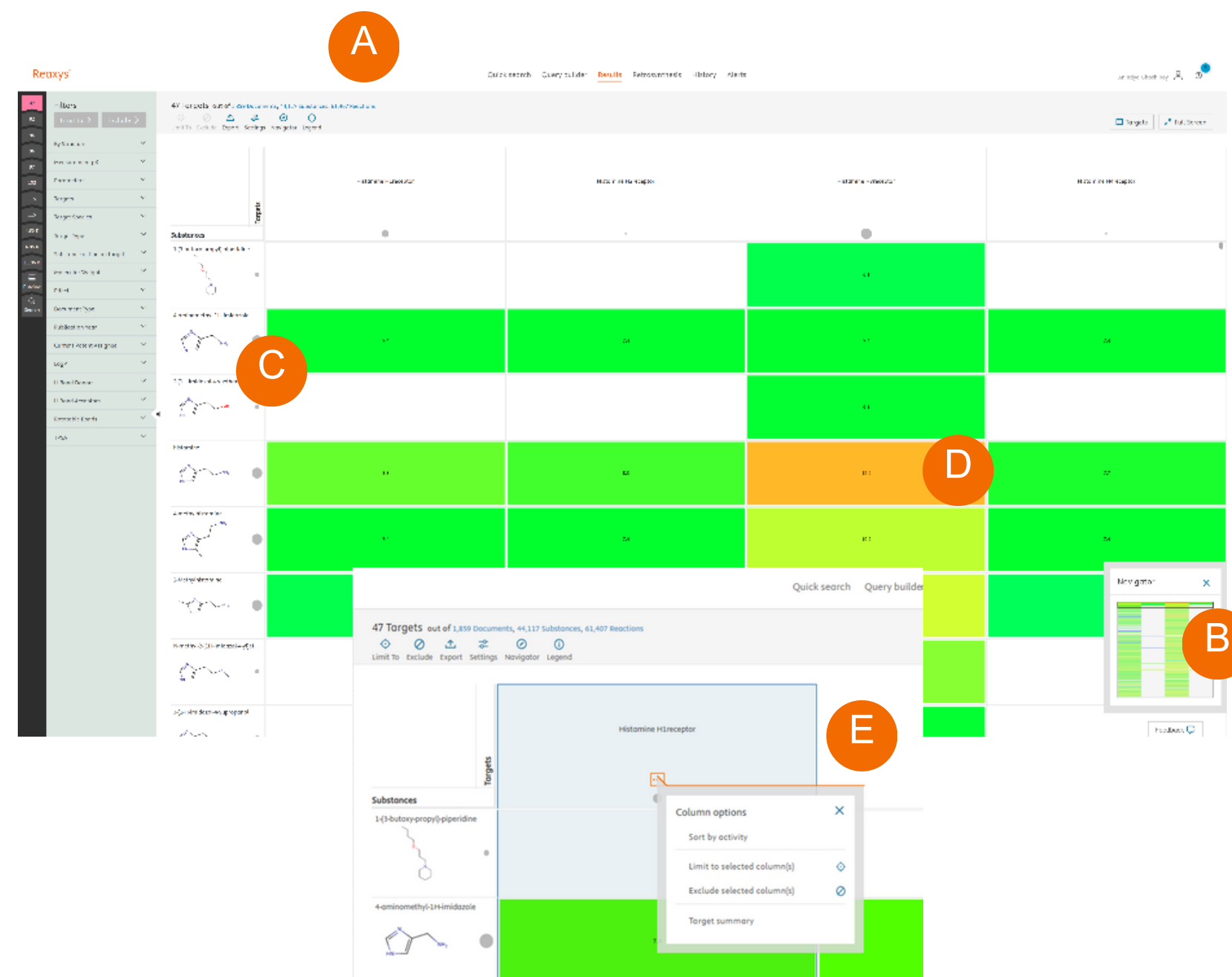
Current Patent Assigned: MPERICAL CHEMICAL INDUSTRIES - DE200751, 1970, A1 [Chem.Abstr., 1970, vol. 73, # 129318]

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

Results: Bioactivity Visualization

Use Bioactivity Visualization to explore Structure–Activity Relationships (SAR), compound potency, and target selectivity. Powered by normalized [pX values](#), the interactive matrix reveals differences in 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.
- Use the Navigator panel (bottom right) to jump to regions of interest in large matrices
- Hover over substance or target names to reveal structures, synonyms and identifiers
- Click any cell to unlock detailed bioactivity insights potency, drug-likeness, target validation and linked literature
- Customize your visualization map by excluding columns and rows



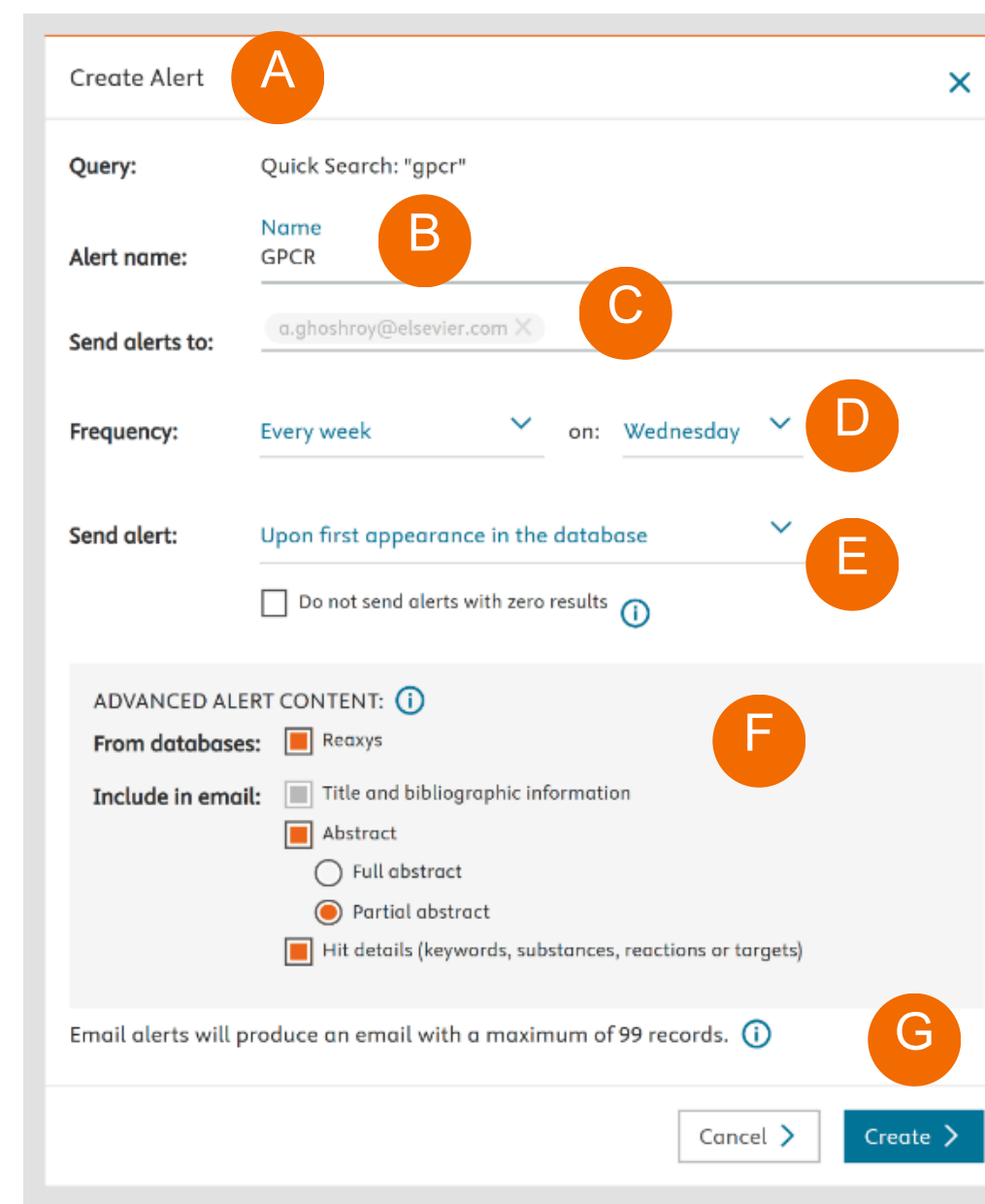
Pro Tip: Use the *Bioactivity Visualization* to spot SAR inflection points — where small structure changes lead to major shifts in potency.



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



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

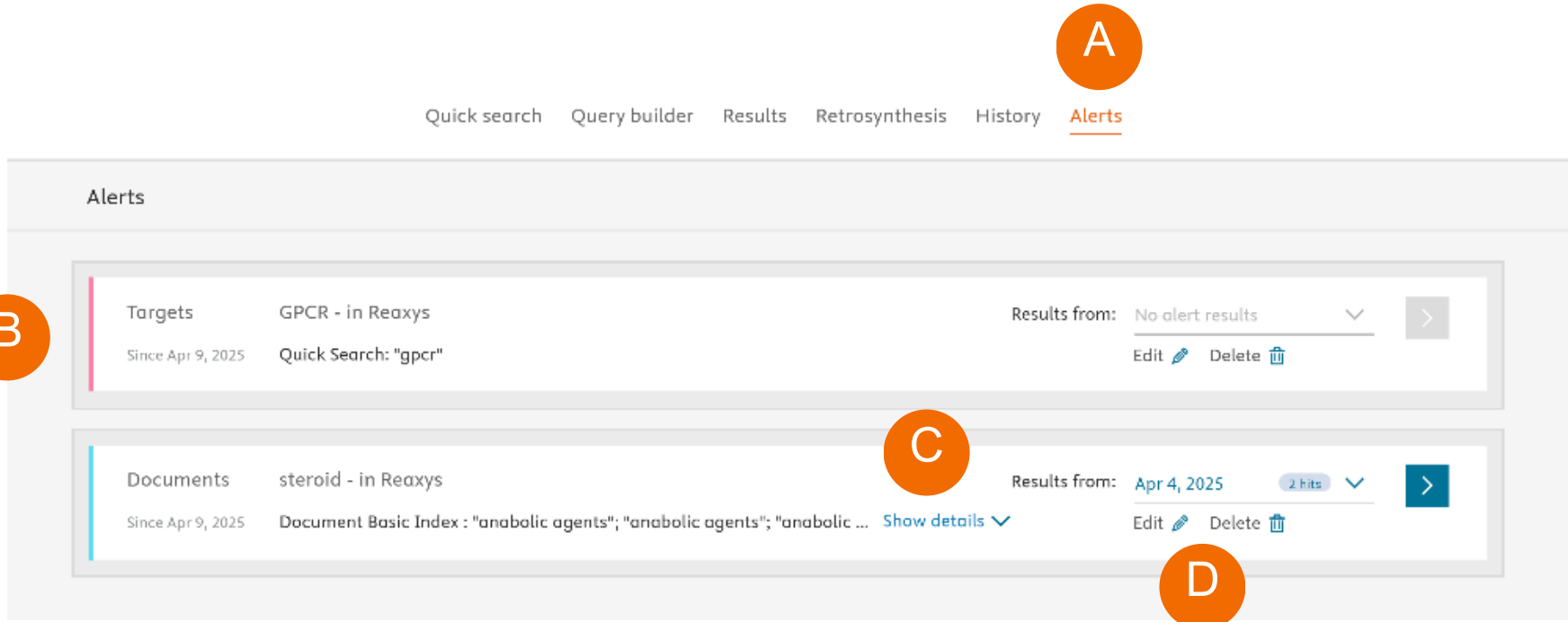
- A**: Title bar 'Create Alert' with a close button.
- Query**: 'Quick Search: "gpcr"'
- B**: 'Alert name:' field with 'GPCR' entered.
- C**: 'Send alerts to:' field with 'a.ghoshroy@elsevier.com' and a remove button.
- D**: 'Frequency:' dropdown set to 'Every week' and 'on:' dropdown set to 'Wednesday'.
- E**: 'Send alert:' dropdown set to 'Upon first appearance in the database'.
- ☐ Do not send alerts with zero results (with an information icon).
- F**: 'ADVANCED ALERT CONTENT:' section with:
 - 'From databases:' with 'Reaxys' selected.
 - 'Include in email:' section with:
 - ☐ Title and bibliographic information
 - ☒ Abstract
 - ☐ Full abstract
 - ☒ Partial abstract
 - ☒ Hit details (keywords, substances, reactions or targets)
- G**: Footer text: 'Email alerts will produce an email with a maximum of 99 records.' with an information icon.
- Buttons: 'Cancel >' and 'Create >'.



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.



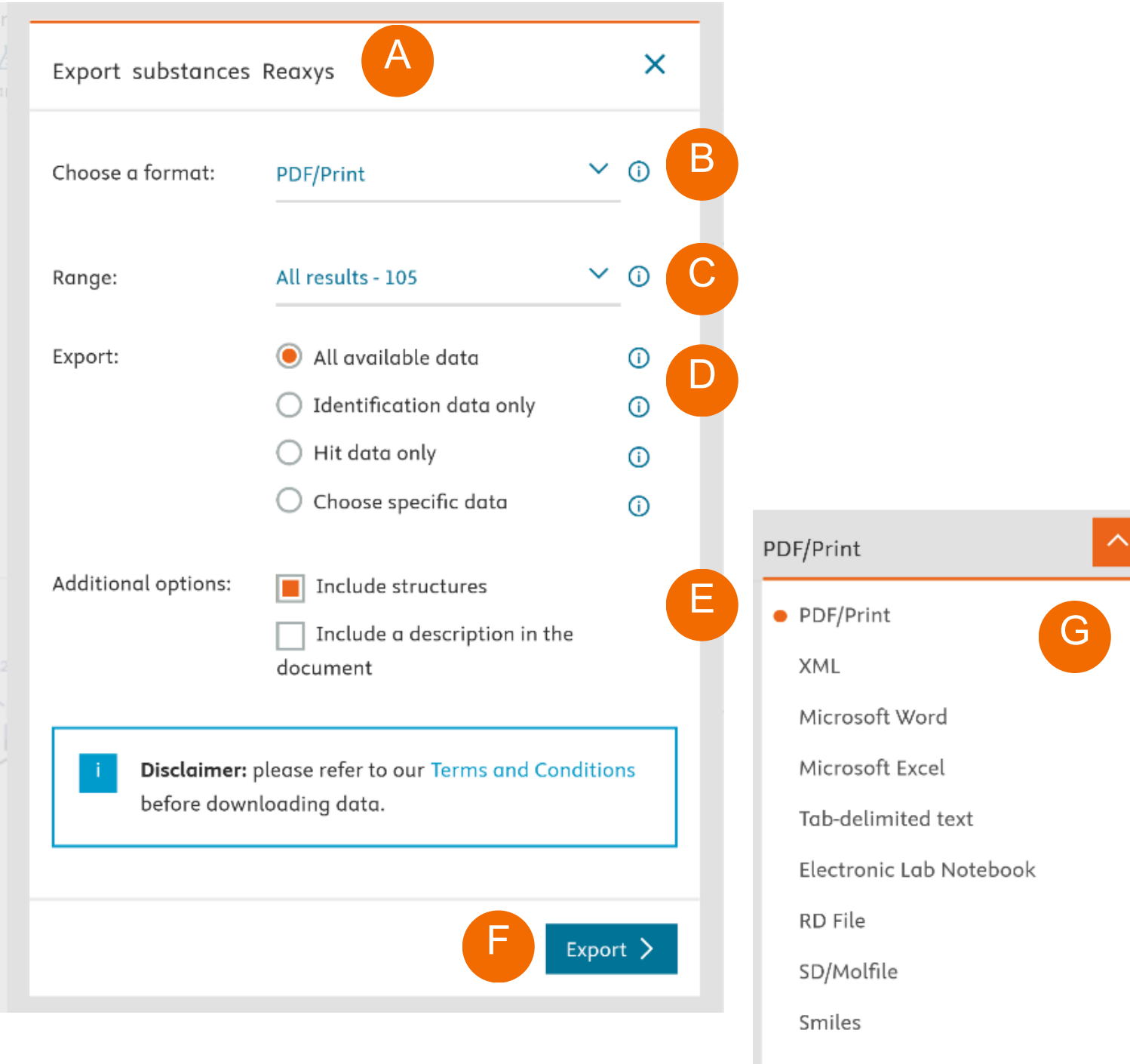
The screenshot shows the 'Alerts' tab in a software interface. At the top, a navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts' (highlighted with an orange circle 'A'). Below the navigation bar, the 'Alerts' section displays a list of alerts. The first alert, labeled with an orange circle 'B', is for 'Targets' with the query 'GPCR - in Reaxys' and 'Quick Search: "gpcr"', created 'Since Apr 9, 2025'. It shows 'Results from: No alert results' and has 'Edit' and 'Delete' buttons. The second alert, labeled with an orange circle 'C', is for 'Documents' with the query 'steroid - in Reaxys' and 'Document Basic Index : "anabolic agents"; "anabolic agents"; "anabolic ..."', also created 'Since Apr 9, 2025'. It shows 'Results from: Apr 4, 2025' with '2 hits' and a 'Show details' link. It also has 'Edit' and 'Delete' buttons. An orange circle 'D' points to the 'Delete' button of the second alert.



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

Results: Export

- Open export window: Click Export from the Results page to access export options
- Select format: Choose the file format (see G), including PDF, Word, Excel, SDfile and others
- Define range: Export all results, selected results or a custom selection
- Choose data to export: Select all data, ID-only, hit-only or specific fields
- Additional options: Include structures or descriptions to enrich reports
- Initiate export: Click Export to start or cancel anytime
- Export formats (inset): Export all results, selected results or a custom selection



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 >

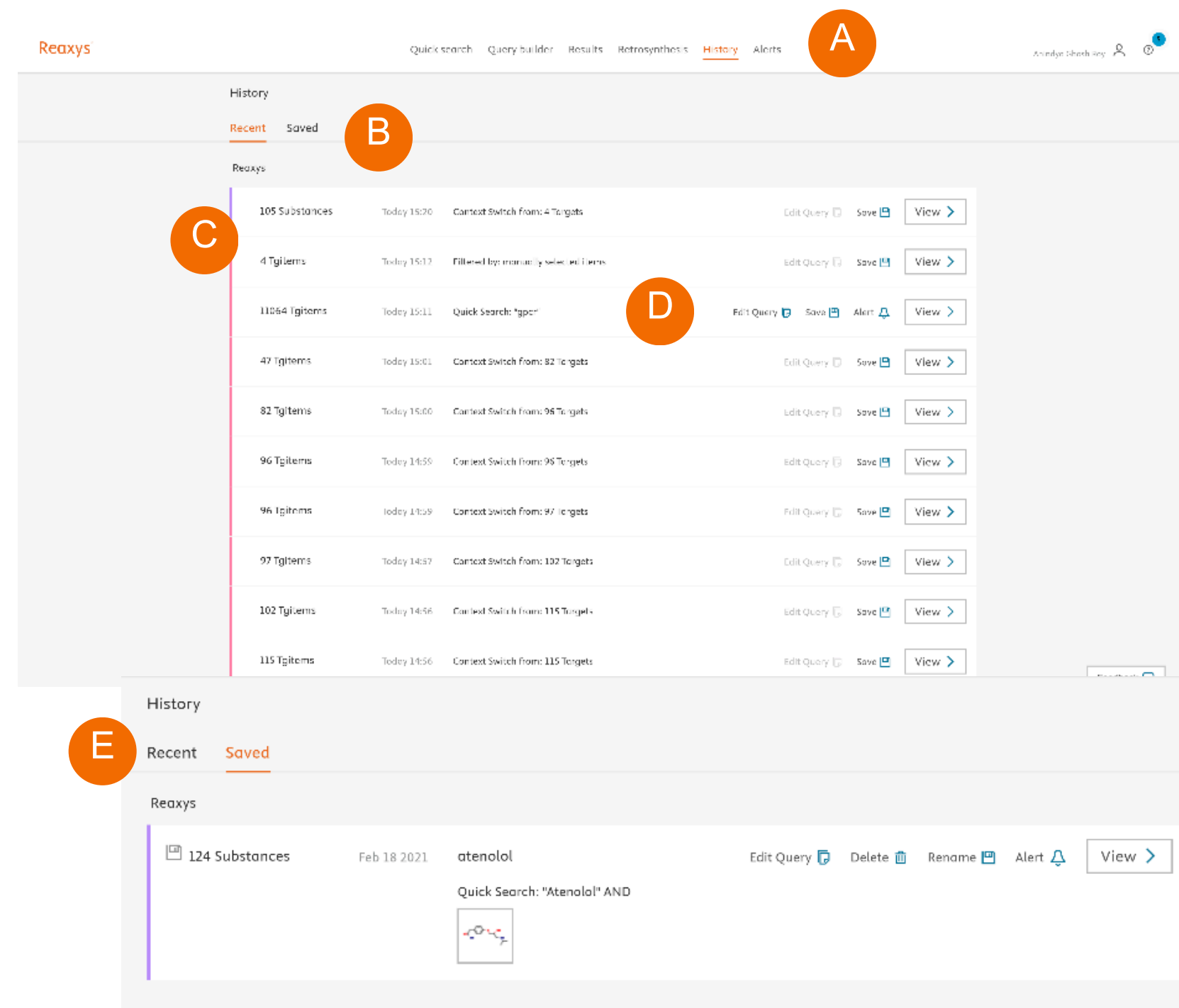
PDF/Print

- PDF/Print
- XML
- Microsoft Word
- Microsoft Excel
- Tab-delimited text
- Electronic Lab Notebook
- RD File
- SD/Molfile
- Smiles

 **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



The screenshot displays the Reaxys interface with the 'History' tab selected. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. Callout A points to the 'History' tab. Callout B points to the 'Recent' sub-tab. Callout C points to the 'Reaxys' section header. Callout D points to the 'Edit Query' button in the recent queries list. Callout E points to the 'Saved' sub-tab in the inset window.

Recent	Saved	
Reaxys		
105 Substances	Today 15:20	Context Switch from: 4 Targets
4 TgItems	Today 15:12	Filtered by manually selected items
11064 TgItems	Today 15:11	Quick Search: "gpc"
47 TgItems	Today 15:01	Context Switch from: 82 Targets
82 TgItems	Today 15:00	Context Switch from: 98 Targets
96 TgItems	Today 14:59	Context Switch from: 98 Targets
96 TgItems	Today 14:58	Context Switch from: 97 Targets
97 TgItems	Today 14:57	Context Switch from: 102 Targets
102 TgItems	Today 14:56	Context Switch from: 115 Targets
115 TgItems	Today 14:56	Context Switch from: 115 Targets

Inset E (Saved queries):

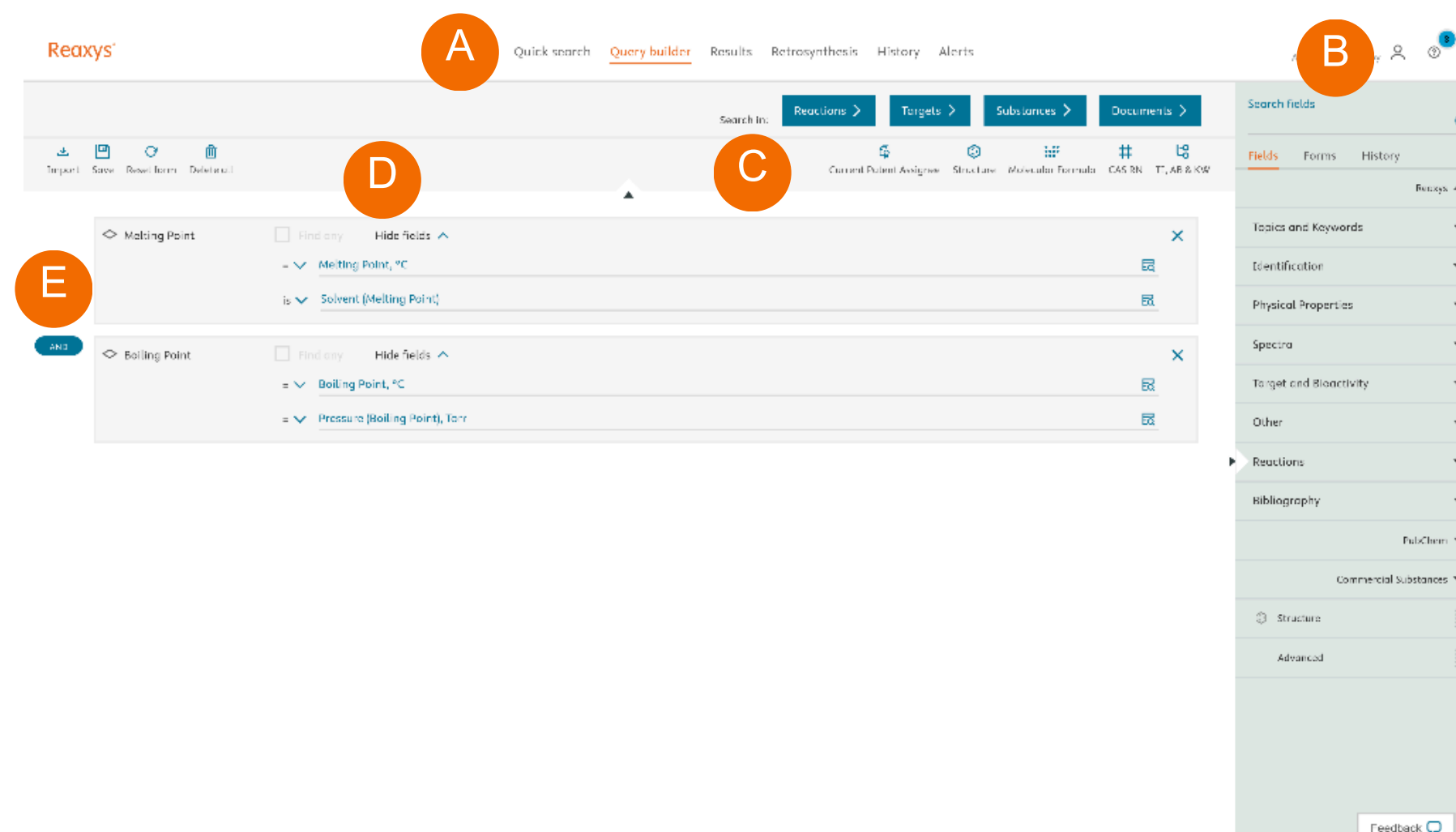
Recent	Saved	
Reaxys		
124 Substances	Feb 18 2021	atenolol
Quick Search: "Atenolol" AND		
		



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

Query Builder

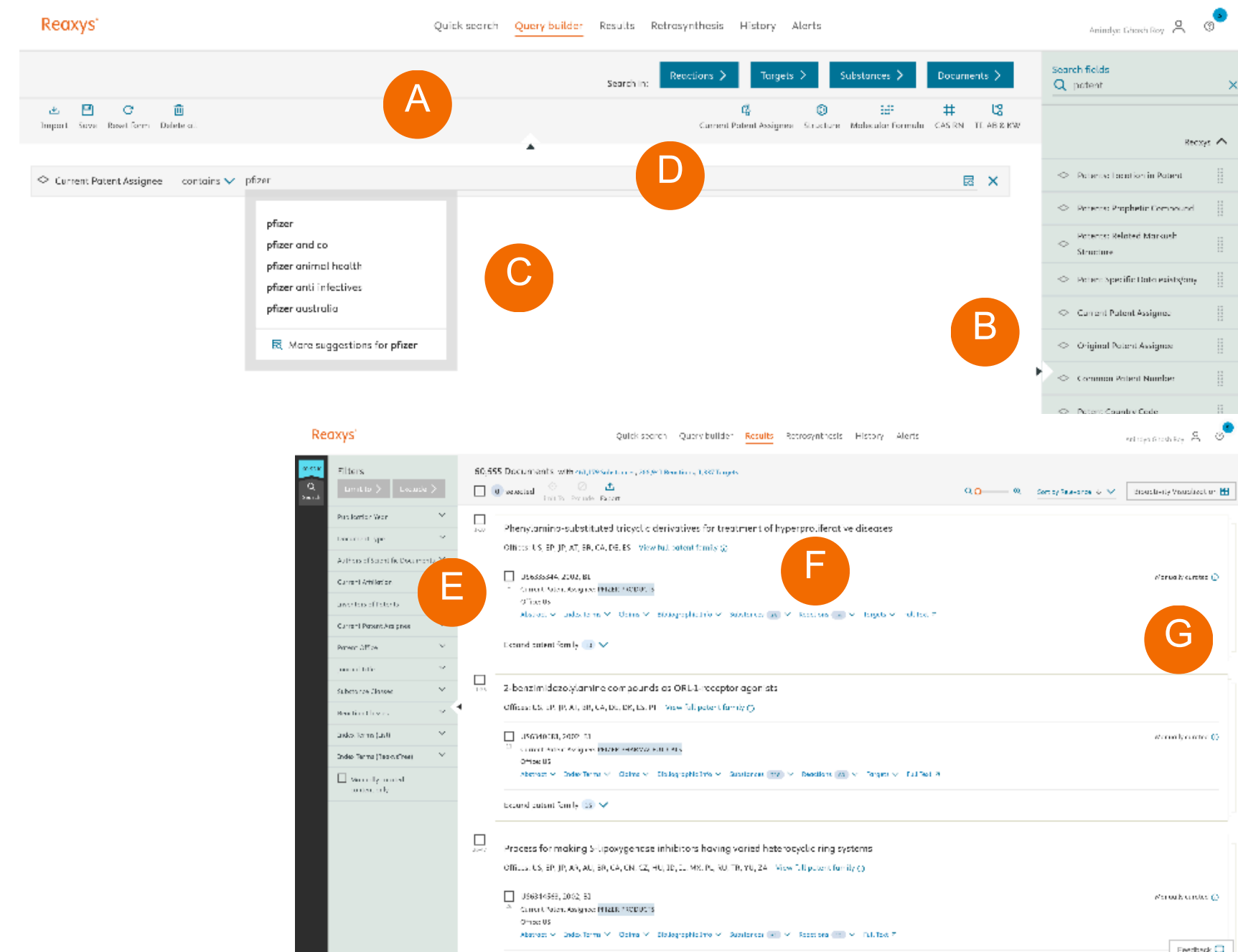
- Open Query Builder: Launch from the top navigation or use Edit Query to customize your search
- Add fields with drag-and-drop: Combine chemical, biological and patent fields (e.g., Melting Point, CAS Numbers, Patent Assignee)
- Combine science and IP data: Find high-potency compounds with known synthesis routes, not patented by competitors
- Save, reuse and set alerts: Save queries for later use and set alerts for new data (substances, reactions, patents)
- 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

- Launch Query Builder from the main navigation
- Select current patent assignee, original assignee or ultimate owner (under Bibliography) to focus on ownership data across substances, reactions and documents
- 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
- Choose result types: Select Substances, Reactions, Targets or Documents to explore data linked to the selected assignee
- Filter and analyze results: Use the Results page to filter by target, structure or property and identify patent-linked compounds, reactions and trends
- View the list of patent families: Click to check the patent entire family cluster
- Data manually curated or automated: See if data is curated manually or automatically generated



The top screenshot shows the Reaxys Query Builder interface. The 'Query builder' tab is active. The search bar contains 'Pfizer'. A dropdown menu shows suggestions: 'Pfizer', 'Pfizer and co', 'Pfizer animal health', 'Pfizer anti-infectives', 'Pfizer australia', and 'More suggestions for Pfizer'. The 'Current Patent Assignee' is set to 'Pfizer'. The 'Search fields' dropdown is set to 'patent'. The 'Results' page shows a list of patent families with details such as 'Phenylamino-substituted triazole derivatives for treatment of hyperproliferative diseases' and 'Benzimidazole compounds as ORL1-receptor agonists'.



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

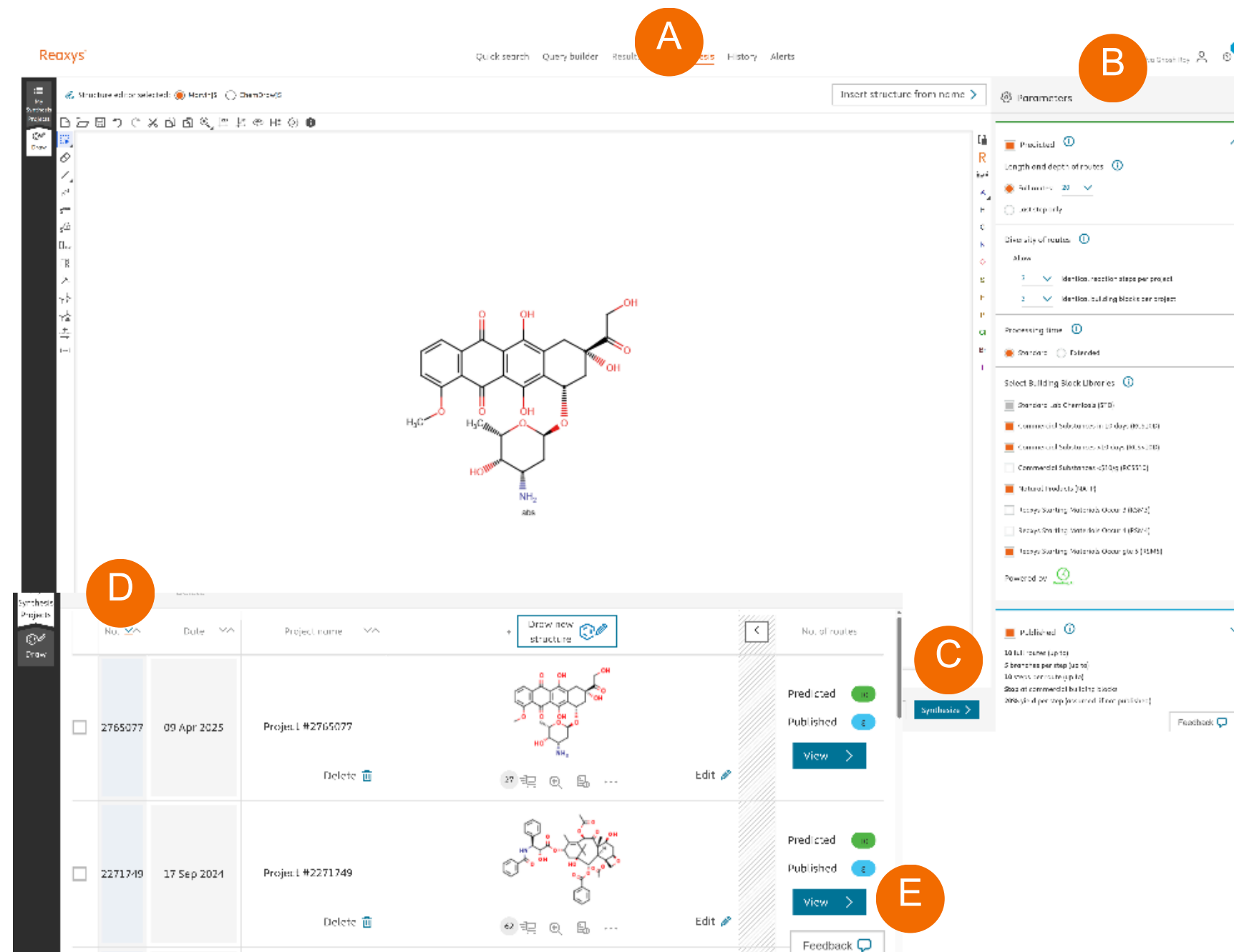


Learn more: [Query builder articles](#)

Retrosynthesis: Published

Set up a Retrosynthesis Query

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



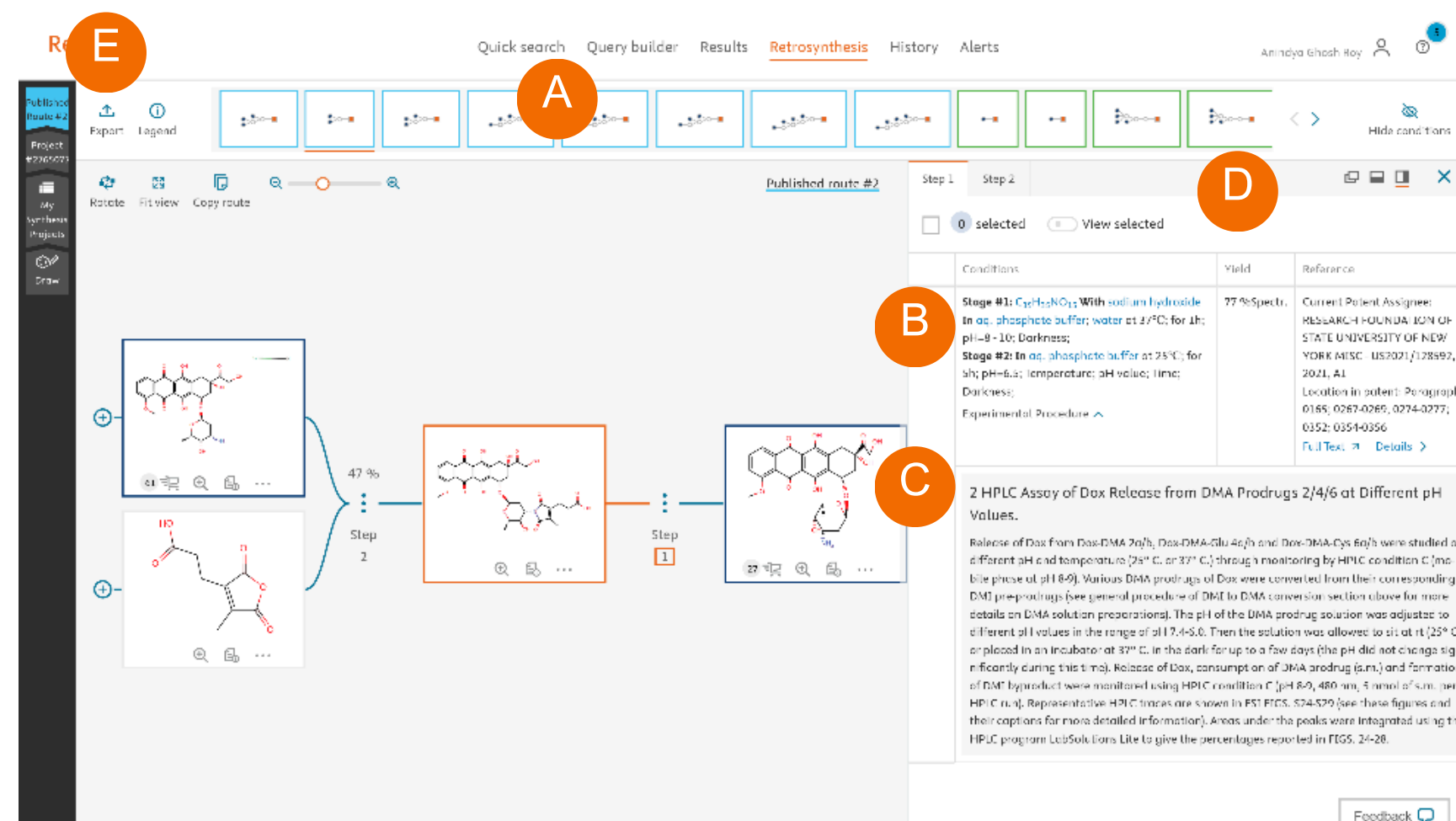
The screenshot displays the Reaxys Retrosynthesis interface. At the top, the 'Structure editor selected' section shows a chemical structure of a complex molecule. The 'Parameters' panel on the right allows users to define search criteria, including 'Published' routes, 'Length and depth of routes', 'Diversity of results', and 'Select Building Block Libraries'. The 'Synthesize' button is prominently displayed. Below the editor, the 'Projects' table lists generated retrosynthetic projects, including their IDs, dates, names, and the number of routes. The table includes columns for 'No.', 'Date', 'Project name', and 'No. of routes'. The first project is 'Project L #2765077' dated '09 Apr 2025', and the second is 'Project L #2271749' dated '17 Sep 2024'. Each project entry includes a 'Delete' button and a 'View' button. The 'View' button for the first project is highlighted with a red circle 'C'. The 'Synthesize' button is highlighted with a red circle 'B'. The 'Structure editor selected' section is highlighted with a red circle 'A'. The 'Projects' table is highlighted with a red circle 'D'. The 'View' button for the second project is highlighted with a red circle 'E'.



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

- Toggle between synthesis routes and reaction steps: Use the navigation buttons to switch between alternative synthesis plans and step-by-step pathways.
- Review experimental conditions: View reaction yields, temperatures, solvents and literature references for each step.
- Access experimental procedures: When available, open full-text procedures to replicate or assess reactions
- Switch layout or use the *Fit View*: Toggle between vertical/horizontal layout and zoom to fit complex pathways more easily
- Export synthesis routes: Download structure diagrams and experimental data, or export directly to ChemDraw for lab planning or collaboration



The screenshot displays the Retrosynthesis software interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Retrosynthesis (selected), History, and Alerts. Below these are buttons for Export, Legend, and a series of icons for navigating between different synthesis routes and steps. The main area shows a reaction pathway for 'Published route #2'. It includes chemical structures for the starting materials, intermediates, and the final product, connected by arrows indicating the reaction steps. A 'Fit View' button is visible. On the right side, there is a table with experimental conditions, yields, and references for the selected step.

Conditions	Yield	Reference
Stage #1: $C_{12}H_{15}NO_{12}$ With sodium hydroxide in ac. phosphate buffer; water at $25^{\circ}C$; for 1h; pH=9-10; Darkness; Stage #2: In ac. phosphate buffer at $25^{\circ}C$; 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 >

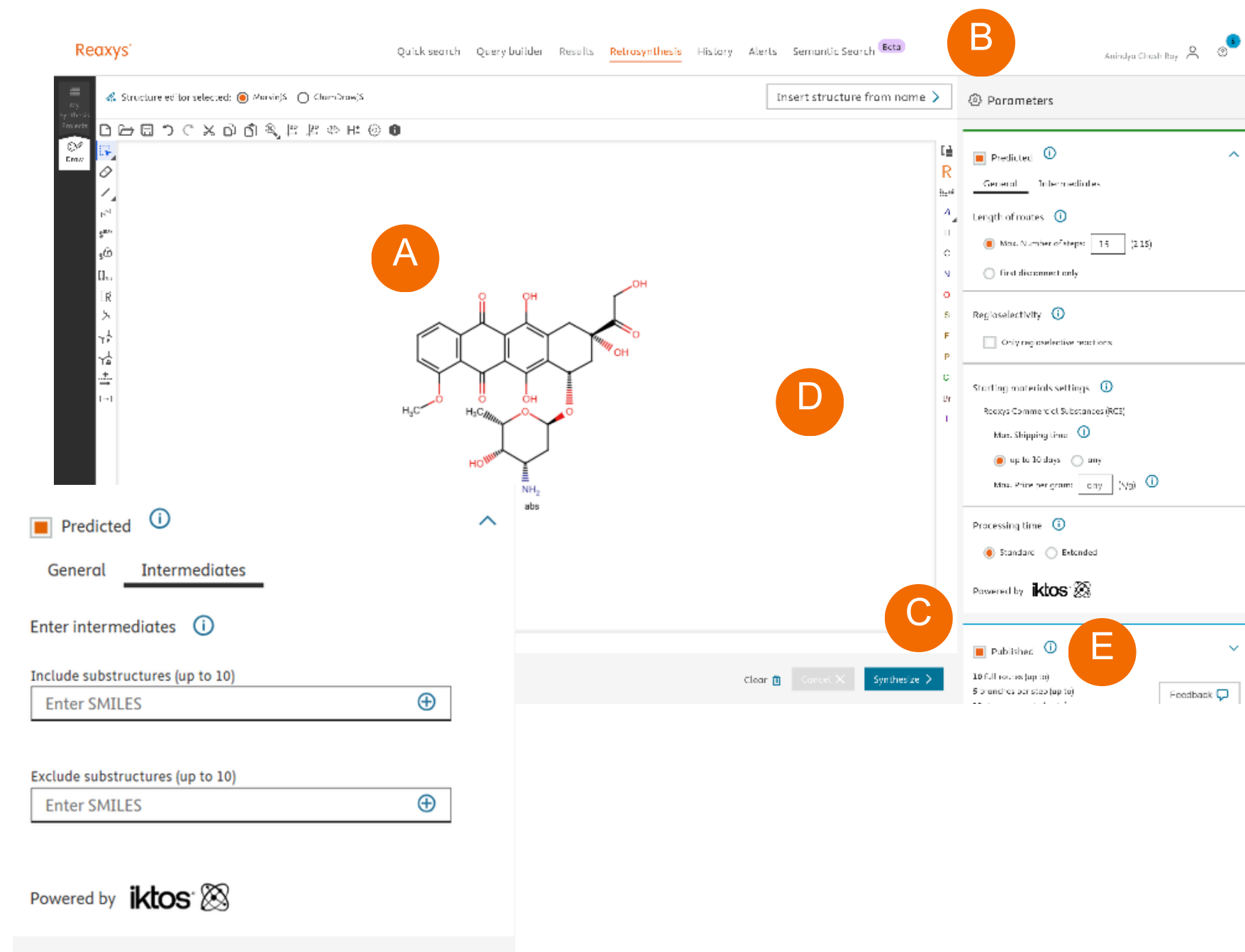
Below the table, there is a section titled '2 HPLC Assay of Dax Release from DMA Prodrugs 2/4/6 at Different pH Values.' which contains detailed text about the assay procedure and results.



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

- Open the Retrosynthesis page and draw your compound. Use the structure editor to sketch or import a compound of interest
- Select Predicted Synthesis Route: Only visible if your institution has access to the Predictive Retrosynthesis module
- Adjust parameters: Customize diversity, speed and building blocks to guide AI output
- Click Synthesize: Generate AI-predicted synthetic routes based on internal algorithms and published knowledge
- 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.

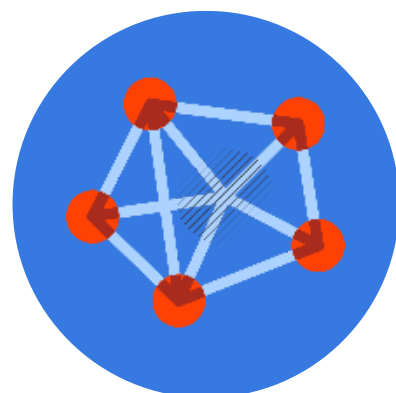
Learn more: [\[Pending AI Guide\]](#) · [\[Iktos Guide\]](#)



4. Reaxys core content

Reaxys core content

Explore the most comprehensive validated chemistry and bioactivity insights



1. Substances

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



2. Reactions

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



3. Documents

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



4. Patents

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



5. Bioactivities

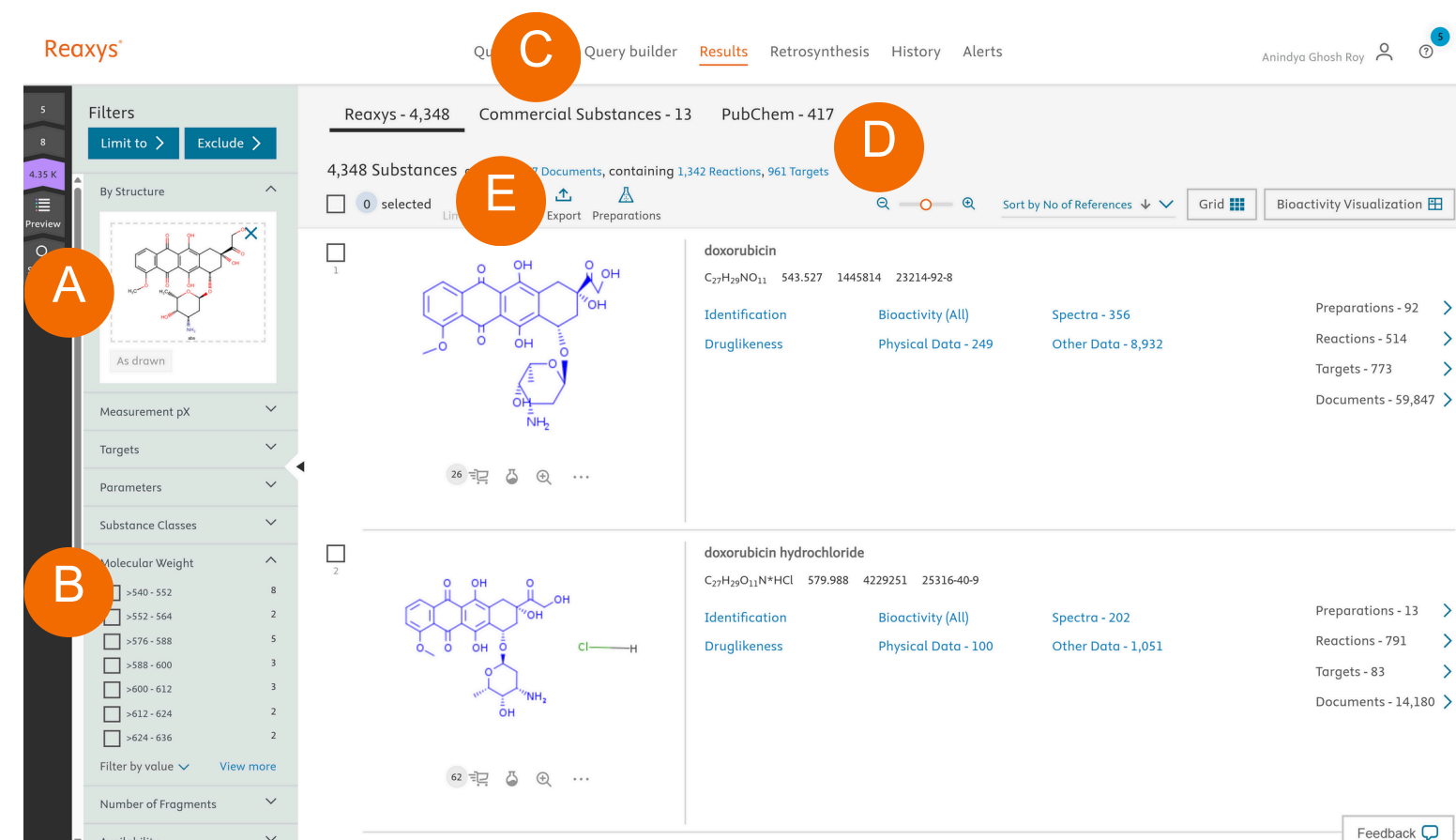
Discover tens of millions of curated bioactivity datapoints — mapped to targets, SAR, MoA and therapeutic outcomes.

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


Substances





Design new molecules with experimentally validated substances.

- Start with chemical structure or name input
- Filter by physicochemical properties (e.g., logP, MW, solubility)
- Toggle supplier availability for sourcing: Explore commercial availability across hundreds of global suppliers — directly linked to Reaxys substance records
- Explore linked reactions, targets and literature
- Export or reuse the curated dataset



The screenshot displays the Reaxys web application interface. On the left, a sidebar (A) contains filters for 'By Structure', 'Measurement pX', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', 'Number of Fragments', and 'Availability'. The top navigation bar (C) includes 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. The main results area (D) shows a list of substances, including 'doxorubicin' and 'doxorubicin hydrochloride'. A detailed view (E) of a substance is shown on the right, displaying its chemical structure, name, molecular formula, and various data points like 'Identification', 'Bioactivity (All)', 'Spectra', and 'Preparations'.

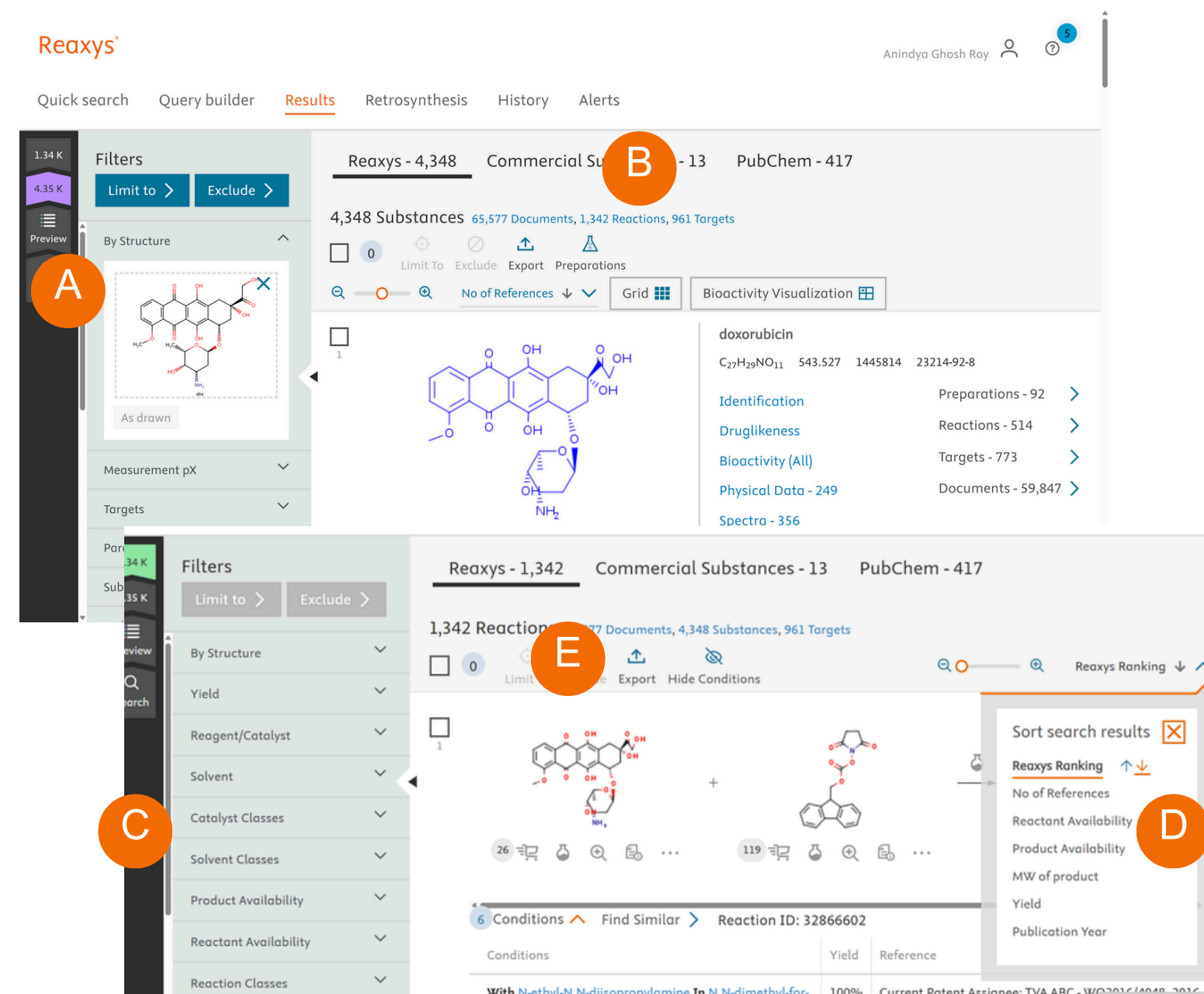
 **Pro Tip:** Use Reaxys to find, validate and source compounds — instantly.

-  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.

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



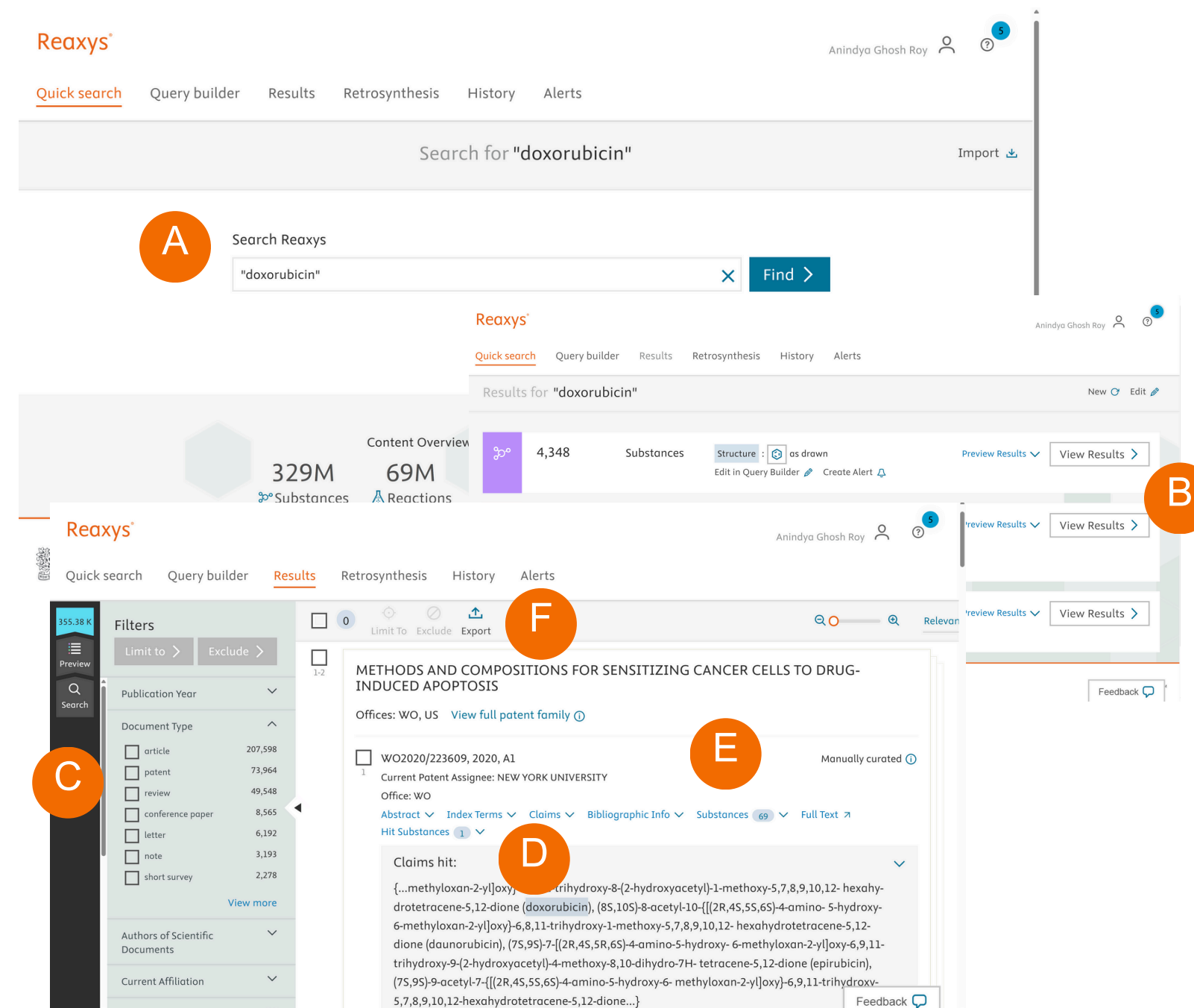
The screenshot displays the Reaxys web application interface. At the top, the user is logged in as Anindya Ghosh Roy. The main navigation bar includes 'Quick search', 'Query builder', 'Results' (highlighted), 'Retrosynthesis', 'History', and 'Alerts'. The search results are categorized by 'Reaxys - 4,348', 'Commercial Substances - 13', and 'PubChem - 417'. The results list shows '4,348 Substances', '65,577 Documents', '1,342 Reactions', and '961 Targets'. A chemical structure of doxorubicin is shown, along with its molecular formula $C_{27}H_{29}NO_{11}$ and various identifiers. A sidebar on the left (A) contains filters for 'By Structure', 'Measurement pX', and 'Targets'. A detailed reaction view (C) shows the synthesis of doxorubicin from its precursors, with a 'Sort search results' dialog (D) open, allowing users to sort results by 'Reaxys Ranking', 'No of References', 'Reactant Availability', 'Product Availability', 'MW of product', 'Yield', and 'Publication Year'. The reaction details include 'Reaction ID: 32866602' and 'Yield: 100%'.

 **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.

- Run a structure, substance or keyword search
- View documents result
- Filter by source type (e.g., journal vs. patent)
- Access highlighted chemical context in the full-text
- Trace back to linked substances, reactions and bioactivity
- Export and reuse filtered references for reporting, compliance or formulation insights



The screenshot displays the Reaxys web interface. At the top, the user is logged in as Anindya Ghosh Roy. The navigation bar includes links for Quick search, Query builder, Results, Retrosynthesis, History, and Alerts. A search bar at the top right contains the text "Search for 'doxorubicin'" with an "Import" button. Below this, a search box labeled "Search Reaxys" contains the text "doxorubicin" and a "Find" button. The results section shows "Results for 'doxorubicin'" with a count of 4,348. It includes a "Content Overview" section with "329M Substances" and "69M Reactions". A list of results is shown, with the first result being a patent document: "METHODS AND COMPOSITIONS FOR SENSITIZING CANCER CELLS TO DRUG-INDUCED APOPTOSIS". The document details include the patent number "WO2020/223609, 2020, A1", the assignee "NEW YORK UNIVERSITY", and the office "WO". The "Claims hit" section is expanded, showing a list of chemical structures and their corresponding patent claims. The interface also features a "Filters" sidebar on the left, a "Limit To" section, and a "Feedback" button at the bottom right.

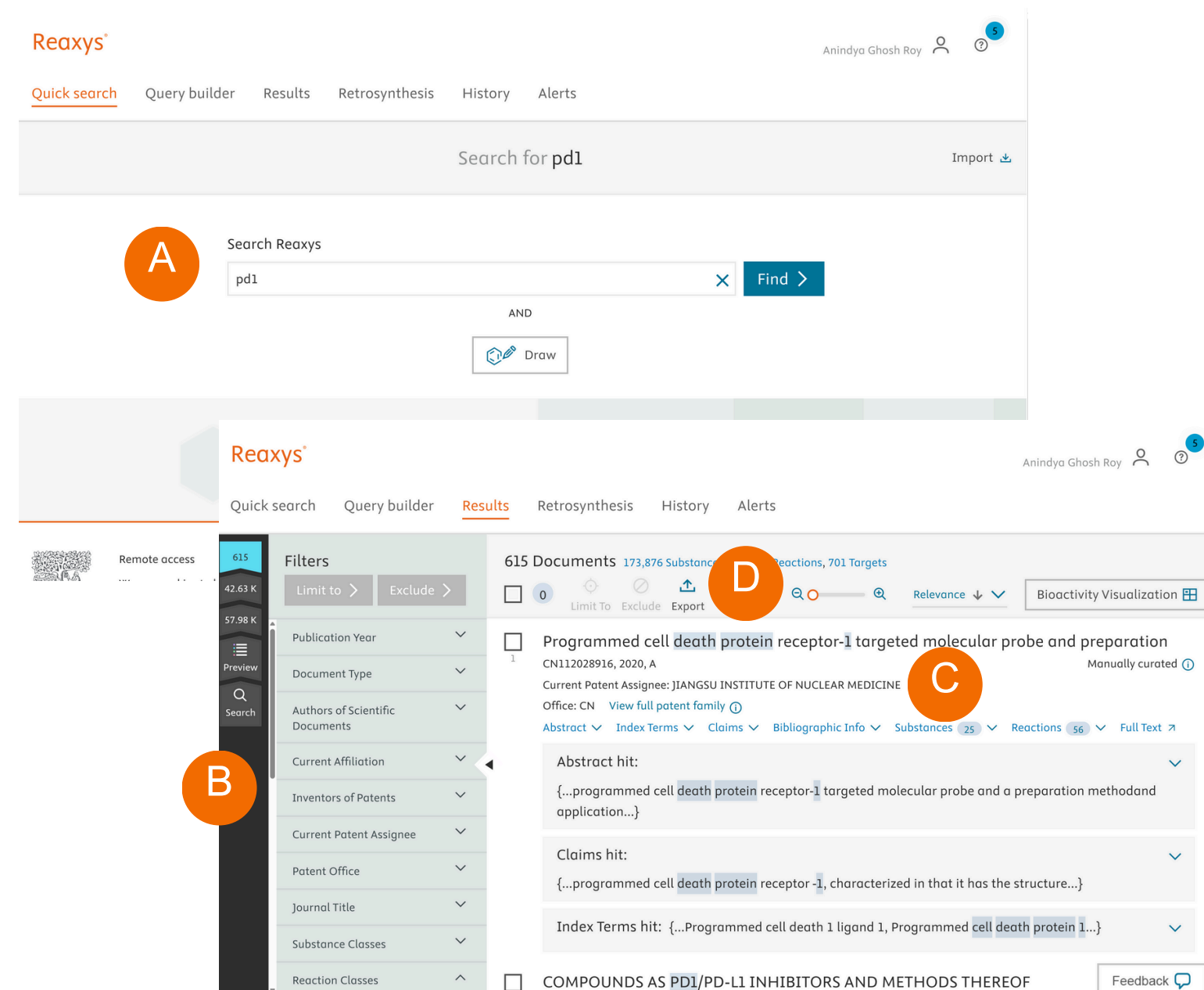


Pro Tip: Link documents directly to compounds and reactions and skip generic keyword mining to access real experimental insights, faster.


Patents


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

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



The screenshot displays the Reaxys patent search interface. At the top, the 'Quick search' tab is active. A search bar contains the keyword 'pd1', with a 'Find' button to its right. Below the search bar, a 'Draw' button is visible. The results section shows 615 documents, 173,876 substances, and 701 targets. A sidebar on the left contains a 'Filters' panel with various criteria like 'Publication Year', 'Document Type', and 'Patent Office'. The main results area displays a list of documents, with the first entry titled 'Programmed cell death protein receptor-1 targeted molecular probe and preparation'. This entry includes an 'Abstract hit', 'Claims hit', and 'Index Terms hit'. A 'Bioactivity Visualization' button is located at the top right of the results section.

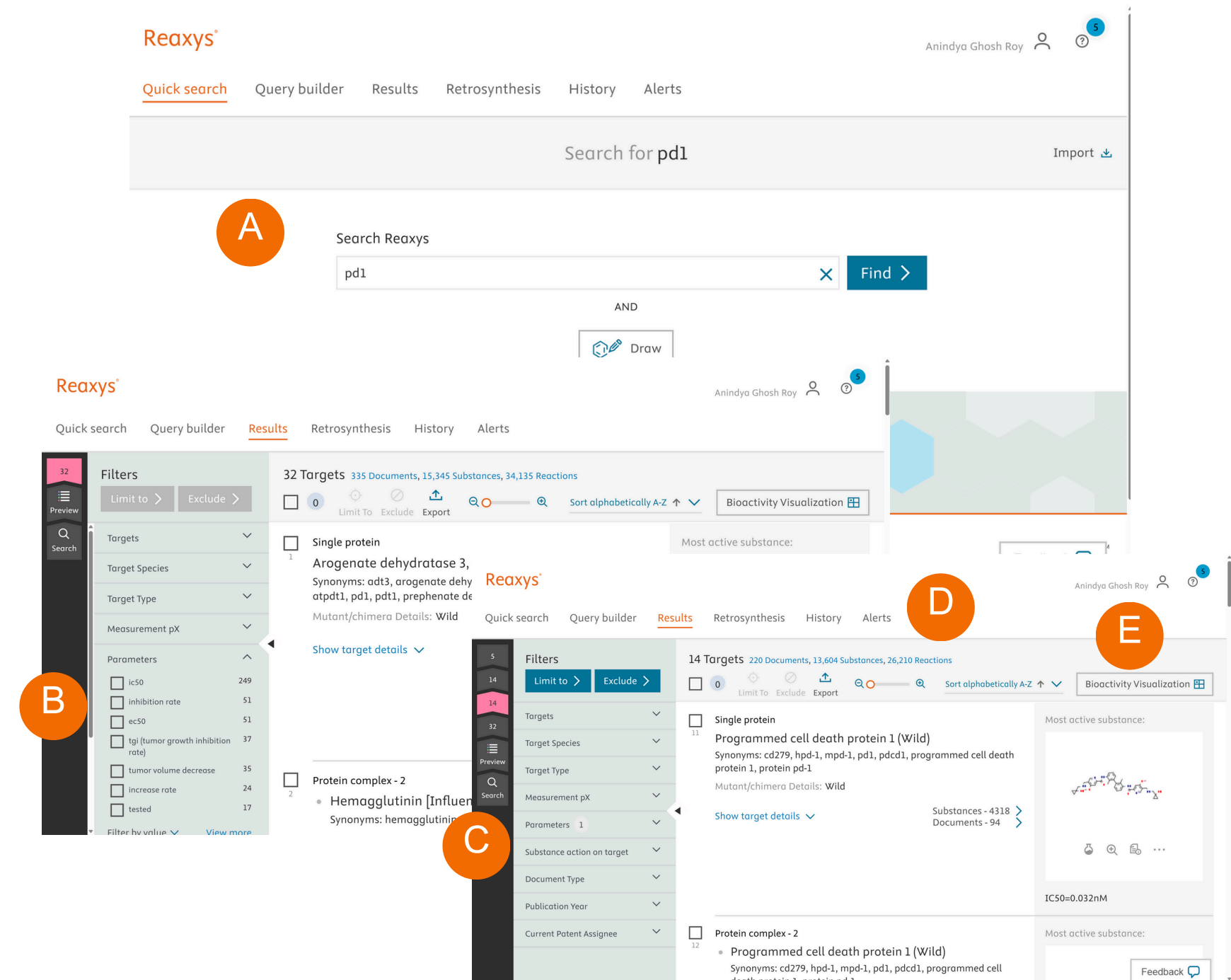
 **Pro Tip:** Mine patent databases to surface novel compounds and reactions, identify therapeutic claims, and compare protected synthetic routes across jurisdictions.

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

Bioactivities


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

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



The screenshots show the Reaxys interface with the following annotations:

- A:** The search bar at the top where 'pd1' is entered.
- B:** The left sidebar filter menu, specifically the 'Parameters' section where 'ic50' is selected.
- C:** The 'Results' page showing a list of targets, including 'Arogenate dehydratase 3' and 'Hemagglutinin [Influenza virus]'. The 'Protein complex - 2' filter is also visible.
- D:** A detailed view of a target, 'Programmed cell death protein 1 (Wild)', showing its structure and associated data.
- E:** The 'Bioactivity Visualization' panel on the right, displaying a graph of bioactivity data.

 **Pro Tip:** Use Reaxys to explore how compounds act on biological targets — and identify therapeutic potential, safety flags, or optimization paths using trusted, experimentally validated bioactivity data.

[Watch Target & Bioactivity expert tips](#)





5 - 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.



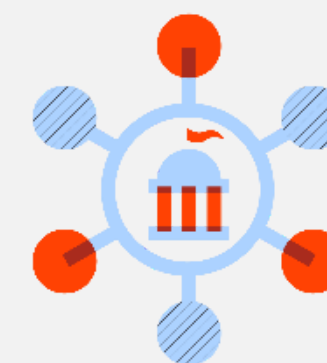
Knowledge

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.

 **Pro Tip:** [Sign in or sign up](#) to access the latest how-to tutorials and articles, courses, insights and product advancements.

Contact support: Having trouble signing in? [Try these steps](#).





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