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Reaxys[®]

Quick reference guide



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Welcome to your quick reference guide to Reaxys and Reaxys Medicinal Chemistry. This document is designed to help users navigate the interface and get started with searching, viewing and filtering results, and using alerts and other personalized features. For advice on using *Query Builder*, *Synthesis Planner* and *Heatmap*, we recommend the [tutorials in the Resource Center](#).

Note: This guide uses screenshots from the combined Reaxys and Reaxys Medicinal Chemistry solution interface. Not all features shown are available to users without a Reaxys Medicinal Chemistry subscription. Please contact your Elsevier representative for more information.

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Navigating the Reaxys home page

The screenshot shows the Reaxys home page with several callout boxes:



- A:** Points to the top navigation bar containing links for Quick search, Query builder, Results, Synthesis planner, History, and Alerts.
- B:** Points to the user profile icon in the top right corner.
- C:** Points to the search bar area, which includes the text "Search substances, reactions, documents and bioactivity data" and a list of databases: "in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, SigmaAldrich and Commercial Substances".
- D:** Points to the search input field with the placeholder text "Search Reaxys" and a "Find >" button.
- E:** Points to the "Draw" button, which is used for structure editors.
- F:** Points to the content overview statistics: "Content Overview | Latest update: 12. May 2021 >" followed by four categories: "148M Substances", "54M Reactions", "61M Documents", and "40M Bioactivities".
- G:** Points to the "Feedback" button in the bottom right corner.


At the bottom of the page, there is an Elsevier logo on the left and a RELX Group logo on the right. The footer text includes: "Copyright © 2021 Elsevier Life Sciences IP Limited. Remote access Terms and Conditions Privacy policy About content Cookies are used by this site. To decline or learn more, visit our Cookies page."

- Use the top bar to navigate between the areas of Reaxys.
- Use the person icon to access your Reaxys profile and settings. Note that if you are not signed into your personal profile, some features (e.g., email alerts, saved search history) are not available. See page 15 for more details.

Use the ? Icon to access the Resource Center.
- Use these links to learn more about the databases that Reaxys searches.
- See page 4 for more on keywords and *Quick search*.
- See page 5 for more on structure editors and *Quick search*.
- See the current document and extracted substance, reaction and bioactivity data point counts for Reaxys.
- Use this *Feedback* feature to give feedback directly to the Reaxys development team.

Using Quick search


Reaxys® **A** Quick search Query builder Results Synthesis planner History Alerts  


Search substances, reactions, documents and bioactivity data **B** Import 
in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, SigmaAldrich and Commercial Substances

Search Reaxys **C** **E** Find >

Reactions, e.g. Suzuki coupling

AND

D  Draw

F Search Reaxys  Find >

St

Chemical Names
 atenolol
 atenolol acid
 atenolol hydrochloride

Target Names
 atendo1
 atendo2
 atendo3
 atendo4
 atendo5

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 Remote access
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- Click here to return to *Quick search* from any other screen.
- Use *Import* to import a previously saved and exported Reaxys query from your desktop or other file library.
- Enter your search terms in this field. As you type, Reaxys Auto Suggest proposes chemical names, target names and concepts (see inset **F**), helping you construct the most accurate query. Note that for patent assignees, we recommend using Query Builder. See pages 16 and 17.
- Click here to open the structure editor and add a structure to your query. See page 5 for more details.
- When your *Quick search* query is ready, click *Find*. This opens the *Results preview* for the query. See page 6.
- Inset showing Reaxys Auto Suggest proposals for “aten”. Selecting one adds it to the query as a phrase.

Using the structure editors for *Quick search*

The screenshot displays the MarvinJS structure editor interface. At the top, the 'Structure editor selected' dropdown is set to 'MarvinJS' (A). To its right is the 'Insert structure from name' button (B). The main workspace (C) contains the MarvinJS logo and a drawing toolbar. On the right, the 'Search this structure as:' panel (D) lists options: 'As drawn' (selected), 'As substructure', 'Similar', 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. At the bottom of the editor, the 'Transfer to query' button is highlighted (E). Below the main interface, a dialog box (F) titled 'Create structure template from name' is open, showing a search input field with the text 'is' and a dropdown menu with options: 'is', 'starts with', 'ends with', and 'contains'.

- Select your preferred structure editor for this query, MarvinJS or ChemDrawJS. You can set your preferred structure editor in your profile settings (see page 15), but you can also change it for any given query.
- Use *Insert structure from name* to open a dialog window (see inset F) that lets you enter a chemical name or identifier and auto-generate a structure.
- Use the tools of the structure editor to create your structure or reaction drawing.
- Add options to the structure query to expand the search to substances fitting the selected parameters.
- When your drawing is ready, click *Transfer to query*.
- Inset showing *Create structure template from name* dialog with options for exact or partial names.

Navigating the *Results preview*

A Search for "atenolol"

B New Edit

C Substances 125 Structure: as drawn Edit in Query Builder Create Alert

D Preview Results View Results

E Documents 32,139 Titles, Abstracts, Keywords: "atenolol" Edit in Query Builder Create Alert

F Commercial Substances 8 Structure: as drawn Edit in Query Builder Create Alert

F Top 3 results

Structure	Identification	Physical Data	Spectra	Reactions	Targets	Documents
<chem>C1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10C11=CC=CC=C11C12=CC=CC=C12C13=CC=CC=C13C14=CC=CC=C14C15=CC=CC=C15C16=CC=CC=C16C17=CC=CC=C17C18=CC=CC=C18C19=CC=CC=C19C20=CC=CC=C20C21=CC=CC=C21C22=CC=CC=C22C23=CC=CC=C23C24=CC=CC=C24C25=CC=CC=C25C26=CC=CC=C26C27=CC=CC=C27C28=CC=CC=C28C29=CC=CC=C29C30=CC=CC=C30C31=CC=CC=C31C32=CC=CC=C32C33=CC=CC=C33C34=CC=CC=C34C35=CC=CC=C35C36=CC=CC=C36C37=CC=CC=C37C38=CC=CC=C38C39=CC=CC=C39C40=CC=CC=C40C41=CC=CC=C41C42=CC=CC=C42C43=CC=CC=C43C44=CC=CC=C44C45=CC=CC=C45C46=CC=CC=C46C47=CC=CC=C47C48=CC=CC=C48C49=CC=CC=C49C50=CC=CC=C50C51=CC=CC=C51C52=CC=CC=C52C53=CC=CC=C53C54=CC=CC=C54C55=CC=CC=C55C56=CC=CC=C56C57=CC=CC=C57C58=CC=CC=C58C59=CC=CC=C59C60=CC=CC=C60C61=CC=CC=C61C62=CC=CC=C62C63=CC=CC=C63C64=CC=CC=C64C65=CC=CC=C65C66=CC=CC=C66C67=CC=CC=C67C68=CC=CC=C68C69=CC=CC=C69C70=CC=CC=C70C71=CC=CC=C71C72=CC=CC=C72C73=CC=CC=C73C74=CC=CC=C74C75=CC=CC=C75C76=CC=CC=C76C77=CC=CC=C77C78=CC=CC=C78C79=CC=CC=C79C80=CC=CC=C80C81=CC=CC=C81C82=CC=CC=C82C83=CC=CC=C83C84=CC=CC=C84C85=CC=CC=C85C86=CC=CC=C86C87=CC=CC=C87C88=CC=CC=C88C89=CC=CC=C89C90=CC=CC=C90C91=CC=CC=C91C92=CC=CC=C92C93=CC=CC=C93C94=CC=CC=C94C95=CC=CC=C95C96=CC=CC=C96C97=CC=CC=C97C98=CC=CC=C98C99=CC=CC=C99C100=CC=CC=C100</chem>	(S)-atenolol C ₁₄ H ₁₇ N ₃ O ₂ 266.31 277925 2622 01 7	Physical Data = 152	Spectra = 113	Reactions = 54	Targets = 123	Documents = 8,002
<chem>C1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10C11=CC=CC=C11C12=CC=CC=C12C13=CC=CC=C13C14=CC=CC=C14C15=CC=CC=C15C16=CC=CC=C16C17=CC=CC=C17C18=CC=CC=C18C19=CC=CC=C19C20=CC=CC=C20C21=CC=CC=C21C22=CC=CC=C22C23=CC=CC=C23C24=CC=CC=C24C25=CC=CC=C25C26=CC=CC=C26C27=CC=CC=C27C28=CC=CC=C28C29=CC=CC=C29C30=CC=CC=C30C31=CC=CC=C31C32=CC=CC=C32C33=CC=CC=C33C34=CC=CC=C34C35=CC=CC=C35C36=CC=CC=C36C37=CC=CC=C37C38=CC=CC=C38C39=CC=CC=C39C40=CC=CC=C40C41=CC=CC=C41C42=CC=CC=C42C43=CC=CC=C43C44=CC=CC=C44C45=CC=CC=C45C46=CC=CC=C46C47=CC=CC=C47C48=CC=CC=C48C49=CC=CC=C49C50=CC=CC=C50C51=CC=CC=C51C52=CC=CC=C52C53=CC=CC=C53C54=CC=CC=C54C55=CC=CC=C55C56=CC=CC=C56C57=CC=CC=C57C58=CC=CC=C58C59=CC=CC=C59C60=CC=CC=C60C61=CC=CC=C61C62=CC=CC=C62C63=CC=CC=C63C64=CC=CC=C64C65=CC=CC=C65C66=CC=CC=C66C67=CC=CC=C67C68=CC=CC=C68C69=CC=CC=C69C70=CC=CC=C70C71=CC=CC=C71C72=CC=CC=C72C73=CC=CC=C73C74=CC=CC=C74C75=CC=CC=C75C76=CC=CC=C76C77=CC=CC=C77C78=CC=CC=C78C79=CC=CC=C79C80=CC=CC=C80C81=CC=CC=C81C82=CC=CC=C82C83=CC=CC=C83C84=CC=CC=C84C85=CC=CC=C85C86=CC=CC=C86C87=CC=CC=C87C88=CC=CC=C88C89=CC=CC=C89C90=CC=CC=C90C91=CC=CC=C91C92=CC=CC=C92C93=CC=CC=C93C94=CC=CC=C94C95=CC=CC=C95C96=CC=CC=C96C97=CC=CC=C97C98=CC=CC=C98C99=CC=CC=C99C100=CC=CC=C100</chem>	(S)-Atenolol C ₁₄ H ₁₇ N ₃ O ₂ 266.31 *21424 9327914 5	Physical Data = 32	Spectra = 24	Reactions = 37	Targets = 16	Documents = 77
<chem>C1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10C11=CC=CC=C11C12=CC=CC=C12C13=CC=CC=C13C14=CC=CC=C14C15=CC=CC=C15C16=CC=CC=C16C17=CC=CC=C17C18=CC=CC=C18C19=CC=CC=C19C20=CC=CC=C20C21=CC=CC=C21C22=CC=CC=C22C23=CC=CC=C23C24=CC=CC=C24C25=CC=CC=C25C26=CC=CC=C26C27=CC=CC=C27C28=CC=CC=C28C29=CC=CC=C29C30=CC=CC=C30C31=CC=CC=C31C32=CC=CC=C32C33=CC=CC=C33C34=CC=CC=C34C35=CC=CC=C35C36=CC=CC=C36C37=CC=CC=C37C38=CC=CC=C38C39=CC=CC=C39C40=CC=CC=C40C41=CC=CC=C41C42=CC=CC=C42C43=CC=CC=C43C44=CC=CC=C44C45=CC=CC=C45C46=CC=CC=C46C47=CC=CC=C47C48=CC=CC=C48C49=CC=CC=C49C50=CC=CC=C50C51=CC=CC=C51C52=CC=CC=C52C53=CC=CC=C53C54=CC=CC=C54C55=CC=CC=C55C56=CC=CC=C56C57=CC=CC=C57C58=CC=CC=C58C59=CC=CC=C59C60=CC=CC=C60C61=CC=CC=C61C62=CC=CC=C62C63=CC=CC=C63C64=CC=CC=C64C65=CC=CC=C65C66=CC=CC=C66C67=CC=CC=C67C68=CC=CC=C68C69=CC=CC=C69C70=CC=CC=C70C71=CC=CC=C71C72=CC=CC=C72C73=CC=CC=C73C74=CC=CC=C74C75=CC=CC=C75C76=CC=CC=C76C77=CC=CC=C77C78=CC=CC=C78C79=CC=CC=C79C80=CC=CC=C80C81=CC=CC=C81C82=CC=CC=C82C83=CC=CC=C83C84=CC=CC=C84C85=CC=CC=C85C86=CC=CC=C86C87=CC=CC=C87C88=CC=CC=C88C89=CC=CC=C89C90=CC=CC=C90C91=CC=CC=C91C92=CC=CC=C92C93=CC=CC=C93C94=CC=CC=C94C95=CC=CC=C95C96=CC=CC=C96C97=CC=CC=C97C98=CC=CC=C98C99=CC=CC=C99C100=CC=CC=C100</chem>	(±)-Atenolol C ₁₄ H ₁₇ N ₃ O ₂ 266.31 *21429 34715 11 6	Physical Data = 29	Spectra = 12	Reactions = 26	Targets = 12	Documents = 12

- See a clear overview of your search results in the *Results preview*, including the number of substance, commercial substance, reaction, target or document results found.
- Click *New* to start a completely new query or *Edit* to edit the existing query.
- Select *Edit in Query Builder* to edit the query using the field-and-form based search interface. See [page 16](#) for details. Select *Create Alert* to generate an email alert for this search. See [page 11](#) for more details.
- Use *Preview Results* to see the top three results for that result category. Inset **F** shows the preview for substances.
- Click *View Results* to see the full view of the results for that category. See [pages 7–10](#) for more details.
- Inset showing the top three results for substances for the query "atenolol".

Navigating a *Results* page — 1

The screenshot shows the Reaxys Results page for 125 substances. The interface includes a filter sidebar (B), a top navigation bar (A), and a main results area with three entries for Atenolol enantiomers. Callout C highlights the 'Export' button, D highlights the database dropdown menu, E shows the expanded dropdown menu with options like 'Reaxys - 125', 'Commercial Substances - 8', 'eMolecules - 4', 'LabNetwork - 2', 'PubChem - 81', and 'SigmaAldrich - 4'. Callout F points to the 'Preparations' link for the first entry, and H points to the 'Reactions' link for the second entry.

A. Use top line to navigate between the displayed category of results for the current search (here, substances) and the other options (here, documents, reactions and targets).

B. Use multiple filters to refine the results list. These can be applied as *Limit to* or *Exclude*. The categories and specific filters displayed are always relevant for the result set, so they change for different searches. See page 10.

C. Select *Export* to open an export dialog window. See page 13 for details.

D. Use the database dropdown menu to change the searched database from *Reaxys* (which encompasses all six databases) to one of the other options (see inset E).

Use the *Sort by* dropdown menu to sort the results list using a category-specific set of options.

E. Inset showing the dropdown menu for database selection.

Navigating a *Results* page — 2

The screenshot displays the Reaxys interface with the following elements:

- Filters Panel (Left):** A vertical sidebar with various filter categories such as 'By Structure', 'Measurement pX', 'Highest Clinical Phases', 'Targets', 'Parameters', 'Substance Classes', 'Molecular Weight', 'Number of Fragments', 'Availability', 'Availability in other databases', 'Available Data', 'Document Type', 'Publication Year', 'Patent Assignee', and 'LogP'.
- Search Results (Center):** A list of substances. Two entries are visible:
 - (R5)-atenolol:** (CH3)2C(NH)CH2CH(OH)CH2OC6H4C... with associated data like 266.34, 2739235, and 29122-68-7.
 - (S)-Atenolol:** C16H19N3O3 with associated data like 266.34, 4234251, and 93179-54-5.
- Inset J (Substance Availability):** A pop-up window showing a list of databases: 'Commercial Substances', 'Accelrys' ACD', 'CambridgeSoft ACX', 'Sigma Aldrich', and 'eMolecules'.
- Inset K (Options):** A pop-up window showing search actions: 'Find Similar', 'View related Markush', 'Copy structure to query', 'Use as filter', and 'Open in database'.
- Annotations:** Orange boxes with letters F, G, H, I, J, and K are placed over specific icons and elements in the interface to indicate their functions.

- F. These options are different for each results category. See page 9 for more details
- G. Use the shopping cart icon to see the substance availability in multiple commercial databases (see inset J).
- Use the pill icon to see druglikeness for the substance.
- Use the magnifying glass icon to zoom into the structure.
- Use the list icon for structure-related searches (see inset K).
- Use the flow icon to create a synthesis plan for the structure.
- H. Use these links to view excerpted data on the substance.
- I. Use these links to access related result sets of the listed types.
- J. Inset showing substance availability databases.
- K. Inset showing options for structure-related search actions.

View options for different *Results* categories

125 Substances out of 8,143 Documents, containing 159 Reactions, 146 Targets

0 selected

Limit To Exclude Export Preparations

Reaxys - 125

Sort by No of References ↓

Grid Heatmap

A. Unique *View* options for substance results include:

- *Preparations* to open the substance's known prep reactions
- *Grid* to toggle between a list and grid view

159 Reactions out of 8,143 Documents, containing 125 Substances, 146 Targets

0 selected

Limit To Exclude Export Syn-Plan Hide Conditions

Reaxys - 159

Sort by Reaxys Ranking ↓

B. Unique *View* options for reaction results include :

- *Syn-Plan* to open synthesis plans for selected substances
- *Hide Conditions* to hide reaction conditions from the results list

146 Targets out of 8,143 Documents, 125 Substances, 159 Reactions

0 selected

Limit To Exclude Export

Reaxys - 146

Sort by Sort alphabetically A-Z ↑

Heatmap

C. Target results have specific *Sort by* options.

8,143 Documents with 125 Substances, 159 Reactions, 146 Targets

0 selected

Limit To Exclude Export

Reaxys - 8,143

Sort by Publication Year ↓

Heatmap

D. Document results offer specific *Sort by* options.

8 Substances

0 selected

Limit To Exclude Export

Commercial Substances - 8

Sort by Commercial Substance ID ↑

Grid

E. Commercial substance results offer specific *Sort by* options and the option to toggle between a list and grid view.

Note: *Heatmap* (see page 19), which shows the relative substance–activity relationships of bioactive substances and targets can be accessed from substance, target or document results, but not from reaction or commercial substance results.

Filter options for different *Results* categories

The categories and specific filters displayed are always relevant for the result set, so they change for different searches. Below are examples of filters specific for substance (A), commercial substance (B), reaction (C), target (D) and document (E) results.

Filters A

Limit to > Exclude >

- By Structure >
- Measurement pX >
- Highest Clinical Phases >
- Targets >
- Parameters >
- Substance Classes >
- Molecular Weight >
- Number of Fragments >
- Availability >
- Availability in other databases >
- Available Data >
- Document Type >
- Publication Year >
- Patent Assignee >
- LogP >

Filters B

Limit to > Exclude >

- By Structure >
- Molecular Weight >
- Number of Fragments >
- Availability in other databases >
- Supplier >
- Supplier Geolocation >
- Usage Classification >
- Package Size >
- Price >
- Purity >
- Stock Availability >
- Shipment Time >
- Shipment Country >

Filters C

Limit to > Exclude >

- By Structure >
- Yield >
- Reagent/Catalyst >
- Solvent >
- Catalyst Classes >
- Solvent Classes >
- Product Availability >
- Reactant Availability >
- Reaction Classes >
- Document Type >
- Publication Year >
- Single step reactions only
- Experimental procedure only

Filters D

Limit to > Exclude >

- Targets >
- Target Species >
- Target Type >
- Measurement pX >
- Parameters >
- Substance action on target >
- Document Type >
- Publication Year >
- Patent Assignee >

Filters E

Limit to > Exclude >

- Index Terms (List) >
- Index Terms (ReaxysTree) >
- Publication Year >
- Document Type >
- Authors >
- Patent Assignee >
- Patent Office >
- Journal Title >
- Substance Classes >
- Reaction Classes >
- Manually processed content only

Creating an alert

Create Alert

Query: Compound: atenolol (exact search), isotopes, tautomer... Show Query

Alert name: Atenolol-Main

Send alerts to: der...om

Frequency: Every week on: Tuesday

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)

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

Cancel Create

Note: You must be signed into your personal account to create alerts.

- A. Use the *Create Alert* option on a *Results preview* line item (see page 6) or *History* line item (see page 14) to open the *Create Alert* dialog window for the query corresponding to that line item.
- B. Enter the unique name of your alert here.
- C. Your registered email address appears here. Enter additional email addresses if needed. Note that the address in the screenshot has been censored.
- D. Select the frequency (weekly, every two weeks, monthly or after every database update) and the weekday or date of the month for the alert.
- E. Choose whether a document should only be included in alerts when it is first added to the database or included every time it is updated.
- F. Advanced alert selections are currently only available for Reaxys database content. The email contains a preview of alert results defined by your selection here.
- G. Click *Create* to create the alert for this query.

Managing your alerts

Reaxys® Quick search Query builder Results Synthesis planner History Alerts

Alerts

Substances	Alert Name	Results from	Actions
Since Apr 21, 2021	Dopamine-Main - in Reaxys Compound: dopamine (exact search), isotopes, tautomers, Include: Stere...	No alert results	Edit Delete
Since Apr 21, 2021	Gabapentin-Main - in Reaxys Compound: gabapentin (exact search), isotopes, tautomers, Include: Stere...	No alert results	Edit Delete
Since Apr 21, 2021	Atenolol-Main - in Reaxys Compound: atenolol (exact search), isotopes, tautomers, Include: Stereo, ...	No alert results	Edit Delete

Note: You must be signed into your personal account to manage your alerts.

- Click *Alert* on any screen to see your alerts.
- Alerts are listed newest to oldest. The listing shows the query type (substances, reactions, targets, documents, commercial substances), date of creation, alert name, database and query details.
- Use the *Results from* dropdown menu to see results from previous iterations of this alert. For example, you could select to see what results were included in the result one month ago.
- Click *Edit* to open the *Edit Alert* dialog window for the selected line item. You can then edit all settings except the query and your email address. Click *Delete* to delete the selected line item.

Exporting results

The screenshot shows the 'Export substances Reaxys' dialog box. It has a title bar with a close button (X) and a label 'A'. The main area contains several sections:

- Choose a format:** A dropdown menu showing 'PDF/Print' with a downward arrow and an information icon (i). Callout 'B' points to this dropdown.
- Range:** A dropdown menu showing 'All results - 480' with a downward arrow and an information icon (i). Callout 'C' points to this dropdown.
- Export:** Four radio button options:
 - All available data (with information icon 'D')
 - Identification data only (with information icon 'D')
 - Hit data only (with information icon 'D')
 - Choose specific data (with information icon 'D')
- Additional options:** Two checkboxes:
 - Include structures (with callout 'E')
 - Include a description in the document

At the bottom, there is an 'Export >' button (callout 'F'). An inset window (callout 'G') is open, showing the 'PDF/Print' format options: PDF/Print (selected), XML, Microsoft Word, Microsoft Excel, Tab-delimited text, Electronic Lab Notebook, RD File, SD/Molfile, and Smiles.

Note: You must be signed into your personal account to export results.

- Use the *Export* option at the top of a *Results* page to open the *Export* dialog window. Note that the options shown depend on the *Results* page type (substances, reactions, targets, documents).
- Select the format using the dropdown menu (see inset **G** for the options).
- Select the range: all results, selected results, or a defined range from the result list.
- Select the data you wish to export. The options may vary based on the export type. Click the information button for more information on the options.
- Choose additional options, which vary based on the export type.
- Click *Export* to start the export. A progress bar is shown at the bottom of the screen. You can cancel the export at any time.
- Inset showing the export format options

Using your query history

The screenshot displays the Reaxys interface with the 'History' tab selected. The main panel shows a list of recent queries:

Results	Time	Action	Options
96 Reactions	Today 11:56	Context Switch from: 15 Substances	Edit Query, Save, View
15 Substances	Today 11:56	Quick Search: "atenolol" "solubility" AND	Edit Query, Save, Alert, View
10 Documents	Today 11:55	Filtered by: Patent Office	Edit Query, Save, View
5,556 Documents	Today 11:55	Quick Search: "HEK293" "phosphorylation"	Edit Query, Save, Alert, View
88 Substances	Today 11:54	Quick Search: "ascorbic acid" "melting" AND	Edit Query, Save, Alert, View

An inset window shows the 'Saved' queries list:

Results	Time	Action	Options
15 Substances	Today 11:56	Atenolol-Solubility	Edit Query, Delete, Rename, Alert, View

- Click *History* to access your recent and saved query lists.
- The *Recent* list shows the queries and actions from this session. The *Saved* list (inset **E**) shows queries that you have saved from this and earlier sessions. Note that you must be signed into your personal account to save queries.
- Queries and actions are listed newest to oldest, showing the type of result (substances, reactions, targets, documents, commercial substances), the date and time; the type (*Quick Search*, *Query Builder*, *Filtered by*, *Context Switch*); and some details of the query or action.
- Use these options to edit the query in *Query Builder* (see slide N); save a recent query to your results list; create an alert (see slide N); or view the query. Note that you cannot edit or create an alert for *Filtered by* or *Context Switch* actions.
- Inset showing saved queries; note that the optional actions are to edit the query, delete or rename the item, or create an alert.

Changing personal settings

The screenshot shows the Reaxys personal settings interface. At the top, there is a navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. A user profile icon is in the top right, labeled 'A'. Below this is a 'Profile' section with tabs for 'Account', 'Profile', and 'Preferences', with 'Preferences' selected and labeled 'B'. The main content area is divided into several sections:

- Default structure/reaction editor settings:** Labeled 'C', it includes a 'Structure Editor' dropdown set to 'ChemAxon's MarvinJS', a 'Search structure as' dropdown set to 'As drawn', and a 'Preferences' section with checkboxes for 'Include Tautomers', 'Include Stereo', 'Include Additional ring closures', 'Include Salts', 'Include Mixtures', 'Include Isotopes', 'Include Charges', and 'Include Radicals'.
- Autoplan:** Labeled 'D', it includes a 'Default settings' section with options for 'Number of plans to create = 5', 'Max. alternative branches = 5', 'Max. number of steps = 5', 'Stop searching if starting material is commercially available', and 'Default yield for reactions without a given yield = 50%'.
- Results per page:** Labeled 'E', it includes a 'Number of results per page' dropdown set to '15'.
- Text and Contrast:** Labeled 'F', it includes 'Text Size' (set to 'A'), 'Contrast' (set to 'A'), and 'Text Color' (set to 'All Black').

A. If you are signed into your personal account, you can access by clicking your name or the person symbol and selecting *Profile*.

B. Select *Account* to see your username, registered email address and password. You can edit your email address and password.

Click *Profile* to see and edit your personal details.

Click *Preferences* to see and edit your query-related settings

C. Among the structure editor settings, you can choose MarvinJS or ChemDrawJS as your preferred editor (see page 5 for more on structure queries) and change the defaults for the query (e.g., include or exclude tautomers, include or exclude salts).

D. Among the settings for *Autoplan* (part of *Synthesis Planner*, see page 18), you can choose how many plans are auto-generated and the maximum number of steps.

E. Set the number of results per page here.

F. Set text size, contrast and text color here.

What is *Query Builder*?

The screenshot shows the Reaxys Query Builder interface. The top navigation bar (A) includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. The search and filter sidebar (B) on the right contains 'Search fields' and 'Search fields forms' sections with various categories like 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. The main workspace (C) is a large area with the text 'Drag & Drop to build a new query'. The inset view (D) shows a detailed query structure with two querylets: 'Melting Point' (containing '56' and 'Solvent (Melting Point)') and 'Boiling Point' (containing 'Boiling Point, °C' and 'Pressure (Boiling Point), Torr'), connected by an AND operator.

Query Builder offers a streamlined drag-and-drop interface that includes all the essential search input: narrowly defined physicochemical properties, including spectra; medicinal chemistry terminology; reaction parameters, such as yield, catalyst and solvent; basic indexes; and more.

- You can open *Query Builder* directly from the top navigation or from various *Edit query* options.
- Create queries from dedicated fields and forms (querylets) with predefined parameter sets that are easy to edit and fill.
- Structure drawings, molecular formulas and CAS registry numbers can also be added to the query.
- Inset showing two querylets (*Melting point* and *Boiling point*) related with the Boolean operator AND.

For more information on *Query Builder*, please see the [tutorials in the Resource Center](#).

Performing a patent assignee search

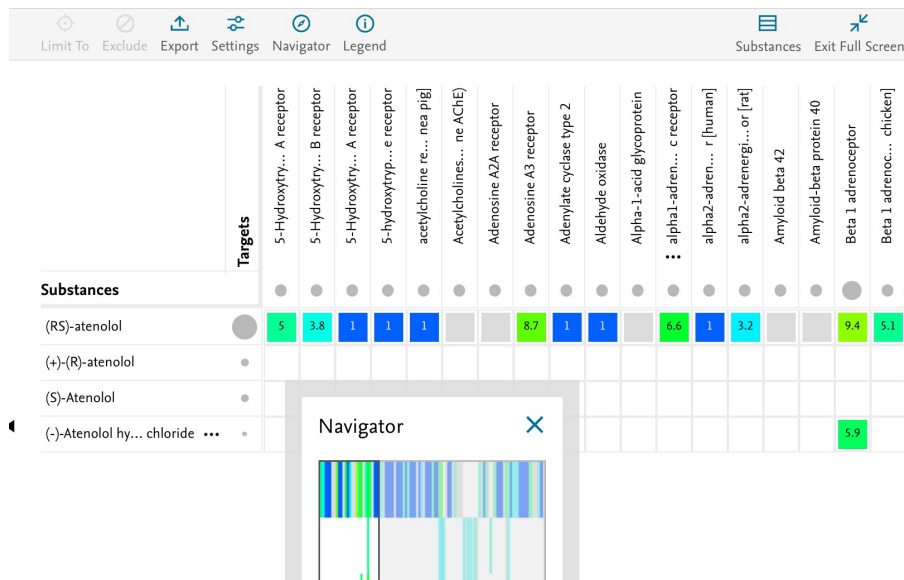
The screenshot shows the Reaxys Query Builder interface. At the top, the 'Query builder' tab is active. The search bar contains 'Pfizer'. The 'Search fields' panel on the right shows the 'Fields' category selected, with 'Patent Assignee' chosen. A dropdown menu shows suggestions for 'Pfizer'. The 'Results' view is shown at the bottom, displaying a list of documents with search results.

Query Builder is currently the best feature to use for patent assignee searches.

- Open *Query Builder* from the top navigation.
- Open the *Fields* category *Bibliography* and select the querylet *Patent Assignee*.
- Enter the company or institution name. Define the field with “contains” rather than “is” for the best return.
- Click the results category of interest (Reactions, Targets, Substances or Documents).
- Inset showing the *Results* view for this search with options to review and filter the results set.

For more information on *Query Builder*, please see the [tutorials in the Resource Center](#).

What is *Heatmap*?



Reaxys Medicinal Chemistry has a Heatmap that provides a clear overview of the relationships between substances and their targets.

Its display includes a color representing the “warmth” of the affinity and a quantifier for this relationship in the form of pX values, which are normalized substance–target affinity values assigned to the data.

Heatmap can be accessed from substance, target or document results, but not from reaction or commercial substance results.

The screenshot shows the *Heatmap* for the affinity of atenolol for a range of targets. The *Navigator* helps navigate to data points of interest. Mouse over any substance or target to see details such as structure, identifiers and synonyms. Click any cell to see the bioactivity detail, including parameters and values for druglikeness and efficacy with the relevant citations.

For more information, see the [tutorials in the Resource Center](#).



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