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Reference guide

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Welcome to your 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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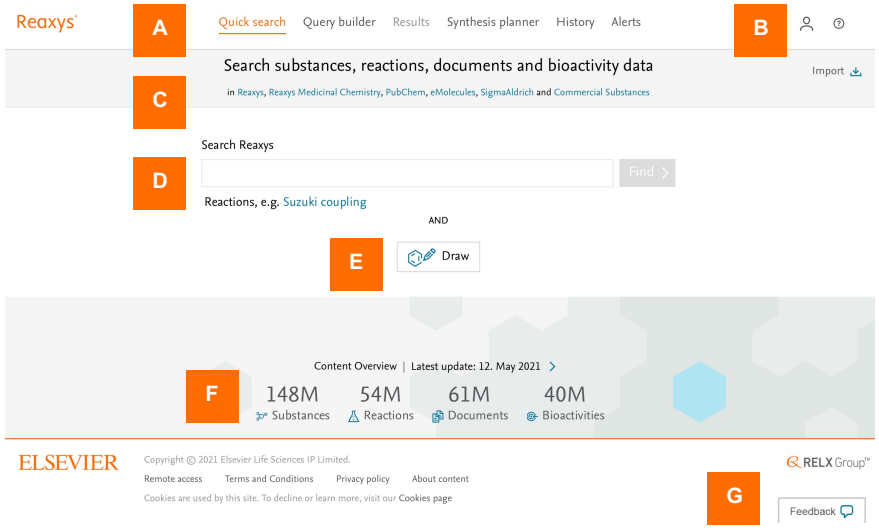
Navigating the Reaxys home page



A. Use the top bar to navigate between the areas of Reaxys.

B. 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.

C. Use these links to learn more about the databases that Reaxys searches.

D. See page 4 for more on keywords and *Quick search*.

E. See page 5 for more on structure editors and *Quick search*.

F. See the current document and extracted substance, reaction and bioactivity data point counts for Reaxys.

G. Use this *Feedback* feature to give feedback directly to the Reaxys development team.

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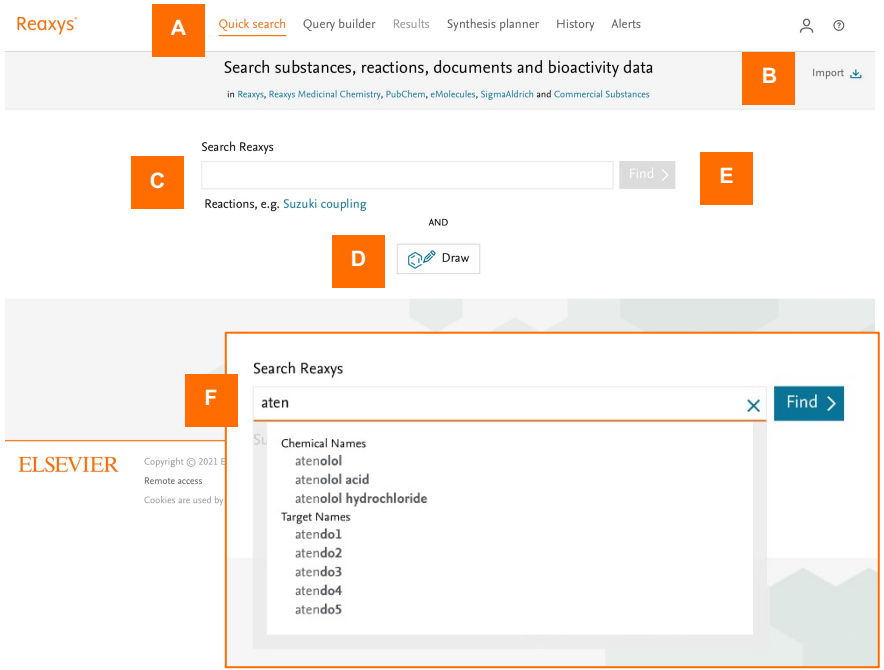
Using *Quick search*



A. Click here to return to *Quick search* from any other screen.

B. Use *Import* to import a previously saved and exported Reaxys query from your desktop or other file library.

C. 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.

D. Click here to open the structure editor and add a structure to your query. See page 5 for more details.

E. When your *Quick search* query is ready, click *Find*. This opens the *Results preview* for the query. See page 6.

F. Inset showing Reaxys Auto Suggest proposals for “aten”. Selecting one adds it to the query as a phrase.

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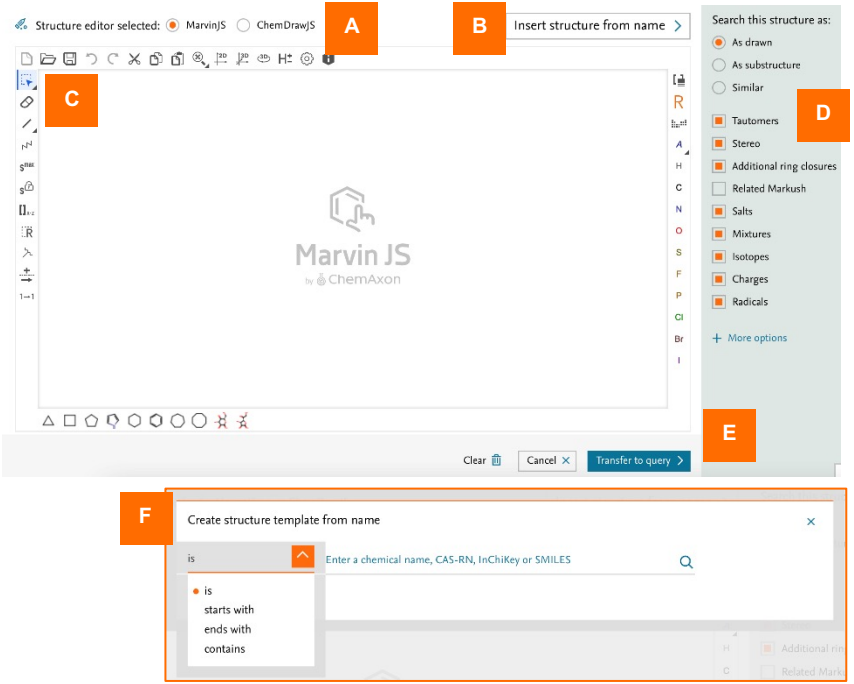
Using the structure editors for *Quick search*



A. 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.

B. 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.

C. Use the tools of the structure editor to create your structure or reaction drawing.

D. Add options to the structure query to expand the search to substances fitting the selected parameters.

E. When your drawing is ready, click *Transfer to query*.

F. Inset showing *Create structure template from name* dialog with options for exact or partial names.

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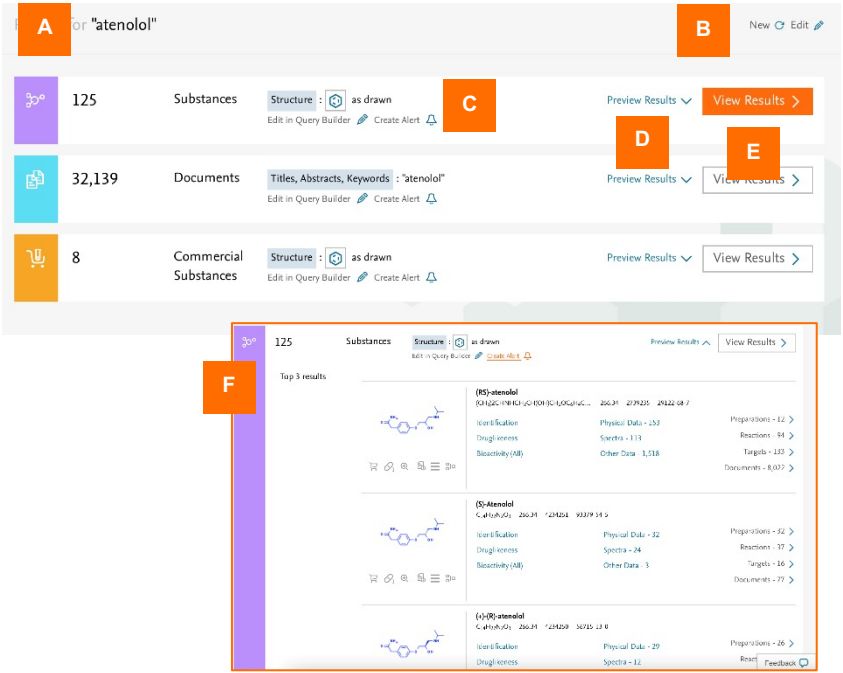
Navigating the *Results preview*



A. 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.

B. Click *New* to start a completely new query or *Edit* to edit the existing query.

C. 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.

D. Use *Preview Results* to see the top three results for that result category. Inset F shows the preview for substances.

E. Click *View Results* to see the full view of the results for that category. See pages 7–10 for more details.

F. Inset showing the top three results for substances for the query “atenolol”.

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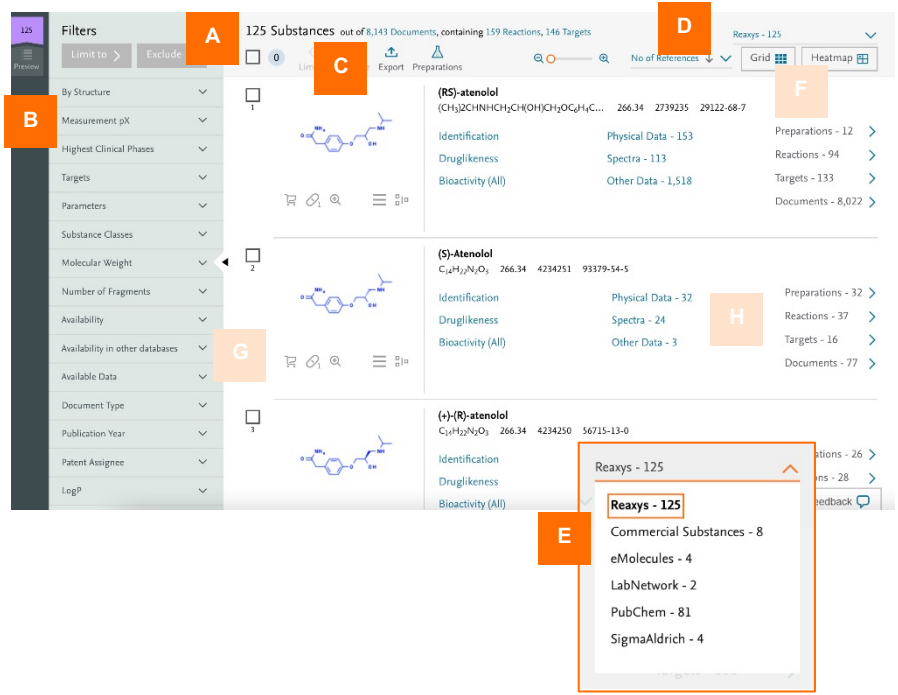
Navigating a *Results* page — 1



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.

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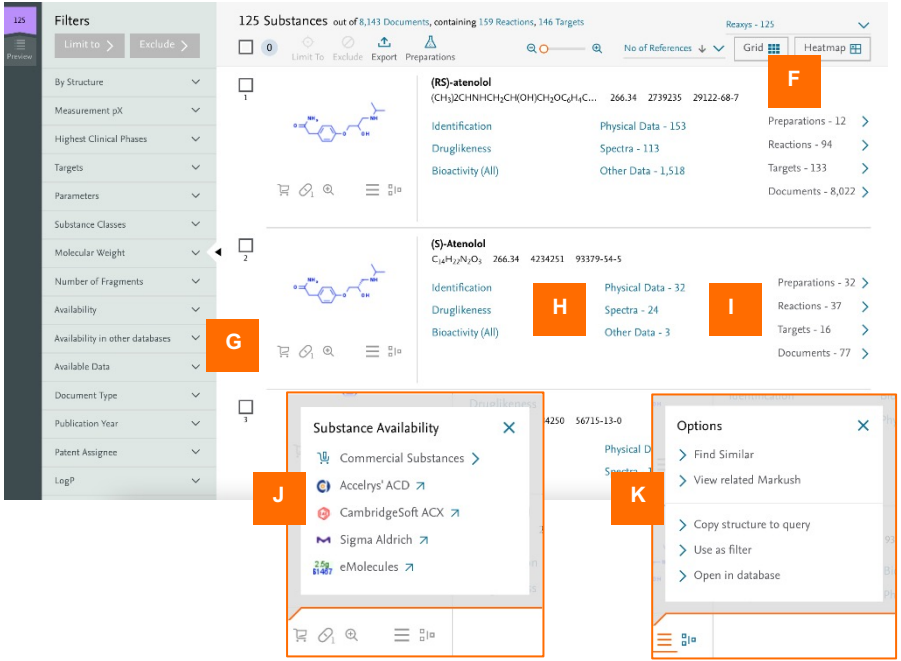
Navigating a *Results* page — 2



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.

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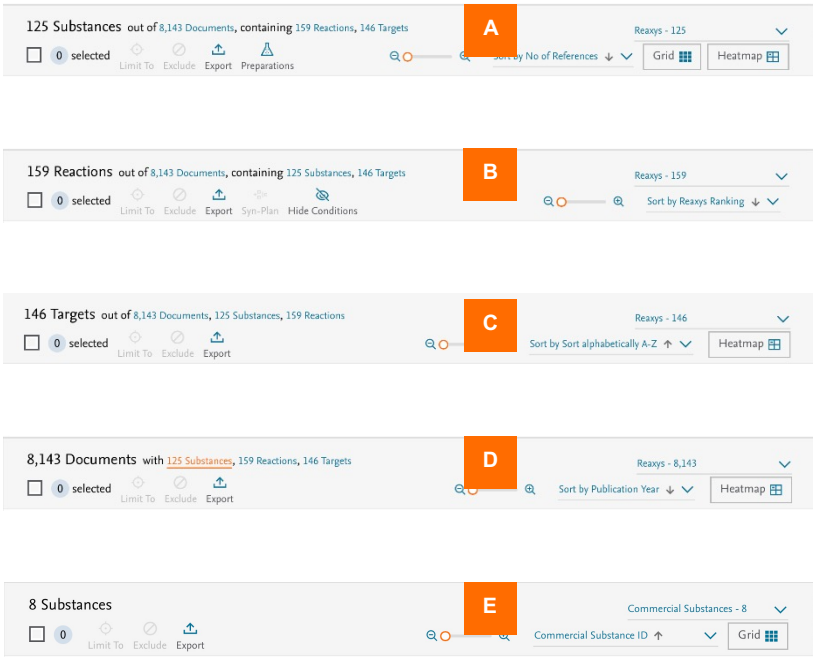
View options for different *Results* categories



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

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

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

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

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.

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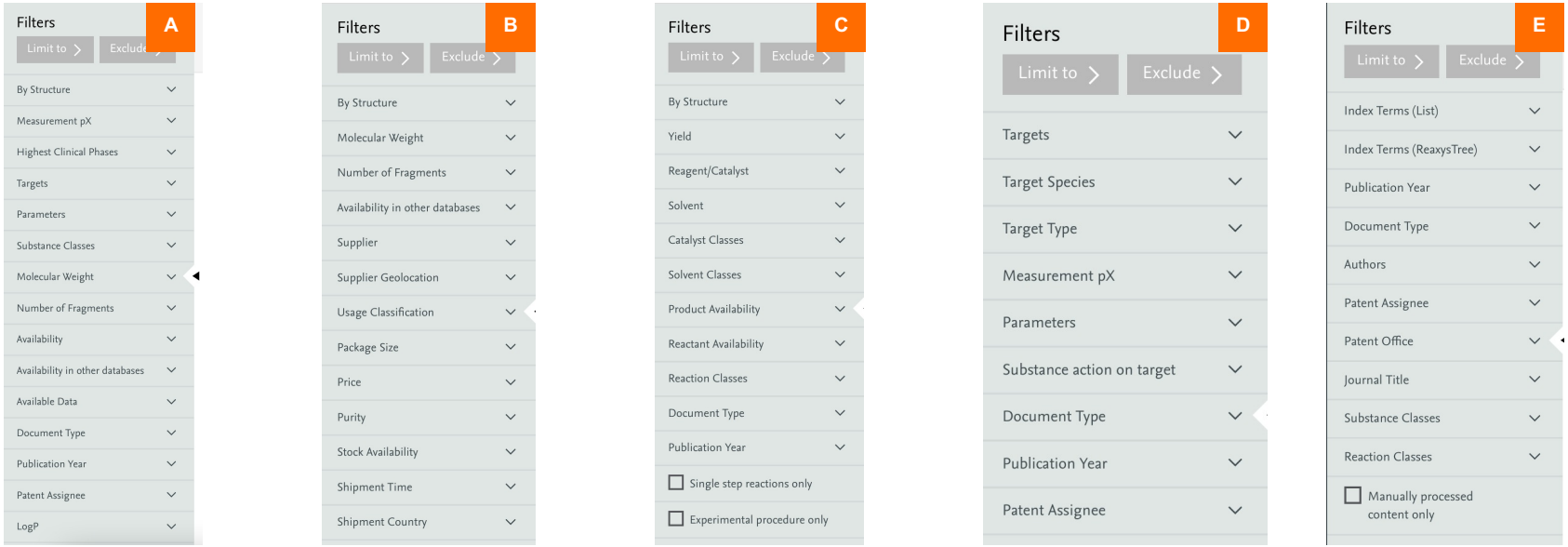
Filter options for different *Results* categories

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.



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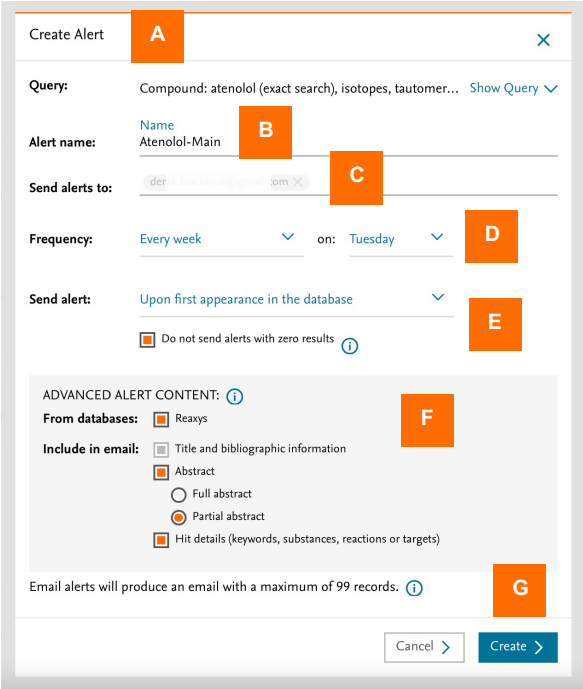
Creating an alert



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.

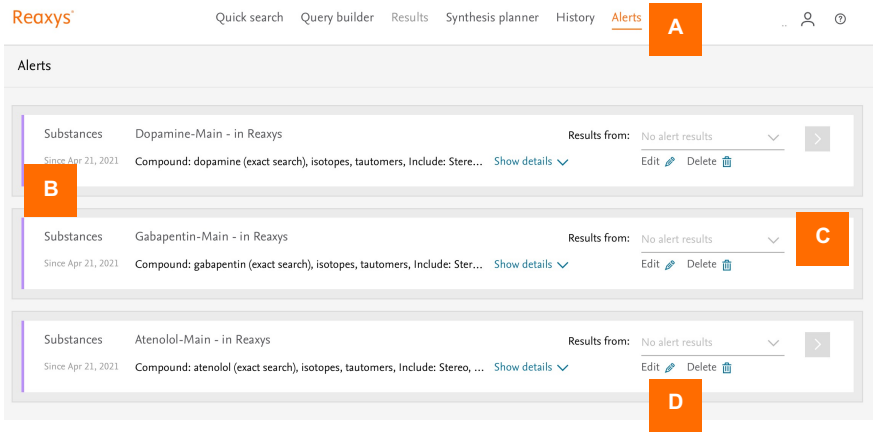
D. Select the frequency (weekly, every two weeks, monthly or after every database update) and the weekday or date of the month for the alert.

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



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

A. Click *Alert* on any screen to see your alerts.

B. 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.

C. 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.

D. 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.

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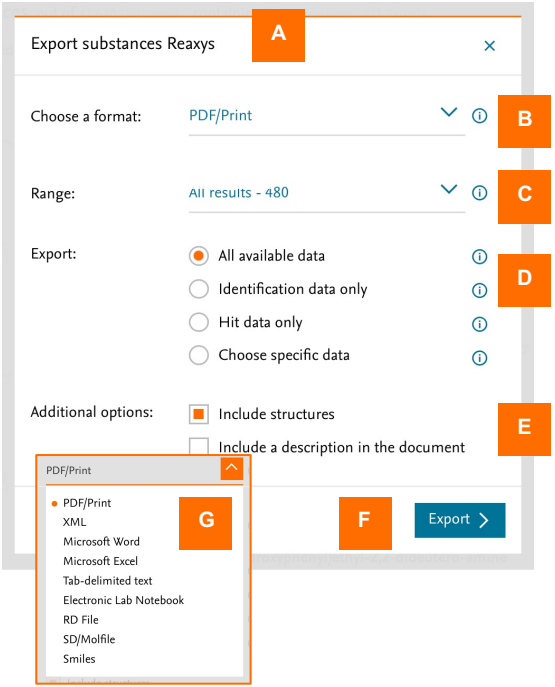
Exporting results



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

A. 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).

B. Select the format using the dropdown menu (see inset G for the options).

C. Select the range: all results, selected results, or a defined range from the result list.

D. 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.

E. Choose additional options, which vary based on the export type.

F. 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.

G. Inset showing the export format options

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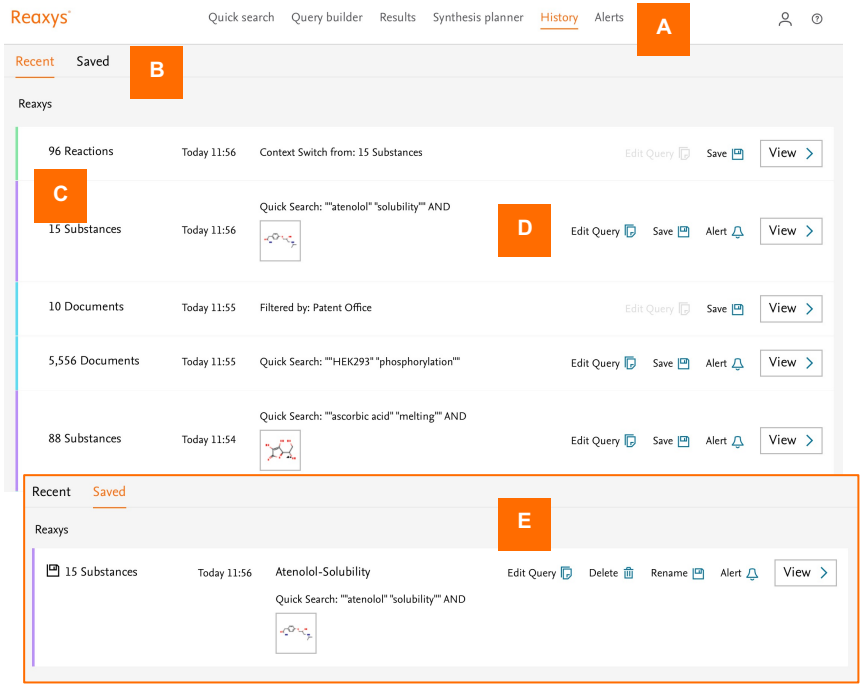
Using your query history



A. Click *History* to access your recent and saved query lists.

B. 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.

C. 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.

D. Use these options to edit the query in *Query Builder* (see page 16); save a recent query to your results list; create an alert (see page 11); or view the query. Note that you cannot edit or create an alert for *Filtered by* or *Context Switch* actions.

E. Inset showing saved queries; note that the optional actions are to edit the query, delete or rename the item, or create an alert.

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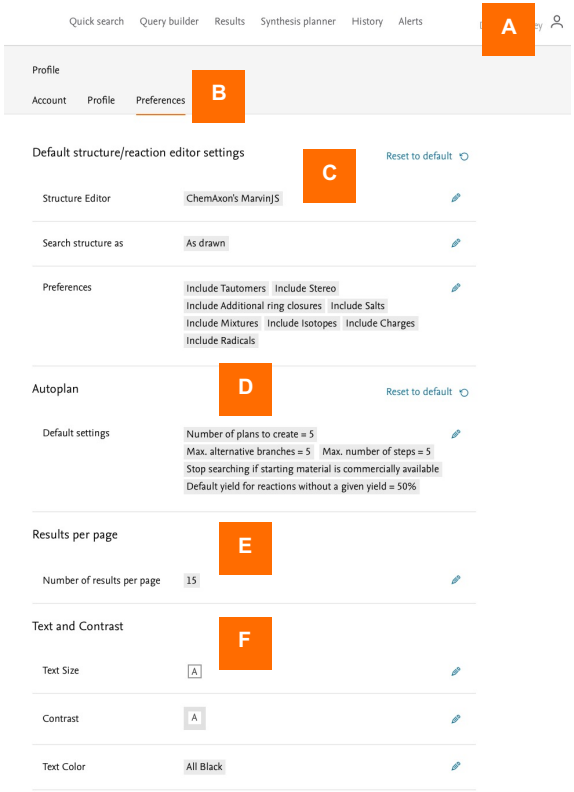
Changing personal settings



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

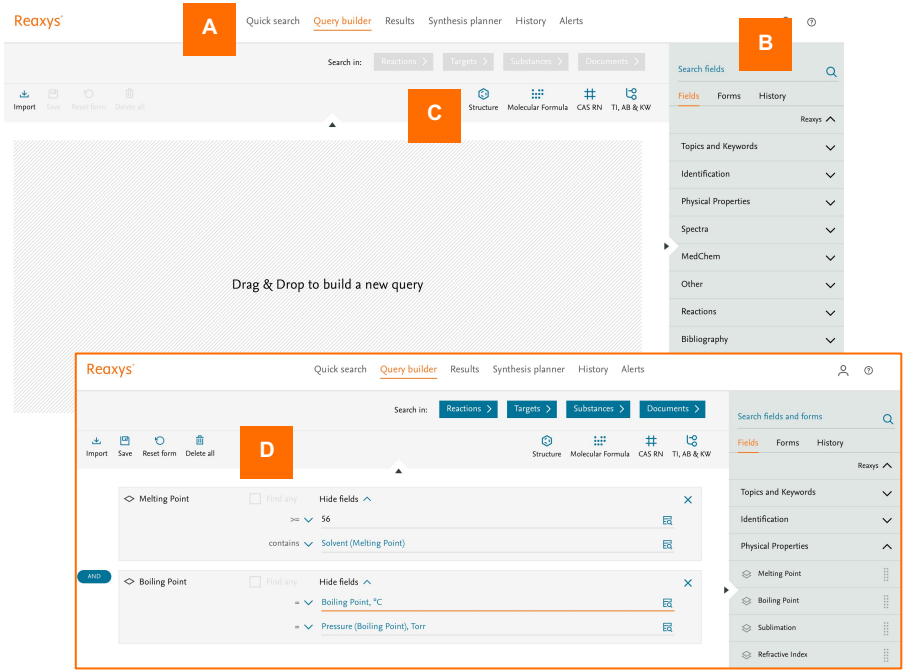
C. Among the structure editor settings, you can choose MarvinJS or ChemDrawJS as your preferred editor (see page 5 for more on structure queries) and change the defaults for the query (e.g., include or exclude tautomers, include or exclude salts).

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*?



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.

A. You can open *Query Builder* directly from the top navigation or from various *Edit query* options.

B. Create queries from dedicated fields and forms (querylets) with predefined parameter sets that are easy to edit and fill.

C. Structure drawings, molecular formulas and CAS registry numbers can also be added to the query.

D. Inset showing two querylets (*Melting point* and *Boiling point*) related with the Boolean operator AND.

For more information on *Query Builder*, please see the tutorial in the Resource Center.

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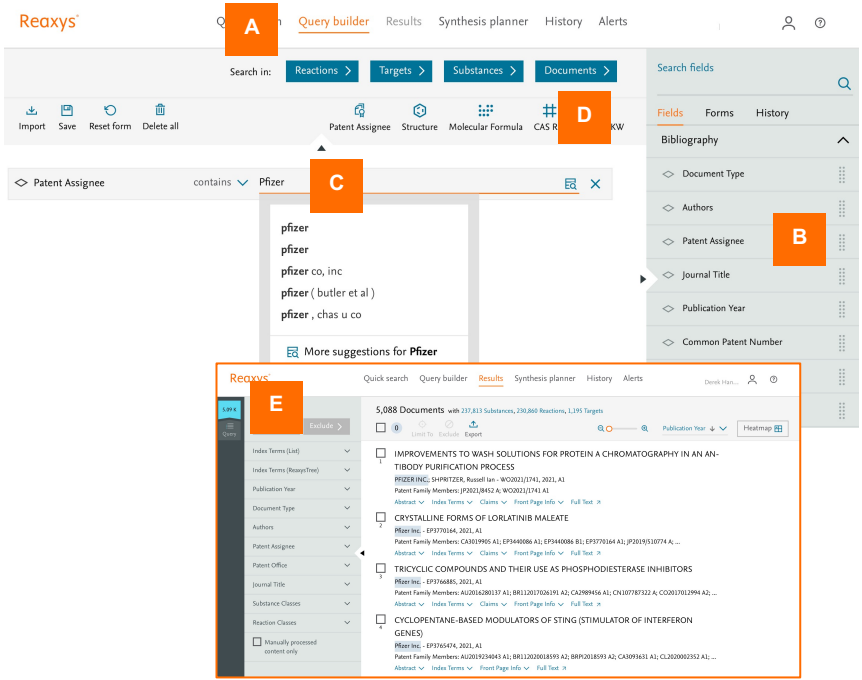
Performing a patent assignee search



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

A. Open *Query Builder* from the top navigation.

B. Open the *Fields* category *Bibliography* and select the querylet *Patent Assignee*.

C. Enter the company or institution name. Define the field with “contains” rather than “is” for the best return.

D. Click the results category of interest (Reactions, Targets, Substances or Documents).

E. 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 tutorial in the Resource Center.

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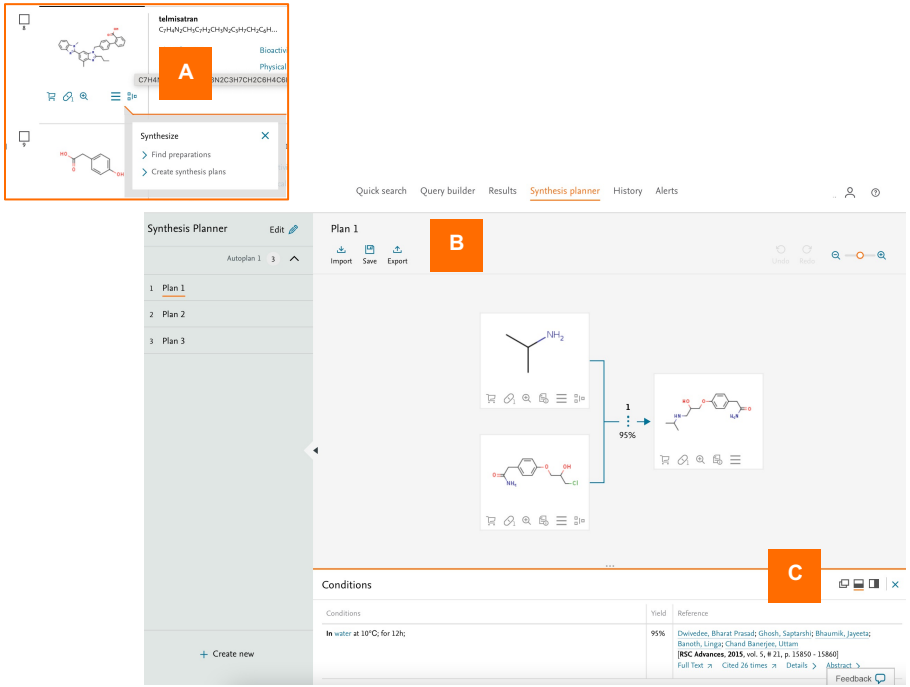
What is *Synthesis Planner*?



Reaxys Synthesis Planner enables you to instantly generate multiple synthesis plans for substances of interest based on information published in peer-reviewed literature.

A. Click on the synthesis icon beside any substance in the results and select *Create synthesis plans*. This opens *Synthesis Planner* (B) which shows the plans.

B. This shows one of three synthesis plans generated for the selected substance. The plan can be saved or exported using the icons at the top left. Other plans can be opened using the menu on the left.

C. The reaction conditions, yield and references are shown under the plan in this example. Using the icons, you can change the display position.

For more information on *Synthesis Planner*, please see the tutorial in the Resource Center.

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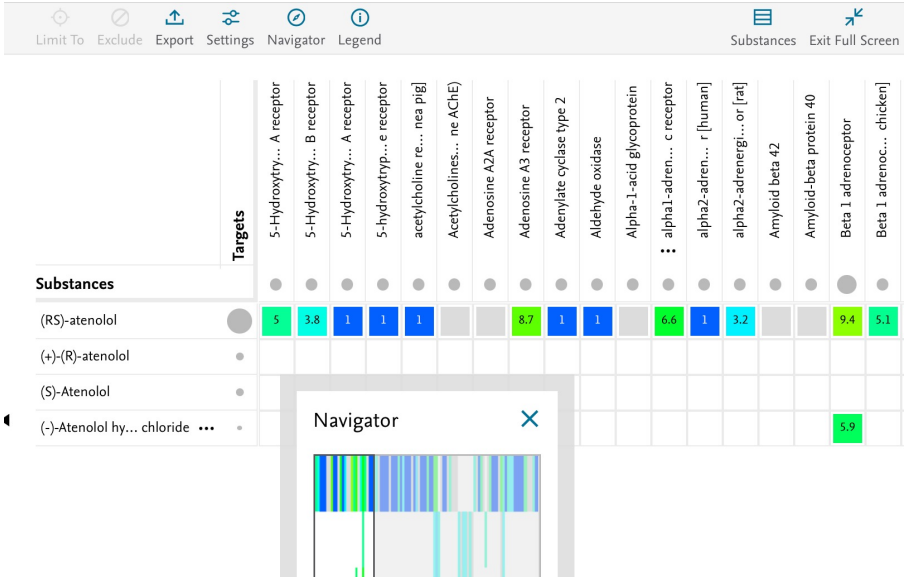
What is *Heatmap*?



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 Resource Center.

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Sign into Reaxys