



Reaxys[®]

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

The screenshot shows the Reaxys home page interface. Callout boxes are placed as follows:

- A:** Points to the top navigation bar containing links like [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 with 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 includes a chemical structure icon.
- F:** Points to the statistics section showing counts: 148M Substances, 54M Reactions, 61M Documents, and 40M Bioactivities.
- G:** Points to the "Feedback" button in the bottom right corner.

Other visible elements include the Elsevier logo, copyright information (© 2021 Elsevier Life Sciences IP Limited), and a RELX Group™ logo.

- 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

The screenshot shows the Reaxys Quick search interface. At the top, the Reaxys logo is on the left, and navigation links (Quick search, Query builder, Results, Synthesis planner, History, Alerts) are in the center. On the right, there are user and account icons. Below the navigation bar, a search bar is labeled 'Search substances, reactions, documents and bioactivity data' with a subtext 'in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, SigmaAldrich and Commercial Substances'. To the right of the search bar is an 'Import' button. Below the search bar is a text input field labeled 'Search Reaxys' with a 'Find >' button. Below the input field, there is a section for 'Reactions, e.g. Suzuki coupling' with an 'AND' operator and a 'Draw' button. An inset window, labeled 'F', shows a search for 'aten' with a list of suggestions under 'Chemical Names' and 'Target Names'. The suggestions include 'atenolol', 'atenolol acid', 'atenolol hydrochloride', 'atendo1', 'atendo2', 'atendo3', 'atendo4', and 'atendo5'. The inset also has a close button and a 'Find >' button.

A Quick search Query builder Results Synthesis planner History Alerts

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

Import

Search Reaxys

Find >

Reactions, e.g. Suzuki coupling

AND

Draw

F

Search Reaxys

aten

Chemical Names

- atenolol
- atenolol acid
- atenolol hydrochloride

Target Names

- atendo1
- atendo2
- atendo3
- atendo4
- atendo5

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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 shows the MarvinJS structure editor interface. At the top, there are buttons for selecting the structure editor (MarvinJS or ChemDrawJS), labeled 'A'. To the right is a button to 'Insert structure from name', labeled 'B'. The main workspace is a large drawing area with a toolbar on the left, labeled 'C'. On the right side of the workspace is a panel for searching the structure, labeled 'D', which includes options like 'As drawn', 'As substructure', 'Similar', 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. At the bottom right of the workspace is a button to 'Transfer to query', labeled 'E'. Below the main workspace is a dialog box labeled 'F' titled 'Create structure template from name', which contains a search input field and a list of search 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*

The screenshot displays the Reaxys search results for the query "atenolol". The interface is organized into three main sections: Substances (125 results), Documents (32,139 results), and Commercial Substances (8 results). Each section includes a "Structure" dropdown set to "as drawn", a "Create Alert" button, and a "Preview Results" dropdown. A red box labeled 'A' highlights the search bar containing the query "atenolol". A red box labeled 'B' highlights the "New" and "Edit" buttons. A red box labeled 'C' highlights the "Edit in Query Builder" button. A red box labeled 'D' highlights the "Preview Results" dropdown. A red box labeled 'E' highlights the "View Results" button. A red box labeled 'F' highlights a detailed preview of the top three results for Substances, showing chemical structures, names, and various data points like Physical Data, Spectra, Reactions, Targets, and Documents.

- 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 displays the Reaxys Results page for a search of 125 Substances. The interface includes a left sidebar with filters, a top navigation bar, and a main results area. Annotations A through H highlight key navigation and filtering elements.

Annotations:

- A:** Top navigation bar showing the current category (Substances) and other options (Documents, Reactions, Targets).
- B:** Filter buttons: Limit to > and Exclude.
- C:** Export button.
- D:** Database dropdown menu (Reaxys - 125).
- E:** Dropdown menu options: Reaxys - 125, Commercial Substances - 8, eMolecules - 4, LabNetwork - 2, PubChem - 81, SigmaAldrich - 4.
- F:** View options: Grid and Heatmap.
- G:** Preparations button.
- H:** Documents button.

- 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).
- 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](#).
- Select *Export* to open an export dialog window. See [page 13](#) for details.
- 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.
- Inset showing the dropdown menu for database selection.

Navigating a *Results* page — 2

The screenshot displays the Reaxys Results page. On the left is a 'Filters' sidebar with categories like 'By Structure', 'Measurement pK', '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'. The main area shows a list of 125 substances. Two substances are highlighted: (R)-atenolol and (S)-Atenolol. Each entry includes a chemical structure, name, formula, and various data links. Two inset windows are shown: 'Substance Availability' (Inset J) listing databases like Accelrys' ACD, CambridgeSoft ACX, Sigma Aldrich, and eMolecules; and 'Options' (Inset K) listing actions like Find Similar, View related Markush, Copy structure to query, Use as filter, and Open in database. Various icons are overlaid on the interface: 'F' (Shopping cart), 'G' (Pill icon), 'H' (Magnifying glass), 'I' (List icon), 'J' (Substance Availability inset), and 'K' (Options inset).

- 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

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

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	▼
<input type="checkbox"/> Single step reactions only	
<input type="checkbox"/> 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	▼
<input type="checkbox"/> Manually processed content only	

Creating an alert

Create Alert

Query: Compound: atenolol (exact search), isotopes, tautomer... [Show Query](#) ✓

Alert name:

Send alerts to:

Frequency: on:

Send alert:

☐ 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.

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

- 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.
- Enter the unique name of your alert here.
- Your registered email address appears here. Enter additional email addresses if needed. Note that the address in the screenshot has been censored.
- Select the frequency (weekly, every two weeks, monthly or after every database update) and the weekday or date of the month for the alert.
- 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.
- Advanced alert selections are currently only available for Reaxys database content. The email contains a preview of alert results defined by your selection here.
- Click *Create* to create the alert for this query.

Managing your alerts

Reaxys® Quick search Query builder Results Synthesis planner History Alerts

Alerts

Substances	Dopamine-Main - in Reaxys	Results from: No alert results	>
Since Apr 21, 2021	Compound: dopamine (exact search), isotopes, tautomers, Include: Stere...	Show details	Edit Delete
Substances	Gabapentin-Main - in Reaxys	Results from: No alert results	>
Since Apr 21, 2021	Compound: gabapentin (exact search), isotopes, tautomers, Include: Stere...	Show details	Edit Delete
Substances	Atenolol-Main - in Reaxys	Results from: No alert results	>
Since Apr 21, 2021	Compound: atenolol (exact search), isotopes, tautomers, Include: Stereo, ...	Show details	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 'Export substances Reaxys' (A). The main area contains several sections: 'Choose a format:' with a dropdown menu showing 'PDF/Print' (B); 'Range:' with a dropdown menu showing 'All results - 480' (C); 'Export:' with four radio button options: 'All available data' (selected), 'Identification data only', 'Hit data only', and 'Choose specific data' (D); and 'Additional options:' with two checkboxes: 'Include structures' (checked) and 'Include a description in the document' (E). At the bottom, there is an 'Export >' button (F). An inset window (G) is open, showing a list of export formats: 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 'History' tab. The main interface shows a list of recent queries. The first query is '96 Reactions' from 'Today 11:56', categorized as 'Context Switch from: 15 Substances'. Below it is a query for '15 Substances' from 'Today 11:56' with a 'Quick Search: "atenolol" "solubility" AND' and a chemical structure icon. Other queries include '10 Documents' (Filtered by: Patent Office), '5,556 Documents' (Quick Search: "HEK293" "phosphorylation"'), and '88 Substances' (Quick Search: "ascorbic acid" "melting" AND'). Each entry has options to 'Edit Query', 'Save', 'Alert', and 'View'. An inset window at the bottom shows the 'Saved' list, highlighting a query titled 'Atenolol-Solubility' from 'Today 11:56' with a 'Quick Search: "atenolol" "solubility" AND' and a chemical structure icon. This inset also includes 'Edit Query', 'Delete', 'Rename', 'Alert', and 'View' options.

- 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 [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.
- 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 'Profile' settings page in Reaxys. At the top, a navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. A user profile icon is in the top right corner, labeled 'A'. Below the navigation bar, the 'Profile' tab is selected, labeled 'B'. The page is divided into several sections, each with a 'Reset to default' link. The 'Default structure/reaction editor settings' section contains 'Structure Editor' (set to 'ChemAxon's MarvinJS', labeled 'C'), 'Search structure as' (set to 'As drawn'), and 'Preferences' (a list of checkboxes including 'Include Tautomers', 'Include Stereo', 'Include Additional ring closures', 'Include Salts', 'Include Mixtures', 'Include Isotopes', 'Include Charges', and 'Include Radicals'). The 'Autoplan' section contains 'Default settings' (a list of checkboxes including '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%', labeled 'D'). The 'Results per page' section contains 'Number of results per page' (set to '15', labeled 'E'). The 'Text and Contrast' section contains 'Text Size' (set to 'A', labeled 'F'), 'Contrast' (set to 'A'), and 'Text Color' (set to 'All Black').

- If you are signed into your personal account, you can access by clicking your name or the person symbol and selecting *Profile*.
- 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
- 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).
- 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.
- Set the number of results per page here.
- Set text size, contrast and text color here.

What is *Query Builder*?

The screenshot displays the Reaxys Query Builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted with an orange box A), 'Results', 'Synthesis planner', 'History', and 'Alerts'. Below this is a search bar with tabs for 'Reactions', 'Targets', 'Substances', and 'Documents'. The main workspace is a large grey area with the text 'Drag & Drop to build a new query' (highlighted with an orange box C). On the right, a sidebar contains 'Search fields' and a list of categories: 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography' (highlighted with an orange box B). An inset window shows a query being built with two querylets connected by an AND operator. The first querylet is 'Melting Point' with a value of 56 and a solvent. The second querylet is 'Boiling Point' with a value of 100 and a pressure. The inset is highlighted with an orange box D.

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 [tutorial in the Resource Center](#).

Performing a patent assignee search

The screenshot illustrates the Reaxys Query Builder interface for a patent assignee search. The interface is divided into several sections:

- Top Navigation:** Includes 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'.
- Search Fields:** A sidebar on the right lists various search fields under the 'Fields' category, including 'Bibliography', 'Document Type', 'Authors', 'Patent Assignee', 'Journal Title', 'Publication Year', and 'Common Patent Number'.
- Search Criteria:** The main search area shows a criteria set for 'Patent Assignee' with the value 'Pfizer'. A dropdown menu is open, showing suggestions like 'pfizer', 'pfizer co, inc', 'pfizer (butler et al)', and 'pfizer, chas u co'.
- Results View:** An inset window shows the 'Results' view, displaying a list of search results with options to 'Limit To', 'Exclude', and 'Export'. The results list includes titles like 'IMPROVEMENTS TO WASH SOLUTIONS FOR PROTEIN A CHROMATOGRAPHY IN AN AN-TIBODY PURIFICATION PROCESS' and 'CRYSTALLINE FORMS OF LORLATINIB MALEATE'.

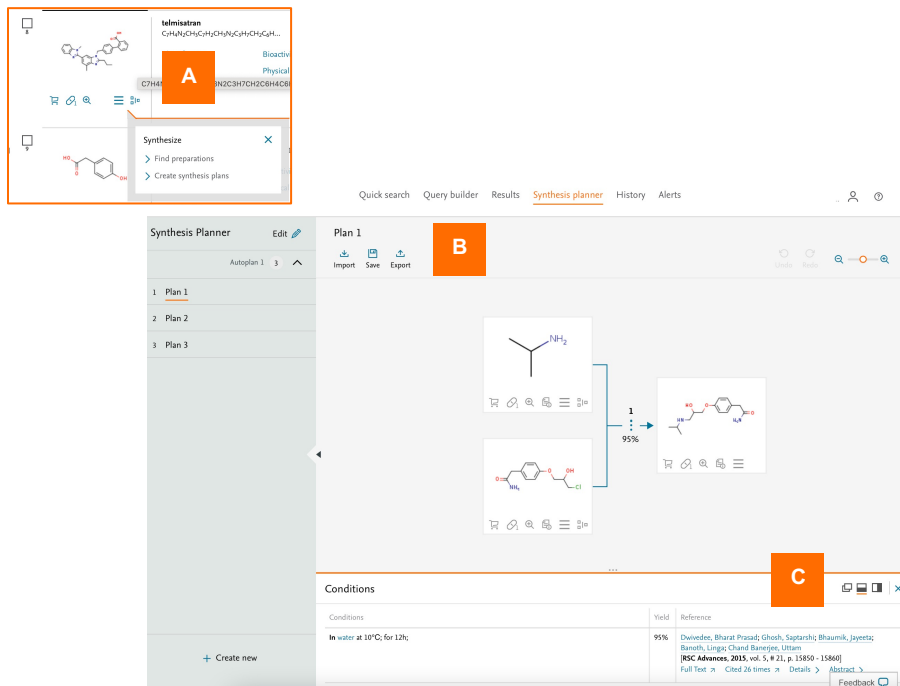
Query Builder is currently the best feature to use for patent assignee searches.

- 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 [tutorial in the Resource Center](#).

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What is *Synthesis Planner*?



The screenshot displays the Reaxys Synthesis Planner interface. At the top left, a red box labeled 'A' highlights the 'Synthesize' button. Below it, a red box labeled 'B' highlights the 'Plan 1' tab. The main workspace shows a chemical reaction scheme with a yield of 95%. At the bottom, a red box labeled 'C' highlights the 'Conditions' and 'References' table.

Conditions	Yield	Reference
In water at 10°C; for 12h;	95%	Davidek, Bharat Prasad; Ghosh, Saptarshi; Bhaumik, Jayanta; Banerji, Linga Chand Banerjee, Uttam [RSC Advances, 2015, vol. 5, # 21, p. 13808 - 13860] Full Text > Cited 34 times > Details > Abstract >

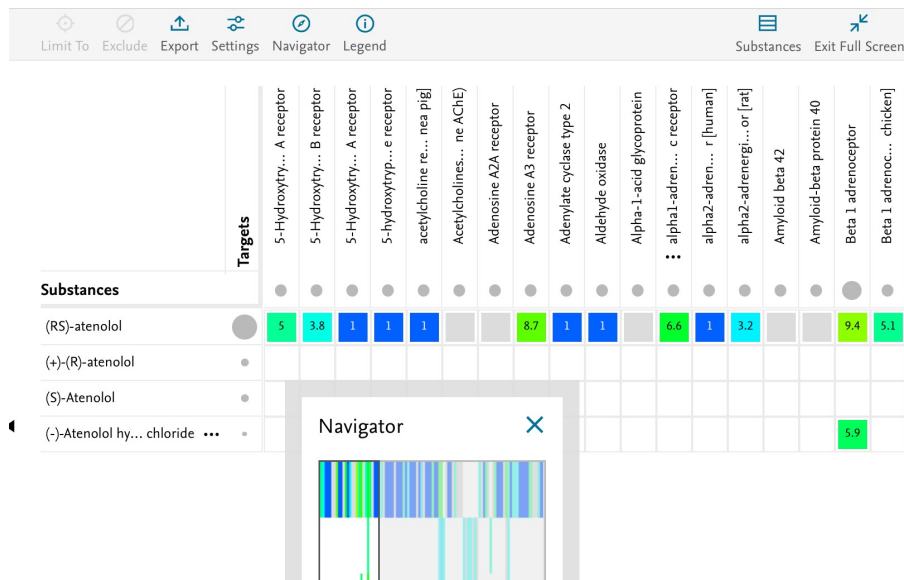
Reaxys Synthesis Planner enables you to instantly generate multiple synthesis plans for substances of interest based on information published in peer-reviewed literature.

- 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.
- 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.
- 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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