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Reaxys[®]

Quick reference guide



Table of contents

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.

Navigating the Reaxys home page	3	Managing your alerts	12
Using <i>Quick search</i>	4	Exporting results	13
Using the structure editors for <i>Quick search</i>	5	Using your query history	14
Navigating the <i>Results preview</i>	6	Changing personal settings	15
Navigating a <i>Results</i> page	7	What is <i>Query Builder</i>?	16
View options for different <i>Results</i> categories	9	Performing a patent assignee search	17
Filter options for different <i>Results</i> categories	10	What is <i>Retrosynthesis</i>?	18
Creating an alert	11	What is <i>Heatmap</i>?	19

Navigating the Reaxys home page

The screenshot shows the Reaxys home page interface. At the top, a navigation bar (A) contains links for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. A user profile icon (B) is located in the top right corner. Below the navigation bar is a search header (C) with the text 'Search substances, reactions, documents and bioactivity data' and a sub-header 'In Reaxys, Reaxys Medicinal Chemistry, PubChem, SigmaAldrich and Commercial Substances'. A search input field (D) is present with the text 'Substance ADME, e.g. Pharmacokinetic of Imatinib' and a 'Find >' button. A 'Draw' button (E) is located below the search field. A statistics section (F) displays 'Content Overview | Latest update: 30, August 2021 >' and four categories: '157M Substances', '56M Reactions', '68M Documents', and '41M Bioactivities'. A 'Feedback' button (G) is located in the bottom right corner. The RELX Group logo is also visible in the bottom right area.

- 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 latest document, substance, reaction and bioactivity data points indexed in Reaxys.
- G. 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, there is a navigation bar with 'Quick search' highlighted (A). Below it, a search bar contains the text 'ADME, e.g. Pharmacokinetic of Imatinib' (C). To the right of the search bar is an 'Import' button (B). Below the search bar is a 'Draw' button (D). To the right of the search bar is a 'Find' button (E). Below the search bar, there is a 'Content Overview' section showing '157M' and '56M' items. An inset window (F) shows search suggestions for 'aten', including 'atenolol', 'atenolol acid', 'atenolol hydrochloride', and target names 'atendo1' through 'atendo5'.

- 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, a dropdown menu (A) allows selecting between 'MarvinJS' and 'ChemDrawJS'. To the right, a button (B) labeled 'Insert structure from name' opens a search dialog. The main workspace (C) contains a drawing toolbar and a central area with the Marvin JS logo. On the right side, a search options panel (D) includes checkboxes for 'As drawn', 'As substructure', 'Similar', 'Tautomers', 'Stereo', 'Additional ring closures', 'Related Markush', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. At the bottom, a 'Transfer to query' button (E) is visible. An inset dialog box (F) titled 'Create structure template from name' shows 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*

The screenshot shows the search results for "atenolol" in the Reaxys interface. The main results list is at the top, and a detailed preview for substances is shown below.

Callout A: Search for "atenolol"

Callout B: New Edit

Callout C: Structure: as drawn

Callout D: Preview Results

Callout E: View Results

Callout F: Top 3 results

Substances Results:

Substance	Chemical Formula	Physical Data	Proprietary Data
(R)-atenolol	C ₁₄ H ₁₉ N ₃ O ₂	297925 29422 01 7	Proprietary - 12 Reactions - 54 Targets - 113 Documents - 8,000
(S)-Atenolol	C ₁₄ H ₁₉ N ₃ O ₂	297925 93279 14 5	Proprietary - 52 Reactions - 37 Targets - 16 Documents - 77
(±)-R)-atenolol	C ₁₄ H ₁₉ N ₃ O ₂	297925 16729 12 8	Proprietary - 26 Reactions - 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 a search of 125 substances. The interface includes a filters sidebar (B), a top navigation bar (A), and a main results area. The results area displays three entries for Atenolol: (R)-atenolol, (S)-Atenolol, and (+)-(-)-atenolol. Each entry includes a chemical structure, identification information, and links to various data categories like Physical Data, Spectra, and Bioactivity. A database dropdown menu (D, E) is open, showing the current database 'Reaxys - 125' and other options like Commercial Substances, eMolecules, LabNetwork, PubChem, and SigmaAldrich. Other callouts (F, G, H) point to specific UI elements like the 'Export' button, search filters, and document links.

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 a search results page. On the left, a 'Filters' sidebar is visible. The main area shows two substance entries: (R)-atenolol and (S)-atenolol. Each entry includes a chemical structure, name, and various data links. Two inset windows are shown: 'Substance Availability' (Inset J) listing databases like Accelrys' ACD and Sigma Aldrich, and 'Options' (Inset K) listing actions like 'Find Similar' and 'View related Markush'.

- 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.

D. Document results offer 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

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

8 Substances

0 selected

Limit To Exclude Export

Commercial Substances - 8

Commercial Substance ID

Grid

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:

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.

- 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
Dopamine-Main - in Reaxys	Since Apr 21, 2021 Compound: dopamine (exact search), isotopes, tautomers, Include: Stere... Show details	No alert results	Edit Delete
Gabapentin-Main - in Reaxys	Since Apr 21, 2021 Compound: gabapentin (exact search), isotopes, tautomers, Include: Stere... Show details	No alert results	Edit Delete
Atenolol-Main - in Reaxys	Since Apr 21, 2021 Compound: atenolol (exact search), isotopes, tautomers, Include: Stereo, ... Show details	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 (A). The main area contains several sections: 'Choose a format:' with a dropdown menu (B) currently set to 'PDF/Print'; 'Range:' with a dropdown menu (C) set to 'All results - 480'; 'Export:' with radio button options: 'All available data' (selected, D), 'Identification data only', 'Hit data only', and 'Choose specific data'; and 'Additional options:' with checkboxes for 'Include structures' (checked, E) and 'Include a description in the document'. At the bottom right is an 'Export >' button (F). An inset window (G) titled 'PDF/Print' 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 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 [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' page in Reaxys, with the 'Preferences' tab selected. The page is divided into several sections, each with a 'Reset to default' link. Annotations A-F point to specific elements:

- A:** Points to the user's name 'A' and the person symbol in the top navigation bar.
- B:** Points to the 'Profile' tab in the sub-navigation bar.
- C:** Points to the 'Structure Editor' setting, which is currently set to 'ChemAxon's MarvinJS'.
- D:** Points to the 'Autoplan' section, which contains settings for the number of plans to create, maximum alternative branches, maximum number of steps, and default yield.
- E:** Points to the 'Results per page' setting, which is currently set to 15.
- F:** Points to the 'Text and Contrast' section, which includes settings for text size, contrast, and text color.

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.

- 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.
- Patent Assignee, structure drawings, molecular formulas and CAS registry numbers can 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

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](#).

Set up a Retrosynthesis query

Quick search Query builder **A** Retrosynthesis History Alerts

Structure editor selected: MarvinJS ChemDrawJS Insert structure from name >

B Parameters

C Synthesize >

D

No.	Date/Time	Project name	Draw new structure	No. of routes
3662	31 Aug 2021 03:49	Project #3662		Predicted ● In progress Published ● View >
3515	31 Aug 2021 07:17	Project #3515		Predicted ● Published ● View >

E

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

- Click on the Retrosynthesis page and draw a compound using the structure editor, as explained in page 5.
- Define your search parameters for published and predicted routes (if you are a customer of Predictive Retrosynthesis module)
- Click on *Synthesize* to obtain retrosynthetic routes.
- A new retrosynthetic route is added to the synthesis projects page, remember to sign-in or register to save your queries.
- Click on *View* to analyse routes.

See more on next page

Analyse Retrosynthesis results

The screenshot displays the Reaxys Retrosynthesis interface. On the left, a vertical sidebar contains icons for 'Export', 'Legend', 'Rotate', and 'Draw'. The main area shows a 'Published route #1' with 'Step 1' selected. A table on the right provides details for the reaction step, including conditions, yield, and a reference. A table below the table lists reagents and experimental procedures. The interface also features a 'Tree view' and 'Table view' toggle, and a search bar at the top.

Conditions	Yield	Reference
With palladium diacetate; triethylamine; 4,5-bis(diphenylphosphino)-9,9-dimethylxanthene In 1,4-dioxane at 50°C; under 760.051 Torr; for 36h; Reagent/catalyst; Solvent; Temperature; Inert atmosphere; Experimental Procedure	95.8%	Shandong Huihai Pharmaceutical And Chemical Co., Ltd.; Hou Xuhui; Zhang Hai; Zhang Shifeng; Fu Dexiu; Jiang Fuyuan; Tian Xixing CN112125882, 2020, A Location in patent: Paragraph 0033; 0041-0048 Full Text Details Abstract

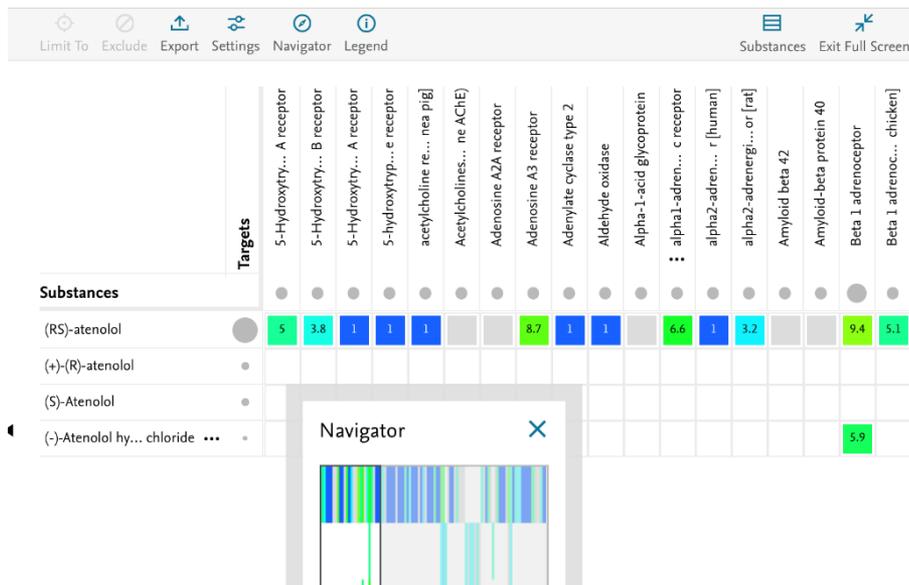
1-4 Example 3
 N-(5-amino-2-methylphenyl)-4-(pyridin-3-yl)pyrimidin-2-amine 0.1mol, 1-[(4-bromophenyl)methyl]-4-methyl piperazine 0.1mol of piperazine, 5mmol of palladium acetate, 5mmol of 4,5-bisdiphenylphosphine-9,9-dimethylxanthene and 0.18mol of triethylamine were added to 200mL of dioxane and replaced with nitrogen twice, Replace it with carbon monoxide twice, and heat to 50° C. under a carbon monoxide atmosphere (1 atm) with stirring for 36 hours. After the reaction is completed, the temperature is

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

- A. Toggle between proposed routes. Toggle between each proposed reaction step for a given route.
- B. Review the different experimental conditions, yield and literature reference for a given reaction step.
- C. Access experimental procedures if available.
- D. Toggle between vertical and horizontal view of reaction information.
- E. Export routes including structures and experimental procedures

For more information on *Retrosynthesis*, please see the videos [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 Resource Center](#).



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Reaxys[®]

An expert-curated chemistry database

Go to www.reaxys.com

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