Reaxys®

Quick Reference Guide

1. The Query Page

THE QUERY OPTIONS

There are several ways to begin your search.

Ask Reaxys – Interprets search keywords written in natural language and retrieves the most relevant results.

Reactions – Open the **Reactions** query theme to access data fields such as Yield, Solvent (Reaction Details), Reagent/Catalyst and Reaction Type. These fields can be searched with or without a chemical structure, which can be drawn using Structure Editors, imported using the Import button in the upper right corner or generated from the name or identifier of the structure.

Substances, Names, Formulas – Open the **Substances** query theme to access data fields such as Molecular Formula (which includes a Formula Builder), CAS Registry Number and Chemical Name. These fields can be searched with or without a chemical structure.

Medicinal Chemistry – Open the **Medicinal Chemistry** query theme to access searchable data fields such as Target Name, Substance Action on Target, Bioassay Category, Bioassay Animal Model, Cells/Cell Lines and Measurement pX. These fields can be searched with or without a chemical structure.

Literature – Open the **Literature** query theme to access a form containing fields such as Authors, Patent Number and Publication Year.

ReaxysTree – Open the **ReaxysTree** option to browse hierarchies of terms, particularly those relating to chemical transformations and substance properties. This helps users to make connections between seemingly disparate aspects of chemistry and make it easier to search the literature.

Physical – Open the **Physical** query theme to access a form containing fields such as Melting Point, Boiling Point and Refractive Index.

Spectra – Open the **Spectra** query theme to access a form containing fields such as NMR Spectroscopy, IR Spectroscopy and Mass Spectrometry.

Natural Product – Open the **Natural Product** query theme to access a form designed to retrieve information about natural products and their isolation.

Advanced – Open the **Advanced** query theme and click on **Show Property List**. This provides access to the data structure and allows detailed bibliographic, data and keyword searches. Searches can be done with or without a chemical structure. The Property List allows the building of a query from field definitions, search terms and data operators.

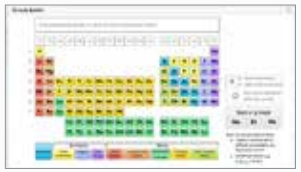
2. Constructing Queries

Feature	Comment
Ask Reaxys	Examples: “synthesis of p-phenylnitrobenzene”, “Suzuki coupling”, “adler phenol oxidation”
Create a structure template from the substance name	 1. The input field for creating a structure based on a chemical identifier Open the **Reactions** query theme and then click the red link below the **Structure** box. Enter the name, CAS number or other identifier for the product, reactant or catalyst of interest in the popup window that appears(1) and click **Submit.**
Search forms	 2. The popup window for precise search terms for solvents  3. The popup window for customization of the Reactions query theme Open the **Reactions** query theme and then use the **Reaction Data** form below the structure box. Select the role of the compound of interest (Product, Starting material, Reagent/ Catalyst or Any role). Fill the fields Product Name, Yield, Reaction Type, etc. Click **Lookup** to open a popup window (2) that allows browsing and selection of precise search terms from the Reaxys taxonomy.
Structure editors	 4. The structure box Open the Reactions query theme and then click the Structure Editors button in the structure box and select one of the 3 options. Click the Help link for information about using ChemDraw, AccelrysDraw ISISDraw or ICEdit.

Substances

Feature	Comment
Ask Reaxys	Enter a chemical name or CAS number. Examples: “quinolone”, “91-22-5”
Create a structure template from the substance name	 1. The input field for creating a structure based on a chemical identifier Open the **Substances** query theme and then click the red link below the **Structure** box. Enter the name, CAS number or other identifier for the compound of interest in the popup window that appears (1) and click **Submit**.
Search forms	 2. The popup window for precise search terms for chemical names  3. The popup window for customization of the Reactions query theme Open the **Reactions** query theme and then use the **Reaction Data** form below the structure box. Select the role of the compound of interest (Product, Starting material, Reagent/ Catalyst or Any role). Fill the fields Product Name, Yield, Reaction Type, etc. Click **Lookup** to open a popuptm the Reaxys taxonomy.
Structure editors	 4. The structure box Open the **Substances** query theme and then click the Structure Editors button (4) in the structure box and select one of the 3 options. Click the Help link for information about using ChemDraw, AccelrysDraw ISISDraw or ICEdit.

2. Constructing Queries

Feature	Comment	
Formula Builder	 1. The input field for creating a structure based on a chemical identifier	Open the **Substances** query theme and then click on Formula Builder button to open the periodic table-based formula builder to build the inorganic or organometallic compound formula of interest. Click an element and use arrows to add a range for the element count. Use the displayed abbreviations to add groups from the periodic table and other options shown on the right side of the Formula Builder.

Medicinal Chemistry

Feature	Comment	
Ask Reaxys		Enter search terms for bioactive compounds, targets or bioactivity data. Examples: “5-ht1a inhibitor”, “Na channel”, “CXCR4 inhibitor”, “Lupeol”
Search forms	 1. The popup window for precise search terms for substance actions on targets  2. The popup window for customization of the Medicinal Chemistry query themee	Open the **Medicinal Chemistry** query theme and then use the **Bioactivities** form. Fill the fields Target Name, Substance Action on Target, Bioassay Category, etc. Click **Lookup** to open a popup window (1) that allows browsing and selection of precise search terms from the Reaxys taxonomy.
Structure editors	 3. The structure box	Open the **Medicinal Chemistry** query theme and click the Structure link in the lower toolbar. The structure box will open at the top of the query theme. Use the Structure Editors button (3) in the structure box and select one of the 3 options. Click the Help link for information about using ChemDraw, AccelrysDraw ISISDraw or ICEdit.

1. Constructing Queries

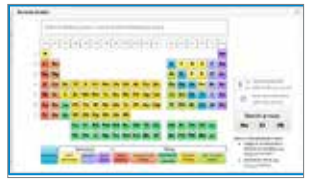
2.1. Literature

Feature	Comment
Ask Reaxys	Enter search terms. Examples: “publications about quasicrystals”, “published by Schrock”, “Tetrahedron, 2014, 70, 2343”
Ask Reaxys	Open the **ReaxysTree** query theme (1). Open folders to find a topic for searching the chemical literature or type a term into the search box, click **Search** and uncheck boxes for unwanted topics. Click **Search Literature**.
Search forms	 2. The popup window for precise search terms for keywords  3. The popup window for customization of the Literature query theme  4. The Structure box Open the Literature query theme and then use the Bibliographic Data form to enter queries for Document Type, Authors, Journal Title and Publication Year. Click Lookup to open a popup window (2) that allows browsing and selection of precise search terms. Add a structure to a Literature query Open the Literature query theme and click the Structure link in the lower toolbar. The structure box will open at the top of the query theme. Use the Structure Editors button (4) in the structure box and select one of the 3 options. Click the Help link for information about using ChemDraw, AccelrysDraw ISISDraw or ICEdit.

2.2. Properties

Feature	Comment
Ask Reaxys	Enter search terms for physical properties. Examples: “boiling point of benzene”, “density of quinoline”
Search forms	Open the **Physical** or **Spectra** query theme and then use the appropriate form. Click **Lookup** to open a popup window that allows browsing and selection of precise search terms. Click **Add/Remove fields** below the form to customize the query theme
Add a structure to a Property query	Open the **Physical** or **Spectra** query theme and click the Structure link in the lower toolbar. The structure box will open at the top of the query theme. Use the Structure Editors button in the structure box and select one of the 3 options. Click the Help link for information about using ChemDraw, AccelrysDraw ISISDraw or ICEdit.
Molecular Formula and Alloy Searches	Open the **Substances** query theme. Click one of the links in the toolbar at the bottom of the page.

Molecular Formula (1): Click an element and use arrows to add a range for the element count. Use the displayed abbreviations to add groups from the periodic table and other options shown on the right side of the Formula Builder.



1. The Formula Builder

Alloy (2): Select the percentage type from the dropdown menu. Add elements in the columns on the left. Note that they are case sensitive. Add percentages (or ranges) in the columns on the right. Check the box for Additional Components if needed.

2. The form for creating alloy searches

2. Constructing Queries

2.3. Natural Products

Feature	Comment	
Ask Reaxys	Enter search terms for natural products. Examples: “isolation from olives”, “nmr of luteolin”, “luteolin patents”	
Search forms	 1. The popup window for precise search terms for natural products	Open the **Natural Product** query theme. The **Isolation from Natural Product** field accepts the names of natural products. Click **Lookup** to open a popup window (1) that allows browsing and selection of precise search terms. The **Literature** query theme can also be very useful for finding citations about natural products. Open it and use the **Bibliographic Data** form to enter queries for Document Type, Authors, Journal Title and Publication Year. Click **Lookup** to open a popup window that allows browsing and selection of precise search terms. **Add a structure to a natural product query** Open the **Natural Product** query theme and click the Structure link in the lower toolbar. The structure box will open at the top of the query theme. Use the Structure Editors button in the structure box and select one of the 3 options. Click the Help link for information about using ChemDraw, AccelrysDraw ISISDraw or ICEdit.

3. Results

3.1. Filters

Feature	Comment	
Filter Results		Filter by categories are displayed on the left side of the results page (1). Opening a category shows all the filters within that category. Multiple categories can be applied to a result set. Some filters have a by value or by group tab allowing a term to be typed in (2). Other filters have a More link allowing more details to be added in a popup window (3), creating a more detailed filter.

3. Results

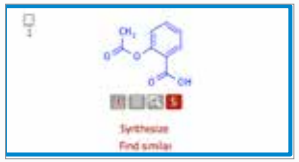
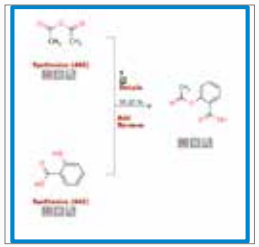
3.2. Analysis View

Feature	Comment
Analyze results using **Analysis View**	 1. Open Analysis View button  2. The base histograms of the Analysis View Reaxys Analysis View lets users select analysis criteria to get a sense of the relationships between results. For example, it permits quick discovery of the individuals and organizations that are active in a particular area of research, sorts results according to yield, or reveals the catalysts or solvents for a particular reaction class. The Open Analysis View button at the top of the results list (1) opens the panel with the analysis histograms for that result set (2). Select a category for Histogram A from its dropdown menu. The number of relevant results in the hitset for that category will be displayed in red in the histogram. Select a category for Histogram B from its dropdown menu. The number of hits per category that are a subset of the Histogram A list will be displayed in yellow in the histogram. The relationships between various categories can be assessed. To limit the hitset to the results of interest, click **Limit to**. To remove irrelevant results, click **Exclude.**

3.1. Filters

Feature	Comment
Analyze compound–target affinity relationships using Heatmap	The Heatmap provides a clear overview of the relationships between compounds and their targets in terms of key parameters to enable rapid identification of the most relevant interactions. Its parameter settings are flexible: changing them reveals new relationships between compounds and protein targets or cell lines. e Heatmap button at the top right of the results list opens the Heatmap (1). Substances are displayed on the Y-axis and Targets are displayed on the X-axis by default. This can be changed using the dropdown menu under the icon Axis Values. Click the Structure icon to display the structures. Click the dropdown menu on any given structure for details about the substance and for copy options. Click the column header line to adjust the width of the column and display larger structures. Click the Navigator icon to display a data map. Click within the map to jump to different data within the hitset. Click the Data Density icon to highlight the columns containing the most data. Click the dropdown arrow on any given column for deleting and sorting options. Select columns by clicking the column headers and then use the Limit to and Exclude options to refine the Heatmap. The pX values in Reaxys are normalized values for compound–target affinity calculated from experimental data points to enable the comparison data from different sources and assays. Use the pX Value sliders to limit results to a particular pX range. The color on the slider indicates the affinity, with blue showing the lowest affinity and red showing the highest. Exclude data coming from the GVK Bio GoSTAR databases by checking ExcludeGoSTAR data.

3. Results

Feature	Comment	
	3.4. Synthesis Plans	
Build a retrosynthetic synthesis plan	 1. The Synthesize link under a structure in the Substances result set  2. The Synthesize, Add and Remove links in the synthesis plan.	Synthesis plans are always started from the Results screen from a structure. Click the Synthesize link (1) under a substance in the Reactions, Substances or Citations results to display the three options for synthetic route generation: Manually – Allows the selection reactions from the bottom of the Synthesis Plans page. by AutoPlan – Automatically creates up to 10 synthetic routes based on preselected options. by AutoPlan (with options) – Automatically creates up to 10 plans based on options that are presented to the user. To edit a synthesis plan, click the Synthesize link under any of the substances in the plan (2). The options Manually, by AutoPlan and by AutoPlan (with options) will be displayed, functioning as described above. There is also the by Query option, which opens a structure query form. Click the Add link to add and compare alternative routes and click Remove to delete part of a plan (2). Click the Details link in the plan to display the reaction conditions. Click Save to save the plan as an .xml file. Click Output to export the plan in various formats. Click the red triangle to save the plan to the Report page.

4. Saving, printing, exporting and sending reports

Save a query – Click Save in the upper right corner of the query page

Save a result list – Click the History button and click the Store link on the right side of the page

Print the current page – Click the Print icon located on the toolbar toward the left side.

Export results – Click the Output icon. Select the desired format, range and content.

Add data to a Report – Mouse over a result (structure, data point, substance, reaction, synthesis route).

Click the red triangle that appears near it. Select from the options that appear.

View a Report – Click Report. Arrange the items using the Show, Move up, Move down and Remove links. Add text using the Annotate link.

Send a Report via email – Click the Send icon on the Report page and fill in the form. The Report will be sent as a zipped .html attachment.