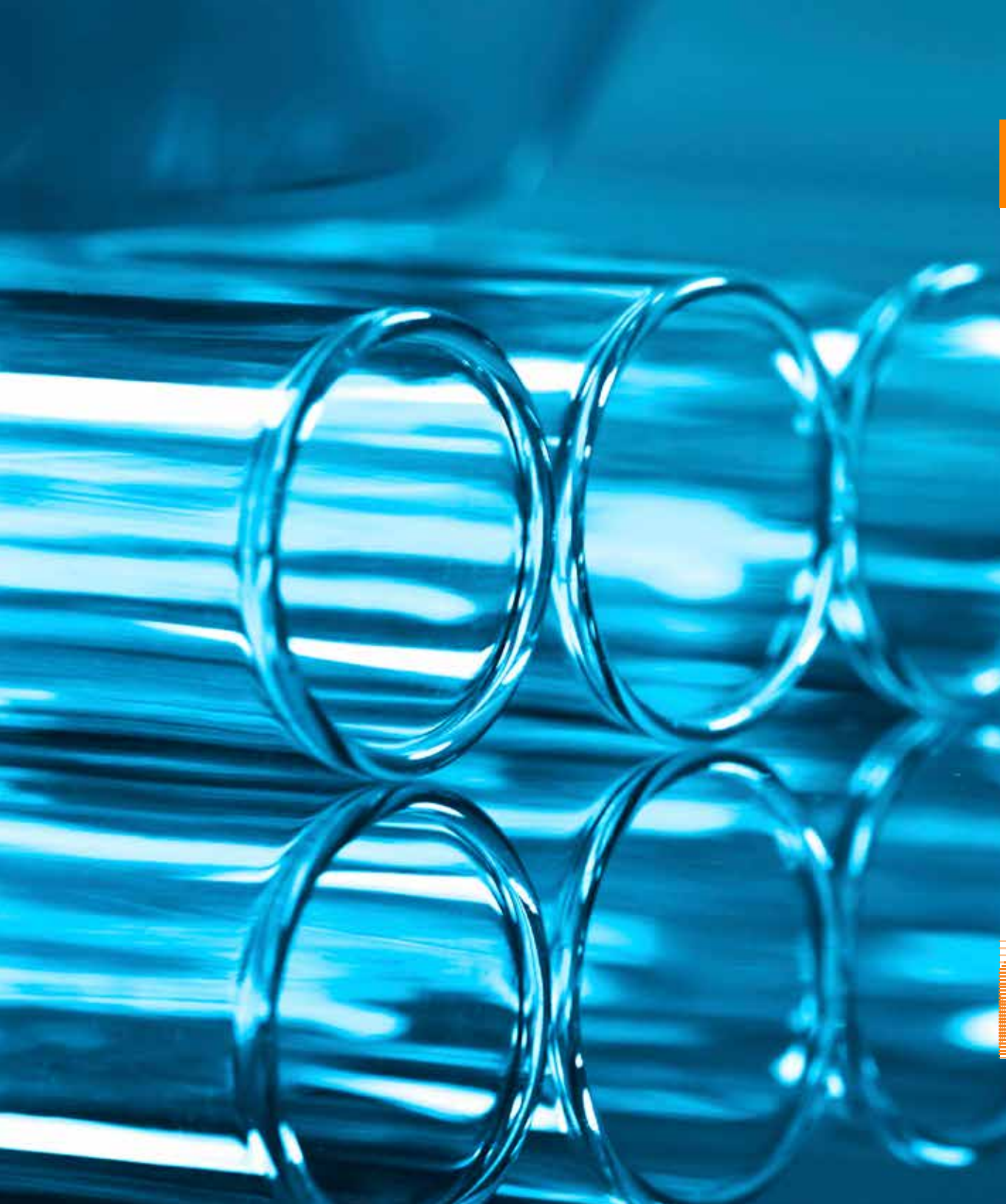

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Reaxys®

Quick Reference Guide

ELSEVIER

Contents

1. The Query Page

There are several ways to begin your search (see Figure 1).

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

Reactions – Select **Reactions** to access data fields such as *Yield, Solvent Reaction Details, Reagent/Catalyst* and *Reaction Type.*

Substances, Names, Formulas – Select **Substances** to access data fields such as *Molecular Formula, CAS Registry Number* and *Chemical Name.*

Medicinal Chemistry – Select **Medicinal Chemistry** to access searchable data fields such as *Target Name, Substance Action on Target, Bioassay Category, Bioassay Animal Model, Cells/Cell Lines* and *Measurement pX.*

Literature – Select **Literature** to access a form containing fields such as *Authors, Patent Number* and *Publication Year.*

ReaxysTree – Select **ReaxysTree** to browse hierarchies of terms, particularly those relating to chemical transformations and substance properties. This helps to make connections between seemingly disparate aspects of chemistry and makes it easier to retreive literature.

Physical – Select **Physical** to access data fields such as *Melting Point, Boiling Point* and *Refractive Index.*

Spectra – Select **Spectra** to access data fields such as *NMR Spectroscopy, IR Spectroscopy* and *Mass Spectrometry.*

Natural Product – Select **Natural Product** to access a form designed to retrieve information about natural products and their isolation.

Advanced – Select **Advanced** and click on **Show Property List**. This provides access to the data structure and allows detailed bibliographic, data and keyword searches. The **Property List** allows the building of a query from field definitions, search terms and data operators.

Note: Reactions, Substances, Medicinal Chemistry and Advanced searches can be performed with or without a chemical structure, which can be: drawn using the **Structure Editors**; imported using the **Import** button in the upper right corner of the screen; or generated from the name or identifier of the structure.

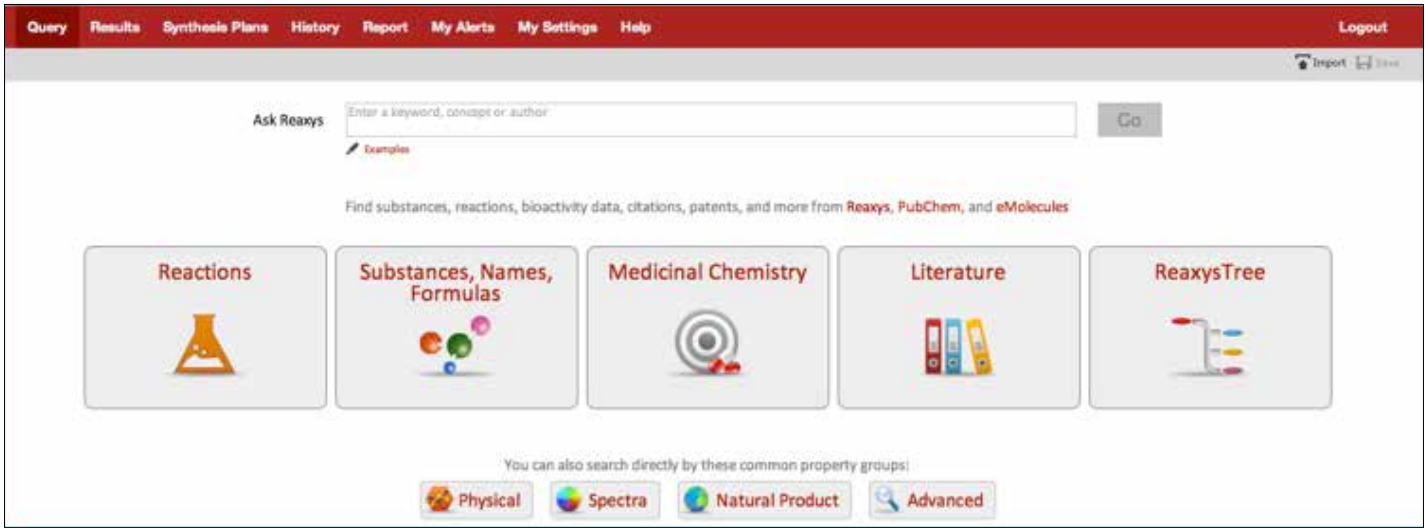
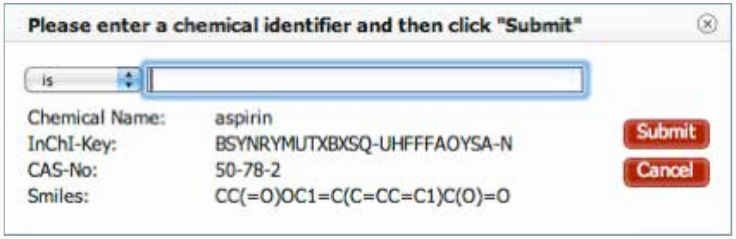


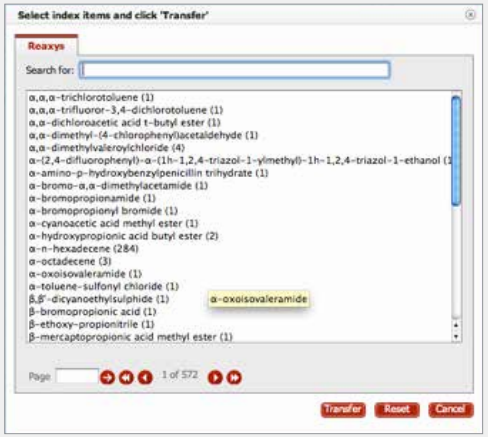
Figure 1.
The Query Page

2. Constructing Queries: Reactions

Feature	Comment
Ask Reaxys	Enter search terms in natural language. Examples: “synthesis of p-phenylnitrobenzene”, “Suzuki coupling”, “adler phenol oxidation”
Create a structure template from the substance name	Select **Reactions** and 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 input field (1) and click **Submit.**
Search forms	Select **Reactions** and 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 menu (2) with precise search terms from the Reaxys taxonomy. Click **Add/Remove** below the form to open a menu for customization of the search form (3).
Structure editors	Select **Reactions** and click the **Structure Editors** button in the structure box and select one of the options. **Reaxys Help** has more information on using structure editors.



1. The input field for creating a structure based on a chemical identifier

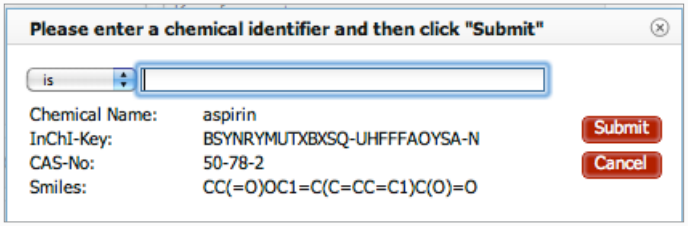


2. The browsing menu for search terms (in this example: solvents)

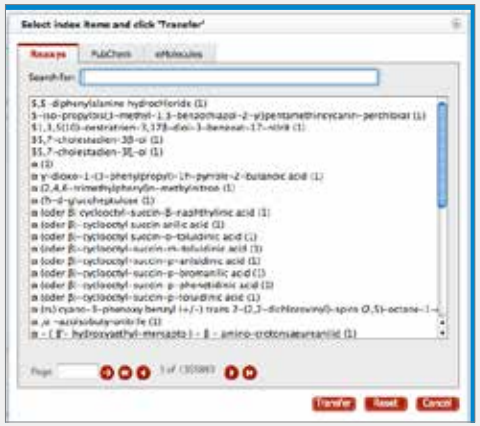
3. The menu for customization of the **Reaction Data** seach form

2. Constructing Queries: 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	Select **Substances** and click the red link below the **Structure** box. Enter the name, CAS number or other identifier for the compound of interest in the input field (1) and click **Submit**.
Search forms	Select **Substances** query theme and use the **Identification** form below the **Structure** box. Fill the fields *Reaxys Registry Number*, *CASRegistry Number*, *Chemical Name*, etc Select the role of the compound of interest (*Product*, *Starting material*, *Reagent/Catalyst* or *Any role*). Click **Lookup** to open a menu (2) with precise search terms from the Reaxys taxonomy. Click **Add/Remove fields** below the form to open a menu for customization of the search form (3).
Structure editors	Open **Substances** and click the **Structure Editors** button in the structure box and select one of the options. **Reaxys Help** has more information on using structure editors.



1. The input field for creating a structure based on a chemical identifier

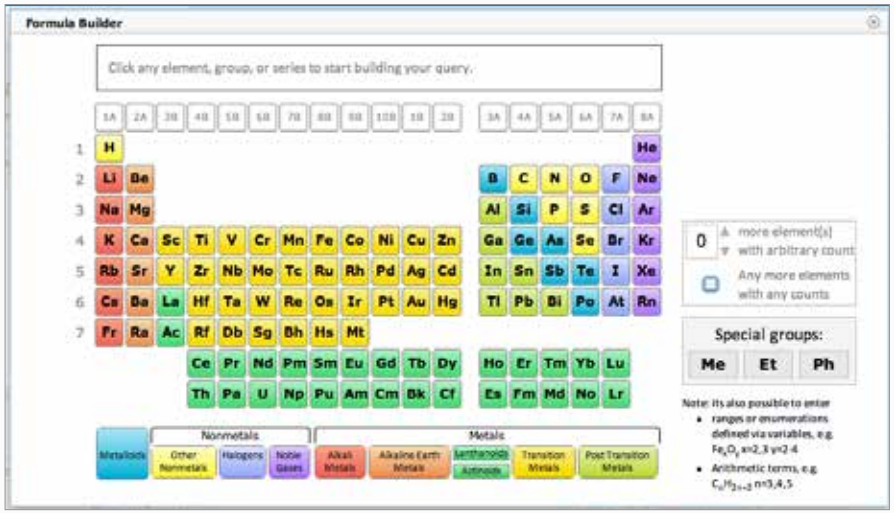


2. The browsing menu for search terms (in this example: chemical names)

3. The menu for customization of the **Identifications** search form

2. Constructing Queries: Substances

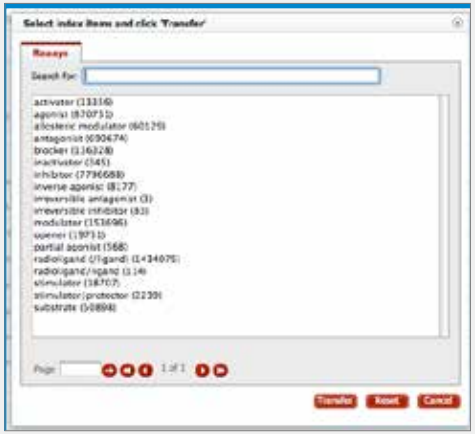
Feature	Comment
Formula Builder	To facilitate the construction of inorganic or organometallic formulas, Reaxys includes a periodic table-based formula builder (1). Select **Substances** and click on **Formula Builder.** Click an element and use arrows to add a range for the element count. Use the displayed abbreviations to add groups from the periodic table and other options shown on the right side (1).



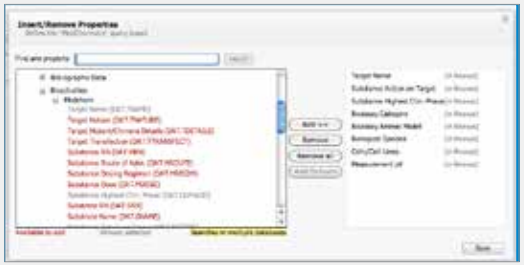
1. Formula Builder

2. Constructing Queries: 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	Select **Medicinal Chemistry** and use the **Bioactivities** form. Fill the fields *Target Name*, *Substance Action on Target*, *Bioassay Category*, etc. Click **Lookup** to open a menu (1) with precise search terms from the Reaxys taxonomy. Click **Add/Remove fields** below the form to open a menu for customization of the search form (2).
Structure editors	Select **Medicinal Chemistry** and click the **Structure** link in the lower toolbar. The structure box will open at the top of the search form. Use the **Structure Editors** button and select one of the options. **Reaxys Help** has more information on using structure editors.



1. The browsing menu for search terms (in this example: substance actions on targets)



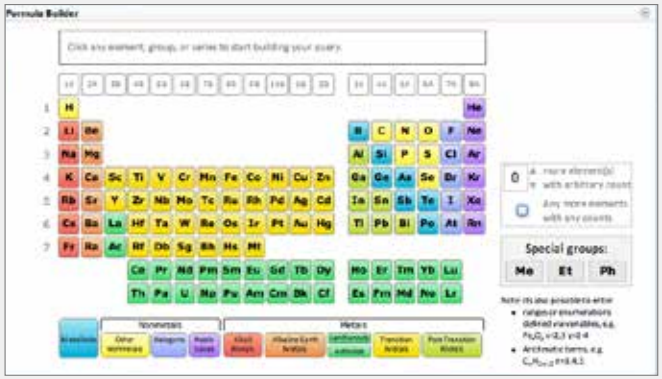
2. The menu for customization of the **Bioactivities** search form

2. Constructing Queries: Literature

Feature	Comment
Ask Reaxys	Enter search terms. Examples: “publications about quasicrystals”, “published by Schrock”, “Tetrahedron, 2014, 70, 2343”
ReaxysTree	Select **ReaxysTree** (1). Open folders to find a topic of interest or type a term into the search box, click **Search** and uncheck boxes for unwanted topics. Click **Search Literature**.  1.ReaxysTree
Search forms	Select Literature and then use the **Bibliographic Data** form to enter queries for *Document Type*, *Authors*, *Journal Title* and *Publication Year*. Click **Lookup** to open a menu (2) with precise search terms. Click **Add/Remove fields** below the form to open a menu for customization of the search form (3).  2. The browsing menu for search terms (in this example: keywords)  3. The browsing menu for customization of the **Bibliographic Data** form
Add a structure to a Literature query	Select **Literature** and click the **Structure** link in the lower toolbar. The structure box will open at the top of the search form. Use the **Structure Editors** button and select one of the options. **Reaxys Help** has more information.

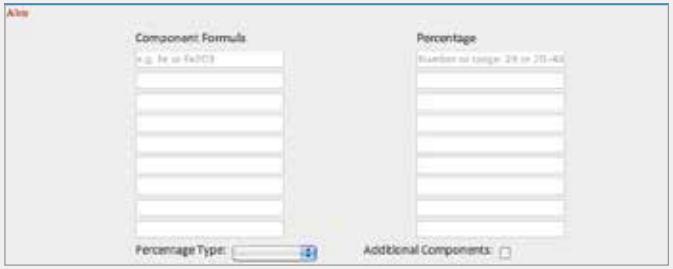
2. Constructing Queries: Properties

Feature	Comment
Ask Reaxys	Enter search terms for physical properties. Examples: “boiling point of benzene”, “density of quinoline”.
Search forms	Select **Physical** or **Spectra** and then use the appropriate form. Click **Lookup** to open a menu with precise search terms. Click **Add/Remove fields** below the form to customize the query theme.
Add a structure to a Properties query	Select **Physical** or **Spectra** 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 and select one of the options. **Reaxys Help** has more information on using structure editors.
Molecular formula and alloy searches	Select **Substances**. Click one of the links in the toolbar at the bottom of the page.



1. The Formula Builder

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.

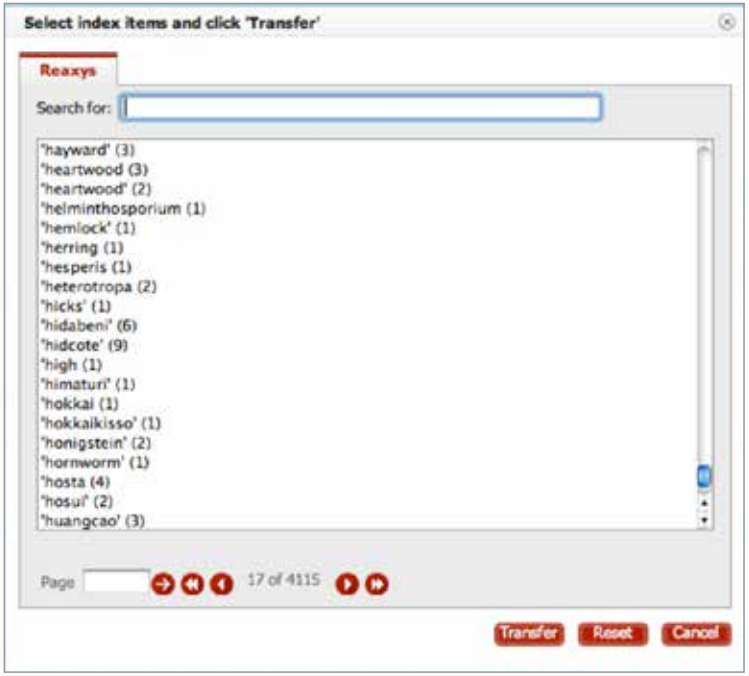


2. The form for creating alloy searches

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. Constructing Queries: Natural Products

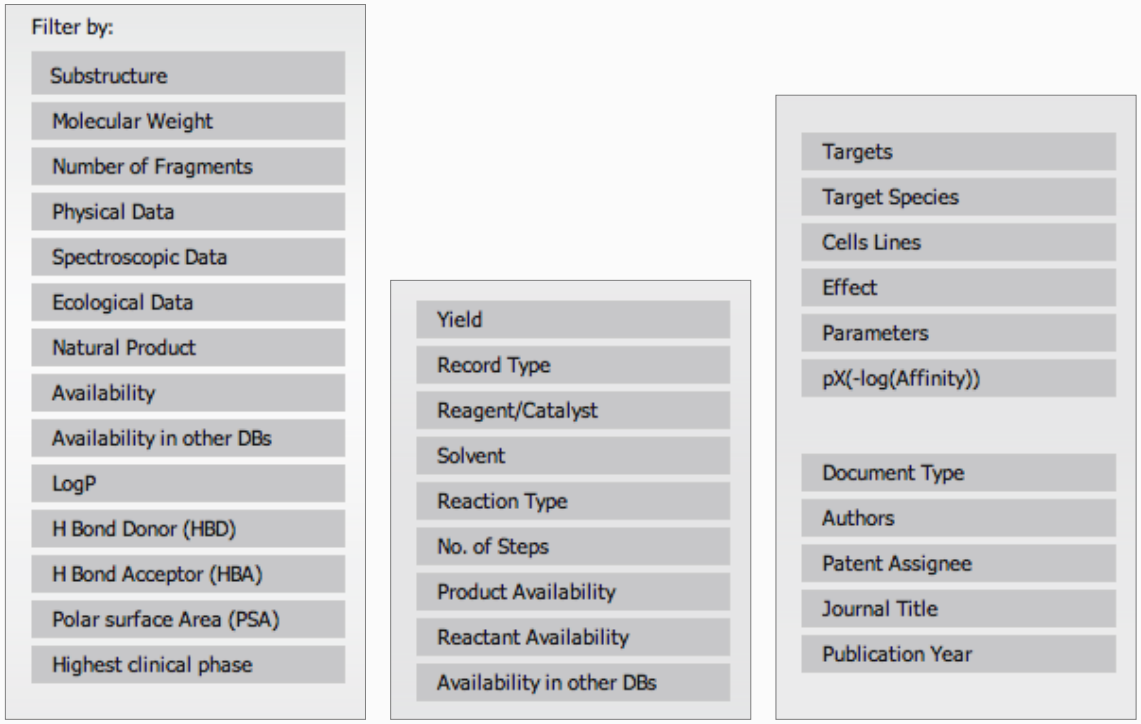
Feature	Comment
Ask Reaxys	Enter search terms for natural products. Examples: “isolation from olives”, “nmr of luteolin”, “luteolin patents”
Search forms	Select **Natural Product**. The **Isolation from Natural Product** field accepts the names of natural products. Click **Lookup** to open a menu (1) with precise search terms. The Literature query theme can also be very useful for finding citations about natural products. See section on literature searches on page 6 for more information.
Add a structure to a natural product query	Select the **Natural Product** and click the **Structure** link in the lower toolbar. The structure box will open at the top of the search form. Use the **Structure Editors** button and select one of the options. **Reaxys Help** has more information on using structure editors.



1. The browsing menu for search terms (in this example: natural products)

3. Results: Filters

Task	Comment
Filter results	The filter 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. Other filters have a **More** link allowing more details to be added.



1. The filter categories

3. Results: Analysis View

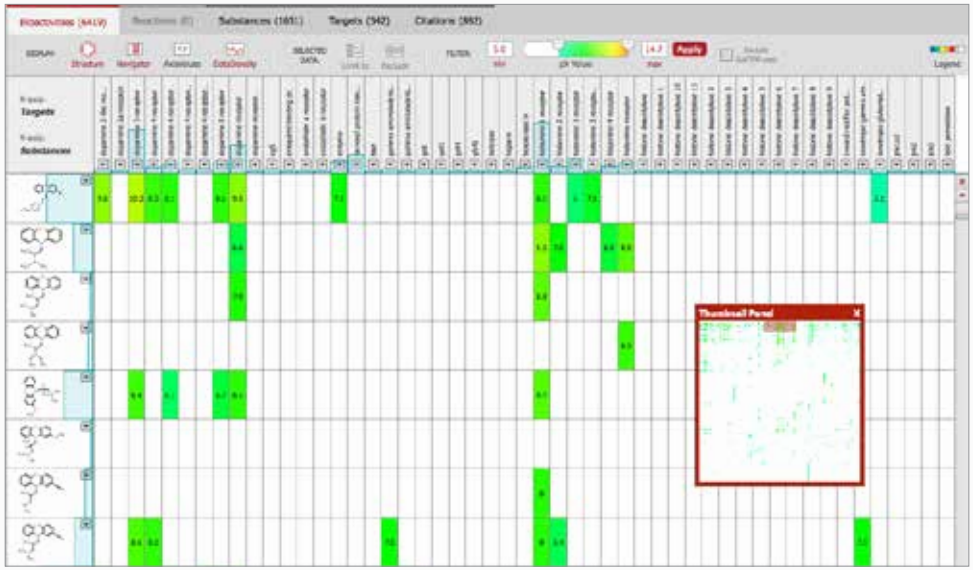
Task	Comment
Analyze results using Analysis View	Reaxys Analysis View lets users select analysis criteria to get a sense of the relationships between results. For example, it permits quick discovery of the individuals and organizations that are active in a particular area of research, sorts results according 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.**

1. The button to open Analysis View is above the results.

2. The base histograms of the Analysis View

3. Results: Heatmap

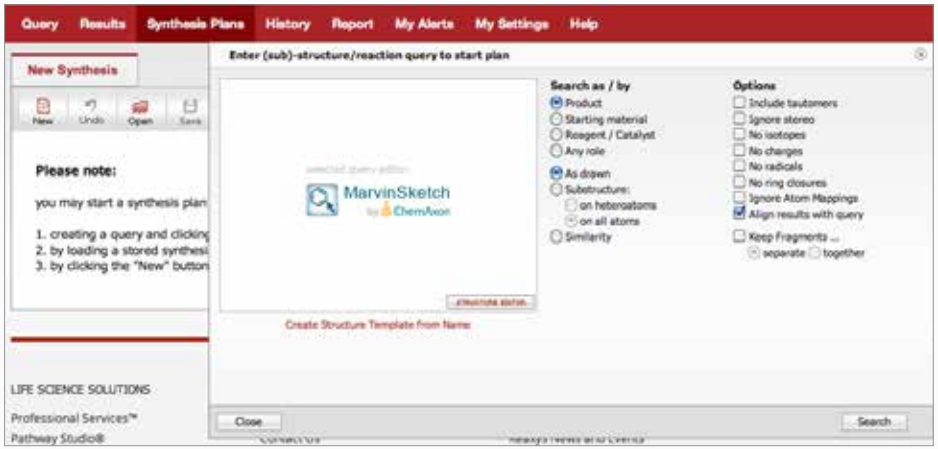
Feature	Comment
Analyze compound-target affinity relationships using Heatmap	The Heatmap provides a clear overview of the relationships between compounds and their targets in terms of key parameters to enable rapid identification of the most relevant interactions. Its parameter settings are flexible: changing them reveals new relationships between compounds and protein targets or cell lines. The **Bioactivities** 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 **Exclude GoSTAR data**.



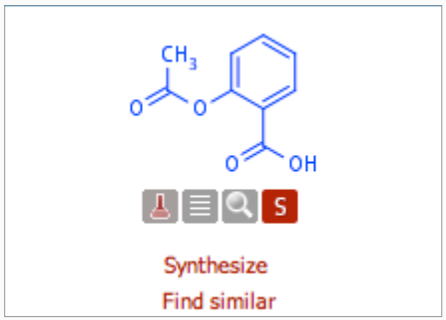
1. The Heatmap

3. Results: Synthesis Plans

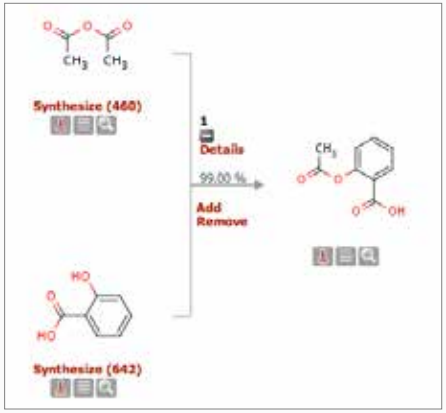
Feature	Comment
Build a retrosynthetic synthesis plan	There are two ways to build a synthesis plan: A. Select **Synthesis Plans** in the top navigation. Click **New** and enter a structure or reaction query to start a plan (1). B. From the **Results** screen, choose the compound of interest from the Reactions, Substances or Citations tab and click the **Synthesize** link (2). This will display the three options for synthetic route generation: **Manually** – Allows the selection of 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 (3). 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. 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.



1. Generating a new Synthesis Plan



2. The **Synthesize** link under a structure in the **Substances** result set



3. The **Synthesize, Add** and **Remove** links in the synthesis plan.

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 (1).

Print the current page – Click the **Print** icon located on the toolbar toward the left side (2).

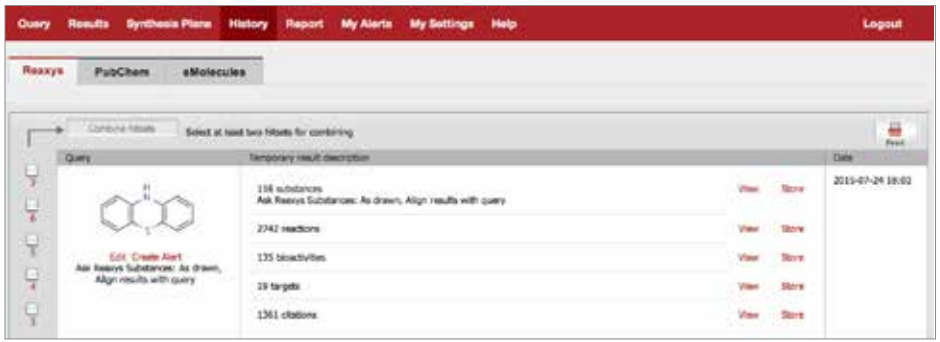
Export results – Click the **Export** icon (2). Select the desired format, range and content.

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

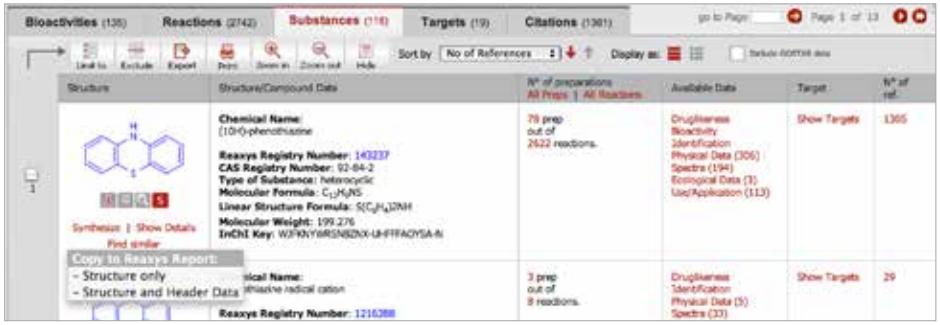
Click the red triangle that appears near it (2). Select from the options that appear.

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

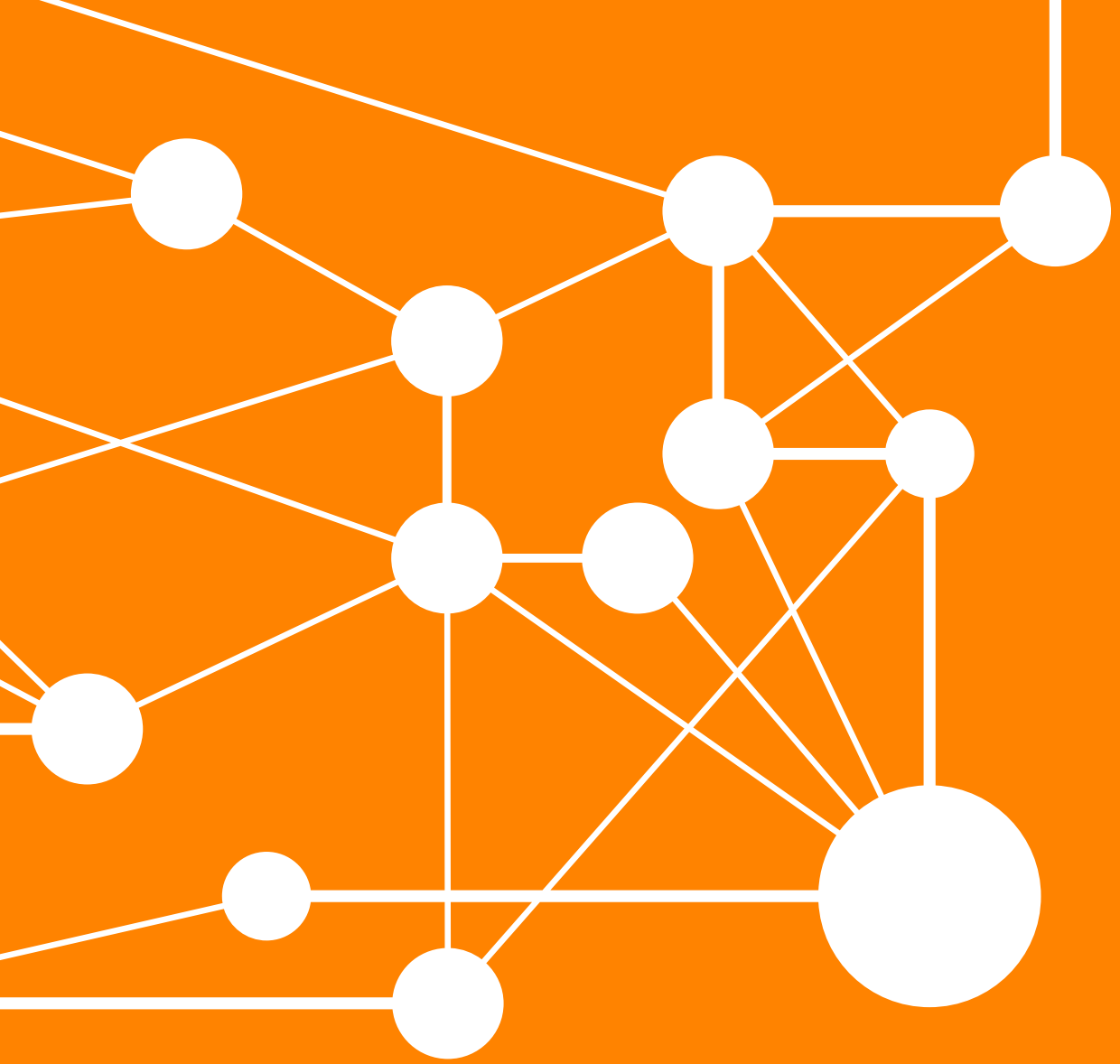
Send a Report via email – Click the **Send** icon on the **Report** page and fill in the form. The **Report** will be sent as a zipped .html attachment.



1. The **Store** link is in the search



2. The **Print** and **Export** icons are at the top of the results list.
The options for adding data to a report are shown.



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