ELSEVIER

Reaxys® Medicinal Chemistry

QUICK START GUIDE

WELCOME TO YOUR QUICK START GUIDE FOR REAXYS MEDICINAL CHEMISTRY.

Reaxys Medicinal Chemistry is a Java-free web solution that runs on modern browsers. The various available browsers present a complex landscape. The Reaxys team has tested the system on the following browser versions.

- Firefox (version 49 or higher)
- Chrome (version 53 or higher)
- Edge (version 14 or higher)
- Safari (version 9 or higher)
- Internet Explorer (version 11)

We recommend using one of these browsers to achieve best performance. While Reaxys Medicinal Chemistry may work on other browsers, some features and functionalities may not work properly.

Please contact us if you have question regarding browser support.

NOTE to Reaxys Medicinal Chemistry users in China: We noticed a significant performance increase if Google Chrome is used. If you encounter any performance issues, then try switching to Google Chrome.

NOTE to all users: We recommend not using addins and plugins or at least reducing their number to the absolutely necessary minimum. All such components influence the performance and memory usage of a browser.

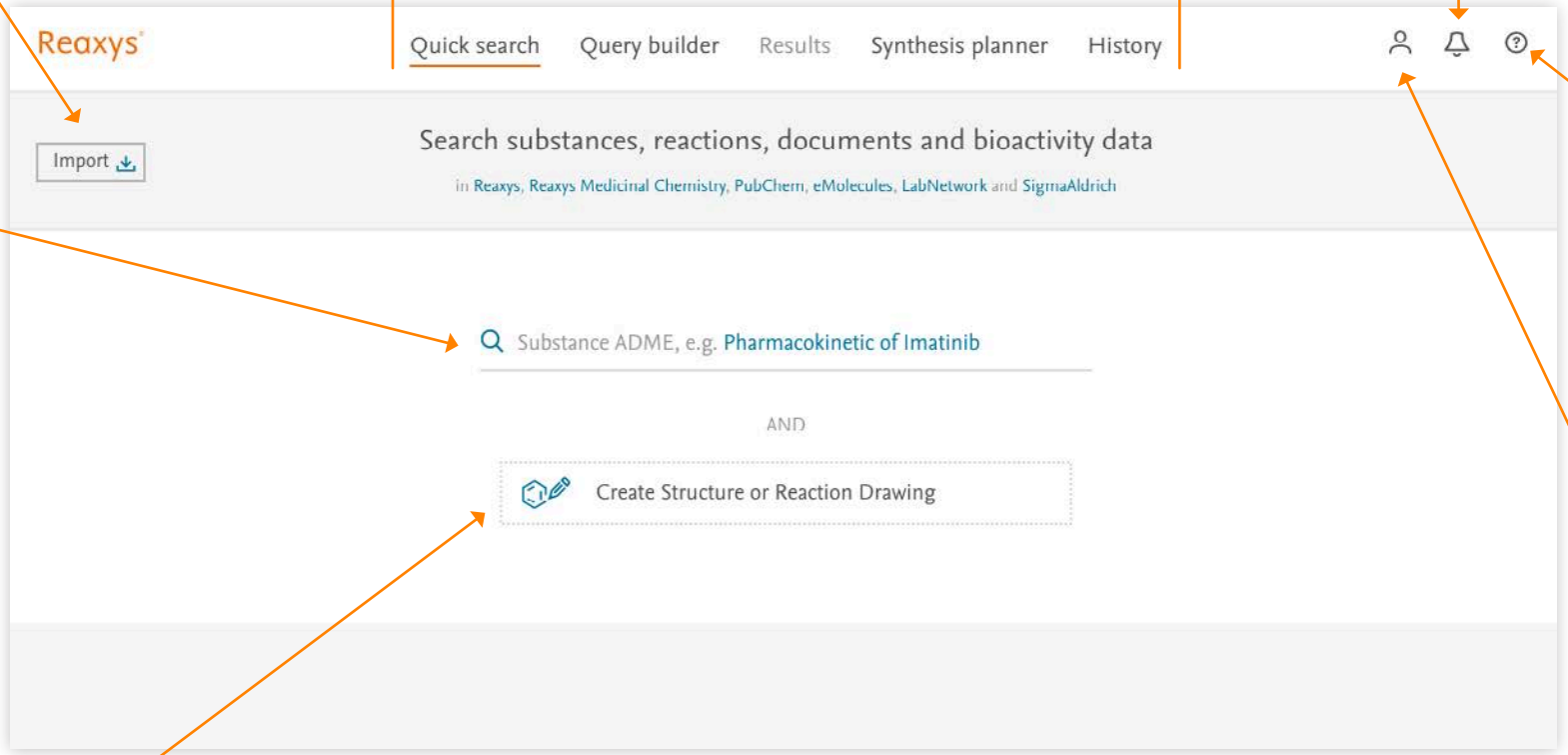
NOTE to Google Chrome users: Please ensure that you have at least 2 Gb of free hard disk space to get the optimum performance from Reaxys.

QUICK SEARCH

Drag your structure file or click here to browse and import it.

Navigate easily between Quick search, Query builder, Results, Synthesis planner and History.

Click the bell icon to access alerts created from the results of your queries.



Click the question mark to access Reaxys Help, with guides, training material and the FAQ.

The Quick Search text option accepts natural language keywords.

Truncations and wildcards are accepted.

Create a user profile to enable customized results displays (hits per page) as well as alerts and saved searches.

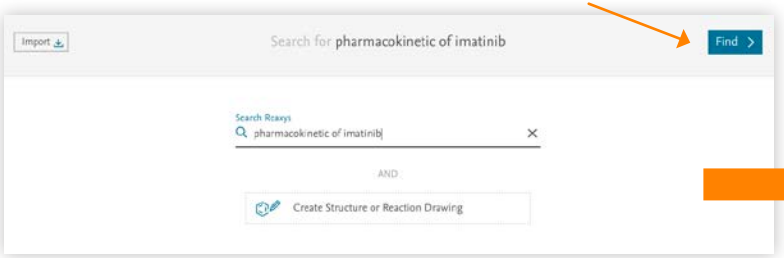
Structure Search enables the creation of structure and reaction drawings.

Use these as the main query or combine them with keywords for added search power.

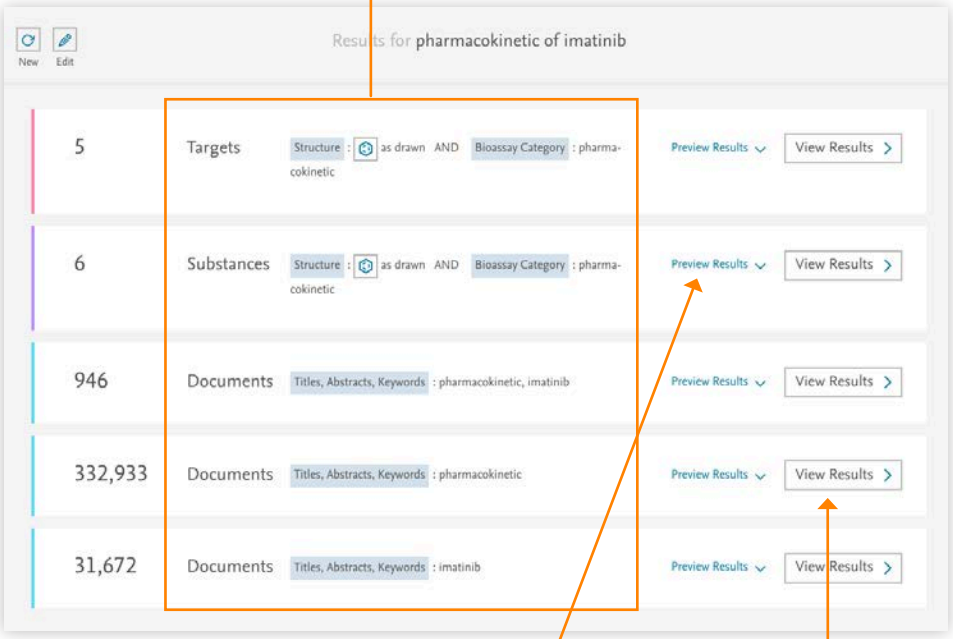
See the Reaxys Quick Start Guide for more information on using structure and reaction drawings.

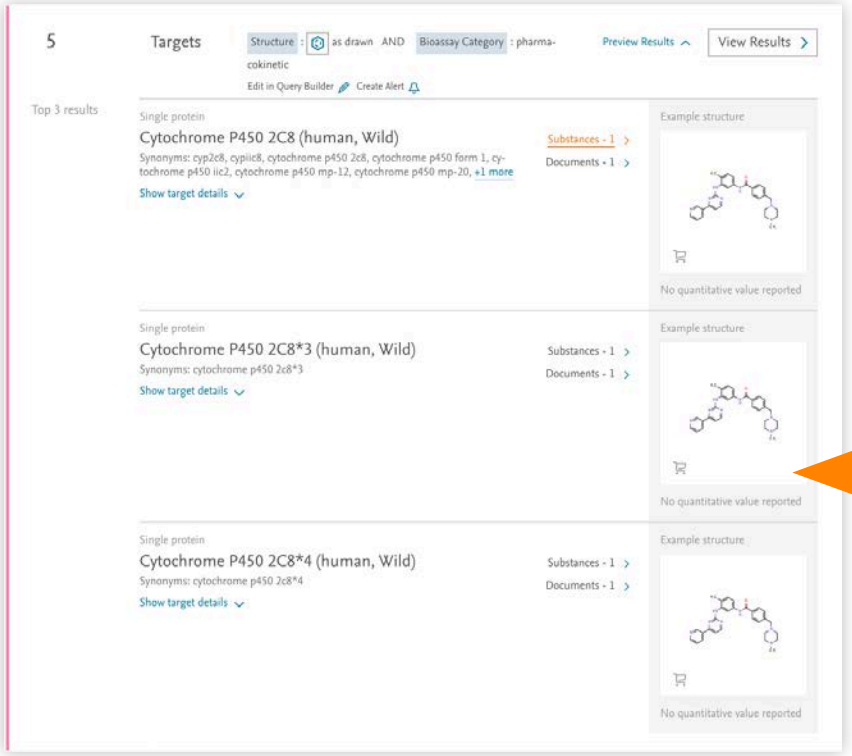
QUICK SEARCH RESULTS PREVIEW

When the query is ready, click Find.



Reaxys analyzes the Quick search query input and provides options based on query interpretation (Targets, Substances and/or Documents in this case; Reactions results are also returned with the appropriate search terms).





Click Preview Results to view the top three results for that result set.

Click View Results to view all results for that result set.

QUERY BUILDER FIELDS, FORMS AND HISTORY PANEL

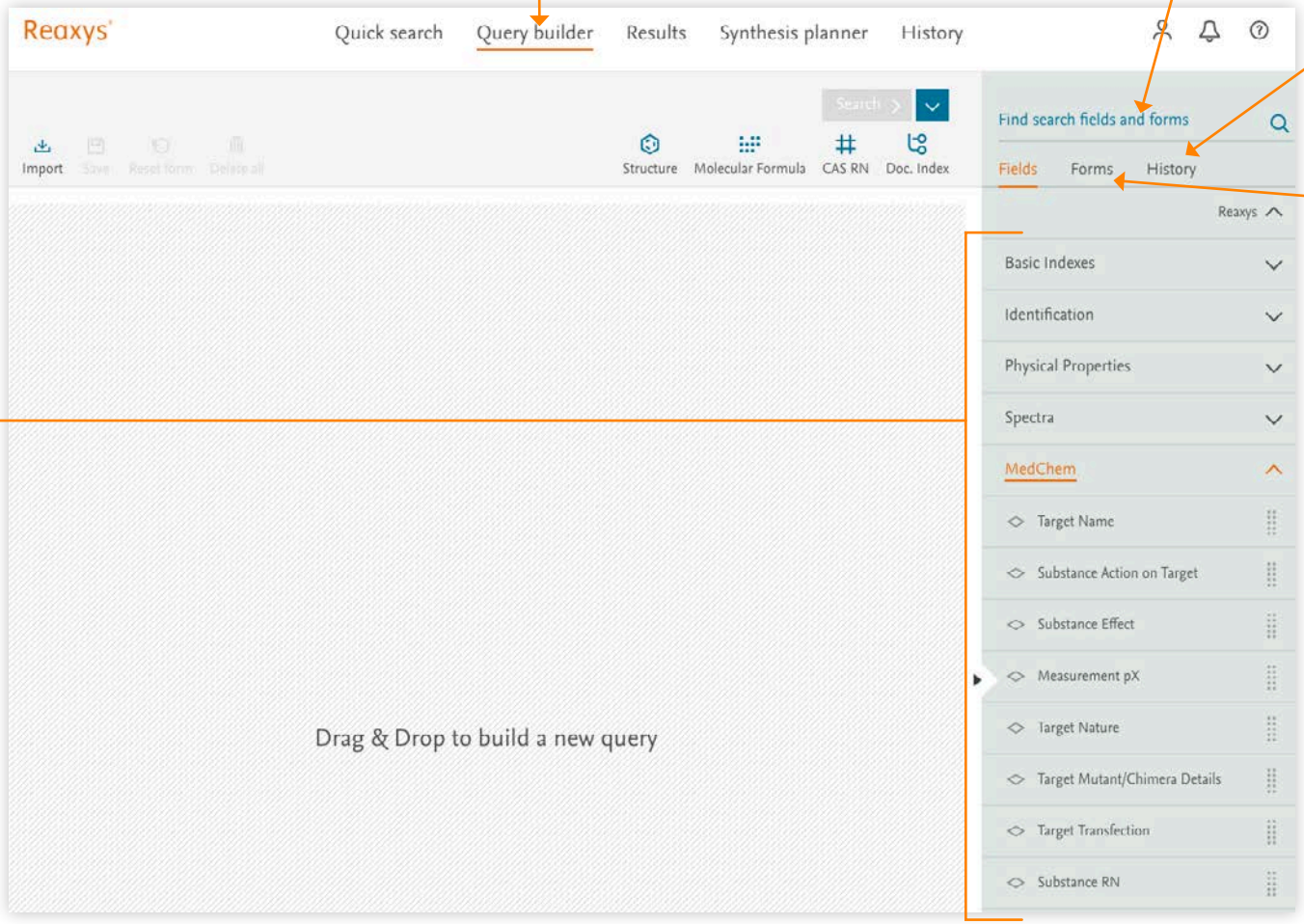
Click here to open Query builder.

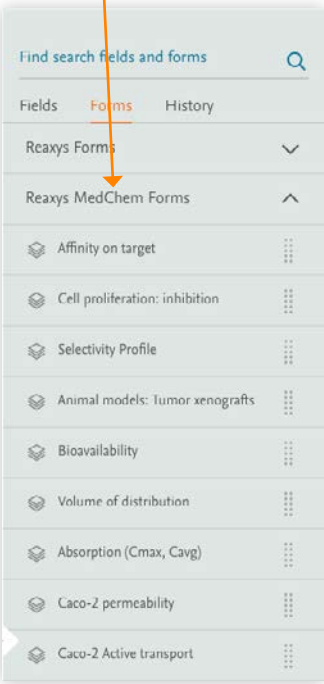
To find search Fields or Forms, enter keywords here. For example, "target" would help to find all fields related to targets.

Click History to display Recent and Saved searches that can be used in Query builder in combination with each other or with other search fields.

Click Forms to access predefined or customized search forms, including a number of forms focused on medicinal chemistry-relevant topics.

The initial view shows the search field categories. There is a wide range of medicinal chemistry search fields with paramaters designed to ensure accuracy of data retrieval.

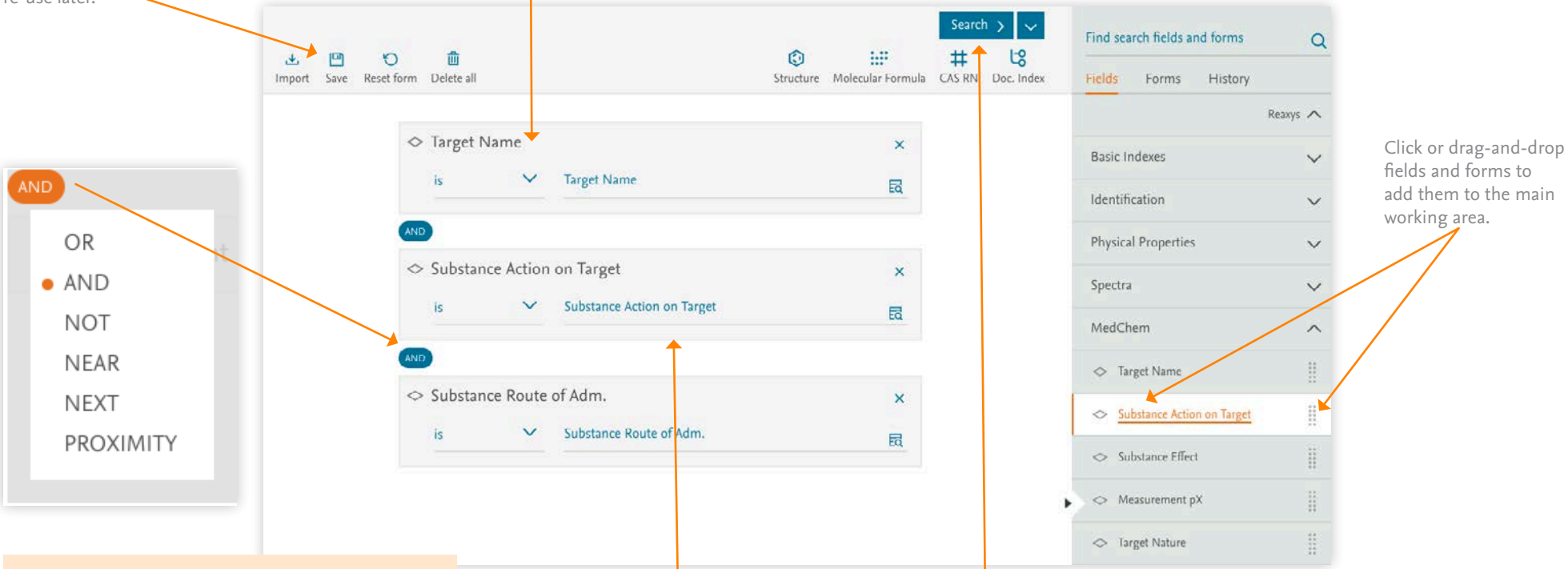




QUERY BUILDER

Save enables the user to save the query for re-use later.

Chosen fields and forms appear in the main working area for Query builder.



Click or drag-and-drop fields and forms to add them to the main working area.

Define the search criteria

Click Search when the query is ready.

CLICK TO ADD BOOLEAN OPERATORS:

- **OR**: contains data from at least one of the fields
- **AND**: contains data from both fields
- **NOT**: contains the first field's data and excludes the second's
- **PROXIMITY**: ensures the content of both fields relate to each other (typically used with parameter fields, e.g., melting point and solvent)

Note: If a field or form consists of multiple parameters, they are automatically combined using the PROXIMITY operator.

DOCUMENT RESULTS PAGE

Use Filters and Analysis options to narrow your results.

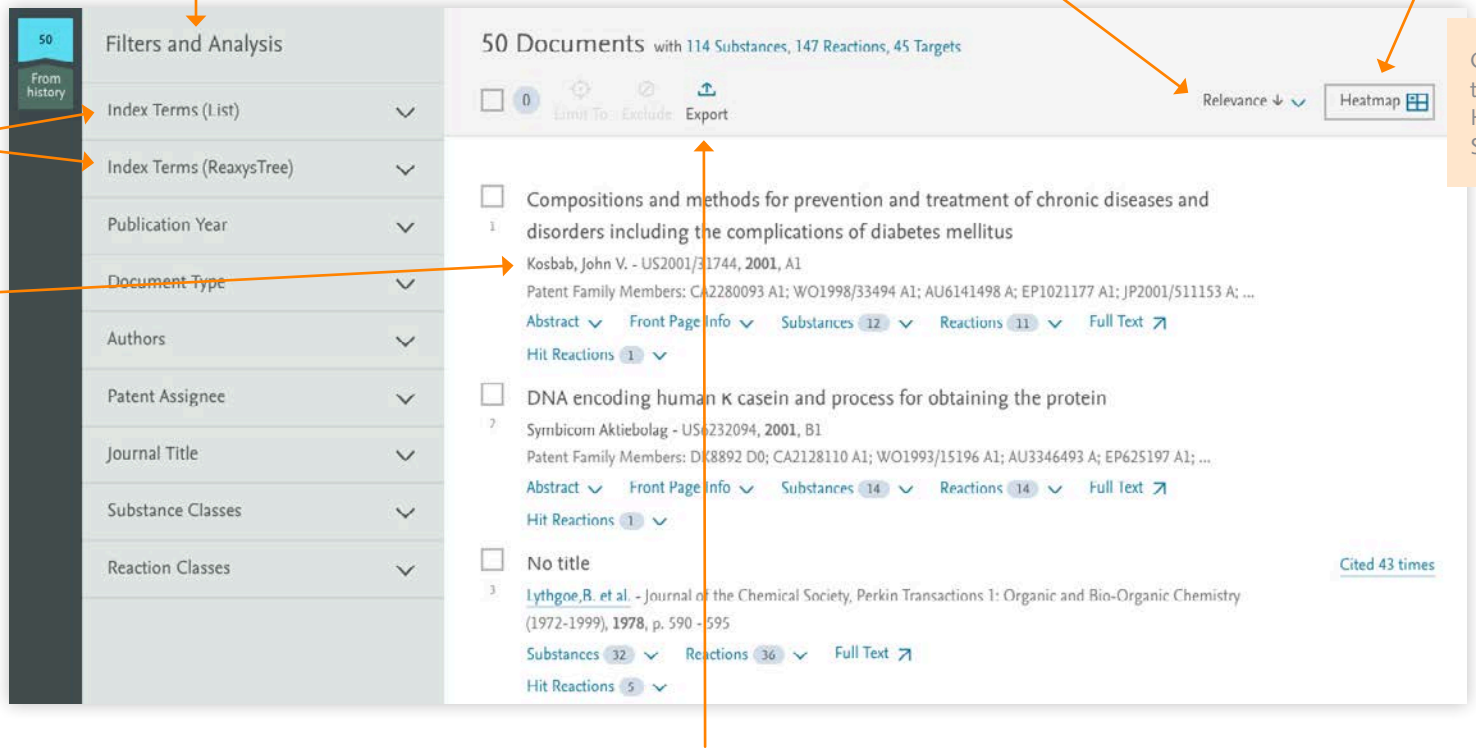
Default sorting is by descending relevance, but other options are available:

- Publication Year.
- Document Type.
- Cited By.

Click here to open the Heatmap for the target(s) and substance(s) in these documents

Use Index Terms (List) and/ or IndexTerms (ReaxysTree) to filter documents by topic.

Click an author's name to explore details about their publications and get additional analysis options in Scopus®.



Click **here** to download Heatmap Quick Start Guide.

To export results:

- Click Export in the toolbar (if the export button is not visible, click Options)
- Define Format, Range, Export data and Additional options
- Click Export – the progress will be displayed in the lower right of the screen
- When the export is complete, click Download

Note: Use the checkboxes beside the results to select individual results and only export those.

TARGETS RESULTS PAGE

Click here to open the Heatmap on the target(s) and substance(s).

Click **here** to download Heatmap Quick Start Guide.

Click text or ⌄ to expand a fliter.

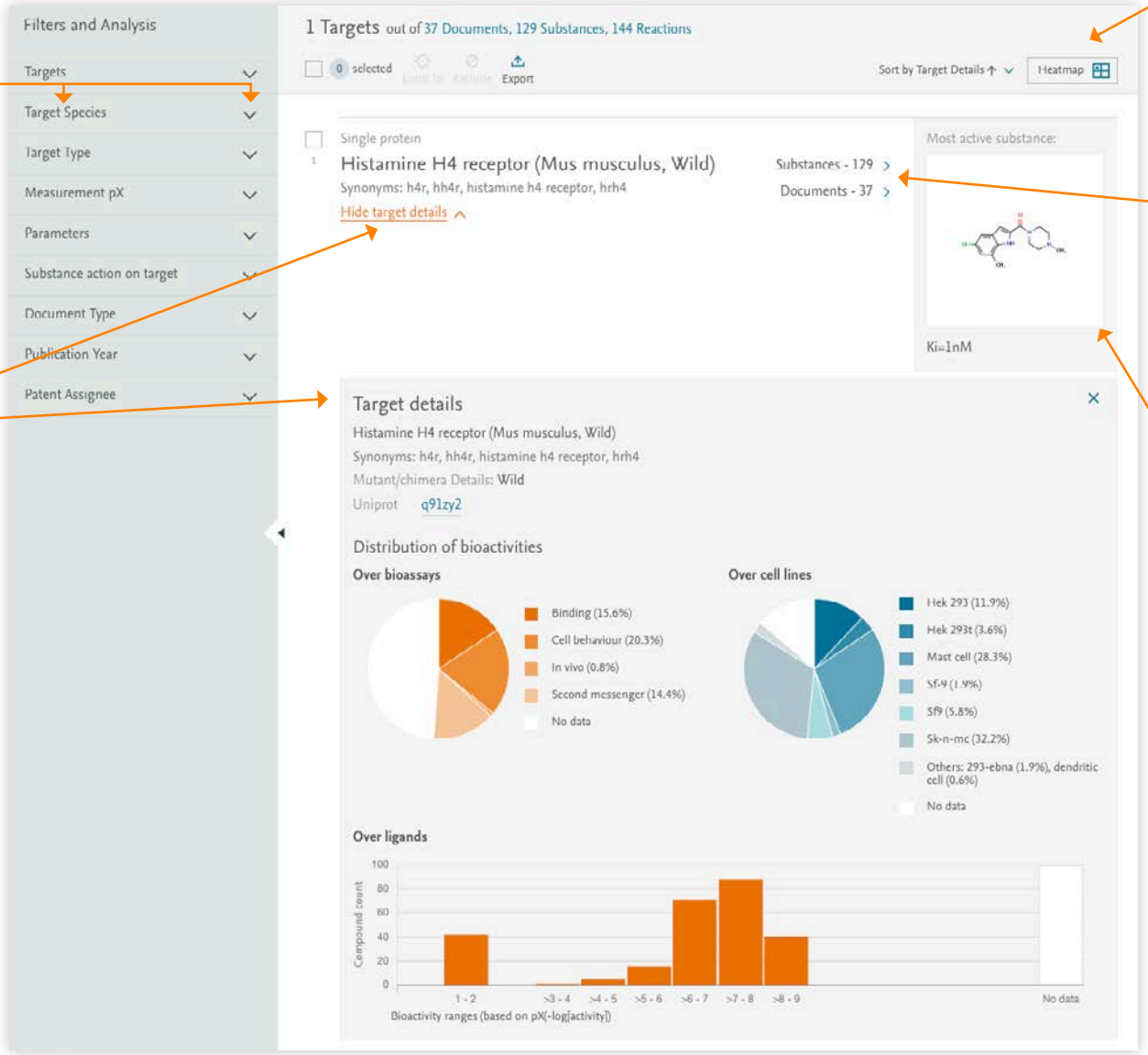
Use these links to go directly to the substance referred to in this record or the source documents for this information.

Click Show target details to see the distribution of bioactivities for a given compound.

Mouse over this structure to reveal the shopping cart, Synthesize link and other options.

Click the shopping cart to see availability information for this substance.

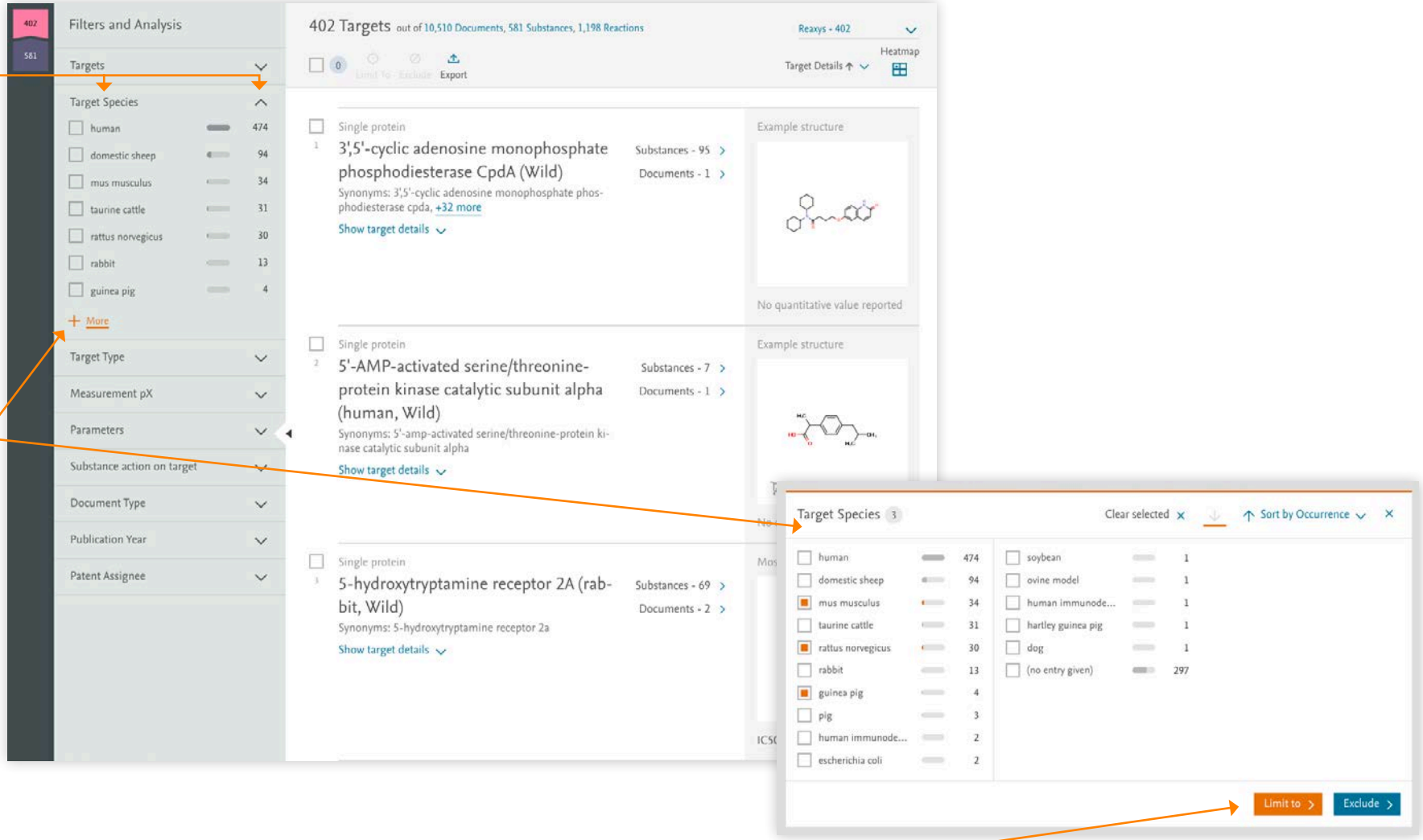
Click Synthesize to access manual or automated planning options for synthesis of this substance.



USING FILTERS

1. Click text or ⌄ to expand the filter.

2. Click More to display additional filter options.

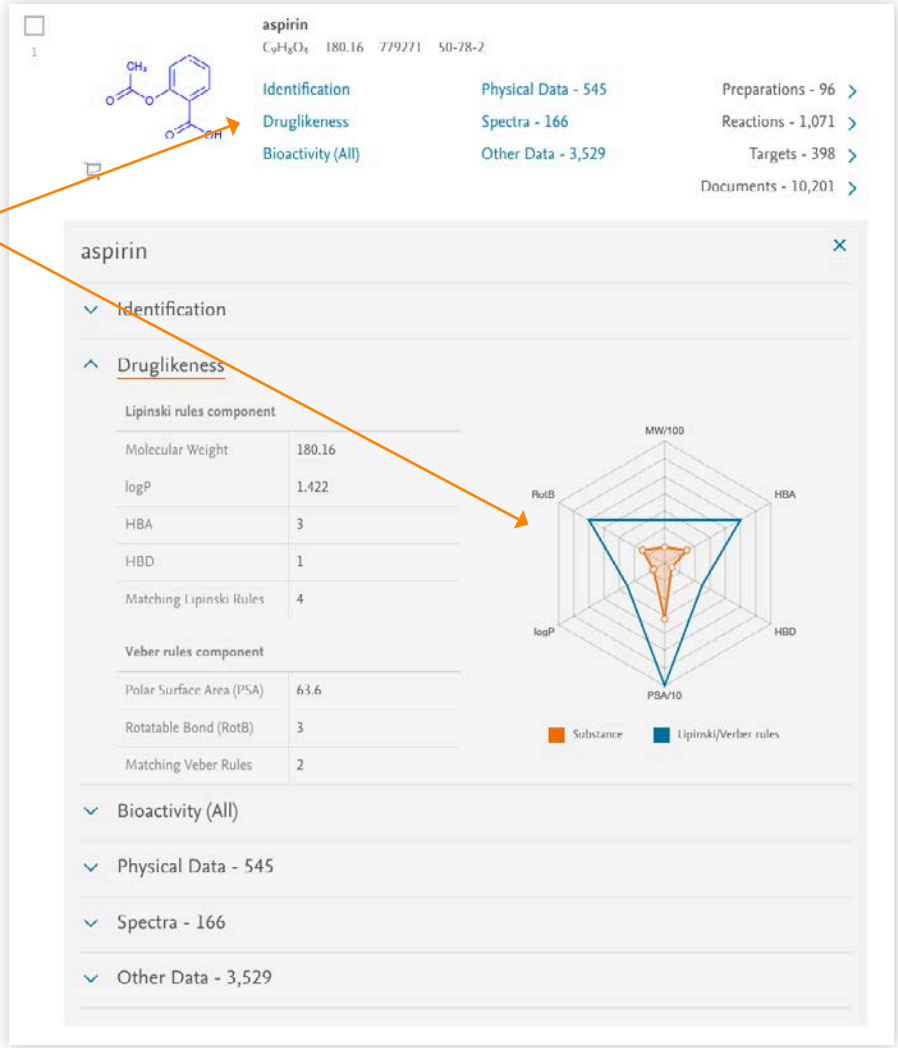


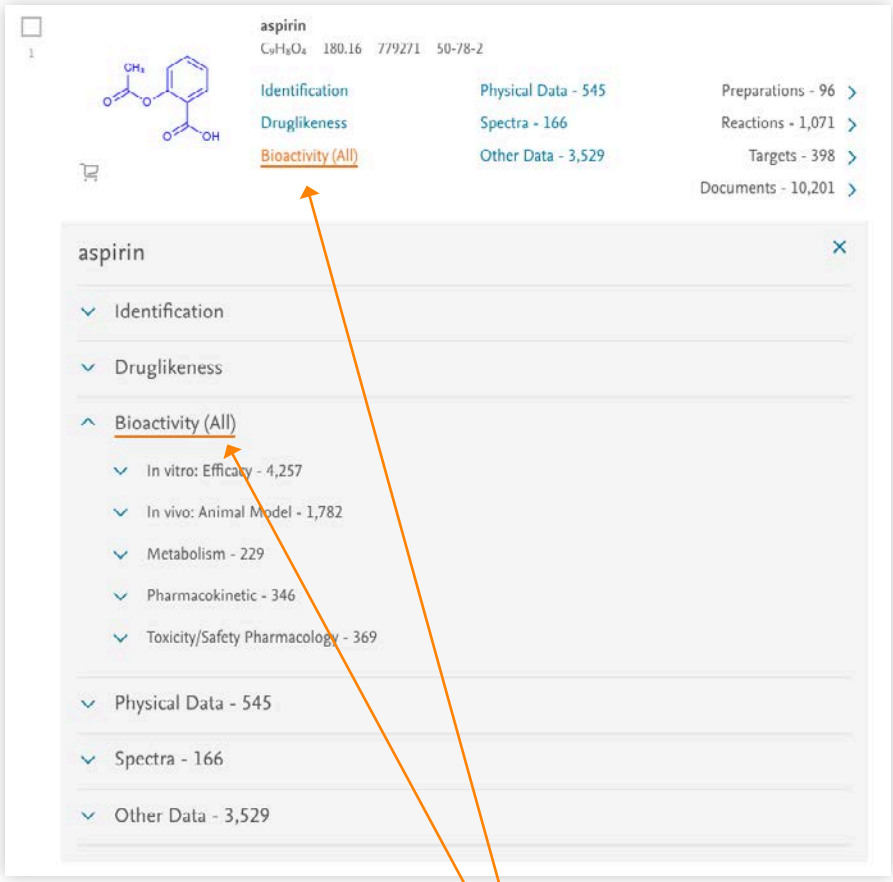
3. Click Limit To to see just the results for rodents or Exclude to see all results except for rodents.

Click **here** to learn more about Filters

SUBSTANCE BIOACTIVITY INFORMATION

In a substance record, click Druglikeness for data on drug-like properties, including a graphic representation of the Lipinski/Verber rules





Click Bioactivity to see the efficacy, toxicity, metabolic profile and pharmacokinetics of the substance.

HEATMAP

A number of options to work with the Heatmap are given, including limiting to and excluding selected columns, exporting the results, changing the displai settings, turning on or off the Navigator panel, and turning on or off the legend explaining the pX value colors.

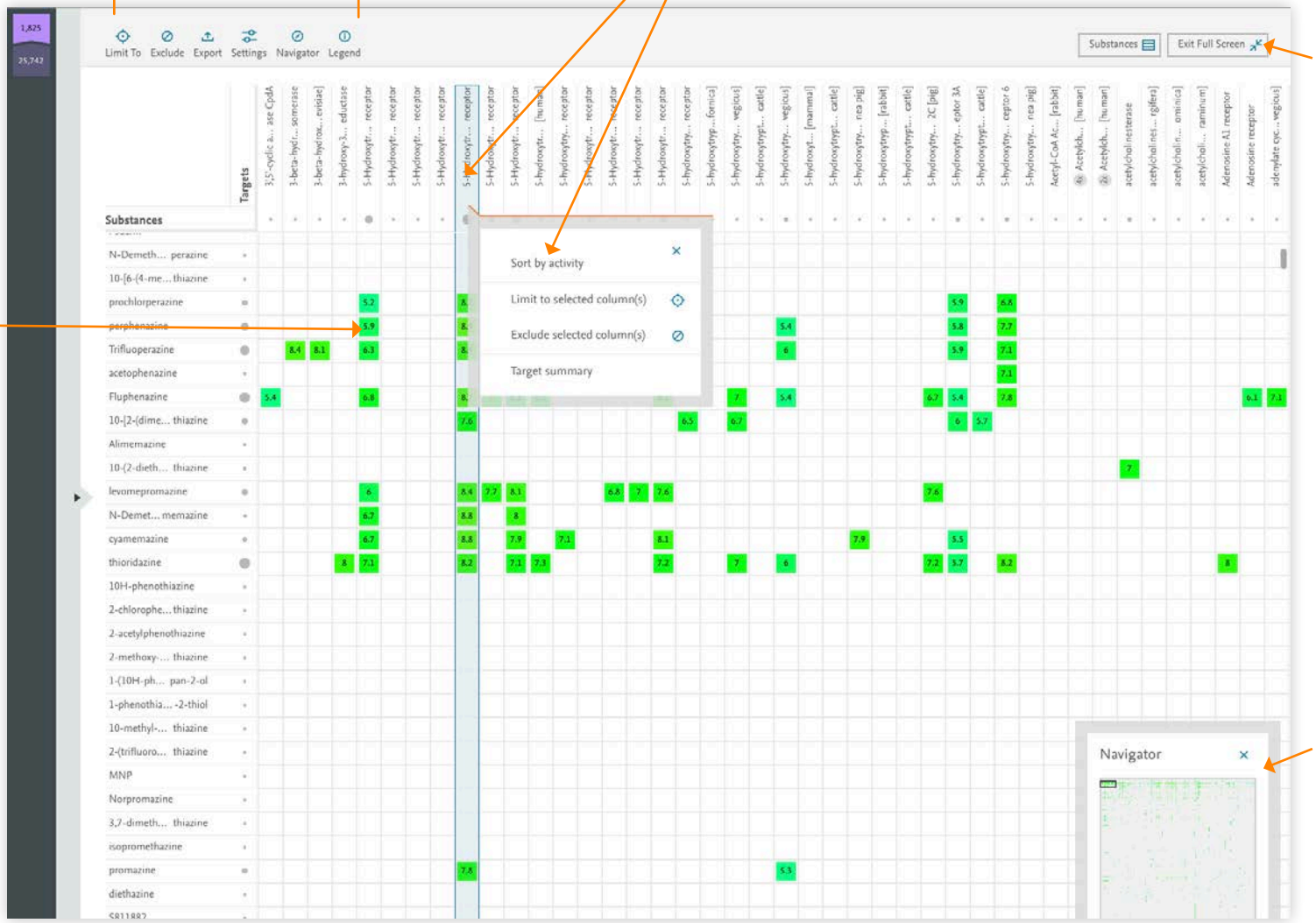
Select a target or substance to highlight its column or row. Clicking on the three dots beside the target or substance name exposes options to sort the Heatmap by activity, limit to the selected column(s), exclude the selected column(s), or call up a summary of the substance or target information.

Heatmap relates Substances (shown here on the Y-axis) to Targets (shown here on the X-axis) in terms of the strength of their interaction (relative affinity)

In the Heatmap, all substances are assigned standardized pX values that represent the relative of that substance for a given target.

If no published interactions between a substance and target are known, no value is given.

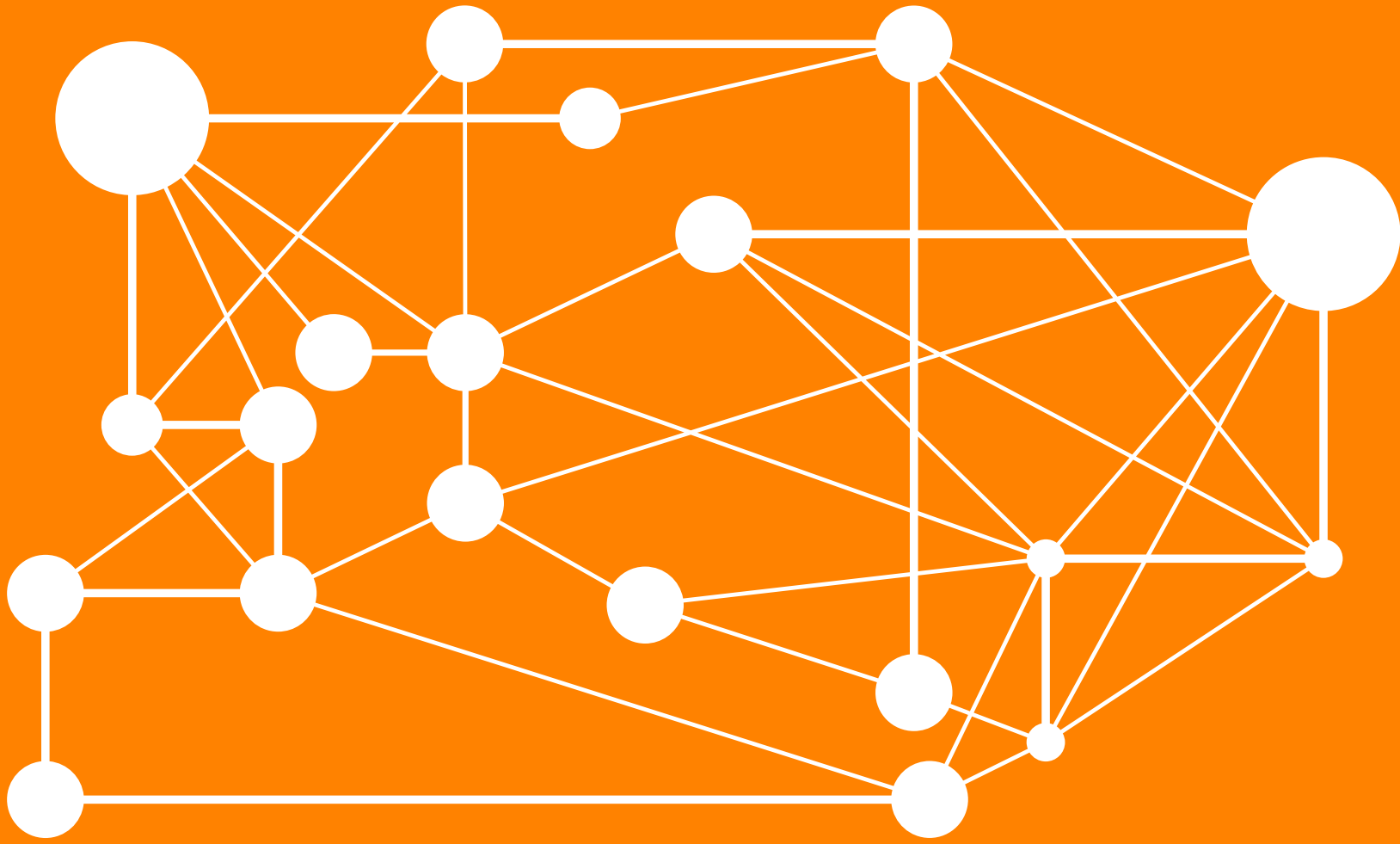
The color of the pX value visualizes the relative affinity, with “hotter” colors representing greater affinity.



Toggle in and out of full screen view or back to the Substances or Reactions results here.

Exiting full screen view will open the Filters panel at the left of the screen.

The Navigator panel shows the full Heatmap and allows users to navigate to areas with interesting clusters of results.



REAXYS MEDICINAL CHEMISTRY

Visit **https://www.reaxys.com** to log in.

Visit the **Reaxys Support Center** for more helpful information about using Reaxys

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