

The new release of Reaxys includes now Reaxys Medicinal Chemistry capabilities.

## Reaxys Medicinal Chemistry Release Notes

### Search

Searches in the new Reaxys Medicinal Chemistry (RMC) can be performed using:

- **Quick search**
  - This supports medicinal chemistry topics (e.g. target names, synonyms, gene name, UNIPROT ID, pdb ID etc.).
  - This also supports chemical structure searches (exact, sub-structure, family, similarity).
- **Query builder**
  - This incorporates new pre-defined RMC forms that support medicinal chemistry workflows (e.g. *Affinity on target*, *Selectivity Profile*, *Cell proliferation: inhibition*, *Animal models: Tumor xenografts*, *Cardiotoxicity* etc.). There are 19 pre-defined forms, with the required values and parameters pre-filled.
  - Taxonomy searches are also accessible through the query builder.

### Results display

- **Bioactivity table for substances**
  - Dynamic table display is now available.
  - Researchers can show/hide columns as desired.
  - Table settings apply to the whole session, so once selected; you don't have to re-work the tables to get the same results.
- **Heatmap**

This provides an overview of the structure activity relationship by displaying by default chemical substances (Y-axis) vs. biological targets (X-axis) and activity potency as pX (Cells).

  - Settings can be changed by accessing the heatmap settings button in the menu bar.
  - A Navigator view (*Navigator* button) provides an overview and a quick navigation method in the heatmap.
  - The colors in the heatmap (*Legend* Button) and in the navigator panel refer to the potency of a substance based on pX values.
  - Full screen display – Click “*Exit fullscreen*” to move to the normal display of the heatmap (filters and menu bar will be visible).
  - Data Density: the circle size relates to the amount of cells filled in the row or the column.
  - Filters are available in the Heatmap view.
  - Cell – Click to display Bioactivity details. Displayed numbers are pX, a value calculated from experimental data points. The pX value is hyperlinked to the real data. If multiple data points are available for an assay/target, select Max, Min, Median, or Average. Use the filters to limit results to a particular pX range.
- **Target display**

This provides an overview on targets that interact with substances and biological processes including:

  - Monomeric as well as Heteromeric targets that consists of multiple proteins (sub-units).
  - Target Names and synonyms including gene names and abbreviation based on Uniprot.
  - Most active substance on the target based on highest pX. When pX is not available for substances tested on the target, a substance is displayed randomly.
  - Link to Uniprot.
  - Link to PDB is provided when available.
    - Graphs displaying type of bioassays where the target was involved and Cell lines used for testing the target are provided.
    - Potency of substances tested on target.

## Export

- Export of medicinal chemistry data is available from the Substances, Targets, Documents and Heatmap pages.
- Three formats are supported for MedChem export Excel (Preferred), SD and XML.
- Whatever the pages where the export is performed the following MedChem data are exported:
  - Substances (Names, Smiles etc.)
  - Targets (Names, Species, mutations etc.)
  - Cell lines
  - Bioassays
  - Bioactivities (pX, IC50, Ki etc.)

### Remark on Heatmap export:

Only Raw data that are used to construct and display the heatmap can be exported, not the heatmap itself as a picture or directly into excel.

## Reaxys Release Notes

### Structure Queries

- The *"Create structure template from name"* feature can now add structures to already existing structures in the editor rather than replacing them. This enables users to create structure queries by merging multiple structures or reaction queries with reactants or reagent/catalysts

### Quick Search

- Graphical searches of Reagents/Catalysts are now supported: if a structure is positioned above a reaction arrow then it will be searched for as a reagent/catalyst.
- *"Edit Query"* has been renamed to *"Edit in Query Builder"* to avoid misunderstandings.

### Results Preview

The results preview layout and click path has been updated to provide a better navigation between quick search and result page:

- When users start typing any query term(s), the header is reflecting this input and remains available on the results preview.
- The search button has been moved into the header and has been renamed to *"Find"* so that it is better recognizable and accessible.
- The results preview is showing a *"New"* and an *"Edit"* button allowing users to return to the *Quick search* page from the results preview.
- If users click the *Quick search* menu link on the results page, then they will return to the *Quick search* page and not to the result preview anymore.

### Substance Results View

- The substance data table display has been improved:
  - It is possible to modify the layout for a given table within a session using the new feature *"Show/Hide columns"*.
  - The layout has been optimized to always show the reference column.
- Clicking *"Show All"* in data tables will now add all available rows if less than 100 rows are available. A *"Show Less"* button has been added at the bottom of the screen during navigation in order to reduce the list to the default as desired to facilitate faster scrolling.
- The Filter *"Availability in other databases"* has been added.

**Document Results Page**

- Some elements on the documents results page have been updated to provide a more condensed view and better data visibility, e.g. all authors are now displayed, if the number of authors does not exceed 10, cited by counts are separated from the text to become more visible and the header has been condensed to save space.

**General Known Limitations**

- **Performance in Target and Reaction results page display**
  - If you have changed the default setting of showing the number of hits per page and you encounter performance issues in displaying data on the result pages, then please revert back to the standard default setting of nine hits per page, max 30 hits per page.
- **Performance of searches in Taxonomy lookups**
  - Searching in taxonomies can take more than 20 seconds if the search retrieves many items.
- **Quick Search**
  - Reaction types/conditions are being search phrase-wise instead of word-wise, which may result in lesser number of result hits than in previous versions. This will be fixed in the next maintenance update.
- **Documents Results Page**
  - Author-link to Scopus does not work if the author name is highlighted/marked as hit.