Reaxys® release notes for July 28, 2017

New Features

3D Zooming

- Zoom for each structure now includes rotate, cleaning, 3D rotate and 3D zooming features.

Alerts

- New Reaxys now supports alert creation from search results or history items so that users can be kept informed on changes in the result of any given query.

Batch Searching

- New Reaxys now supports batch searching for molfiles, SMILES and any advanced query with up to 1,000 queries per batch (batch query files size limit is 50 Mb).

CAS Registry Numbers (CAS RNs)

- CAS RNs are now searchable across all the integrated databases with a single query.

Export: Documents

- Abstracts can be included in Excel exports using the “Include Abstracts” option.

Filters

- A new taxonomy tree view has been implemented for taxonomy-based filters, e.g. IndexTerms (ReaxysTree) in document results or Reaction Classes in reaction results or target names in target results for Reaxys Medicinal Chemistry. Click “IndexTerms (ReaxysTree)” in Document Results and the “More” button will provide a tree view of the matching terms from ReaxysTree, enabling more rapid navigation of large result sets.

- It is now possible to keep applied filters open. This helps to keep an overview of which filters have been used on the result set.

- The structure filter can now be applied to reactions, including the structures of reagents and catalysts. Draw the desired structure and place it above a reaction arrow and it will be treated as a reagent or catalyst

- The option “Copy structure from query” enables users to take the structure from the query as a template for structure filters on the Substance Results and Reactions Results pages.

History

- History items from the previous version of Reaxys are now visible in New Reaxys, facilitating the migration of users who stored large amounts of result sets through the previous interface.

Link-In

- New Reaxys can now also be accessed through a parametrized URL. This facilitates the integration of New Reaxys into in-house systems via implementation of a simple link.

Query Builder

- Querylets/Forms can now be added to Query Builder by simply clicking them rather than always needing to drag and drop them. This improves the speed of complex query creation.
- The search performance for taxonomy lookups has been improved, especially in **Reaxys Medicinal Chemistry** target name taxonomy.
- Query Builder now allows users to create and save their own forms, so they can build their own preferred query forms for quicker and easier searches.

Quick Search

- Name-to-structure translation for inorganic salts and stereochemistry has been improved.
- Searches in documents for substance names, CAS numbers, molecular formulas and INCHI-Keys are now enriched with substance synonyms, resulting in more documents for a given substance name search, if applicable.
- It is now possible to combine searches for drawn substances with text input for bioactivity query types, such as target names.
- It is now possible to combine drawn reagents and/or catalysts with text input in queries.

Results Page General

- Customized Availability Icons are now supported, allowing customers to link Reaxys with their in-house procurement system for commercially available compounds.
- Citations in reaction details and substance properties displays now also have a hyperlink to the titles and abstracts of the given reference. A click opens a moveable window displaying the title and abstract of the document allowing users to see the data in context.

Document Results

- Document results can be sorted using “Cited by” to more quickly show the most-cited references.

Reaction Results

- Reaction results now has a zoom feature. It is available through the Toolbar.
- Reaction IDs are displayed for each reaction.
- The reaction data display design has been updated and streamlined to facilitate navigation into the details.
- The structure filter can now be applied to reactions, including the structures of reagents and catalysts. Draw the desired structure and place it above a reaction arrow and it will be treated as a reagent or catalyst.

Substance Results

- Substance results can now be sorted by Reaxys Registry Number.
- The options menu for Markush structures has been extended to find all related compounds.
- Modification details are now also displayed to make it easier to distinguish compounds from each other while scrolling through a result set.
- Next to the table with Lipinsky and Veber rules, we also display the druglikeness spider graph, which shows how well a given substance fits into the druglikeness space defined by the given rules.

Fixed Previous Limitations

Heatmap

- In Internet Explorer 11, not all columns and rows were displayed in the Heatmap scroll. This has been fixed.
- In Firefox and Internet Explorer 11, structure drawings on the X-axis were displayed squeezed. They are now displayed normally.
- The Access Token was shown instead of the chemical name for specific substances without structures. Chemical names are now shown.
- The loading animation for columns headers was misplaced. This has been fixed.

Quick Search

- The issue with the capitalization of letters in words next to substance names causing incorrect annotations has been fixed.
- Citation Basic Index Searches were missing brackets around terms with overlaps. This issue has been fixed.

Document Results

- The link to Scopus from highlighted author names was not working. This has been fixed.

Target Results

- The most active substances did not have availability links. This has been fixed.
- On the Targets Results page, it was not possible to scroll up after clicking “Show Less” for results with large number of synonyms. This has been fixed.

Known Limitations

Heatmap

- Heatmap in normal mode is not displayed completely if the browser window width is less than 1024 pixels.

Results Page General

- The “Export” button turns orange.
- In Internet Explorer 11, the Substance Availability tooltip tail is misplaced for the most active substances in Target Results displays

Document Results

- Some nodes are incorrectly displayed as folders in the taxonomy view for Index Terms (ReaxysTree).

Reaction Results

- The word ‘steps’ is missing in multi-step reaction details.

Substance Results

- In Internet Explorer 11, the Druglikeness section cannot be opened for some substances.