

Reaxys release for April 2019

To ensure the best user experience for researchers, the Reaxys development team has implemented a range of new features that increase efficiency or improve usability.

A quicker way to find more relevant documents

Concept searching, also known as phrase searching, helps you retrieve more relevant documents more quickly. This has been implemented in **Quick Search** and in **Query Builder** with this release.

In the **Quick Search** query bar, put quotation marks around two or more words to create a search concept or phrase (A). Reaxys will combine the terms within the quotes using a NEXT{1} operator. This means that all the terms in the concept or phrase must be next to each other in the result set, thus increasing the precision of a search and resulting in more relevant hits.

In addition, we have changed the default setting for NEAR and NEXT operators in **Query Builder**. When used without curly bracket qualifiers, they are interpreted as NEAR{1} and NEXT{1}, respectively instead of NEAR{3} NEXT{3}, respectively. Please note that Reaxys supports a qualifier range of 1-10.

The top screenshot shows the Reaxys 'Quick search' interface. The search bar contains the text "heart attack" in quotes. Below the search bar, the results are displayed, showing 340,271 Documents. A 'New' button and an 'Edit' button are visible, labeled with an orange 'B'. The bottom screenshot shows the 'Results' page. On the left, there is a 'Filters' sidebar with a 'Preview' button labeled with an orange 'C'. The main results area shows a list of documents, with the first document titled 'Modern semi-automatic set-up for testing cell migration' and the abstract mentioning 'myocardial infarction'.

Easier navigation between query and results pages

The *New* and *Edit* buttons (B) in the **Results Preview** have been refined to improve the navigation from back to **Quick Search** to start a new query or edit the current one. A new *Preview* button (C) has been added to the **Results** pages to enable navigation from the **Results** page back to the **Results Preview**.

Improved pharmaceutical, bioactivity and disease query construction

Thanks to a newly added disease taxonomy and the **(Clinical) findings / disease** querylet, Reaxys Medicinal Chemistry users can now search for diseases and clinical findings.

The screenshot displays the Reaxys Query Builder interface. At the top, there are tabs for 'Quick search', 'Query builder' (selected), 'Results', 'Synthesis planner', and 'History'. Below these are buttons for 'Reactions', 'Targets', 'Substances', and 'Documents'. A search bar on the right contains the text 'disease'. The main query area shows a querylet '(Clinical) findings /...' with a dropdown menu set to '(Clinical) findings / disease'. Below this, a detailed view of the '(Clinical) findings / disease' querylet is shown, featuring a tree structure of categories and their corresponding counts.

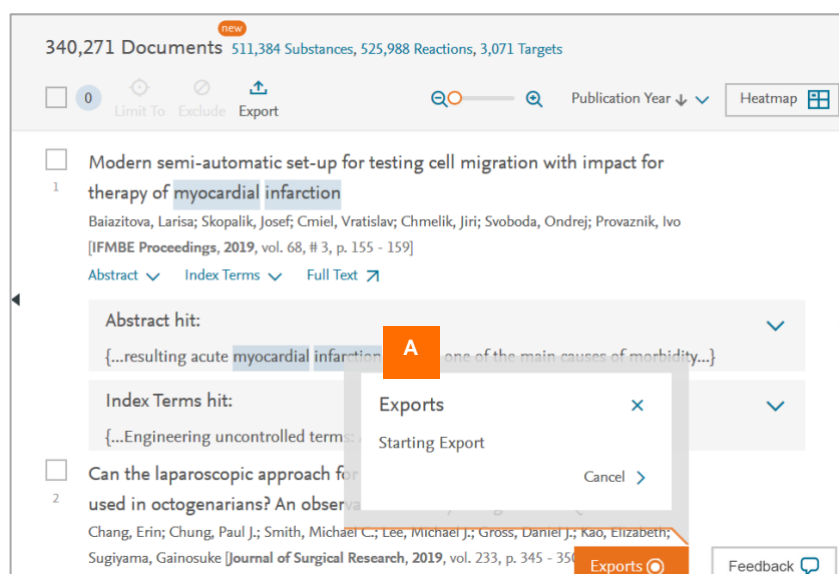
Category	Count
Experimental Disease	550,327
diseases	142,797
animal disease	186
general aspects of disease	13,206
mental disease	8,634
physical disease	126,450
plant disease	96
nonpathological finding	400,934
clinical finding	311
drinking history	504
fertility history	353
sexual desire history	643

In addition, for the following Reaxys Medicinal Chemistry querylets, we have changed the default operator so more terms can be found more quickly.

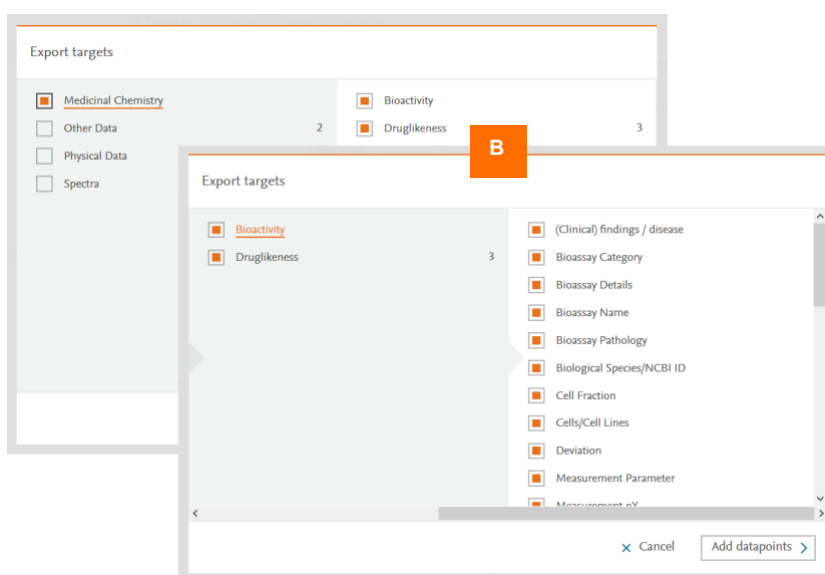
- **Cell / Cell line** — the new default operator is “starts with”
- **Substance route of Adm.** — the new default operator is “starts with”
- **Bioassay/Animal model** — the new default operator is “contains”
- **Measurement Parameter** — the new default operator is “contains”

Improved export options

The export dialog (A) shows immediately to ensure that the export status is clear.

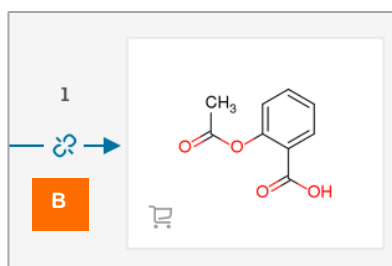
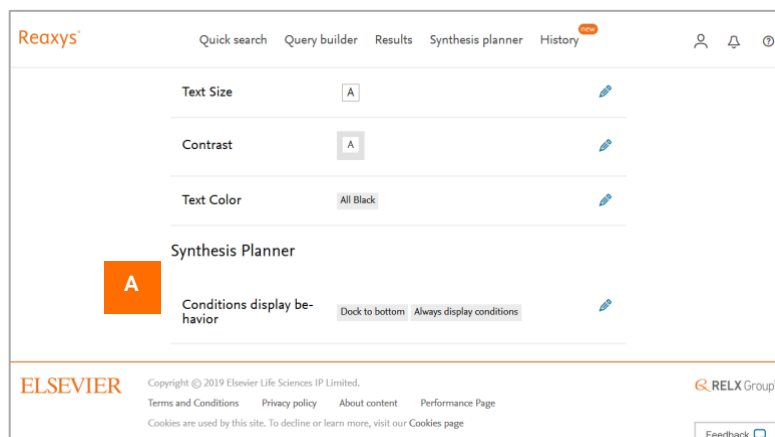


In addition, a new export option has been added to Reaxys Medicinal Chemistry. Users can select individual bioactivity data fields (B), meaning greater flexibility to export data that are relevant to medicinal chemistry workflows.



Improved Synthesis Planner options

In their user profile, registered and logged in users can choose their default for how and where reaction conditions are displayed in **Synthesis Planner** (A). Options include below or beside the synthesis plan; and always displayed or only displayed on request.



A tooltip has been added for the *broken link* icon (B) in **Synthesis Planner**. The icon is shown if the selected target substance does not have a preparation reaction in Reaxys and a similar molecule has been selected for propagating a synthesis path instead. It indicates that the synthesis plan shown will create a different substance to the desired one. The tooltip helps users to remember the meaning of the icon.

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