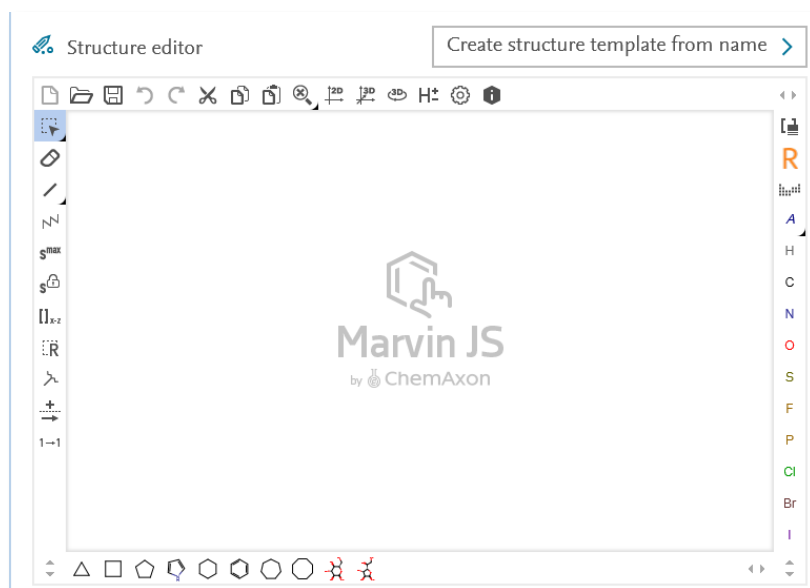


Reaxys release for March 2018

How has structure query generation improved?

The latest update to the Java-free structure editor MarvinJS enables easier and faster generation of structure queries. These changes align with user requests and are fully integrated in the structure editor. Improved functions include substitution count handling and atom editing. New functions include atom locking and manual mapping. Additional templates are also available.



How has manual synthesis planning improved?

Auto suggest, which is familiar to users of popular search engines is now available in Reaxys. Based on your text input, our auto suggest gives you suggestions for chemical names and for concepts in chemistry and biomedicine. It can make searching faster. It's designed to help you get a sense of what Reaxys can offer, possibly directing you to a search you might not have considered. If you pick a suggested term, Reaxys also searches all available synonyms for it. Any query can be viewed and edited in Query Builder as usual, so the search is still fully in your control.

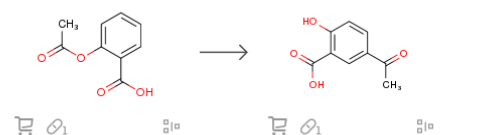
Can I start building a synthesis plan from a reaction?

Users can generate a synthesis plan from any substance visible in a Result View (Substances, Reactions, Citations) or from any reaction visible in a Reaction Result View. This option allows users to select a single reaction or multiple reactions and create synthesis plans based on the selection.

1,217 Reactions 12,000 Documents 631 Substances, 410 Targets Reaxys - 1,217

Limit To Exclude Export Syn-Plan

Reaction ID: 800599

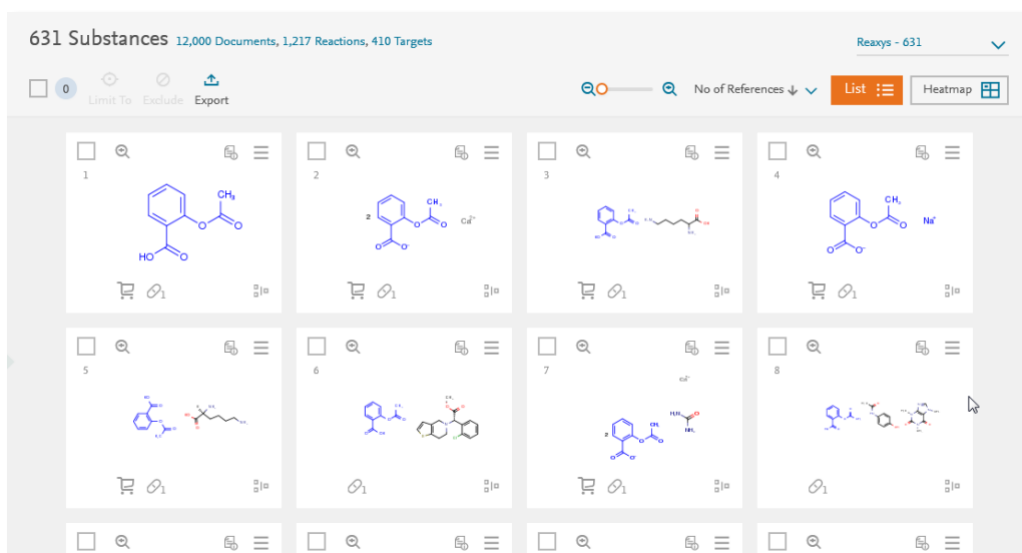


4 Conditions Find Similar

Yield	Conditions	References
82%	With aluminium trichloride In nitrobenzene for 1h;	Leclerc, Gerard; Bizet, Jean Claude; Bieth, Nicole; Schwartz, Jean - Journal of Medicinal Chemistry, 1980, vol. 23, # 7, p. 738 - 744 Full Text Details Abstract
78%	With aluminum (III) chloride In neat (no solvent) at	Puttaswamy, Naveen; Pavan Kumar; Al-Ghorbani, Mo-

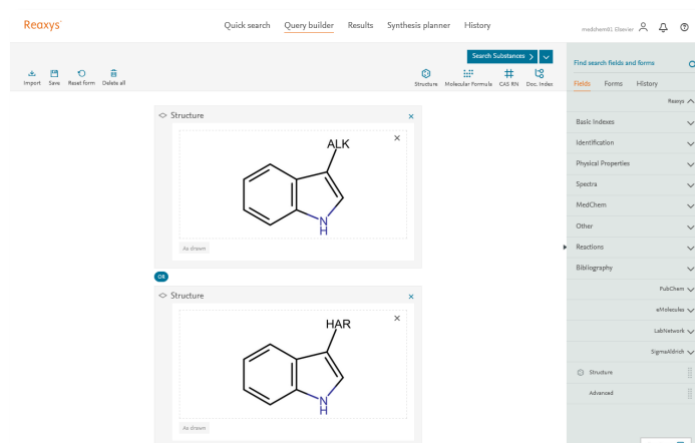
How can I quickly review a large set of substances?

The Substance Results View has a feature that enables users to toggle between the standard list view and a grid view. The grid view serves as a quick overview of large result sets, making it much easier to scroll through. This saves time in identifying the interesting substances. Access this feature by clicking on the Grid button and toggle back using the List button.



Are multi-structure querylets now supported in Query Builder?

Query Builder now supports the entry of multiple structure querylets in a single query. They can be combined using the Boolean operators AND, OR or NOT. This provides more flexibility for the creation of structure-related queries and reduces the need to create combined searches via the search history. To use this feature, simply create the structures one by one, each time selecting the Boolean operator that should link them by clicking on the default AND to display the options.



How have results displays been improved?

Substance options are always displayed

In all Results Views (Substances, Reactions, Citations), when a substance is shown, the icons for all related functions (expand, purchase options, synthesize, etc.) are always displayed. Previously, it was necessary to hover over the substance. This provides quicker access to the options.

Reaction ID: 1636875

Chemical reaction scheme showing the synthesis of a substituted indole derivative from 3-methylindole and an allyl bromide derivative.

Yield	Conditions	References
93%	With potassium carbonate in N,N-dimethyl-formamide at 20°C; for 10h; regioselective reaction; Experimental Procedure	Senthikumar, Kumaraja - Catalysis Communications, 2015, vol. 70, p. 86 - 89 Full Text Cited 1 times Details Abstract
64%	With sodium hydride in N,N-dimethyl-formamide at 0 - 20°C; for 0.5h; Inert atmosphere;	Smith, Andrew J.; Young, Allan; Rohrbach, Simon; O'Connor, Erin F.; Allison, Mark; Wang, Hong-Shuang; Poole, Darren L.; Tuttle, Tell; Murphy, John A. - Angewandte Chemie - International Edition, 2017, vol. 56, # 44, p. 13747 - 13751; Angew. Chem., 2017, vol. 129, p. 13935 - 13939,5 Full Text Details Abstract
	With lithium diisopropyl amide 1) THF / 0 deg C 2) r.t.; Yield given. Multistep reaction;	Odile, Roy; Blevins, Burke; Ratcliff, Matt; Hegedus, Louis S. - Journal of Organic Chemistry, 1980, vol. 45, # 13, p. 2709 - 2710 Full Text Details Abstract

+ Show all conditions 3 out of 7

Substance details preview available in Reactions and Citations View

Use the new **View details** icon above any substance to open the substance details preview, which shows its CAS number(s) and available data. This icon is shown above all substances in the Reactions and Citations Results Views, enabling quick access to the property information from those screens. It is not needed in the Substance Results View as this view already contains this information.

Reaction ID: 1636875

Chemical reaction scheme showing the synthesis of a substituted indole derivative from 3-methylindole and an allyl bromide derivative.

3-Methylindole
C₉H₈N 131-177 111296 83-34-1

Identification	Physical Data - 184	Preparations - 226
Druglikeness	Spectra - 275	Reactions - 1,128
Bioactivity (A6)	Other Data - 41	Targets - 30
		Documents - 1,938

View Details

Yield	Conditions	References
93%	With potassium carbonate in N,N-dimethyl-formamide at 20°C; for 10h; regioselective reaction; Experimental Procedure	Senthikumar, Kumaraja - Catalysis Communications, 2015, vol. 70, p. 86 - 89 Full Text Cited 1 times Details Abstract
64%	With sodium hydride in N,N-dimethyl-formamide at 0 - 20°C; for 0.5h; Inert atmosphere;	Smith, Andrew J.; Young, Allan; Rohrbach, Simon; O'Connor, Erin F.; Allison, Mark; Wang, Hong-Shuang; Poole, Darren L.; Tuttle, Tell; Murphy, John A. - Angewandte Chemie - International Edition, 2017, vol. 56, # 44, p. 13747 - 13751; Angew. Chem., 2017, vol. 129, p. 13935 - 13939,5 Full Text Details Abstract
	With lithium diisopropyl amide 1) THF / 0 deg C 2) r.t.; Yield given. Multistep reaction;	Odile, Roy; Blevins, Burke; Ratcliff, Matt; Hegedus, Louis S. - Journal of Organic Chemistry, 1980, vol. 45, # 13, p. 2709 - 2710 Full Text Details Abstract

+ Show all conditions 3 out of 7

Sticky header makes it easier to access important functions

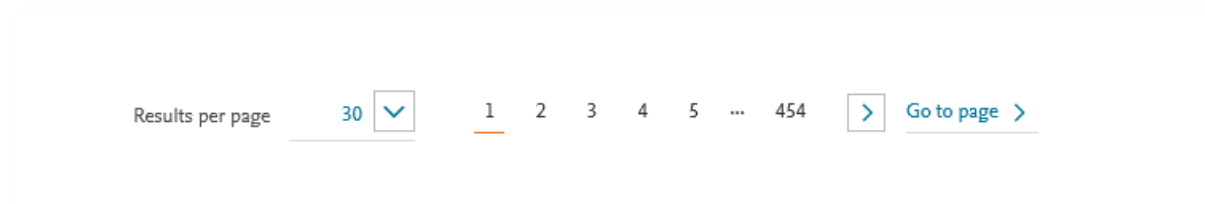
The header bar has been made sticky so that it is always visible to the user, no matter how far down the results set they scroll. This keeps important functions (e.g., limit setting, export, zoom, sorting) accessible.

How can I see CAS numbers and substance property data availability outside the Substances Results View?

Use the new **View details** icon above any substance to open the substance details preview, which shows its CAS number(s) and available data. This icon is shown above all substances in the Reactions and Citations Results Views, enabling quick access to the property information from those screens. It is not needed in the Substance Results View as this view already contains this information.

How do I change the results shown per page?

The default is to display 30 results per page of any given Results View. This can be changed with the dropdown option shown in the bar with the pages of results. Note that users who have registered accounts can save their new default in their preferences. You must be logged in to save the new preference.

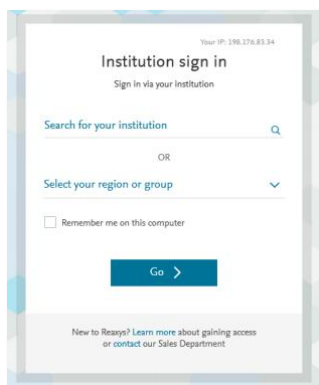


Are CAS registry number searches now performed across all integrated databases?

If a CAS registry number (RN) is entered in Quick Search, the search is now executed in all integrated databases that may contain CAS RNs. This increases the hit rate and saves users time, since only one search is needed.

Can I search for my institution when using institutional login?

Users can quickly search for their institution with a dedicated search function rather than using a long scroll-through list. In addition, Reaxys remembers the last selected institutes for a quick login.



For more information, please visit elsevier.com/reaxys.

Reaxys is a trademark of Elsevier Life Sciences IP Limited, used under license.
Copyright © 2018, Elsevier B.V.