

Reaxys release for November 2018

We have some great new developments in Reaxys this month. They're designed to make Reaxys simpler and more intuitive to use. This release includes some improvements requested by users because Reaxys is developed in an agile and customer-responsive manner.

The improvements include changes to Quick Search, Query Builder, our structure editor options and Synthesis Planner. See below for more details.

Check the latest database update from the Quick Search page

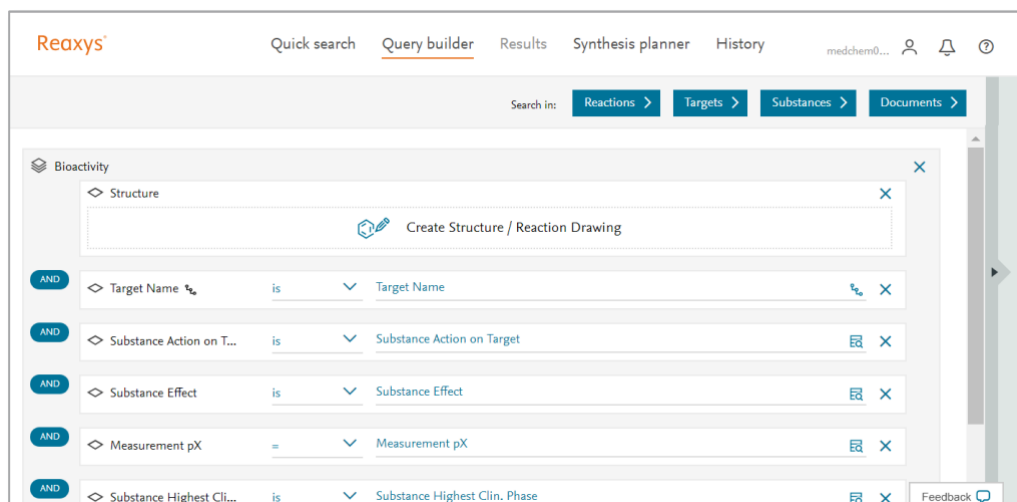
On the Quick Search page, you can now see information about the latest Reaxys database update. Click the hyperlink to find out more about updates to all the other integrated databases. This helps you check how current the content in Reaxys is, so you always know exactly what your search covers.

Get more term suggestions in Quick Search

We're pleased to announce that our auto suggest feature now includes millions of CAS numbers alongside the existing chemical concepts and names. These additional terms will help construct more precise Quick Search queries.

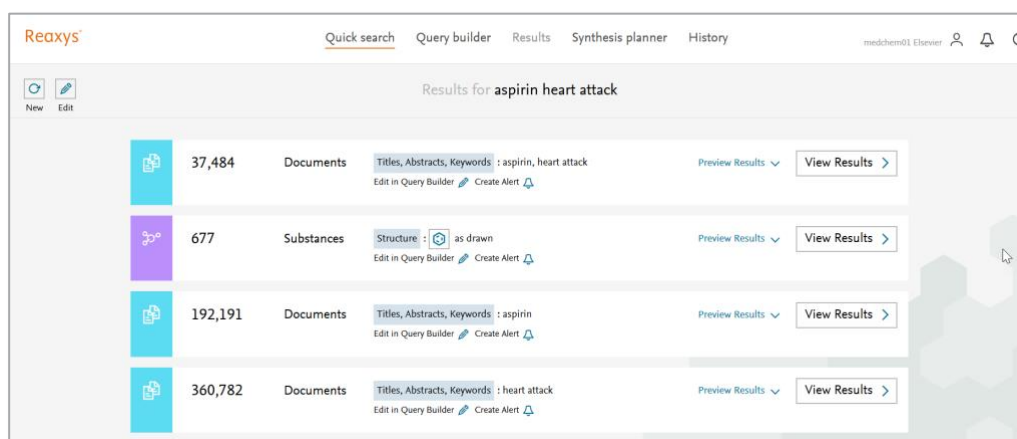
Build queries more efficiently with the new-look Query Builder

For an even better search experience, we've refined the look and feel of Query Builder. The resized querylets let you fit more search fields in the visible window. Collapsed querylets now display a summary of their fields. You can also edit the group name for combined querylets.



Make faster decisions on search options using the results preview

To enable the simultaneous quick review of more than one search query option, we've added a new feature. Search suggestions that include a structure or reaction query typically include a special icon. Click on it to show the enlarged query in a dialog box. You can move the dialog box so you can investigate other search suggestions without losing that suggestion. This adds to the flexibility of your search experience.



Note that we've also refined the relevance sorting for search options so that you'll always see the most relevant option at the top of the list. This helps with more efficient searching.

Choose your preferred structure editor: Marvin JS, ChemDraw JS or Chem Draw 18

Which structure editor do you prefer using within Reaxys: Marvin JS or ChemDraw JS? Now you can decide and even set your favorite as your default. Simply sign into your registered account to change the preference.

The availability of ChemDraw JS as an integrated feature in Reaxys is thanks to a close collaboration between Elsevier and PerkinElmer. In addition to the possibility to use ChemDraw JS in Reaxys, you can also access Reaxys via ChemDraw 18: the desktop version of the software now contains a search feature allowing you to run Reaxys searches on structures with a single click.

See why a document is relevant to your text-based query with Hit View

To give Reaxys users the best sense of why a document is relevant to a text-based query, we've implemented a Hit View feature in Reaxys. It shows the first abstract and index term item(s) that match your search term(s) and includes a few words before and after the term to give context. This hit information aids in assessing why the document was retrieved as a hit, helping you more efficiently select the right documents for your further research.

Navigate reaction information faster on the new Reactions page

Get an instant overview of result sets on the new Reactions page! The refined page groups structure icons below the substance, provides vertical separators within the condition table and puts the Reaction ID next to the 'Find Similar' option. This makes it easier to navigate the retrieved information.

The screenshot shows the Reaxys Reactions page. The top navigation bar includes 'Quick search', 'Query builder', 'Results' (selected), 'Synthesis planner', and 'History'. The user is 'Peter van Straat...'. The main header indicates '556,448 Reactions' out of 480,398 documents containing 309,320 substances and 2,112 targets. A sidebar on the left shows 'Filters and Analysis' with various filters like 'By Structure', 'Reagent/catalyst', 'Document type', 'Publication year', 'Reaction classes', and 'Solvent'. The main content area displays a chemical reaction scheme. Below the reaction, there are 'Hits in 6 Conditions' and a 'Find Similar' button. A table lists conditions and references for the reaction.

Conditions	Yield	References
Stage #1: iron(II) chloride tetrahydrate; iron(III) chloride hexahydrate With ammonium hydroxide In water at 20°C for 1h; Stage #2: In water at 99.84°C; for 4h; Experimental Procedure	100%	Shah, Arpan K.; Prathap, K. Jeya; Kumar, Manish; Kureshy, Rukhsana I.; Khan, Noor-ul H.; Bajaj, Hari C [Applied Catalysis A: General, 2014, vol. 469, p. 442 - 450] Details > Full Text > Abstract > Cited 11 times >
With ammonium hydroxide In water at 20°C Experimental Procedure		Kim, Sung-Eun; Lee, Sang-Wha Materials Research Bulletin, 2012, vol. 47, # 10, p. 269 - 273 Details > Full Text > Abstract > Cited 11 times >
Stage #1: iron(II) chloride tetrahydrate; iron(III) chloride hexahydrate With hydrogenchloride at 45°C; Inert atmosphere Stage #2: With sodium hydroxide at 45°C; for 0.5h; Inert atmosphere;		Mandal, Samir; Chatterjee, Nabanita; Das, Subhadip; Saha, Krishna Das; Chaudhuri, Keya RSC Advances, 2014, vol. 4, # 39, p. 20077 - 20085 Details > Full Text > Abstract > Cited 11 times >

More easily review conditions during synthesis planning

In Synthesis Planner, we've activated a more flexible display of the conditions of each synthesis step. The conditions can still be shown in a movable dialog box, but you can also choose to "dock" the conditions display at the bottom or right side of the screen. For users with large or multiple monitors, this makes it really easy to scroll through the conditions of the various steps of the plan.

The screenshot shows the Reaxys Synthesis planner page. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner' (selected), and 'History'. The user is 'medchem0...'. The main header indicates 'Synthesis plan 1'. Below the header, there are 'Import', 'Save', and 'Export' buttons. The main content area displays a chemical reaction scheme. Below the reaction, there is a 'Conditions' table with a docked view.

Yield	Conditions	Reference
90%	Fries method;	Hercouet; Le Corre - [Tetrahedron, 1981, vol. 37, # 16, p. 2867 - 2873] Full Text > Cited 55 times > Details > Abstract >
90%	With aluminium trichloride at 120 - 140°C; for 0.25h;	Sudha; Shashikanth; Khanum, Shaikh Ara - [Heterocyclic Communicat] 10, # 1, p. 85 - 88 Feedback >

Export structure images for substances

Thanks to the new Excel format for exports, you can download structure images for substance result sets. Note that the old Excel format is now named 'Tab-delimited text'. The default export limit is 1,000 for all file types. Remember to sign into your registered account to get a higher limit.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
	Structure: image	SMILES	Substance	Links to Re	Data Count	CAS Registr	Chemical N	Linear Strui	Molecular I	Molecular Y	Type of Sub	Type and N	InChI Key	Compositio	Compositio	Compositio	Field Availa	Number of	Number of	References
1		<chem>CC(=O)OC1=CC=CC=C1C(=O)O</chem>	779271	https://nev (1 of 680)	50-78-2	aspirin; ace	C6H4OCC	C9H8O4	180.16	isocyclic			BSYNRYMU				Identificati	1184	16028	
2		<chem>[Ca++].CC(=O)OC1=CC=CC=C1C(=O)[O-]</chem>	3755901	https://nev (2 of 680)	69-46-5	calcium O-	2C9H7O4[1	2C9H7O4*	398.382	isocyclic			BFFDNWBX				Identificati	8	90	
3		<chem>NCCCCC(N)C(=O)OCC1=CC=CC=C1C(=O)Cl</chem>	5690287	https://nev (3 of 680)	62952-06-1	lysine Acet	C9H8O4*Cl	C6H14N2O	326.349	isocyclic			JJBCTGUC				Identificati	1	81	
4		<chem>[Na+].CC(=O)OC1=CC=CC=C1C(=O)[O-]</chem>	3919633	https://nev (4 of 680)	493-53-8	sodium O-	Na(1+)*C6	C9H7O4*N	202.142	isocyclic			JZLOKWGV				Identificati	44	51	
5																				

Faster result page loading

Reaction and substance result pages now load more quickly thanks to the implementation of a faster structure rendering method.

New options for login

If users sign out, a logout page is now displayed to allow users to restart Reaxys with different credentials and options.

If desired, Reaxys can now also display some customer-specific text on the login page. This can be used to make users aware of available in-house support resources (customer-specific help pages or intranet support pages).

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

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