

Reaxys release for June 2020

To help users stay up-to-date on new information relevant to their searches, we've further enhanced the alert service for Reaxys users. The emails now contain more details about the results, making it easier to establish their relevance to your current work. In addition, you have much greater flexibility in the alert settings. Alongside this major enhancement, we've also made it easier to build queries, review structure results and more.

How enhanced Reaxys email alerts benefit you

1. A more streamlined workflow

Alert emails set up for the Reaxys database now include greater detail, including bibliographic details (A) and information related to your search, e.g., substances (B), making it easier to establish the relevance of the new information.

Each alert email will contain up to 99 results or 10 Mb of content. Note that for reactions, substances and targets, only up to 3 examples will be shown to keep the size of the emails manageable. As always, you can easily view all the hits by following the convenient link to Reaxys.

Reaxys

Dear Customer,
your alert gave new hits:

Alert name: "Cyclic peptides research project"
Last Run: 2019-May-15
Results: 9 new hits
Query: Quick search: "cyclic peptides"

[View all new documents in Reaxys](#) [Edit or see overview of all alerts in Reaxys](#)

Preview of new results:

1. Non-melanoma skin cancer as a possible adverse event due to anti-interleukin-6 treatment
Dierckx, Hoge, Pfeiffer-Jensen, Lorenzen [Scandinavian Journal of Rheumatology, 2019, vol. 48, p. 82 - 86]

Index Terms hit: [...] certolizumab pegol, cyclic citrullinated peptide antibody, folic acid...

Abstract
No Abstract available

[View document in Reaxys](#) [Full text](#)

2. Adrenomedullin: Continuing to explore cardioprotection
Tsuruda, Toshihiro; Kato, Juhji; Kuwatsuka, Kenji; Kitamura, Kazuo [Peptides, 2019, vol. 111, p. 47 - 54]

Abstract
Adrenomedullin (AM), a peptide isolated from an extract of human pheochromocytoma, comprises 52 amino acids with an intramolecular disulfide bond and amidation at the carboxy-terminus. AM is present in various tissues and organs in rodents and humans, including the heart. The peptide concentration increases with cardiac hypertrophy, acute myocardial infarction, and overt heart failure in the plasma and the myocardium. The principal function of AM in the cardiovascular system is the regulation of the vascular tone by vasodilation...

[View document in Reaxys](#) [Full text](#)

3. Clinical significance of serum B cell chemokine (CXCL13) in early rheumatoid arthritis patients
Allen, Shadia L.; Salem, Rehab A.; Elghamry, Dina M.; El-Ghazew, Aïf F. [Egyptian Rheumatologist, 2019, vol. 41, p. 13-14]

Abstract
Background: The diagnosis of early rheumatoid arthritis (RA) is challenging. B-cell chemokine (CXCL13) plays a critical role in the disease pathogenesis. Aim of the work: To assess the diagnostic value of serum CXCL13 in early RA and compare it with rheumatoid factor (RF) and anti-citrullinated peptide (anti-CCP) antibodies. Patients and methods: The study included 60 RA patients; 30 early, 20 established RA and 30 healthy controls.

Reaxys

Dear Customer,
your alert gave new hits:

Alert name: "Cyclic peptides research project"
Last Run: 2019-May-15
Results: 9 new hits
Query: Quick search: "cyclic peptides"

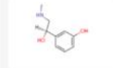
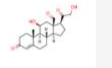
[View all new documents in Reaxys](#) [View all new substances in Reaxys](#)
[Edit or see overview of all alerts in Reaxys](#)

Preview of new results:

1. Non-melanoma skin cancer as a possible adverse event due to anti-interleukin-6 treatment
Dierckx, Hoge, Pfeiffer-Jensen, Lorenzen [Scandinavian Journal of Rheumatology, 2019, vol. 48, p. 82 - 86]

Abstract
No abstract available

Hit Substances

[View document in Reaxys](#) [View hit substances in Reaxys](#) [Full text](#)

2. Adrenomedullin: Continuing to explore cardioprotection
Tsuruda, Toshihiro; Kato, Juhji; Kuwatsuka, Kenji; Kitamura, Kazuo [Peptides, 2019, vol. 111, p. 47 - 54]

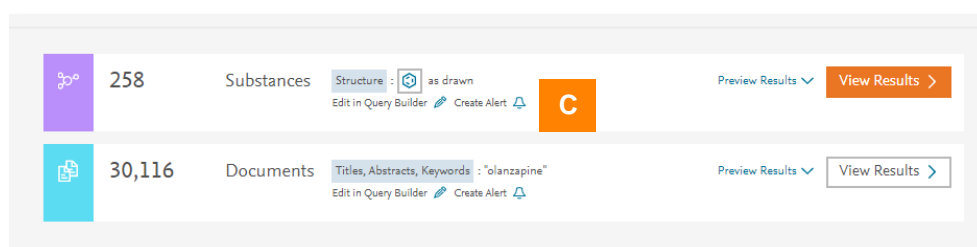
Abstract
Adrenomedullin (AM), a peptide isolated from an extract of human pheochromocytoma, comprises 52 amino acids with an intramolecular disulfide bond and amidation at the carboxy-terminus. AM is present in various tissues and organs in rodents and humans, including the heart. The peptide concentration increases with cardiac hypertrophy, acute myocardial infarction, and overt heart failure in the plasma and the myocardium. The principal function of AM in the cardiovascular system is the regulation of the...

Note also that you must be logged into your Reaxys account to set up email alerts.

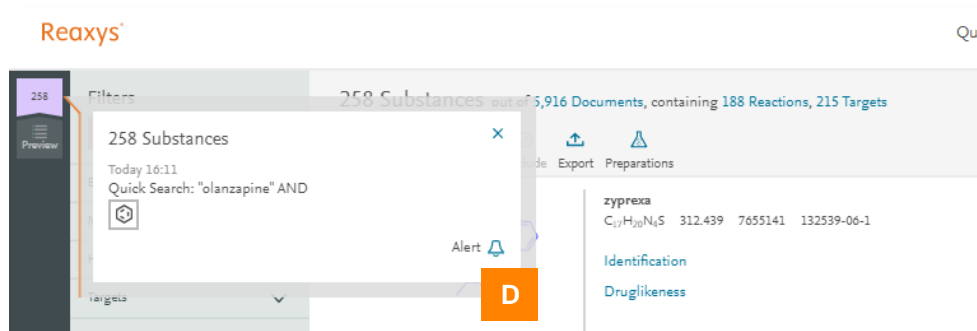
2. A more personalized experience

You now have broad customization options for your alert. This includes full flexibility in naming the alert, setting the frequency, determining the information included in the email, and defining the regularity of alerts about a single document. The details of these options are given below.

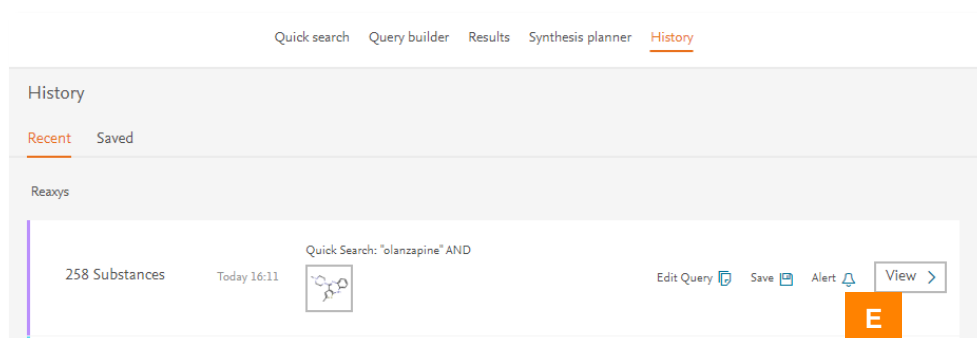
You can create alerts from the **Quick search results preview** (C), the **Results** page left bar (D) or your search history (E).



This screenshot shows the top section of the Reaxys interface. It displays two search results: '258 Substances' and '30,116 Documents'. The 'Substances' result is highlighted with a purple icon and includes a 'Create Alert' button. The 'Documents' result is highlighted with a blue icon. Both results have 'Preview Results' and 'View Results' links. A red letter 'C' is placed over the 'Create Alert' button for the substances result.



This screenshot shows the detailed view of the '258 Substances' result. The left sidebar contains a 'Filters' section with a 'Quick Search: "olanzapine" AND' query. The main area displays the chemical structure of zyprexa (C₁₇H₁₉N₄S) and its identification details. A red letter 'D' is placed over the 'Alert' button in the sidebar.



This screenshot shows the 'History' page in the Reaxys interface. It displays a list of recent searches, including the 'Quick Search: "olanzapine" AND' query. The 'Alert' button is visible next to the search entry. A red letter 'E' is placed over the 'Alert' button.

In the alerts pop-up, you can set the following preferences: the alert name (F); the email address(es) of the recipient(s) (G); the frequency, with options including every week, every two weeks, every month and after each update as well as the weekday (H); and the regularity of the alert for each document (on its first appearance only or after every update) (I). You can also choose whether you receive email alerts even if there are no new results matching your query (J) and what to include in the email, such as the title, bibliographic information and hit details (K).

Create Alert

Query:

Quick Search:

Alert name:

Name

Coupling reaction

F

Send alerts to:

user@company.com

X

G

Frequency:

Every week

▼

on: Monday

H

Send alert:

Upon first appearance in the database

I

i

☐ Do not send alerts with zero results

J

ADVANCED ALERT CONTENT: i

From databases:

☒ Reaxys

K

Include in email:

☐ Title and bibliographic information

☒ Abstract

☐ Full abstract

☒ Partial abstract

☒ Hit details (keywords, substances, reactions or targets)

Email alerts will produce an email with a maximum of 99 records. i

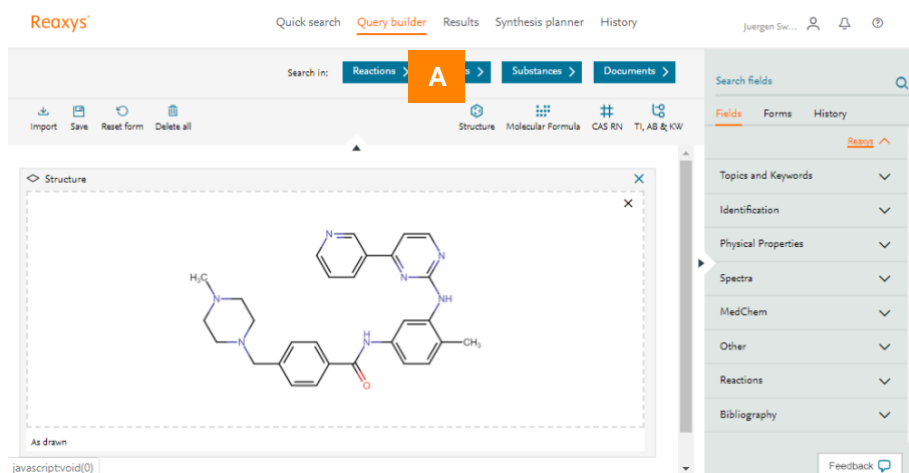
Cancel >

Create >

Improving your user experience

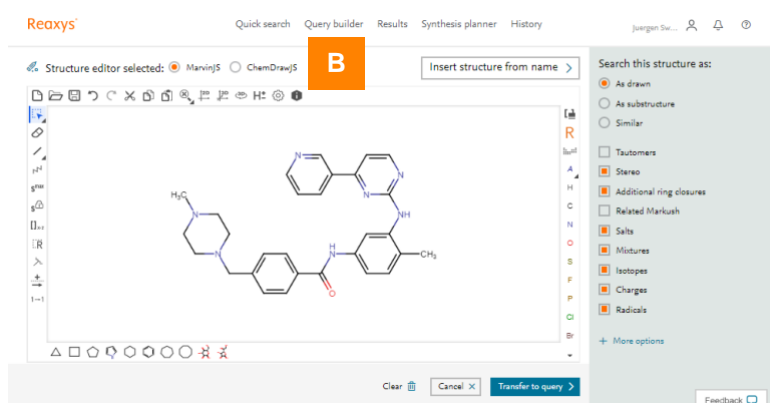
Retrieve all reactions for a structure with one query

Use this new reaction search option when you need to assess all the options for making or modifying a substance of interest. Open the *Structure* querylet, draw your structure and click to search in *Reactions* (A). Reaxys will retrieve all reactions with that structure as starting material, reagent or product. To search for the structure in a specific role, simply add a reaction arrow (before the structure for a product search; after the structure for a starting material search; and below the structure for a reagent search). This improvement greatly increases the flexibility of reaction searches.



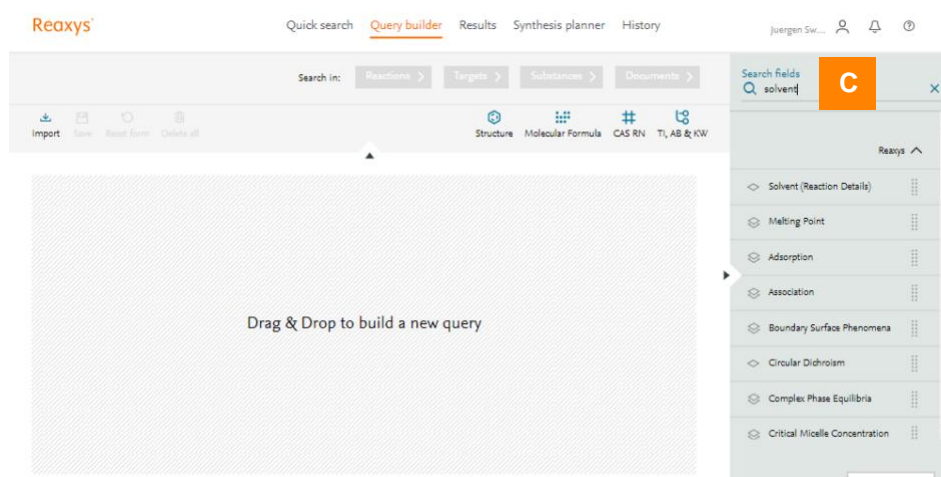
Easily select your preferred structure editor

It's now much easier to choose your preferred structure editor for a given query. Radio button selection for MarvinJS and ChemDrawJS is now enabled (B), replacing the previous dropdown menu. You can still save your preferred editor in your profile. This interface refinement simply makes it easier to see the options.



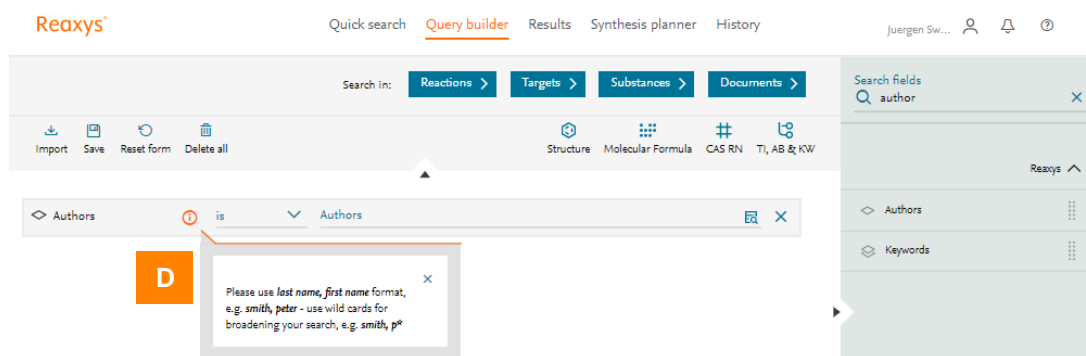
Find the querylet you want more easily

Query Builder contains hundreds of search fields. Some parameter search fields (e.g., solvent) have similar names in relation to various facts (e.g., reaction details, melting point(s), adsorption, association). To make it easy to find the querylet with the right attributes for your search, we've refined the list of querylets that appears when you use the search field (C). This improves the efficiency of search construction and the accuracy of search results.



Gain additional insights for successful author searching

Query Builder supports searches for detailed bibliographic information. Query formulation for journal titles and other bibliographic information is straightforward, but searching for authors can require some additional insights. The new help feature (D) in the *Authors* querylet supports the creation of successful searches with explanations of how best to build your search.



See the best structural representation of substances of interest

Accurate 3D structural representation of substances can be important for your investigations. To support this need, we've added a *View in 3D* option (E) to the *Zoom* feature for structure results. The zoom is typically sufficient for 2D structures, but this new 3D option is ideal for cleaning of 3D coordinates and rotating the structure to view it from different angles.

The screenshot displays the Reaxys web interface. On the left is a 'Filters' sidebar with various search criteria like 'By Structure', 'Measurement pX', and 'Molecular Weight'. The main area shows search results for '1 Substances'. A chemical structure of a tungsten complex is highlighted. An orange box with the letter 'E' is overlaid on the 'Structure' tab, indicating the 'View in 3D' function. The structure itself is a tungsten atom coordinated by two 2,6-dichlorophenoxide ligands and two chlorine atoms. The interface also includes a top navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. A right sidebar lists related data like 'Spectra - 2', 'Other Data - 3', 'Preparations - 1', 'Reactions - 5', and 'Documents - 6'. The RELX Group logo is visible in the bottom right corner.

Understand the impact of the latest update from the homepage

Reaxys content updates occur twice a week. To quickly review the most recent update and understand its impact on your searches, simply click on the *Latest update* link (F) on the Reaxys homepage.

The screenshot shows the Reaxys homepage. At the top, there's a navigation bar with 'Reaxys' logo, 'Quick search' (highlighted), 'Query builder', 'Results', 'Synthesis planner', and 'History'. On the right, there's a user profile 'Juergen Sw...', a bell icon for notifications, and a circular icon. Below this is a search bar with the placeholder 'Search substances, reactions, documents and bioactivity data' and a link to 'Import'. A secondary search bar below it has the placeholder 'Search Reaxys' and a 'Find' button. Below the search bar, there's a section for 'Substance Properties, e.g. solubility of vitamin D3' with an 'AND' operator and a 'Draw' button. The main content area features a 'Content Overview' section with a 'Latest update: 11. February 2020' and a button labeled 'F'. Below this, there are four statistics: '118M Substances', '49M Reactions', '59M Documents', and '37M Bioactivities'. The footer includes the 'ELSEVIER' logo, copyright information 'Copyright © 2020 Elsevier Life Sciences IP Limited.', links for 'Terms and Conditions', 'Privacy policy', 'About content', and 'Performance Page', and a note about cookies. The 'RELX Group' logo is also present.

Enjoy other improvements to your user experience

Also in this release:

- We've refined the way long field names are displayed in Query Builder to ensure they do not obscure other fields or information. The name is displayed with a truncation. Simply mouse over it to see the full name.
- The *Feedback* button is important, because it allows you to contact the Reaxys team easily. However, on smaller screens and in some browsers, it sometimes obscured other features. We've adjusted this in the current release.
- The *Preferences* tab of your Profile displays your user preferences (e.g., preferred search type, preferred structure editor and AutoPlan settings). Its layout has been refined to make it easier to see what you've saved as your settings.

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