

YOUR GUIDE
TO WHAT'S NEW
IN REAXYS

new

 **REAXYS**[®]

HOW YOU THINK HOW YOU WORK



In consultation with expert chemists, we have redesigned the Reaxys user interface and expanded its content to make it better than ever.

Reaxys is the chemistry workflow solution that chemists prefer to use, and now supports your complete information workflow.

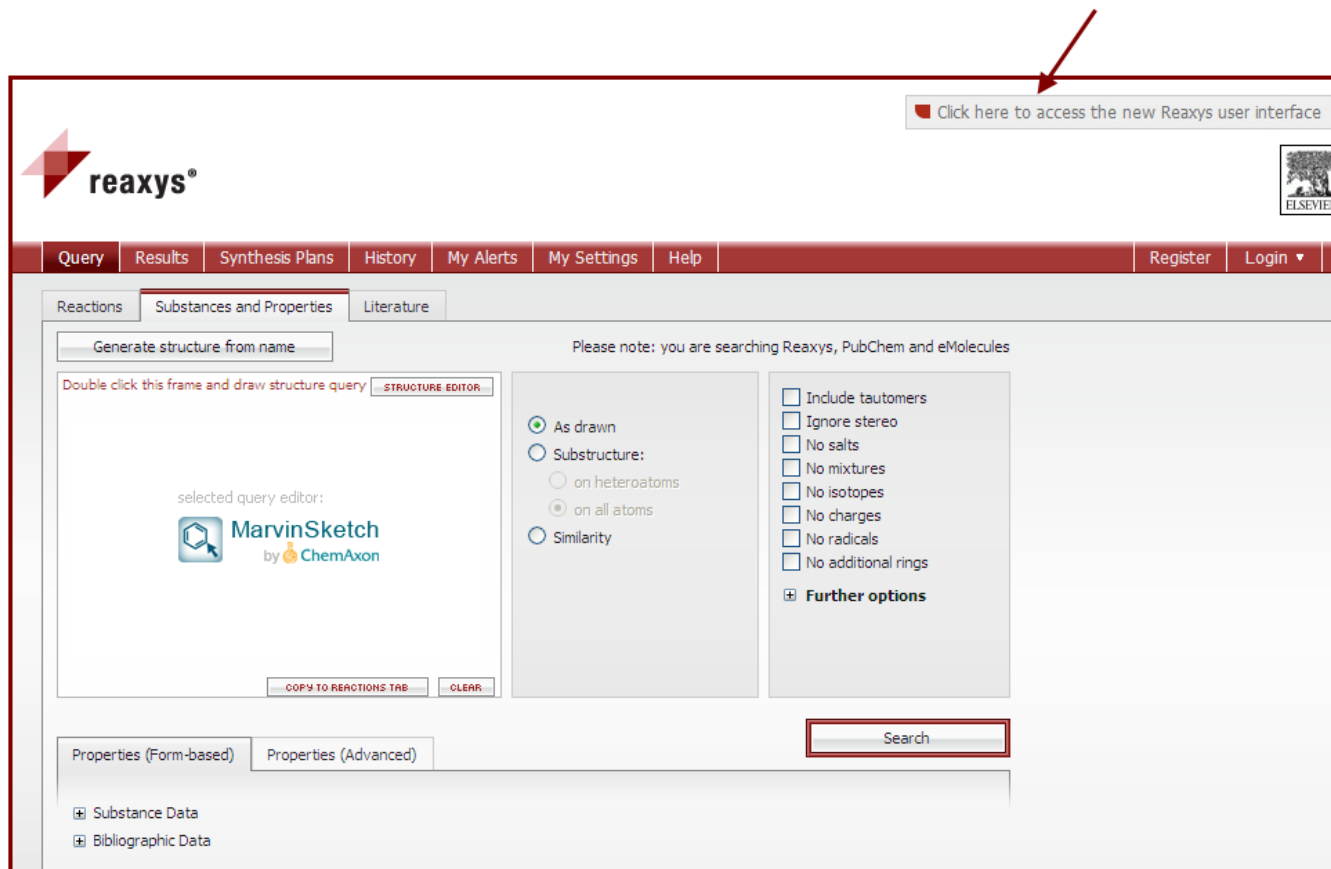
This quick guide to what's new in Reaxys covers some of the main changes to the user interface and content.

1. ACCESSING THE NEW REAXYS

We're making the new Reaxys user interface with all its great new features available to you from **April 2, 2013**. Click the link in the top right of the Start screen to experience the power and versatility of the new Reaxys user interface.

See how the expanded content broadens your search range. Enjoy the ease of the optimized query forms and reporting and communication functions. Discover the benefits of new features like Autoplan and Analysis View.

The old Reaxys user interface will remain available until June 1, 2013. A link in the top right of the new interface Start screen allows you to switch back.



The screenshot displays the Reaxys web application interface. At the top right, a red arrow points to a button labeled "Click here to access the new Reaxys user interface". The main interface features a navigation bar with tabs for "Query", "Results", "Synthesis Plans", "History", "My Alerts", "My Settings", and "Help", along with "Register" and "Login" options. Below this, there are tabs for "Reactions", "Substances and Properties", and "Literature". The "Substances and Properties" tab is active, showing a search area with a "Generate structure from name" input field and a "STRUCTURE EDITOR" section. The structure editor contains a "selected query editor" with the MarvinSketch logo by ChemAxon. To the right of the editor are search options: "As drawn" (selected), "Substructure:" (with sub-options "on heteroatoms" and "on all atoms"), and "Similarity". Further options include checkboxes for "Include tautomers", "Ignore stereo", "No salts", "No mixtures", "No isotopes", "No charges", "No radicals", and "No additional rings". A "Search" button is highlighted with a red box. At the bottom, there are tabs for "Properties (Form-based)" and "Properties (Advanced)", with "Substance Data" and "Bibliographic Data" listed below.

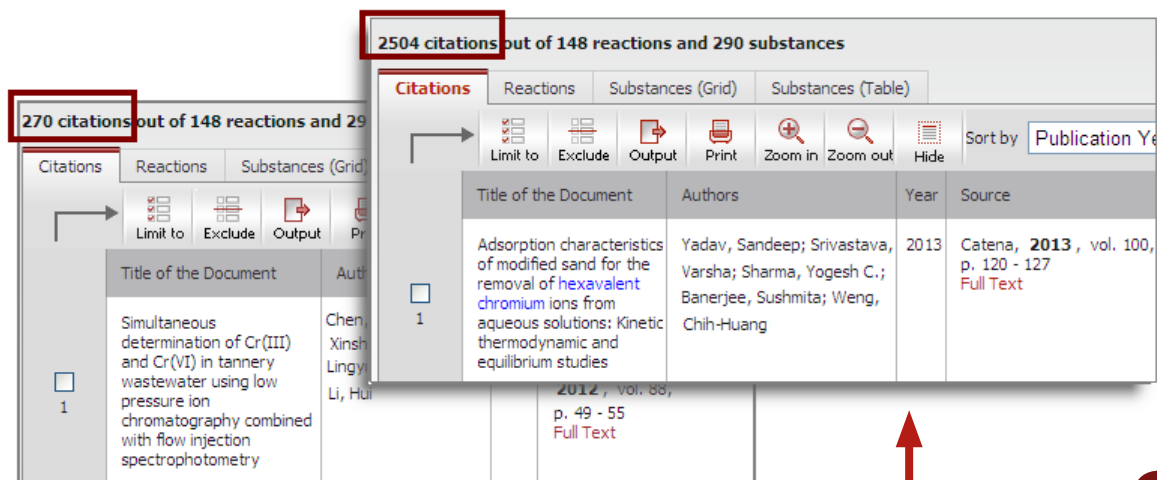
2. EXPANDED CONTENT

The content in Reaxys has been expanded from 400 core chemistry journals and essential chemistry patents to include books, conference proceedings, editorials in fields as diverse as life sciences, engineering, pharmacology, environmental science and many more.

With the **expanded content of over 16,000 periodicals**, Reaxys now offers a whole new dimension in answering your chemistry information needs.

Here is an example of a literature search for hexavalent chromium using the previous version of Reaxys and the same search using Reaxys with the expanded content. The new Reaxys returns 2504 citations from all the essential literature compared to 270 with the older version.

It's easy to see the extent of the added content when you compare the indexes for the **Document Type** fields.

270 citations out of 148 reactions and 29 substances

2504 citations out of 148 reactions and 290 substances

Title of the Document	Authors	Year	Source
Adsorption characteristics of modified sand for the removal of hexavalent chromium ions from aqueous solutions: Kinetic thermodynamic and equilibrium studies	Yadav, Sandeep; Srivastava, Varsha; Sharma, Yogesh C.; Banerjee, Sushmita; Weng, Chih-Huang	2013	Catena, 2013 , vol. 100, p. 120 - 127 Full Text
Simultaneous determination of Cr(III) and Cr(VI) in tannery wastewater using low pressure ion chromatography combined with flow injection spectrophotometry	Chen, Xinhua; Lingyi, Li, Hui	2012	Vol. 88, p. 49 - 55 Full Text

Select index items and click 'Transfer'

Search for:

- book review / secondary ref. (84251)
- journal (3347950)
- patent (819776)

Transfer
Reset
Cancel

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Select index items and click 'Transfer'

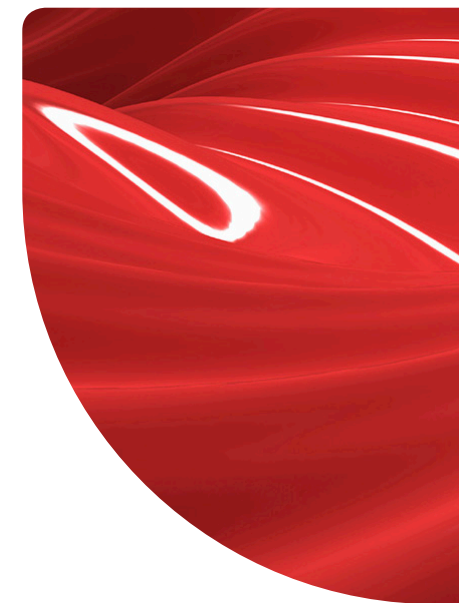
Reaxys

Search for:

- abstract report (15961)
- article (13418436)
- book (2915)
- book review / secondary ref. (84251)
- business article (27364)
- conference paper (2550880)
- conference review (21428)
- editorial (330263)
- erratum (82904)
- letter (351447)
- note (391017)
- patent (819776)
- review (1090916)
- short survey (201394)

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3. OPTIMIZED QUERY FORMS

We have streamlined the user interface to make the key search query forms directly available from the **Start** page. This gives you the fastest possible access to the functions that you need for your workflow.

For structural searches, directly access the **Substance/Reaction** search form, which allows you to use a range of structural editors for your query.

To find substances without having to draw the structure, open the Names and Formulas form with search fields for chemical names, molecular formulas, CAS Registry Number® and more.

When you want to perform a search of all the essential publications, choose the **Literature** search form, with fields such as Authors, Patent Number, and Publication Year.

The screenshot shows the REAXYS search interface. At the top is the REAXYS logo and a navigation bar with tabs: Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below the navigation bar are tabs for 'Standard' and 'Advanced' search, along with 'Query: Import Save' and 'Sources: Reaxys, PubChem, eMolecules.' The main content area is titled 'Start search with:' and features three large search form cards: 'Substances / Reactions' (with a chemical structure of pyridine and 'Elemental from dotmatics'), 'Identification' (with a chemical structure of Salvarsan and 'H2(S,Se)O4'), and 'Literature' (with a book cover 'talanta'). Below these cards are five buttons: 'Reaction Data', 'Physical', 'Spectra', 'Bio Activity', and 'Natural Product'. Red lines connect the buttons to their respective search forms.

Open a structure search form

Search using chemical identifiers

Perform a literature search

4. DATA SEARCH FORMS

The new Reaxys makes it incredibly easy to discover all areas of the rich Reaxys data repository: just open a **subject search form**, enter the term or value you are interested in and click search.

You may even customize the form with more or different search fields: just click "add/remove fields".

The screenshot displays the Reaxys Search Form interface. A modal window titled "Reaxys Search Form" is open, showing a list of physical properties search fields. Each field includes a checkbox for "exists", a dropdown menu for the search operator (currently set to "="), an input field for the value, and a "Lookup" button. To the right of each field, it indicates "In Reaxys" and provides an "Add to form" button. A red box highlights the "Add / Remove fields" button at the bottom right of the modal. Below the modal, the main search interface is visible, showing a query builder with "AND" operators and a list of selected fields: Solubility (MCS), Dissociation Exponent, and Boiling Point (°C). At the bottom, there are buttons for "Substances / Reactions", "Identification", "Literature", "Reaction Data", "Physical", "Spectra", "Bio Activity", and "Natural Product". A red box highlights the "Physical" button. At the very bottom, there are "Reset Form", "Clear Query", and "SEARCH" buttons.

Property	Exists	Operator	Value	Lookup	In Reaxys	Action
Melting Point	<input type="checkbox"/>	=		Lookup	In Reaxys	Add to form
Melting Point (°C)	<input type="checkbox"/>	=		Lookup	In Reaxys	Add to form
Boiling Point	<input type="checkbox"/>	=		Lookup	In Reaxys	Add to form
Boiling Point (°C)	<input type="checkbox"/>	=		Lookup	In Reaxys	Add to form
Density	<input type="checkbox"/>	=		Lookup	In Reaxys	Add to form
Density (gcm ⁻³)	<input type="checkbox"/>	=		Lookup	In Reaxys	Add to form
Solubility (MCS)	<input type="checkbox"/>				In Reaxys	Add to form
Dissociation Exponent	<input type="checkbox"/>				In Reaxys	Add to form
Refractive Index	<input type="checkbox"/>				In Reaxys	Add to form
Optical Rotatory Power	<input type="checkbox"/>				In Reaxys	Add to form
Partition octan-1-ol/water (MCS)	<input type="checkbox"/>				In Reaxys	Add to form

Buttons: Add & Search, Replace & Search, Cancel, Add / Remove fields

Query Builder: AND, AND, Solubility (MCS) exists, Dissociation Exponent exists, Boiling Point (°C) =

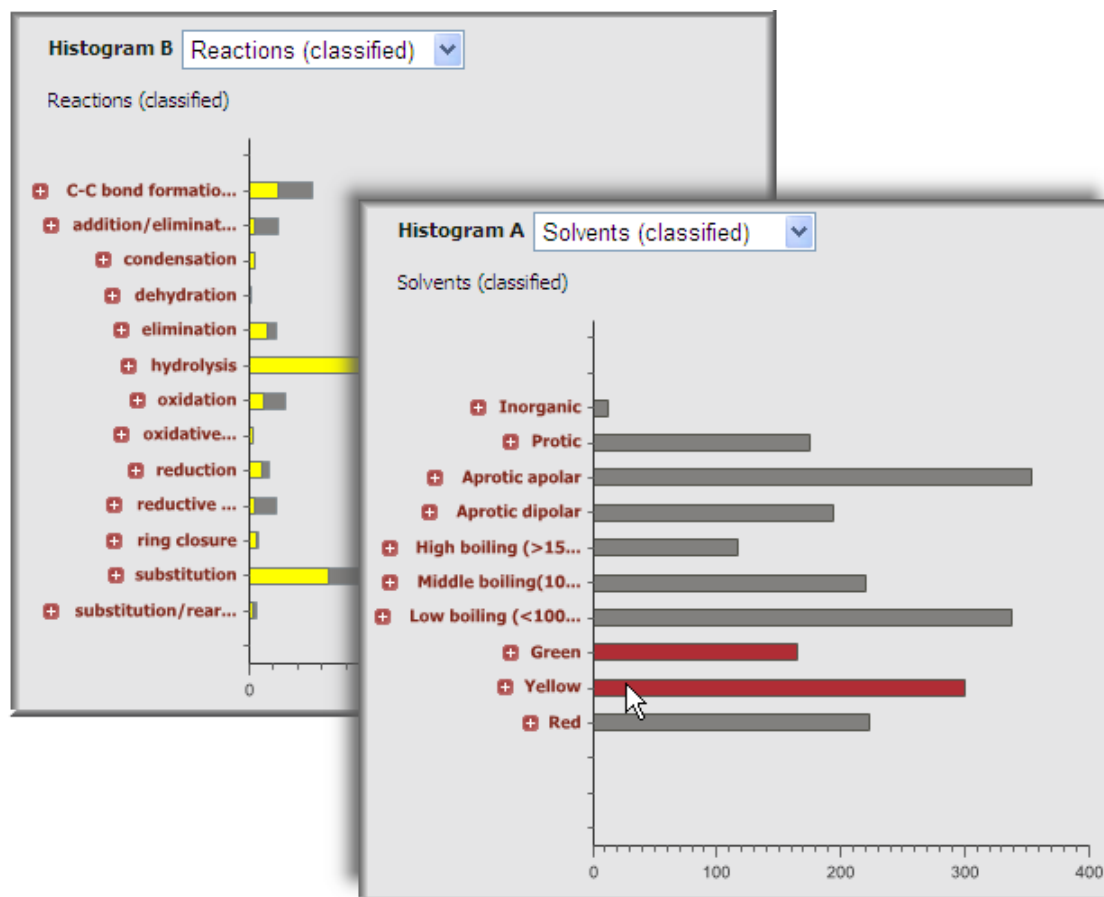
Navigation: Substances / Reactions, Identification, Literature, Reaction Data, Physical, Spectra, Bio Activity, Natural Product

Footer: Reset Form, Clear Query, SEARCH

5. ANALYSIS VIEW

One of our most exciting new features is the **Analysis View**, which is designed to give you a quick and convenient overview of a result set in the form of a histogram. This streamlines your workflow and gives deeper insight into the results. You can select various relevant criteria for histogram creation and then filter and sort from within the histogram.

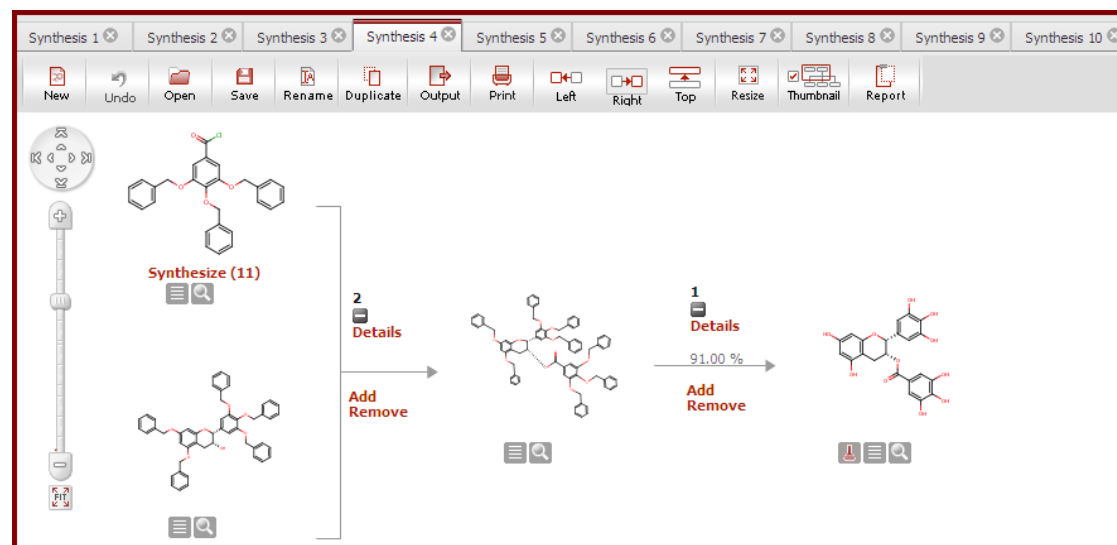
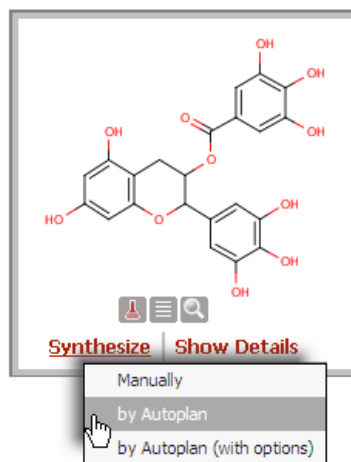
With this sophisticated view into the data, you can see, for example, which companies are patenting particular areas or which catalysts are used in a particular class of reactions and what yields can be expected.



6. AUTOPLAN

AutoPlan automates the underlying processes in creating synthesis routes, removing the often time-consuming, routine work in browsing and selecting single reactions. AutoPlan enables instant retrieval of multiple complete, but alternative synthesis plans providing you with flexible overviews to support your creativity.

Click **Synthesize** when you have the results of a substance or reaction search and select **By AutoPlan**. This will automatically generate multiple synthesis plans. You can still plan out and create your own synthesis plans by manually adding each step to each synthesis plan, but AutoPlan gives you extra options.



7. REPORTING AND COMMUNICATION

The new **Reaxys Report** feature offers you even greater opportunities to exchange data with your colleagues. You can send details from multiple results views to **Reaxys Report** by mousing over a result and selecting the chosen mode of reporting.

The optimized design allows you to instantly select specific results of interest (entire query, citation data, property facts, reaction) and copy them to the report.

You can collect, combine and annotate data across different result sets into a single, shareable report. The **Reaxys Report** supports you in assembling and organizing ideas and to share them with the team.

The screenshot illustrates the workflow for sending a Reaxys Report. At the top, a navigation bar includes tabs for Query, Results, Synthesis Plans, History, Report, and My Alerts. Below this is a toolbar with icons for Print, Undo, Open, Save, Regroup, Send, Send to Elsevier, and Clear all. The 'Send' icon is highlighted with a red box and a red arrow pointing to a 'Send Reaxys Report' dialog box.

The dialog box contains the following fields:

- Your e-mail:** Me@MyCompany
- To:** MyColleague@MyCompany
- Subject:** Reaxys Report

The main text area of the dialog displays: "Here is the report you requested with activity data and synthesis plans." At the bottom, there is a disclaimer: "Please note: Reaxys data is owned and copyright protected by Reed Elsevier Properties SA and used under license." and two buttons: "Cancel" and "Send".

On the left side of the dialog, a 'Copy to Reaxys Report:' menu is shown with three options:

- This fact (highlighted with a red box and a mouse cursor)
- This fact and the structure
- This fact, the structure and header data

Background elements include a 'Dissociation Exponent (pK)' card showing the value 7.68.

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