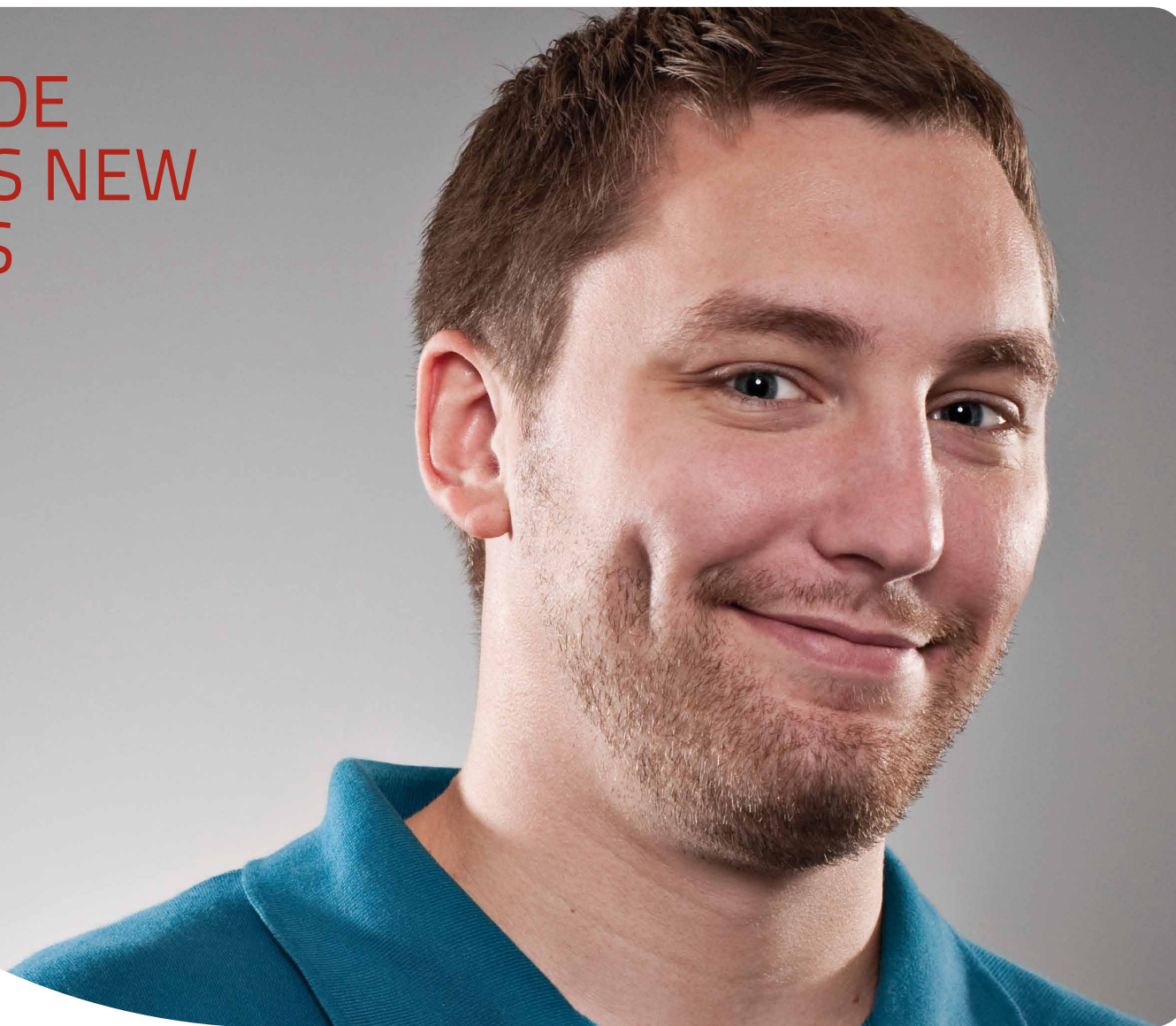


YOUR GUIDE
TO WHAT'S NEW
IN REAXYS





In consultation with expert chemists, we've refined the Reaxys content and added new search options to make it more powerful than ever.

This quick guide to what's new in Reaxys covers all of the improvements that will make finding answers easier. Discover how we've ensured that Reaxys will support every stage of your research.

1. EXPANDED AND INDEXED CONTENT

In 2013, we expanded the content of the Reaxys database to over 16,000 items, which includes essential chemistry journals and patents as well as articles, books, conference proceedings, and editorials in fields as diverse as life sciences, engineering, pharmacology, environmental science, and many more.

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

What's more, all of the content has been fully indexed and organized using the chemistry taxonomy Reaxys Tree to increase searchability.

270 citations out of 148 reactions and 290 substances

2504 citations out of 148 reactions and 290 substances

Citations Reactions Substances (Grid) Substances (Table)

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by Publication Year

Title of the Document	Authors	Year	Source
Simultaneous determination of Cr(III) and Cr(VI) in tannery wastewater using low pressure ion chromatography combined with flow injection spectrophotometry	Chen, Xinhua; Ling, Li, Hui	2012	Vol. 88, p. 49 - 55 Full Text
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

Select index items and click 'Transfer'

Search for:

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

Transfer
Reset
Cancel

Page 1 of 1

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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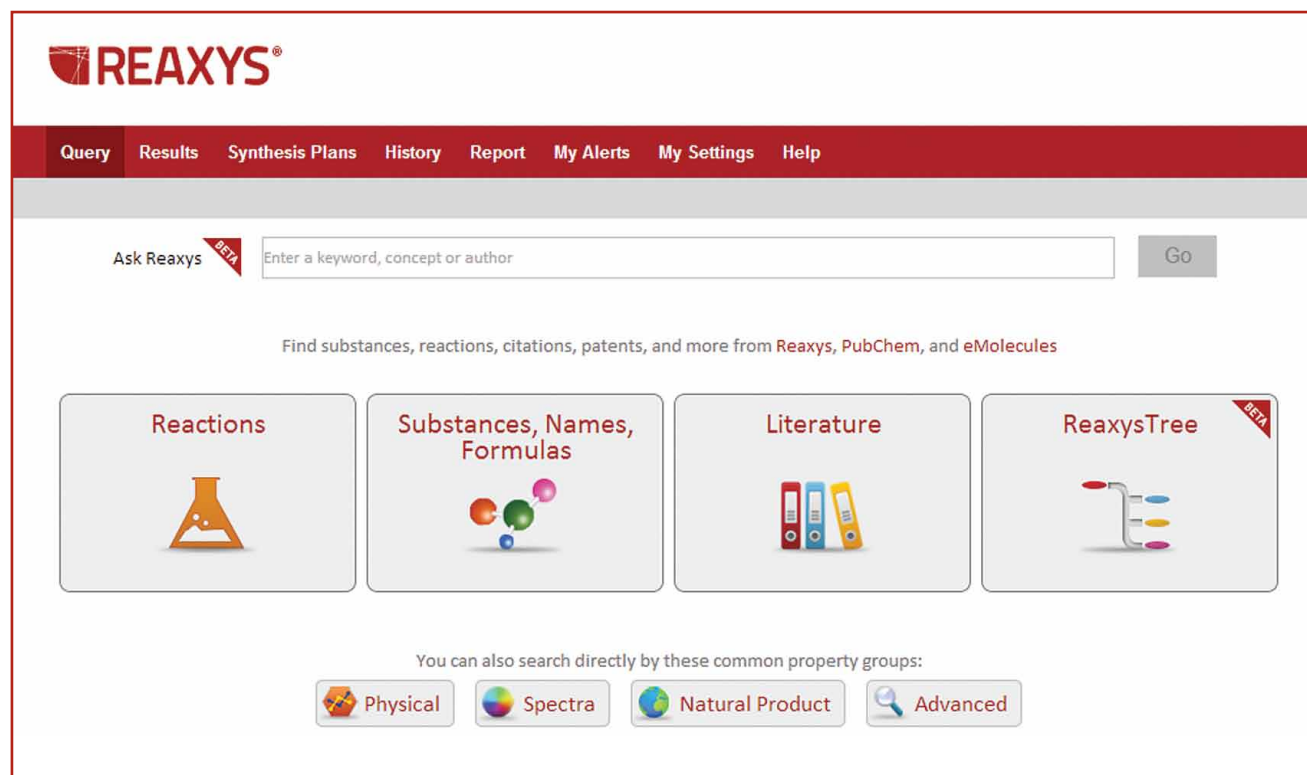
2. OPTIMIZED QUERY THEMES

From the Reaxys start page, you have the choice of three main search categories. Each opens a dedicated, customizable query theme. Reaxys supports text- and chemical structure-based input and includes 500 searchable fields covering more than 130 subject themes.

The **Reactions** query theme supports your investigations into substance synthesis pathways and reactions.

The **Substances, Names and Formulas** theme presents you with pre-defined search fields for chemical identifiers, including chemical structures and names, molecular formulas, and CAS Registry Numbers.

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



3. SEARCH QUERY THEMES

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

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

Furthermore, you can add additional search sub-queries using the formula builder, structural search functions, and more. Reaxys facilitates versatile and flexible searching.

The screenshot shows the Reaxys web interface with the 'Structure' search theme selected. The top navigation bar includes 'Query', 'Results', 'Synthesis Plans', 'History', 'Report', 'My Alerts', 'My Settings', and 'Help'. The 'Ask Reaxys' search bar is at the top. Below it, a row of icons represents different search themes: Reactions, Substances, MedChemistry, Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Structure' theme is active, displaying a 'Structure' editor with a 'MarvinSketch by ChemAxon' logo. To the right of the editor are checkboxes for search options: 'Include tautomers', 'Ignore stereo', 'No isotopes', 'No charges', 'No radicals', 'No ring closures', 'Ignore atom mappings', 'Align results with query', and 'Keep fragments'. Below the editor, a 'Please select role' section has radio buttons for 'Product', 'Starting material', 'Reagent / Catalyst', and 'Any role'. The 'Reaction Data' section contains input fields for Yield (numerical), Solvent, Reagent/Catalyst, Time (h), Temperature (°C), Pressure (Torr), Reaction Type, and Reaction Basic Index, each with a 'Lookup' button. At the bottom, there are buttons for 'Add to Query', 'Structure', 'Molecular Formula', 'Alloy', 'Add/Remove Fields...', and 'Search Reactions'.

The screenshot shows the Reaxys web interface with the 'Physical' search theme selected. The top navigation bar is the same as the previous screenshot. The 'Ask Reaxys' search bar is at the top. Below it, the same row of icons is shown, but 'Physical' is now the active theme. The 'Physical Data' section contains input fields for Melting Point (°C), Boiling Point (°C), Refractive Index, Density, Dissociation Exponent, Dynamic Viscosity (P), Optical Rotatory Power (deg), and log POW, each with a 'Lookup' button. At the bottom, there are buttons for 'Add to Query', 'Structure', 'Molecular Formula', 'Alloy', 'Add/Remove Fields...', and 'Search Substances'.

4. NEW WAYS TO FIND ANSWERS

The new Reaxys has even more options for finding answers. We've made it easier for you to get the information for your research by adding more natural and intuitive ways to search.

Ask Reaxys lets you query the database by typing the way you speak, as if you were using a regular search engine. This lets you search for phrases and concepts in a familiar way. The underlying algorithm will recognize the context and return answers in the most relevant form (e.g., documents, synthesis plans, or substance and property data).

Reaxys Tree visualizes the Reaxys taxonomy and lets you browse the database to make your own connections between seemingly disparate aspects of chemistry. This familiar tree-like data structure is a new and intuitive way to find answers.

The new Reaxys also includes a periodic table-based **Formula Builder** to facilitate inorganic and organometallic chemistry searches. Click and build your compound formula, no matter how complex.

The screenshot displays the Reaxys web application interface. At the top, the Reaxys logo is visible alongside the user status 'Anonymous user (145.36.235.1)'. A navigation bar includes links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below this, a search bar labeled 'Ask Reaxys' prompts the user to 'Enter a keyword, concept or author'. A row of icons represents different search categories: Reactions, Substances, Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Browse Literature' section on the left shows a hierarchical tree of chemical topics, including chemical transformations, physico chemical analysis methods, physico chemical properties, quantum chemical calculation methods, ab initio calculation, coupled cluster theory, electron correlation and CI calculation, electronic band structure model, empirical method, relativistic calculation, semi-empirical NDO calculation, statistical model calculation, and valence bond calculation. On the right, the 'Formula Builder' window is shown, featuring a periodic table where elements can be clicked to build a chemical formula. It includes a search bar for elements, groups, or series, and a 'Special groups' section with buttons for Me, Et, and Ph. A note at the bottom right of the Formula Builder states: 'Note: It is also possible to enter ranges or enumerations defined via variables, e.g. Fe₂O₃, n=2,3 y=2-4. Arithmetic terms, e.g. C₆H_{2n+2} n=3,4,5'.

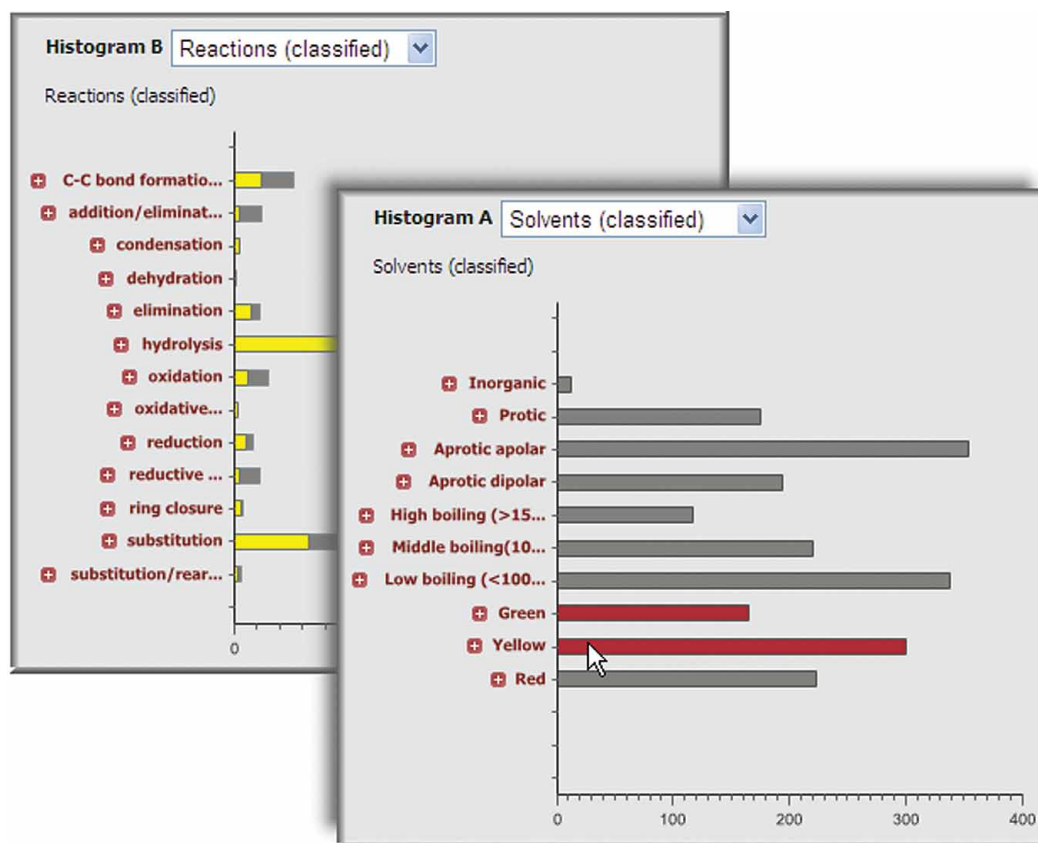
Ask Reaxys and Reaxys Tree are available on the Reaxys Start Page.

The Formula Builder is based on the periodic table.

5. REAXYS ANALYSIS VIEW

Reaxys Analysis View 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.

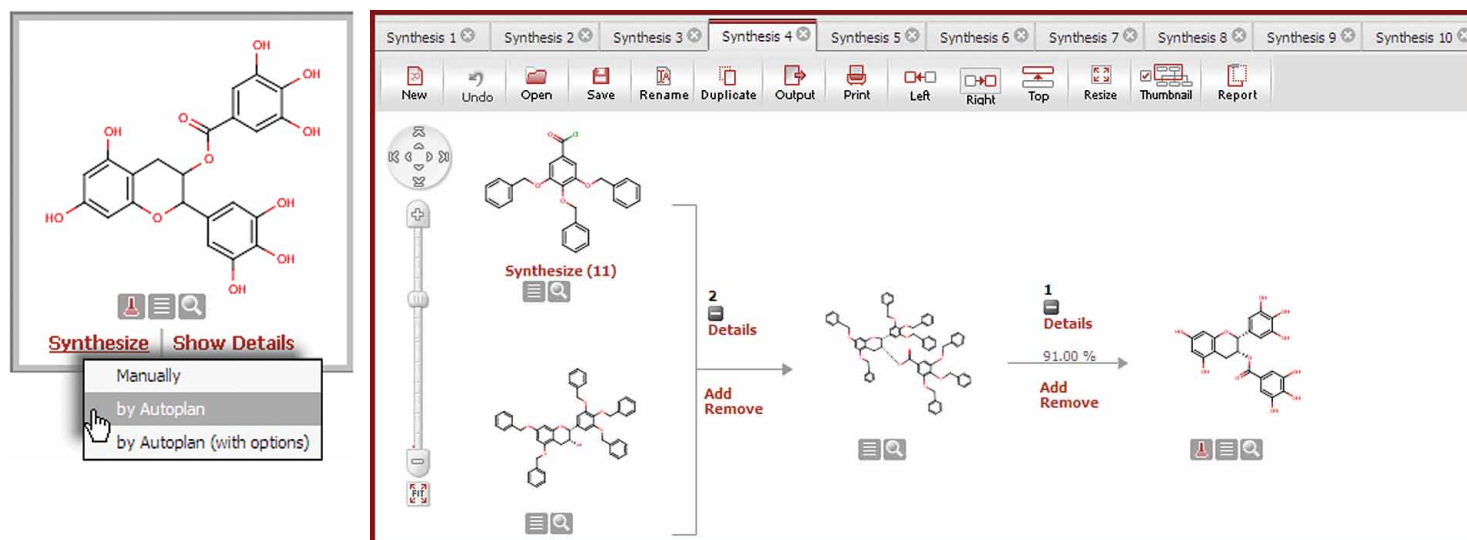
With this sophisticated view into the data, you can see, for example, which individuals or organizations are working in particular areas or which catalysts or solvents are used in a particular class of reactions and what yields can be expected.



6. REAXYS 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.

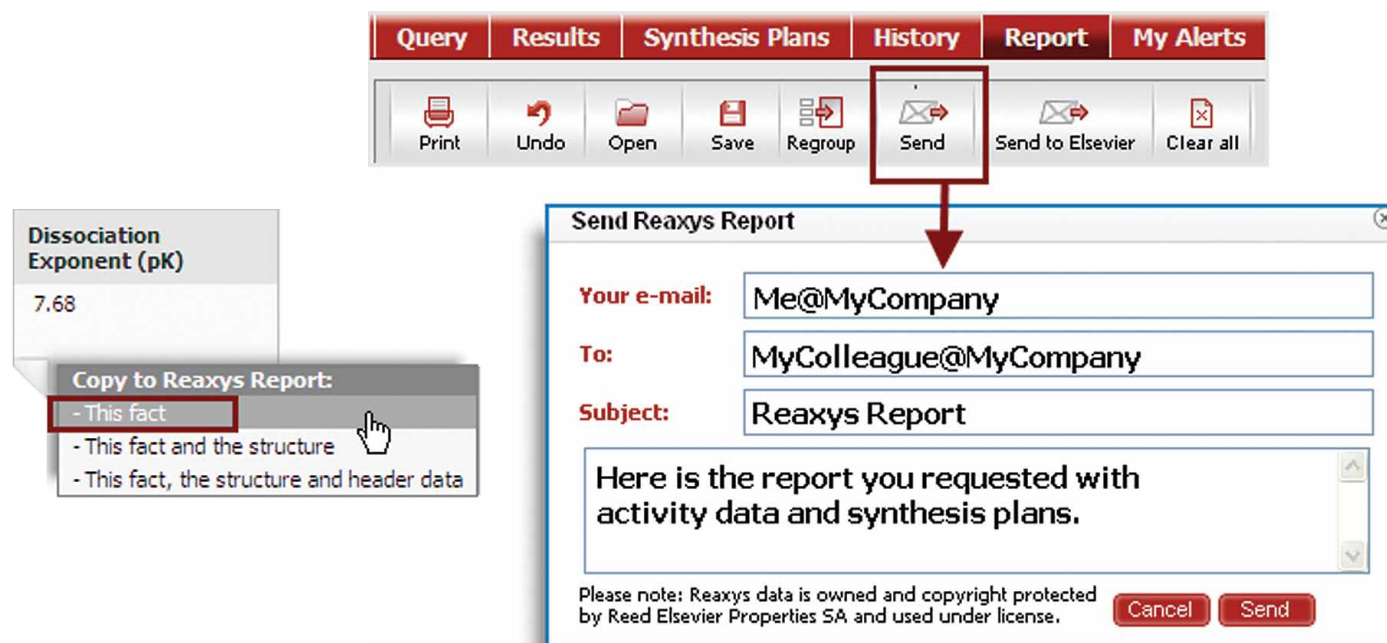


7. REPORTING AND COMMUNICATION

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.



8. FULL INTEGRATION WITH YOUR SYSTEMS

To ensure the smoothest possible working experience, we've worked on ways that you can fully integrate Reaxys into your own systems. These go beyond reporting and data export functions that allow you to share results with your colleagues and enable you to personalize and increase your research power.

The **Reaxys Structure Flat File** allows you to integrate Reaxys into your internal computation workflows or in-house systems.

Reaxys also has an **Application Programming interface** to support the development of specific chemical reaction and substance research applications.

User Interface



Structure Flat File



Application Programming Interface

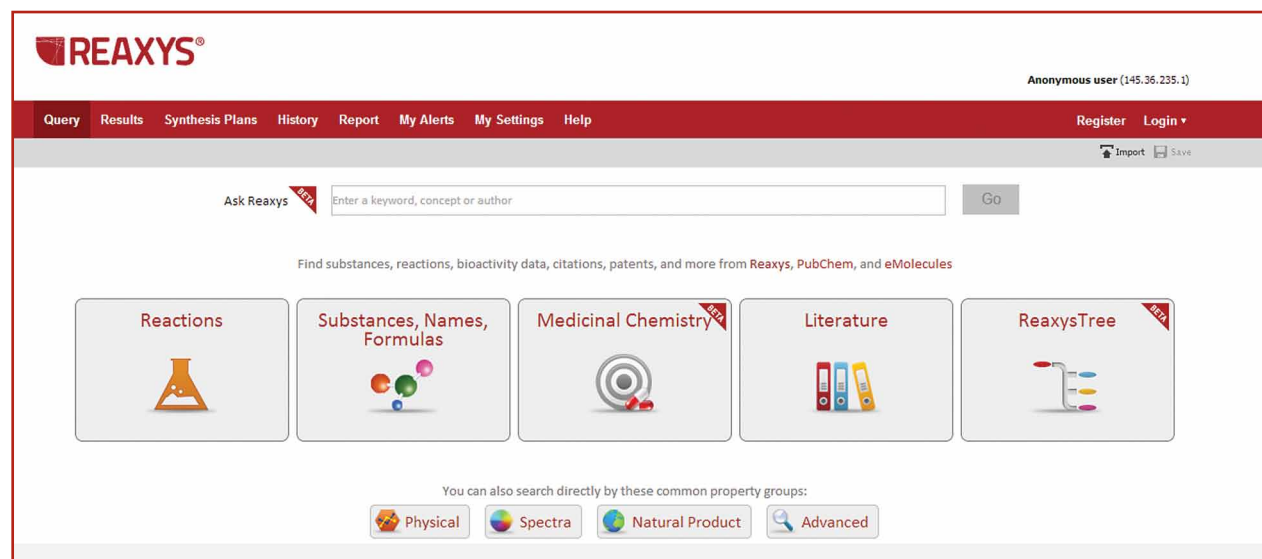


9. THE POSSIBILITY TO INTEGRATE WITH REAXYS MEDICINAL CHEMISTRY

If you're involved in life science research, you may need more information about the interactions between known compounds and target proteins. In particular, if your research includes pharmacokinetic or toxicity studies or you want to know more about the in vitro efficacy of a compound, you may need to go beyond the Reaxys database.

You now have the possibility to access the world's largest database for compound and target interactions. Reaxys can be fully integrated with Reaxys Medicinal Chemistry, allowing you to deeply explore the relationships between compounds of interest, proteins, and bioactivity data.

What's more, if you subscribe to both solutions, you can access the two databases through a single, streamlined user interface.



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