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REAXYS FACT SHEET

INTRODUCTION

Reaxys combines a comprehensive database organized according to chemistry principles with features that support flexible query input, compound synthesis pathway generation, report creation, detailed literature reviews, and more. Reaxys has the answers to all your chemistry questions.

- Does an organic, inorganic, or organometallic compound exist?
- What do we know about this compound in terms of structure, properties and reactions?
- How can I obtain this compound? Should I synthesize or purchase it?
- Who else is working on this compound or reaction type?

FEATURES

Comprehensive, highly organized database

Reaxys excerpts structure and property data from essential journals, patents, and textbook chapters. The core of the database is a comprehensive set of chemistry literature selected for relevance. A further 16 thousand periodicals taken from a broad range of chemistry-related journals, textbooks, and conference proceedings complete the picture. To increase searchability, all of the information is indexed and organized according to the principles of chemistry taxonomy.

The Reaxys database contains:

55 million organic, inorganic, and organometallic compounds

36 million chemical reactions

500 million published experimental facts

This unique collection of data is sourced from:

16,000 chemistry-related periodicals

130 subject themes - more than any other research solution

Over 240 years of chemistry coverage (1771–present)

REAXYS®

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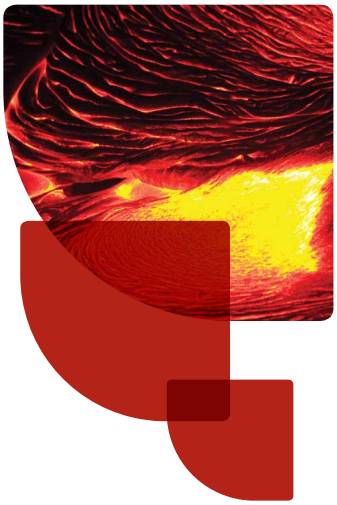
Numbers as of March 1, 2014. Numbers of facts and literature pieces approximate



Flexible search query construction

From the Reaxys start page (Figure 1), you have the choice of 3 main search categories: **literature**; **reactions**; and **substances, names and formulas**. The customizable query themes support text- and chemical structure-based input and include 500 searchable fields covering more than 130 subject themes that include concepts as varied as physico-chemical data, spectra, thermodynamics, electrochemistry, and magnetochemistry. It also includes a periodic table-based **Formula Builder** (Figure 2) to facilitate inorganic and organometallic chemistry searches.

New ways to find answers – Ask Reaxys and Reaxys Tree

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. 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 (Figure 3) and lets you browse the database to make your own connections between seemingly disparate aspects of chemistry.

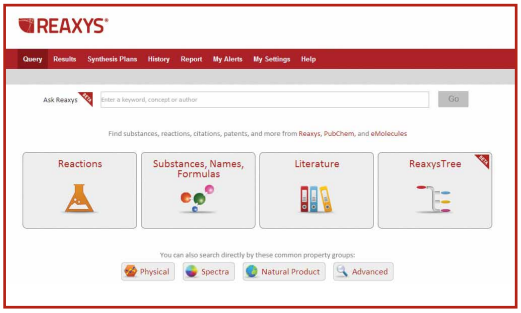


Figure 1. The new Reaxys UI.

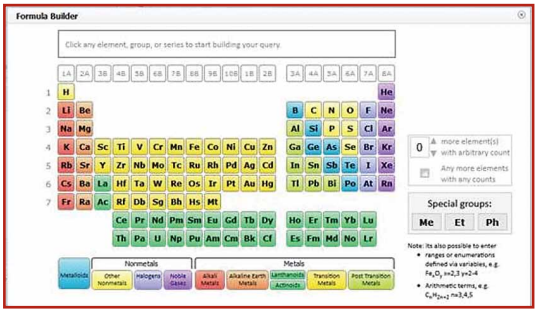


Figure 2. The Reaxys Formula Builder.

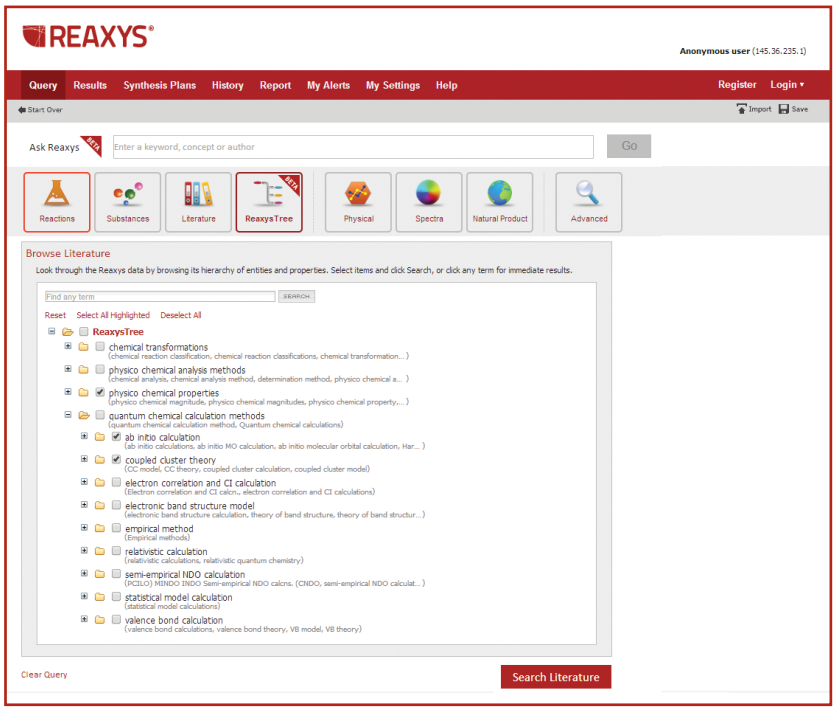


Figure 3. Browse data taxonomically using Reaxys Tree.

Compound synthesis pathway planner with links to purchase information

Reaxys AutoPlan removes the time-consuming aspects of synthesis planning by instantly generating multiple, alternative synthesis pathways for compounds of interest (Figure 4). It includes links to the eMolecules, Accelrys ACD, and PerkinElmer ChemACX databases to give you more information, including the best options for buying the compounds.

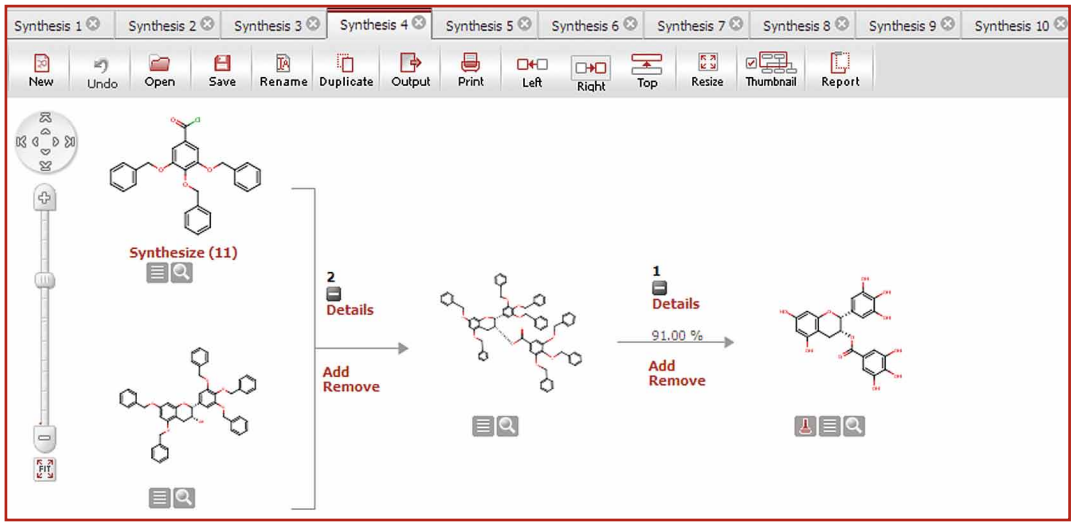


Figure 4. Reaxys AutoPlan generates multiple synthesis pathways for your compound.

Support for search result assessment

Reaxys Analysis View lets you select analysis criteria to get a sense of the relationships between your results. For example, you can quickly discover which individuals or organizations are active in particular fields of research, sort your results according to yield, or assess the catalysts or solvents for a particular reaction class (Figure 5).

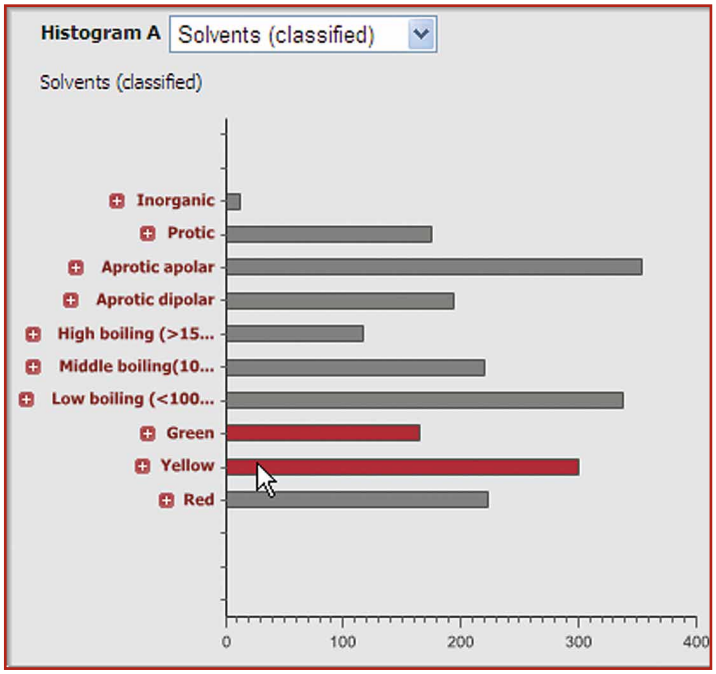


Figure 5. Reaxys Analysis View generates histograms from your hitsets.

Share your findings with your whole organization

To facilitate data sharing with your colleagues, the **Reaxys Report** feature supports annotation and export of search results and synthesis pathways (Figure 6). Reaxys is also compatible with electronic lab notebooks (ELNs) from major suppliers, such as Accelrys, Perkin Elmer, and IDBS.

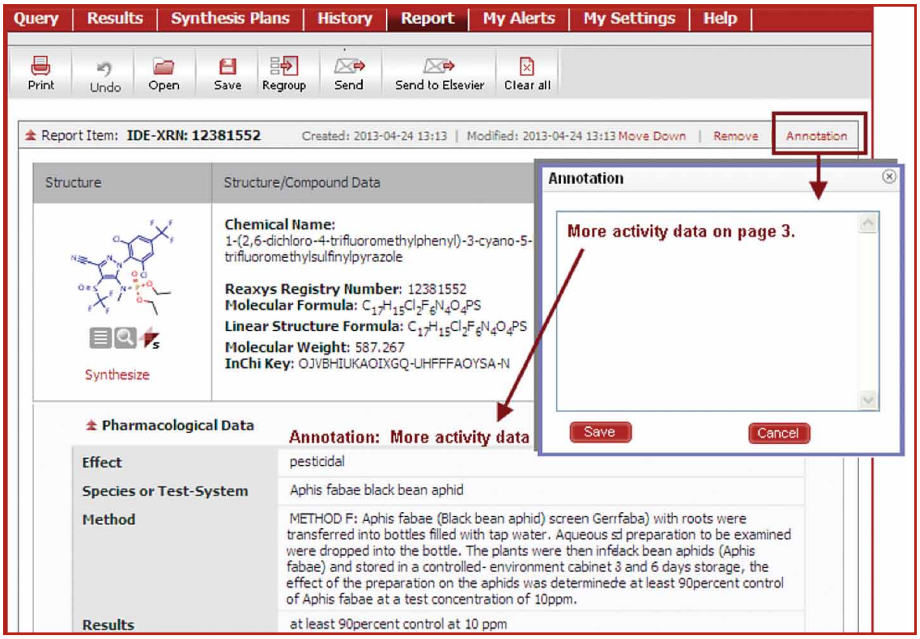


Figure 6. A Reaxys Report showing how annotations can be added.

Integrate Reaxys with your system

The **Reaxys Structure Flat File** allows you to integrate Reaxys into your internal computation workflows or in-house system. There is also an **Application Programming Interface** to support the development of specific chemical reaction and substance research applications, personalizing and increasing your research power.

Explore the largest bioactivity database in the world

Reaxys can be fully integrated with Reaxys Medicinal Chemistry, allowing you to deeply explore the relationships between compounds of interest, proteins, and bioactivity data. If you subscribe to both solutions, you can access them through a single, streamlined user interface.

KEY BENEFITS

What does Reaxys enable?

- Rapid discovery of chemical structures, properties, and reactions
- Flexible query construction that doesn't require specialist knowledge
- Insight into chemistry literature from 1771 to present day
- Confident assessment of compound synthesis and purchase options
- Straightforward, barrier-free data sharing within and outside your organization

Discover more at
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