Fact Sheet

Reaxys®

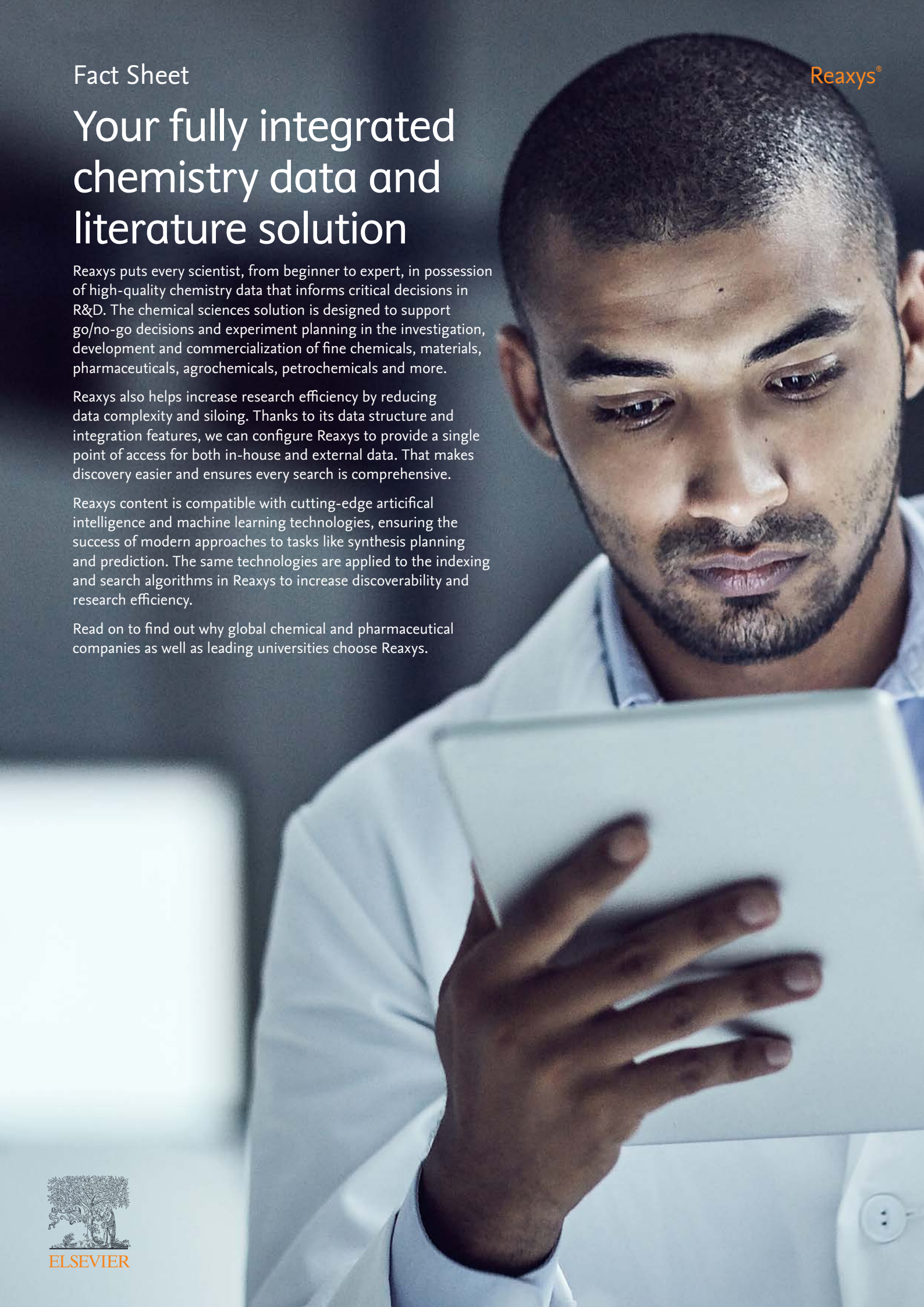
Your fully integrated chemistry data and literature solution

Reaxys puts every scientist, from beginner to expert, in possession of high-quality chemistry data that informs critical decisions in R&D. The chemical sciences solution is designed to support go/no-go decisions and experiment planning in the investigation, development and commercialization of fine chemicals, materials, pharmaceuticals, agrochemicals, petrochemicals and more.

Reaxys also helps increase research efficiency by reducing data complexity and siloing. Thanks to its data structure and integration features, we can configure Reaxys to provide a single point of access for both in-house and external data. That makes discovery easier and ensures every search is comprehensive.

Reaxys content is compatible with cutting-edge articifical intelligence and machine learning technologies, ensuring the success of modern approaches to tasks like synthesis planning and prediction. The same technologies are applied to the indexing and search algorithms in Reaxys to increase discoverability and research efficiency.

Read on to find out why global chemical and pharmaceutical companies as well as leading universities choose Reaxys.



ELSEVIER

Improve productivity and inform decisions with relevant answers

Reaxys provides access to a highly curated database of experimental facts and relevant citations. It is designed to inform critical decisions chemical sciences research and development projects with precise substance property, reaction and synthesis data presented alongside experimental procedures, patent information, citations and details of commercial availability.

By excerpting the broadest range of data types from the literature, Reaxys is unique among chemical sciences research solutions. Over 500 million published experimental facts are readily available with information about the sources of each data point.

Thanks to this unparalleled direct access to essential data, Reaxys helps answer key questions, such as:

- Does this chemical substance exist?
- What is known about its properties and reactions?
- Does it have druglike or bioactive properties?
- How can I synthesize or purchase it?
- Is it being used in novel research?
- Who else has worked on it?
- What patent claims have been made relating to it?

Keep information discoverable — now and in the future

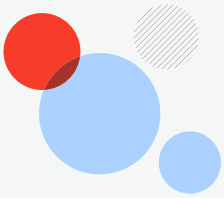
Rapidly evolving technologies produce increasingly diverse types of data. Will current formats of chemical data be relevant in the future? Make sure your research captures insights from across the chemistry information landscape in the same contextual view, whether you're using published, commercial or internal data.

Reaxys is designed to store any type of chemistry data, integrate content across databases, help share insights with collaborators, and make data usable today and in the future.

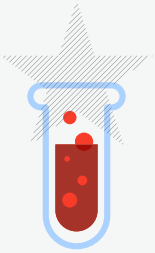
The power of Reaxys in data integration scenarios has been thoroughly tested. In a collaboration with Pistoia Alliance involving pharmaceutical companies and electronic lab notebook (ELN) providers, Elsevier has made the Reaxys data structure available as a unified data model (UDM) to standardize data exchange in synthetic chemistry. In a project with Lundbeck, a fully integrated chemical data solution was created to give one point of access to multiple resources that used to be separate silos.

This approach makes it easier to:

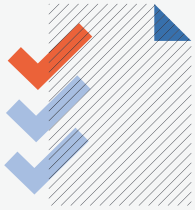
- Discover chemistry data regardless of format used for reporting
- Store, share and explore knowledge in its intended context
- Share research or service outcomes in a universal format



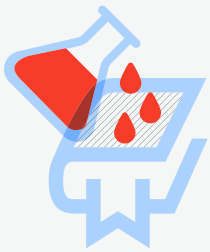
>118M
organic, inorganic and organometallic substances, including data on natural products with their species derivation



>49M
chemical reactions

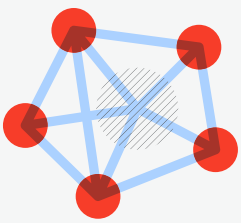


>500M
published experimental facts, including substance property, spectral and reaction data



>59M
documents from a collection of over 16,000 chemistry-related periodicals from multiple publishers

>1.5M
patents from the world, U.S., European, Japanese, South Korean, Chinese and Taiwanese patent offices



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indexing sources for a cross-disciplinary view of chemistry

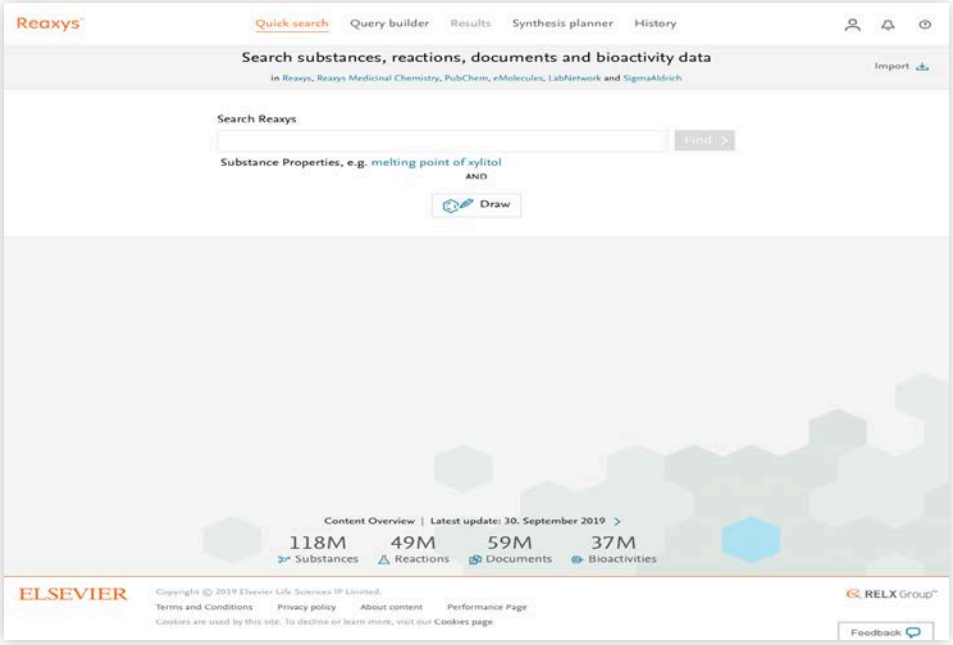


Figure 1. Reaxys *Quick Search* is a highly intuitive search form. Every user can easily build a keyword- or structure-based search to retrieve substance property and reaction data as well as relevant literature.

The Reaxys home screen also includes information about the databases covered by Reaxys and a content overview.

The *Feedback* feature allows users to make suggestions about features and content. It is available on every screen.

Ensure discoverability of answers, regardless of your field or focus

Chemistry is a far-reaching and complex science. Researchers in disciplines as disparate as engineering, geology, pharmacology and medicine require chemistry answers for their investigations.

Since different scientists approach scientific questions from different perspectives, it is essential that modern search engines approach knowledge from multiple angles.

Indexing using terms from taxonomies is how a record is prepared for discovery in a search engine. In Reaxys, each record is indexed with terms from 6 taxonomies to support a truly cross-disciplinary view of chemistry information.

- ReaxysTree (for chemistry)
- Compendex® (for engineering)
- Geobase® (for geology)
- Emtree® and MeSH® (for pharmacology and medicine)
- Scopus® Authors (for researcher name-based searches)

Using these taxonomies, the core chemistry content undergoes deep manual indexing and exceprtion of substance properties, reactions and synthesis procedures. A process of rules-based automated content enrichment based on machine learning technologies is applied to index and excerpt data from a broader range of over 16,000 chemistry-related periodicals. These processes generate the indexed bibliographic records and excerpted substance, reaction and target records that form the unique Reaxys knowledge base. In fact, Reaxys excerpts more types of property and spectral data than any other chemistry research solution — and that includes data points and searchable text-based information.

Access a rich repository of data from peer-reviewed articles, patents and more

Each query from Reaxys *Quick Search* (Figure 1) and *Query Builder* (Figure 3) leverages superior search algorithms to quickly retrieve substance property and reaction data, synthesis options, experimental procedures, patent claims and citations. The comprehensive Reaxys knowledge base covers every type of literature and third-party commerical databases. Integration projects also enable the inclusion of content from internal databases in a Reaxys search. Reaxys accesses:

- A carefully curated collection of ~450 essential journals and textbooks in organic, inorganic and physical chemistry, material science, petrochemistry, pharmacology, and medicinal and computational chemistry
- >16,000 chemistry-related periodicals, including conference abstracts, with minor publications in core fields and major publications in related fields
- Patents with a global range that goes beyond the world, US and European content to include Asian-language patents from the China, Taiwan, Japan and South Korea offices
- Substance databases from leading chemicals and cheminformatics companies, including SigmaAldrich, Advanced Chemistry Development and WuXi AppTec's LabNetwork
- Publicly available substance and literature databases, including reliable links to eMolecules and PubChem

Ensure a user-friendly search experience, regardless of your expertise

The streamlined Reaxys user interface and search algorithms based on cutting-edge artificial intelligence facilitate smart query construction.

Quick Search (Figure 1) accepts natural language-based keyword queries, structure or reaction drawings, and a combination of the two. Keywords can include identifiers such as SMILES and InChiKeys. The chemistry-specific keyword auto suggest feature helps to increase search precision. As you type, it suggests potentially relevant chemical names and terms from the indexing sources ReaxysTree and Emtree.

Each *Quick Search* is answered with a *Results Preview* dialog (Figure 2) where you can choose the result view you wish to focus on first: substances, reactions, targets or documents. You can select to preview the first three results for that category, view the results, start a new query, edit the query in *Quick Search* or *Query Builder*, or even create an email alert for this search. Regardless of which result view you choose, you can easily navigate to the other result views.

Query Builder (Figure 3) offers you a versatile means to construct advanced queries using multiple data fields combined with Boolean operators (AND, OR, NOT, NEAR{n}, NEXT{n} and PROXIMITY). Click or drag-and-drop interactive querylets from an extensive list. You can set the parameters and add all essential input, including precise properties, ranges, structure drawings and molecular formulas. *Query Builder* is developed in consulation with leading research chemists to maintain its relevance to your daily work, and feedback from users is also taken into account.

To ensure the greatest flexibility with structure and reaction drawing, Reaxys users can choose between two popular editors: ChemAxon's MarvinJS and PerkinElmer's ChemDraw. Both support simple and sophisticated structure drawing with easy structure query editing in *Query Builder*. Either one can be set as the default strucure editor for drawing-based queries. What's more, users can start a Reaxys search from ChemDraw Desktop, meaning they can spontaneously check for information about a structure.

Figure 2. The *Results Preview* shows the relevant result types for your Quick Search query and gives a range of options for your next step.

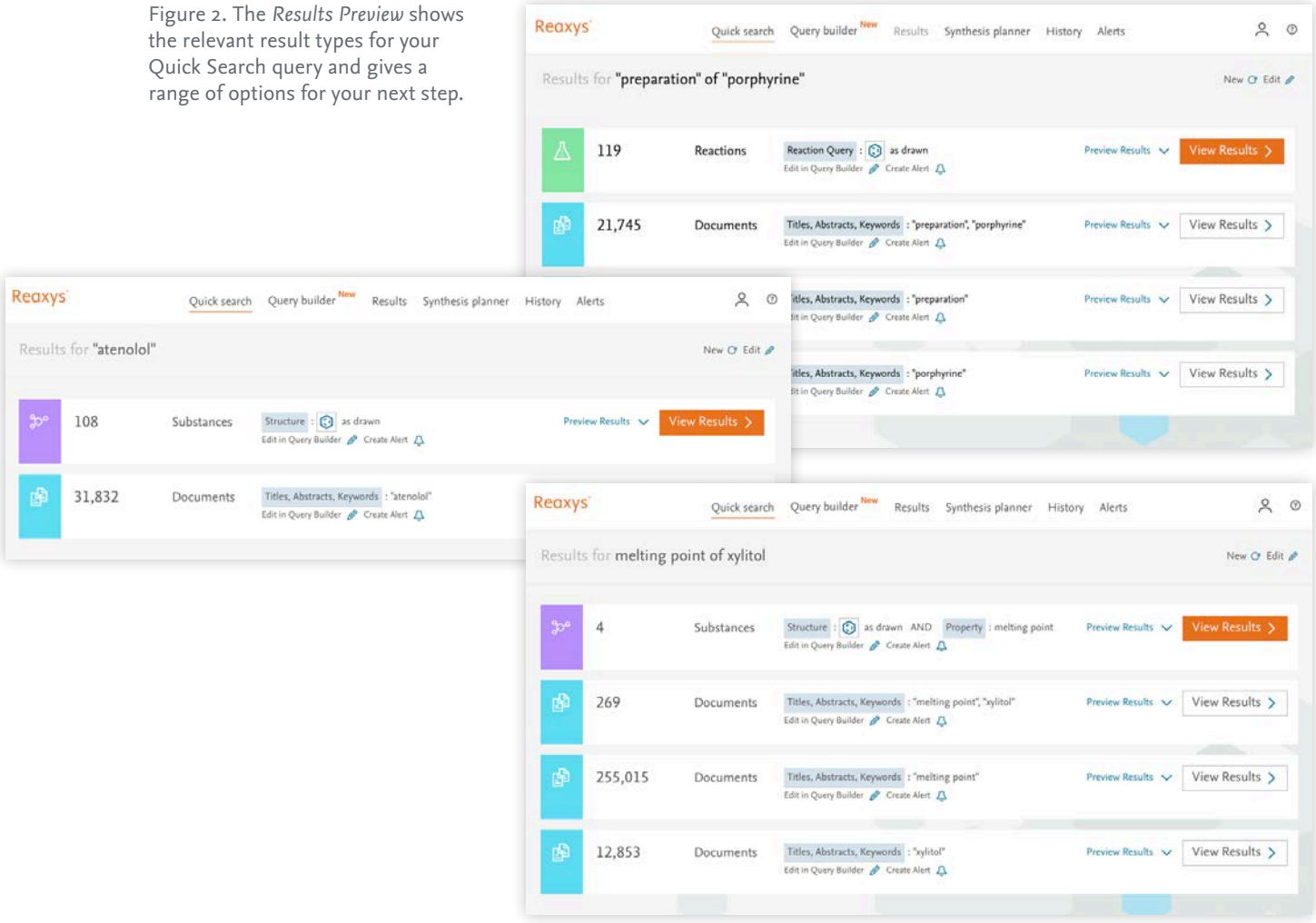
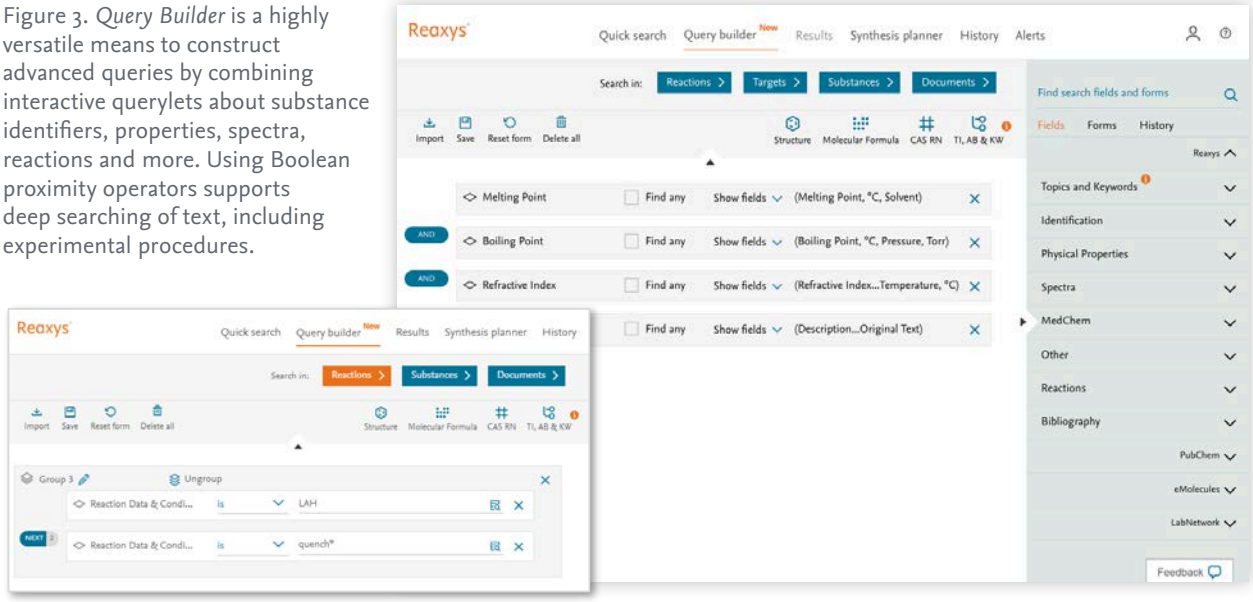


Figure 3. *Query Builder* is a highly versatile means to construct advanced queries by combining interactive querylets about substance identifiers, properties, spectra, reactions and more. Using Boolean proximity operators supports deep searching of text, including experimental procedures.



It is also easy to import load and search for batches of structures as SD or MOL files using the Import feature. This searching mode is designed to simultaneously retrieve substances, reactions and documents for multiple structures with just a few clicks.

Thanks to the proximity operators (NEAR{n}, NEXT{n} and PROXIMITY), Reaxys supports deep searching of text. This includes the possibility to search within experimental procedures to easily discover safety comments, reaction details, substance notes, purification methods and even process-scale reactions.

Reaxys offers a broad range of interactive filter categories and other options for working with results (Figure 4). These have been designed in a user-centric process. Each result set triggers its own list of relevant filter categories. *Limit to* and *Exclude* options for every filter give additional flexibility. In the *Reactions* results view, there are also one-click filters available for experimental procedures and single-step reactions. The interactive filter categories ensure every user can quickly assess even very large result sets, identify the desired results within subsets of a list of reactions, substances, targets or references, and more.

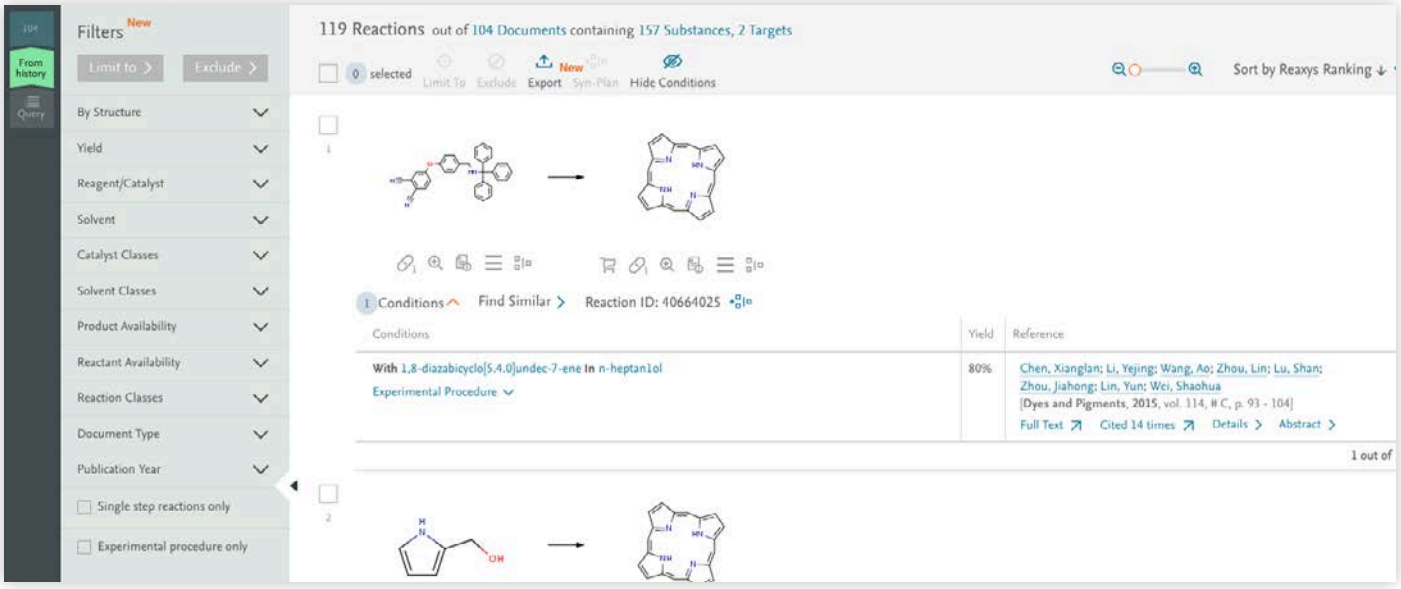


Figure 4. The interactive filters help to quickly refine result sets. In this *Reactions* view, the single-click options *Single-step reactions only* and *Experimental procedures only* are shown at the bottom of the filter list. The remaining filters are also relevant to the result set.

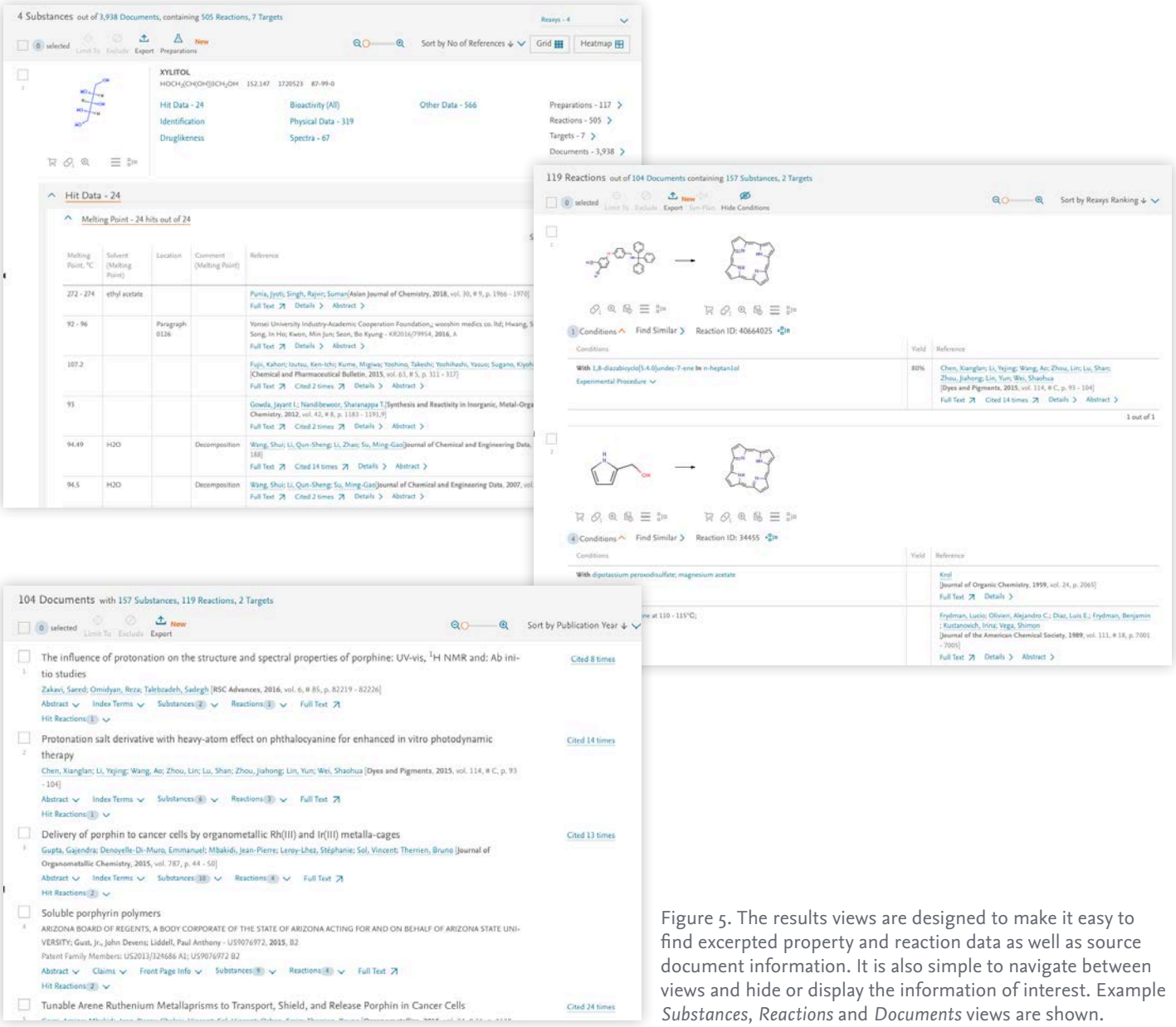


Figure 5. The results views are designed to make it easy to find excerpted property and reaction data as well as source document information. It is also simple to navigate between views and hide or display the information of interest. Example *Substances*, *Reactions* and *Documents* views are shown.

Enjoy clarity in every result set

The *Substances*, *Reactions*, *Documents* and *Targets* results view (Figure 5) are each designed for the optimum display of the excerpted property and reaction data, experimental procedures, patent claims, and other document information.

Each substance is depicted as a structure with relevant identifiers alongside links to information on its identification, druglikeness, bioactivity, physical data, spectra, other data, preparations, reactions, targets, and relevant documents. In addition, links to the substance availability in commercial databases (where possible), options for further searches, and published synthesis options are also provided.

Each reaction is depicted with the option to show or hide the reaction conditions, find similar reactions, and add the reaction to a *Synthesis Planner* working page (Figure 6).

Each document is listed as the title, authors and source along with the option to view the abstract, terms used to index the document, substances mentioned in the document, and a link to the full text.

Each target is described with the relevant identifiers, an example structure, bioactivity charts, and links to relevant substances and documents.

To support prior art investigations and reduce the amount of time spent searching through long patents, if a result includes claims containing one of the search terms, the information is displayed with the term highlighted as the *Claims hit*. Where relevant, you can also use a single-click option to expand the claims information into a full list of the claims in the order they appear in the patent.

Easily investigate synthesis routes based on published reactions and conditions

Synthesis Planner (Figure 6) removes the time-consuming aspects of synthesis planning. Click the *Synthesize* icon and choose the manual or Autoplan option for any substance in a subtance or reaction record to open this feature. Autoplan is particularly efficient: it instantly generates multiple, alternative synthesis pathways for compounds of interest. This synthetic blueprinting is based on reactions described in multiple source documents, allowing you to build the best synthesis route for your purposes. Reaction conditions can be displayed in the position most convenient for you, including in a separate window. As in the *Substances* and *Reactions* results views, where possible, links to substance availability in commercial databases are included for each substance. This supports synthesize-or-purchase decisions by ensuring all the relevant information is available through one interface.

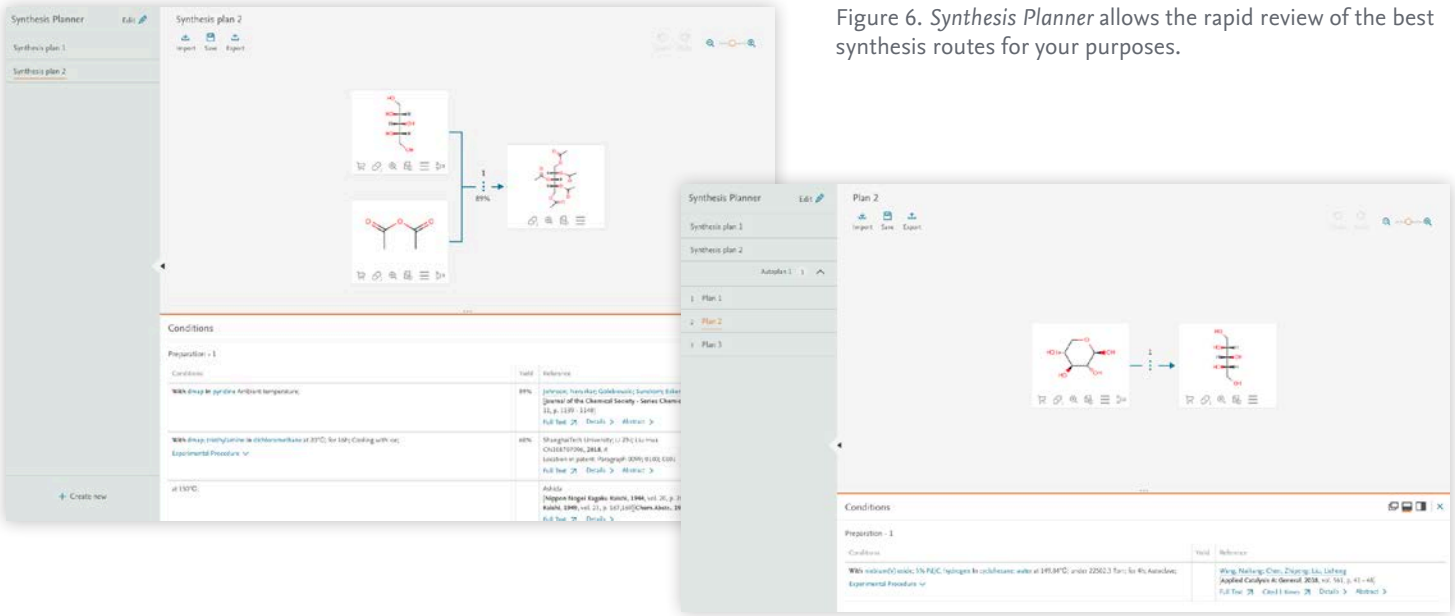


Figure 6. *Synthesis Planner* allows the rapid review of the best synthesis routes for your purposes.

Integrate Reaxys into existing workflows

The seamless integration of Reaxys into existing workflows sets it apart from other chemistry research solutions. Reaxys already provides multiple options that align with this goal:

- Flexible data export options, including the Structure Flat File, allowing data to be used in other cheminformatics and analytics systems (e.g., for structural analog searching or uniqueness assessments)
- Compatibility with ELNs from major suppliers, including Accelrys, Perkin Elmer and IDBS, for greater flexibility of working with data
- The Reaxys Application Programming Interface (API), which, with the support of our Professional Services Team, supports the querying of Reaxys from in-house search interfaces
- The HopInto feature, which can be integrated into in-house systems, supports the smooth continuation of a work query by transfering the user from the system to Reaxys
- Interoperability with other Elsevier solutions, including Scopus, Mendeley® and ScienceDirect®, guaranteeing streamlined and seamless workflows that are not available with any other chemistry research solution

Key benefits

Reaxys is a unique and powerful solution that supports chemical sciences research and development. The rapid and reliable access to comprehenisve substance data and relevant literature supports the best-informed decisions in every project. Its versatile features enable researchers to:

- Search de-siloed internal and external databases
- Discover chemical structures, properties and reactions
- Compare in-house and external data more easily
- Increase research efficiency and R&D productivity
- Make properly informed go/no-go decisions
- Leverage artificial intelligence technologies for chemistry investigations, including predictive retrosynthesis

Reaxys

Reaxys delivers relevant substance property and reaction data, synthesis options, experimental procedures, patent information, and citations. It helps chemicals and pharmaceuticals businesses develop commercially successful products. It provides an integrated view of the data and literature that informs decisions and allows companies to more easily combine in-house and external data for highly efficient research.

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