R&D SOLUTIONS FOR PHARMA & LIFE SCIENCES

Reaxys® Medicinal Chemistry

Fact Sheet

Essential data for lead identification and optimization

Reaxys Medicinal Chemistry empowers early discovery in drug development with normalized substance–target affinity data and comprehensive pharmacokinetic, efficacy, toxicity, safety and metabolic profiles. It is designed to enable beginners and experts to create equally powerful searches, revealing the potential activity of a substance as part of a range of in silico modeling workflows.

Introduction

Reaxys Medicinal Chemistry empowers **hit identification** and **lead optimization** with normalized substance–target affinity data and comprehensive pharmacokinetic, efficacy, toxicity, safety and metabolic profiles. It combines the world's largest and best-organized substance bioactivity data with tools for hitset assessment and the possibilities to export data to existing computational environments, facilitating harmonized analysis of in-house and external data.

Reaxys Medicinal Chemistry helps to answer critical research questions:

- What are all the substances that interact with my target?
- What types of interaction occur between my substance and my target?
- What interactions do other substances with similar structures have?
- What is the comparative affinity of different substances for my targets?
- What phenotypic screening has been done on similar substances?
- Which of my drug candidates has the highest chance of success?
- Who are the key researchers working on similar substances and targets?

The Reaxys Medicinal Chemistry Database contains:

>35.2M bioactivity data points	**>6.8M** unique substances with bioactivity	**>27K** unique targets	**>65K** species

This unique collection of data is sourced from:

>133K medicinal chemistry patents	**>370K** medicinal chemistry articles	**>5K** drug discovery and pharmacology journals

FEATURES

The world's largest & best-organized medicinal chemistry database

Content includes:

- Structure–activity relationship (SAR) profiles
- Data from in vivo animal studies
- In vitro efficacy, pharmacokinetic, toxicity and safety data
- In vitro metabolic profiles

All the data, including content from third-party databases, are harmonized using Reaxys standards for chemicals, targets and bioactivities. Elsevier life science experts normalize the data; map concepts and glossaries; and remove inconsistent data and duplicate citations.

Quick and intuitive search capabilities

To facilitate rapid retrieval of bioactivity data and citations, Reaxys Medicinal Chemistry offers users Quick Search: an intuitive interface that accepts queries consisting of natural **keywords and/or substance structure or reaction drawings** (Figure 1). The intelligent search algorithms understand and interpret the text, offering users a preview of the types of result their query will return (Figure 2). This enables beginners and experts alike to quickly find answers to drug discovery questions.

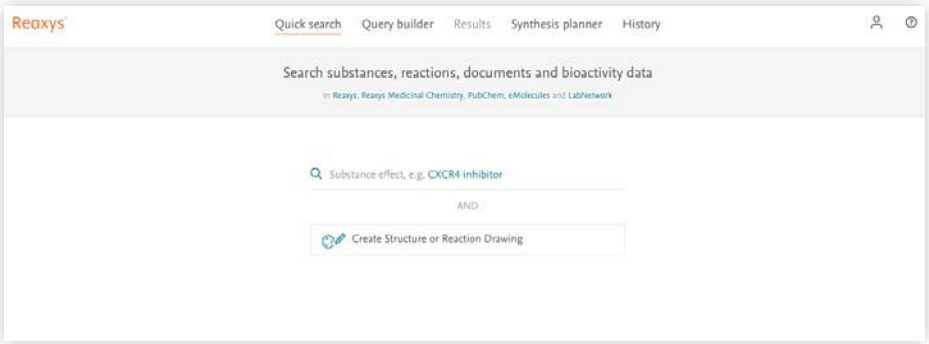


Figure 1. Quick Search accepts and interprets keyword and/or structure queries

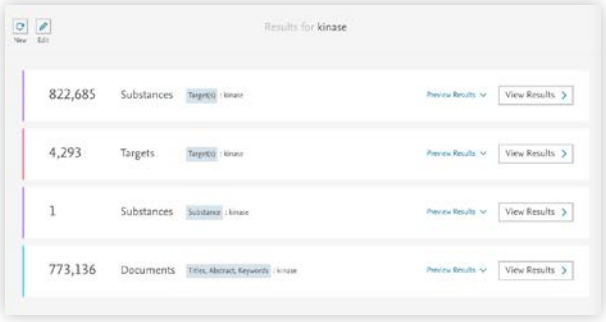


Figure 2. The results preview helps users get directly to the information they require

Flexible and powerful query construction

The user interface provides an intuitive Query Builder (Figure 3) that enables **straightforward drag-and-drop construction of advanced queries**, using text input and chemical structure drawings. It also includes 19 dedicated query forms for lead optimization searches. By making it easy to precisely define the parameters of the query and retrieve the relevant answers, Reaxys Medicinal Chemistry puts powerful search capabilities in the hands of all users.

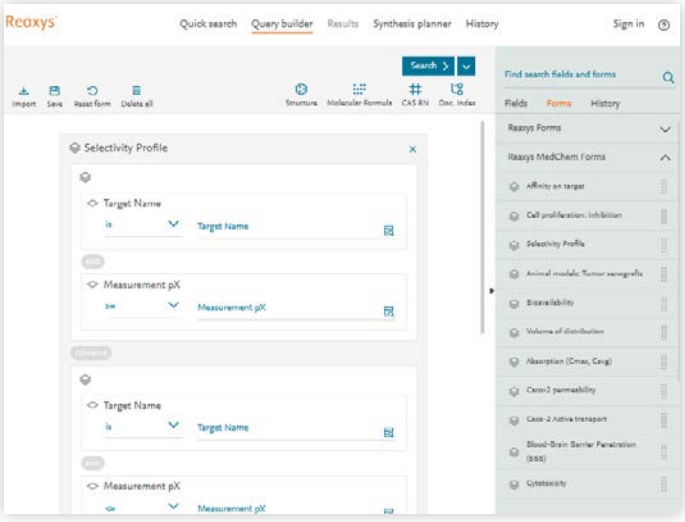


Figure 3. Query Builder enables straightforward construction of advanced queries and includes 19 dedicated query forms for major lead optimization search workflows

Easy access to detailed information

Results are displayed in an easy-to-read manner. Filters (Figure 4A) enable quick refinement of the hitset to focus in on the most relevant substances, targets or literature. It is straightforward to drill down to get precise information about physical, chemical and bioactive properties about substances (Figure 4A and B) and target details (Figure 4C).

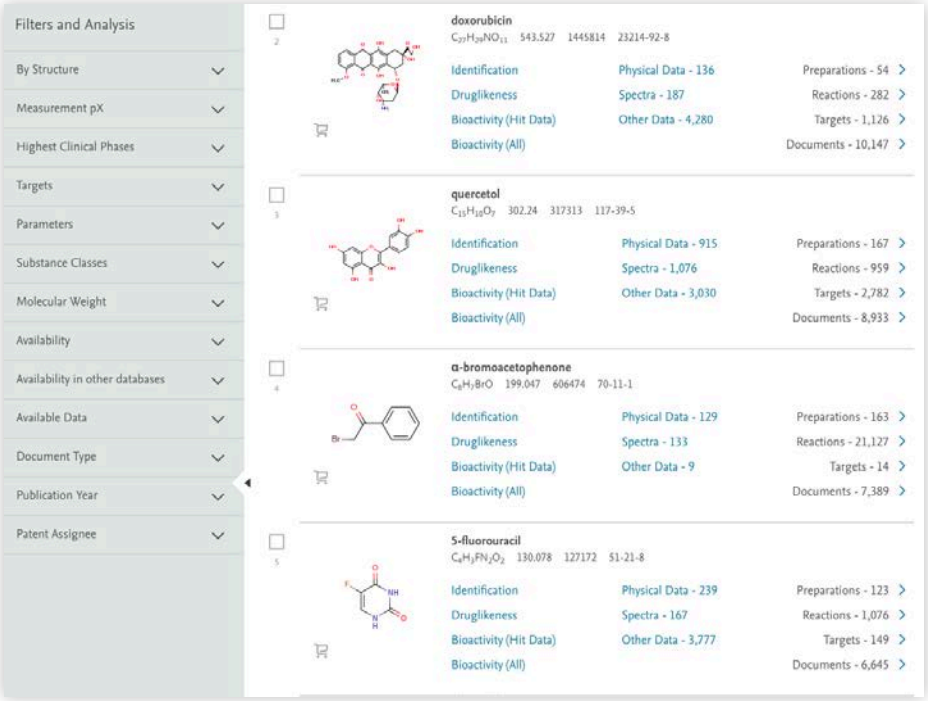


Figure 4A. Results are displayed with obvious filter and drill-down options

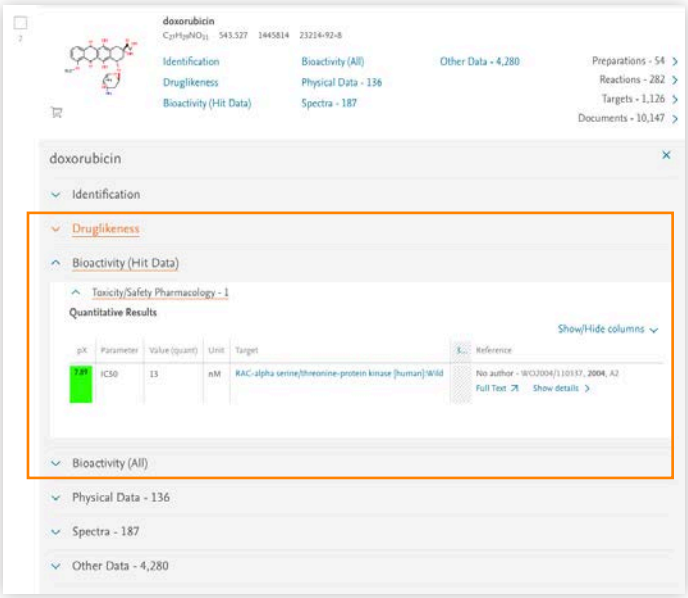


Figure 4B. Substance details include a drug likeness display and quantitative bioactivity information displayed in an interactive table

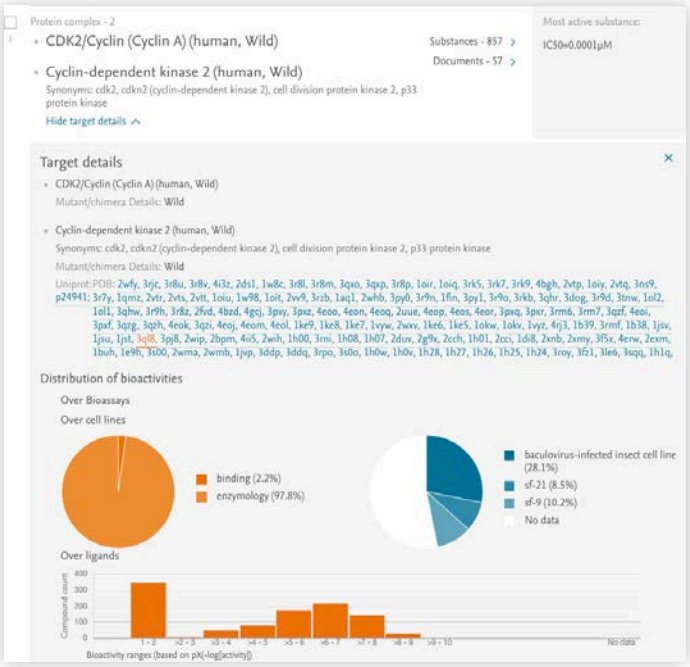


Figure 4C. Target details include easy-to-read charts of bioactivity distributions

Rapid assessments of substance and target interactions

Heatmap (Figure 5) provides a clear overview of the relationships between substances and their targets in terms of key parameters. This enables rapid identification of the most relevant interactions. Its parameter settings are flexible: changing them reveals new relationships between substances and protein targets or cell lines.

Figure 5. Heatmap enables rapid assessment of substance–target interactions

Clear quantification of substance and target affinities

To facilitate comparisons of biodata from different publications and assay types, all the data points in Reaxys Medicinal Chemistry have **pX values**. These are normalized values assigned to the data to enable easy quantification of substance–target affinity and comparison of information from all around the world. They are displayed in Heatmap View (Figure 5) for convenient reading.

Share discoveries with colleagues and external collaborators

Reaxys Medicinal Chemistry allows export of search results in multiple formats that are fully compatible with modeling, workflow and data visualization software from major suppliers. It is also possible to annotate results and send them directly to fellow researchers.

Integrate Reaxys Medicinal Chemistry into existing workflows

The **Application Programming Interface** (API) allows flexible information delivery and real-time programming access to the content and system (Figure 6). The Flat File delivers structures, related reaction data and bioactivity information for in-house usage, e.g., QSAR/QSPR modeling and chemical space analysis. Elsevier's R&D Solutions Professional Services team stands ready to ensure that Reaxys Medicinal Chemistry can operate seamlessly within an existing environment of tools.

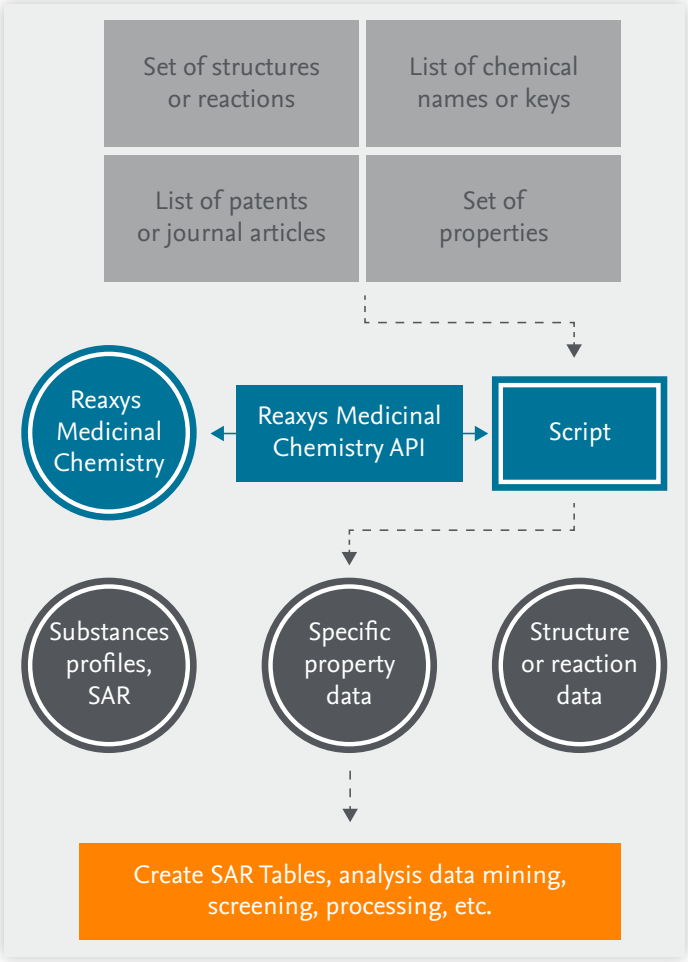


Figure 6. A schematic showing how Reaxys Medicinal Chemistry can be integrated into an existing research workflow using the Application Programming Interface

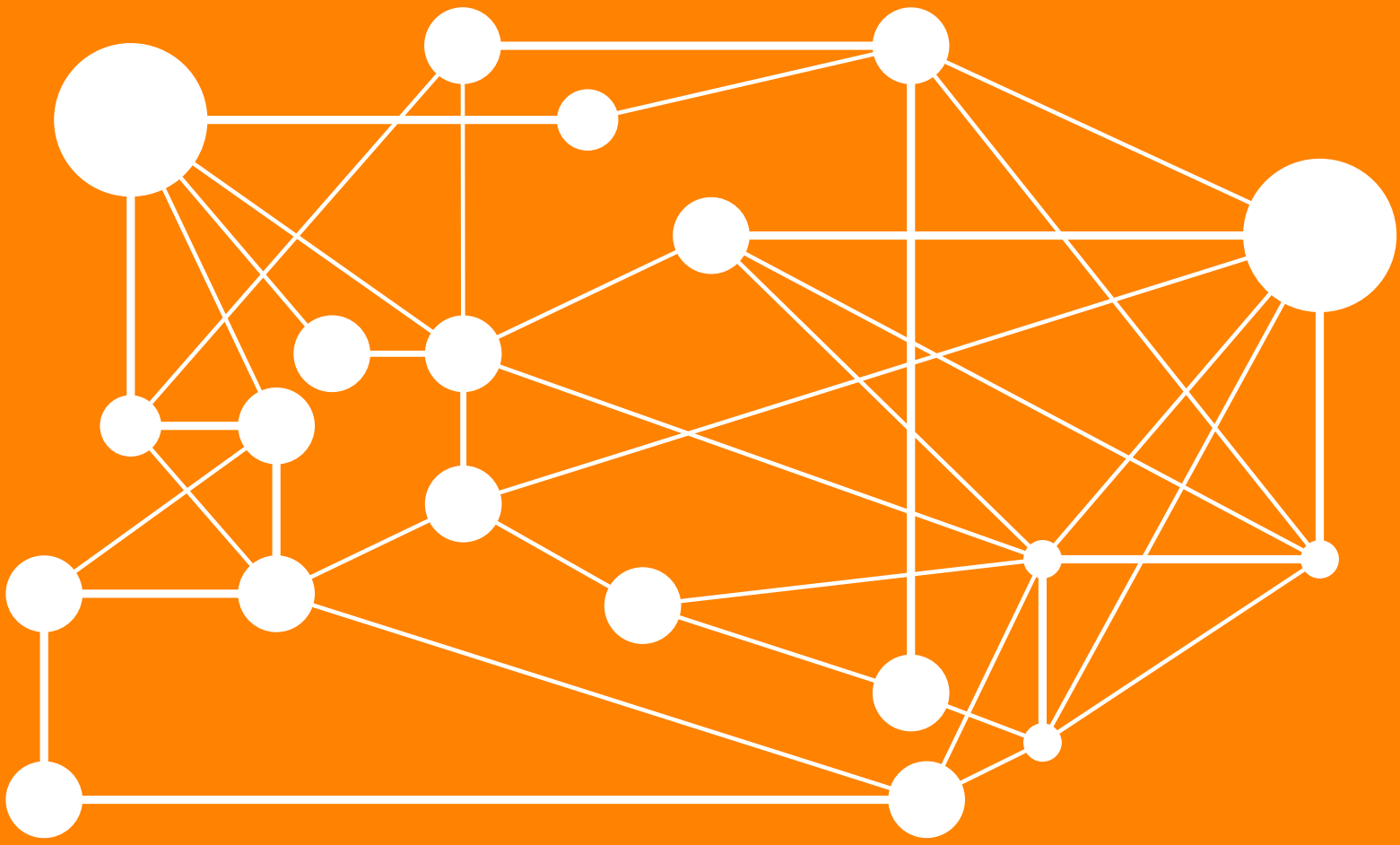
Explore synthesis routes and chemical properties

Reaxys Medicinal Chemistry can be fully integrated with Reaxys, enabling deep exploration of the structures and physicochemical properties of known compounds and providing access to reaction data and synthesis route information. Subscribers to the two solutions can access them through a single, streamlined user interface.

Key benefits

What does Reaxys Medicinal Chemistry enable?

- Confident assessment of compound effects on target proteins
- Quantification of compound and target affinities
- Rapid assessment of large hitsets
- Direct data use without need for normalization
- Excellent overviews of the research environment



Reaxys Medicinal Chemistry

Reaxys Medicinal Chemistry helps customers achieve more efficient hit identification and lead optimization by providing the shortest path to normalized substance–target affinity data and comprehensive pharmacokinetic, efficacy, toxicity, safety and metabolic profiles

LEARN MORE

To request information or a product demonstration, please contact us at elsevier.com/reaxys-medicinal-chemistry.

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