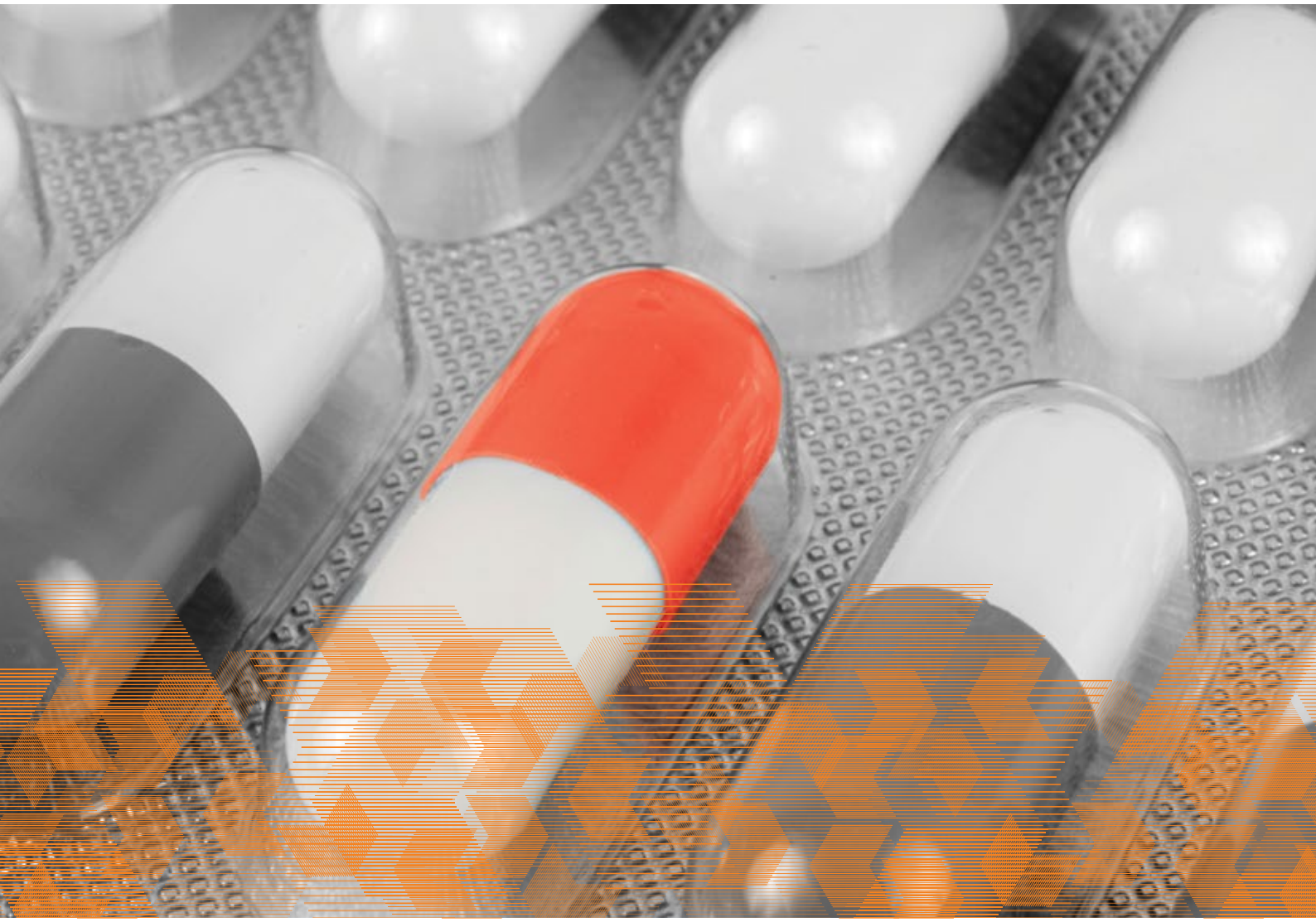
Reaxys® Medicinal Chemistry

Fact Sheet



DATA FOR LEAD IDENTIFICATION AND OPTIMIZATION

Reaxys Medicinal Chemistry empowers early discovery in drug development with access to the world's largest compound bioactivity database. All of the data are normalized to enable accurate compound-target affinity assessments.

ELSEVIER

Reaxys® Medicinal Chemistry

Fact Sheet

Introduction

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

BY DELIVERING ACCURATE EXPERIMENTAL FACTS, REAXYS MEDICINAL CHEMISTRY HELPS TO ANSWER CRITICAL RESEARCH QUESTIONS IN EARLY DRUG DEVELOPMENT:

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

The Reaxys Medicinal Chemistry database contains:

>30.5 MILLION bioactivity data points	**>6.2 MILLION** compounds with bioactivity	**>13,600** total targets	**>9,440** species

This unique collection of data is sourced from:

>108,000 medicinal chemistry patents	**>349,000** medicinal chemistry articles and others	**>5,000** drug discovery and pharma 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, which includes content from third-party databases, is harmonized using Reaxys standards for chemicals, targets and bioactivities. Elsevier life science experts normalize data; map concepts and glossaries; and remove inconsistent data and duplicate citations.

ASK REAXYS

This innovative feature provides an intuitive way to quickly search for bioactivity data and citations. **Ask Reaxys** understands and interprets text (Figure 1) and retrieves specific information in the most relevant form. By bridging the user-friendly input that resembles natural language and the abstract technical language of the database, it makes information more accessible.

Figure 1. Ask Reaxys accepts and interprets text queries

FLEXIBLE SEARCH QUERY CONSTRUCTION

The user interface for Reaxys Medicinal Chemistry provides access to key search query options: **medicinal chemistry, substances** and **literature** (Figure 2). Text input and chemical structure generation are supported and dedicated filters allow users to refine result sets (Figure 3).

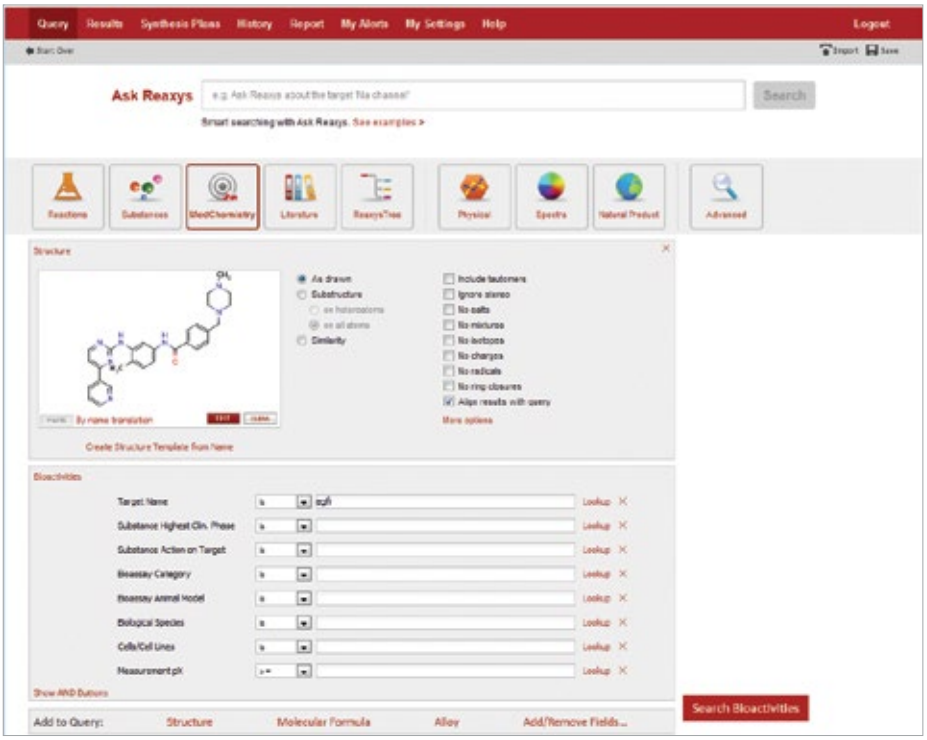


Figure 2. Versatile search queries are constructed via the user-friendly interface

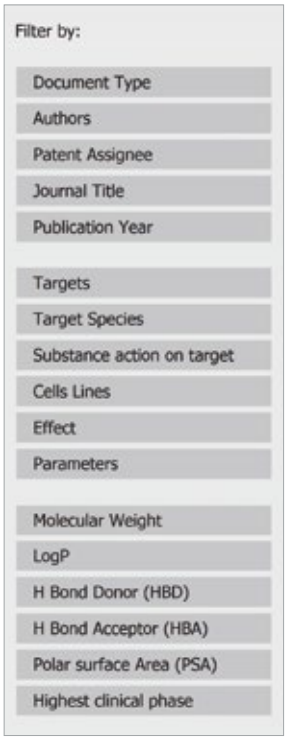


Figure 3. Hitsets can be refined using dedicated filters

EASILY ASSESS COMPOUND INTERACTIONS

Heatmap View (Figure 4) provides a clear overview of the relationships between compounds and their targets in terms of key parameters to enable rapid identification of the most relevant interactions. Its parameter settings are flexible: changing them reveals new relationships between compounds and protein targets or cell lines.

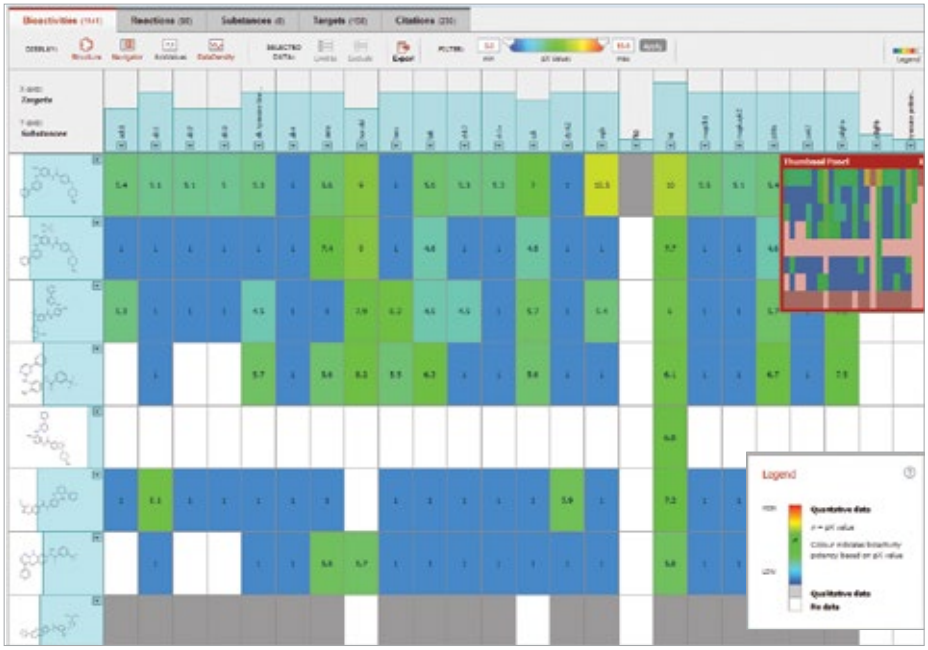


Figure 4. Use Heatmap View to rapidly assess compound–target interactions

QUANTIFY COMPOUND 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 compound–target affinity and comparison of information from all around the world. They are displayed in Heatmap View (Figure 4) for convenient reading.

SHARE DISCOVERIES WITH COLLEAGUES AND EXTERNAL COLLABORATORS

Reaxys Medicinal Chemistry allows **flexible 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** allows flexible information delivery and real-time programming access to the content and system (Figure 5). 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 R&D Solutions Professional Services team stands ready to ensure that Reaxys Medicinal Chemistry can operate seamlessly within an existing environment of tools.

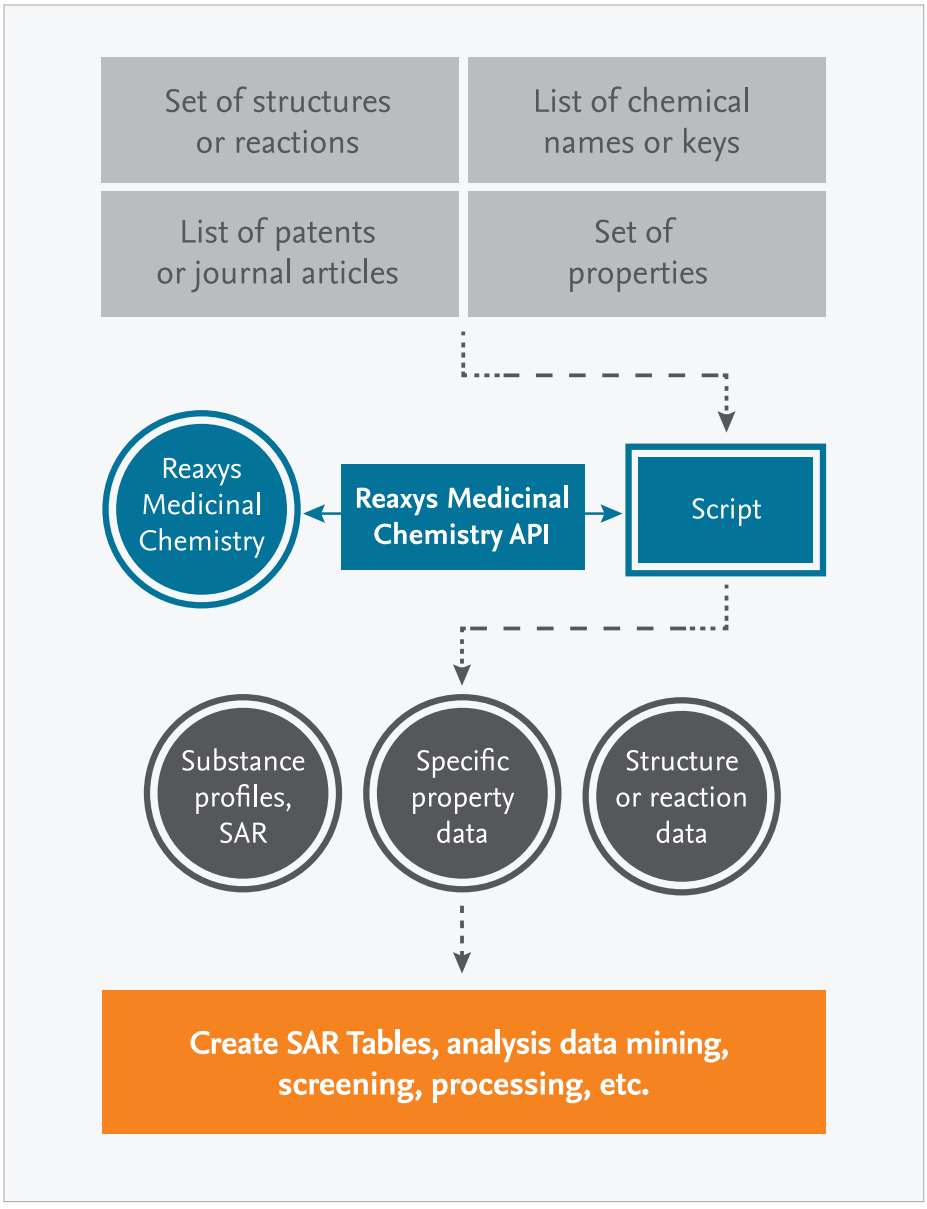


Figure 5. A schematic showing how Reaxys Medicinal Chemistry can be integrated into an existing research workflow via the API.

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.

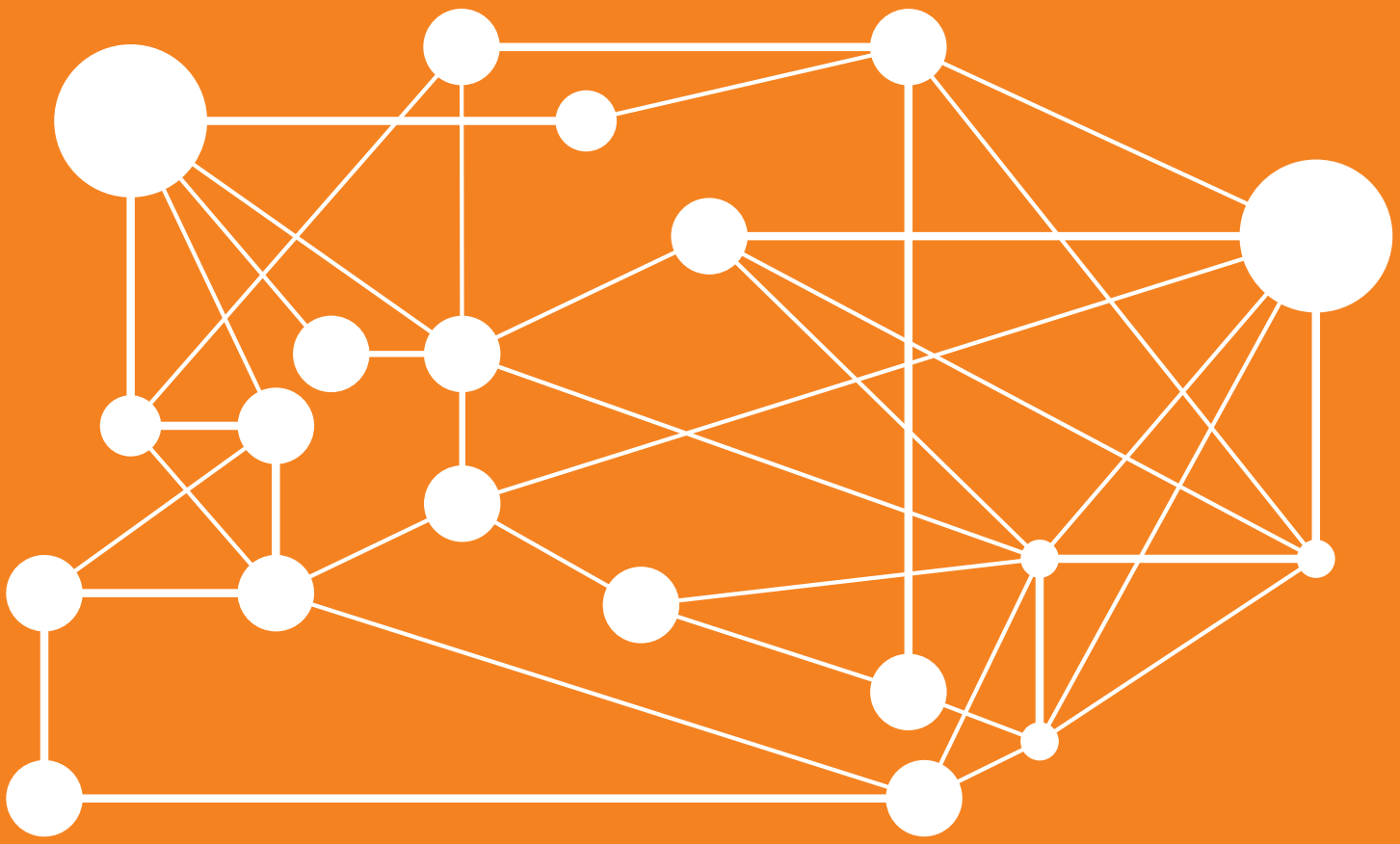
KEY BENEFITS

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

GET STARTED

To learn more about how Reaxys Medicinal Chemistry empowers successful drug development, contact your Elsevier sales representative or visit **elsevier.com/reaxys**



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Visit www.elsevier.com/rd-solutions or contact your nearest Elsevier office.

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