Reaxys

Sygnature Discovery *accelerates target assessment* with Reaxys

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Advancing human progress together

Sygnature Discovery embeds Reaxys into its multidisciplinary workflows to streamline access to bioactivity and target data. This reduces manual searching and *enables faster, more confident recommendations* for first- and best-in-class discovery programs.

Background

Organizations seeking to develop first-in-class novelty or best-in-class therapies face increasing complexity in identifying and prioritizing viable drug targets. Bioactivity data is often dispersed across patents and literature in inconsistent and unstructured formats. With rising pressure to accelerate early drug discovery, research scientists need tools that deliver fast, reliable access to target information, while preserving the scientific nuance and context needed to make confident, data-driven decisions.

"Reaxys automates bringing data together so our scientists can focus on analysis and making more confident decisions."

Colin Sambrook Smith
Director of Computational Sciences and Informatics, Sygnature Discovery

Introduction

Sygnature Discovery is one of the largest integrated drug discovery contract research organizations in the UK and North America with more than 750+ scientists from over 50 countries. It supports a global client base that spans major pharmaceutical companies, biotechs, VC-backed start-ups and non-profits. With no internal drug programs, Sygnature is differentiated by focusing entirely on their customers' priorities, ensuring confidentiality and dedicated expertise. Their interdisciplinary Target Identification and Prioritization Team features members with diverse backgrounds across Bioinformatics, Biosciences, Computational Chemistry and Medicinal Chemistry. This co-located expertise is a major strength of Sygnature, which has a robust history of delivery on standalone and integrated projects through comprehensive drug discovery capabilities. By blending AI-powered workflows with scientific judgment from experts, Sygnature ensures high-confidence and context-aware target recommendations.

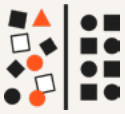
Client projects typically fall into two categories. For some clients, Sygnature generates and refines a long list of potential targets based on a disease area under study. Other clients bring an existing shortlist and rely on Sygnature to assess, rank and recommend targets based on scientific and commercial risk. To continue serving clients' needs effectively, Sygnature sought a solution that could accelerate access to high-quality bioactivity and target data, while ensuring no critical insights were missed.

Sygnature selected Reaxys, Elsevier's chemistry intelligence platform, for its curated patent and chemical structural data, transparent search capabilities and trustworthy excerpted content. Embedded into multidisciplinary workflows, Reaxys is one of a suite of purpose-built solutions that enable Sygnature to accelerate target assessments across the business.

With Reaxys, Sygnature's teams can extract and analyze bioactivity and target data in *days rather than weeks*.

Sygnature's challenges

Supporting first-in-class and best-in-class discovery requires Sygnature to uncover all relevant insights related to a potential target. Meeting this demand posed challenges for multidisciplinary teams to confidently deliver evidence-based recommendations.



Challenge 1: Manual, fragmented access to target and bioactivity data in patents

Effective target identification relies on fast access to a wide range of high-quality data sources, especially when companies are aiming to break new ground or compete in crowded spaces. Retrieving target and bioactivity data manually from multiple sources is a time-consuming process and comes with increased risks.

One of the richest but most complex data sources is patents, where novel chemical structures often appear before being published elsewhere. Chemical compounds are among the most frequently patented inventions, with millions of unique structures documented across global filings. Pharmaceuticals and medical technologies made up 12.6% of all patent families[1] filed between 2010 and 2020 across the five largest IP offices (covering the US, Europe, China, Japan and South Korea). That means more than one in eight patent families was related to pharma or medical technologies.

Alongside the volume of patents is the complexity. Documents are long, often untranslated to English and inconsistently indexed. Many patents list numerous related compounds alongside the one that is relevant to the search and a single character error may lead to chemists investigating the wrong compound. Timely access to patent data is essential for preventing project delays and ensuring teams understand novelty, competitive activity and known liabilities of compounds.

Challenge 2: Time-intensive manual workflows

Target identification requires scientific context, expert interpretation and iterative exploration. Sygnature uses automation to aggregate data but always reserves final judgment for its scientists. Legacy tools sometimes made it challenging to fully understand how search results were generated.

Without visibility into how a search was constructed or the ability to edit and refine it, teams couldn't easily troubleshoot or trust the results. Chemists had to ask follow-up questions or manually trace how a compound was linked to a target. Sygnature sought a tool that would give scientists the ability to build and refine complex queries with confidence and provide an audit trail for search results.

Challenge 3: Aligning complex query searches with multidisciplinary teams

Sygnature's drug discovery model brings together medicinal chemists, DMPK specialists, bioscientists and computational experts to assess and prioritize targets. Discrepancies in search terms, structure queries or synonym coverage could result in different teams working from different baselines.

To support streamlined decision-making, Sygnature sourced a platform that enabled all users to execute the same complex queries with shared visibility and traceability.

[1] Nicola Grassano, Robert M'Barek, Trends in Patents in Life Sciences: focus on Pharmaceuticals and Medical Technologies, JRC Publications Repository, European Commission, 2025, https://publications.jrc.ec.europa.eu/repository/handle/JRC142609

"Reaxys gives us the ability to query and download structures, link them to bioactivity data, and explore structure-activity relationships. With this scientific data, combined with curated patent information and translations across languages, Reaxys gives us confidence we won't miss critical insights."

Dr Christine Richardson
Principal Scientist, Sygnature Discovery

Solution

With Reaxys, Sygnature accelerates access to critical data while giving its scientists full control over how data is searched, interpreted and applied.

Why Sygnature selected Reaxys

- Curated bioactivity and target data, from literature and patents
- Breadth of patent coverage and automated translation of patent title, abstract and claims into English
- Excerpted content, no need to read full documents to find key data
- Transparent, editable querying with full visibility into search logic
- Ability to combine structure- and text-based searches
- Fast export of data into SD files for downstream analysis
- Secure access and behind firewall search, supporting client confidentiality
- User-friendly and intuitive interface
- Flexibility to add in-house data from clients

Using Reaxys, chemists can build complex queries across bioactivity, target and patent data, with full visibility into how each search is constructed. Rather than relying on time-consuming manual methods, teams can review and refine each step, ensuring results align with evolving project needs and enabling reproducible workflows across teams.

Equally valuable has been Reaxys' structure-based search, which connects chemical compounds to relevant publications, reaction data and more than 47 million indexed patents from 105 patent offices.

"In Reaxys, each biological target is mapped to its broader family and all known synonyms. This helps our scientists identify the right entity even when naming conventions differ. We've found that some targets are referenced under many different aliases, so Reaxys' depth of indexing has been essential to ensuring completeness and avoiding missed data at the earliest stage of discovery," adds Dr Richardson.

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Dr Christine Richardson
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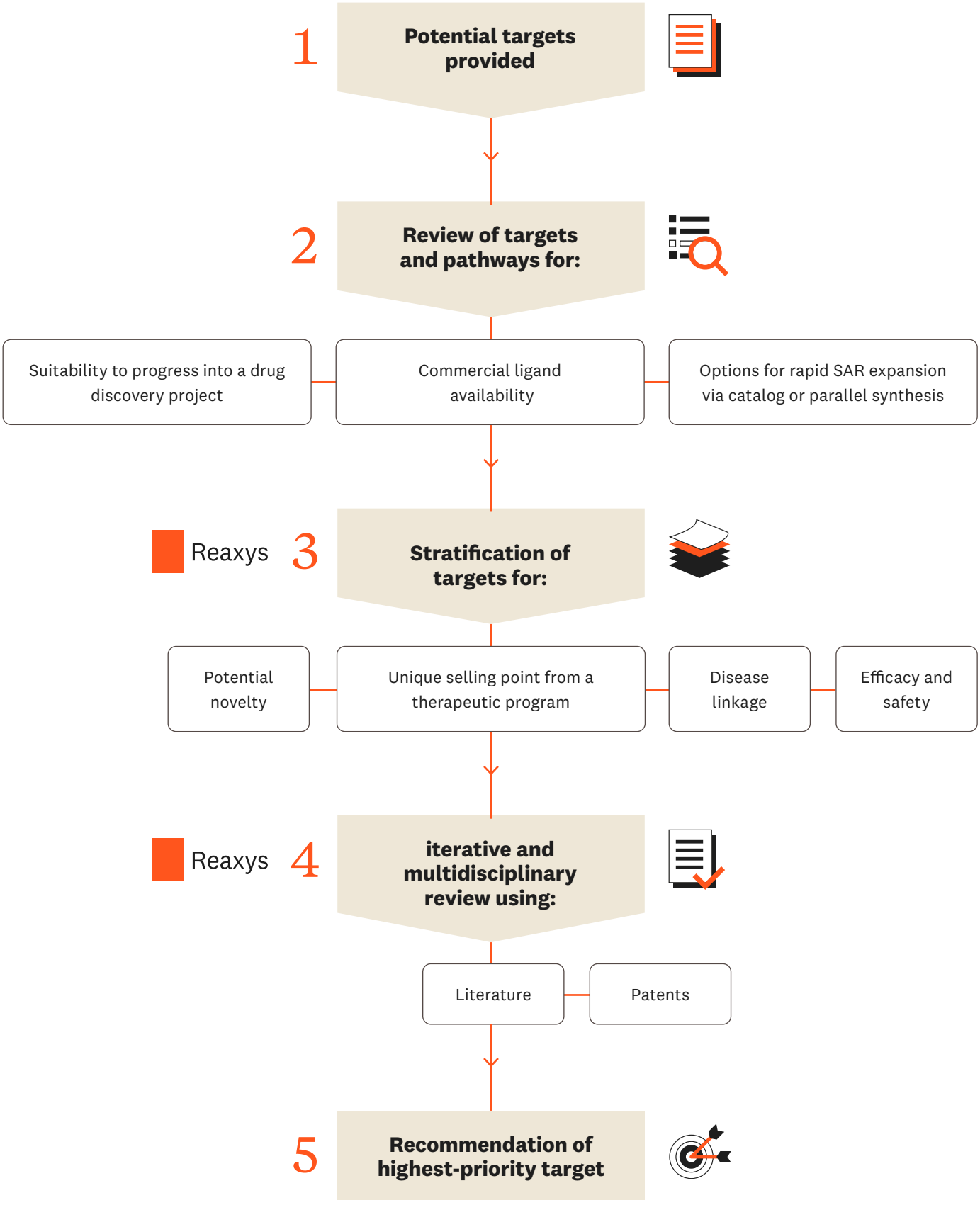
Target prioritization project

The value of Reaxys was clear during a target prioritization project for a US biotech company.



Impact for Sygnature

By embedding Reaxys into its cross-functional, semi-automated workflows, Sygnature can access curated bioactivity and target data in seconds and explore competitive IP with confidence. Reaxys supports target identification and prioritization for more than 400 users at Sygnature, including bioscience, DMPK, chemistry, and computational teams. Scientists report more confident decisions, driven by Reaxys' transparency, curated data, and cross-disciplinary usability.

"By replacing time-intensive manual workflows with intelligent search and data integration, Reaxys has reduced the burden on our expert reviewers, freeing up their time for strategic analysis," concludes Dr Richardson.

Optimize chemistry research with Reaxys, a comprehensive chemistry database delivering critical insights from over a billion trusted data points combined with innovative technology.

Reaxys helps chemists easily explore chemical, bioactivity and toxicity data from literature and patents, so you can accelerate synthesis planning, competitive analysis and the DMTA cycle.

Learn more about Reaxys elsevier.com/reaxys

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