ARTICLE

Enabling Data-Based Decision-Making for Successful Drug Development

FROM MORE DATA TO INCREASED SUCCESS

How does Elsevier ensure that the data available through its research solutions is of sufficiently high quality and easily discoverable? Using the example of Reaxys® Medicinal Chemistry, which is focused on answers needed for critical decisions in early drug discovery, we look at how providing high-quality information by curating, normalizing and integrating data impacts R&D productivity.

ELSEVIER

Elsevier has put considerable effort into ensuring that Reaxys Medicinal Chemistry meets the bioactivity data needs of the pharma industry.

"The goal of Reaxys Medicinal Chemistry is to facilitate the development of 'smarter leads' – leads with optimal affinity, selectivity and ADMET properties; leads that will not fail in preclinical and clinical phases for reasons that could have been predicted. This requires access to data that must be laboriously extracted by hand from the overwhelmingly large body of published literature. For that, we have established a methodical and unrivalled production process."

– Dr. Olivier Barberan,

Product Manager for Reaxys Medicinal Chemistry

The recent exponential growth of chemical and biological data enabled by new technology has not given the promised significant impact on pharmaceutical productivity. The issue is that a wealth of information alone cannot improve decision-making in drug discovery or increase productivity and success. If the data does not come in well-organized infrastructure that makes it easily accessible, it can even slow the research process down.

In the development of all its R&D Solutions for Pharma & Life Sciences, Elsevier's aim is to increase information discoverability so that researchers can quickly find the information they need for critical decisions and move back into the lab. Data is carefully curated and deeply indexed and provided through user-friendly interfaces that allow searches for specific data as well as original literature. Since early discovery is a particularly important phase for success in drug development, considerable effort goes into ensuring that Reaxys Medicinal Chemistry meets the bioactivity data requirements of the pharmaceutical industry.

IMPROVING DISCOVERABILITY

Reaxys Medicinal Chemistry is a tool that lets scientists easily convert large amounts of information into a thorough understanding of drug candidates, targets, mechanisms, and safety concerns, and make good decisions based on this understanding. It includes data on affinity, potency, specificity, synthesis, pharmacokinetics, toxicity, off-target activity, metabolism, transport and more. To ensure that the data does not overwhelm researchers and slow their progress, each piece of information undergoes four stages of careful curation (Figure 1).

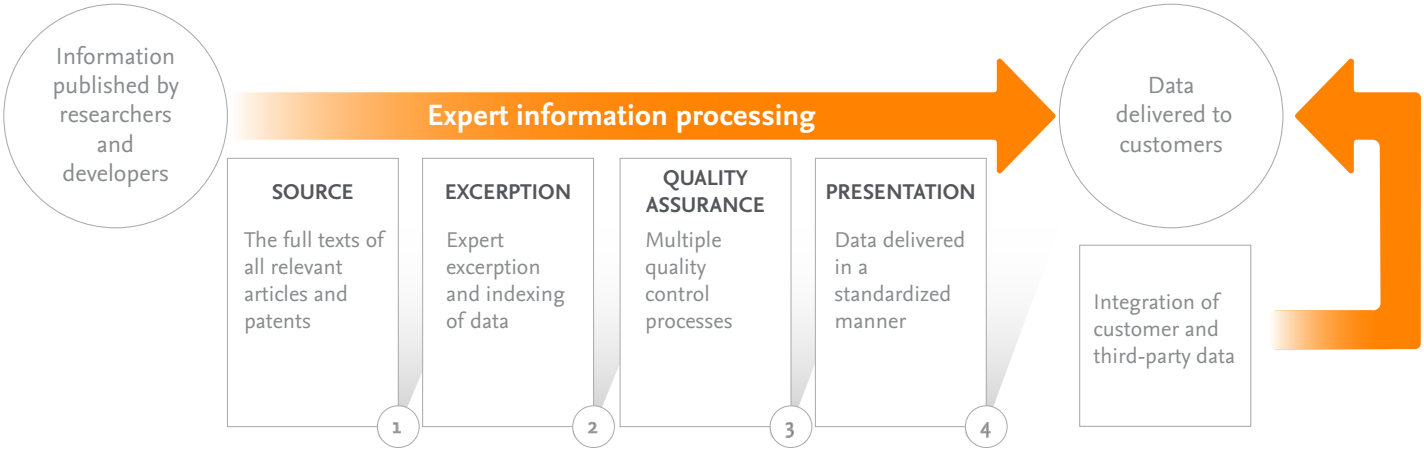


Figure 1. Four pillars in the production process contribute to the value of data in Reaxys Medicinal Chemistry. The resulting high-quality information can be integrated with researchers' own data to enable search and assessment of all available content in a single environment.

PILLAR 1: THE MOST COMPREHENSIVE SOURCE OF HIGH-QUALITY BIOACTIVITY DATA

Reaxys Medicinal Chemistry provides a comprehensive overview of all small-molecule bioactivity, regardless of where the data were published.

Sources for core data

A text-mining and ranking process identifies documents likely to contain extractable data from the entire Embase® literature collection and from all patent classes from the USPTO, WIPO and EPO. Roughly 800,000 articles along with 800,000 to 1 million patents are evaluated each year for inclusion, with approximately 2,000 full-text publications selected for excerption each month. The database currently includes over 31.7 million bioactivity datapoints pertaining to over 6.2 million compounds.

PILLAR 2. EXCERPTED DATA ORGANIZED FOR QUICK RETRIEVAL

The excerpted data are presented clearly and concisely as extracted experimental facts, so scientists can quickly assess the relevance and use the information to move their projects forward. Searching for buried information in original publications is inefficient, especially when the documents might not be pertinent to the query. Excerption adds high value to the content and lets the information be immediately used to support informed decision-making.

Users can quickly retrieve such highly relevant results because the content is structured within a comprehensive classification system. The concepts and terms for indexing are organized in hierarchical taxonomies that accommodate the high level of data granularity and connect in ways that reflect the current knowledge. The indexing is regularly revised to ensure it develops in tune with pharmaceutical industry needs.

PILLAR 3. SUPERIOR QUALITY ASSURANCE

A series of quality assurance checks guarantee that the data are accurate and that the database functions properly. They include inspection of samples of the data to confirm that data points are precise and that no data was missed. Prior to publishing, over 4,000 automatic queries make sure that the new data do not conflict with the database architecture or performance, and extensive manual queries assess retrieval speed, results and correct functionality.

PILLAR 4. EASILY ACCESSIBLE INFORMATION READY FOR USE

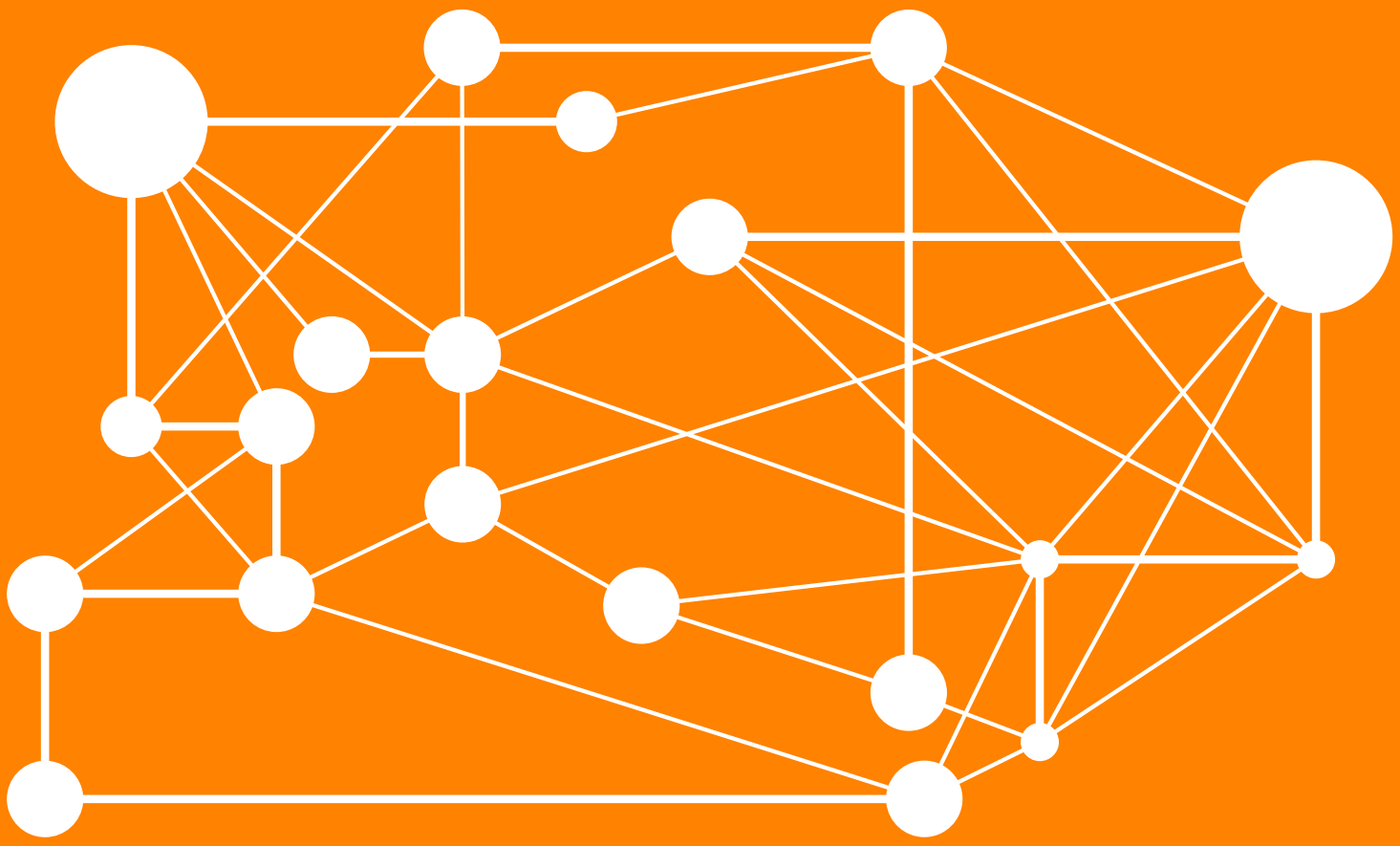
In early drug development, it is critical to know how the affinity of one drug structure for a target compares with that of another. Thanks to the standardized and normalized data in Reaxys Medicinal Chemistry, experimental results from multiple sources can be meaningfully compared.

Normalization reduces the data to a common form and organizes them to minimize redundancy. Standardization places the data on comparable scales to equalize parameter range and data variability for each bioactivity parameter. Thus, data are directly useful as input for any type of analysis, including in silico structural or statistical modeling and analysis in external data analysis platforms.

THE SINGLE SOURCE FOR MEANINGFUL BIOACTIVITY DATA

Reaxys Medicinal Chemistry aims to be the single source for the most detailed and high-quality data on small molecules that are relevant and meaningful to early drug development. The ease with which users can access and use this information equips them to make well-informed decisions quickly and early and avoid going too far down the wrong research path, thus advancing projects and increasing success.

Thanks to its Application Programming Interface, Reaxys Medicinal Chemistry can be fully integrated into an existing environment of data, tools and processes. This means that researchers can assess their own experimental results together with our high-quality, curated data using a single search interface as well as tools like Pipeline Pilot and KNIME. Such integration supports faster identification of essential data for critical decisions and facilitates a comprehensive range of in silico profiling applications.



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