Chemistry & Bioactivity data from Reaxys®

Chemical structure, reaction, and bioactivity data that has been experimentally validated

Example use cases

- Integrate trusted chemistry data into custom applications and third-party tools
- Support customized reporting and alerting within internal search tools
- Search for implementations of items based on individual properties
- Build, train, validate and optimize models for predictive retrosynthesis, synthetic feasibility, reaction conditions, reaction optimization and more
- Create a graph database of reaction paths
- Perform protein-ligand binding QSAR
- Assemble reference data for FEP calculations
- Facilitate SEA models
- Conduct polypharmacology analytics
- Undertake chemical structure analytics
- Create reporting dashboards with different views of Reaxys data
- Combine Reaxys data with business analytics to prioritize projects
- Augment internal datastores and fortify knowledge graphs with Reaxys data

Improve chemical R&D productivity with expertly curated structure, property and reaction data, experimental procedures and chemistry literature. Reaxys empowers hit identification and lead optimization with normalized substance-target affinity data and pharmacokinetic, efficacy, toxicity, safety and metabolic profiles.

The data set currently encompasses:

- 179+ million substances
- 57+ million reactions
- 86+ million documents
- 41+ million bioactivities
- 32+ thousand unique targets
- 54+ thousand species

Up-to-date counts for substances appear on the reaxys.com homepage, along with details of the latest update.

Chemists curate this chemistry knowledge from:

- 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
- 105 patent offices and 170 IPC classes.
- 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.

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Reaxys®

Available data sets

We offer any one, or more, of the following options:

All Reaxys data files via API:

- Direct access to Reaxys content
- Knime nodes and Pipeline Pilot nodes (generic and PSG versions) with example workflows and documentation
- Simple Python SDK and examples
- Documentation of Reaxys database fields and technical API manual
- Structure search supports MDL format

Reaction Data Flat File:

- 20 million organic and organometallic, single-step, full reactions
- Conditions (reagent, catalyst, solvent chemical names, temperature, duration, pressure, etc.), description of experimental procedure, yields
- Associated references
- Chemical structures for reactants and products in MDL format
- Documentation

Bioactivity Data Flat file:

- 7 million substances with associated bioactivities
- Chemical structures in MDL format
- Fact availability list
- Bioactivity data points, target information, assay information
- Associated references
- Documentation

Structure Data Flat file:

- 34 million substances
- Chemical structures in MDL format
- Fact availability list
- Associated references for patents only (patent numbers, year, kind code, family members)
- Documentation

Reaxys data files are delivered by API

Programmatic access using a programming language or KNIME and Pipeline Pilot nodes.

Reactions data via flat file

- Delivered via AWS S3 as files in RDF and UDM format (XML)

Bioactivity data via flat file

- Delivered via AWS S3 as files in SDF and OpenPHACTS format (XML)

Structure data via flat file

- Delivered via AWS S3 as files in SDF and Reaxys XML format

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