

BIOVIA BIOACTIVITY DATABASES

Datasheet

BIOVIA Bioactivity Databases accelerate scientific research by delivering insight into druggability and intelligence on investigational drugs. By providing easy access to integrated, cross-referenced data from multiple sources, BIOVIA enables you to search and explore comprehensive information, when and how you want, in the context of your laboratory workflows - saving time, reducing costs, and enhancing decision confidence.

BIOVIA MDDR

MDDR contains over 260,000 biologically relevant compounds and well-defined derivatives. Updates add about 10,000 substances a year to the database. MDDR, jointly produced by BIOVIA and Clarivate Analytics, covers patent literature, journals, meetings, and congresses.

Medicinal chemists, pharmacologists, and molecular modelers use the database to create SAR tables (matching chemical structure to pharmacological effect) and find competitive information about compounds similar to their lead compounds.

- MDDR provides:
- Chemical structure
- Calculated properties based on chemical structure
- 3D models
- Compound name – trademarks and company codes
- CAS registry number
- Biological activity based on the Prous classification system
- Description of therapeutic action containing ED50, LD50, inhibition values, etc.
- Patent information including patent number, title, source, priority number and inventors' names
- Literature references hyperlinked to primary literature (full text, abstracts, patents, conference proceedings, etc.)
- Company codes, generic names, trade names and trademark names
- Originating company
- Development phase in the R&D process

BIOVIA COMPREHENSIVE MEDICINAL CHEMISTRY (CMC)

CMC helps medicinal chemists, pharmacologists, and molecular modelers validate new pharmacophores, plan combinatorial libraries, develop and corroborate structure-based calculators and predictors, and perform structure-activity relationship (SAR) analyses.

CMC provides:

- 2D and 3D chemical structures
- Biological activity
- Drug class
- pKa
- Calculated logP and Measured logP (CMC on BIOVIA DiscoveryGate has calculated logP values only)
- Calculated compound-based properties (with CMC Finder)
- Generic name
- CAS registry number
- Originating company
- Literature references

BIOVIA TOXICITY

Toxicity Database includes the contents of the Registry of Toxic Effects of Chemical Substances (RTECS) database, the GENE-TOX database (US Environmental Protection Agency) and the Chemical Carcinogenesis Research Information System database (National Cancer Institute).

The structure-searchable bioactivity database of toxic chemical substances contains data from in vivo and in vitro studies of:

- Acute toxicity
- Mutagenicity
- Tumorigenicity and carcinogenicity
- Skin and eye irritation
- Reproductive effects
- Multiple dose effects

Scientists from a variety of disciplines use the database:

- Toxicologists at pharmaceutical and chemical companies
- Drug Safety scientists, both discovery and preclinical development
- Drug metabolism and pharmacokinetics (DMPK) scientists
- Medicinal chemists
- Clinical toxicologists
- Safety officers in pharmaceutical companies – especially in synthesis scale up and production facilities

The Registry of Toxic Effects of Chemical Substances (RTECS) Database

The Registry of Toxic Effects of Chemical Substances (RTECS®) database is a comprehensive collection of basic toxicity information for over 160,000 compounds including: prescription and non-prescription drugs, food additives, pesticides, fungicides, herbicides, solvents, diluents, chemical wastes, reaction products of chemical waste and substances used in industrial and household situations.

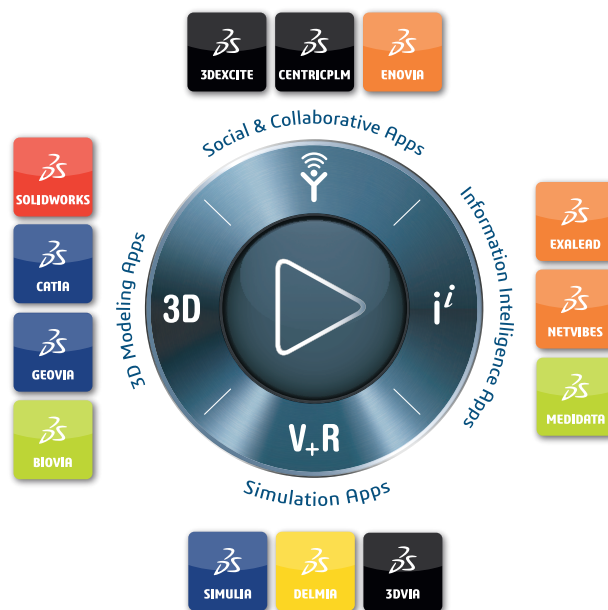
Originally built and maintained by the National Institute of Occupational Safety and Health (NIOSH) in 1971, BIOVIA now produces the RTECS files using existing data selection criteria and rules they established. The database covers six categories of toxicity data—acute toxicity, tumorigenicity, mutagenicity, skin and eye irritation, reproductive effects and multiple dose effects.

As well as being available from BIOVIA, RTECS is also offered for purchase by several value-added resellers including:

- Atrion International, Inc.
- Canadian Center for Occupational Health and Safety
- ChemADVISOR, Inc.
- Chemical Abstracts Service (CAS)
- ChemSoft Limited
- Personal Care Products Council (PCPC)
- DIALOG
- Expert Publishing, LLC.
- Leadscope, Inc.
- SiteHawk
- RightAnswer
- Wolters Kluwer (Croner)
- Decernis
- Environmental Working Group

Our 3DEXPERIENCE® Platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the 3DEXPERIENCE® Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes' collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 250,000 customers of all sizes in all industries in more than 140 countries. For more information, visit www.3ds.com.



©2020 Dassault Systèmes. All rights reserved. 3DEXPERIENCE®, the Compass icon, the 3DS logo, CATIA, BIOVIA, GEOVIA, SOLIDWORKS, 3DVIA, ENOVIA, EXALEAD, NETVIBES, MEDIDATA, CENTRIC PLM, 3DEXCITE, SIMULIA, DELMIA, and FVAE are commercial trademarks or registered trademarks of Dassault Systèmes, a French "société européenne" (Versailles Commercial Register # B 322 306 440), or its subsidiaries in the United States and/or other countries. All other trademarks are owned by their respective owners. Use of any Dassault Systèmes or its subsidiaries trademarks is subject to their express written approval.