BIOVIA

3DEXPERIENCE®

BIOVIA DIRECT

Datasheet

The BIOVIA Direct chemistry data cartridge enables researchers to register, search and retrieve molecules, reactions and chemically modified biomolecules in a fully integrated, relational Oracle® environment and on AWS hosted environments using Oracle®, including Amazon RDS Custom. It combines industry-proven BIOVIA chemistry capabilities with fast search indexes that provides the best overall performance and scalability for structure and reaction queries and registration. BIOVIA Direct, BIOVIA Pipeline Pilot and the **3D**EXPERIENCE® platform use the same chemistry engine delivering harmonized results regardless of the workflow – The Same Chemistry Everywhere.

DASSAULT SYSTEMES

COMPREHENSIVE CHEMICAL STORAGE

- Small molecule drug-like structures
- Reactions including reagent information, atom numbering and reaction bond role
- Chemically modified biomolecules (CMB), including:
  - Biologics e.g., antibody-drug conjugates (ADCs)
  - Peptides and recombinant proteins
  - Oligonucleotides
  - Formats for CMBs include:
    - Full chemistry
    - Biopolymer (including expanded/contracted residues)
    - Self-Contained Sequence Representation (SCSR), a highly compressible version of the molfile format that contains all the sequence information needed to transport across systems
- Polymers
- Mixtures and formulations
- R groups / Markush
- Stereochemistry and enhanced stereochemistry (ABS, OR, AND) for:
  - Tetrahedral: carbon, nitrogen, sulphur and phosphorus
  - Axial stereochemistry
    - Allene
    - Atropisomer/biaryl systems
  - Cis/trans double bonds
  - Higher order: trigonal bipyramidal, square planar, octahedral (stereochemistry only)
- Other bond types
  - Organometallic/haptic bond (dative and coordination)
  - Hydrogen bonds
  - Variable attachment (aka Markush bonds)
  - Homology groups (for example, includes HAC- heteroaromatic, ARY- aromatic all carbon)

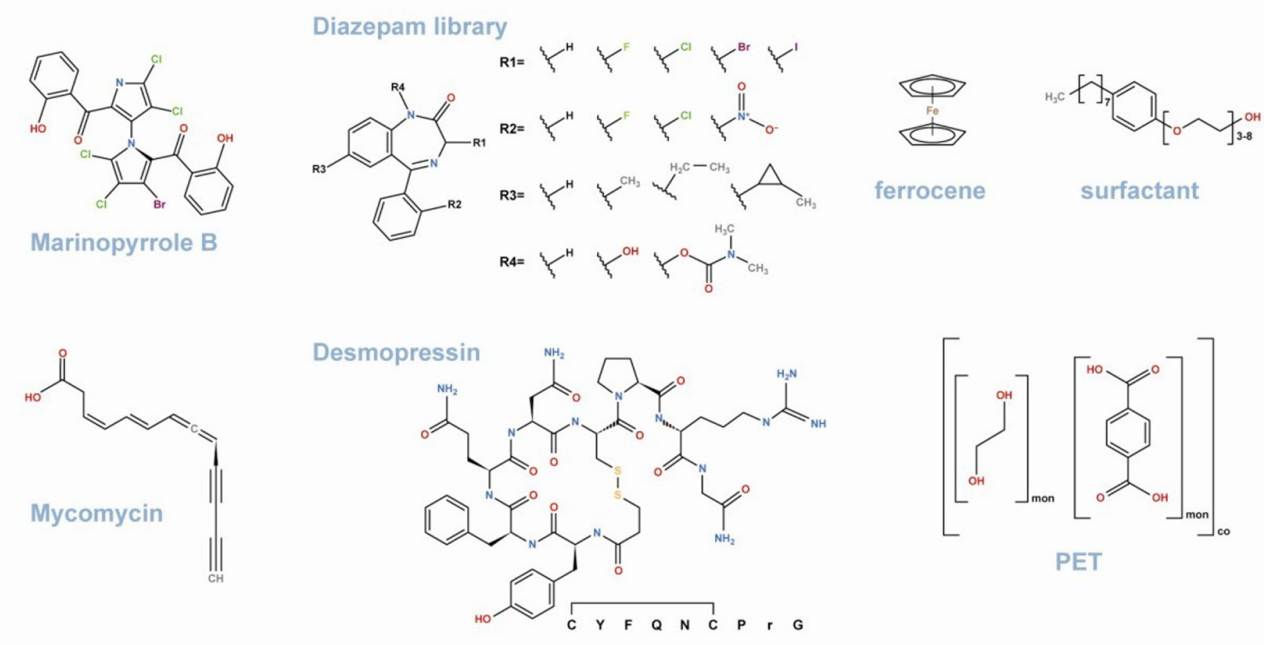


Figure 1. Examples of the many chemical representation styles supported by BIOVIA Direct

PREMIERE CHEMISTRY SEARCHING

- Molecule and Reaction
  - SSS - Substructure search with the option to:
    - Ignore stereochemistry
    - Include tautomers (molecule only)
    - Ignore pi-system charges (haptic bonded systems)
  - Exact search
  - Flexmatch (including numerous parameters to ignore/ include mixtures, tautomers, stereochemistry and more)
  - SIM – similarity search
  - FMLA (molecular formula searching syntax)
  - Query atoms (A, Q, X, M, R, Rx Z), as well as atom lists (for example; in N, C, O, also NOT N, C, O)
  - Query bonds (any, aromatic, single/double and many more)
- Reaction only
  - Reaction bond role (make bond, break bond, reacting center etc.)
  - Atom mapping in reactions
- Chemically modified biomolecules
  - Cyclic peptides (-C-A-L- same as -L-A-C-)
  - Search with any format (full chemistry, biopolymer, SCSR) and retrieve your expected results (requires the Direct Admin to enable this advanced indexing capability)
  - Sequence text, search for natural residues in your CMBs (can be combined with chemistry or sequence features)
  - Include/exclude phosphate (RNA/DNA searches)

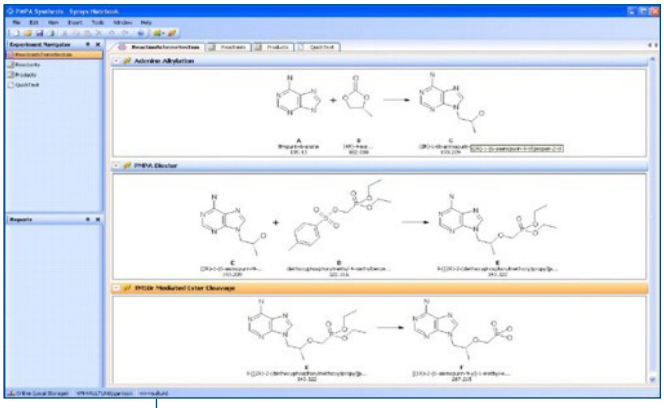


Figure 2. The BIOVIA Direct chemistry engine powers the multidisciplinary BIOVIA Workbook, BIOVIA Notebook, BIOVIA Chemical and Biological Registration and BIOVIA Insight.

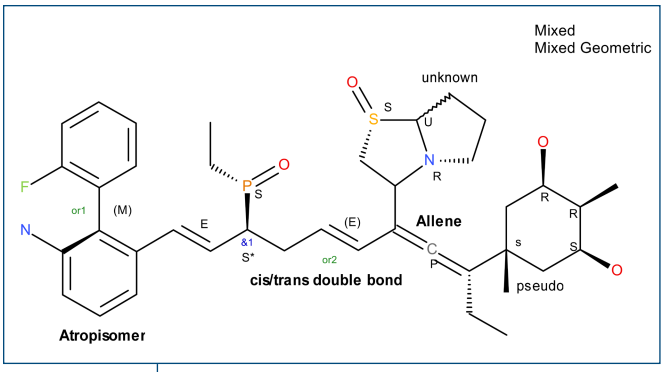


Figure 3. Comprehensive stereo and enhanced stereochemistry support.

SUPPORT FOR INDUSTRY-STANDARD FORMATS

- One cartridge for both molecules and reactions
- SDfiles and RDfiles
- Molfiles and rxnfiles
- Chimestrings
- Canonical SMILES strings
- InChI and RInChI
- NEMA key
- Hierarchical editing language for macromolecules (HELM) string and XHELM
- Monoisotopic formula masses
- Formula masses for isotopically enriched structures
- UniProt for sequences
- Can index small molecules and CMBs in the same data source
- Reaction and molecule fast search index, speeds searching, especially for large databases (100M's of records)
- 24/7 operation
- Tested and proven with databases containing over 17 million reactions and over 2 billion structures
- Direct can be installed and run on AWS hosted environments using Oracle®, including Amazon RDS Custom
- Oracle partitioning: partition domain indexing for larger databases and partitioning of large tables to improve search speeds
- Direct boost files (faster I/O) and multi-threading support (more CPU) improves performance

EMBEDDED IN ORACLE TECHNOLOGY

BIOVIA Direct makes chemical databases accessible to researchers and developers working directly with standard Oracle SQL syntax. With this technology, scientists can manage fully relational molecule structure and reaction databases while integrating other enterprise data in an open, flexible Oracle environment. For example, one of the advantages of Oracle technology is the ability to include multiple domain indexes in tables. The system is not constrained by arbitrary limits and supports multiple molecule/reaction tables with as many molecule/reaction columns as needed.

EASY DATA INTEGRATION

Open integration enables developers to use standard relational database development tools from Oracle, Microsoft and other vendors. Developers can also use industry-standard database connection tools including Open Database Connectivity (ODBC), Java® Database Connectivity (JDBC) or SQL*Net® for reaction and chemical structure searching.

FLEXIBLE APPLICATION DEVELOPMENT

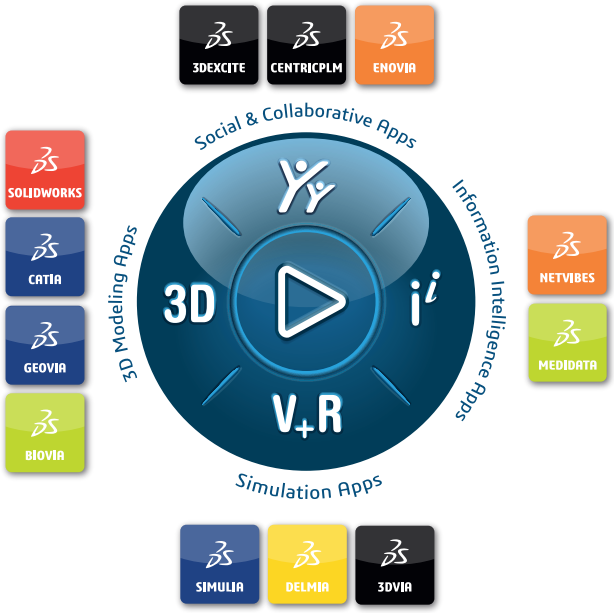
BIOVIA Direct powers cheminformatics applications that manage structures, chemically modified biomolecules and chemical reactions using industry standard BIOVIA Pipeline Pilot, Java®, Visual Basic®, NET® and C++ development environments. Because it is data model independent, the cartridge permits exceptional flexibility in the design of applications and the management of proprietary reaction and molecule information.

LEARN MORE

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

Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit **www.3ds.com**.



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