DASSAULT SYSTEMES

BIOVIA

BIOVIA DIRECT

Datasheet

The BIOVIA Direct chemistry data cartridge enables researchers to register, search and retrieve molecules and reactions in a fully integrated, relational Oracle® environment—combining industry-proven BIOVIA chemistry capabilities with fast search indexes that provide the best overall performance and scalability for structure and reaction queries and registration. BIOVIA Direct and BIOVIA Pipeline Pilot use the same chemistry engine delivering harmonized results regardless of the workflow – The Same Chemistry Everywhere.

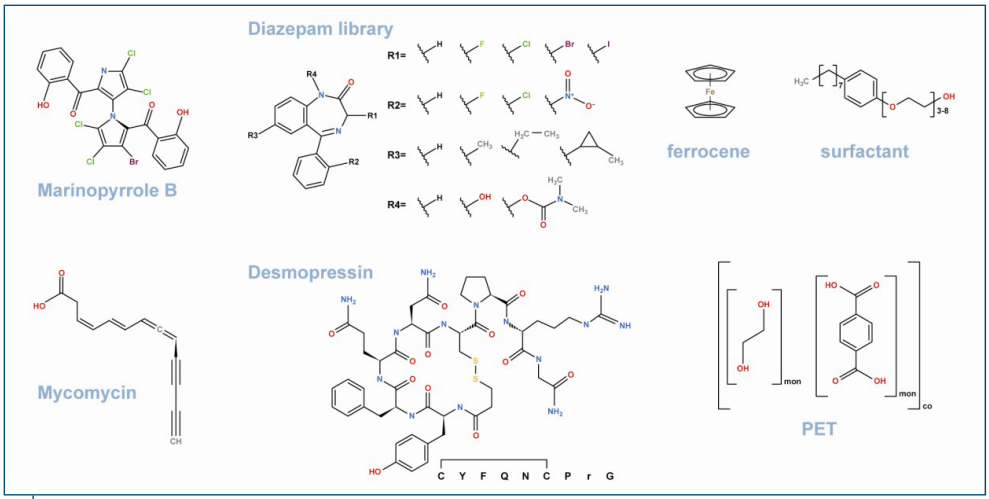

Figure 1: Examples of the many chemical representation styles supported by BIOVIA Direct

PREMIERE CHEMISTRY SEARCHING

- Markush (generic) structure registration and searching
- Markush homology group searching
- Non-Specific structure (NONS) registration and Searching
- Registration and searching of organometallics with haptic bonding, and structures with hydrogen bonding
- Option to search Organometallics ignoring pi-system charges
- Flexmatch for exact-match, stereochemistry, tautomer, isomer and salt searches
- Similarity searches, including searches for smaller and larger compounds
- Molecular weight, formula, Rgroup, Sgroup, polymer and mixture queries
- Extensive query tuning to enable focused hit sets
- Enhanced stereochemistry for structures and queries
- Non-tetrahedral stereochemistry support for allenes and biphenyls, and two-ring systems in general
- Storage and retrieval of chemically modified sequences - antibody-drug-conjugates, peptides, oligonucleotides, and oligosaccharides

SUPPORT FOR INDUSTRY-STANDARD FORMATS

- SDfiles and RDfiles (including other RDF formats)
- Canonical SMILES strings
- Chimestrings, molfiles, and rxnfiles
- InChI names and keys including "Enhanced Stereochemistry" naming
- NEMA key
- Hierarchical Editing Language for Macromolecules (HELM) String and XHELM
- Monoisotopic formula masses
- Formula masses for isotopically enriched structures
- UniProt for sequences
- One cartridge for both molecules and reactions
- Reaction and molecule fast search index speeds searching, especially for large databases
- 24/7 operation
- Tested and proven with databases containing over 17 million reactions and over 69 million structures
- Oracle Partitioning: Partition Domain Indexing for larger databases and partitioning of large tables.
- Direct boost files (faster I/O) and Multi-threading support (more CPU)

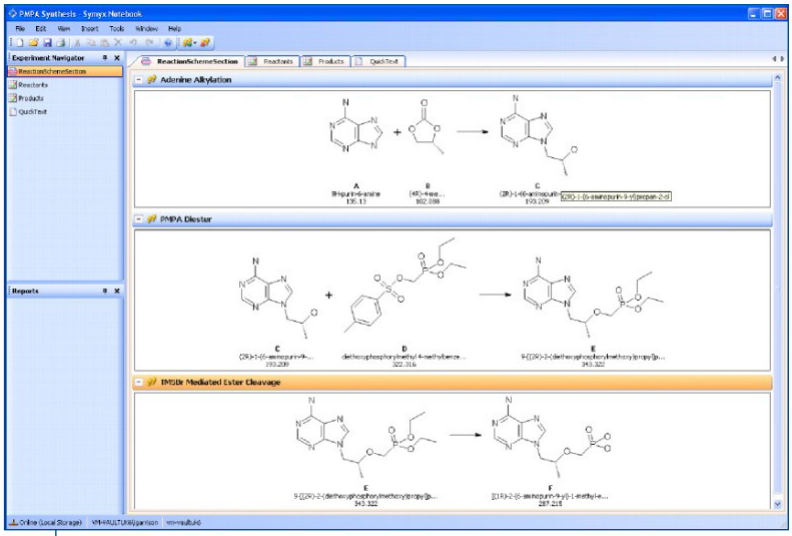

Figure 2: The BIOVIA Direct chemistry engine powers the multidisciplinary BIOVIA Workbook, BIOVIA Notebook and BIOVIA Insight.

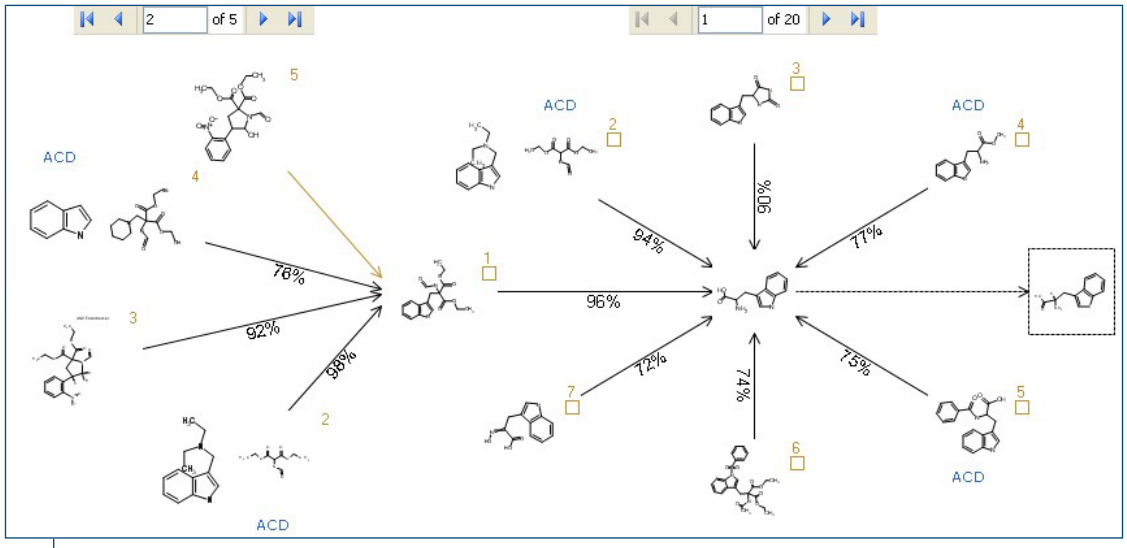

Figure 3: The performance of BIOVIA Direct enables the construction of reaction plans in seconds and provides availability information on each structure.

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 ActiveX® Data Objects (ADO), 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 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.

ISIS-TO-BIOVIA DIRECT MIGRATION

BIOVIA Direct is compatible with the ISIS system. R&D organizations working with legacy ISIS molecule databases can upgrade these databases to BIOVIA Direct and continue to access them through their existing ISIS/Host applications as they pursue a phased upgrade path from ISIS to BIOVIA Direct. BIOVIA Direct also enables ISIS customers to take advantage of advances in BIOVIA chemical representation, stereochemistry and chemical Fastsearch capabilities.

To learn more about BIOVIA Direct, go to 3dsbiovia.com/BIOVIA-direct

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