

# Symyx Direct Cheminformatics

The Symyx Direct chemistry data cartridge enables researchers to register, search and retrieve molecules and reactions in a fully integrated, relational Oracle® environment—combining industry-proven Symyx chemistry capabilities with fast search indexes that provide the best overall performance and scalability for structure and reaction queries and registration.

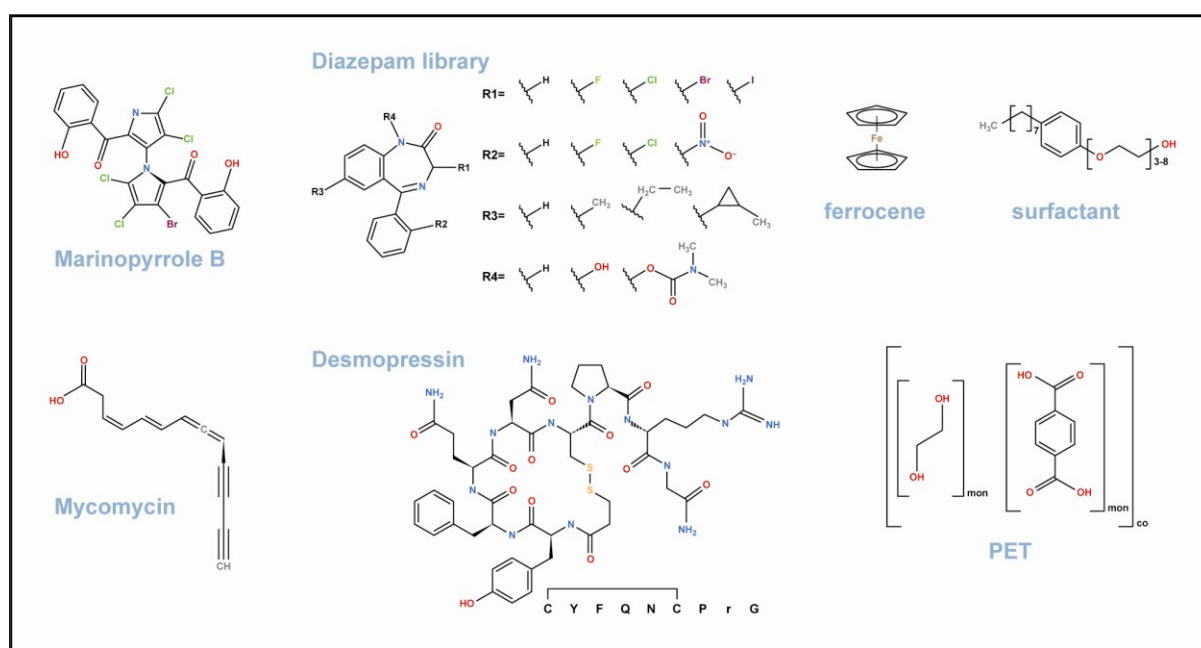


Figure 1: Examples of the many chemical representation styles supported by Symyx Direct

## Premiere chemistry searching

- Markush (generic) structure registration and searching
- 2D and 3D exact and substructure searches
- Flexmatch for exact-match, tautomer, isomer and salt searches
- Similarity searches, including searches for smaller and larger compounds
- Molecular weight, formula, Rgroup, Sgroup, polymer and mixture queries
- Reaction substructure/reaction similarity searches
- Extensive query tuning to enable focused hit sets
- Enhanced stereochemistry for structures and queries
- Non-tetrahedral stereochemistry support for allenes and biphenyls
- Storage and retrieval of sequences—peptides, oligonucleotides and oligosaccharides

## Support for industry-standard formats

- SDFfiles, RDFfiles and XDFfiles
- Canonical SMILES strings
- Chime strings, Molfiles
- InChi names and keys
- NEMA key
- Monoisotopic formula masses
- Formula masses for isotopically enriched structures
- UniProt for sequences

## Performance

- 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 five million reactions and over 27 million structures

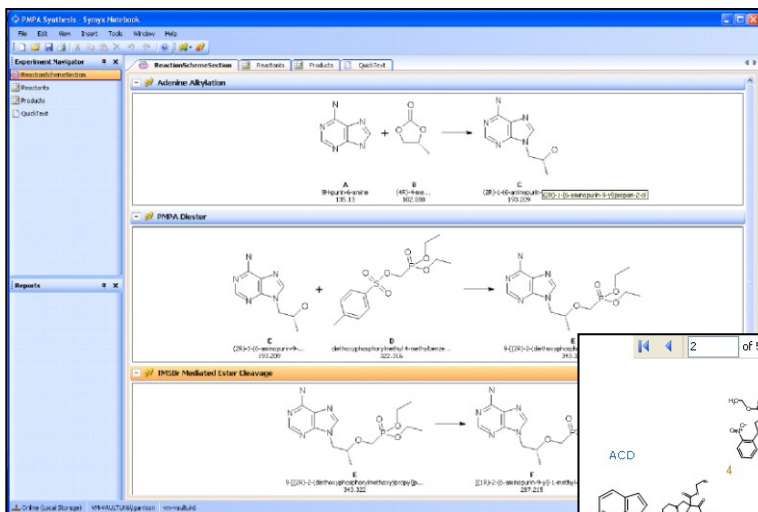
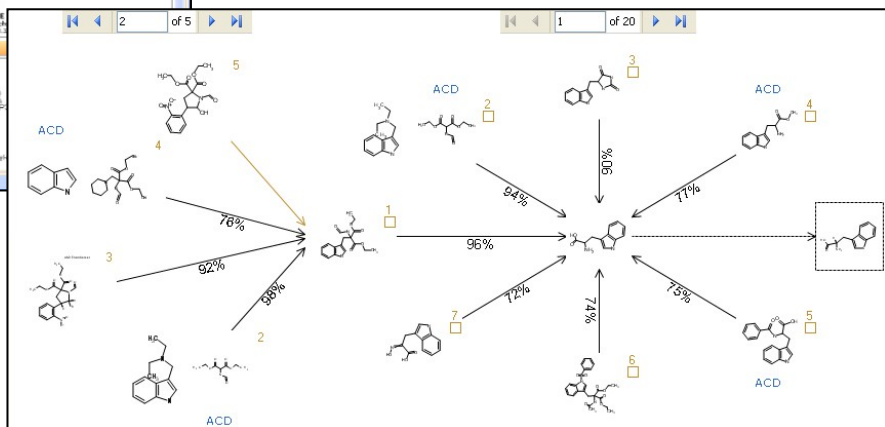


Figure 2: The Symyx Direct chemistry engine powers the enterprise Symyx Notebook.

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



### Embedded in Oracle technology

Symyx 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<sup>®</sup> Data Objects (ADO), Open Database Connectivity (ODBC), Java<sup>®</sup> Database Connectivity (JDBC) or SQL\*Net<sup>®</sup> for reaction and chemical structure searching.

### Flexible application development

Symyx Direct powers cheminformatics applications that manage structures and chemical reactions using industry-standard methods and tools such as Java<sup>®</sup>, Visual Basic<sup>®</sup>, .NET<sup>®</sup> and C++. 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-Isentris migration

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