

# ACCORD CHEMISTRY CARTRIDGE

By defining a new chemistry data type, the Accord Chemistry Cartridge seamlessly integrates the Accord Chemistry engine into Oracle® databases. This object-relational extension is designed to enable scientists to store, index and search chemical moieties alongside numbers and text within one underlying relational database server.

As you would expect from the world's leading provider of chemical component software solutions, Accord Chemistry Cartridge provides the industry's next-generation, scalable, high performance chemical server solution by working with Oracle, the leading provider of relational database technology worldwide.

## PROGRAMMING INTERFACES

Because the Accord Chemistry Cartridge implements up-to-date indexing algorithms within the underlying Oracle database server, chemical searching is fast and reliable. Accord is revolutionary in enabling chemistry to be treated as a first class data type within an industry-standard SQL framework. Users can seamlessly combine chemical substructure, reaction and

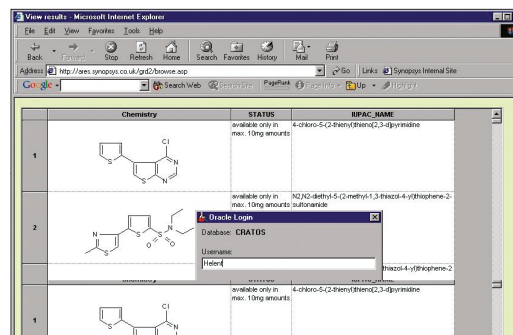
exact structure searching with numeric and text SQL or PL/SQL terms.




The Accord Chemistry Cartridge can be used via SQL and PL/SQL. You can submit searches and browse the database from web pages, VB-forms and any ODBC/JDBC compliant programming language.

Because the Accord Chemistry Cartridge tunes Oracle into chemistry from the ground up, complex issues such as query optimizations and index lookups are all taken care of by the system. Different indexing options are available to optimize storage space requirements versus the speed of registration. Indexes can be updated or re-built online, optimized for the number of records or the number of hours of indexing time, with no downtime for maintenance.

```
SELECT id, chemistry
FROM chemistrytable
WHERE chemistrymatches (chemistry,
SSSConst. MatchSub, query_chemistry ) = 1;
```

Where chemistry is a database column of type BLOB, CLOB, or VARCHAR2 containing any combination of Accord Chemistry, Molfiles, ISIS Sketch data, ChemDraw data, SMILES, etc. Similarly query\_chemistry can be BLOB, CLOB or VARCHAR2 in any chemistry format.



Chemistry	STATUS	RFPAC_NAME
	available only in max. 10mg amount	4-chloro-5-(2-phenylphenoxy)-2,3-dipyrindine
	available only in max. 10mg amount; subversive	4-(2,6-dichloro-5-O-methyl-1,3-thiazol-4-yl)thiazene-2-
	available only in max. 10mg amount	4-chloro-5-(2-phenylphenoxy)-2,3-dipyrindine

An Accord Chemistry Cartridge database as viewed using the Accord Grid Control in Internet Explorer

a wide range of organic, organometallic and inorganic molecules and reactions; features such as isotopes, charges, radicals, and delocalized pi-systems are all accounted for by the software. Accord understands aromaticity the way chemists do using the Hückel rule. Accord interprets a comprehensive range of stereochemical designations, both chiral and geometric. It also provides full support for reaction information and atom mapping, and a wide range of chemical formats, including Rxnfiles and SMILES strings. Text can be associated with atoms, bonds or structures.

## ACCORD DEVELOPMENT TOOLS

Accelrys offers a comprehensive range of component-based client/server application development tools to complement those provided natively by Oracle.

The Accord Chemistry Control and the Accord Grid Control can be utilized within client-side container applications and the web to phrase chemical queries and display search results. And with the Accord Software Development Kit, developers can create their own structure-savvy applications in C/C++, Visual Basic or Delphi. The Accord SDK allows you to modify structures through PL/SQL. This is how Accelrys develops chemistry modules. It also allows you to calculate physical or chemical properties, and to import and export a variety of formats.

Accord Enterprise Informatics and all modules of the Accord product family are based on the Accord Chemistry engine, and developed using the Accord SDK and the Accord chemistry controls.

## KEY SOLUTION BENEFITS

Chemical indexing ensures fast SQL exact, substructure similarity and reaction comparison operators.

- Matching options allow relaxed searches such as FRAMEWORK or TAUTOMER
- PL/SQL procedures can call Accord Chemistry SDK functions, as required, to create business rules and registration scripts.
- Handles the full range of chemical representation and query features, including stereochemistry and pi-systems.
- Compounds and reactions are handled in one cartridge, even in the same table and column if required.
- Searchable for reaction changes with full support for atom or bond mapping.
- Support for a multitude of formats – existing databases can be indexed without a conversion of existing data. Chemistry data even stay in the same column in the same table
- Reads and writes a host of chemical formats, including SD and RD files. Web and thick or thin client-server development support right out of the box.
- Has been used productively with libraries in excess of 8 million structures.

To learn more about Informatics, go to [accelrys.com/informatics](http://accelrys.com/informatics)