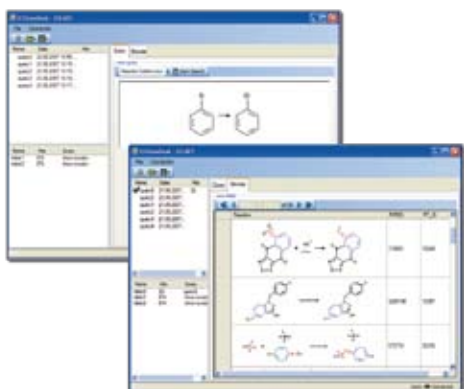




InfoChem's Chemistry Cartridge ICARTRIDGE is a powerful software module, designed to integrate storage and retrieval of chemical structures and reactions in a relational Oracle® environment. ICARTRIDGE uses one of the fastest search and indexing algorithms for structures and reactions.

New developments in version 2.6 prove InfoChem's expertise in meeting the requirements of modern chemists in a more and more complex scientific world.



Use the new front-end application ICHEMDESK for easy access to your chemical data.

Extended SQL Interface

Based on the standard Oracle® SQL syntax, ICARTRIDGE introduces new SQL operators and index types to access your molecules and reactions.

Chemical Structures

The new SQL search operators offer a large spectrum of search options:

- Comprehensive query feature support
- Various exact structure search modes
- Substructure search (SSS)

- R-group search (exact, substructure)
- Inverse substructure search
- Sophisticated chemical formula search
- Similarity search
- All-in-one structure search (SSA)

The new operator SSA retrieves all significant records in one result set ordered by relevance from exact to similar hits.

Chemical Reactions

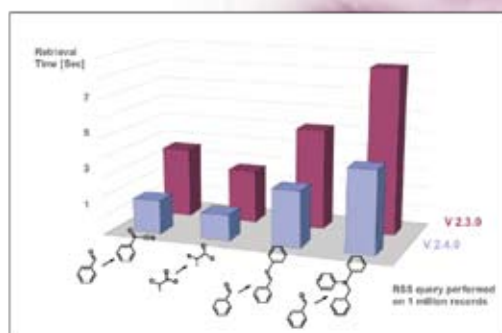
ICARTRIDGE provides specific SQL operators for

- Comprehensive query feature support
- Various exact reaction and role searches
- Reaction substructure search (RSS)
- Various reaction type searches (based on InfoChem's ClassCodes)

Performance

Built on InfoChem's fast search algorithm IC_{FSE}, ICARTRIDGE offers one of the fastest search engines for structures and reactions currently available. It is developed and tested for more than 20 million structures and over 4 million reactions!

Furthermore the search performance of ICARTRIDGE has been substantially enhanced since version 2.3.



ICARTRIDGE performance enhancement in version 2.4.0

Integration

ICARTRIDGE takes advantage of Oracle®'s basic technologies. Structural and factual data can be seamlessly integrated in an unrestricted, open Oracle® environment.

Easy access is granted via various database connection standards like ADO, ODBC and JDBC.

Chemical standard formats like MOL, RXN and SMILES are supported.

Any existing Oracle® database with structure or reaction data in LOB column and standard format can be indexed immediately – no data conversion is necessary. Unicode support is provided.

Import / Export

Structures, reactions and all associated data can be imported simultaneously from files in standard MDL® SDF / RDF format into any relational data model.

Chemistry Toolbox

In addition, ICARTRIDGE offers advanced chemistry tools, accessible via standard SQL or PL/SQL interfaces:

- Calculation of InChI and InChI key
- Calculation of unique structure identifiers
- Standardization of chemical structures and reactions
- Calculation of stereo descriptors
- Calculation of various molecular masses and chemical formulas
- Highlighting of query in structure and reaction records

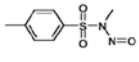

Unique Features of ICARTRIDGE

- Full integration of InfoChem's reaction classification algorithm CLASSIFY

- Enhanced Atom/Atom mapping (reaction center identification)
- Handling of partially defined structures (variable points of attachment, generic structures; support of Markush-structures under development)

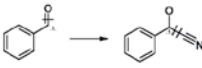
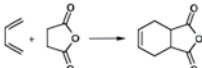
Examples

```
SELECT COUNT(*) FROM STRUCTURES a
WHERE SSS(a.MOL, iccart.readMolFile(..), 'MOL') = 1;
```

Query	Hits	Time
	22	0.1 sec
	10560	1.6 sec

Results for **substructure** queries on one million records.

```
SELECT COUNT(*) FROM REACTIONS a
WHERE RSS(a.REACTION, iccart.readRxnFile(..), 'RXN') = 1;
```

Query	Hits	Time
	223	1.2 sec
	374	0.2 sec

Results for **reaction substructure** queries on one million records.

Supported Systems

Operating systems:

- Win XP, Win 2003 Server
- Sun Solaris 8 or higher (64 Bit)
- Linux RHEL (64 Bit)

Database systems:

- ORACLE 9.2
- ORACLE 10
- ORACLE XE

32 / 64 Bit for SUN / Linux

32 Bit for Windows

Unicode systems are also supported