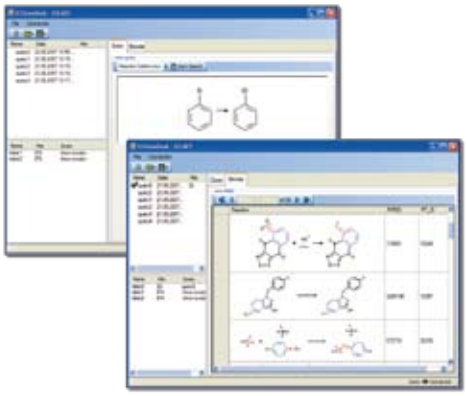
IC CARTRIDGE

InfoChem

InfoChem's Chemistry Cartridge IC*CARTRIDGE* is a powerful software module, designed to integrate storage and retrieval of chemical structures and reactions in a relational Oracle® environment. IC*CARTRIDGE* 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 IC*CHEMDESK* for easy access to your chemical data.

Extended SQL Interface

Based on the standard Oracle® SQL syntax, IC*CARTRIDGE* 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

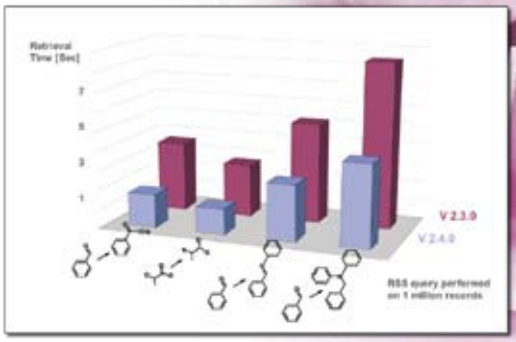
IC*CARTRIDGE* provides specific SQL operators for

- 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*, IC*CARTRIDGE* 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 IC*CARTRIDGE* has been substantially enhanced since version 2.3.



IC*CARTRIDGE* performance enhancement in version 2.4.0

Integration

IC*CARTRIDGE* 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, IC*CARTRIDGE* offers advanced chemistry tools, accessible via standard SQL or PL/SQL interfaces:

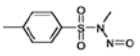
- Calculation of InChI and InChI key
- Calculation of unique structure identifiers
- Standardization of chemical structures and reactions
- Calculation of stereo descriptors
- Calculation of various molecular masses and chemical formulas
- Highlighting of query in structure and reaction records

Unique Features of IC*CARTRIDGE*

- 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)

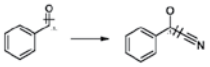
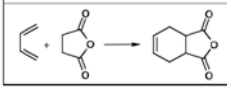
Examples

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

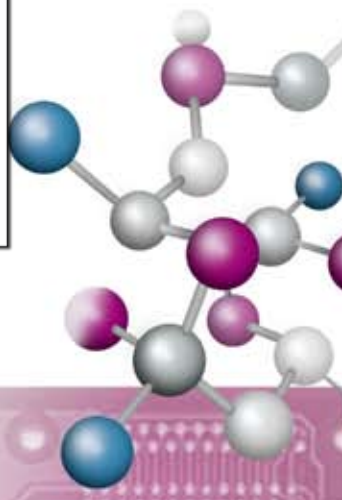
Query	Hits	Time
	22	0.1 sec
	10560	1.6 sec

*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

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