

JChem Extensions

- ChemAxon's tool for KNIME workflow -



4th KNIME Users Group Meeting and Workshop
Zurich, Switzerland

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Overview

- INFOCOM
- JChem Extensions
- New Features
- Future Developments

INFOCOM

- IT Business company of Teijin Group



- Offering wide varieties of IT services & solutions

- ◆ Head office: Tokyo, JAPAN

- ◆ Capital: 1.59 billion yen (ca. \$15M)

- ◆ No. of employees:

- 683 (stand-alone) / 1,151 (consolidated) , as of March 31, 2010

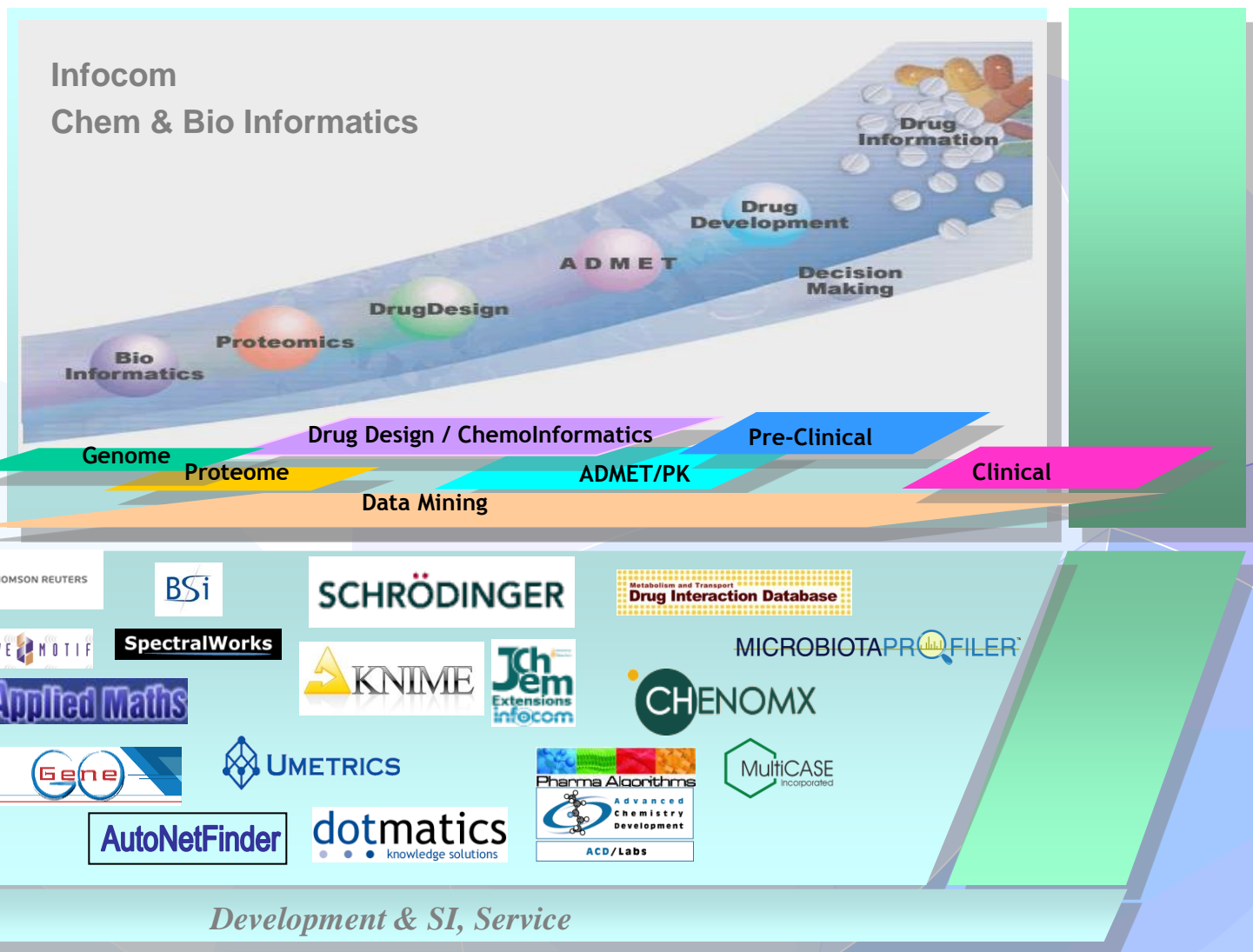
- Chem & Bio Informatics Department

- ◆ for life science market in Japan

- ◆ for more than 25 years

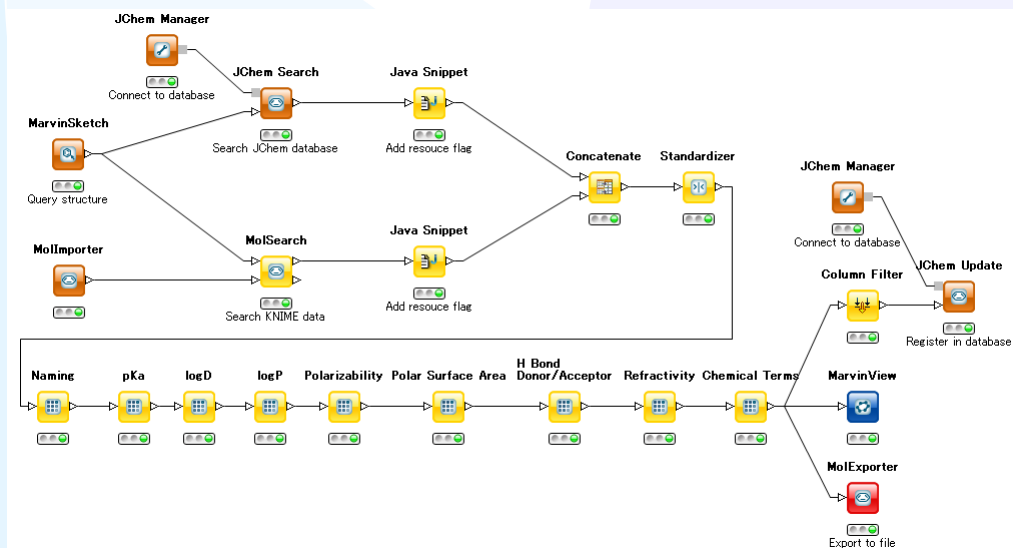
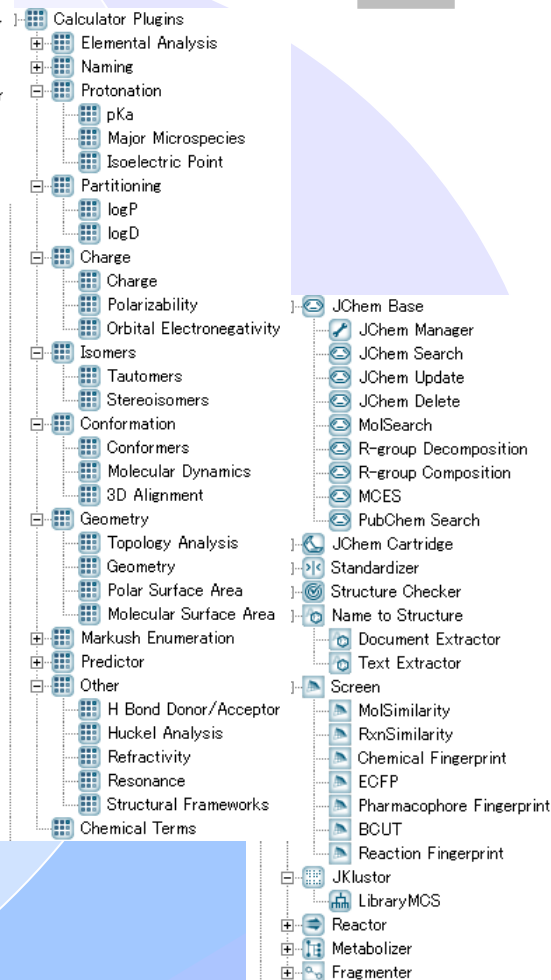
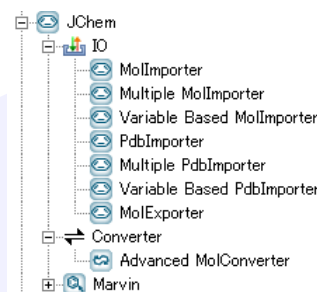


Our Business (Life science area)



JChem Extensions

- Extensions of ChemAxon's tool for KNIME workflow
- Infocom implement it with the support of ChemAxon
- Contains over 90% of ChemAxon's cheminformatics functionality
- New version coming soon!



ChemAxon's cheminformatics functionality

Visualization



Marvin

Structure, query & reaction editor, viewer & visualization

Property Prediction



Calculator Plugins

Structure property prediction & calculation

Selected calculations listing

- pKa, Major microspecies
- logP, logD
- Charge
- Tautomerization
- Stereoisomer
- Conformation and 3D alignment
- Topology Analysis
- Molecular Surface Area
- Markush Enumeration
- Hydrogen bond donor/ acceptor
- Structural Frameworks
- Structure to Name
- etc...

Add-ons



Markush Search

Store & search Markush structures

Chemical DB – toolkit



JChem Cartridge

JChem/Oracle integration



JChem Base

Structure searching & db access



Standardizer

Chemical business rules processing

Structure checker

Batch structure file validation and correction

Chemical DB – desktop



Instant JChem

Structure db management, search & prediction



JChem for Excel

Enabling chemistry in Excel



JChem Webservices

Web services integration interface

Nomenclature



Name to Structure

Import & search chemical names

Enumeration



Reactor

Enumeration via reaction modelling

Library analysis



JKlustor

Clustering & diversity analysis



Fragmenter

Decomposition to fragments and R-groups

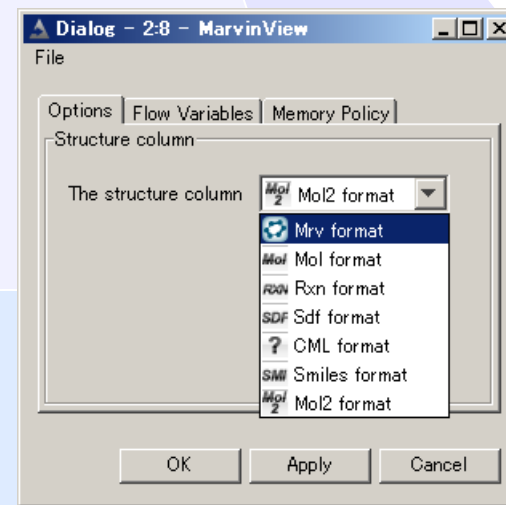
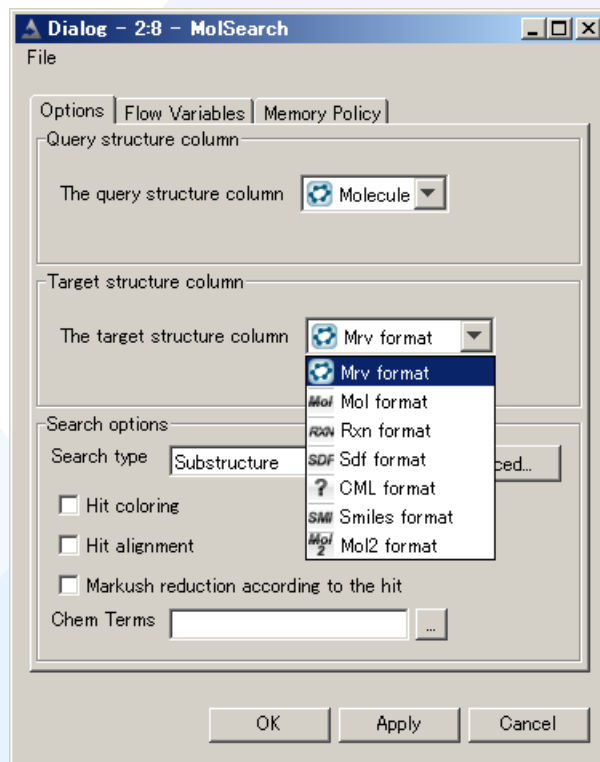
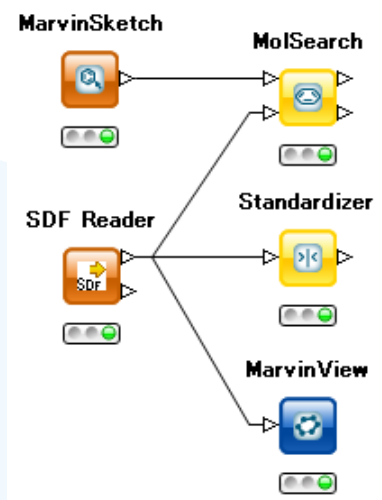


Screen

HT pharmacophore screening

New Features

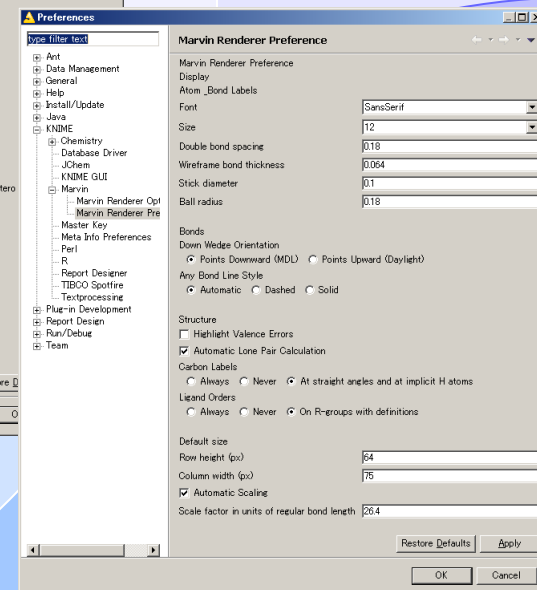
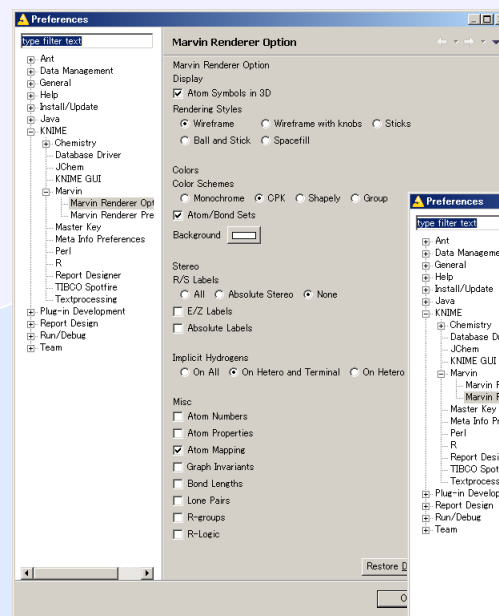
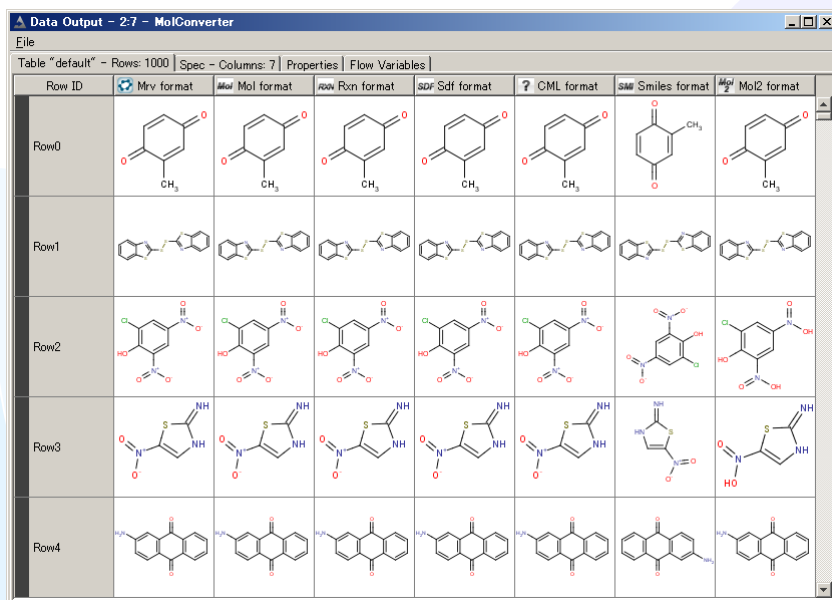
- Accepts input data in a wide variety of formats
 - ◆ Easy to create workflows with other partner's extensions
 - ◆ No need to use convertor node



New Features (Cont.)

■ New Marvin Renderer

- ◆ The rendering of wide variety of formats is supported
- ◆ Various options can be specified



New Features (Cont.)

■ New Nodes

◆ Structure Checker

- Filtering drawing mistakes or special structural elements

◆ MCES

- Finds the largest common substructure of two molecules

◆ Predictor

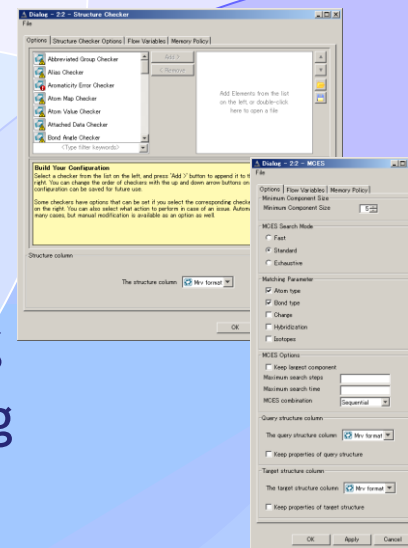
- Molecular property prediction as the sum of atomic contributions

■ Improvements

◆ Marvin/JChem 5.4.1.1 are used.

◆ Performance improvements in structural searching

◆ Performance improvements in importing/exporting



Future Developments

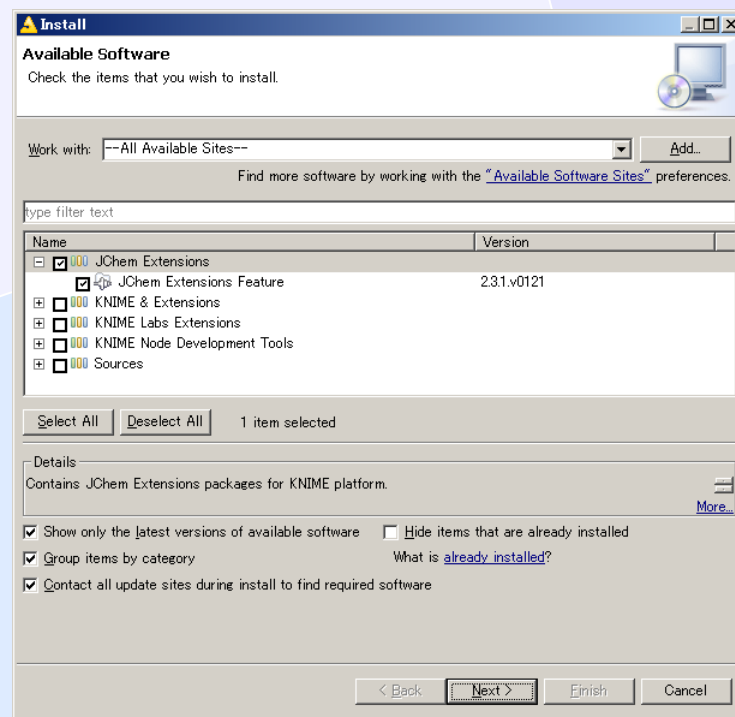
- Integrate with JChem For Excel
 - ◆ Export to the JC4XL format.
- Integrate with Instant JChem
 - ◆ Connect to the IJC database
 - ◆ Execute workflow from IJC
- Etc...

We need your suggestions!!

Let's try

■ JChem Extensions:

- ◆ http://www.infocom.co.jp/bio/develop/jchemextension_en.html
- ◆ http://www.infocom.co.jp/bio/develop/jchemextension_update_en.html
- ◆ Download and Install via the update site
 - Update Site : <https://www.infocom.co.jp/bio/knime/update>



■ KNIME:

- ◆ <http://www.knime.org/>
- ◆ <http://www.knime.com/>

■ E-MAIL:

- ◆ info-science@infocom.co.jp

Acknowledgements



- Infocom development team
- ChemAxon
- KNIME organization

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