

ChemAxon's JChem Nodes on KNIME workbench



ChemAxon
European User Group Meeting
Visegrad, Hungary
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United Innovation
info.com group

- INFOCOM
- KNIME
- JChemExtensions
 - nodes
 - relational db
 - combination with other party's node
 - bench mark
 - future plan

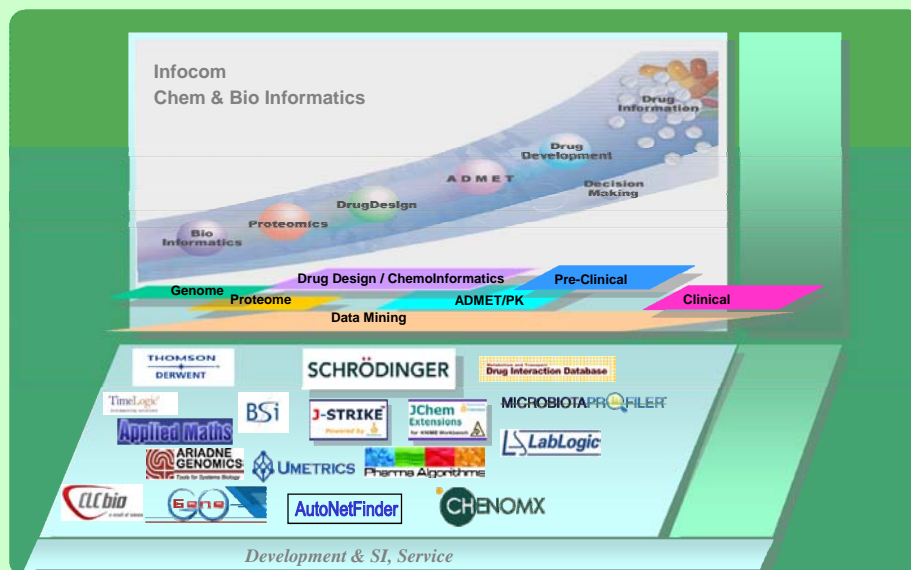
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INFOCOM

- IT Business company of Teijin Group
TEIJIN *Human Chemistry, Human Solutions*
- Offering wide varieties of IT services & solutions
 - Head office: Tokyo, JAPAN
 - Capital: 1.59 billion yen (ca. \$15M)
 - No. of employees: 603 (non-consolidated)
1,111 (consolidated) as of March 2007
- Chem & Bio Informatics Department
 - for life science market in Japan
 - for more than 20 years
- J-STRIKE: powered by ChemAxon
 - Web Based chemical structure database management systems
 - Launched 2007



Our Business (Life science area)



KNIME

The Konstanz Information Miner

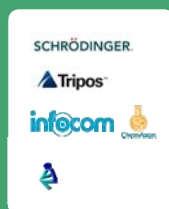


- **KNIME (naim):**
 - Workflow & Data mining platform
 - Developed at the University of Konstanz, Germany.
 - Open Source / Eclipse
 - Free of charge !
 - Knime, CDK, R, Weka ...
 - Commercial suppliers & partners join in
 - Schrödinger, Tripos, etc



KNIME & Extensions

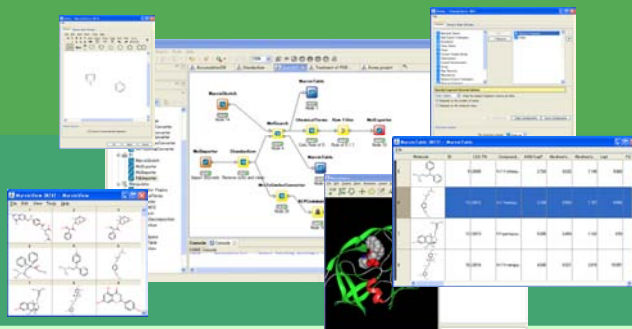
- **KNIME Node**
 - KNIME (Basic node)
 - KNIME Chemistry Feature (CDK)
 - KNIME Data Mining (Weka) Feature
 - KNIME JFreeChart Feature
 - and more Plug-in
- **Partners' Node**
 - Schrödinger Knime Extensions
 - Tripos Chemistry Extensions
 - Infocom JChem Extensions (ChemAxon's tools)
 - Trewaren Consultants Ltd
 - ...
- **Customize Node**



JChemExtensions

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- Extensions of ChemAxon's tool for Knime workflow
- Infocom implement it with the support of ChemAxon
- Release: Jan 31st 2008
- 38 novel nodes (May 2008)
- Free for academic



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JChemExtensions for KNIME Workbench

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Converter

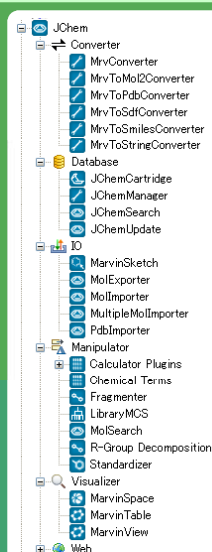
Database

IO

Manipulator

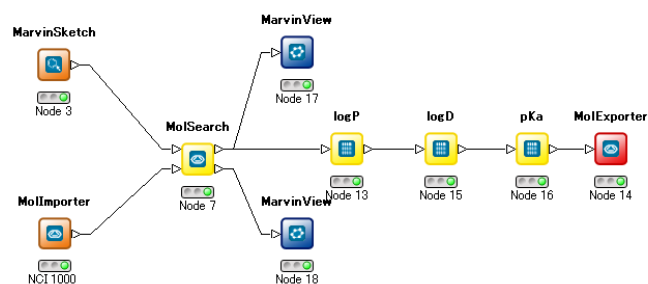
Visualizer

Planning...



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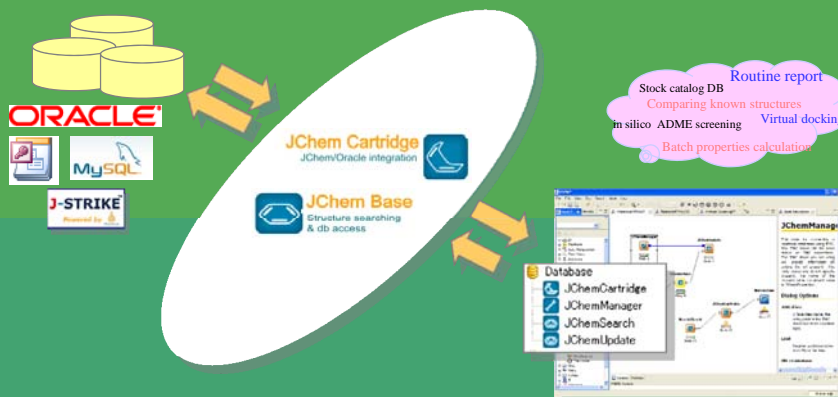
JChemExtensions (Workflow sample)



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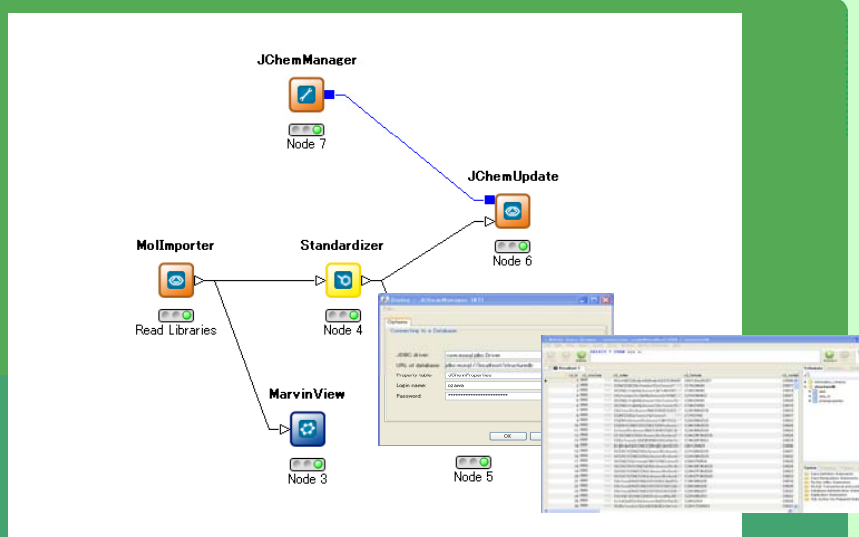
JChemExtensions & Relational DB

- Improve the usefulness of chemical structures in Knime, on your desktop.



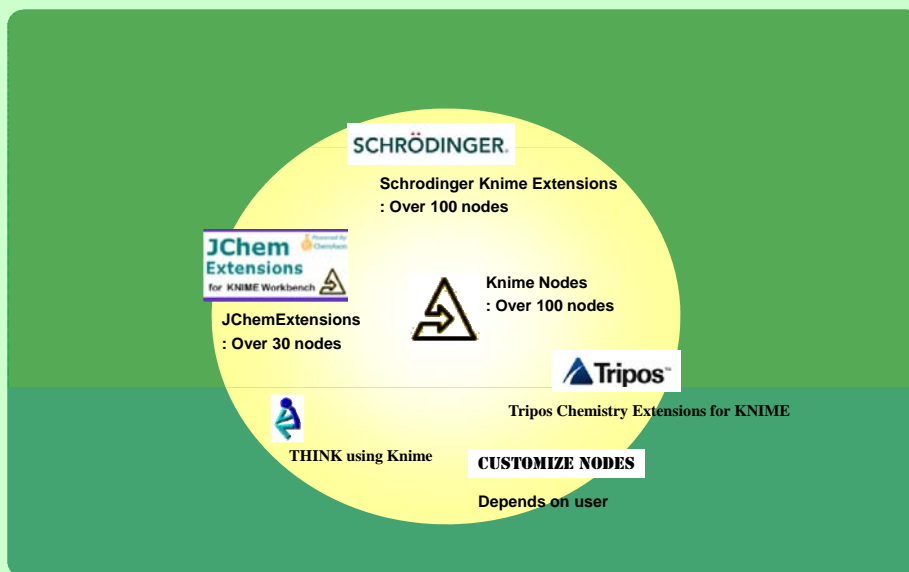
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JChemExtensions & Relational DB (Workflow sample:MySQL)



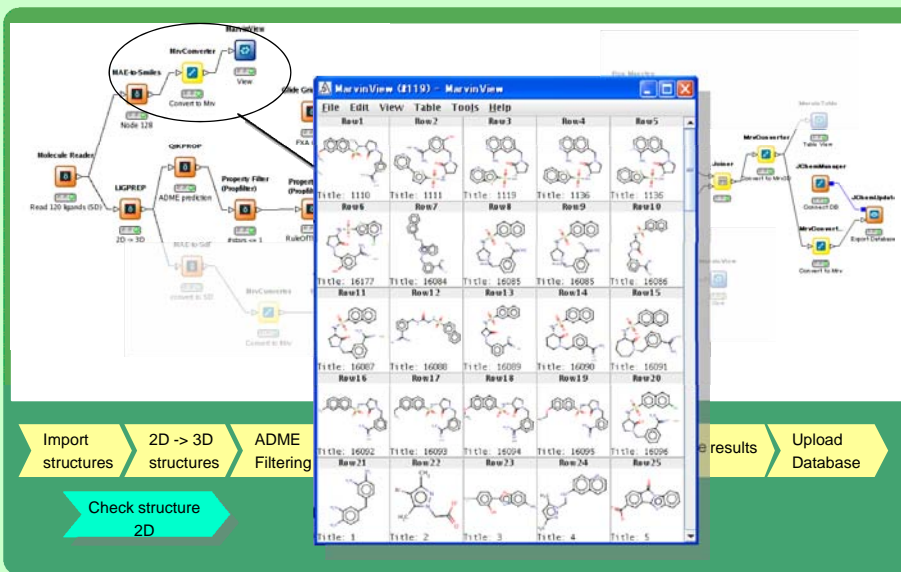
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Combination with other parties



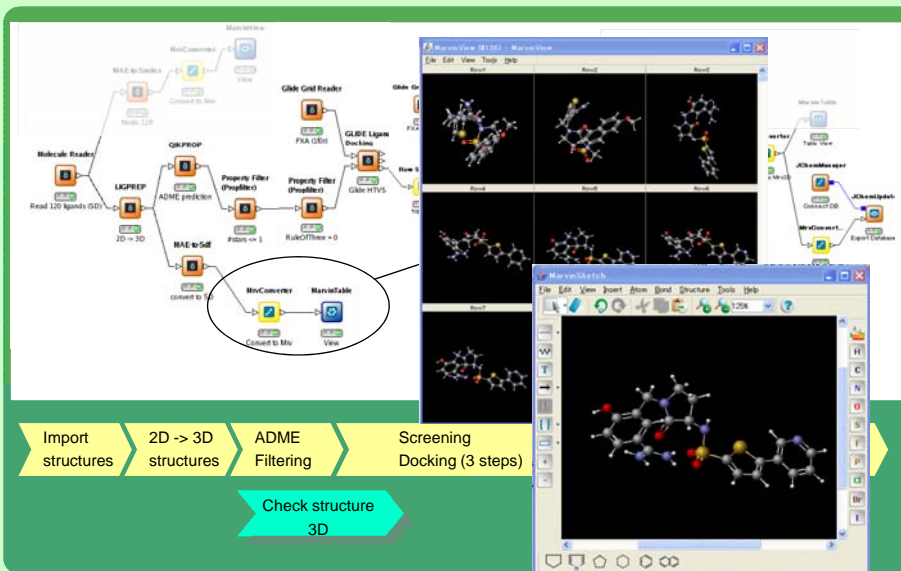
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Combination with other parties (Workflow sample with Schrödinger)



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Combination with other parties (Workflow sample with Schrödinger)



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Combination with other parties (Workflow sample with Schrödinger)

Import structures

Round up the results

Upload Database

Check structure 2D or 3D

Combination with other parties (Workflow sample with Schrödinger)

Import structures

2D -> 3D structure

Set & Upload DB

Bench Mark

- In preparation

Feature plan

- Implement other ChemAxon tools
- Connect to Public Database
 - E.g. PubChem...
 - See Mr. Ohshima's poster
- Web based version
 - But , it depends on Knime development plan
- JChemExtensions: server service
 - Processing huge data
 - E.g standardizer...

Let's try

JChemExtensions:

- Academic version
- Evaluation version



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Knime :



www.knime.org

ChemAxon :



www.knime.org

Thanks