

JChem Extensions - ChemAxon's tool for KNIME workflow -



ChemAxon 2010 European UGM
Budapest, Hungary

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Overview

- INFOCOM
- JChem Extensions
- New Features
- Marvin Family Nodes
- 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

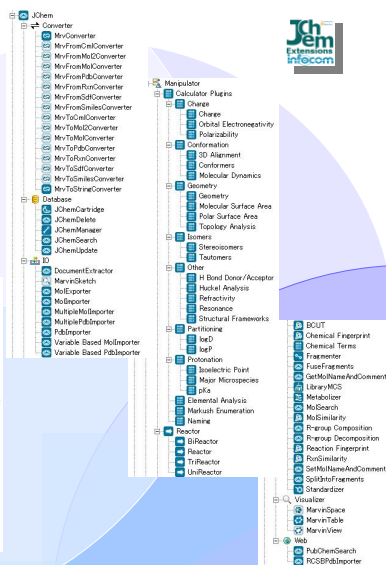
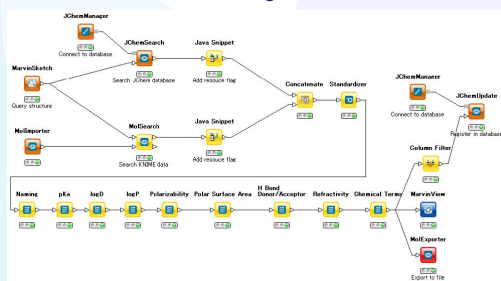
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JChem Extensions

- Extensions of ChemAxon's tool for KNIME workflow
- InfoCom implement it with the support of ChemAxon
- 1st Release / 26Nodes: Jan 31st 2008
- 2nd Release / 70Nodes: Jul 13th 2009
- New version coming soon!



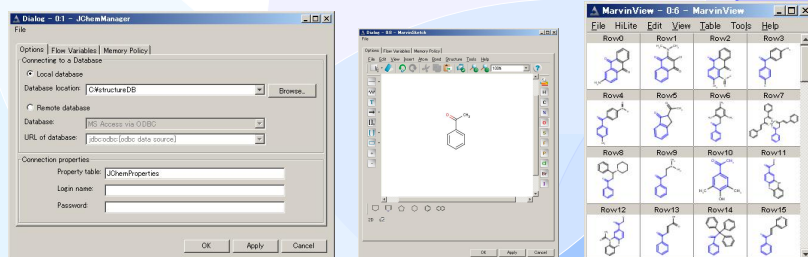
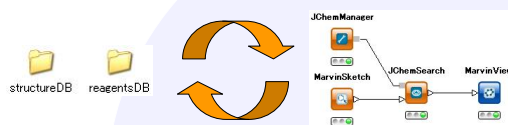
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New Features

- Local database
 - Create local database
 - Structural search and update from KNIME work flow



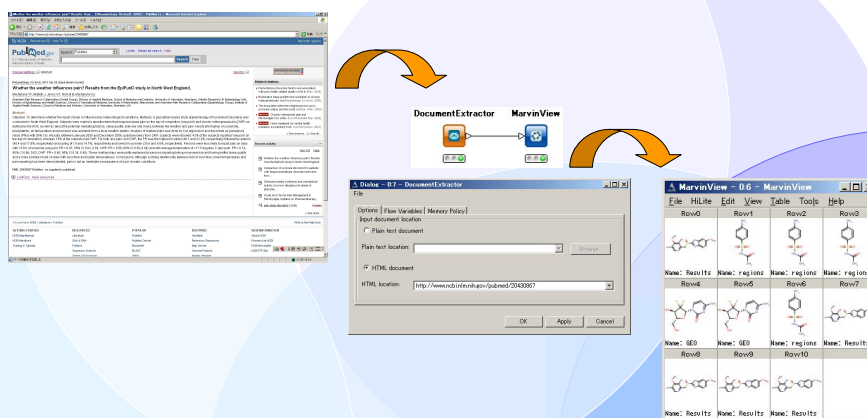
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New Features (Cont.)

- DocumentExtractor
 - Extract structure from plain text or web site
 - Using "Name to structure"



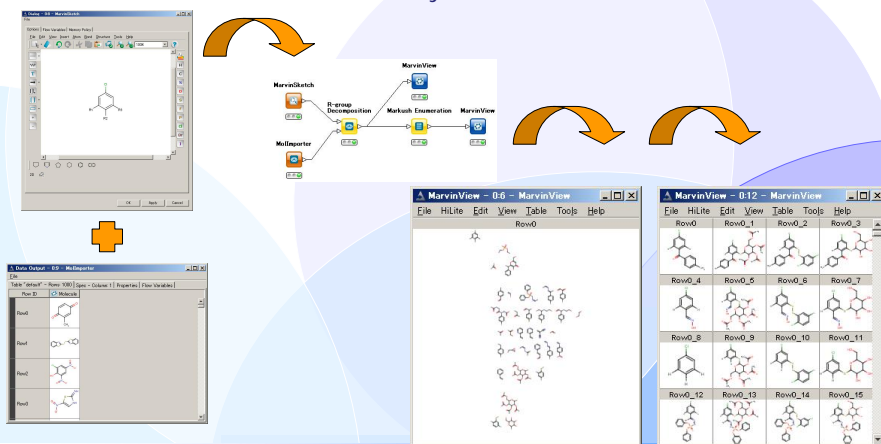
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New Features (Cont.)

- R-group Decomposition + Markush Enumeration
 - ◆ R-group Decomposition node outputs Markush structure
 - ◆ Enumerate structures directly in the workflow







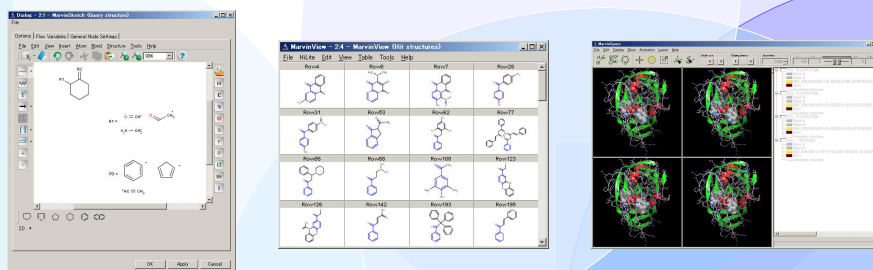
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Marvin Family Nodes are FREE !

- What are “Marvin Family Nodes” ?
 - ◆ Marvin Sketch node 
 - ◆ Marvin View node 
 - ◆ Marvin Space node 
 - ◆ Converter nodes 
- Some basic nodes of JChem Extensions
- Free of charge for ALL customers!!



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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
- MarvinView node
 - ◆ Support Color Attribute of Color Manager node
- Etc...

We need your suggestions!!

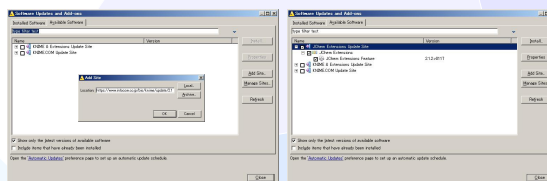
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Let's try

- 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

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Thanks

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