KNIME Nodes History of Changes

Oct 15th, 2019: Version 4.0.0.v192100

For KNIME 4.0.0 and JChem 19.21.0 (System requirement: KNIME 4.0.0 or later)

New Features and improvement

Marvin/JChem 19.21.0 are used.

Bugfixes

- **JC4XL Writer, JC4O Writer**
  - Could not output to local file.

Sep 24th, 2019: Version 4.0.0.v192000

For KNIME 4.0.0 and JChem 19.20.0 (System requirement: KNIME 4.0.0 or later)

New Features and improvement

Marvin/JChem 19.20.0 are used.

Improvements

- **Chemical Terms**
  - Support 2D Array output.

Jun 28th, 2019: Version 4.0.0.v191500

For KNIME 4.0.0 and JChem 19.15.0 (System requirement: KNIME 4.0.0 or later)

Note

The update site url has been changed as below.
https://www.infocom-science.jp/knime/update/4.0

New Features and improvement

Marvin/JChem 19.15.0 are used.

Mar 1st, 2019: Version 3.6.0.v190600

For KNIME 3.6.0 and JChem 19.6.0 (System requirement: KNIME 3.6.0 or later)

Note

The update site url has been changed as below.
https://service.infocom.co.jp/knime/update/3.6

New Features and improvement

Marvin/JChem 19.6.0 are used.

Sep 20th, 2018: Version 3.6.0.v0902, Version 3.5.0.v0804

For KNIME 3.6.0 and JChem 18.22.0 (System requirement: KNIME 3.6.0 or later)
For KNIME 3.5.0 and JChem 18.22.0 (System requirement: KNIME 3.5.0 or later)

New Features and improvement

Marvin/JChem 18.22.0 are used.

Improvements

- **MolExporter**
  - Add 'The output option' options.

Jul 12th, 2018: Version 3.6.0.v0901

For KNIME 3.6.0 and JChem 18.13.0 (System requirement: KNIME 3.6.0 or later)

New Features and improvement

No changes. (Just update for KNIME 3.6.0)

Jun 15th, 2018: Version 3.5.0.v0803

For KNIME 3.5.0 and JChem 18.13.0 (System requirement: KNIME 3.5.0 or later)

New Features and improvement

Marvin/JChem 18.13.0 are used.

Mar 16th, 2018: Version 3.5.0.v0802

For KNIME 3.5.0 and JChem 18.8.0 (System requirement: KNIME 3.5.0 or later)

New Features and improvement

Marvin/JChem 18.8.0 are used.

Feb 19th, 2018: Version 3.5.0.v0801

For KNIME 3.5.0 and JChem 18.4.0 (System requirement: KNIME 3.5.0 or later)

New Features and improvement

Marvin/JChem 18.4.0 are used.

Improvements

- **Elemental Analysis**
  - Add 'Recognize formula in pseudo labels' options.
  - Calculating molecular weight from molecular formula.

Dec 18th, 2017: Version 3.5.0.v0800

For KNIME 3.5.0 and JChem 17.28.0 (System requirement: KNIME 3.5.0 or later)

Bugfixes

- There was compatibility problem on Mac update.

Nov 16th, 2017: Version 3.4.2.v0701

For KNIME 3.4.2 and JChem 17.28.0 (System requirement: KNIME 3.3.0 or later)

New Features and improvement

Marvin/JChem 17.28.0 are used.

Bugfixes

- **R-group Decomposition**
  - Clean up the configuration dialog.
- **ComplianceChecker**
  - Moved under the ChemAxon / Infocom > JChem repository tree.

Sep 29th, 2017: Version 3.3.2.v0602

For KNIME 3.3.2 and JChem 17.24.0 (System requirement: KNIME 3.3.0 or later)

New Features and improvement

Marvin/JChem 17.24.0 are used.

Bugfixes

- **PubChem Search**
  - Some query structure could not be worked as XML issue.

Aug 28th, 2017: Version 3.3.2.v0601

For KNIME 3.3.2 and JChem 17.21.0 (System requirement: KNIME 3.3.0 or later)

New Features and improvement

Marvin/JChem 17.21.0 are used.

New Nodes

- **ComplianceChecker**
  - This node checks all chemical structures provided in a given column of the input DataTable against ComplianceChecker's rule set. It's included in free extensions.
- **JChem PostgreSQL Cartridge**
  - Search data by structure, substructure and similarity through extensions to PostgreSQL's native SQL language.

Improvements

- **MarvinRenderer**
  - Show missing value as difference from empty structure.
- **JChem Search**
  - Output cd_id value option has been added.
- **JChem Update**
  - Update option (with selected cd_id) has been added.

Bugfixes

- **Standardizer**
  - Some configurations could not be worked as SAX parser issue

Jun 6th, 2017: Version 3.3.2.v0600

For KNIME 3.3.2 and JChem 17.10.0 (System requirement: KNIME 3.3.0 or later)

New Features and improvement

Marvin/JChem 17.10.0 are used.

New Nodes

- **Recalculate Table**
  - Recalculate structure tables of relational databases.
- **Scalar Descriptor**
  - Calculate the Scalar Descriptor.

Improvements

- **Marvin Cell**
  - KNIME's Java Snippet node can be used to work with Marvin Cell data types like ChemAxon Molecule object.
- **MarvinRenderer**
  - Wireframe with knobs display option has been eliminated.
- **Markush Composer**
  - 'Ignore input molecules not containing the scaffold' has been added.

- 'Keep all of multiple results or only the most relevant one' has been added.

Bugfixes

- **Chemical Terms**
  - Some functions could not be worked.

Feb 3rd, 2017: Version 3.1.0.v0506

For KNIME 3.1.0 and JChem 17.1.30.0 (System requirement: KNIME 3.1.0 or later)

New Features and improvement

Marvin/JChem 17.1.30.0 are used.

New Nodes

- **CNMR Prediction**
  - Calculate the CNMR Prediction.
- **HNMR Prediction**
  - Calculate the HNMR Prediction.

Improvements

- **Advanced MolConverter**
  - Support Image formats.

Bugfixes

- **MarvinView**
  - MarvinView node caused KNIME to hang on the Mac.
- **MolSimilarity**
  - MolSimilarity node could not be used without Molecular Descriptors license.
- **PubChem Search**
  - PubChem Search node could not access to the PubChem Power User Gateway via HTTP protocol.

Nov 29th, 2016: Version 3.1.0.v0505

For KNIME 3.1.0 and JChem 16.11.21.0 (System requirement: KNIME 3.1.0 or later)

New Features and improvements

Marvin/JChem 16.11.21.0 are used.

New Nodes

- **JC4O Reader**
  - Reads the contents of an Office file created with JChem For Office.
- **JC4O Writer**
  - Writes the incoming data table contents to a JChem For Office compatible docx and pptx file.

Improvements

- **MolConverter, Advanced MolConverter**
  - Add 'Remove small fragments' options.
  - Add 'Cleaning' options.
- **JChem Search, MolSearch**
  - The default Vague Bond Level has changed.
- **Marvin Renderer**
  - Add 'S-group Attachment' options.

Bugfixes

- **DocumentExtractor**
  - OSR external tool option could not be off.

Sep 30th, 2016: Version 3.1.0.v0504

For KNIME 3.1.0 and JChem 16.9.26.0 (System requirement:KNIME 3.1.0 or later)

New Features and improvements

Marvin/JChem 16.9.26.0 are used.

Apr 15th, 2016: Version 3.1.0.v0503

For KNIME 3.1.0 and JChem 16.4.11.0 (System requirement: KNIME 3.1.0 or later)

New Features and improvements

Marvin/JChem 16.4.11.0 are used.

Improvements

- The node icon has been changed.

Feb 19th, 2016: Version 3.1.0.v0502

For KNIME 3.1.0 and JChem 16.2.15.0 (System requirement: KNIME 3.1.0 or later)

New Features and improvements

Marvin/JChem 16.2.15.0 are used.

Improvements

- **The following nodes have supported concurrent processing.**
  - Converter nodes
  - Marvin nodes (in part)
  - Calculator Plugins nodes (in part)
  - Standardizer
  - Screen nodes (in part)
- **Marvin Renderer**
  - Add 'Transparent' options.

Dec 9th, 2015: Version 3.1.0.v0501

For KNIME 3.1.0 and JChem 15.12.7.0 (System requirement: KNIME 3.1.0 or later)

New Features and improvements

Marvin/JChem 15.12.7.0 are used.

Improvements

- **All nodes and renderer.**
  - Support adaptor type cell (e.g. CDK, RDKit) which contains structural data type.

Sep 25th, 2015: Version 2.8.2.v0306

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x, 2.12.x) and JChem 15.9.21.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 15.9.21.0 are used.

Sep 11th, 2015: Version 2.8.2.v0305

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x, 2.12.x) and JChem 15.9.7.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 15.9.7.0 are used.

New Nodes

- **Markush Composer**
  - Automatically generate Markush structures based on a set of compounds.

Improvements

- **DocumentExtractor, TextExtractor**
  - Extract option has been enhanced.

- **Structure Checker**
  - Output Fixes Applied, Problems Remaining information.
- **Markush Enumeration**
  - Node repository tree has been moved to JChem > Markush.

Bugfixes

- **Standardizer, Structure Checker**
  - Sometimes the full interface did not display.
- **Structure Checker**
  - In some case, the node did not work correctly.

Sep 4th, 2015: Version 2.8.2.v0304

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x, 2.12.x) and JChem 15.8.31.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 15.8.31.0 are used.

New Nodes

- **Markush Overlap**
  - Calculates the overlapping space between two Markush structures.

Improvements

- **DocumentExtractor, TextExtractor**
  - Extract option has been enhanced.
- **Markush Viewer, R-group Decomposition, R-group Composition**
  - Node repository tree has been moved to JChem > Markush.

Jul 30th, 2015: Version 2.8.2.v0303

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x) and JChem 15.7.20.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 15.7.20.0 are used.

New Nodes

- **HLB**
  - Calculate the hydrophilic-lipophilic balance number (HLB number).

Improvements

- **JChem Search, JChem Update, JChem Cartridge**
  - Support Boolean, DateAndTime and BinaryObject type cell
- **Tautomers**
  - Improving and modifying the tautomerization options.
- **logP**
  - Improving and modifying the logP calculation methods.
- **logD**
  - Improving and modifying the logD calculation methods

Apr 8th, 2015: Version 2.8.2.v0302

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x) and JChem 15.3.30.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 15.3.30.0 are used.

New Nodes

- **Maccs Fingerprint**
  - The fingerprints encode the Maccs Key. It is based on the following information. https://www.chemaxon.com/forum/ftopic8138.html
- **Atom Selection**
  - Handle atom selection information.

Improvements

- **MolSearch**
  - Add hit atom indexes option has been added.
- **Marvin Renderer**
  - Add 'Margin size' options.

Feb 17th, 2015: Version 2.8.2.v0301

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x) and JChem 15.2.9.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 15.2.9.0 are used.

Improvements

- **All nodes and renderer.**
  - Support adaptor type cell (e.g. CDK, RDKit) which contains structural data type.

Bugfixes

- **Standardizer, Structure Checker**

    - The previous version could not work in headless environment (KNIME Batch Mode).
- **MarvinSpace**
    - Close the view the whole application will close.

Dec 8th, 2014: Version 2.8.2.v0300

For KNIME 2.8.2 (also KNIME 2.9.x, 2.10.x, 2.11.x) and JChem 14.11.24.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 14.11.24.0 are used.

New Nodes

- **Aqueous Solubility**
    - Calculate the solubility.

Improvements

- **JC4XL Writer**
    - Supports ImageCell(PNGImageCell).
- **Marvin Renderer**
    - Automatic Scaling option has been enhanced.

Jul 7th, 2014: Version 2.8.2.v0205

For KNIME 2.8.2 (also KNIME 2.9.x) and JChem 6.3.1.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 6.3.1.0 are used.

Improvements

- **All nodes and renderer.**
    - Support adaptor type cell (e.g. CDK, RDKit) which contains structural data type.

Bugfixes

- **MarvinSpace**

- The previous version could not work due to OpenGL libraries version issue.

May 23rd, 2014: Version 2.8.2.v0204

For KNIME 2.8.2 (also KNIME 2.9.x) and JChem 6.3.0.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 6.3.0.0 are used.

Improvements

- **Tautomers, Conformers, Stereoisomers, Molecular Dynamics**
  - Keep input columns option has been addded.
- **MCS**
  - Ring handling mode option has been added.
- **Reactor**
  - The Reactor nodes can use input data as reaction schemes.
  - Generate synthesis code option has been added.
- **Fragmenter, Screen nodes**
  - Example config files are bundled and added to a file list.

Bugfixes

- **JChem Search, JChem Update**
  - The unnecessary data field was outputted.

Apr 2nd, 2014: Version 2.8.2.v0203

For KNIME 2.8.2 (also KNIME 2.9.x) and JChem 6.2.1.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 6.2.1.0 are used.

Improvements

- **Sphere Exclusion**
  - Clustering method option has been added.

Bugfixes

- **JChem Cartridge**
  - SQLException was thrown, if SQL statement has multi line breaks.
- **All nodes**
  - The previous version could not work on Mac environment due to java version issue.

Feb 6th, 2014: Version 2.8.2.v0202

For KNIME 2.8.2 (also KNIME 2.9.x) and JChem 6.2.0.0 (System requirement: KNIME 2.8.0 or later)

New Features and improvements

Marvin/JChem 6.2.0.0 are used.

Improvements

- **MolConverter**
  - Support Inchi data type.
- **DocumentExtractor, TextExtractor**
  - Extract option has been enhanced.
- **Marvin Renderer**
  - Support Inchi data type.
- **All nodes**
  - Skip weird cases and keep the execution of workflow.

Bugfixes

- **JChem Update**
  - Bits to be set for patterns could not be more than 3.
- **Sphere Exclusion**
  - Sphere Exclusion could not work with Chemical Fingerprints
- **All nodes**
  - The previous version could not work on Mac environment due to java version issue.

Nov 12th, 2013: Version 2.7.4.v0201

For KNIME 2.7.4 (also KNIME 2.8.x) and JChem 6.1.3.0 (System requirement: KNIME 2.7.0 or later)

New Features and improvements

Marvin/JChem 6.1.3.0 are used.

New Nodes

- **Sphere Exclusion**
  - Calculate the Sphere Exclusion.

Improvements

- **MolImporter, MolExporter**
  - Performance of I/O was increased by using concurrent processing in molecule import /export.
- **MolExporter**
  - 'Including data types of properties' option has been added.
- **JC4XL Writer**
  - Support xlsm file for appending data.
- **Advanced MolConverter**
  - Support binary data type (SKC, CDX format).
- **Topology Analysis**
  - 'Fsp3' option has been introduced
- **Standardizer**
  - Standardizer GUI has been updated based on JChem / Marvin updated.
  - StandardizerResult output has been added.
- **Structure Checker**
  - Structure Checker GUI has been updated based on JChem / Marvin updated.
- **Library MCS**
  - Library MCS uses the newly developed MCS module.
  - Add 'Structure output is split in level' option (output is Collection Column).
- **Metabolizer**
  - Metabolizer GUI has been updated based on JChem / Marvin updated.
  - Metabolizer uses the newly developed Metabolizer module.
- **Marvin Renderer**
  - Add 'IUPAC Numbering' option.
- **The following nodes have supported part of streaming processing.**
  - MolImporter, MolExporter
  - JC4XL Reader, JC4XL Writer
  - Fuse Fragments, Join Reaction
  - MolSearch, Formula Search
  - Document Extractor
  - LibraryMCS
  - Reactor
  - Metabolizer

Bugfixes

- **JChem Search, JChem Update**
  - The unnecessary data field was outputted.

Jul 3rd, 2013: Version 2.6.3.v0200

For KNIME 2.6.3 (also KNIME 2.7.x) and JChem 6.0.2.0 (System requirement: KNIME 2.5.0 or later)

New Features and improvements

Marvin/JChem 6.0.2.0 are used.

New Nodes

- **MCS**
  - The MCS finds the maximum common substructure (MCS) of two molecules.
- **Similarity Calculator**
  - Calculate the similarity based on a Fingerprint.

Improvements

- **JC4XL Writer**
  - 'Append / Overwrite' option has been added.
- **JChem Search, MolSearch**
  - Advanced option has been enhanced.
- **Topology Analysis**
  - 'Aromatization method' option has been added.
- **Reactor**
  - 'Mark reaction center' option has been added.
- **MolSimilarity, RxnSimilarity**
  - If query and target structures are from same data, only a half is outputted to reduce execution time.
- **FingerPrint**
  - A result can be outputted as a bit format.

Bugfixes

- **MolSimilarity, RxnSimilarity**
  - Preprocessing time has been reduced.
- **FingerPrint**
  - The length of the result as binary format was not fixed.

May 20th, 2013: Version 2.6.3.v0138

For KNIME 2.6.3 (also KNIME 2.7.x) and JChem 5.12.4.0 (System requirement: KNIME 2.5.0 or later)

New Features and improvements

Marvin/JChem 5.12.4.0 are used.

Bugfixes

- **JChem Search**
  - If search time takes longer than 6 seconds, the search stops as time out error.

Apr 25th, 2013: Version 2.6.3.v0137

For KNIME 2.6.3 (also KNIME 2.7.x) and JChem 5.12.3.0 (System requirement: KNIME 2.5.0 or later)

New Features and improvements

Marvin/JChem 5.12.3.0 are used.

New Nodes

- **Screen3D**
  - Calculate the three dimensional similarity comparison of molecular pairs.
- **MolFragmenter**
  - Molecule fragmenter.

Improvements

- **The following nodes have supported streaming processing.** (requirement:KNIME 2.7.4 and DataRush 6.1.0-18)
  - Converter nodes
  - Set MolName And Comment, Get MolName And Comment, Split Into Fragments, Split Reaction, RCSB PdbImporter
  - Calculator Plugins nodes
  - Standardizer
  - Structure Checker
  - Text Extractor
  - Fragmenter, MolFragmenter
  - Screen nodes (except for MolSimilarity, MolSimilarity, Screen3D)
- **Multiple MolImporter, Multiple PdbImporter**
  - In order to delete a file, multiple files can be selected.
- **Isoelectric Point**

    - 'Keep explicit hydrogens' option has been added.
- **Molecular Dynamics**
    - New MMFF94 forcefield implementation has been introduced.
- **JChem Search, MolSearch**
    - Advanced option has been enhanced.
- **R-group Decomposition**
    - 'Include scaffold in the output' option has been added.
- **Fragmenter**
    - Some Fragmenter options have been added.

Bugfixes

- **Database nodes**
    - Database nodes did not recognize non-standard character sets such as MacRoman.
- **MolSimilarity**
    - If there were two or more query structures, the result was not correct.

Nov 1st, 2012: Version 2.6.3.v0135

For KNIME 2.6.3 and JChem 5.11.3.0 (System requirement: KNIME 2.5.0 or later)

New Features and improvements

Marvin/JChem 5.11.3.0 are used.

New Nodes

- **Dipole Moment Calculation**
    - Calculate the Dipole moment.

Improvements

- **MarvinSketch**
    - Output molecule properties that are added in MarvinSketch GUI.
- **pKa, Major Microspecies**
    - 'Keep explicit hydrogens' option has been added.
- **LibraryMCS**
    - 'Keep properties of structure' option has been added.

Sep 6th, 2012: Version 2.6.0.v0134

For KNIME 2.6.0 and JChem 5.10.3.0 (System requirement: KNIME 2.5.0 or later)

Bugfixes

- **JC4XL Reader**
  - Since the unnecessary log was outputted, processing speed was slow.
- **JC4XL Reader, JC4XL Writer**
  - In the KNIME 2.6.1, could not work correctly.
- **Join Reaction, MolExporter, Reactor, R-group Composition**
  - In Windows 7 and Linux, dialog layout was broken.

Aug 24th, 2012: Version 2.6.0.v0133

For KNIME 2.6.0 and JChem 5.10.3.0 (System requirement: KNIME 2.5.0 or later)

New Features and improvements

Marvin/JChem 5.10.3.0 are used.

New Nodes

- **Shape Descriptor**
  - Shape descriptor implements a 3D alignment based similarity calculation.
- **Join Reaction**
  - Join reaction from reactants and products.

Improvements

- **Marvin Renderer**
  - Add 'Peptide Display' options.
- **MarvinSketch**
  - Add 'Outputting multiple fragments' options.
- **MolExporter**
  - Add 'Export empty (missing) structure' options.
- **Reactor**
  - Outputs both of successful products / reactions and failed reactants.
- **MolSearch**
  - Add 'Add match count to the search result' options.

Bugfixes

- **MolImporter**
  - MolImporter nodes did not recognize non-standard character sets such as MacRoman.
- **JC4XL Reader**
  - If there are some blank or error cells on an Excel sheet, then they were not ignored.

- **JC4XL Writer**
  - Empty (missing) data was not written correctly.
- **logP, logD**
  - Selected Method was not recognized correctly.

May 10th, 2012: Version 2.5.4.v0132 and Version 2.4.2.v0132

For KNIME 2.5.4 and JChem 5.9.3.0 (System requirement: KNIME 2.5.0 or later)

For KNIME 2.4.2 and JChem 5.9.3.0 (System requirement: KNIME 2.3.4 or later)

Bugfixes

- **MolImporter, (also other nodes that have file path parameter)**
  - File path parameter would be blank in case of importing older workflows. This version can load an older workflow which is built at 2.5.0.v0127 or later.
- **JChem Cartridge**
  - IOException was thrown by saving / loading an executed workflow, if SQL statement which is an INSERT, UPDATE, or DELETE statement.
- **3D Alignment**
  - NullPointerException was thrown, if the alignment type was "atom pairs",

Backward compatibility

We have also created JChem Extensions version 2.4.2.v0132.
All of features are same except for the sortable table feature of MarvinTable node.

Apr 26th, 2012: Version 2.5.4.v0131 and Version 2.4.2.v0131

For KNIME 2.5.4 and JChem 5.9.3.0 (System requirement: KNIME 2.5.0 or later)

For KNIME 2.4.2 and JChem 5.9.3.0 (System requirement: KNIME 2.3.4 or later)

New Features and improvements

Marvin/JChem 5.9.3.0 are used.

Improvements

- **MolImporter**
  - Support the common office document formats.
  - Add 'Add the input file name' option.

- **MolExporter**
  - Add 'Encoding' option.
  - Support URL as file path to export structural file.
- **JC4XL Writer**
  - Support URL as file path to write xlsx file.
- **pKa**
  - Add 'Number of acidic pKa / basic pKa' options.
- **R-group Decomposition**
  - Add 'Undefined R-atom matches' option.
- **R-group Composition**
  - Add 'Filter out duplicate structures on each rgroup set' option.
  - Add 'Add selected rgroup structures to all rgroup set' option.
- **JChem Cartridge**
  - GUI has been improved.
  - Add 'Database Schema Browser'.
  - Add 'SQL Statement' which supports DML (SELECT, INSERT, UPDATE, DELETE) SQL statement with input data and variable.
- **Document Extractor / Text Extractor**
  - Support the common office document formats.
  - Add 'Accept elements / generic names / ions' options.
- **ECFP/FCFP**
  - Node name has been renamed.
  - Add 'Substructure' output type.
- **Reactor**
  - Add 'Reaction rules' options.
- **MarvinSketch**
  - The information on the selected atoms and bonds can be stored in MRV format.
- **Marvin Cell**
  - Unique Smiles is used for comparison of data.
  - This affects the GroupBy, Sorter nodes.

Bugfixes

- **Importer / Exporter**
  - If the extension of structural file is upper case, could not work.
- **JC4XL Writer**
  - The result sheet was grouped with the structure data sheet (hidden sheet).
  - The result file did not recalculate the formula (for rendering structure).
- **Chemical Fingerprint / Reaction Fingerprint**
  - If input data has missing cell, could not work continual.
- **All nodes**
  - GUI has been improved.
  - Support resizing the window.
  - Node color has been improved.

Backward compatibility

We have also created JChem Extensions version 2.4.2.v0131.

All of features are same except for the sortable table feature of MarvinTable node.

Jan 24th, 2012: Version 2.5.1.v0129 and Version 2.4.2.v0129

For KNIME 2.5.1 and JChem 5.8.0.0 (System requirement: KNIME 2.5.0 or later)

For KNIME 2.4.2 and JChem 5.8.0.0 (System requirement: KNIME 2.3.4 or later)

New Features and improvements

Marvin/JChem 5.8.0.0 are used.

New Nodes

- **Markush Viewer**
  - Markush Viewer is a application of ChemAxon to view the various R-group definitions of Markush structures in an organized way.

Improvements

- **Marvin Renderer**
  - Add 'Quality' options.
  - Add 'Coordinate Bond Line Style' options.

Bugfixes

- **MolImporter, (also other nodes that have file path parameter)**
  - File open/save dialog could not work correctly.
- **JChemSearch**
  - Always returned no hit results.

Backward compatibility

We have also created JChem Extensions version 2.4.2.v0129.
All of features are same except for the sortable table feature of MarvinTable node.

Dec 8th, 2011: Version 2.5.0.v0128 and Version 2.4.2.v0128

For KNIME 2.5.0 and JChem 5.7.0.0 (System requirement: KNIME 2.5.0 or later)

For KNIME 2.4.2 and JChem 5.7.0.0 (System requirement: KNIME 2.3.4 or later)

New Features and improvements

Improvements

- **Document Extractor**
  - Support URL as file path to extract file document.

Bugfixes

- **MolImporter, (also other nodes that have file path parameter)**
  - When using with KNIME Server, could not work correctly.

Backward compatibility

We have also created JChem Extensions version 2.4.2.v0128.
All of features are same except for the sortable table feature of MarvinTable node.

Dec 5th, 2011: Version 2.5.0.v0127

For KNIME 2.5.0 and JChem 5.7.0.0 (System requirement: KNIME 2.5.0 or later)

New Features and improvements

Marvin/JChem 5.7.0.0 are used.

New Nodes

- **JC4XL Reader**
  - Reads the contents of an Excel file created with JChem For Excel.
- **JC4XL Writer**
  - Writes the incoming data table contents to a JChem For Excel compatible xlsx file.

Improvements

- **MolImporter, PdbImporter**
  - Support URL as file path to import structural file.
- **MolConverter, Advanced MolConverter**
  - Support output (export) options.
- **Structure Checker**
  - Support output to separate port (Fixed and unfixed structures).
- **Document Extractor, Text Extractor**
  - Add 'Lookup of CAS numbers' options.
- **MarvinView**
  - Support hilite filter features (HiLite > Filter menu).

- **MarvinTable**
  - Sort data in table view by clicking the column header (based on KNIME feature).

Bugfixes

- **MolExporter**
  - When using with KNIME Server, could not work correctly.
- **JChem Manager, JChem Cartridge**
  - When using with KNIME Server (Web Portal), workflow credential could not work correctly.
- **LibraryMCS**
  - The 'Maximum level count' option on the 'Clustering' tab can not be set smaller than 5.

Aug 9th, 2011: Version 2.4.1.v0125

For KNIME 2.4.1 and JChem 5.5.1.0 (System requirement: KNIME 2.3.4 or later)

New Features and improvements

Marvin/JChem 5.5.1.0 are used.

New Nodes

- **Split Reaction**
  - Splitting products and reactants from reaction.
- **Formula Search**
  - Filters molecules based on sophisticated chemical formula search.

Improvements

- **JChem Cartridge, JChem Manager**
  - Support workflow credential for "User name and password" to connect to the database.
- **MCES**
  - Support matrix type output.
  - Output MCS Distance.
- **MolExporter**
  - Support multiple structural columns to export the file.
- **JChem Manager**
  - Support added JDBC driver file in Preference dialog of KNIME File > Preferences menu.
- **Split Into Fragments**
  - Add 'Split into columns as collection' options.

Bugfixes

- **MarvinSpace**
  - Support MacOS 64 bit.
- **Marvin Renderer**
  - Empty data issue has been fixed.
- **All nodes**
  - Calculating requirement and dependency could not work correctly and it has been fixed.
  - Executing workflow in KNIME batch mode could not work and it has been fixed.

Removed nodes

- MrvConverter
- MrvFromCmlConverter
- MrvFromMol2Converter
- MrvFromMolConverter
- MrvFromPdbConverter
- MrvFromRxnConverter
- MrvFromSdfConverter
- MrvFromSmilesConverter
- MrvToCmlConverter
- MrvToMol2Converter
- MrvToMolConverter
- MrvToPdbConverter
- MrvToRxnConverter
- MrvToSdfConverter
- MrvToSmilesConverter
- MrvToStringConverter

Use the 'MolConverter' node instead.

May 25th, 2011: Version 2.3.4.v0124

For KNIME 2.3.4 and JChem 5.4.1.1

New Features and improvements

- Marvin/JChem 5.4.1.1 are used.
- Node repository tree has been changed based on JChem/Marvin products.

New Nodes

- **Structure Checker**
  - Filtering drawing mistakes or special structural elements.

- **Predictor**
  - Molecular property prediction as the sum of atomic contributions.
- **Pharmacophore Fingerprint**
  - Pharmacophore Fingerprint descriptors.
- **ECFP**
  - Extended-Connectivity Fingerprints descriptors.

- **MCES**
  - Find the largest common substructure of two molecules.
- **TextExtractor**
  - Extract chemical names from text (in KNIME table) and converts them to chemical structures.

Improvements

- **Marvin Renderer**
  - Support other structure format than MrvType.
  - Various options/preferences can be specified in Preference dialog of KNIME File > Preferences menu.
- **MolImporter, MolExporter**
  - Performance improvements in importing/exporting.
  - Export image files.
- **Fuse Fragments**
  - Add 'Fragments per molecule/No. of fuse molecules' options.
  - Add 'Arrange molecules in a 2D square lattice/Number of colums' options.
- **Calculator Plugins**
  - Modify GUI and features based on JChem/Marvin updating.
- **JChemSearch, JChemUpdate, JChemDelete**
  - The accessible tables are listed based on the database connection information.
- **JChemSearch, MolSearch**
  - Performance improvements in structural searching.
  - Add 'Markush reduction according to the hit' option.
  - Add 'Allow duplication of the search result' option.
  - Add 'Add query data to the search result' option.
- **R-group Decomposition**
  - Add 'Generate Markush output' option.
  - Add 'Process all hits' option.
  - Add 'Hit ordering' option.
  - Add 'Allow duplication of the search result' option.
  - Add 'Add query data to the search result' option.
- **R-group Composition**
  - Add 'Scaffold modification' option.
- **Document Extractor**
  - Support PDF, XML formats.
- **MolSimilarity, RxnSimilarity**
  - Add 'Descriptors' options.
  - Add 'Dissimilarity metric' options.
- **Chemical Fingerprint, ECFP, Pharmacophore Fingerprint, BCUT, Reaction Fingerprint**

    - Output fingerprint as Integer data type.
- **Reactor**
    - Add 'Generate Unsuccessful reactions' option.
- **All nodes**
    - Some nodes (For instance, MarvinSketck, MolImporter, JChemSearch) that have output port support other structure format than MrvType.
    - All of node that have input port support other structure format than MrvType.

Bugfixes

- **Reactor**
    - If check the 'Keep properites' option, the columns order in output table are changed automatically.
- **Markush Enumeration**
    - Markush library size returns a wrong value, therefore, the return type is changed from IntCell to LongCell.
- **All nodes**
    - Workflow process speed might be dramatic slowdown on KNIME2.3 or later.

Deprecated nodes

- MrvConverter
- MrvFromCmlConverter
- MrvFromMol2Converter
- MrvFromMolConverter
- MrvFromPdbConverter
- MrvFromRxnConverter
- MrvFromSdfConverter
- MrvFromSmilesConverter
- MrvToCmlConverter
- MrvToMol2Converter
- MrvToMolConverter
- MrvToPdbConverter
- MrvToRxnConverter
- MrvToSdfConverter
- MrvToSmilesConverter
- MrvToStringConverter

Will be removed. Use the 'MolConverter' node instead.