Pipeline Pilot Components History of Changes

History of Changes for the Frequent Release branch. For LTS branches please click here.

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NOTE: For the sake of brevity only versions with significant changes
are listed here.
The appropriate versions are available for all released JChem versions.



Version 20.1, January 14, 2020
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- New component: "ChemAxon Major Microspecies"


Version 19.18, August 4, 2019
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- Bugfix: "Marvin JS" compatibility with Internet Explorer 11 restored


Version 19.17, July 16, 2019
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- Bugfix: "ChemAxon Reactor" threw exception for reactions containing
R-groups


Version 19.7, March 12, 2019
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- Bugfix: configuration property names were not read properly in some
cases



Version 19.1, January 14, 2019
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- Compound Registration:
  > Advanced registration options added
  > Compatible with Compound Registration version Carbon.2 (18.22.2)
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Version 18.28, November 28, 2018

- "ChemAxon Document Extractor", "ChemAxon Name to Structure" and "ChemAxon Structure to Name" :
  Parameter names and legal values relating to CAS Registry Numbers® have been modified due to legal request.
  NOTE: Incompatible changes. Please update all usages of "ChemAxon Document Extractor" and "ChemAxon Name to Structure"
    by right-click and "Replace with Latest Version", and if needed set the relevant option to True again.
    Notice about CAS Registry Numbers® : https://docs.chemaxon.com/pages/viewpage.action?pageId=72515588

Version 18.20, August 21, 2018

- "JChem for Office Writer" bugfix: did not run with default Document Style

Version 18.13, June 12, 2018

- Required Compound Registration version: 18.5.14

- "Insert to JChem Table" bugfix: inserting of non-string type additional data fixed

Version 18.8, March 14, 2018

- Marvin Applets are no longer supported

- "ChemAxon HTML Molecular Table Viewer"
  > Opens default browser, with option to override
  > On click always pop-up image
  > ChemAxon rendering is default
  > Pipeline Pilot image options updated

- "MarvinSketch Applet" component removed

Version 17.29.0, December 8, 2017

- Pipeline Pilot 17.2.0 or later is required.
  For earlier versions the 17.24.x LTS releases are available (bugfixes only).

- Fixed Marvin JS installation instructions (reverse proxy setting could be lost)

- Bugfix: fixed example "JChem Base Insert and Search"

Version 17.27.0, October 26, 2017

- Bugfix: some components did not remove some properties in certain cases

Version 17.26.0, October 20, 2017

- Pipeline Pilot 9.5 or later is required.

Version 17.23.0, September 16, 2017

- Minimum required JChem Web Services version: 17.2.6.0

- "JChem Web Services Search" : advanced search options string added

Version 17.16.0, July 22, 2017

- "ChemAxon Calculator" : new options added for logP and logD calculations
  > Calculation method
  > Consider tautomers

Version 17.15.0, July 15, 2017

- "JChem PSQL Cartridge Search" : Similarity Search support added

- Required JChem PostgreSQL Cartridge version: 2.9 or later

Version 17.14.0, July 7, 2017

- "Compliance Checker" no longer blocks in filter mode until all records finished

- Bugfix: "JChem for Office Writer" image quality fixed

Version 17.2.13.0, February 15, 2017

- Minimum required Pipeline Pilot version : 9.2

- Minimum required Internet Explorer version : 11

- Bugfix: JVM crash in certain cases during error reporting ("No server process") fixed.

Version 17.1.30.0, February 4, 2017

- "JChem for Office Writer", "JChem for Office Reader":
  regular page breaks are exported and recognized for Word documents from now on.

Version 17.1.9.0, January 14, 2017

- New components:
  > "JChem for Office Reader"
  > "JChem for Office Writer"

Version 17.1.2.0, January 3, 2017

- "Marvin JS" component: compatibility fix for newer FireFox versions

Version 16.12.5.0, December 8, 2016

- "ChemAxon Molecular Table Viewer" component removed (obsolete)

Version 16.11.7.0, November 16, 2016

- External documentation links fixed/updated for several components

Version 16.10.24.0, October 26, 2016

- New component: "JChem Web Services Search"

Version 16.10.3.0, October 5, 2016

- New components for Compliance Checker integration:
  > "Compliance Checker"
  > "Compliance Checker Categories"

Version 16.9.5.0, September 7, 2016

- "Chemical Terms Calculator" : molecule type results are allowed

Version 16.8.15.0, August 16, 2016

- Marvin JS is now included as integral version of the package for simplified installation

- Upgraded and simplified installation instructions

- "ChemAxon HTML Molecular Table Viewer" bugfix: did not find applet if it was selected for pop-up

Version 16.6.20.0, June 21, 2016

- "JChem for Excel Writer" bugfix: exception when conditional formatting was missing fixed

Version 16.6.6.0, June 7, 2016

- New options for "JChemSearch" and "JChem Oracle Cartridge Search":
  > Homology Narrow Translation
  > Homology Broad Translation

- "MolConverter" bugfix: exception if "Keep Properties" parameter is used

Version 16.5.30.0, May 31, 2016

- New component: "MarvinSketch Applet":
  Completely re-written component, earlier prototypes removed.

Version 16.5.23.0, May 25, 2016

- New component: "JChem PSQL Cartridge Search"

Version 16.4.18.0, April 20, 2016

- "ChemAxon Name to Structure" : added option to allow CAS lookup by web service,
    new default is disabled

Version 16.3.28.0, April 4, 2016

- New components for compound registration:
    > "Registration Connection"
    > "Registration Auto Register"
    > "Registration Get Structure by ID"
    > "Registration Structure Search"

Version 16.3.21.0, March 23, 2016

- The default Vague Bond Level has changed for "JChemSearch", "JChem Cartridge Search"
    and "ChemAxon Structure Search Filter" components according to JChem changes:
  > Vague bond level "Default" (Level 1) option renamed to "Ligands and bridging bonds of aromatic rings"
  > The new default vague bond level is "Ambiguous aromaticity 5 membered rings" (Level Half)

- "ChemAxon Tautomerization"
  > "Generic Tautomer" option removed
  > New options added: normal tautomers, protect ester groups, ring-chain tautomers

Version 16.2.22.0, February 26, 2016

- "ChemAxon Structure to Name" : added option to generate CAS numbers

Version 16.2.15.0, February 20, 2016

- "Drop JChem Base Table" : Added "Ignore Missing Table" option

- "Molecule from IUPAC Name (ChemAxon)" renamed to "ChemAxon Name to Structure"

- "Molecule to IUPAC Name (ChemAxon)"
  > Renamed to "ChemAxon Structure to Name"
  > Added option to generate traditional names
  > "Z" atoms treated as attachment points (not as carbon)

Version 16.1.25.0, February 5, 2016

- "Marvin JS" component:
  > Web services URL have to be set centrally in chemaxon.conf, GUI options removed.
  > Option for embedded or popup mode
  > Multiple instances per form supported

Version 15.11.16.0, November 26, 2015

- New component: "Marvin JS"

Version 15.9.28.0, September 30, 2015

- Error reporting and logging has been improved

Version 15.9.21.0, September 24, 2015

- "JChem Cartridge Search"
  > Retrieval of hits is faster in most cases
  > Coloring and alignment is now off by default
  > Bugfix: in version 15.9.14.0 incorrect vague bond level was applied for previous cartridge versions (Level 1 instead of Half)

Version 15.9.7.0, September 10, 2015

- "ChemAxon Document Extractor":
  > CAS lookup default changed to off (bugfix),
     but extra interactive warning of web service usage was removed
  > Options added to enable/disable systematic and common names;
elements, ions and groups
  > Options added to retrieve the context of hits
  > Document section information (for USPTO XML patents)

Version 15.8.24.0, August 26, 2015

JChem Cartridge Search bugfix:
  - "ORA-01000: maximum open cursors exceeded" for larger result sets
fixed

Version 15.5.18.0, May 20, 2015

- "JChem for Excel Writer" component:
  > Conditional Formatting Expression option added
  > NOTE: became subprotocol, GUID changed

Version 15.3.9.0, March 13, 2015

- Configuration file "chemaxon.conf" file instead of
  environment variables for global settings:
  > license location
  > log directory
  > OSR tools
- Default log directory changed to "logs" directory inside package

Version 15.1.26.0, January 29, 2015

- New component: "JChem for Excel Reader"

- Component "ChemAxon Fragmenter" removed (discontinued product)

Version 15.1.12.0, January 13, 2015

- JChem Cartridge components: backwards compatibility tested and set
to minimum version 6.1.0
- "ChemAxon Standardize" bugfixes:

  > Did not work with configuration string and configuration file (only with simple actions)
  > Relative path for custom Standardizer configuration file was not resolved properly
  > Order changed for simple actions: Clean 2D and 3D moved to the end of list, Dearomatize moved up

Version 15.1.5.0, January 8, 2015

- "JChemSearch", "JChem Cartridge Search":
  "Remove Unused R-group Definitions" option added, unused groups no longer removed by default
- "Insert to JChem Table" : rejected empty structures no longer considered as an "error"
  (i.e. no error message, does not affect "Halt on Error" option)
- "JChemSearch" bugfix: dissimilarity values were not returned
- "JChem Cartridge Search" bugfixes:
    > Filter Query caused exception in certain cases
    > removed unused (ineffective) option "Ordering"
- "Create JChem Base Table" bugfix : relative path for custom Standardizer
  configuration file was not resolved properly

Version 14.12.15.0, December 18, 2014

- "ChemAxon HTML Molecular Table Viewer": "Display R-Logic" option added
- "ChemAxon Image from Molecule": "Display R-Logic" option added
- "ChemAxon Structure Search Filter"
  > Bugfix: ineffective "Markush Hit Representation" option removed.
    Markush search is not supported by this component, please use the JChemSearch component.
  > Bugfix: illegal default value for Tautomer Search removed

Version 14.12.8.0, December 10, 2014

- "ChemAxon MolConverter" bugfix: file input property selection was not effective in case of file output
- "ChemAxon Structure Checker":
  > "Ignore OCR Errors" option removed in line with JChem changes as separate option.
    Use the OCR checker("ocr") in the configuration instead.
  > Bugfix: Structures with no remaining issues were not fixed properly
  > Bugfix: Fixes are always executed for checkers with fix mode "Ask" (e.g. action strings)

Version 14.11.17.0, November 20, 2014

- External documentation links updated due to ChemAxon website changes.

- "Create JChem Base Table" bugfix: default fingerprint parameters were incorrect for Reaction and Markush table types.

Version 14.11.03.0, November 5, 2014

- New components:
  > "JChem Cartridge Search"
  > "JChem Cartridge Information"

- "JChemSearch" and "ChemAxon Structure Search Filter" components:
  > New "Default" Vague Bond Level option corresponding to new default Level 1 in JChem.
  > New "Stereo Search" option "Enantiomer Search", other stereo options renamed
  > Bugfix for "Stereo Search", "Charge Matching", "Isotope Matching", "Radical Matching":
    The "Default" option was not incorrect default for "Duplicate" search type,
    as non-specific query could match specific targets.
    New "Default" option changes behavior to Exact matching in case of "Duplicate" search.

  NOTE: Please update usages of "JChemSearch" and "ChemAxon Structure Search Filter"
        components by right-click and "Replace with Latest Version"

Version 14.9.29.0, October 2, 2014

- Pipeline Pilot 9.0 or later is required.

Version 14.9.22.0, September 24, 2014

- "ChemAxon Markush Filter" Prototype component removed, no advantage
    over "Chemaxon Chemical Terms Filter" since Pipeline Pilot 8.5

Version 14.8.4.0, August 9, 2014

- Some "Advanced" parameters were converted to normal in several

components, so they will not behave "Hidden" in Pipeline Pilot 9.0

Version 14.7.7.0, July 23, 2014

- "ChemAxon Reactor" component : "Generate Unsuccessful Reactions" option added

Version 2.9, July 10, 2014

- New component: "JChem Table Information"

- "Create JChem Base Table":
  > New options added: fingerprint parameters, custom standardization,
    absolute stereo, duplicate filtering, tautomer duplicate filtering

- "Insert to JChem Table" component:
  > Duplicate filtering is table option, with override option for compatibility

- "Delete from JChem Base Table" component:
  > Bugfix: backward compatibility fix

Version 2.8.1, May 16, 2014

- Supported JChem versions:
  > 6.3.x : 6.3.0 and above
  > 6.2.x : 6.2.0 and above

- "ChemAxon Calculator" component:
  > Bugfix: backward compatibility fix for pKa "Mode" option

Version 2.8, April 27, 2014

- "ChemAxon Reactor" component : temporary disk space usage significantly reduced

- "Create JChem Base Table": extra fields can be specified for table creation

- "Delete from JChem Base Table": can accept cd_id values as input data

- "JChemSearch" component:

  > Bugfix: cd_id values were not returned if neither molecular structure
            nor data fields were requested

Version 2.7.1, February 13, 2014

- Supported JChem versions:
    > 6.2.x : 6.2.0 and above
    > 6.1.x : 6.1.0 and above

- "ChemAxon Document Extractor": support added for multiple File/URL input

- "ChemAxon HTML Molecular Table Viewer": aromatization option did not work for ChemAxon image option

- "ChemAxon HTML Molecular Table Viewer" and "ChemAxon Image from Molecule":
    Option "ChemAxon Image Options (De)aromatization" renamed to "ChemAxon Image Options Aromatization"

Version 2.7, January 10, 2014

- "ChemAxon Document Extractor" upgraded (in 6.1.x version only):
    > Support for a total 3 OSR tools (CLiDE, OSRA, Imago)
    > NOTE: parameter OSRA on/off parameter removed (!),
        replaced by "OSR Tool" with multiple options
    > Several new options added: start page, end page, OSR filtering,
        OSR timeout, acronyms, OLE object conversion and more
- "ChemAxon Document Extractor" fix:
    > Better compatibility for extraction from certain web sites

Version 2.6.4, September 29, 2013

- Supported JChem versions:
    > 6.1.x : 6.1.0 and above
    > 6.0.x : 6.0.0 and above

- "LibMCS Clustering" component updated (in 6.1.x version only):
    > Uses new clustering algorithm, faster execution time
    > New atom matching options: Radicals, Isotopes
    > Clustering method options changed: please "Replace with Latest Version"

Version 2.6.3, July 29, 2013

- Pipeline Pilot 8.5 or newer is required

- "ChemAxon HTML Molecular Table Viewer" component:
    > Bugfix: did not work with structure source property

Version 2.6.2, June 6, 2013

- "JChem for Excel Writer" component:
    > Vertical Alignment option added

Version 2.6.1, May 30, 2013

- "JChem for Excel Writer" component:
    > Bugfix: style setting for mixed case properties did not work

- "ChemAxon Calculator" component:
    > Option for micro pKa calculation (6.0 version only)

Version 2.6, May 23, 2013

- Supported JChem versions:
    > 6.0.x : 6.0.0 and above
    > 5.12.x : 5.12.0 and above

- "JChem for Excel Writer" component:
    > Option for overwrite / append behaviour
    > Options for formatting:
        - column width
        - horizontal alignment
        - text wrapping

- "ChemAxon Calculator" component:
    > Option for pKa correction library file (6.0 version only)

- "ChemAxon HTML Molecular Table Viewer" component:
    > Bugfix: exception in case the input contained no molecule

Version 2.5.2, April 16, 2013

- "JChem for Excel Writer" component:
    > Option for controlling the relative position of the structure column

    > Bugfix: data columns did not keep order

Version 2.5.1, March 7, 2013

- Supported JChem versions:
    > 5.12.x : 5.12.0 and above
    > 5.11.x : 5.11.0 and above

- "JChemSearch" component:
    > String parameter added for advanced search options

-"ChemAxon Standardize" component:
    > Also accepts molecule source as input

Version 2.5, December 25, 2012

- New component:
    > "ChemAxon Structure Checker"

Version 2.4.1, November 20, 2012

- JChem Base "Insert" component:
    > support for binary input formats added

Version 2.4, October 22, 2012

- Supported JChem versions:
    > 5.11.x : 5.11.0 and above
    > 5.10.x : 5.10.0 and above

- Pipeline Pilot 8.0 or newer is required

- New component:
    > "JChem for Excel Writer"

- "ChemAxon Structure Search Filter" bugfix:
    explicit H removal was not disabled during query structure standardization

- Support for binary structure formats in:
    "ChemAxon MolConverter", "ChemAxon Image From Molecule", "ChemAxon HTML Molecular Table Viewer"

- Example protocols updated / fixed

Version 2.3.3, June 29, 2012

- Supported JChem versions:
    > 5.10.x : 5.10.0 and above
    > 5.9.x : 5.9.0 and above

Version 2.3.2, April 20, 2012

- Improved error handling in "ChemAxon Calculator" and "Chemical Terms Calculator"

Version 2.3.1, March 15, 2012

- Improved error handling in "ChemAxon Ionize Molecule at pH"

Version 2.3, March 6, 2012

- Supported JChem versions:
    > 5.9.x : 5.9.0 and above
    > 5.8.x : 5.8.0 and above

- "ChemAxon Document Extractor" upgraded (in 5.9 version only):
    > Optical Structure Recognition support via OSRA
    > More options and result properties

- "Create JChem Base Table" creates the JChem property table if does not exist

- "Connection" accepts empty login and password

Version 2.2, February 18, 2012

- Supported JChem versions:
      > 5.8.x : 5.8.0 and above
      > 5.7.x : 5.7.0 and above

- New component:
      > "Delete from JChem Base Table"

Version 2.1, November 29, 2011

- Supported JChem versions:
    > 5.6.x : 5.6.0.1 and above
    > 5.7.x : 5.7.0 and above

- New component:
    > "ChemAxon Document Extractor"

Version 2.0, October 17, 2011

- New component:
    > "ChemAxon Formula Search Filter"

- "ChemAxon Reactor" component : speedup by multi-threading and more efficient reactant selection

- "ChemAxon Structure Search Filter" : improved error handling

- "ChemAxon Calculator" : more options for pKa data export and visualization

- "JChemSearch" : BigDecimal return type support added for hit data retrieval

Version 1.9, May 12, 2011

- Supported JChem versions:
    > 5.4.x : 5.4.0.1 and above
    > 5.5.x : 5.5.0 and above

- New component:
    > "ChemAxon Structure Search Filter"

- Added error handling options for Naming components

- "LibMCS Clustering" component: reduced memory need

- Minor improvements in error handling, installation, system information dialog

Version 1.8.1, January 17, 2011

- Restored Pipeline Pilot 7.5 compatibility

- "ChemAxon Reactor"

      > Fused reaction output option added
      > Reactant ratio option added
      > "ChemAxon_Last_Record_Tag" temporary property wasn't removed (bugfix)

- Obsolete component "CTAB from Molecule" removed

Version 1.8, December 21, 2010

- Requires JChem 5.3.0 or newer, JChem 5.4.x support added

- Pipeline Pilot 8.0 or newer is required

- New component:
      > "ChemAxon Fragmenter"

- Markush Enumeration options added:
      > coloring (scaffold, R-group)
      > homology group enumeration
      > MRV source output

- JChemSearch:
      > Markush hit reduction option (with homology expansion)
      > threw exception if NULL value was found in exported data columns (bugfix)

- "Create JChem Base Table": support for various table types

- Reactor: Synthesis Code also enabled for reaction output

- JChem Base "Insert" component:
      > structure source input did not work (bugfix)
      > did not accept Pipeline Pilot reactions (bugfix)

Version 1.7, July 1, 2010

- New components:

      > "ChemAxon Image From Molecule"

      > "ChemAxon HTML Molecular Table Viewer"

- "JChemSearch" (JChem Base):

    > Query-filtering (flow-trough) mode

    > Hit coloring and alignment

    > Various output options: PP molecule, MRV source, Original source

    > Search modes renamed according to new JChem terminology

    > "Duplicate" search type added

    > Fetching data fields of hit records from JChem Base table

    > Stereo search option updated

  - "Insert" (JChem Base):

    > Option to continue on error, problem structures directed to Fail port

    > Option to enable empty structures

  - "Chemical Terms Calculator" : byte[] result type supported

Version 1.6.2, February 18, 2010

- "ChemAxon MolConverter":

    > able to use ByteArray input as ASCII source (e.g. obtained from cd_structure field)

    > threw exception on properties not convertible to String ot StringArray (bugfix)

Version 1.6.1, January 8, 2010

- "ChemAxon Reactor" : keeps properties of reactants in products (option added)

- "ChemAxon MolConverter" : keeps properties also in file output

Version 1.6, August 31, 2009

- "ChemAxon 3D Conformers" component added

Version 1.5.1, June 9, 2009

- JChemSearch component returns result structures faster after search

Version 1.5, May 29, 2009

- Requires JChem / Marvin 5.1.3 or newer

- New components:

    > "ChemAxon MolConverter"

    > "ChemAxon Tautomerization"

    > "ChemAxon Markush Enumeration"

- "Chemaxon Reactor" component can now skip errors

- Error reporting was further improved. Error log always present at a default location.

- "Show ChemAxon Environment" component improved (displays info in Notepad).

Version 1.4, November 24, 2008

- "LibMCS Clustering" component added

- "Molecule to IUPAC Name" component added

- "Molecule from IUPAC Name" component added

- "ChemAxon Reactor" component:
    > New options added:
        - Synthesis Code generation
        - Unambiguous only (single) mode
        - Output reaction mapping
        - Options to ignore 3 types of reaction rules
    > Bugs fixed:
        - reaction output always contained all products
        - premature termination with "No Server Process" message for large input sets

- Utility protocol added for displaying ChemAxon software properties

Version 1.3.1, October 22, 2008

- Bugfix: ChemAxon Reactor only returned the first set of products for a
  given pair of reactants resulting in fewer products in certain cases.
- Bugfix: ChemAxon Calculator threw exception for inconsistent input
  structures in some cases
  (instead of just adding an error tag, and letting processing go on).

Version 1.3, July 11, 2008

 - Chemical Terms Calculator component added

 - New error reporting system: more informative error text, ability to write
   detailed error log to file if CHEMAXON_PP_LOG_DIR environment variable set.

 - Collection recompiled for Marvin / JChem 5.1 compatibility
   (while still maintaining JChem 3.2 / Marvin 4.1.2 backwards compatibility)

Version 1.2, March 5, 2008

 - ChemAxon Reactor component added

 - ChemAxon Standardize component upgraded:
      > more simple actions (checkboxes)
      > also accepts configuration string and configuration file for advanced
        tasks

 - JChem Base Insert:
      > Duplicate filtering option (using Pass and Fail ports)
      > Returns cd_id (primary key) values
      > Two input modes:
          - read structure source from a specified property
          - if property not specified uses PP input molecule
      > Insert into additional data fields (only for string column types yet)

  - JChemSearch
      > Several search options were added
      > Easier protocol integration and better performance due to concentrated
        functionality

- Create JChem Base Table component added
- Drop JChem Base Table component added

- General documentation upgrade of most components