JChem Base History of Changes

November 29th, 2019: JChem Base 19.25.0

No changes.

November 15th, 2019: JChem Base 19.24.0

No changes.

November 8th, 2019: JChem Base 19.23.0

No changes.

October 21th, 2019: JChem Base 19.22.0

Bugfixes

- **Search Engine**
  - Order sensitive search of reaction structures did not retrieve all hits.
  - Nitrogen in marked stereo configuration matched unmarked chiral center.
  - Small ring cis double bond stereo configurations were recognized as trans in case of trans perspective drawing in 3D.

Regeneration

Regeneration of Markush structures type tables is needed to use JChem 19.22.0. Please, regenerate Markush structures JChem tables after upgrade. The new table version is 19.22.0.0.

The version number of the other types of JChem tables has not changed.

Long Term Supported Release - December 9th, 2019: JChem Base 19.21.2 (Europium.2)

Long Term Supported Release - October 18th, 2019: JChem Base 19.21.1 (Europium.1)

October 7th, 2019: JChem Base 19.21.0

Regeneration

Full regeneration is needed to use JChem 19.21.0. Please, regenerate all JChem tables after upgrade. The new table version is 19.21.0.0

September 18th, 2019: JChem Base 19.20.0

Bugfixes

- **Search Engine**
  - Nitrogen in marked tetrahedral stereo chiral center matched Nitrogen in unmarked chiral center.

September 2nd, 2019: JChem Base 19.19.0

Regeneration

Full regeneration is needed to use JChem 19.19.0. Please, regenerate all JChem tables after upgrade. The new table version is 19.19.0.0

August 3rd, 2019: JChem Base 19.18.0

No changes.

July 16th, 2019: JChem Base 19.17.0

Regeneration

Full regeneration is needed to use JChem 19.17.0. Please, regenerate all JChem tables after upgrade. The new table version is 19.17.0.0

July 4th, 2019: JChem Base 19.16.0

No changes.

June 27th, 2019: JChem Base 19.15.0

No changes.

June 24th, 2019: JChem Base 19.14.0

No changes.

June 17th, 2019: JChem Base 19.13.0

No changes.

June 3rd, 2019: JChem Base 19.12.0

No changes.

May 21st, 2019: JChem Base 19.11.0

No changes.

May 7th, 2019: JChem Base 19.10.0

Bugfixes

- **JChem Base - DB functionalities**
  - Structures couldn't be inserted to the database if formula or sorted formula is very large.
  - CD_SMILES column may contain valence info as extended data, MolImporter cannot read such entries
- **Installation**
  - *jcman* and *jcmanager* gave false JVM version warnings for openjdk8.

Regeneration

Full regeneration is needed to use JChem 19.10.0. Please, regenerate all JChem tables after upgrade. The new table version is 19.10.0.0

April 8th, 2019: JChem Base 19.9.0

No changes.

March 18th, 2019: JChem Base 19.8.0

No changes.

Long Term Supported Release - July 30th, 2019: JChem Base 19.7.3 (Deuterium.3)

Long Term Supported Release - June 3rd, 2019: JChem Base 19.7.2 (Deuterium.2)

Long Term Supported Release - April 11th, 2019: JChem Base 19.7.1 (Deuterium.1)

March 8th, 2019: JChem Base 19.7.0

Improvements

- **Installation**
  - com.fasterxml.jackson.core:jackson-databind:2.9.8 dependency was removed from JChem Base

Regeneration

Regeneration of Markush structures type tables is needed to use JChem 19.7.0. Please, regenerate Markush structures JChem tables after upgrade. The new table version is 19.7.0.0.

The version number of the other types of JChem tables has not changed.

February 28th, 2019: JChem Base 19.6.0

No changes.

February 13th, 2019: JChem Base 19.4.0

No changes.

February 4th, 2019: JChem Base 19.3.0

No changes.

January 23rd, 2019: JChem Base 19.2.0

No changes.

January 11th, 2019: JChem Base 19.1.0

Bugfixes

- **JChem Base - DB functionalities**
  - Reaction fingerprint parameters at database import were not cached and caused slowdown

December 14th, 2018: JChem Base 18.30.0

Bugfixes

- **JChem Base - DB functionalities**

- Reactions that can't be mapped upon database import were repeatedly mapped during searching.

December 6th, 2018: JChem Base 18.29.0

No changes.

November 28th, 2018: JChem Base 18.28.0

No changes.

November 14th, 2018: JChem Base 18.27.0

No changes.

November 12th, 2018: JChem Base 18.26.0

No changes.

October 31st, 2018: JChem Base 18.25.0

No changes.

October 9th, 2018: JChem Base 18.24.0

No changes.

September 25th, 2018: JChem Base 18.23.0

No changes.

Long Term Supported Release - July 22nd, 2019: JChem Base 18.22.6 (Carbon.6)

Long Term Supported Release - May 8th, 2019: JChem Base 18.22.5 (Carbon.5)

Long Term Supported Release - February 1st, 2019: JChem Base 18.22.4 (Carbon.4)

Long Term Supported Release - December 19th, 2018: JChem Base 18.22.3 (Carbon.3)

Long Term Supported Release - November 29th, 2018: JChem Base 18.22.2 (Carbon.2)

Long Term Supported Release - September 25th, 2018: JChem Base 18.22.1 (Carbon.1)

September 7th, 2018: JChem Base 18.22.0

No changes.

August 29th, 2018: JChem Base 18.21.0

No changes.

August 21st, 2018: JChem Base 18.20.0

No changes.

August 10th, 2018: JChem Base 18.19.0

Bugfixes

- **JChem Web Services**
  - Substructure Checker results overwrote each other.

August 3rd, 2018: JChem Base 18.18.0

Regeneration

Full regeneration is needed to use JChem 18.18.0. Please, regenerate all JChem tables after upgrade. The new table version is 18.18.0.0

July 24th, 2018: JChem Base 18.17.0

No changes.

July 9th, 2018: JChem Base 18.16.0

No changes.

June 28th, 2018: JChem Base 18.15.0

Bugfixes

- **Search Engine**
  - False hits could be received when searching molecules with axial stereo information.

June 22th, 2018: JChem Base 18.14.0

Bugfixes

- **Search Engine**
  - Structural keys with explicit hydrogens and a single heavy atom caused missing hits when searching with queries with atom/bond list.

June 12th, 2018: JChem Base 18.13.0

No changes.

June 1st, 2018: JChem Base 18.12.0

Bugfixes

- **Search Engine**
  - Searching with alkenyl query homology atom could throw StackOverflowError.

May 23th, 2018: JChem Base 18.11.0

Bugfixes

- **Search Engine**
  - The hit display of a similarity search showed the query instead the target in some cases.
  - Queries with explicit H were searched far longer in isMatching than in findFirstHit.

April 13th, 2018: JChem Base 18.10.0

Bugfixes

- **Search Engine**
  - Search did not stop if totalSearchTimeoutLimit was reached.

April 4th, 2018: JChem Base 18.9.0

No changes.

Long Term Supported Release - November 29th, 2018: JChem Base 18.8.3 (Barium.3)

Long Term Supported Release - August 3rd, 2018: JChem Base 18.8.2 (Barium.2)

Long Term Supported Release - April 6th, 2018: JChem Base 18.8.1 (Barium.1)

March 14th, 2018: JChem Base 18.8.0

Regeneration

Full regeneration is needed to use JChem 18.8.0. Please, regenerate all JChem tables after upgrade. The new table version is 18.8.0.0

February 27th, 2018: JChem Base 18.5.0

Regeneration

Full regeneration is needed to use JChem 18.5.0. Please, regenerate all JChem tables after upgrade. The new table version is 18.5.0.0

February 13th, 2018: JChem Base 18.4.0

Bugfixes

- **Search Engine**
  - Structural keys were useless in screening as the structural fingerprint was always zero.

Known issues

- Missing hits can occur when a structural key contains explicit Hydrogen(s) and IMPLICIT_H_MATCHING_IGNORE search option is applied.

January 30th, 2018: JChem Base 18.3.0

Bugfixes

- **JChem Base - DB functionalities**
  - Creating a molFormat("smiles") CT column with JChemManager GUI was throwing an error.

January 18th, 2018: JChem Base 18.2.0

No changes.

January 12th, 2018: JChem Base 18.1.0

Improvements

- **Installation**
  - Oracle jdbc driver has been upgraded to ojdbc8-12.2.0.1
- **Search Engine**
  - Reaction search is sped up in cases of queries without reaction properties and mapping.
- **JChem Base - DB functionalities**
  - Command line tool *duplicatecheck* is provided for checking duplicates present in tables. Documentation

Bugfixes

- **Search Engine**
  - Cancelling a search query did not stop the search running in the background at Reaction and Markush type tables.
- **JChem Base - DB functionalities**
  - NullPointerException was thrown during the database import in case of some tetrahedral stereo molecules containing explicit Hydrogen atom on the stereo centers.
  - In Oracle, regeneration from pre 17.24.0 releases to 17.27.0, 17.28.0 and 17.29.0 fails; to 18.1.0 works.
- **JChem Web Services**
  - Data type of customer added columns for chemical terms automatically changed to predefined but not appropriate data types.

December 8th, 2017: JChem Base 17.29.0

Improvements

- **Installation**
  - JChem runs in Java 8 Environment from now on. Documentation

Bugfixes

- **Search Engine**
  - Duplicate structures could be inserted into tables with duplicate filtering true option if there were too many structures with the same hash code already in the database.
- **JChem Base - DB functionalities**
  - Known issue relating invalid SYS_* indexes on JCHEMPROPERTIES table in Oracle has been fixed.

Known issues

- In Oracle, upgrade of older versions than 17.24.0 can be executed only in two steps. 1st step: upgrade to 17.24.0 (or 17.25.0 or 17.26.0); 2nd step: upgrade to 17.29.0

Regeneration

Full regeneration is needed to use JChem 17.29.0. Please, regenerate all JChem tables after upgrade. The new table version is 17.29.0.0

November 9th, 2017: JChem Base 17.28.0

Bugfixes

- **Search Engine**
  - Peptide sequence file format was not handled correctly in the searches. From now on the 3-letter peptide format works in searches.
  - Duplicate search was extremely slow when the target structure contained charged hydrogen atom.

Known issues

- Invalid SYS_* indexes must be manually rebuilt on JCHEMPROPERTIES table in Oracle.
- In Oracle, upgrade of older versions than 17.24.0 can be executed only in two steps. 1st step: upgrade to 17.24.0 (or 17.25.0 or 17.26.0); 2nd step: upgrade to 17.28.0

October 26th, 2017: JChem Base 17.27.0

Improvements

- **JChem Base - DB functionalities**
  - In Oracle, the data type of the PROP_VALUE_EXT column in the JCHEMPROPERTIES table has been changed from LONG RAW to BLOB.

Bugfixes

- **Search Engine**
  - ArrayIndexOutOfBounds exception was thrown when an R-group-containing-molecule with polymers was searched with polymer matching option switched on.

Known issues

- Invalid SYS_* indexes must be manually rebuilt on JCHEMPROPERTIES table in Oracle.

- In Oracle, upgrade of older versions than 17.24.0 can be executed only in two steps. 1st step: upgrade to 17.24.0 (or 17.25.0 or 17.26.0); 2nd step: upgrade to 17.27.0

October 19th, 2017: JChem Base 17.26.0

No changes.

October 13th, 2017: JChem Base 17.25.0

Bugfixes

- **Search Engine**
  - Similarity search was slow when Chemical Terms filter was used.
  - Endless searches could happen with some homology groups in rare cases.

Long Term Supported Release - February 23th, 2018: JChem Base 17.24.3 (Argon.3)

Long Term Supported Release - February 16th, 2018: JChem Base 17.24.2 (Argon.2)

Long Term Supported Release - October 18th, 2017: JChem Base 17.24.1 (Argon.1)

September 22th, 2017: JChem Base 17.24.0

Bugfixes

- **Search Engine**
  - Tautomer duplicate search could give false results when aromatic rings were part of the tautomer region.
  - Stereo search could give false results in case of quaternary stereo centers where only one wedge bond was indicated.

Known issues

- Image generation in JChem Web Services might be very slow.

Regeneration

Full regeneration is needed to use JChem 17.24.0. Please, regenerate all JChem tables after upgrade. The new table version is 17.24.0.0

September 14th, 2017: JChem Base 17.23.0

Bugfixes

- **Search Engine**
  - In tables where tautomerize standardizer action was set, tautomer search could result missing hits.

Regeneration

Full regeneration is needed to use JChem 17.23.0. Please, regenerate all JChem tables after upgrade. The new table version is 17.23.0.0

September 1st, 2017: JChem Base 17.22.0

Bugfixes

- **Search Engine**
  - Duplicate / full fragment search combined with tautomer search could result failing hits.

Regeneration

Full regeneration is needed to use JChem 17.22.0. Please, regenerate all JChem tables after upgrade. The new table version is 17.22.0.0

August 18th, 2017: JChem Base 17.21.0

Improvements

- **Search Engine**
  - New separate homology groups has been introduced: Aryl, Heteroaryl, Heteroalicyclyl, Fusedheteroaryl, Fusedheteroalicyclyl. Documentation

Bugfixes

- **Search Engine**
  - Additional text notes of HeterosubstitutedAlkyl, Hydroxyalkyl and Haloalkyl homology groups were not handled correctly.

Regeneration

Regeneration of "Markush" type tables is needed to use JChem 17.21.0. Please, regenerate the "Markush" type JChem tables after upgrade. Their new table version is 17.21.0.0.

August 9th, 2017: JChem Base 17.20.0

No changes.

JChem Base 17.19.0

Not released.

August 3rd, 2017: JChem Base 17.18.0

No changes.

July 25th, 2017: JChem Base 17.17.0

No changes.

July 21st, 2017: JChem Base 17.16.0

No changes.

July 14th, 2017: JChem Base 17.15.0

No changes.

July 6th, 2017: JChem Base 17.14.0

Regeneration

Full regeneration is needed to use JChem 17.14.0. Please, regenerate all JChem tables after upgrade. The new table version is 17.14.0.0

June 20th, 2017: JChem Base 17.13.0

Bugfixes

- **Markush Search**
  - Existence of haloAlkyl, hydroxyAlkyl, or heteroSubstitutedAlkyl in Markush target blocked finding substructure search hits if the matching substructure was outside the homology region.

June 15th, 2017: JChem Base 17.12.0

No changes.

June 8th, 2017: JChem Base 17.11.0

No changes.

June 1st, 2017: JChem Base 17.10.0

Bugfixes

- **Search Engine**
  - Tautomer duplicate search missed hits in some rare cases. Versions 17.5.0 - 17.9.0 need manual regeneration in order to fix database searches influenced by this bug.

May 26th, 2017: JChem Base 17.9.0

No changes.

May 9th, 2017: JChem Base 17.8.0

No changes.

May 5th, 2017: JChem Base 17.7.0

Bugfixes

- **Search Engine**
  - Filtered search with maximum hit count caused missing hit.
  - Superstructure search could give missing or additional hits when query properties were present.

April 26th, 2017: JChem Base 17.6.0

Bugfixes

- **Search Engine**
  - The use of FilterQuery search option with FINE or more detailed logging failed with ArrayIndexOutOfBoundsException.

April 20th, 2017: JChem Base 17.5.0

Improvements

- **Installation**
  - New version numbering system has been introduced. Blog

Bugfixes

- **JChem Base - DB functionalities**
  - UpdateHandler sometimes changed autoCommit mode of Postgres connections.

Regeneration

Full regeneration is needed to use JChem 17.5.0. Please, regenerate all JChem tables after upgrade. The new table version is 17.5.0.1

April 3rd, 2017: JChem Base 17.4.3

Improvements

- **Installation**
  - Bundled MySQL JDBC driver changed to MariaDB JDBC driver.

March 27th, 2017: JChem Base 17.3.27

No changes.

JChem Base 17.3.20

Not released.

March 13th, 2017: JChem Base 17.3.13

Bugfixes

- **Search Engine**
  - Double bond stereo was not always taken into account in tautomer duplicate search of molecules containing H atoms with stereo information.
  - Tautomer duplicate search could give false negative results when valence property was present on an atom within the tautomer region.

JChem Base 17.3.6

Not released.

February 27th, 2017: JChem Base 17.2.27

No changes.

February 20th, 2017: JChem Base 17.2.20

No changes.

February 13th, 2017: JChem Base 17.2.13

No changes.

February 6th, 2017: JChem Base 17.2.6

No changes.

January 30th, 2017: JChem Base 17.1.30

No changes.

January 23rd, 2017: JChem Base 17.1.23

No changes.

January 16th, 2017: JChem Base 17.1.16

No changes.

January 9th, 2017: JChem Base 17.1.9

No changes.

January 2nd, 2017: JChem Base 17.1.2

Bugfixes

- **Search Engine**
  - Tautomer duplicate search, tautomer full structure and tautomer full fragment search in database could result missing hits.

Regeneration

Full regeneration is needed to use JChem 17.1.2. Please, regenerate all JChem tables after upgrade. The new table version is 17.1.2.0.

December 26th, 2016: JChem Base 16.12.26

No changes.

December 19th, 2016: JChem Base 16.12.19

Regeneration

Full regeneration is needed to use JChem 16.12.19. Please, regenerate all JChem tables after upgrade. The new table version is 16.12.19.0.

December 12th, 2016: JChem Base 16.12.12

No changes.

December 5th, 2016: JChem Base 16.12.5

Improvements

- **Search Engine**
  - Speed of database search has been increased by improving the selectivity in the screening search phase, especially in case of query structures with Generic query atoms or with Any bonds.

Regeneration

Full regeneration is needed to use JChem 16.12.5. Please, regenerate all JChem tables after upgrade. The new table version is 16.12.5.0.

November 28th, 2016: JChem Base 16.11.28

No changes.

November 21st, 2016: JChem Base 16.11.21

No changes.

November 14th, 2016: JChem Base 16.11.14

Bugfixes

- **Search Engine**
  - The tautomer duplicate and full structure search could have been very slow in case of large, highly symmetrical, and stereo configured molecules.

November 7th, 2016: JChem Base 16.11.7

New features and Improvements

- **Installation**
  - New installers are provided which differ from the old installers (up to version 16.10.31).
    - The new installer does not upgrade JChem installations created by any old installer, they must be uninstalled manually.
    - New home directory of JChem is called JChemSuite, by default.
    - No desktop icons are created for the GUI applications.
    - JChem Manager GUI can be started by JChemSuite/bin/jcmanager.exe.

October 31st, 2016: JChem Base 16.10.31

No changes.

October 24th, 2016: JChem Base 16.10.24

No changes.

October 17th, 2016: JChem Base 16.10.17

No changes.

October 10th, 2016: JChem Base 16.10.10

No changes.

October 3rd, 2016: JChem Base 16.10.3

Bugfixes

- **JChem Base - DB functionalities**

- Database import froze for molecules containing extreme number of rings.

September 26th, 2016: JChem Base 16.9.26

Bugfixes

- **Search Engine**
  - Similarity search for reactions returned false results.

Regeneration

Full regeneration is needed to use JChem 16.9.26. Please, regenerate all JChem tables after upgrade. The new table version is 16.9.26.0.

JChem Base 16.9.19

Not released.

September 12th, 2016: JChem Base 16.9.12

No changes.

September 5th, 2016: JChem Base 16.9.5

No changes.

August 29th, 2016: JChem Base 16.8.29

Bugfixes

- **Search Engine**
  - Wedge bonds were not always recognized within the rings causing missing hits in search.

Regeneration

Full regeneration is needed to use JChem 16.8.29. Please, regenerate all JChem tables after upgrade. The new table version is 16.8.29.0.

August 22th, 2016: JChem Base 16.8.22

No changes.

August 15th, 2016: JChem Base 16.8.15

No changes.

August 8th, 2016: JChem Base 16.8.8

Bugfixes

- **R-group decomposition**
  - Tetrahedral stereo information at the attachment points of the R-groups was lost.

August 1st, 2016: JChem Base 16.8.1

Bugfixes

- **JChem Base - DB functionalities**
  - Reacting center query properties were not correctly persisted in the database.

Regeneration

Regeneration of "Query structures" and "Any structures" type tables is needed to use JChem 16.8.1. Please, regenerate the "Query structures" and "Any structures" type JChem tables after upgrade. Their new table version is 16.8.1.0.

July 25th, 2016: JChem Base 16.7.25

No changes.

July 18th, 2016: JChem Base 16.7.18

No changes.

July 11th, 2016: JChem Base 16.7.11

No changes.

July 4th, 2016: JChem Base 16.7.4

Regeneration

Full regeneration is needed to use JChem 16.7.4. Please, regenerate all JChem tables after upgrade. The new table version is 16.7.4.0.

June 27th, 2016: JChem Base 16.6.27

New features and Improvements

- **Search Engine**
  - Support of undefined R-atoms around tetrahedral stereo centers on query side is introduced.

June 20th, 2016: JChem Base 16.6.20

No changes.

June 13th, 2016: JChem Base 16.6.13

No changes.

June 6th, 2016: JChem Base 16.6.6

No changes.

May 30th, 2016: JChem Base 16.5.30

Bugfixes

- **JChem Base - DB functionalities**
  - Cache registrations were not removed if multiple caches became invalid at the same time.

May 23th, 2016: JChem Base 16.5.23

New features and Improvements

- **JChem Web Services**
  - Searching by JChem Oracle Cartridge is supported from now on.

Regeneration

Full regeneration is needed to use JChem 16.5.23. Please, regenerate all JChem tables after upgrade. The new table version is 16.5.23.0.

May 16th, 2016: JChem Base 16.5.16

Bugfixes

- **Search Engine**
  - Syn, anti, endo, exo information were calculated for ambiguous cases resulting inconsistent search results.
  - Chemical elements with valence 1 were handled incorrectly in searches on query side, resulting loss of hits.

Regeneration

Full regeneration is needed to use JChem 16.5.16. Please, regenerate all JChem tables after upgrade. The new table version is 16.5.9.0.

May 2nd, 2016: JChem Base 16.5.2

No changes.

April 25th, 2016: JChem Base 16.4.25

Bugfixes

- **Search Engine**
  - 'Duplicate keys in cache' error has been fixed. Affected versions are from 15.5.11.

April 18th, 2016: JChem Base 16.4.18

No changes.

April 11th, 2016: JChem Base 16.4.11

No changes.

April 4th, 2016: JChem Base 16.4.4

No changes.

March 28th, 2016: JChem Base 16.3.28

No changes.

March 21st, 2016: JChem Base 16.3.21

No changes.

March 14th, 2016: JChem Base 16.3.14

Bugfixes

- **Search Engine**
  - *Substitution count* query property on atoms was not correctly handled causing missing hits in duplicate search.

March 7th, 2016: JChem Base 16.3.7

Bugfixes

- **Search Engine**
  - Properties of homology groups were not checked during duplicate search.

February 29th, 2016: JChem Base 16.2.29

No changes.

February 22nd, 2016: JChem Base 16.2.22

Bugfixes

- **JChem Base - DB functionalities**
  - Import of chemical structures in InChI format could have been frozen in case of incorrect structures.
  - Due to a bugfix in the aromatization, full regeneration is needed.

Regeneration

Full regeneration is needed to use JChem 16.2.22. Please, regenerate all JChem tables after upgrade. The new table version is 16.2.22.0.

February 15th, 2016: JChem Base 16.2.15

No changes.

February 8th, 2016: JChem Base 16.2.8

Bugfixes

- The **Known issues** of version 16.2.1 has been fixed.

February 1st, 2016: JChem Base 16.2.1

Known issues

- Some slowdown in import and in searches can be experienced.
- Tables must be regenerated if tautomer duplicate and tautomer full structures searches are planned to be executed.

January 25th, 2016: JChem Base 16.1.25

No changes.

January 18th, 2016: JChem Base 16.1.18

Bugfixes

- **Search Engine**
  - Duplicate search with *ignoreCumuleneOrRingCisTransStereo:n* or *ignoreAxialStereo:n* could have caused ArrayIndexOutOfBondsException if the query molecule contained an explicit hydrogen.
  - An ArrayIndexOutOfBoundsException could have been thrown for duplicate search with molecule containing a link node if this node had more than two ligands.

January 11th, 2016: JChem Base 16.1.11

No changes.

January 4th, 2016: JChem Base 16.1.4

Bugfixes

- **Markush Search**
  - Homology aliases were not handled correctly in duplicate search.

December 14th, 2015: JChem Base 15.12.14

No changes.

December 7th, 2015: JChem Base 15.12.7

No changes.

November 30th, 2015: JChem Base 15.11.30

- License is no longer required for creating Markush tables, only for importing structures.

November 23rd, 2015: JChem Base 15.11.23

Bugfixes

- **Search Engine**
  - Aromatic stereo bonds were not imported properly from SMARTS strings.

Regeneration

Full regeneration is needed to use JChem 15.11.23. Please, regenerate all JChem tables after upgrade. The new table version is 15.11.23.0.

November 16th, 2015: JChem Base 15.11.16

No changes.

November 9th, 2015: JChem Base 15.11.9

Bugfixes

- **Search Engine**
  - Duplicate search did not consider link node outer atoms.
  - Some hits were missing when there was s<n> query property on explicit hydrogen atom.
  - False hits were resulted in duplicate and full structure search in the case of target structures with separated hydrogen ion/molecule fragments.

November 2nd, 2015: JChem Base 15.11.2

No changes.

October 26th, 2015: JChem Base 15.10.26

No changes.

October 19th, 2015: JChem Base 15.10.19

No changes.

October 12th, 2015: JChem Base 15.10.12

No changes.

October 5th, 2015: JChem Base 15.10.5

Regeneration

Regeneration of "Reactions" type tables is needed to use JChem 15.10.5. Please, regenerate the "Reactions" type JChem tables after upgrade. Their new table version is 15.10.5.0.

September 28th, 2015: JChem Base 15.9.28

Regeneration

Regeneration of "Query structures" type tables is needed to use JChem 15.9.28. Please, regenerate the "Query structures" type JChem tables after upgrade. Their new table version is 15.9.28.0.

September 21th, 2015: JChem Base 15.9.21

No changes.

September 14th, 2015: JChem Base 15.9.14

Improvements

- **Search Engine**
  - The default value of the search option *vague bond level* is modified. Its new default is *half*. Documentation

September 7th, 2015: JChem Base 15.9.7

No changes.

August 31st, 2015: JChem Base 15.8.31

Bugfixes

- **Search Engine**
  - False positive polymer hits could be experienced when searching with particular ring structures.
  - IndexOutOfBoundsException was thrown by targets with attached data and monomer group.

August 24th, 2015: JChem Base 15.8.24

Bugfixes

- **Search Engine**
  - Pseudo atom with *UnknownGroup* alias string was not recognized as homology group.

August 17th, 2015: JChem Base 15.8.17

No changes.

August 10th, 2015: JChem Base 15.8.10

Bugfixes

- **Search Engine**
  - Query structures having atoms with explicit hydrogen and any atom (A) neighbours could result false positive hits.

August 3rd, 2015: JChem Base 15.8.3

No changes.

July 27th, 2015: JChem Base 15.7.27

Bugfixes

- **JChem Base - DB functionalities**
  - Date type data from an sdf file could not be imported into Date type column of a JChem table in Oracle.
- **Search Engine**
  - ClassCastException was thrown at search when a target reaction in an *Any structures* type table contained R-groups.

July 20th, 2015: JChem Base 15.7.20

Improvements

- **JChem Base - DB functionalities**
  - Search speed up can be achieved in JChem tables filled with numerous structures having small, stereo-configured rings. To attain this speed-up, manual table regeneration is needed.

- **Search Engine**
  - R-group bridges are supported in Markush and query structures.
  - Reserved memory of database search engine have been increased from 10 - 100 MB to 250 - 1000 MB. API documentation

July 13th, 2015: JChem Base 15.7.13

No changes.

July 6th, 2015: JChem Base 15.7.6

Improvements

- **Search Engine**
  - New homology group - Heterocyclyl - is introduced. Documentation

June 29th, 2015: JChem Base 15.6.29

Bugfixes

- **Markush Search**
  - Search hit coloring was inaccurate in case of Markush targets with position variation bonds.
- **Search Engine**
  - JChemSearch could block for searches throwing exception.

Deprecations

- **Removals**
  - Function UpdateHandler#getPreferredTableType(Molecule) is removed. Please read our documentation in order to select the table type to use.

June 22nd, 2015: JChem Base 15.6.22

Bugfixes

- **JChem Base - DB functionalities**
  - NumberFormat exception was thrown during import in case of molecule with large coordinate value.
- **Search Engine**
  - Query atom property '(A)' was removed by default standardizer action 'aromatize:g' causing false search results.
  - Searches reaching their timeout limits could run into deadlock situation.

Deprecations

- **Search Engine**
  - JChemSearch#setTimeout(int seconds) has been deprecated. JChemSearchOptions#setTotalSearchTimeoutLimitMilliseconds(int milliseconds) should be used instead. **Note**: the new method handles its parameter as milliseconds.
  - JChemSearch#getTimeout() has been deprecated. JChemSearchOptions#getTotalSearchTimeoutLimitMilliseconds() should be used instead. **Note**: the new method returns milliseconds instead of seconds.
  - Previously deprecated method JChemSearchOptions#setMaxTime() should be replaced by JChemSearchOptions#setTotalSearchTimeoutLimitMilliseconds() in order to limit the total timeout on multiple targets. The timeout limit for a search on a single target should be set via SearchOptions#setTimeoutLimitMilliseconds().
  - Previously deprecated method JChemSearchOptions#getMaxTime() should be replaced by JChemSearchOptions#getTotalSearchTimeoutLimitMilliseconds() in order to retrieve the total timeout limit on multiple targets. The timeout limit for a search on a single target should be retrieved via SearchOptions#getTimeoutLimitMilliseconds().

June 15th, 2015: JChem Base 15.6.15

No changes.

June 8th, 2015: JChem Base 15.6.8

Upgrade

- IKVM.NET version has been upgraded to 7.4.

June 1st, 2015: JChem Base 15.6.1

Bugfixes

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search may have frozen for big tables.

May 25th, 2015: JChem Base 15.5.25

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

May 18th, 2015: JChem Base 15.5.18

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

May 11th, 2015: JChem Base 15.5.11

Bugfixes

- **JChem Base - DB functionalities**
  - Cache load was slow on big tables in some cases.

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

May 4th, 2015: JChem Base 15.5.4

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

April 27th, 2015: JChem Base 15.4.27

Bugfixes

- **JChem Base - DB functionalities**
  - JChem now accepts yyyy-mm-dd date format too during import and not only mm/dd /yyyy.
- **Search Engine**
  - ArrayIndexOutOfBoundsException may have occurred when handling molecules containing multiple groups.

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

April 20th, 2015: JChem Base 15.4.20

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

April 13th, 2015: JChem Base 15.4.13

Bugfixes

- **Search Engine**
  - Parallel execution of StandardizerMolSearch with the same query instance could cause NullPointerException.

Known issues

- **Installation**
  - Four needless jar files are included in the installers: hamcrest-core-1.3.jar, jackson-core-asl-1.9.13.jar, jackson-mapper-asl-1.9.13.jar, and junit-4.11.jar.

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

April 6th, 2015: JChem Base 15.4.6

Improvements

- **Search Engine**

- Molecular descriptor caching can be switched on resulting in a 1-2 orders of magnitude speed-up of similarity search with molecular descriptors. Documentation

Bugfixes

- **Search Engine**
  - HitDisplayTool.getHitIndexes() method returned null instead of correct atom indexes.
  - Descriptor similarity search always used the first metric of the descriptor. Now the dissimilarity metric option is considered.

Deprecations

- **Removals**
  - Public constants in chemaxon.jchem.version.VersionInfo were removed; use public functions of the same class instead.

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

March 30th, 2015: JChem Base 15.3.30

Deprecations

- **Search Engine**
  - JChemSearchOptions#setMaxTime() and JChemSearchOptions#getMaxTime() has been deprecated.

Known issues

- **JChem Base - DB functionalities**
  - Import with duplicate filtering or duplicate search might be frozen for big tables.

March 23th, 2015: JChem Base 15.3.23

Bugfixes

- **Search Engine**
  - The known slow-down in similarity search from previous week has been eliminated.

Known issues

- **JChem Base - DB functionalities**

- Import with duplicate filtering or duplicate search might be frozen for big tables.

March 16th, 2015: JChem Base 15.3.16

Known issues

- **Search Engine**
  - Similarity search has a slow-down of about 50-60% compared to the previous releases.

March 9th, 2015: JChem Base 15.3.9

Regeneration

Full regeneration is needed to use JChem 15.3.9. Please, regenerate all JChem tables after upgrade. The new table version is 15.3.9.0.

March 2nd, 2015: JChem Base 15.3.2

Regeneration

Full regeneration is needed to use JChem 15.3.2. Please, regenerate all JChem tables after upgrade. The new table version is 15.3.2.0.

February 23th, 2015: JChem Base 15.2.23

Bugfixes

- **Search Engine**
  - Mapped reactions did not hit unmapped ones in case of memory searches.

February 16th, 2015: JChem Base 15.2.16

Bugfixes

- **Markush Search**
  - Coloring of bonds in R-groups of Markush hits was not correct.

February 9th, 2015: JChem Base 15.2.9

No changes.

February 2nd, 2015: JChem Base 15.2.2

Bugfixes

- **Search Engine**
  - Mapped reactions did not hit unmapped ones in case of memory searches.
  - Query structure having double bond in symmetric ring system and explicit Hydrogen atom on the ring system failed to match to the corresponding structure without the explicit Hydrogen atom using FULL match, stereo search type set to STEREO_SPECIFIC, double bond stereo matching set to DBS_ALL, and stereo model set to STEREO_MODEL_GLOBAL.

January 26th, 2015: JChem Base 15.1.26

Improvements

- **Search Engine**
  - Combined searches have been speed-up. Blog

Bugfixes

- **JChem Base - DB functionalities**
  - UnsupportedOperationException was thrown in database import of peptide sequences containing amino acids with three attachment points.

- **Search Engine**
  - Reaction search on reaction tables caused missing hits in case of basic aromatization.
- **JChem API**
  - The accidental API change of the previous release which rendered the constants of `chemaxon.jchem.db.TableTypeConstants` unusable in `switch` statements (since they became non-compile time constants) has been reverted.

January 19th, 2015: JChem Base 15.1.19

Bugfixes

- **JChem Base - DB functionalities**
  - Targets that have list atoms or not-list atoms with empty definition lists caused errors during search. These structures won't be allowed to be imported/indexed.

- **Search Engine**
  - [!#1;!#6] smarts atom matched isotopic hydrogens.
  - NullPointerException was thrown during search when disconnected R-group definitions were found in a target structure.

Known issues

- **JChem API**
  - An accidental API breaking change has been introduced in `chemaxon.jchem.db.TableTypeConstants` which may cause compile error if table type constants are used in the `case` clause of `switch` statements. This change will be reverted in the next release.

January 12th, 2015: JChem Base 15.1.12

No changes.

January 5th, 2015: JChem Base 15.1.5

Bugfixes

- **Search Engine**
  - JChemSearch.getHitsAsMolecules() returned standardized structures for Superstructure search.

December 15th, 2014: JChem Base 14.12.15

No changes.

December 8th, 2014: JChem Base 14.12.8

No changes.

December 1st, 2014: JChem Base 14.12.1

Bugfixes

- **Search Engine**
  - NullPointerException was thrown when search contained Markush structure with R-atom in a ring system with bicyclo stereo information.

November 24th, 2014: JChem Base 14.11.24

No changes.

November 17th, 2014: JChem Base 14.11.17

No changes.

November 10th, 2014: JChem Base 14.11.10

Bugfixes

- **JChem Base - DB functionalities**
  - Molfiles with brackets in their first line could be erroneously imported into JChem tables.

November 3rd, 2014: JChem Base 14.11.3

Bugfixes

- **Search Engine**
  - Some structures with multiple syn-anti stereo configurations didn't match themselves.

Deprecations

- **Removals from the public API**
  - Methods with NOV_01_2014 RemovalDate were removed. The following classes are affected:
    - `chemaxon.jchem.db.Exporter`
    - `chemaxon.jchem.db.StructureTableOptions`
    - `chemaxon.jchem.db.TableInfo`

October 27th, 2014: JChem Base 14.10.27

No changes.

October 20th, 2014: JChem Base 14.10.20

Bugfixes

- **Markush search**
  - Hydrogen atoms in nested R-group definitions were not correctly handled in full searches and searches with queries having s* property.
  - False hits could be resulted in Markush searches when atoms of the query structure had s* query atom property and position variation bonds were present in the target structures. The previous solution was further improved.

Regeneration

Full regeneration will be required in case of "Any structures" and "Query structures" type JChem tables after upgrade. Their new table version will be 14.10.20.0.

October 13th, 2014: JChem Base 14.10.13

Bugfixes

- **Search Engine**
  - Hydrogen query properties of atoms within tetrahedral stereo configuration were not exported correctly to SMARTS causing false hits.

Regeneration

Full regeneration is needed in case of specific tables to use JChem 14.10.13. Please, regenerate "Any structures" and "Query structures" type JChem tables after upgrade.

October 6th, 2014: JChem Base 14.10.6

Bugfixes

- **Installation/deployment**
  - JChem Manager could not be launched by 'jcman.bat' on Windows Prompt.
- **Markush search**
  - False hits could be resulted when atoms of the query structure had s* query property and position variation bonds were present in the target structures.

September 29th, 2014: JChem Base 14.9.29

Bugfixes

- **Installation/deployment**
  - Command line options (switches) of 'jcman.bat' did not work correctly on Windows Prompt.

Known issues

- **Installation/deployment**
  - JChem Manager cannot be launched by 'jcman.bat' on Windows Prompt. Recommended workaround: apply the desktop icon of JChem Manager or start by JChemManager.exe.

September 22th, 2014: JChem Base 14.9.22

New features and Improvements

- **Search Engine**
  - The performance of tautomer search has been increased resulting even 100% speed-up in some cases of tautomer substructure search.

Bugfixes

- **JChem Base - DB functionalities**
  - ConnectionHandler incorrectly stated that it closes open connection in its finalize() method - warning message has been changed.

September 15th, 2014: JChem Base 14.9.15

No changes.

September 8th, 2014: JChem Base 14.9.8

Bugfixes

- **Search Engine**
  - Matching of structures with ring cis/trans stereo configuration could fail. Forum topic
  - Searching with query side homology groups could cause ClassCastException in version 14.9.1

September 1st, 2014: JChem Base 14.9.1

Bugfixes

- **JChem Base - DB functionalities**
  - Oracle locking exception during database modification in JChem version 14.8.25 fixed.

Regeneration

Full table regeneration is needed to use JChem 14.9.1. Please, regenerate all JChem tables after upgrade. The new table version is 14.9.1.0.

August 25th, 2014: JChem Base 14.8.25

No changes.

August 18th, 2014: JChem Base 14.8.18

No changes.

August 11th, 2014: JChem Base 14.8.11

Bugfixes

- **JChem Base - DB functionalities**
  - Not fully mapped reactions could be imported incorrectly.

August 4th, 2014: JChem Base 14.8.4

New features and Improvements

- **JChem Base - DB functionalities**
  - Oracle 9i is not supported anymore.
- **Search Engine**
  - The accuracy of Maximum Common Substructure (MCS) search was improved in case of connected mode.

Bugfixes

- **Search Engine**
  - Reaction center bond query properties were not correctly handled during the evaluation of exact bond matching.
  - Stereo marking "marked" of double bonds was not checked during searching with exact bond matching option.

July 28th, 2014: JChem Base 14.7.28

Bugfixes

- **Search Engine**
  - Some structures could not find an identical structure if axial stereo search option was switched on. Forum topic

July 21st, 2014: JChem Base 14.7.21

No changes.

July 14th, 2014: JChem Base 14.7.14

No changes.

July 7th, 2014: JChem Base 14.7.7

New features and Improvements

- **JChem Base - DB functionalities**
  - Support of VMN format of Markush structures is disabled.
  - JTF format is not supported anymore.
- **Search Engine**
  - New homology groups - heterosubstitutedAlkyl, haloalkyl, and hydroxyalkyl - are introduced. Documentation
  - Allene stereo search option is renamed to cumulene or ring cis-trans stereo as this describes the behavior of the option better. Documentation
  - Full structure and full fragment structure search is not allowed on query table type.
  - Markush MCS search type has been removed from JChem Base search types.

Bugfixes

- **JChem Base - DB functionalities**
  - Export from big JChem tables threw out of memory exception on PostgreSQL database.
  - NullpointerException was thrown during chemical terms calculation in database.
  - Any (A) and hetero (Q) atoms could not be saved in Markush tables.
- **Search Engine**
  - Explicit H sometimes did not match AH, MH, QH in case of markush searches.
  - Any (A) and hetero (Q) atoms could not be used on the target side in memory Markush searches.
  - Structures with explicit hydrogen could throw exception for allene and axial searches

Regeneration

Full table regeneration is needed to use JChem 14.7.7. Please, regenerate all JChem tables after upgrade. The new table version is 14.7.7.0.

Older versions

Please visit this page for History of changes relating older JChem versions.