

Standardizer History of Changes

LTS Release - October 18th, 2019: 19.21.1 Standardizer (Europium.1)

No changes

October 7th, 2019, Standardizer 19.21.0

Bugfixes

- HashMap creation in the constructor slowed down standardization and the map wasn't used in most of the use cases

September 2nd, 2019, Standardizer 19.19.0

Bugfixes

- Cloning Clean2DAction will now create a proper clone of TemplateBasedClean

June 20th 2019, Standardizer 19.14

Bugfixes

- NullPointerException is thrown for some D-substituted compounds during standardisation
- Valence checking error causes normal canonical tautomer generation to fail during standardisation of some salt compounds

May 30th 2019, Standardizer 19.12.0

Bugfixes

- Fixes for the normal canonical tautomer generation

May 3rd 2019, Standardizer 19.10.0

Bugfixes

- False negative tautomer search hit for some molecules due to incorrect generic tautomer pairs

LTS Release - April 11th, 2019: 19.7.1 Standardizer (Deuterium.1)

No changes

April 8th 2019, Standardizer 19.9.0

Bugfixes

- Incorrect generic tautomer pairs where generated during tautomer search for certain molecules

March 8th 2019, Standardizer 19.7.0

No changes

February 1st 2019, Standardizer 19.4.0

Bugfixes

- Improved canonical tautomer generation

December 13th 2018, Standardizer 18.30.0

Bugfixes

- Incorrect standardized forms of some ChemBL compounds and salts
- Fixing some Exception in charge calculations during standardization

LTS Release - September 25th, 2018: 18.22.1 Standardizer (Carbon.1)

September 5th 2018, Standardizer 18.22.0

Bugfixes

- Incorrect Exception is thrown when molecule with valence error is standardized

August 24th 2018, Standardizer 18.21.0

Bugfixes

- Amine compounds lose stereo flags during tautomerization in standardization processes (in Standardizer)
- H atom is added to the generated resonant structure of heterocyclic compounds during standardization (in Standardizer)
- Incorrect standardized (normal canonical tautomer) forms of stereoisomers of sulphur compounds

August 1st, 2018: Standardizer 18.18.0

Bugfixes

- De-aromatization of a large ring with N fails
- Standardization (tautomerization) results of the same molecule coming from DB sources are different

February 13th, 2018: Standardizer 18.4.0

Bugfixes

- Command Line Interface problem: Only the user interface can be started from command prompt.

December 5th, 2016: Standardizer 16.12.5

Bugfixes

- Strip salts action can be applied to exact matches considering also the explicit H cases.

November 28th, 2016: Standardizer 16.11.28

Bugfixes

- Strip salts action was changed to remove salts only in case of exact isotope matching.

July 25th, 2016: Standardizer 16.7.25

Bugfixes

- Error in template based clean of reactions was fixed.

September 14th, 2015: Standardizer 15.9.14

Improvements

- Standardizer command line application returns proper exit status code if Standardizer license is missing or is invalid.

June 22th, 2015: Standardizer 15.6.22

Bugfixes

- Strip salts action doesn't remove all components from the molecule. It leaves at least one component, even if it is a salt defined in the salt dictionary.

May 11th, 2015: Standardizer 15.5.11

Bugfixes

- Mixture brackets were removed when *Transform* action modified a structure inside the mixture brackets.

April 13th, 2015: Standardizer 15.4.13

Bugfixes

- *Ungroup S-groups* action removed coordinate bonds from ferrocene.

February 2nd, 2015: Standardizer 15.2.2

Bugfixes

- Bugfixes in *Clean 2D* action.

January 19th, 2015: Standardizer 15.1.19

Bugfixes

- *Partial 2D clean* (*Clean 2D* action) did not work.
- *Clean 3D* action did not work in Standardizer application and Standardizer command line application. *Clean 3D* did not work via API when final clean was invoked.

November 17th, 2014: Standardizer 14.11.17

Bugfixes

- *Clean 2D* action options were not shown in Standardizer configuration editor.

November 10th, 2014: Standardizer 14.11.10

Bugfixes

- Renaming *Transform* actions did not work in some cases. [\[error report\]](#)

August 4th, 2014: Standardizer 14.8.4

Bugfixes

- Some standardizer actions (*Transform*, *Strip Salts*, *Remove Solvents*) required *Structure Search* license besides *Standardizer* license.

July 21th, 2014: Standardizer 14.7.21

New features and Improvements

- *Convert Wedge Interpretation* standardizer action was removed from Standardizer. Remove it from all of your standardizer configurations.

July 7th, 2014: Standardizer 14.7.7

New features and Improvements

- More convenient solvent removal with the new *Remove Solvents* action.

Bugfixes

- Standardizer requires significantly less memory. Occasional out of memory errors were eliminated.
- GUI layout fixes.

Please visit [this page](#) for History of changes relating older JChem versions.