

Structure Checker History of Changes

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

No changes

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

No changes

October 9th, 2018: Structure Checker 18.24.0

Bugfixes

- Pipe errors of Structure Checker

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

No changes

February 13th, 2018: Structure Checker 18.4.0

Bugfixes

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

August 1st, 2017: Structure Checker 17.18.0

Bugfixes

- Overlapping Atom Checker does not detect those atoms which are just too close but actually do not overlap.

October 3rd, 2016: Structure Checker 16.10.3

Bugfixes

- *Multicenter Checker* will not detect the endpoint of a position variation bond as multicenter.

September 26th, 2016: Structure Checker 16.9.26

Improvements

- A list of **excluded** atom labels can be specified for *Pseudo Atom Checker*.

November 9th, 2015: Structure Checker 15.11.9

Improvements, deprecations

- *Wedge Error Checker* was replaced by [Incorrect Tetrahedral Stereo](#), [Non-standard Wedge Scheme](#), and [Non-stereo Wedge Bond](#) checkers.
- *Wedge Error Checker* is deprecated.

August 24th, 2015: Structure Checker 15.8.24

Improvements

- Additional improvements in *Wedge Error Checker* and *Clean Wedge Fixer*.

August 3rd, 2015: Structure Checker 15.8.3

API changes

- `chemaxon.checkers.runner.BasicCheckerRunner` was removed from the public API. Use [AdvancedCheckerRunner](#).

July 6th, 2015: Structure Checker 15.7.6

Bugfixes

- *Wedge Error Checker* didn't detect non-stereo wiggly bonds.

Improvements

- *Clean Wedge Fixer* converts non-stereo wiggly bonds to single bonds.

June 22th, 2015: Structure Checker 15.6.22

Bugfixes

- *Solvent Checker* threw exception if input molecule couldn't be converted to SMILES format.

April 13th, 2015: Structure Checker 15.4.13

New features

- New checker: [Brackets Checker](#).

January 26th, 2015: Structure Checker 15.1.26

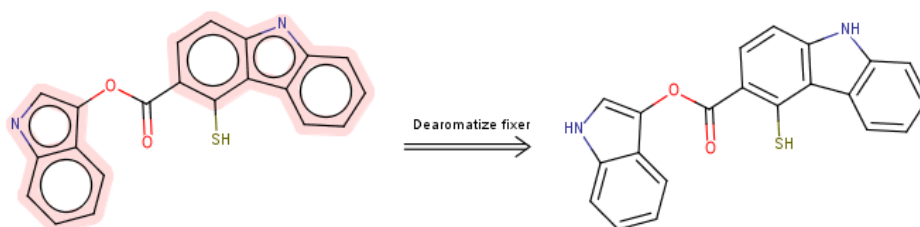
Bugfixes

- *Wedge Error Checker* didn't always agree with *Wedge Clean Fixer*. From now on the molecules fixed by *Wedge Clean Fixer* are accepted as correct by *Wedge Error Checker*.

January 12th, 2015: Structure Checker 15.1.12

Improvements

- Aromaticity error fixing improvements: *Dearomatize* and *Rearomatize* fixers can fix aromaticity errors in heteroaromatic rings (containing only carbons and nitrogens) in unambiguous cases.



Bugfixes

- *Bond Angle Checker* did not accept some bond angles as correct. Bonds connected to a ring were affected.

January 5th, 2015: Structure Checker 15.1.5

Bugfixes

- From now on *Rare Element Checker* will not detect deuterium (D) and tritium (T) as rare element.

November 17th, 2014: Structure Checker 14.11.17

Bugfixes

- *Chiral Flag Error Checker* did not report invalid chiral flag on achiral molecules.

October 27th, 2014: Structure Checker 14.10.27

New features and Improvements

- New checker: *R-group Bridge Error Checker*.
- *R-group Attachment Error Fixer* improvements:

- removes superfluous attachment points,
- can fix errors in R-group definitions having multiple equivalent candidates for the addition or removal of the attachment point(s),
- can fix structures containing contracted abbreviated groups,
- can handle R-group bridges.

October 6th, 2014: Structure Checker 14.10.6

Bugfixes

- *Circular R-group Reference Checker* failed to identify some circular references
- *Missing R-group Checker* did not identify unnumbered R-group as missing

July 21th, 2014: Structure Checker 14.7.21

New features and Improvements

- *OCR Error Checker* was improved, now it identifies optical structure recognition errors better
- "Discard OCR errors" option was removed from Structure Checker application and `structurechecker` command line application. Use OCR Error Checker.

Bugfixes

- *Overlapping Bond Checker* detected some non-overlapping bonds as overlapping [[error report](#)]

July 7th, 2014: Structure Checker 14.7.7

New features and Improvements

- Less invasive fix of bond length errors and bond angle errors with newly introduced *Bond Length Fixer* and *Bond Angle Fixer*.

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