# Calculator Plugins History of Changes

## 11th July 2019, Calculator Plugins, 19.17

### New features and improvements

- New Required HLB calculation in the HLB Predictor and its integration into MarvinSketch and cxcalc

## 20th June 2019, Calculator Plugins, 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

### New features and improvements

- Varying assignment of close $pK_a$ values in symmetric molecules with many $pK_a$ values

## 30th May 2019, Calculator Plugins, 19.12.0

### Bugfixes

- fixes for the normal canonical tautomer generation

## 17th May 2019, Calculator Plugins, 19.11.0

### New features and improvements

- Improved MolecularFormulas and Elemental Analysis API

## 3rd May 2019, Calculator Plugins, 19.10.0

### Bugfixes

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

## 29th March 2019, Calculator Plugins, 19.9.0

### Bugfixes

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

### New features and improvements

- Improved pKa and tautomer calculations for certain molecules

## 25th February 2019, Calculator Plugins, 19.6.0

### New features and improvements

- the *Protect Charge* option of the tautomer generation is automatically adjusted in the case of dynamic $pK_a$ calculation

## 11th February 2019, Calculator Plugins, 19.4.0

### Bugfixes

- Quaternary pyridine effect on phenol is improved for the $pK_a$ calculation
- Improved canonical tautomer generation
- Incorrect generated normal canonical form is fixed for certain molecules

## 18th January 2019, Calculator Plugins, 19.2.0

### Bugfixes

- LogD calculation with considered tautomerization does not terminate for casein
- Compound chemical formulas of molecules without C atoms are not listed alphabetically

### New features and improvements

- Improving the predicted $pK_a$ values of certain CH acids

## 13th December 2018, Calculator Plugins, 18.30.0

### Bugfixes

- Elemental Analysis Plugin handles repeating unit groups incorrectly during calculation
- Incorrect standardized forms of some ChemBL compounds and salts
- Strongest basic pKa value of cytosine needs some correction based on experimental data
- Fixing some Exception in charge calculations during standardization
- Inconsistent $pK_a$ values of ionised and neutral form of boronic acids

## 30th October 2018, Calculator Plugins, 18.25.0

### Bugfixes

- Microspecies table of the $pK_a$ Plugin does not change when $pK_a$ is calculated at different temperatures

## 5th September 2018, Calculator Plugins, 18.22.0

### Bugfixes

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

## 24th August 2018, Calculator Plugins, 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

## 1st August 2018, Calculator Plugins, 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

## 17th July 2018, Calculator Plugins, 18.17.0

### Bugfixes

- Incorrect $pK_a$ value of a *pyrimidine* ring N atom of a compound

## 7th June 2018, Calculator Plugins, 18.13.0

### Bugfixes

- Elemental Analysis Plugin calculates properties for molecules with position variation bonds incorrectly

## 18th May 2018, Calculator Plugins, 18.11.0

### Bugfixes

- Inconsistent $pK_a$ values with changing min/max calculation options

- Inconsistent isoelectric point calculation for *iminodiacetic acid*
- Incorrect isoelectric point calculation for *omeprazole*
- Update/Fix $pK_a$ value for *carbonic acid/bicarbonate*

## 9th March 2018, Calculator Plugins, 18.8.0

### Bugfixes

- Wrong generic tautomer forms in some cases

### New features and improvements

- Improving the $pK_a$ calculation and the logD values for some bioisosteric compounds

## 10th January 2018, Calculator Plugins, 18.1.0

### New features and improvements

- Adding *Recognize pseudo formula in pseudo labels* option to the ElementalAnalyzerPlugin node in KNIME

### Bugfixes

- Topology Analysis outputs incorrect values for some molecules

## 6th December 2017, Calculator Plugins, 17.29.0

### Bugfixes

- Solubility Predictor calculates different solubility values for the same molecule in neutral and ionized forms
- Generic tautomer forms of a molecule pair with negative charge are incorrect
- Exception is thrown during pKa calculation for tricyclic bromine compounds

## 23rd October 2017, Calculator Plugins, 17.27.0

### New features and improvements

- Calculating molecular weight from molecular formula. See the API doc page of this feature.

## 16th October 2017, Calculator Plugins, 17.26.0

### Bugfixes

- Incorrect tautomerization of some heterocyclic molecules during standardization
- Incorrect tautomerization of zwitterionic sydnone compounds

## 18th September 2017, Calculator Plugins, 17.23.0

### Bugfixes

- Incorrect normal canonical tautomer forms of sulfanone derivatives

## 28th August 2017, Calculator Plugins, 17.20.0

### Bugfixes

- Different dominant tautomer distribution of the same molecule with a rotated bond
- Different normal canonical form of the same molecule

## 7th August 2017, Calculator Plugins, 17.18.0

### Bugfixes

- Stereoisomer generation in KNIME throws exception for some molecules

## 3rd July 2017, Calculator Plugins, 17.14.0

### New features and improvements

- The Isoelectric Point Plugin is improved so that it handles quaternary amine salts as a microspecies carrying +1 charge (instead of neutral)
- Modifying table text of the exported PDF file in the Solubility Predictor

### Bugfixes

- Major tautomer calculation at pH 7.4 throws exception for specific molecules
- $pK_a$ calculation in cxcalc throws exception for a specific molecule

## 3rd July 2017, Chemical Terms, 17.14.0

### New features and improvements

- *maximalprojectionsize* and *minimalprojectionsize* functions are introduces in Chemical Terms

## 30th May 2017, Calculator Plugins, 17.10.0

### Bugfixes

- Tautomer pair has slightly different generic tautomers
- Predicted $pK_a$ value of sorbic acid is off in the new Chemicalize (requires fine-tuning)

## 3rd May 2017, Calculator Plugins, 17.7.0

### Bugfixes

- $pK_a$ values of the N1 atom of adenosine predicted with the new version of Chemicalize were quite off compared to the experimental results

### New features and improvements

- Only practically justified isoelectric points (when the input molecule has a certain $pK_a$ and charge distribution threshold) will be printed on the output of the Isoelectric Point Plugin

## 10th April 2017, Calculator Plugins, 17.04.10.

### Bugfixes

- Molecules stored in SD and CXSMILES/CXSMARTS format have different generic tautomer forms

## 6th March 2017, Calculator Plugins, 17.03.06

### New features and improvements

- Re-placing the Resonance Plugin under the Isomers plugin group

### 27th February 2017, Calculator Plugins, 17.02.27

### Bugfixes

- Incorrect $pK_a$ and pH-dependent solubility predicted for the indigo (CAS 482-89-3) molecule
- Wrong output after filtering generated 3D stereoisomers in the StereoIsomer Plugin
- Input molecule (with the predicted properties) does not appear correctly in the output window of some protonation-type plugins (e.g. $pK_a$, HBDA)
- Incorrect Elemental Analysis calculations results (e.g. mass, formula) for larger molecules with S-groups
- Alignment Plugin throws an exception when there are no input molecules on the canvas

## 20th February 2017, Calculator Plugins, 17.02.20

### Bugfixes

- Incorrect tautomer distribution predicted for some *thioamide* compounds in the Tautomer Plugin
- Incorrect tautomer distribution predicted for some *nitroparaffin* compounds in the Tautomer Plugin

- Incorrect normal canonical tautomers calculated for some heterocyclic compounds in the Tautomer Plugin
- Input molecules don't appear in the result window of the NMR Predictor. The molecules only appeared after hitting the Update button of the viewer.
- Input molecule appears small and translated in the result window of the Solubility Predictor even after pressing the Update button of the viewer.

#### 13th February 2017, Calculator Plugins, 17.02.13

#### New features and improvements

- Charged and isotope atoms are recognized in formula during Elemental Analysis calculations (e.g. mass)

### 23rd January 2017, Chemical Terms, 17.01.23

#### New features and improvements

- New Largest Conjugated System calculation functions are available in Chemical Terms
- New Chemical Terms demo site is available

### 16th January 2017, Calculator Plugins, 17.01.16

#### Bugfixes

- Matching normal canonical forms of some molecules to the ones found in the literature

### 9th January 2017, Calculator Plugins, 17.01.09

#### Bugfixes

- Incorrect van der Waals radius of the radon atom used for van der Waals volume calculation

### 2nd January 2017, Calculator Plugins, 17.01.02

#### Bugfixes

- Generic tautomer form of some molecules change after CXSMILES export and import

### 26th December 2016, Calculator Plugins, 16.12.26

#### Bugfixes

- Incorrect results with stereoisomer generation for some molecule
- Some modifications in the StereoisomerSettings API

## 19th December 2016, Calculator Plugins, 16.12.19

### Bugfixes

- Strange generic tautomer forms for some molecules
- Incorrect tautomer distributions for different tautomer forms of the same molecule

## 21st November 2016, Chemical Terms, 16.11.21

### New features and improvements

- Introducing name export options for the *name()* function

## 14th November 2016, Calculator Plugins, 16.11.14

### Bugfixes

- Incorrect pKa values are calculated for MINA and DAM (acetone derivative) compounds
- OutOfMemoryError was thrown during conformer generation

### 17th October 2016, Calculator Plugins, 16.10.17

### Bugfixes

- Solubility values for the same molecule represented by different SMILES codes were different

## 10th October 2016, Chemical Terms, 16.10.10

### Bugfixes

- Incorrect dominant tautomer forms are generated for some azide-type molecules using the *dominantTautomer()* function

## 3rd October 2016, Chemical Terms, 16.10.3

### Bugfixes

- Incorrect dominant tautomer forms are generated for some molecules containing Se using the *dominantTautomer()* function

## 5th September 2016, Calculator Plugins, 16.9.5

### Bugfixes

- Incorrect logP atomic increments are calculated by the *getAtomlogPIncrement()* function for some molecule

**New features and improvements**

- Large molecules make the pH-dependent solubility calculation slow down. Calculation was speeded up.

## 29th August 2016, Chemical Terms, 16.8.29

**Bugfixes**

- Incorrect dominant tautomer forms and distributions are generated using the *dominantTautomer()* function

## 29th August 2016, Calculator Plugins, 16.8.29

**Bugfixes**

- Incorrect isotope handling during tautomerization: isotope atoms vanish in result tautomer forms

### 18th July 2016, Calculator Plugins, 16.7.18

**Bugfixes**

- Carbanions appear in the major microspecies form at pH 7.4 with some molecules in the Major Microspecies Plugin

## 4th July 2016, Calculator Plugins, 16.7.4

**Bugfixes**

- Some molecules are not standardized correctly due to tautomerization

## 13th June 2016, Calculator Plugins, 16.6.13

**Bugfixes**

- Atomic charges don't add up to total charge in the Charge Plugin for some molecule
- Normal canonical tautomer generation throws Exception for some molecules during standardization
- Incorrect standardized form of cyanidine due to wrong tautomerization

## 10th May 2016, Calculator Plugins, 16.5.10

### Bugfixes

- Elemental Analysis Plugin calculates basic properties for molecules with double variation bonds incorrectly

## 3rd May 2016, Calculator Plugins, 16.5.3

### New features and improvements

- Some properties and calculation option are removed from the Elemental Analysis Plugin, and the plugin window is re-organized based on some user feedback

## April 25th 2016, Calculator Plugins, 16.4.25

### Bugfixes

- Precision of calculations does not work as expected in the Analysis Box in MarvinSketch

### April 18th 2016, Calculator Plugins, 16.4.18

### New features and improvements

- Groups written in pseudo labels are recognized in Elemental Analysis calculations

## May 16th 2016, Calculator Plugins, 16.5.16

### Bugfixes

- Incorrect tautomerization of some pyridine derivatives

### February 22nd 2016, Calculator Plugins, 16.2.22

### Bugfixes

- Exception was thrown during generic tautomer calculation for a specific molecule.

## January 18th 2016, Calculator Plugins, 16.1.18

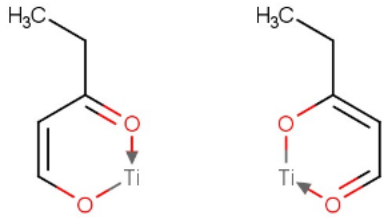
### Bugfixes

- Incorrectly calculated $pK_a$ values for the molecule with CAS number 1224844-38-5.

## January 11th 2016, Calculator Plugins, 16.1.11

### New features and improvements

- New feature in the Tautomerize Plugin: canonical tautomerization of organic molecules containing metal atoms. See an example of tautomer pairs below:




## January 11th 2016, Chemical Terms, 16.1.11

### New features and improvements

- Improving the following Chemical Terms functions to handle atom index *arrays* as input parameters: *formalCharge(), hCount(), connections(), valence(), radicalCount(), atno(), map().*

### Bugfixes

- Improving the *matchCount()* function to handle molecules with query Hs.

## December 14th 2015, Calculator Plugins, 15.12.14

### Bugfixes

- Bugfix for the Tautomerization Plugin: the plugin gave back different canonical tautomers from what were expected for oxim-type molecules.
- Bugfix for the NMR Plugin: calculating NMR spectra for highlighted molecules did not work.

## November 9th, 2015, Calculator Plugins, 15.11.9

### Bugfixes

- Bugfix for the Refractivity Plugin: refractivity failed for a molecule throwing exception. See the forum topic for details.
- Bugfix for the $pK_a$ Plugin: inconsistent calculated values for the same molecule represented in different atom order. See the forum topic for details.
- Bugfix for the 3D Alignment Plugin: molecule selecting function did not work properly during the alignment process. See the forum topic for details.

## November 2nd, 2015, Calculator Plugins, 15.11.2

### Bugfixes

- Bugfixes for the Tautomer Plugin: bugs in the dominant tautomer distribution calculation for molecules containing P. See the forum link for details.
- Bugfix for the Solubility Predictor: calculated solubility at pH 7.4 was not the same in cxcalc and MarvinSketch

## October 26th, 2015, Calculator Plugins, 15.10.26

### Bugfixes

- Bugfix for aromatization/de-aromatization: errors in conversion between aromatic and Kekulé forms.

## October 12th, 2015, Chemical Terms, 15.10.12

### Bugfixes

- Bugfix for calculating chemical properties for agents in ReactionContext: evaluating Chemical Terms functions for reaction agents threw Exception

## October 5th, 2015, Calculator Plugins, 15.10.5

### Bugfixes

- Bugfix for the $pK_a$ calculation: improving calculated values in relation to the log*D* training. See the forum link for details.
- Bugfixes for the Tautomer Plugin: bugs in the dominant tautomer distribution calculation in cxcalc. See the forum link for details.
- Bugfix for the steric hindrance calculation in Metabolizer: slow-down of generation of 3D conformers for molecules with fused rings fixed. See the forum link for details.

## September 14th, 2015, Calculator Plugins, 15.9.14

### Bugfixes

- Bugfix for the MCS-based Alignment method in the Alignment Plugin. See the forum link for details.

## August 24th, 2015, Calculator Plugins, 15.8.24

### Bugfixes

- Bugfix for major microspecies calculation in cxcalc: fix for lost SD properties in the output.
- Bugfix for the log*P*/log*D* plugin: correct error message shown for cation/anion concentration setting

## August 10th, 2015, Calculator Plugins, 15.8.10

### Bugfixes

- pKa calculation fixes for amide structures. See the forum link for details.
- Fix for solving the pKa calculation slow-down and JVM break.

## August 3rd, 2015, Calculator Plugins, 15.8.3

### New features and improvements

- Calculating chemical properties for highlighted structures: it is possible to run the calculators for highlighted structures in MarvinSketch.
- Solubility results/plot is automatically updated when the molecule is modified on the canvas in MarvinSketch.
- New HLB node in KNIME is now available. See the KNIME release notes for details.

## July 20th, 2015, Calculator Plugins, 15.7.20

### Bugfixes

- Bugfix for tautomerization: tautomer generation for molecules with explicit Hs wasn't working properly.

## July 13th, 2015, Calculator Plugins, 15.7.13

### Bugfixes

- Bugfix for rendering acidic/basic pKa values: red/blue representation wasn't working.

## June 29th, 2015, Calculator Plugins, 15.6.29

### Bugfixes

- Bugfixes for tautomerization: various bugs in the tautomerization of the Standardizer KNIME node; tautomerization of indazole for its pKa calculation was incorrect.
- Bugfix for geometry optimization with MMFF94 in the Geometry Plugin

## June 8th, 2015, Calculator Plugins, 15.6.8

### Bugfixes

- Bugfix for the Tautomer Plugin: tautomerization of 4-hydroxycoumarin wasn't correct.

## June 1st, 2015, Calculator Plugins, 15.6.1

### Bugfixes

- Bugfix for the Tautomer Plugin: bad oxo-enol tautomerization for a molecule.
- Bugfix for the Tautomer Plugin: calculating dominant tautomer distribution in cxcalc didn't behave well for certain molecules.

## May 18th, 2015, Calculator Plugins, 15.5.18

### New features and improvements

- Releasing the new HLB Predictor in MarvinSketch. See the documentation here.

### Bugfixes

- Bugfix for calculating the pKa for carbanions. See the forum topic about the bug here.

## April 27th, 2015, Calculator Plugins, 15.4.27

### New features and improvements

- Releasing the new HLB Predictor in cxcalc, its API and in Chemical Terms. See the documentation here.

## April 13th, 2015, Calculator Plugins, 15.4.13

### New features and improvements

- Improving and modifying the tautomerization options in the Tautomerization Plugin. See the documentation for details.
- Improving and modifying the log*P* calculation methods in the log*P* Plugin. See the documentation for details.
- Improving and modifying the log*D* calculation methods in the log*D* Plugin See the documentation for details.

## March 23rd, 2015, Calculator Plugins, 15.3.23

### Bugfixes

- Bugfix for the Solubility Plugin: plugin froze in Marvin for compounds with hashed bond

## March 16th, 2015, Calculator Plugins, 15.3.16

### Bugfixes

- Fixes for the pKa plugin

## March 9th, 2015, Calculator Plugins, 15.3.9

### Bugfixes

- Fixes in the Generic Tautomer generation method in the Tautomer Plugin

## February 16th, 2015, Calculator Plugins, 15.2.16

### Bugfixes

- Fixes in the Canonical Tautomer generation method in the Tautomer Plugin

## February 9th, 2015, Calculator Plugins, 15.2.9

### Bugfixes

- Fixes for the Tautomer Plugins

## February 2nd, 2015, Calculator Plugins, 15.2.2

### Bugfixes

- Functionality fixes for the Elemental Analysis Plugin
- Fixes for cyano compounds in the $pK_a$ Plugin

## January 19th, 2015, Calculator Plugins, 15.1.19

### Bugfixes

- Minor fixes for the $pK_a$ and the Tautomer Plugin

## January 5th, 2015, Calculator Plugins, 15.1.5

### New features and improvements

- Stiochiometry in chemical formulae is shown in subscripts. Subscripts are now correctly displayed in the Elemental Analysis Plugin.

## December 15th, 2014, Calculator Plugins, 14.12.15

### Bugfixes

- msdistr bugfix
- stereoisomer calculation bugfix
- Solubility Predictor: result view fix

## December 8th, 2014, Calculator Plugins, 14.12.08

### New features and improvements

- Solubility node in KNIME

### Bugfixes

- Canonical tautomer calculation bugfix

## November 24th, 2014, Chemical Terms, 14.11.24

### Bugfixes

- Mass calculation from formula

## November 17th, 2014: Calculator Plugins, 14.11.17

### Bugfixes

- Valence fix for $S^{2-}$

## November 3rd, 2014: Calculator Plugins, 14.11.03

### New features and improvements

- ADME predictors have been removed.

### Bugfixes

- cxcalc minor issues fix

## October 20th, 2014: Calculator Plugins, 14.10.20

### Bugfixes

- logP/logD calculation improvement

## October 13th, 2014: Calculator Plugins 14.10.13

### Bugfixes

- Setting of the measurement unit of the Solubility Predictor (unit could not be set in MSketch, issue fixed)

## September 22nd, 2014: Calculator Plugins 14.9.22

### New features and improvements

- Chemical Terms stereoAnalysis() function has been improved. Documentation.

## September 15th, 2014: Calculator Plugins 14.9.15

### New features and improvements

- New Solubility Predictor API has been released. API doc.
- Chemical Terms logS() function has been improved. Documentation.

## August 18th, 2014: Calculator Plugins 14.8.18

### New features and improvements

- New calculation in Elemental Analyser Plugin: mass spectrum (Documentation).
- 'Grouped dot disconnected formula' has been added to Elemental Analyser Plugin.

## August 11st, 2014: Calculator Plugins 14.8.11

### Bugfixes

- Bugs reactant() and product() functions in Chemical Terms have been fixed.
- 'Setting radius' option in Geometry Plugin has been removed.

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

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