Name to Structure History of Changes

November 8th, 2019: Name to Structure 19.23

Improvements

- The common names of 220 more pesticides have been added to the dictionaries.

October 21st, 2019: Name to Structure 19.22

Bug fixes

- The stereochemistry of some substituted D-amino-acids was incorrect.

September 2nd, 2019: Name to Structure 19.19

Improvements

- Some CAS Registry Numbers are now converted with more precise information. In particular, some metal complexes that were previously disconnected now contain the relevant coordinate bonds.

July 16th, 2019: Name to Structure 19.17

Bug fixes

- Stereochemistry was missing in the structures converted from some CAS Registry Numbers®.

July 4th, 2019: Name to Structure 19.16

Improvements

- Some CAS Registry Numbers that were converted to a structure with only aliases representing the amino-acid 3 letter codes, for instance 98059-61-1. The underlying chemical meaning of each amino-acid is now automatically added when absent.

June 27th, 2019: Name to Structure 19.15

New features

- EC numbers are now detected and converted using a third-party webservice.

June 24th, 2019: Name to Structure 19.14

Improvements

- The common name dictionaries have been updated.

May 7th, 2019: Name to Structure 19.10

Bug fixes

- Between versions 19.2 and 19.9, the automated proxy configuration was happening at the first use of naming, instead of at the first use of the network for CAS Registry Number lookup.

February 28th, 2019: Name to Structure 19.6

Bug fixes

- "Names" with only semicolons and NULL (0) control characters were imported as empty structures.

January 23rd, 2019: Name to Structure 19.2

Improvements

- The common name dictionary has been significantly updated and extended with 30 thousand new names and synonyms.
- For CAS Registry Numbers(R), when one of the remote webservices is unavailable, the conversion will not block for as much time as before.

January 11th, 2019: Name to Structure 19.1

Bug fixes

- Some CAS Registry Number lookups were incorrectly cached in version 18.30.
- Some CAS Registry Numbers were converted to invalid structures in version 18.30.

December 14th, 2018: Name to Structure 18.30

Improvements

- All rebaudiosides are now supported.

Bug fixes

- Some CAS Registry Numbers that started to fail around December 13th are now fixed.

November 28th, 2018: Name to Structure 18.28

Bug fixes

- Invalid structures were generated for names containing "monomethylene".

November 12th, 2018: Name to Structure 18.26

Improvements

- The carbonimidoyl group name is now supported.

October 31st, 2018: Name to Structure 18.25

Improvements

- Derivatives of cycloalkyl (e.g. cycloalkoxy) are now recognized.

Bug fixes

- Carbon count ranges where misinterpreted when separated from the main carbon group, for instance in c1-3-halocycloalkyl.

August 3rd, 2018: Name to Structure 18.18

New features

- A custom dictionary can now be specified as a remote URL. For technical reasons the ':' character cannot be used in format options, so a '=' should be used instead, for instance `name:dict=https=//myserver/dict.smi`

June 12th, 2018: Name to Structure 18.13

New features

- The common name dictionary has been extended with 15 thousand common names (including synonyms) for 5 thousand polymers.

Bug fixes

- In some rare cases, a structure could be generated with invalid bonds.

May 23rd, 2018: Name to Structure 18.11

New features

- The common names of 5 thousand herbicides and pesticides are now included in the dictionary.
- Some additional CAS Registry Numbers are supported.

Improvements

- CAS Registry Numbers starting with a 0 are now reported as invalid.

Bug fixes

- CAS Registry numbers with invalid check digits are now consistently reported.

April 13th, 2018: Name to Structure 18.10

Improvements

- Structures imported from a CAS Registry Number are now always in Kekulé form.

April 4th, 2018: Name to Structure 18.9

Improvements

- Name with incorrect dashes after brackets (OCR errors) can now be interpreted, for instance: 2-(-4-(-2-aminobenzyl)phenyl)acetic acid

March 14th, 2018: Name to Structure 18.8

Bug fixes

- The primes in locants such as 1'-O were ignored.

February 27th, 2018: Name to Structure 18.5

Improvements

- Some common names were wrongly converted to the imidic form instead of the amide form.

February 13th, 2018: Name to Structure 18.4

Improvements

- Names containing a 'dehydro' corresponding to a triple bond are now supported.
- Names containing the term 'carboaryl' are now converted using the corresponding homology group instead of the broader group 'aryl'.

January 30th, 2018: Name to Structure 18.3

Bug fixes

- Some names with E/Z descriptors without locants were ignored or misinterpreted.

January 12th, 2018: Name to Structure 18.1

Improvements

- For all capitals input like ASPIRIN where the input format is not specified but detected by the system, the input is now detected as name when possible, not a one letter aminoacid sequence.

December 8th, 2017: Name to Structure 17.29

Improvements

- A different exception class is used when a name is simply unknown to a custom webservice compared to when the connection to the webservice failed.

Bug fixes

- Some names containing "ylidene" were converted to an invalid structure.

November 9th, 2017: Name to Structure 17.28

Improvements

- More CAS registry numbers are supported.

October 19th, 2017: Name to Structure 17.26

Bug fixes

- Name to Structure could use a large amount of memory at startup if it was used simultaneously in a large number of threads.

October 13th, 2017: Structure to Name 17.25

Bug fixes

- Isotope descriptors were missing for the carbon atom of some characteristic groups (carboxylic acid, carboxamide, ...) on a cyclic parent.

September 22nd, 2017: Name to Structure 17.24

Bug fixes

- Some names containing "epoxy" were converted to an invalid structure.

September 14th, 2017: Name to Structure 17.23

Bug fixes

- Polyalenes (for instance pentalene, octalene, ...) are now supported.

September 1st, 2017: Name to Structure 17.22

Bug fixes

- Charges were missing on some metals: nickel, zinc, ...

August 9th, 2017: Name to Structure 17.20

Improvements

- Longer common names are now supported.
- CAS Registry Numbers with invalid check digits are now reported as errors with a specific error message. This happens in particular for CAS Numbers which have been entered with a typo.
- String of the form X-XX-X were wrongly recognized as CAS Registry Numbers.

August 3rd, 2017: Name to Structure 17.18

New features

- The common name dictionary is extended to include INCI names (International Nomenclature of Cosmetic Ingredients).
- The new nameField format option can be used to set which field/property stores the original name (instead of the molecule title).

July 6th, 2017: Name to Structure 17.14

Improvements

- Nucleoside substituents such as adenosyl are now supported.

Bug fixes

- Some nucleosides and nucleotides had incorrect stereochemistry.
- CAS number conversion was failing since version 17.9 in .NET 32 bit applications.
- The homology group haloalkyl is now represented more accurately.

May 31st, Name to Structure 17.10

Improvements

- The conversion of some sugars has been improved.

Bug fixes

- Names with a numbered C locant before a homology group, such as "1-C-acyl..." were not converted.

May 26th, 2017: Name to Structure 17.9

New features

- When converting CAS Registry Numbers, a more advanced detection of network proxy settings is now in place. This includes supporting the proxy auto-configuration (PAC) and the Web Proxy Autodiscovery Protocol (WPAD) protocols.

May 5th, 2017: Name to Structure 17.7

Bug fixes

- More ASCII syntaxes are supported for superscript numbers in bridged ring system names.
- The name format was not detected for names contain the special "soft-hyphen" character.

Name to Structure 17.02.20

Bug fixes

- CAS registry number resolution failed when the ChemAxon user home directory did not exist. This could happen exceptionally, such as running under the NetworkService system account in Windows.

Name to Structure 17.02.06

Improvements

- Generic structures now get assigned the type 'generic' even when imported from a common name, such as "ester", "fatty acid", ...

Name to Structure 17.01.30

Improvements

- All character entities are now recognized in the USPTO XML format.

Bug fixes

- CAS number resolution using the remote webservice works again in Java versions lower than 8 and in .NET applications such as JChem for Office.

Name to Structure 17.01.16

Improvements

- The webservice call for CAS number resolution never uses an HTTP redirection, resulting in faster response time.

Name to Structure 16.12.26

Improvements

- More OCR error correction is performed in alkyl ranges.

Name to Structure 16.12.05

Improvements

- Improvements when processing names with added spaces.

Name to Structure 16.11.28

Improvements

- Ring fusions involving multiple bonds are now supported.
- The traditional steroid numbering of cyclopenta[a]phenanthrene is now supported in addition to the IUPAC numbering.

Name to Structure 16.11.21

Improvements

- The numbering of complex fused ring systems is now supported.

Name to Structure 16.10.31

Improvements

- Capital S- is now understood as sym- where appropriate.
- Names with added space characters are better recognized.
- More fused names are understood.

Name to Structure 16.10.24

Bug fixes

- Metals and some other element names were imported with an unneeded zero valence property.

Name to Structure 16.10.10

Improvements

- More disconnected structures are now supported, for instance pyridine acetate.
- More complex ethers are now supported.

Name to Structure 16.10.03

Improvements

- Non-strictly IUPAC forms of Hantzsch-Widman names are now recognized.

Bug fixes

- Names separated by ';' were not detected from arbitrary text formats. This affected in particular JChem for Excel.
- Some salts and esters were not recognized.

Name to Structure 16.09.26

Improvements

- The N^{...} syntax for superscript locants is now supported.
- More OCR errors are corrected.

Name to Structure 16.09.12

Bug fixes

- Some names with multiplied suffixes were not converted.

Name to Structure 16.09.05

Improvements

- The common name dictionary received a significant update.

Name to Structure 16.08.22

Improvements

- The homology group heterocycloalkyl is now supported.

Bug fixes

- Some names containing bond modifiers with non-consecutive locants were not supported, for instance: 1,3,5(10)-Estratriene.

Name to Structure 16.08.08

Improvements

- The iso form of chains, such as isodecyl, is now better supported.

Name to Structure 16.08.01

Bug fixes

- Some element names were wrongly detected and represented as structures.
- Some names containing "ano" lead to corrupt structures.

Name to Structure 16.07.11

Improvements

- Higher order fusions with omitted primed locants are now supported.

Name to Structure 16.07.04

Improvements

- Fused ring systems with higher-order attached components are now supported.

Name to Structure 16.06.27

Improvements

- Fused ring systems with multiple first-order attached components are now supported.

Bug fixes

- "Fatty acid" had an overly broad representation.

Name to Structure 16.06.20

Improvements

- HTTP proxy configuration is now described in the logging system and in the stack trace when an HTTP connection fails. This is useful in particular when investigating why a CAS number resolution failed.

Bug fixes

- Some incomplete names used to be converted to impossible aromatic structures.

Name to Structure 16.05.23

Bug fixes

- The webservice call for CAS number resolution was using an HTTP redirection, resulting in slower response time.

Name to Structure 16.05.16

Bug fixes

- The conversion of Japanese element names was enabled by disabling common name conversion.

Name to Structure 16.03.14

Bug fixes

- Some group types (for example ethoxy, propargyl, C1-C8-alkoxycarbonyl, ...) that were generated as complete structures are now generated with an attachment point.

Name to Structure 16.02.15

Bug fixes

- Names containing a substituent to a formohydrazido group were not converted.

Name to Structure 16.02.01

Improvements

- The support for Japanese chemical names found in Japanese legal documents has been vastly improved.

Bug fixes

- Some syntaxes for benzofused ring systems were not supported.

Name to Structure 16.01.18

Improvements

- The support for functional groups containing Selenium and Tellurium atoms has been improved.
- Chain ester names used as substituents are now recognized.

Name to Structure 16.01.11

Improvements

- All locants are now supported in tryptamine.

Name to Structure 15.12.14

Improvements

- Support has been added for more cases of accidental spaces in name (often caused by OCR), such as "m ethyl".
- Support has been improved for parent names starting with a symbol, such as *s*- and *as*-indacene.

Name to Structure 15.11.23

Improvements

- Additional OCR error correction allows to convert more names from scanned documents and patents.

- Spiro names that mistakenly lack a prime on the second spiro atom locant are now automatically fixed.
- The accuracy in the conversion of Chinese names to structures is improved.

Name to Structure 15.11.16

Bug fixes

- The numbering of flavanone has been fixed.

Name to Structure 15.10.05

Improvements

- Multiple custom dictionaries can be specified using the 'dict' format option: dict=<dictionary_path_1>;<dictionary_path_2>

Name to Structure 15.08.31

Bug fixes

- The 'systematic' name format option does not disable the conversion of other name types anymore.

Name to Structure 15.08.24

Improvements

- Names containing the keyword "substituted" are now supported, for instance: "2,4-disubstituted pyridine".

Name to Structure 15.08.17

Improvements

- More syntaxes for carbon count in homology groups are recognized, for instance "(C1-6) alkyl".

Name to Structure 15.07.20

Improvements

- The "Heterocyclyl" homology group is now supported.
- Fix new OCR error in Japanese.

Name to Structure 15.05.25

Bug fixes

- CAS Registry Numbers can now be converted when entered with extra whitespace before or after the number. This is especially useful when using copy-paste in end-user applications.

Name to Structure 15.05.04

Improvements

- Several improvements increase the conversion of systematic names.
- Names with small typographical errors, such as added spaces or missing dashes, are better supported. This especially improves the extraction of names from lower quality sources, such as patent texts generated by OCR.

Bug fixes

- Esters of nitric acid were imported with a radical instead of the C-O bond.

Name to Structure 15.04.20

Improvements

- Some additional OCR error correction is performed in Chinese.

Name to Structure 15.04.06

Bug fixes

- Some lists of names improperly separated lead to extremely long processing time.
- -alanine wrongly had a chiral stereocenter.

Name to Structure 15.03.02

Improvements

- The file size of the naming component has been reduced by 10%, leading to reduced startup time in the applet.

Name to Structure 15.02.16

Bug fixes

- Japanese names with fullwidth full stop characters were not supported.

Name to Structure 15.02.09

Bug fixes

- Some E/Z and R/S stereodescriptors were not honored correctly.

Name to Structure 15.01.19

Improvements

- Some more rarer acids are now supported, including those based on an Antimony atom.

Bug fixes

- Names containing the "sulfonato" prefix were converted incorrectly.

Name to Structure 15.01.05

Bug fixes

- Japanese names containing the '=' separator character (for instance in esters) were not supported.

Name to Structure 14.12.08

Improvements

- Support was added for acetimidamides and the imidamido suffix.

Name to Structure 14.10.27

Improvements

- Failures from a custom naming webservice are now reported as an exception, to make it easier to solve misconfiguration of the service.

Name to Structure 14.10.20

Improvements

- Conversion of systematic names is improved by supporting more functional groups.

Name to Structure 14.10.13

Improvements

- Added support for the olato suffix in inorganic nomenclature.

Name to Structure 14.09.29

Improvements

- Parent homology groups such as alkyl or hydroxyalkyl are now generated with an attachment point.

Name to Structure 14.09.15

Improvements

- Custom name to structure webservice and CAS number resolution now try to use the system HTTP proxies, when available.

September 8th, 2014: Name to Structure 14.09.08

New Features and Improvements

- Naming webservice URLs can now contain a [DOMAIN] parameter that get replaced by the Windows domain name of the machine, or by the network domain name on non-Windows computers. This information can be used by the webservice, for instance for simple access control or user-based customization of the result.

Bug Fixes

- Japanese and Chinese names with full-width curly braces were not supported.

August 18th, 2014: Name to Structure 14.8.18

New Features and Improvements

- Corporate IDs (registry numbers) can be converted using the API and class chemaxon.naming.n2s.DatabaseNameConverter.

August 4th, 2014: Name to Structure 14.8.4

New Features and Improvements

- Support for organo-metallic names was extended.
- Support for CAS names was improved.

July 14th, 2014: Name to Structure 14.7.28

New Features and Improvements

- Halonium ions are imported correctly.
- Substituted ferrocene and analogues are now supported.

Bug Fixes

- CAS number conversion and naming webservice calls could run for a long time or even not return if the webservice was not responsive.

July 14th, 2014: Name to Structure 14.7.14

New Features and Improvements

- OCR error correction is improved.
- Lowercase d- and l- stereo-descriptors are now interpreted as D- and L-, since names are sometimes (wrongly) converted to all lowercase. This is correct most of the time since the old usage of d- and l- for optical activity (dextrorotatory and levorotatory) is out of use and replaced by (+) and (-).

July 7th, 2014: Name to Structure 14.7.7

New Features and Improvements

- Names with (r) and (s) pseudo-asymmetric stereo centers are now fully supported.
- Chinese name to structure coverage was improved by about 3 percentage points.

- Additional OCR error correction is performed.

Bug Fixes

- Some names designating multiplied fused systems failed to be converted.
- Some names referring to the locant of spiro atoms were failing to be converted to structure or were missing stereochemistry on those atoms.
- Some partially saturated polyacenes and polyaphenes were not supported.
- Some Chinese and Japanese chemical names with punctuation characters were were not supported by the automatic format recognizer.
- Double bonds in large rings that are part of fused systems had unknown stereochemistry. They now have cis stereochemistry.

June 4th, 2014: Name to Structure 6.3.1

Bug Fixes

- Some substituents separated by a space from an acid parent were wrongly interpreted as esters.
- The naming webservice was not working in the applet.