Structure to Name History of Changes

October 7th, 2019: Structure to Name 19.21

Bug fixes

- Name generation failed for structures with enhanced stereochemistry markers on atropisomerism centers.

June 27th, 2019: Structure to Name 19.15

New features

- EC numbers can now be generated using a third-party webservice by using the `name:EC#` format option.

June 24th, 2019: Structure to Name 19.14

Improvements

- The common name dictionaries have been updated.

May 7th, 2019: Structure to Name 19.10

Bug fixes

- The fusion letter generated for a fusion bond immediately adjacent to another one was wrong, for instance in dodecahydrocyclopenta[e]quinoline.

January 23rd, 2019: Structure to Name 19.2

Improvements

- The common name dictionary has been significantly updated and extended with 30 thousand new names and synonyms.

September 24th, 2018: Structure to Name 18.23

Bug fixes

- Name generation was failing for some structures with unknown M/P stereochemistry.

September 7th, 2018: Structure to Name 18.22

Bug fixes

- Name generation was failing for compounds containing a methaneselone or methanetellone group.
- Name generation was failing on substituted trivalent iodine.

May 23rd, 2018: Structure to Name 18.11

Improvements

- Synonyms returned by the "name:common,all" export option are now listed in decreasing order of importance.
- The export option "name:common,all,en" can be used to exclude Asian names from the list of synonyms.

April 4th, 2018: Structure to Name 18.9

Bug fixes

- Some very long phrases were sometimes included in the list of all synonyms for a structure.

March 14th, 2018: Structure to Name 18.8

Bug fixes

- Radicals in cyclic components were sometimes ignored.

February 27th, 2018: Structure to Name 18.5

Improvements

- Name generation is generally about 10% faster. Importantly, it is dramatically faster (hundred of times) on some large and highly symmetrical structures such as dendrimers. Such structures used to sometimes lead to long pauses or failures due to timeout, while they are now almost instantaneous.

Bug fixes

- Cyclopeptides were given incorrect names. They are now named using the systematic IUPAC nomenclature for the underlying structure.

February 13th, 2018: Structure to Name 18.4

Improvements

- Structures with triple bond in an otherwise aromatic ring are now named using the 'dehydro' descriptors. For instance, the structure with traditional name benzyne is now given the correct IUPAC name: 1,2-didehydrobenzene.

Bug fixes

- The traditional name generator (name:t) was sometimes incorrectly returning Chinese names.

January 30th, 2018: Structure to Name 18.3

Improvements

- Bond E/Z stereochemistry is now included in Hantzsch-Widman ring names.

Bug fixes

- Name generation failed for an isotopic modification of a ketone group.

January 12th, 2018: Structure to Name 18.1

Improvements

- The groups tellurinyl and telluronyl and now supported.
- The IUPAC name generated for [O-][O+]=O (ozone) is now 'trioxygen' instead of '2?-trioxida-1,2-diene'. The name 'ozone' is generated with the "traditional" option.

Bug fixes

- A wrong name was generated for acyl halides when using the ASCII option, in particular in MarvinSketch.

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.

August 9th, 2017: Structure to Name 17.20

Bug fixes

- Some dictionary common names contained "HCl" for structures without hydrochloride.

May 26th, 2017: Structure to Name 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.

Structure to Name 17.04.03

Bug fixes

- Conversion to CAS Registry Number now also works on Java 6, Java 7 and .NET.

Structure to Name 17.03.13

Bug fixes

- Correct systematic names are now generated for phosphorus-based groups with non-standard valence (for instance pentamethoxy-?-phosphane)

Structure to Name 17.02.06

Bug fixes

- Some traditional names were in Chinese or Japanese instead of English.

Structure to Name 16.11.14

Bug fixes

- Names were generated for some structures with query bonds.

Structure to Name 16.10.31

New features

- Stereogenic axes (M/P) are now featured in generated names.

Improvements

- Fused names are generated in more cases, instead of the more complex bridged names.

Structure to Name 16.10.24

Bug fixes

- Vowels inside brackets were sometimes not elided when required.
- The term "ion" was incorrectly included in compound names.
- The name generated for some chemical element was fixed.
- Use the 1- locant to indicate substitution on the carbon atom of methanamine, as specified by IUPAC.

Structure to Name 16.10.17

Bug fixes

- The lookup of CAS Registry Numbers was failing for some structures with stereocenters of undefined chirality.

Structure to Name 16.10.10

Improvements

- IUPAC names are now generated for acids partially modified by halogens, for instance carbonobromidic acid.

Structure to Name 16.10.03

Bug fixes

- Some groups contained an unneeded 'carbo' prefix when applied to chains, for instance propanecarboximidate instead of the correct form: propanimidate.

- The names of some complex deeply substituted structures could depend on the specific input representation.

Structure to Name 16.09.26

Bug fixes

- The common name of some structures with bridged cycle stereochemistry was not found.

Structure to Name 16.09.12

Bug fixes

- Fused names with a long cyclic parent of length above 26 could contain invalid characters.

Structure to Name 16.08.22

Bug fixes

- Names were generated for some query structures with atom lists.

Structure to Name 16.08.01

New features

- Names such as "2-arylnaphthalene" are now generated for structures with simple homology groups.

Structure to Name 16.07.25

New features

- Names such as "N-substituted benzamide" are now generated for structures with simple R groups.

Bug fixes

- Incorrect names were generated for some esters when the "ascii" option was used.

Structure to Name 16.07.04

Improvements

- Some common names are now better chosen among the list of synonyms.

Bug fixes

- Traditional name generation (name:t) did not find common name for structures imported from common name when the structure contained a salt which had a dictionary name by itself.
- Primed locants for skeletal replacement were not always listed in the right order.

Structure to Name 16.06.27

Bug fixes

- The retained IUPAC names hydroxyl and hydroperoxyl are now generated.

Structure to Name 16.06.20

Bug fixes

- Some common names were not found when generating names with the traditional ("name:t") option.

Structure to Name 16.06.06

New features

- A new option, name:singleCAS#, has been introduced. While name:CAS# fetches all CAS Registry Numbers associated with the structure, singleCAS# returns the lowest one (historically assigned earlier). This option also uses a public internet webservice.

Bug fixes

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

Structure to Name 16.02.22

Improvements

- When using the API to conver a structure to common name (format option "name:common") or to CAS registry number (format option "name:cas#"), an exception of class

chemaxon.naming.s2n.NoKnownNameException is now thrown when no common name or CAS registry number is known for the structure. This is intended to make it easier for programs to distinguish those situations from failures.

Structure to Name 15.11.16

Bug fixes

- Saturated rings inside fused ring systems are now correctly named based on the insaturated ring names (for instance pyrazine instead of piperazine) together with hydro prefixes.

Structure to Name 15.10.26

Bug fixes

- In structures with sulfonamides (and similar groups) connected to a cyclic parent and N-substituted with some complex acyclic components, the wrong parent was selected, leading to incorrect IUPAC names.

Structure to Name 15.07.27

Improvements

- Correct IUPAC names are now generated for simple inorganic molecules of two identical atoms such as dinitrogen and dichlorine.

Structure to Name 15.07.06

New features

- IUPAC Names are now generated for ring assemblies of size 2, such as biphenyl, bifuran, bicyclohexane, ...

Structure to Name 15.06.29

Improvements

- The group carbodithioate is now recognized.

Bug fixes

- Some multiplied substituents were missing surrounding parentheses.

Structure to Name 15.06.08

Improvements

- The group sulfinimidoyl is now recognized.

Structure to Name 15.05.18

Bug fixes

- Substituted benzyl was used in generated names, while this is not allowed by the IUPAC rules. These structures now get names based on substituted phenyl connected to a methyl parent, following the IUPAC rules.

Structure to Name 15.04.20

Bug fixes

- Some ring substituents were missing locants for their own substituents.

Structure to Name 15.04.06

Improvements

- When using the "ascii" option, non-standard valences will be indicated using "lambda..." instead of "$l^{...}" so that the name is easier to read.

Structure to Name 15.03.02

New features

- Reaction molecules are now named by separating the reactents, reagents and products. For instance, `molconvert name:t -s '[C].O=O>>O=C=O'` returns "`carbon + dioxygen ? carbon dioxide`".

Structure to Name 15.02.23

Bug fixes

- The "carbonylimino" group was wrongly named as "amido".

Structure to Name 14.12.15

Improvements

- IUPAC compliant names are now generated for racemic mixtures, such as rac-(2R,3R)-3-bromobutan-2-ol.

Bug fixes

- Name generation could fail on instances of the RgMolecule class when assertion checking is enabled.

Structure to Name 14.12.08

Improvements

- Following the new 2013 IUPAC rules, use locants N,N'',N' for guanidine instead of the previously used locants 1,2,3.
- Adopt the new IUPAC 2013 rules for parentheses. This leads to slightly more parentheses in some cases, where this is useful to avoid any ambiguity.

Bug fixes

- Structures with a cis/trans double bond resulting of the substitution of a parent functional group were named with an unnecessary and invalid "ene" suffix.
- Structures with a radical on a chalcogen atom (O, S, ...) connect to a cyclic component were named incorrectly (ignoring the radical and substituents)
- Some common names failed to be recognized depending on irrelevant factors, such as the atom order in the input structure.
- Some structures with multiple identical functional groups were sometimes assigned different names depending on irrelevant factors, such as the atom order in the input structure.

July 28th, 2014: Structure to Name 14.7.28

New Features and Improvements

- IUPAC names are generated for halonium ions, such as bromanium, chloranium, ...

July 7th, 2014: Structure to Name 14.7.7

New Features and Improvements

- A novel nomenclature for enhanced stereochemistry has been introduced to name structures with multiple independent OR groups.
- IUPAC names are now generated for phosphorothioic acid, phosphonothioic acid, and their derivatives, including their esters.
- Significant improvements in parent selection, resulting in a stricter adherence to IUPAC rules, especially for amines and imines.
- The name succinamide is now used in traditional mode.
- Use unicode superscript representation for interior fusion atoms, for instance in 3a¹H-phenalene.

Bug Fixes

- Wrong locants (typically N instead of N') were generated for some structures with a substituted multiplied suffix.
- Name generation was failing on some structures with isotopes.
- For structures with isotopes, generated names used to contain non-ASCII Unicode characters even when the ASCII option was used.
- A valid but suboptimal numbering was chosen in some cases, for instance (3S,4R)-2,5-diamino-3,4-dimethylhexanedioic acid instead of (3R,4S)-2,5-diamino-3,4-dimethylhexanedioic acid.
- Fixed stack overflow when generating a name in the rare case of a *-O=N-* configuration.
- Structures containing an ester and a separate fragment were named as if they were a single fragment. They are now named separately using the ';' fragment name separator.