

What's New in InChI Software Version 1.01

Compatibility

Identifiers produced by the InChI version 1 software version 1.01 are same as those produced by released in April 2005 InChI version 1 provided that both were generated with the same InChI options.

AuxInfo could be different for some of the structures containing "Either" (wavy) single stereo bonds or "aromatic" bonds.

A more detailed analysis of "aromatic" bonds may produce a new error message: "Cannot process aromatic bonds."

Ordinal numbers of `__stdcall` entry points exported from Win32 `inchilib.dll` with `__declspec(dllexport)` have changed. Ordinal numbers of `__cdecl` entry points remain unchanged.

New Features

New software features

The new software features are turned on by command line options summarized in the following table.

Command line option (without / or - prefix)	Explanation
InChI2InChI	Check input InChI string for significant syntax errors; may remove layers; the result is an InChI string. Meaningful additional options: FixedH, RecMet (keep these layers), Snon (remove stereo layer), NoLabels, Tabbed, STUDIO, Compress.
InChI2Struct	Convert input InChI string into a 0D structure. cInChI-1 outputs structure in AuxInfo; InChI software library produces a binary connection table. A description of differences in comparing the input InChI and InChI generated out of the reconstructed structure are in a log file and (in case of InChI software library) in bitmaps related to InChI layers. If AuxInfo containing coordinates is available in the input then cInChI-1.exe would display the reconstructed structure in case of options <code>d</code> and <code>dcr</code> .
SPXYZ	Treat Phosphines as stereogenic
SAsXYZ	Treat Arsines as stereogenic
FixSp3bug or FB	Activate fixes of two known bugs in stereochemical sp^3 (/t) segment

None of these options are available in wInChI-1.exe except FB, which is always turned on. All of them are available in cInChI-1 and in InChI software library, libinchi.dll/libinchi.so, where new entry points were added for the first two options.

InChI validation protocol

The purpose of InChI validation is to verify that InChI code included in an application or InChI code ported to a particular compiler or operating system produces same InChI as the software distributed by IUPAC, cInChI-1, software version 1.01.

Bugs Fixed

Several bugs have been fixed. Most of the bugs were discussed at InChI-discuss,

<https://lists.sourceforge.net/lists/listinfo/inchi-discuss>

The elimination of the following two bugs in creating stereochemical sp³ (/t) segment may lead to identifiers different from those produced by InChI version 1 software version 1.00:

- A stereocenter connected by 3 bonds in a 2D structure could be undetected if an average bond length is greater than 20.
- A parity of a stereocenter connected by 4 bonds in a 2D structure such that a stereobond exactly overlaps with another single bond may become “undefined” depending on the order of the atoms in the structure.

To maintain compatibility with software version 1.00, the fix for these bugs is activated by a new command line option, FixSp3bug or FB.

Processing Files Greater Than 2 Gigabytes

To process files greater than 2 GB with cInChI-1 the output of a problem file should be suppressed. To do that, the output and log file names should be included in the command line; the name of the problem file should be NUL, for example:

```
cInChI-1 /NEWPS /FB input.sdf output.txt logfile.log NUL
```

wInChI-1.exe cannot process files greater than 2 GB.

Running wInChI-1 under Linux

Reportedly, wInChI-1.exe could be run under WINE build 20050524 running on Mandrake 10.1

Suppressing cInChI-1 console output

Standard redirection may be used to suppress cInChI-1 console output.

Under Windows:

```
cInChI-1 /NEWPS /FB input.sdf output.txt logfile.log NUL 2>NUL
```

Under Linux:

```
clnChl-1 -NEWPS -FB input.sdf output.txt logfile.log NUL 2>/dev/null
```

“>” or “1>” redirects standard output, “2>” redirects standard error output.