

# IUPAC InChI and InChIKey

## IUPAC InChI format

ChemAxon applications are able to import and export IUPAC InChI files, and export IUPAC InChIKey files. This function does not work in the applets (except signed ones).

The export makes an InChI with AuxInfo by default. The import requires an InChI string (AuxInfo is optional). Without AuxInfo, the generated molecule does not include coordinates.

At the moment Linux, Windows and Mac platforms are supported.

Since Version 5.5 the InChI 1.03 version is integrated, jni-inchi sourceforge project is used to call the native C code. Since Version 5.2.5 InChIKey export format is also included.

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| <i>Code:</i> <b>inchi,</b><br><b>inchikey</b> |
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| <b>See also</b> |
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| InChI and<br>InChIKey export<br>options |
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## Known Issues

- Allenes and cumulenes are not supported yet.

## JNI-InChI

JNI-InChI is Copyright 2006-2010, Sam Adams. JNI-InChI is free software: you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version. (See [GPL](#), [LGPL](#) licence.)

The modified source, that we use in our program to locate and download dlls, is available [here](#).

The compiled version (jni-inchi\_07.jar) is in the lib directory of the installed marvin. If you find any bugs, we recommend asking for a bugfix on our technical support forum, instead of modifying the source.

## References

- [iupac.org](http://iupac.org)
- [www.iupac.org/inchi](http://www.iupac.org/inchi)
- [sourceforge.net/projects/inchi](http://sourceforge.net/projects/inchi)
- <http://jni-inchi.sourceforge.net>

InchiExport uses the *InChI format*, InChITM Material is © IUPAC 2005