

IUPAC InChI, InChIKey, RInChI and RInChIKey

IUPAC InChI and RInChI format

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

The export makes an InChI with AuxInfo or RInChI with RAuxInfo by default. The import requires an InChI or RInChI string (AuxInfo and RAuxInfo are optional).

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

Since Version 19.11 the InChI 1.05 version and RInChI 1.00 are integrated. Since Version 19.11 InChIKey export and RInChIKey export are also included.

Code: **inchi,**
inchikey

See also

[InChI and
InChIKey export
options](#)

Known issues

In case of RInChI the export of reaction agents to RInChI and RInChIKey are not supported yet.

Native InChI and RInChI libraries

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References

- iupac.org
- www.iupac.org/inchi
- sourceforge.net/projects/inchi