



INTERNATIONAL UNION OF  
PURE AND APPLIED CHEMISTRY

## InChI Software 1.01 Summary

The IUPAC International Chemical Identifier, InChI version 1, was released in August 2006. The whole package includes:

- InChI version 1 software version 1.01 documentation, and Windows and Linux (i386) executable programs
- InChI version 1.01 source code and Application Program Interface (API)
- InChI validation protocol
- What 's new in InChI software version 1.01

This release includes the following new features:

- InChI validation protocol to establish whether software that includes the InChI algorithm produces valid InChI
- InChI reversal: InChI to structure conversion (connection table, bond orders, charges, stereochemical parities; the resultant structures have no coordinates; success rate on average is 99.7 percent)
- Several bug fixes that eliminate known InChI failures
- Several minor additional features

For more detail, see the [Whats\\_New.pdf](#) included in the package.

### Q&A

Q: Why is the InChI version in this package 1, not 1.01?

A: The version of the chemical identifier (as a string of characters derived from a chemical structure) is the same, only the software and documentation were updated. Therefore, the InChI version is still version 1.

We express our gratitude to those who discovered and helped fix various problems with the software and validation protocol.

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