

Summary

The current version of InChI Identifier is 1; the current version of InChI software is 1.04 (August 2011). Previously released software versions 1.01 (2006), 1.02-beta (2007), 1.02-standard (2009), and 1.03 (June 2010) as well as all earlier versions are now considered obsolete.

The current software is able of producing both standard and non-standard InChI/InChIKey.

The summary of the features of the distributed package is as follows:

- the software licence is changed from GNU Lesser General Public Licence, LGPL version 2.1 to the more permissive IUPAC/InChI-Trust Licence for the International Chemical Identifier (InChI) Software version 1.0;
- the software now supports the chemical elements up to 112, copernicium (the last one which is currently recognised by IUPAC; support for elements 105-112 is newly added);
- the possibility of processing multiple input files at a single run is added to the inchi-1 executable (both Windows and Linux versions); the common file name wildcards are recognized;
- the support for CML input files is no longer provided; related source codes were removed ;
- several minor bugfixes/changes were made to the source codes;
- InChI executable and InChI API library binaries are supplied in 32 and 64 bit versions for both Windows and Linux.