The IUPAC International Chemical Identifier (InChI)

http://www.iupac.org/inchi
http://inchi.sourceforge.net

InChI FAQ: http://wwmm.ch.cam.ac.uk/inchifaq

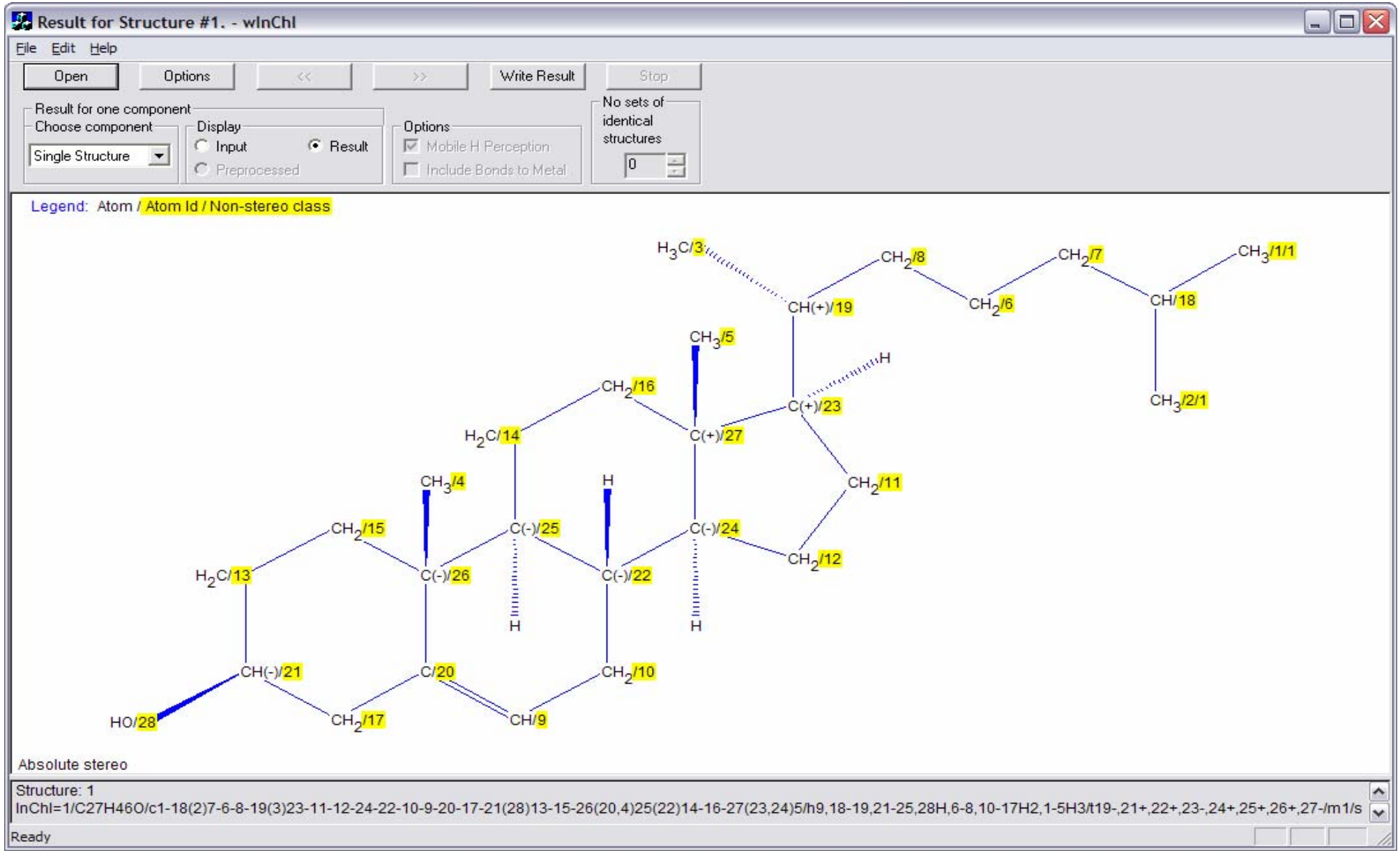
InChI:

- an Open Source, non-proprietary, public-domain identifier for chemicals
- a string of characters uniquely representing a specified molecular structure
- a precise, robust, IUPAC-approved chemical substance tag
- independent of the way the chemical structure is drawn
- indexed by internet search engines
- usable in both printed and electronic data sources
- enables reliable structure recognition and easy linking of diverse data compilations

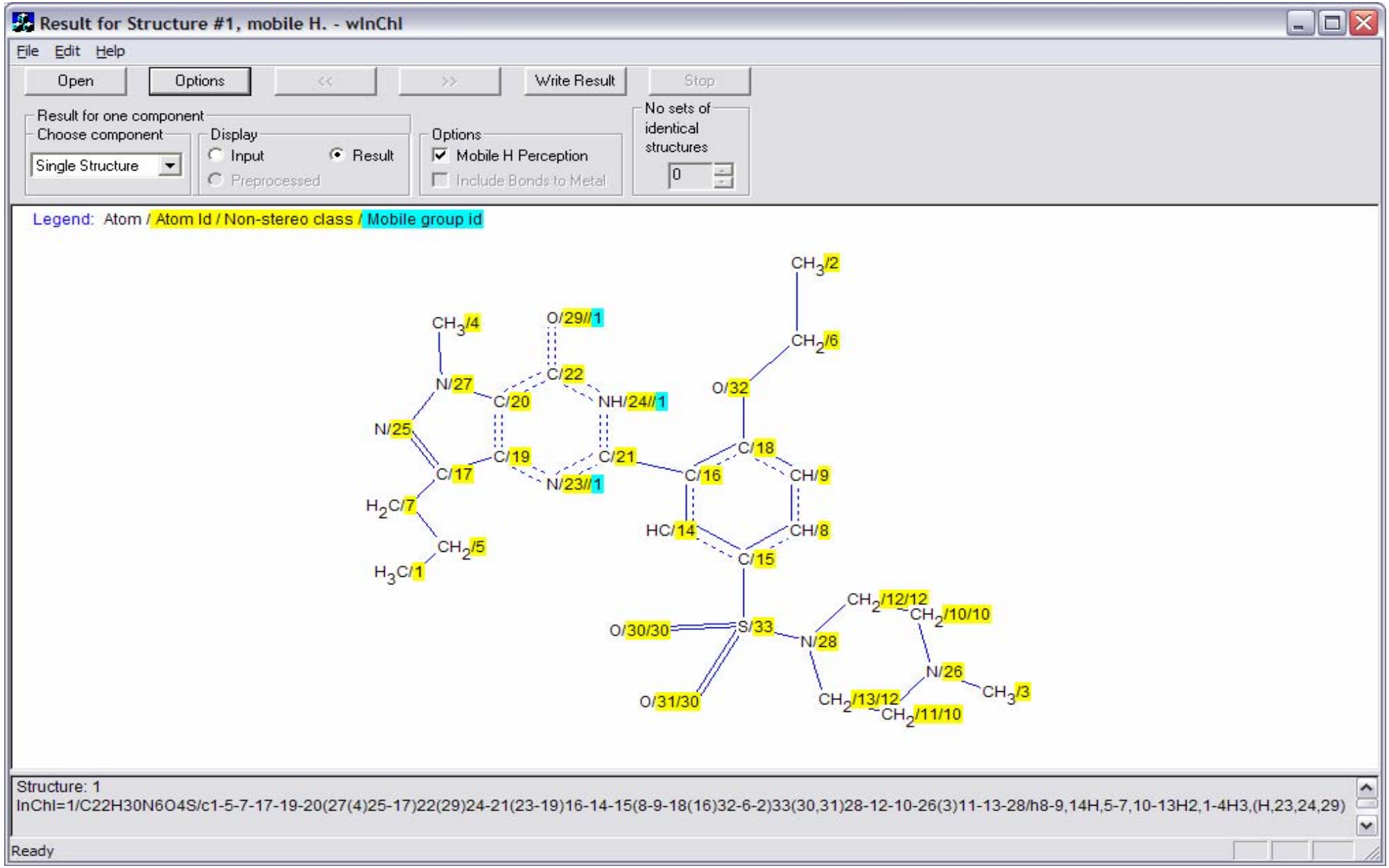
InChI software:

- accepts input in the form of MOLfiles (or SDfiles) and CML files
- is integrated with ACD ChemSketch
- accepts structures generated by cut-and-paste from ChemDraw, Marvin, and BKChem
- deals with organic compounds with *Z*/*E* and sp^3 configurations, tautomers, and isotopes as well as salts, organometallic compounds and protonated forms
- regenerates the original structure from InChI output

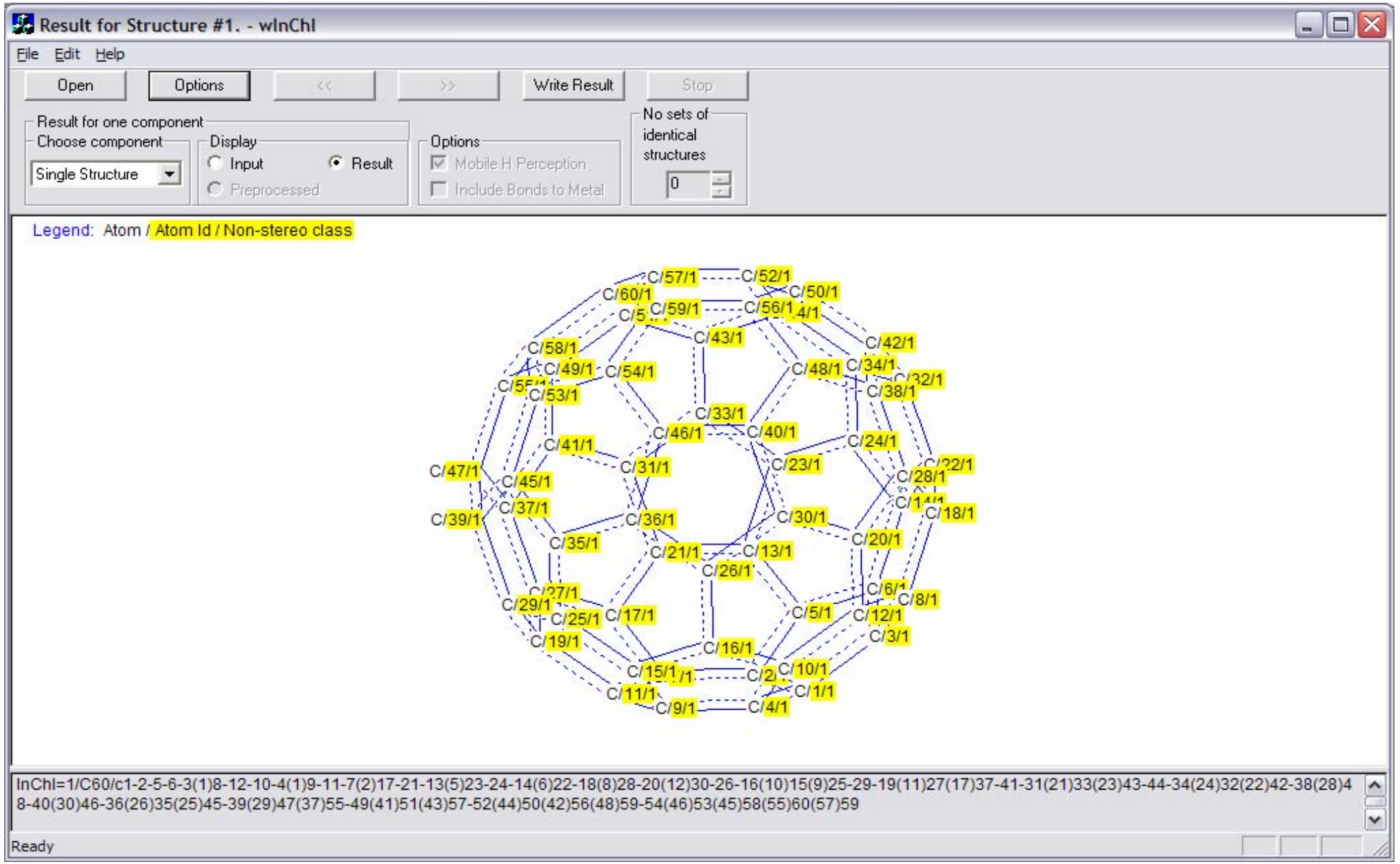
InChI for cholesterol



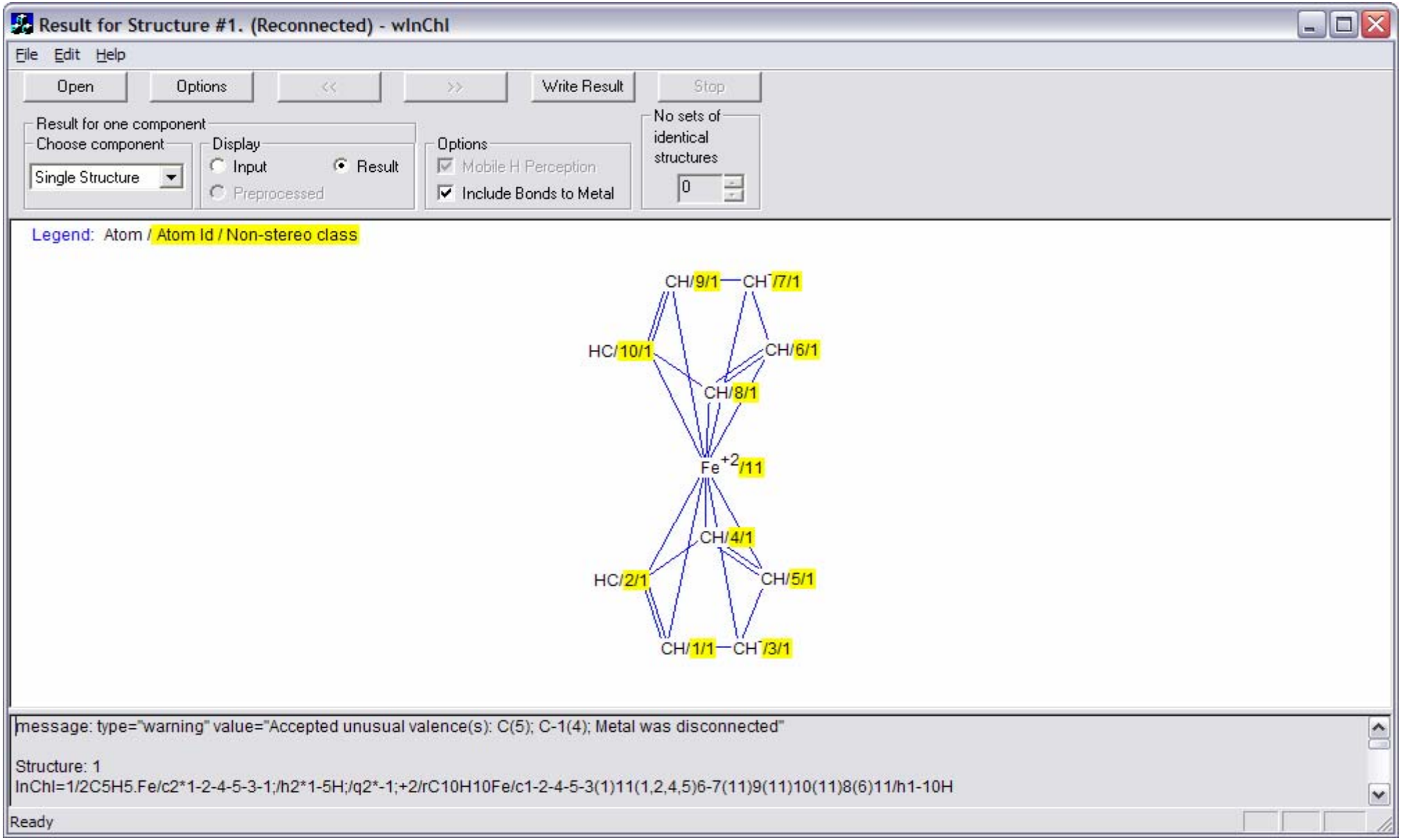
InChI for Viagra



InChI for C_{60} fullerene



InChI for ferrocene



InChI data layers:

1. **Formula (standard Hill sorted)**
2. **Connectivity (no formal bond orders)**
   i. **disconnected metals**
   ii. **connected metals**
3. **Isotopes**
4. **Stereochemistry**
   i. **double bond (*Z*/*E*)**
   ii. **tetrahedral (sp^3)**
5. **Tautomers (on or off)**

Charges are not part of the basic InChI, but are added at the end of the InChI string.

InChI symbolism:

/c connectivity-1.1 (excluding terminal H)

/h connectivity-1.2 (locations of terminal H, including mobile H attachment points)

/p proton balance

/t sp^3 (tetrahedral) parity

/m parity inverted to obtain relative stereo (1 = inverted, 0 = not inverted, . = unaffected by inversion)

/s stereo type (1 = absolute, 2 = relative, 3 = racemic)

/i isotopic specification

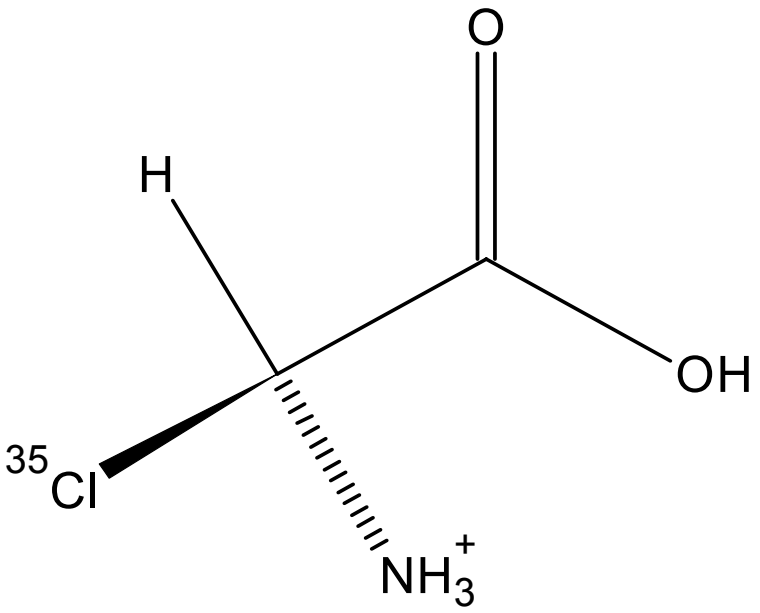
/f chemical formula of the fixed-H structure if different

/h connectivity-2 (locations of fixed mobile H)

/q charge

/r chemical formula of “connected metal” structure

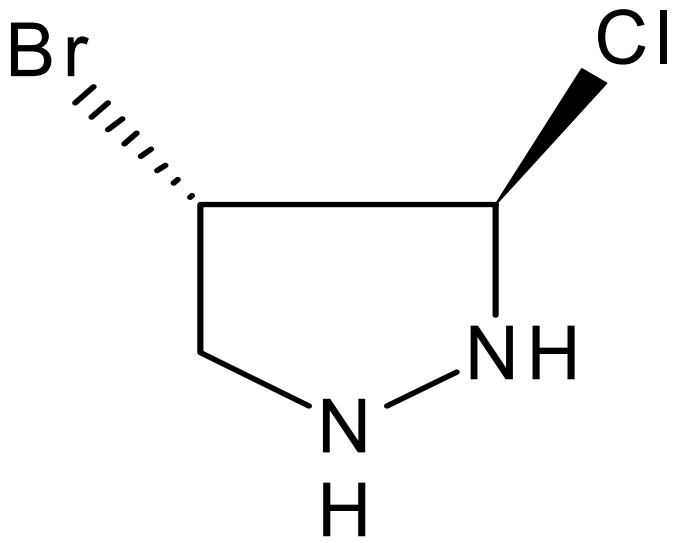
Chloroalaninium InChI layers



InChI=1/C2H4ClNO2/c3-1(4)2(5)6/h1H,4H2,(H,5,6)/p+1/t1-/m1/s1/i3+0/fC2H5ClNO2/h4-5H/q+1

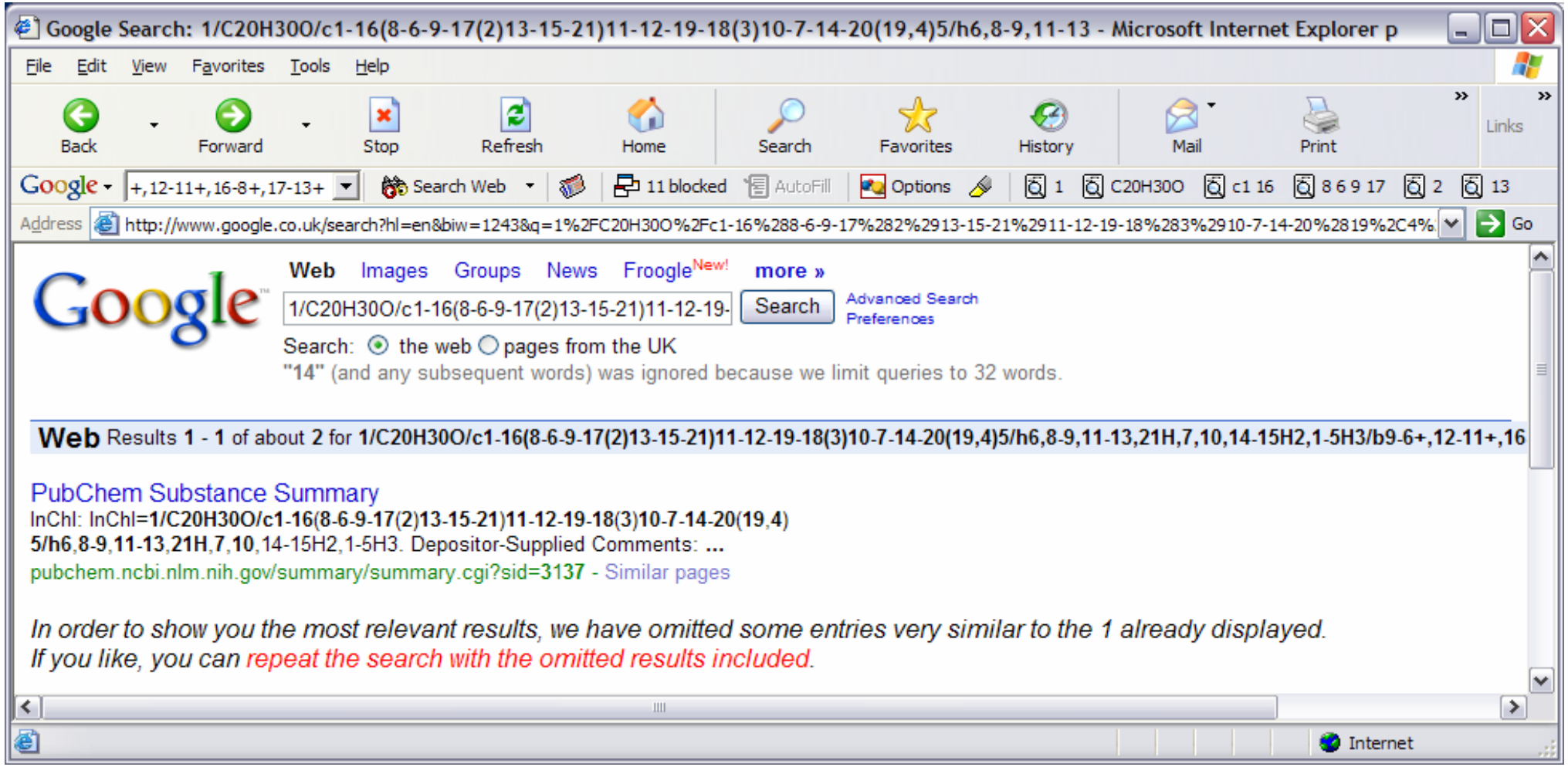
Main layer:	**C2H4ClNO2/c3-1(4)2(5)6**
Proton balance layer:	**p+1**
Stereo layer:	**t1-/m1/s1**
Isotopic layer:	**i3+0**
Fixed-H layer:	**fC2H5ClNO2/h4-5H**
Charge layer:	**q+1**

Configuration



Abs. chirality: InChI = 1/C3H6BrClN2/c4-2-1-6-7-3(2)5/h2-3,6-7H,1H2/t2-,3-/m0/s1
Rel. chirality: InChI = 1/C3H6BrClN2/c4-2-1-6-7-3(2)5/h2-3,6-7H,1H2/t2-,3-/s2
Racemic: InChI = 1/C3H6BrClN2/c4-2-1-6-7-3(2)5/h2-3,6-7H,1H2/t2-,3-/s3

Web search for retinol InChI



InChI early users:

US National Institute of Standards and Technology – 150,000 structures

US National Center for Biotechnology Information: PubChem project – 800,000+ structures

US National Cancer Institute – 23 million+ structures

US Environmental Protection Agency – DSSTox database – 1450 structures

Kyoto Encylopedia of Genes and Genomes (KEGG) database – 9584 structures

University of California at San Francisco ZINC database – 3.3 million structures

BRENDA enzyme information system (University of Cologne) – 36,000 structures

Chemical Entities of Biological Interest (ChEBI) database of the European Bioinformatics Institute – 5000 structures

Nature Chemical Biology

Under consideration:

ISI – 2 million+ structures

Beilstein Journal of Organic Chemistry

European Patent Office

US Patent and Trademark Office

Selected literature:

Stephen E. Stein, Stephen R. Heller, and Dmitrii Tchekhovskoi, "An Open Standard for Chemical Structure Representation: The IUPAC Chemical Identifier", *in Proceedings of the 2003 International Chemical Information Conference (Nimes)*, Infonortics, pp. 131-143; http://www.hellers.com/steve/resume/p157.html

Michael Freemantle, "Unique Labels for Compounds", *C&EN*, Vol.80, No. 48, 2 Dec 2002

David Adam, "Chemists synthesize a single naming system", *Nature*, 23 May 2002

Peter Murray-Rust, Henry S. Rzepa and Yong Zhang, "Googling for INChIs; A remarkable method of chemical searching", *W3C Workshop on Semantic Web for Life Sciences*, 27-28 October 2004, Cambridge, Massachusetts USA; http://lists.w3.org/Archives/Public/public-swls-ws/2004Oct/att-0019/

Simon J. Coles, Nick E. Day, Peter Murray-Rust, Henry S. Rzepa, and Yong Zhang, "Enhancement of the chemical semantic web through the use of InChI identifiers", *Org. Biomol. Chem.*, 2005, 3(10), 1832 – 1834

M. D. Prasanna, Jiri Vondrasek, Alexander Wlodawer, T.N. Bhat, "Application of InChI to Curate, Index, and Query 3-D Structures", *PROTEINS: Structure, Function and Bioinformatics*, 2005, 60:1-4

Aurélien Monge, Alban Arrault, Christophe Marot and Luc Morin-Allory, "Analysis of a Set of 2.6 Million Unique Compounds gathered from the Libraries of 32 Chemical Providers", presented at the 10th Electronic Computational Chemistry Conference, April 2005; http://www.univ-orleans.fr/icoa/eposter/eccc10/monge/

Bea Perks, "International chemical identifier goes online", *Chem. World*, 16 May 2005

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IUPAC General Assembly

Beijing

2005

Pages layout for poster

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