Why Librarians will love InChI

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The main web sites for the IUPAC InChI project are:
http://www.iupac.org/inchi
and
http://www.inchi-trust.org **6/14/2011**

Slides are available at http://www.hellers.com/steve/pub-talks/sla-6-11.pdf

Outline

1. Background/History/Objective/Why InChI?
2. InChI and Librarians
3. InChI Technical Details and Examples
4. InChI Trust
5. Current and Future InChI activities
6. Acknowledgements

Chemists use diagrammatic representations to convey structural information, and these are sometimes supplemented by verbal descriptions of structure. Conventional chemical nomenclature is a means of specifying a chemical structure in words, and systematic nomenclature provides an unambiguous description of a structure, a diagram of which can be reconstructed from its systematic name. The IUPAC International Chemical Identifier, or InChI, which is currently being developed, is a machine-readable string of symbols which enables a computer to represent the compound in a completely unequivocal manner. InChIs are produced by computer from structures drawn on-screen, and the original structure can be regenerated from an InChI with appropriate software. An InChI is not directly intelligible to the normal human reader, but InChIs will in time form the basis of an unequivocal and unique data base of all chemical compounds.

Objective

The objective of the IUPAC Chemical Identifier Project is to create a unique label, the IUPAC Chemical Identifier (InChI), which will be an Open Source, freely available, non-proprietary identifier for well defined chemical substances that can be used in printed and electronic data sources thus enabling easier LINKING of and working with diverse data and information compilations.

Why InChI? - Too Many Identifiers

Structure diagrams
- various conventions
- contain 'too much' information

Connection Tables
- MolFiles, Smiles, ROSDAL, …

Pronounceable names
- IUPAC, CAS 8th CI name, CAS 9th CI name, trivial, WHO INN

Index Numbers
- EINECS, FEMA, DOT, RTECS, CAS, Beilstein, USP, RTECS, EEC, RCRA, NCI, UN, USAF , EC

CML and InChI

CML (Chemical Markup Language) is an approach to managing molecular information using tools such as XML and Java.

CML is capable of supporting a wide range of chemical concepts including:

MOLECULES
reactions
spectra and analytical data
computational chemistry
chemical crystallography and materials

InChI fits within CML framework and structure and is the way molecules are described.

Why Use InChI ?

For publishers, database providers, organizations, and librarians with one or more databases and with customers and stakeholders needing to access this information, using InChI gives one an advantage being able to LINK and FIND content from multiple sources. It offers librarians and their stakeholders the ability to more easily FIND existing information and data by easily being able to integrate, remix, and retell. InChI is a small, but vital, part of new organization models and technologies involving chemicals that will lead to improved efficiencies new discoveries. Combinability increases the value of information and data.

InChI will save time and money!

Critical factors for the success of InChI project

1. Technically competent staff
2. Fulfill a real community need
3. Political and Financial Support

Technical: **InChI is a unique representation/identifier for defined chemical structures. Probably marginally better than previous ones. The InChI algorithm was built on the shoulders of giants, starting with Euler in 1736.**
http://en.wikipedia.org/wiki/Graph_theory

Practical: **InChI and the related hash-code compressed InChIKey are the ONLY available universal LINKs for in-house and public databases of defined chemical structures. The adoption and use of InChI by the vast majority of publishers and database providers assure it is and will continue to be widely used.**

Why InChI is becoming a success

1. Organizations need a structure representation for their content (databases, journals, patents, chemicals for sale, products, and so on) so that their content can be found and LINKED to and combined with other content on the Internet.

2. InChI is a public domain algorithm that anyone, anywhere can freely use. The other major representations are proprietary and hence not affordable for the world-wide community.

3. InChI is not a replacement for any internal structure representations. InChI is IN ADDITION to what one uses internally. Its value to most organizations is in LINKING information.

How do we know the InChI project is beneficial?

Success is uncoerced adoption

InChI – What is missing?

While we believe InChI covers some 99% of the chemicals found in computer readable databases, there are areas of chemistry not yet covered by the InChI algorithm. Some are currently being addressed, while others of lesser importance will be addressed in the next few years. But these gaps have not impeded the widespread adoption and support of InChI.

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InChI have some advantages over other chemical identifiers developed before:

(1) They are freely useable and non-proprietary.

(2) They allow a more advanced representation of chemical information than other codes (such as the SMILES code).

(3) They are unambiguous, i.e. conversion of chemical structures using standardized algorithms only leads to one InChI. (see next slides)

(4) They are precisely indexed by major search engines such as Google.

However, InChI are not applicable to generic formats often disclosed in patent literature, such as Markush structures, since they were rather designed to represent specific chemical structures and compounds. InChI therefore are not yet useful for comprehensive retrieval of patent literature.

Excerpt taken from:
Full-text prior art and chemical structure searching in e-journals and on the internet – A patent information professional's perspective
World Patent Information, Volume 31, Issue 4, December 2009, Pages 278-284
Maik Annies (Syngenta)

Re: [CHMINF-L] Inchi and chemical databases

You forwarded this message on 9/15/2010 5:37 PM.

CHEMICAL INFORMATION SOURCES DISCUSSION LIST [CHMINF-L@LISTSERV.INDIANA.EDU] on behalf of Ian A Watson

Sent: Wednesday, September 15, 2010 3:24 PM

To: CHMINF-L@LISTSERV.INDIANA.EDU

Interesting example of Caffeine smiles on the web site. I was able to generate 172 different smiles for the Caffeine molecule (email me if you'd like them). Presumably each one of these could be a unique smiles in somebody's implementation.

But when I converted each of those 172 different smiles to InChI, I got the exact same InChI string for each one. That's exactly how things are supposed to work. Nice.

Ian Watson

```
c1(=O)c2c(n(C)c(=O)n1C)ncn2C
c12c(n(C)c(=O)n(C)c1=O)ncn2C
O=c1n(C)c(=O)c2c(ncn2C)n1C
Cn1c2c(nc1)n(C)c(=O)n(C)c2=O
c12c(ncn1C)n(C)c(=O)n(c2=O)C
O=c1c2c(ncn2C)n(c(=O)n1C)C
c12c(n(cn1)C)c(=O)n(C)c(=O)n2C
Cn1c2c(nc1)n(c(=O)n(c2=O)C)C
c12c(ncn1C)n(c(=O)n(C)c2=O)C
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c12c(n(C)cn1)c(=O)n(c(=O)n2C)C
Cn1c(=O)c2c(ncn2C)n(c1=O)C
n1cn(C)c2c1n(c(=O)n(c2=O)C)C
n1cn(c2c1n(C)c(=O)n(c2=O)C)C
c12c(c(=O)n(c(=O)n1C)C)n(C)cn2
c1nc2c(n1C)c(=O)n(C)c(=O)n2C
c1(=O)n(C)c(=O)c2c(ncn2C)n1C
O=c1n(c(=O)c2c(ncn2C)n1C)C
Cn1cnc2c1c(=O)n(C)c(=O)n2C
n1(c(=O)n(c(=O)c2c1ncn2C)C)C
c1(=O)n(C)c(=O)c2c(n1C)ncn2C
O=c1n(c2c(n(cn2)C)c(=O)n1C)C
Cn1c2c(n(cn2)C)c(=O)n(c1=O)C
Cn1c(=O)c2c(n(c1=O)C)ncn2C
Cn1cnc2c1c(=O)n(c(=O)n2C)C
c1nc2c(c(=O)n(C)c(=O)n2C)n1C
c12c(ncn1C)n(c(=O)n(c2=O)C)C
c1nc2c(n1C)c(=O)n(c(=O)n2C)C
Cn1c2c(n(cn2)C)c(=O)n(C)c1=O
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n1(C)c2c(nc1)n(C)c(=O)n(c2=O)C
n1(c(=O)c2c(n(c1=O)C)ncn2C)C
n1(c(=O)c2c(n(C)c1=O)ncn2C)C
Cn1c(=O)n(c2c(c1=O)n(C)cn2)C
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c1(=O)n(C)c(=O)c2c(ncn2C)n1C
n1(cnc2c1c(=O)n(c(=O)n2C)C)C
n1(C)c(=O)n(C)c2c(n(cn2)C)c1=O
n1(c2c(n(cn2)C)c(=O)n(C)cn2)C
n1(C)cnc2c1c(=O)n(C)c(=O)n2C
O=c1c2c(n(C)c(=O)n1C)ncn2C
n1(c2c(nc1)n(c(=O)n(c2=O)C)C)C
n1(C)c(=O)c2c(n(c1=O)C)ncn2C
n1(c2c(c(=O)n(c1=O)C)ncn2C
n1cn(C)c2c1n(C)c(=O)n(c2=O)C
c12c(c(=O)n(C)c(=O)n1C)n(cn2)C
Cn1c2c(n(C)cn2)c(=O)n(c1=O)C
n1(c(=O)n(C)c2c(n(cn2)C)c1=O)C
n1cn(c2c1n(C)c(=O)n(C)c2=O)C
c1(=O)n(c2c(c(=O)n1C)C)n(cn2)C
Cn1c(=O)n(c(=O)c2c1ncn2C)C
O=c1n(c(=O)c2c(n(C)cn2)C)C)C
n1(c2c(c(=O)n(c1=O)C)n(C)cn2)C
c12c(n(cn1)C)c(=O)n(c(=O)n2C)C
c12c(c(=O)n(C)c(=O)n1C)n(C)cn2
Cn1c(=O)c2c(n(C)c1=O)ncn2C
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```
c1(=O)n(C)c2c(n(cn2)C)c(=O)n1C
O=c1n(C)c2c(c(=O)n1C)n(C)cn2
n1(C)c2c(c(=O)n(C)c1=O)n(C)cn2
n1cn(c2c1n(c(=O)n(C)c2=O)C)C
O=c1n(c(=O)n(C)c2c1n(cn2)C)C
c1(=O)c2c(n(c(=O)n1C)C)ncn2C
c1(=O)n(c2c(n(cn2)C)c(=O)n1C)C
Cn1c2c(c(=O)n(c1=O)C)n(cn2)C
c1(=O)n(c(=O)c2c(n1C)ncn2C)C
O=c1n(c(=O)c2c(n1C)ncn2C)C
n1cn(C)c2c1n(c(=O)n(C)c2=O)C
n1(c(=O)n(C)c2c(c1=O)n(C)cn2)C
O=c1c2c(ncn2C)n(C)c(=O)n1C
n1cnc2c1c(=O)n(C)c(=O)n2C)C
n1(C)cnc2c1c(=O)n(C)c(=O)n2C)C
n1cn(C)c2c1n(C)c(=O)n(C)c2=O
O=c1n(C)c(=O)n(C)c2c1n(C)cn2
n1(C)c(=O)n(c2c(c1=O)n(C)cn2)C
Cn1c(=O)c2c(ncn2C)n(C)c1=O
n1(c2c(n(cn2)C)c(=O)n(c1=O)C)C
n1(C)c2c(n(C)c(=O)n(c1=O)nc1
Cn1c2c(n(c(=O)n(c2=O)C)C)nc1
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O=c1n(C)c2c(n(C)cn2)c(=O)n1C
n1(C)c2c(n(cn2)C)c(=O)n(C)c1=O
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O=c1n(c2c(c(=O)n1C)n(cn2)C)C
Cn1c2c(n(C)c(=O)n(C)c2=O)nc1
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Cn1c2c(n(c(=O)n(C)c2=O)C)nc1
c1(=O)n(c(=O)n(C)c2c1n(C)cn2)C
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n1(c(=O)c2c(n(C)cn2)C)c(=O)n1C
n1(C)c2c(n(C)cn2)c(=O)n(c1=O)C
n1(C)c2c(nc1)n(C)c(=O)n(c2=O)C
n1(C)c2c(n(cn2)C)c(=O)n(c1=O)C
n1(C)c2c(c(=O)n(C)c1=O)n(cn2)C
n1(c(=O)n(c2c(n(C)cn2)c1=O)C)C
n1(c(=O)n(c2c(c1=O)n(cn2)C)C)C
n1(C)c2c(n(C)cn2)c(=O)n(C)c1=O
n1(C)c2c(c(=O)n(c1=O)C)n(cn2)C
n1(C)c2c(n(c(=O)n(C)c2=O)C)nc1
n1(C)c2c(nc1)n(c(=O)n(c2=O)C)C
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O=c1c2c(n(c(=O)n1C)C)ncn2C
O=c1n(C)c2c(n(cn2)C)c(=O)n1C
n1(C)c(=O)n(c2c(n(C)cn2)c1=O)C
n1(C)c2c(c(=O)n(c1=O)C)n(cn2)C
Cn1c2c(c(=O)n(C)c1=O)n(C)cn2
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n1(C)c2c(nc1)n(c(=O)n(C)c2=O)C
Cn1c(=O)n(C)c2c(c1=O)n(C)cn2
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n1(C)c2c(n(c(=O)n(C)c2=O)C)nc1
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n1(C)c2c(c(=O)n(c1=O)C)n(C)cn2
n1(C)c2c(n(c(=O)n(C)c2=O)C)nc1
n1(C)c2c(nc1)n(c(=O)n(c2=O)C)C
```

What is in it for the Librarian?

The particular value of InChI to the library community is simple. The justification (or perhaps a better way to put it - the return on investment - ROI) is that the librarians and their stakeholders can more easily and cost effectively, find the information they need. This will improve quality and the quantity of the results they obtain. There are no other notations now being used, e.g., SMILES or CAS numbers, that can make this statement, since both are proprietary, not widely readily available, and not likely to ever be non-proprietary.

Put very explicitly, today there already are more InChIs in databases and information resources than any other chemical identifier because of two factors. One is that InChIs are free. The second is that the Internet allows one to find information associated with an InChI.

Besides these practical and political benefits, as librarians begin to use InChIs in their everyday activities and training, it will show vision and leadership to your organization and stakeholders.

How difficult is it to create an InChI?

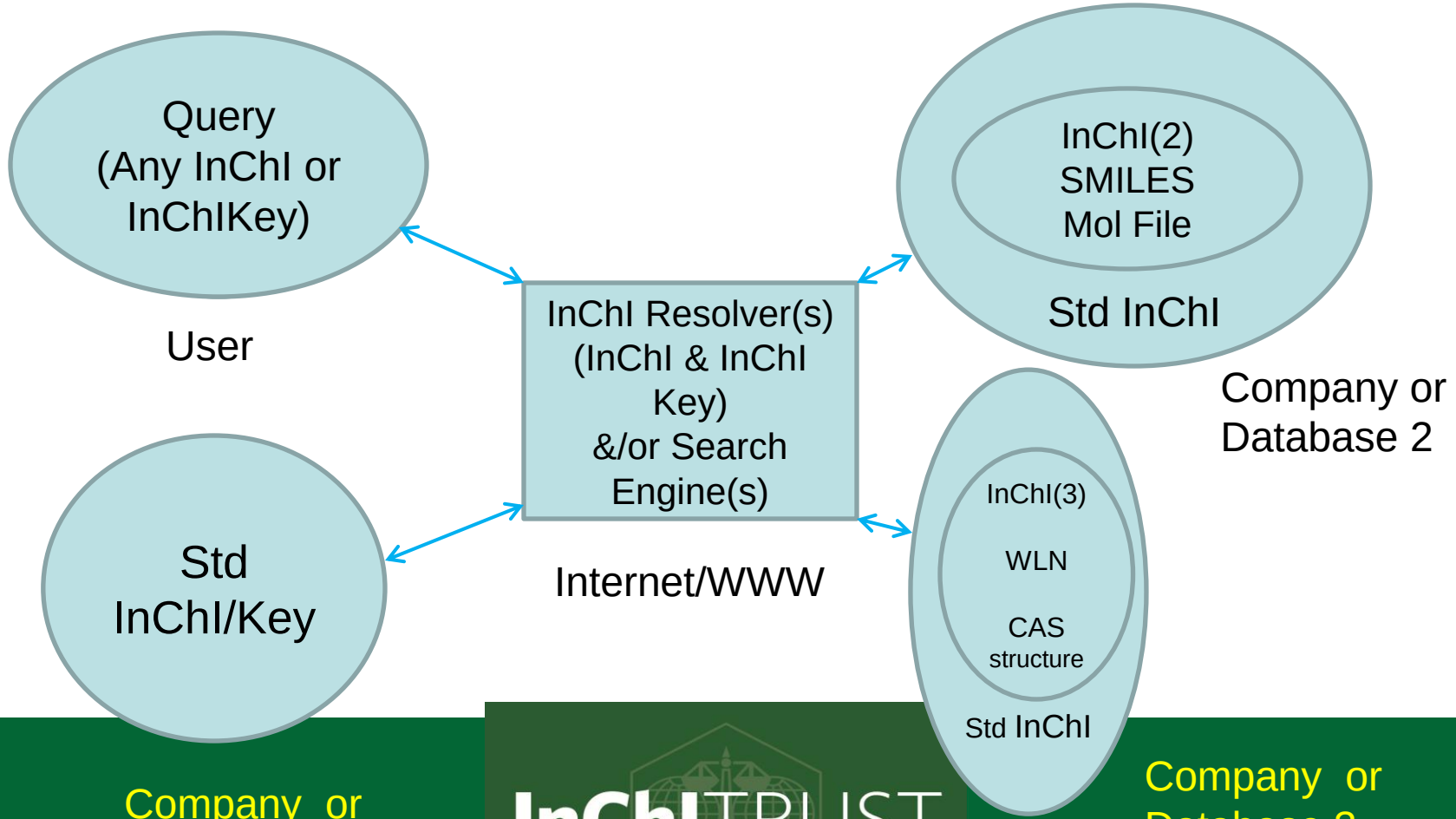
Today, all the major structure drawing programs (ChemDraw, MDL/Symyx/Accelrys Draw, ISIS Draw, ChemAxon Marvin Sketch, ACD Labs ChemSketch, Jmol and so on) have incorporated the InChI algorithm in their products, with usually an "InChI" button for generating the InChI.

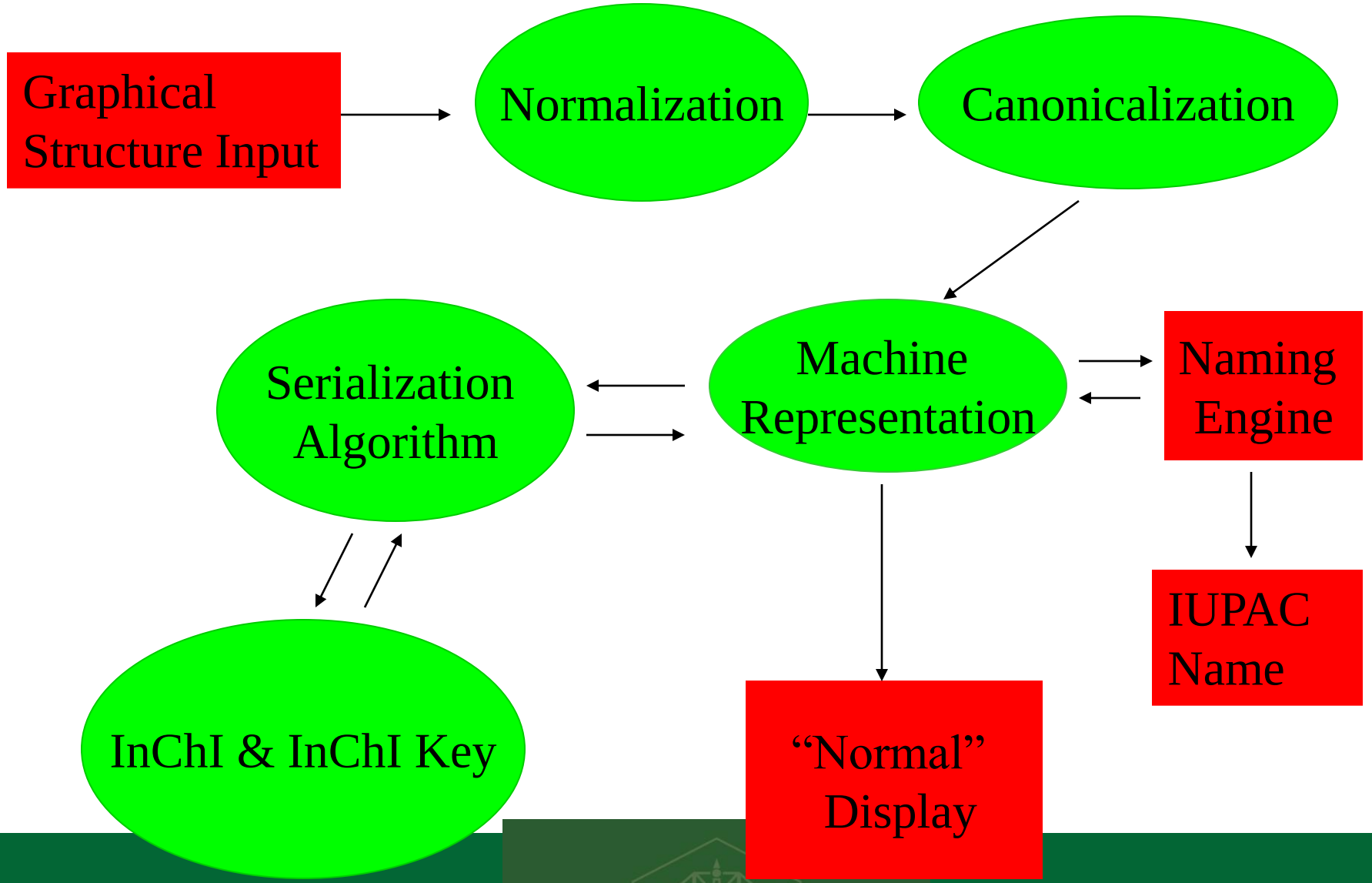
Who uses/searches InChIs?

InChIs are now found in virtually all major chemical databases, particularly in the very large ones. Databases such as Reaxys (30 million structures), NIH/PubChem (25 million structures), NIH/NCI (60 million structures), and SciFinder (55 million structures) all have InChIs and allow for InChIs as input for a search.

The next slide shows different databases from different organizations can link together and find ALL available information ONLY by using InChIs.

The LINKED and Interoperable and Combinable World of InChI




Graphical Structure Input
Normalization
Canonicalization
Machine Representation
Serialization Algorithm
Naming Engine
IUPAC Name
InChI & InChI Key
"Normal" Display

SHORT DESCRIPTION OF THE InChI

The conversion of structural information to its InChI is based on a set of IUPAC structure conventions and the rules for normalization and canonicalization (conversion to a single, predictable sequence) of a structure representation. The resulting InChI is simply a series of characters that serve to identify uniquely the structure from which it was derived. This conversion of a graphical representation of a chemical substance into the unique InChI character string can be carried out automatically by anyone using the freely available programs, and the facility can be built into any program dealing with chemical structures. The InChI uses a layered format to represent all the available structural information relevant to compound identity. InChI layers are listed below. Each layer in an InChI representation contains a specific type of structural information. These layers, automatically extracted from the input structure, are designed so that each successive layer adds additional detail to the Identifier. The specific layers generated depend on the level of structural detail available and whether or not allowance is made for tautomerism. Of course, if there are any ambiguities or uncertainties in the original structure representation, these will remain in the InChI.

This layered structure design of an InChI offers a number of advantages. If two structures for the same substance are drawn at different levels of detail, the one with the lower level of detail will, in effect, be contained within the other. Specifically, if one substance is drawn with stereo-bonds and the other without, the layers in the latter will be a subset of the former. The same will hold for compounds treated by one author as tautomers and by another as exact structures with all hydrogen atoms fixed. This can work at a finer level. For example, if one author includes a double bond and tetrahedral stereochemistry, but another omits stereochemistry, the InChI for the latter description will be contained within that for the former.

InChI layered structure design

The current InChI layers are:

1. **Formula**
2. **Connectivity (no formal bond orders)**
    a. **disconnected metals**
    b. **connected metals**
3. **Isotopes**
4. **Stereochemistry**
    a. **double bond (*Z/E)***
    b. **tetrahedral (sp3)**
5. **Tautomers (on or off)**

Charges are added to end of the string

InChI Characteristics

1. Easy to generate (It will use existing software.)

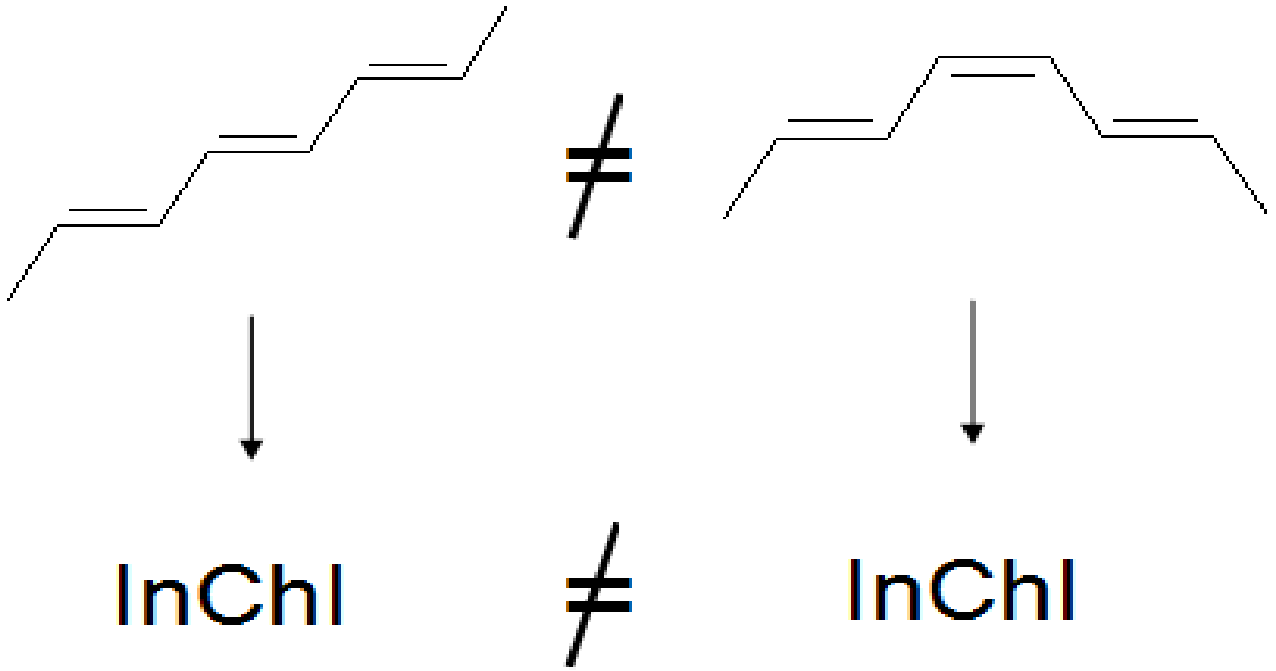
2. Expressive (It will contain structural information.)

3. Unique/Unambiguous

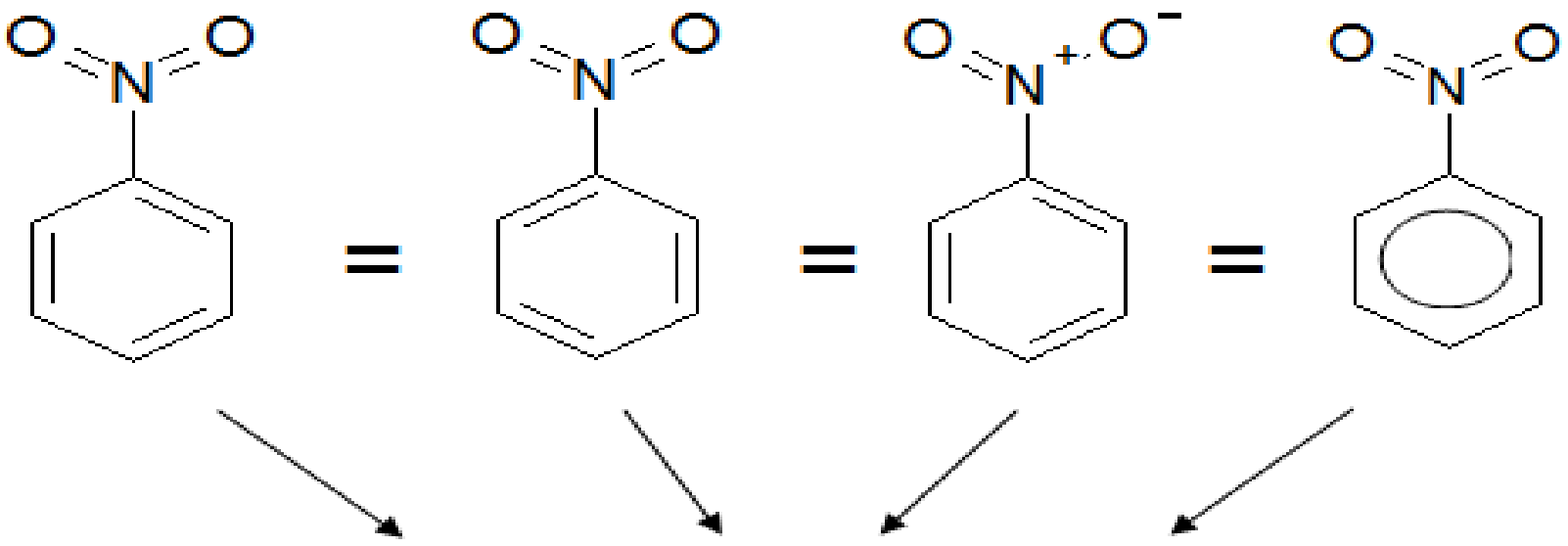
4. Easy to search for structure via Internet search engines (Google, Yahoo, Microsoft Bing, etc.) using the InChI (hash) Key.

5. Think of an InChI as a synonym that can be found in databases on the Internet.

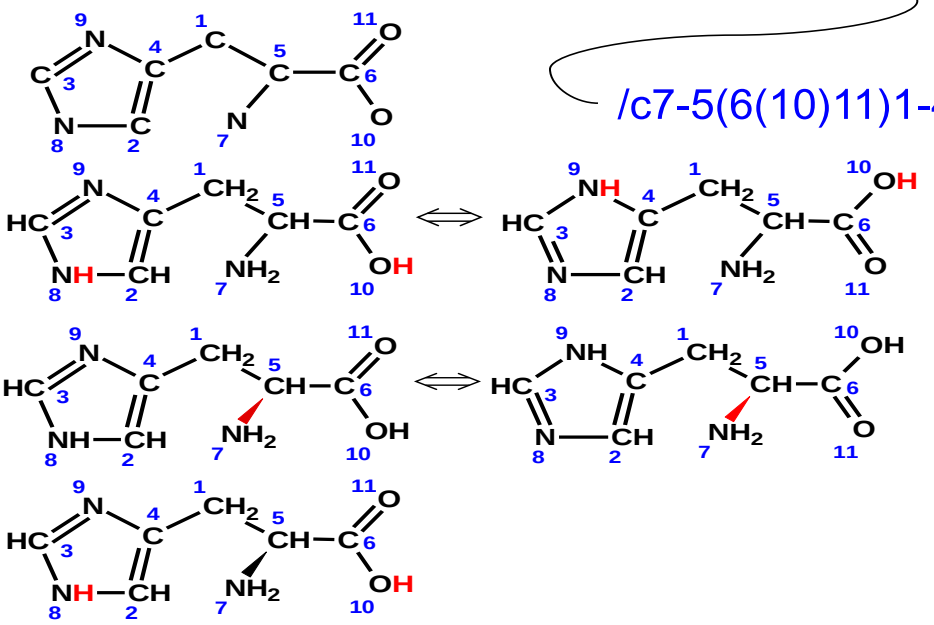
Different geometric or stereo isomers have different identifiers
–All distinguishing structural information is included



One compound has only ONE InChI



InChI Layers: L-Histidine



InChI=1/C6H9N3O2

Formula

Connections

/c7-5(6(10)11)1-4-2-8-3-9-4

Hydrogens (mobile)

/h2-3,5H,1,7H2,(H,8,9)(H,10,11)

Stereo

/t5-/m0/s1

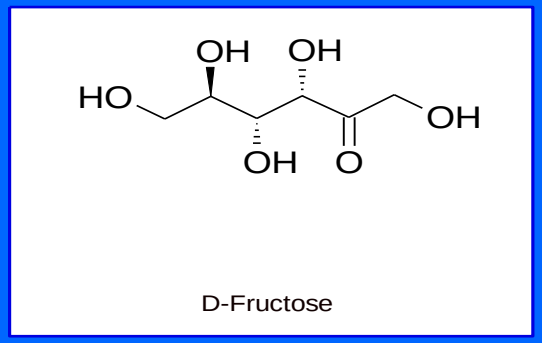
Hydrogens (fixed)

/f/h8,10H

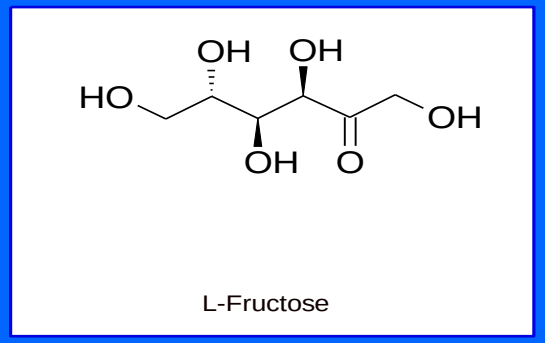
InChI=1/C6H9N3O2/c7-5(6(10)11)1-4-2-8-3-9-4/h2-3,5H,1,7H2,(H,8,9)(H,10,11)/t5-/m0/s1/f/h8,10H

InChIKey=HNDVDQJCIGZPNO-QLMCEAFFNA-N **InChIKey=HNDVDQJCIGZPNO-YFKPBYRVSA-N**

InChI TRUST



D-Fructose



L-Fructose

D-Fructose (natural)

InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3,5-9,11-12H,1-2H2/t3-,5-,6-/m1/s1

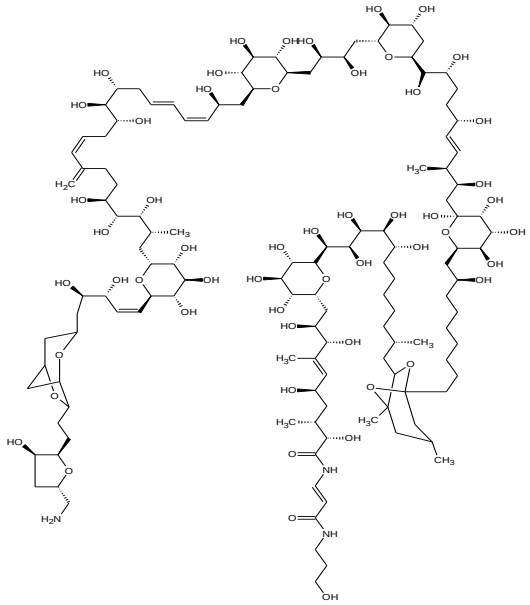
InChIKey=BJHIKXHVCXFQLS-UYFOZJQFSA-N

L-Fructose

InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3,5-9,11-12H,1-2H2/t3-,5-,6-/m0/s1

InChIKey=BJHIKXHVCXFQLS-FUTKDDECSA-N

Really long InChI (Palytoxin)



Palytoxin

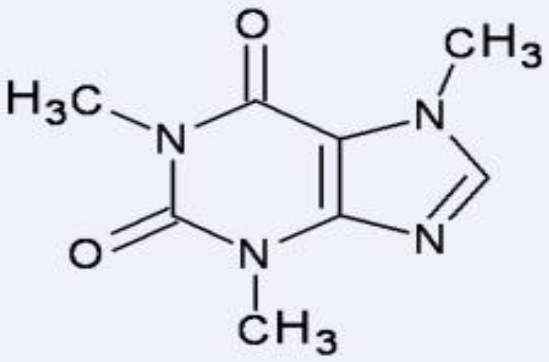
Isolated from Hawaiian soft coral

One of the most toxic non-peptide substances

Contains >70 stereochemical elements

InChI=1S/C129H223N3O54/c1-62(29-33-81(143)108(158)103(153)68(7)47-93-111(161)117(167)110(160)91(180-93)36-35-76(138)82(144)51-73-50-74-53-92(178-73)90(177-74)38-37-89-85(147)52-75(61-130)179-89)23-20-28-78(140)105(155)77(139)26-18-13-16-25-70(135)48-94-112(162)118(168)113(163)97(181-94)55-84(146)83(145)54-95-107(157)87(149)57-96(182-95)106(156)80(142)34-32-69(134)31-30-65(4)88(150)60-129(176)125(174)123(173)115(165)99(184-129)49-71(136)24-15-10-9-11-19-40-128-59-64(3)58-127(8,186-128)100(185-128)44-63(2)22-14-12-17-27-79(141)109(159)116(166)120(170)122(172)124-121(171)119(169)114(164)98(183-124)56-86(148)102(152)66(5)45-72(137)46-67(6)104(154)126(175)132-42-39-101(151)131-41-21-43-133/h13,16,18,20,23,25,30-31,35-36,39,42,45,63-65,67-100,102-125,133-150,152-174,176H,1,9-12,14-15,17,19,21-22,24,26-29,32-34,37-38,40-41,43-44,46-61,130H2,2-8H3,(H,131,151)(H,132,175)/b18-13+,23-20-,25-16-,31-30+,36-35-,42-39+,66-45+/t63-,64?,65-,67+,68+,69+,70+,71-,72-,73?,74?,75-,76+,77+,78+,79+,80+,81-,82+,83+,84+,85+,86-,87+,88-,89+,90?,91+,92?,93+,94-,95+,96-,97+,98+,99+,100?,102+,103+,104-,105-,106?,107-,108+,109-,110+,111-,112-,113+,114-,115-,116-,117-,118+,119+,120+,121-,122-,123+,124?,125+,127?,128?,129-/m0/s1

InChIKey=CWODDUGJZSCNGB-DCBUCRFRSA-N



InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3 (caffeine)

character indicating the number of protons ('N' means neutral)

InChIKey=RYYVLZVUVIJVGH-UHFFFAOYSA-N

flag character for InChI version: 'A' for version 1

First block (14 letters)

Encodes molecular skeleton (connectivity)

Second block (8 letters)

Encodes stereochemistry and isotopes

flag character ('S') indicates standard InChIKey (produced out of standard InChI)

1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3 Search

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InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3**
InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H**,1-3H3 ... reveals an inhibitor of **Mre11**-Rad50-Nbs1 complex , Nature Chemical Biology, 2008 ...
www.chemspider.com/InChIKey=RYYVLZVUVIJVGH-UHFFFAOYAW - Cached - Similar

Caffeine - Wikipedia, the free encyclopedia
1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3. InChI key, RYYVLZVUVIJVGH-UHFFFAOYAW. Properties. Molecular formula, C8H10N4O2 ...
en.wikipedia.org/wiki/Caffeine - Cached - Similar

Compound **7** : Moonlighting proteins Hal3 and Vhs3 form a ...
Nov 1, 2009 ... InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3**. InChIKey: RYYVLZVUVIJVGH-UHFFFAOYAW ...
www.nature.com › Journal home › Archive › Article › Full text

caffeine (CHEBI:27732)
Oct 17, 2009 ... InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3**. InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3** ...
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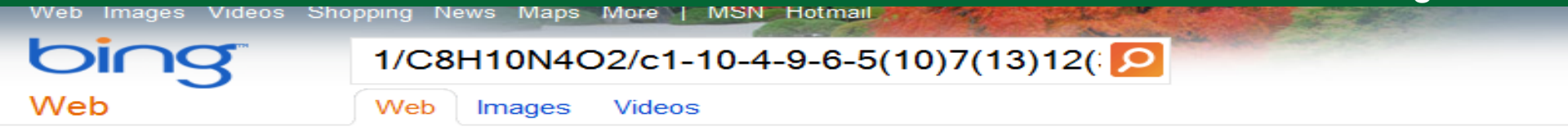
InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3**
InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3**. ... reveals an inhibitor of Mre11-Rad50-Nbs1 complex , Nature Chemical Biology, 2008 ...
mesh.chemspider.com/Chemical-Structure.2424.html - Cached

Caffeine Mass Spectrum
CH$NAME: Caffeine CH$FORMULA: C8H10N4O2 CH$EXACT_MASS: 194.08038 CH$SMILES: ... CH$IUPAC: **1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3** ...
www.massbank.jp/jsp/Dispatcher.jsp?type=disp&id...**1** - Cached - Similar

caffeine 58-08-**2**
Aug 3, 2010 ... IUPAC Name -, 1,3,7-trimethylpurine-2,6-dione. InChI -, InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3** ...
www.thegoodscentscompany.com/data/rw**1014161**.html - Cached - Similar



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NMRanalyst Sample Application: Caffeine
... **1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3** ... 1D Proton Resonances From Web Site: $> cat ...
www.sciencesoft.net/caffeine/index.html · Cached page

ChemSpider News » ChemSpider Integrations
The InChiÂ andÂ InChIKey for caffeine are shown below: InChI=**1/C8H10N4O2 /c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3** InChIKey=RYYVLZVUVIJVGH-UHFFFAOYAW
www.chemspider.com/news/category/integration · Cached page

InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3
Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1.67 estimate) = 0.16 Log Kow (Exper. database match) = -0.07 Exper.
www.chemspider.com/Chemical-Structure.2424.html · Cached page

caffeine 58-08-2
1,3,7-trimethylpurine-2,6-dione: InChI - InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2 /h4H,1-3H3**: InChIKey - RYYVLZVUVIJVGH-UHFFFAOYAW
www.thegoodscentscompany.com/data/rw1014161.html · Cached page

Chemistry and Biology support, KDE/Strigi GSoC project: August 2007
InChI=**1/C8H10N4O2/ c1-10-4-9-6-5(10)7(13) 12(3)8(14)11(6)2/ h4H,1-3H3** The solution was to add a special flag to chemistry.inchi ontology field property that would indicate that a ...
neksa.blogspot.com/2007_08_01_archive.html · Cached page

International Union of Pure and Applied Chemistry
InChI=**1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3** InChIKey=RYYVLZVUVIJVGH-UHFFFAOYAW First block (**14** letters), encodes molecular skeleton (connectivity ...
www.iupac.org/inchi/release102.html · Cached page

Caffeine Mass Spectrum
... name: caffeine ch$formula: c8h10n4o2 ch$exact_mass: 194.08038 ch$smiles: cn(c2)c(c(=o)1)c(n2)n(c)c(=o)n(c)1 ch$iupac: **1/c8h10n4o2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2 /h4h,1-3h3** ...
www.massbank.jp/jsp/Dispatcher.jsp?type=disp&id=PR010011&site=1 · Cached page

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Scientific Articles Mentioning InChI

"The Chemical Translation Service (CTS) - a web-based tool to improve standardization of metabolomic reports"
Gert Wohlgemuth, Pradeep Kumar Haldiya, Egon Willighagen, Tobias Kind, and Oliver Fiehn
Bioinformatics, published 9 September 2010 (Open Access)

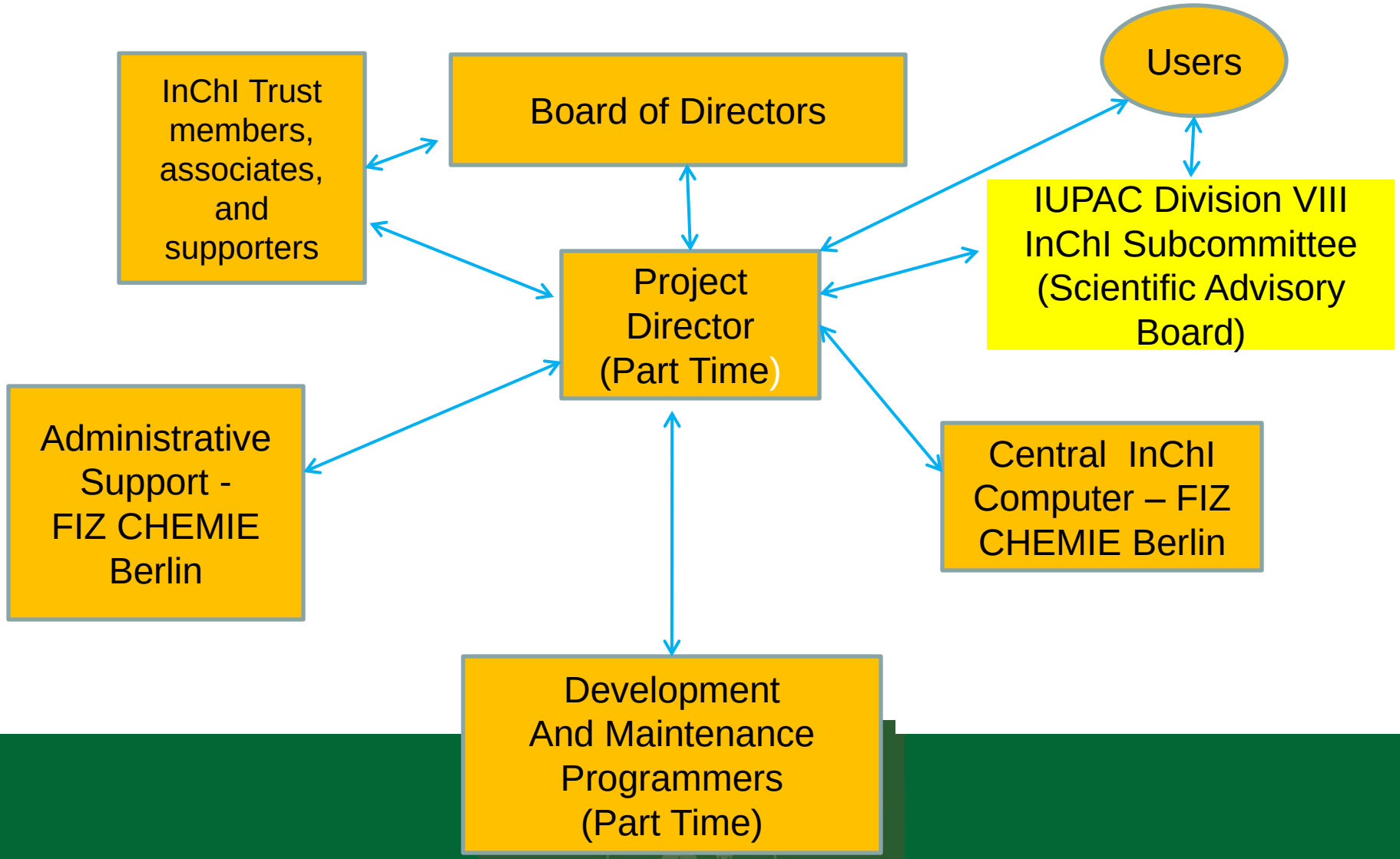
"PathwayAccess: CellDesigner plugins for pathway databases"
John L. Van Hemert and Julie A. Dickerson
Bioinformatics **2010**, *26(18)*, 2345-2346 (Open Access)

"Utopia documents: linking scholarly literature with research data"
T. K. Attwood, D. B. Kell, P. McDermott, J. Marsh, S. R. Pettifer, and D. Thorne
Bioinformatics **2010**, *26(18)*, 568-574 (Open Access)

The InChI Trust

With the requirements met of what areas of chemistry InChIs were needed for NIST databases, and since IUPAC is fundamentally and culturally a volunteer organization, a way had to be found to continue development of InChI, and maintain the InChI algorithm. InChI had to be "institutionalized" and turned over to an entity that would ensure its ongoing activities and be acceptable to the community. It was concluded that a not-for-profit organization would best fit the ongoing and future project needs. Thus the decision to create and incorporate the "InChI Trust". As there is no "free lunch", the Trust needs resources to continue to operate. Membership in the InChI Trust requires annual dues. The income from these revenues will be used exclusively for InChI development, maintenance, and educational activities associated with the project. Membership will entitle a member to influence the direction, priority, and speed of further Trust activities. Those organizations which do not join the InChI Trust will still have free access to the InChI algorithms but will not participate in any decision-making or direction - setting activities.

InChI Trust Organization



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Current IUPAC Working Groups

In Progress:

Organometallics
InChI Resolver
Electronic States
RInChI –InChI for Reactions

Completed:

Markush
Polymers/Mixtures

To be started in 2012:

Inorganics

Possible Future Enhancements

1. Transrutherfordium elements
2. Transition states.
3. Work with IUCr for 3D information
4. Proteins, Peptides & Biopolymers
5. Mac supported version
6. Java version
7. VS2010 .NET compilation support
8. Integrate with Microsoft Chem4Word

The Future

InChI has become mainstream for publishers, databases providers, and software developers. Over the next 5-10 years, publishers will use data mining to create both better abstracts, useful indexing, and concept terms. Search engines will be able to search for appropriate text and structures and direct users to the original (fee or free/Open Access/Open Data) sources.

Acknowledgements

(Primarily members for the IUPAC InChI subcommittee and associated InChI working groups)

Steve Bachrach, Colin Batchelor, John Barnard, Evan Bolton, Steve Boyer, Steve Bryant, Szabolcs Csepregi , Rene Deplanque, Nicko Goncharoff, Jonathan Goodman, Guenter Grethe, Richard Hartshorn, Jaroslav Kahovec , Richard Kidd, Hans Kraut, Alexander Lawson , Peter Linstrom, Bill Milne, Gerry Moss, Peter Murray-Rust, Heike Nau , Marc Nicklaus, Carmen Nitsche, Matthias Nolte , Igor Pletnev, Josep Prous, Hinnerk Rey, Ulrich Roessler, Roger Schenck , Martin Schmidt, Steve Stein, Peter Shepherd, Markus Sitzmann, Chris Steinbeck, Keith Taylor, Dmitrii Tchekhovskoi, Bill Town, Wendy Warr, Jason Wilde, Tony Williams, Andrey Yerin.

Special Acknowledgement: Ted Becker& Alan McNaught for their vision and leadership of the future of IUPAC nomenclature.