The Status of the InChI Project

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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 **8/25/2011**

Slides are available at http://www.hellers.com/steve/pub-talks/nci-8-11.pdf

Outline

1. Background/Objective/Why InChI?
2. History & examples
3. InChI Trust/Membership
4. InChI – Current & Future activities
5. Certification Suite
6. The Future/Summary
7. Acknowledgements

Background

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 arbitrary 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, USAN , EC

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, resources, money – and find information!

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 , private, 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.**

InChI is the worst computer readable structure representation except for all those other forms that have been tried from time to time.

With apologies to Sir Winston Churchill (House of Commons speech on Nov. 11, 1947)

We need to LINK information. InChI is an ADDITION to whatever one is using so that you can LINK. If you have a structure file representation, use it. If not consider InChI as your way to go, along with others -

SMILES, WLN, MolFile, CAS, Rasmol, etc.

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

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 Policy & Culture

Do not go outside our circle of competence.

No mission creep.

Staff is not territorial.

What is in it for the US Government databases?

The particular value of InChI to US Government databases is simple. The justification (or perhaps a better way to put it - the return on investment - ROI) is that the groups and their stakeholders can more easily and cost effectively, find the information they need – internally and externally. 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 more US Government organizations begin to use InChIs in their everyday activities and training, it will show vision and leadership to your organization and stakeholders. It might even make the Tea Party happy.

How difficult is it to create an InChI?

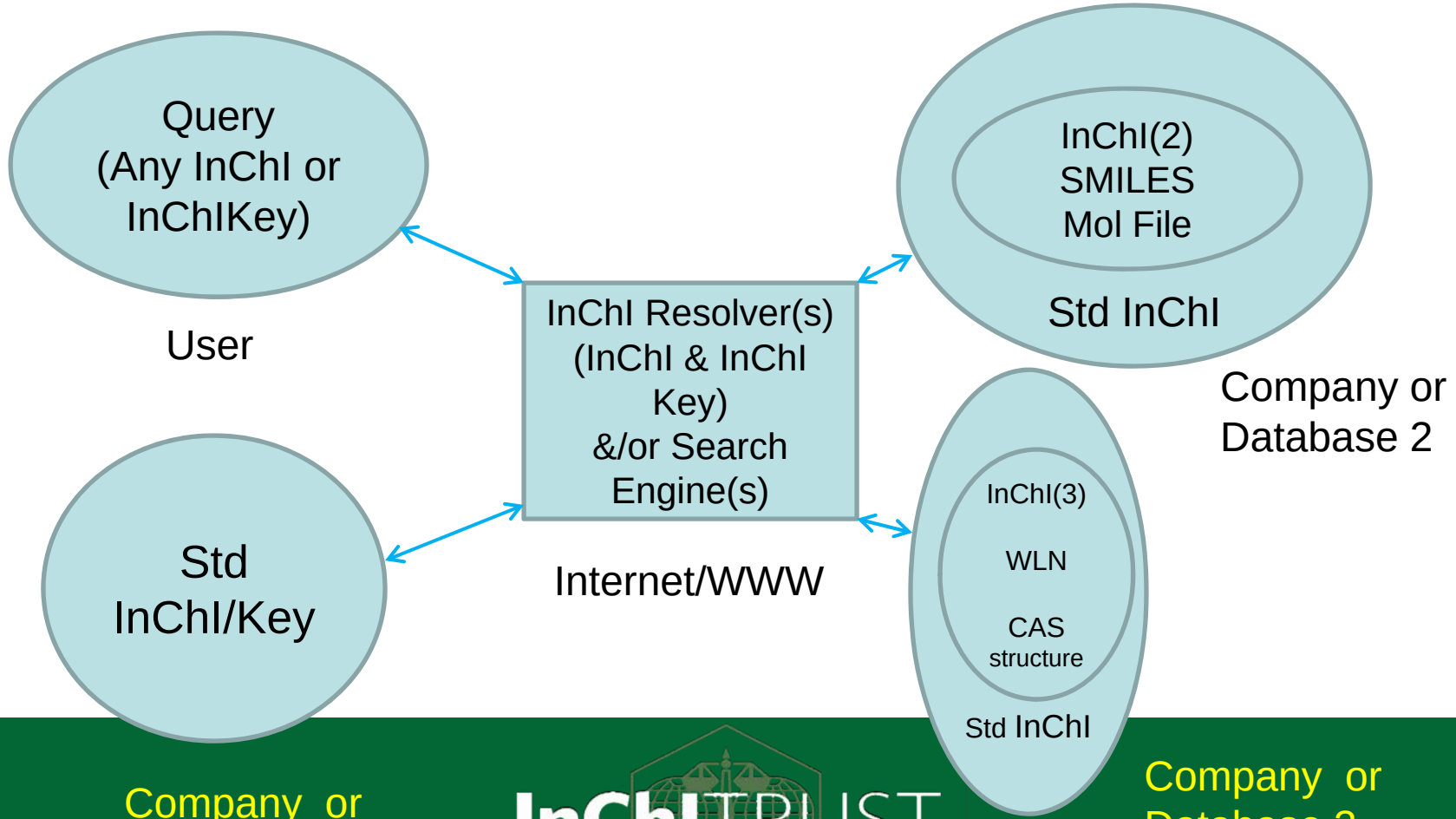
Today, all the major structure drawing programs (ChemDraw, MDL/Symyx/Accelrys Draw, ISIS Draw, ChemAxon Marvin Sketch, ACD Labs ChemSketch, Jmol and so on) have incorporated the InChI algorithm in their products, with usually an "InChI" button for generating the InChI.

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 how different databases from different organizations can link together and find ALL available information. This can be done ONLY by using InChIs.

The LINKED and Interoperable and Combinable World of InChI



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

Reaxys linking

Interoperability between ScienceDirect and Reaxys creates richer, more discoverable chemistry content

A new integration between ScienceDirect and Reaxys, Elsevier's unique web-based chemistry database, improves the discoverability and usefulness of Elsevier scientific chemistry full text content.

Authors submitting articles to selected chemistry journals are invited to contribute structure (MOL) files of their key compounds. These structure files will be used to add compound identifiers (InChI keys) to the article, making both the article and its key compounds more discoverable through mainstream search engines like Google.

In addition, the structure files will also be used to visually display all the key compounds referenced in an article in a single scrollable list. Further functionality, including links to both Reaxys and Google, will be easily accessible within the application.

What are the benefits?

For the author of the article the benefit is better discoverability of the article. Also, the article is further enriched to be even more attractive to the reader.

The researcher benefits from faster digestion of the article, as well as connectivity to relevant other content on the web. The interoperability between ScienceDirect and Reaxys allows researchers to unravel deep layers of information, otherwise hidden in the full text, to further increase research productivity.

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 Characteristics

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

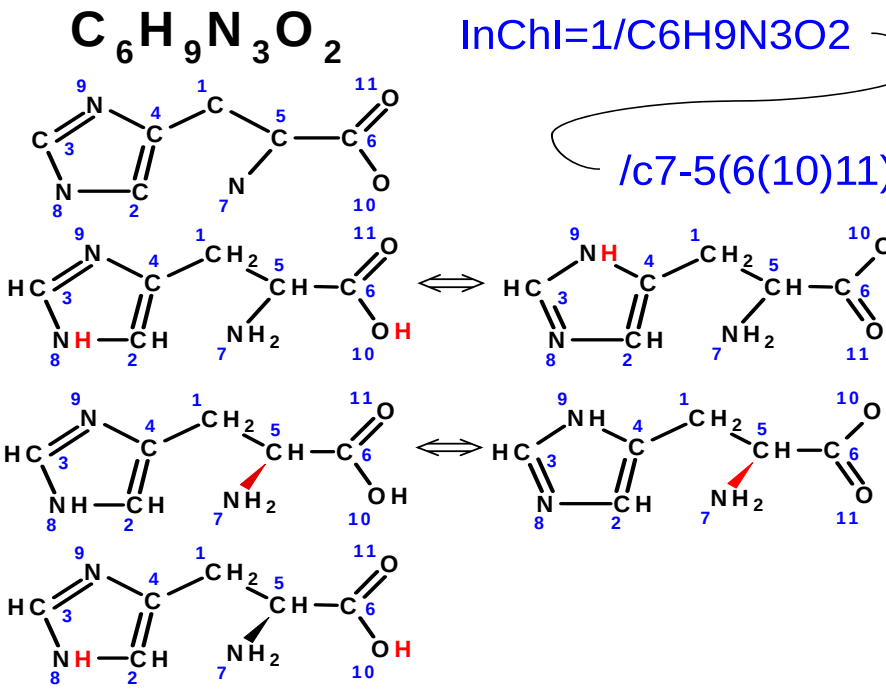
2. Expressive (It will contain structural information.)

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.

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

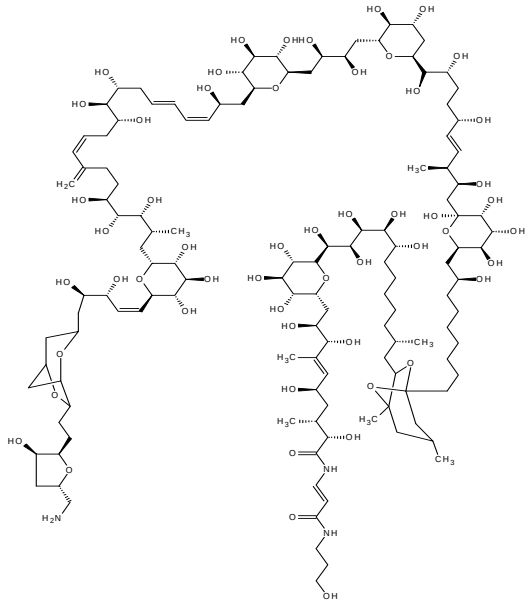
Hydrogens (fixed)

/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

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

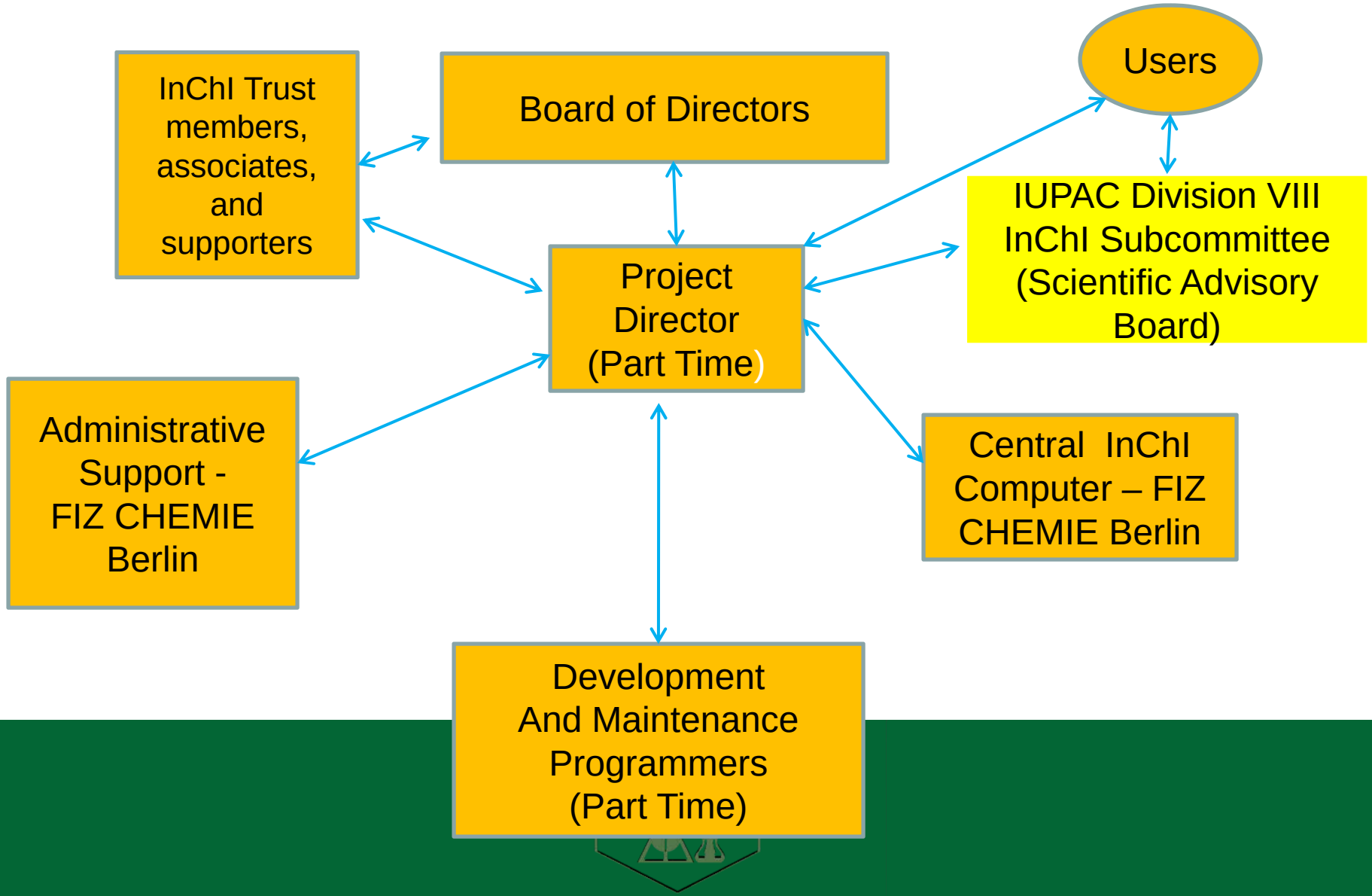
The InChI Trust

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 a UK charity.

The InChI Trust (continued)

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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16 as of 8/25/11

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Too numerous to list

Why join the InChI Trust?

By joining the InChI Trust as a non-paying supporter you will add to the growing list of supporters who believe that the larger the size of supporting organizations, the more likely a vendor, with whom you do business or need information from, will want to add InChIs to their products. The more InChIs in resources, the better you can serve you customers, users, and stakeholders.

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.

Current IUPAC Working Groups & Projects

In Progress:
Organometallics
InChI Resolver
Electronic States
RInChI – InChI for Reactions

Completed:
InChI Certification Suite
Version 1.04 released – 8/11)
Markush (contract to be signed shortly)
Polymers/Mixtures

To be started in 2011/2012:
Revised FAQ's from Cambridge- Nick Day/Peter Murray-Rust
InChI teaching materials
Inorganics

Possible Future Enhancements

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

InChI Certification Suite

The InChI certification suite is a software package developed and designed to check that your installation of the InChI program has been performed correctly. The programs test your installation against a broad set of structures (which are provided with the Suite) to assure the InChIs and InChIKeys are correct and valid..

Once the certification package is run in-house, the results are sent back to the Trust, an "InChI certified" logo will be sent to person/organization. The InChI Trust certification logo can then be put on the pages of the web site for all users to see.

Unlike other Trust products (software and documentation) the Certification Suite is NOT free. It costs $5,000 per year.

The InChI Trust needs financial supporters. If you can't join as a member for administrative/bureaucrat reasons, please support the project by obtaining a copy of the Certification Suite.

The Future/Summary

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.

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