

The InChI Chemical Structure Standard

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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>

4/21/2016

Slides are available at <http://www.hellers.com/steve/nanomolecules-4-16.pdf>

This is a green talk –

**These slides were made from
100% recycled electrons**

InChI – The 30,000 foot view

This presentation will give the background and history of the InChI project.

The goal of this presentation is to show the value of InChI as a **tool**, for creating a notation for defined chemical structures and for linking to and finding more information than one can currently easily obtain.

*Make no little plans;
they have no magic to
stir men's blood and
probably themselves
will not be realized.
Make big plans; aim
high in hope and work.*

~ Daniel Burnham



(With thanks to Francis Collins)

Date: Mon, 15 Nov 1999 18:48:30 -0500 (EST)
From: Stephen R. Heller<srheller@cliff.nal.usda.gov>
To: stein <sstein@enh.nist.gov>
Subject: Re: A strawman proposal

Steve-

First rough draft. Let's talk tomorrow about it.

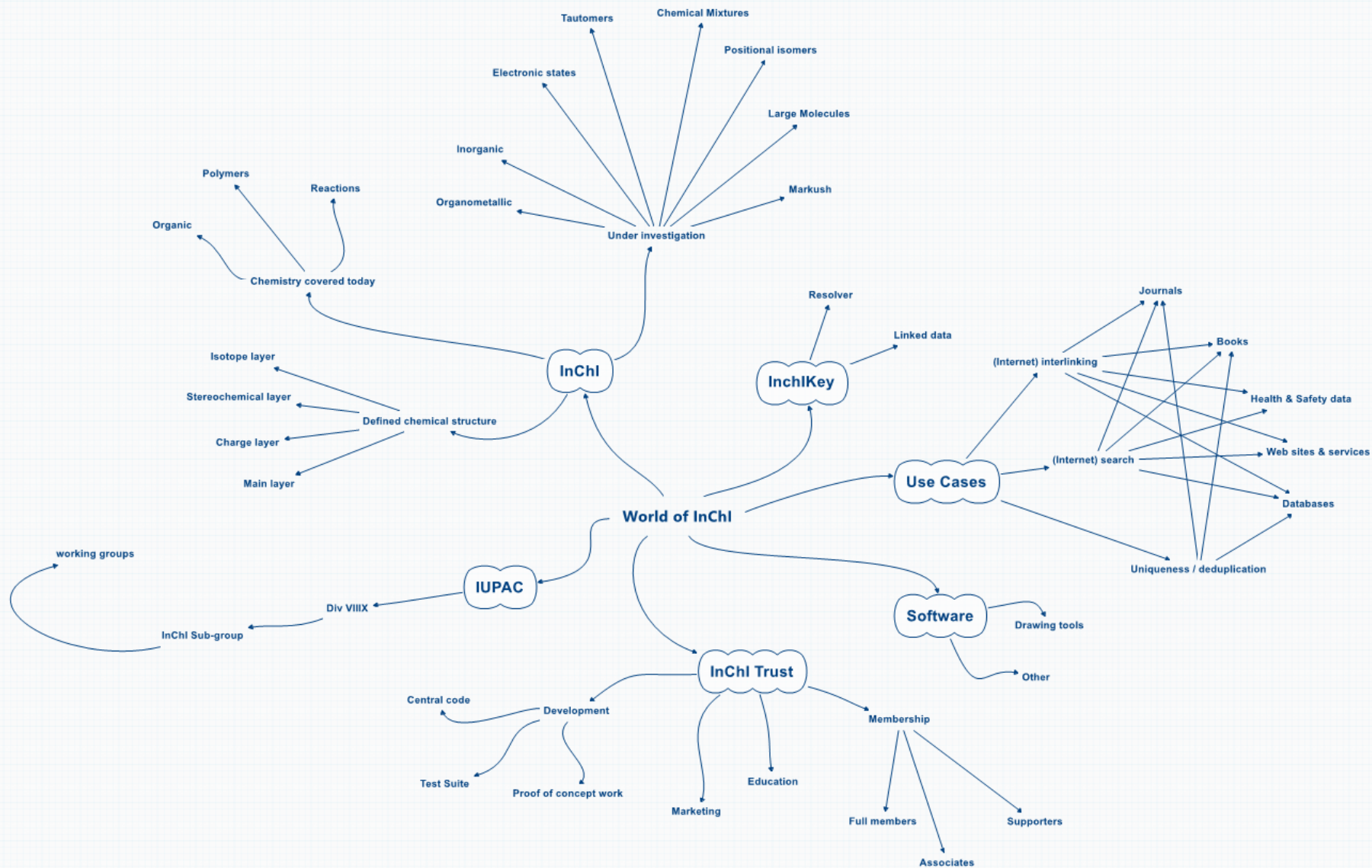
Steve

11/15/99

An IUPAC Chemical Registry System

**In response to the upcoming March 2000 IUPAC meeting -
Representations of Molecular Structure: Nomenclature and its Alternatives
- I would like to propose the creation of an IUPAC public domain chemical
registry system.**

...



Why InChI? - Too Many Good and Excellent Identifiers (“Standards”)

Structure diagrams

- various conventions
- contain ‘too much’ information

Connection Tables/Notations

- MolFiles, SDF, SMILES, SLN, ROSDAL, ...

Pronounceable names (and mostly unpronounceable) and mostly complex names

- IUPAC, CAS 8th CI name, CAS 9th CI name, trivial, trade, WHO INN, ASK, ISO

(Dumb) Index Numbers

EINECS, ELINCS, FEMA, DOT, RTECS, CAS, Beilstein, USP, RTECS, EEC, RCRA, NCI, UN, USAN, EC, ChemSpider ID, REACH, PubChem CID, BAN, NSC, ASK, KEGG, BP, IND, MARTINDALE, MESH, IT IS, RX-CUI, NDF-RT, ATC, AHPA, USP/NF, UNII, MFCD#, ...

“Standards are like toothbrushes – everyone has one but no one wants to use someone else's.”

Phil Bourne, Associate Director for Data Science, NIH

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)**

InChI Project Goal:

To link data about a chemical from many sources with the purpose of creating new information.

Current InChI Status

At present, practically speaking, InChI can handle simple organic molecules, which turns out to cover 99%+ of what people deal with every day. If it did not then the usage of InChI would not be as great as it is.

InChI does not currently handle nanomolecules structures. To date no one or group has shown an interest in creating an approved IUPAC standard for nanomolecules.

InChI will handle nanomolecules. The issue is **when, not if**, and with whom InChI will work with to implement a nanomolecule standard.

What is InChI?

The IUPAC International Chemical Identifier, or InChI, is a non-proprietary, 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 with existing structure drawing software, and the original structure can be regenerated from an InChI with existing structure drawing software.

InChI is really just a synonym.

http://en.wikipedia.org/wiki/International_Chemical_Identifier

InChI Videos

1. What on Earth is InChI?

<http://www.youtube.com/watch?v=rAnJ5toz26c>

2. The Birth of the InChI

<http://www.youtube.com/watch?v=X9c0PHXPfso>

3. The Googlable InChIKey

<http://www.youtube.com/watch?v=UxSNOtv8Rjw>

4. InChI and the Islands

<http://www.youtube.com/watch?v=qrCqJ0o4jGs>

InChI is plumbing. InChI is an (enabling) tool. InChI is a modern enabling technology.

For all but small group of chemists developing it, InChI is not something anyone should want to know about.

All you want to do is use InChI to find information on the web.

InChI is helping scientists to do better work and find/link to the latest information.

InChI is not a replacement for any existing internal structure representations. InChI is in **ADDITION to what one uses internally. Its value to the is in **FINDING** and **LINKING** information**

InChI is for computers

An InChI string is not directly intelligible to the normal human reader. Like Bar Codes, and InChI QR codes - InChIs are not designed to be read by humans.

Or, put another way – never send a human to do a machine's job!

Technology is at its best when it is invisible.

What “*is*” the InChI standard?

The InChI standard programmed into the **algorithm** is an **arbitrary** decision as to how structures are handled. In most cases there is total agreement (e.g., methane). In cases of more complex molecules where there is not agreement among chemists, one representation is chosen. As long as the arbitrarily chosen representation is properly programmed, one will always get the **SAME** result using it – which is what a standard is!

Unique InChI Features

Only IUPAC endorsed International structure standard

Only Open Source structure standard

Only structure standard support by a wide majority of publishers, database producers, and chemistry software companies

Whatever the controversies, InChI has now been more widely adopted than SMILES. In addition three US Government agencies - FDA, NIH, NIST - now have become paying members of the InChI Trust which would seem to indicate more official and institutional support leading to further widespread usage.

Large Databases with InChIs/InChIKeys

NCI – 110 million
PubChem - 91 million (68 million online)
EBI UniChem – 90.5 million
ChemSpider – 34 million
IUPAC – 0 million

Why InChI is a success

1. Organizations need a structure representation for their content (databases, journals, chemicals for sale, products, and so on) so that their content can be **LINKED** to and combined with other content on the Internet. InChI provides an excellent ROI (return on investment). InChI increases productivity!
2. InChI is a public domain **algorithm** that anyone, anywhere can freely use. And they sure use it!

Success is uncoerced adoption

The main reason InChI works so well and at such a low cost is that I consider it a Crowdsourcing project.

The Trust gets the needed services (the creation of InChIs) by the contributions from a large group of people rather than from traditional employees of an organization.

Four Requirements for a Computer Representation Standard

Need
Definition/Specification
Timing/Infrastructure
Acceptance/Use

**An Open Source system
keeps us on our toes. If
things don't work or we don't
respond as needed InChI
won't remain a standard.**

InChI is an international computer readable standard not just for chemists, but rather has very wide technical and non-technical use for **linking and connecting information in many areas of scientific and everyday activities --**

abstracting services

biology/genomics databases

bio-activity databases

books

chemical spills

chemistry databases

clinical trials

company annual reports

drug information

drug overdoses

electronic books

environmental information

food additives

lawsuits

magazines

medical information

medical records

newspapers

patents

packages/bottles/transportation labels/ everyday product labels

scientific journals

toxicological information

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

1(=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)
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)
n1cn(c2c1n(C)c(=O)n(c2=O)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)c(=O)c2c1ncn2C)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(C)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)
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)
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)cn2c1c(=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)
n1(C)c(=O)c2c(n(c1=O)C)ncn2C
n1(c2c(c(=O)n(C)c1=O)ncn2C)C
c12c(n(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)ncn2C
Cn1cnc2c1c(=O)n(c(=O)n2C)C
O=c1n(c(=O)n(c2c1n(cn2)C)C)
n1(c2c(c(=O)n(C)c1=O)ncn2C)C
c12c(n(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)ncn2C
Cn1cnc2c1c(=O)n(c(=O)n2C)C
O=c1n(c(=O)n(c2c1n(cn2)C)C)
n1(c2c(c(=O)n(C)c1=O)ncn2C)C
c12c(n(cn1)C)c(=O)n(c(=O)n2C)C
c12c(c(=O)n(C)c(=O)n1C)ncn2C
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(nc(=O)n1C)ncn2C
c1(=O)n(c2c(n(cn2)C)c(=O)n1C)C
Cn1c2c(c(=O)n(c1=O)C)ncn2C)
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(c1=O)C
n1(c2c(n(cn2)C)c(=O)n(c1=O)C)
Cn1c2c(n(C)c(=O)n(c2=O)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)ncn2)C)
c1(=O)n(C)c(=O)n(c2c1n(cn2)C)C
n1(c2c(n(C)cn2)c(=O)n(c1=O)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)ncn2C
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(=O)n(c2c1n(cn2)C)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)c2c(ncn2C)n(C)c1=O)C
Cn1c(=O)c2c(n(C)c2=O)C)nc1

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)
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)
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)
c1(=O)n(c(=O)n(c2c1n(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)ncn2)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



InChI

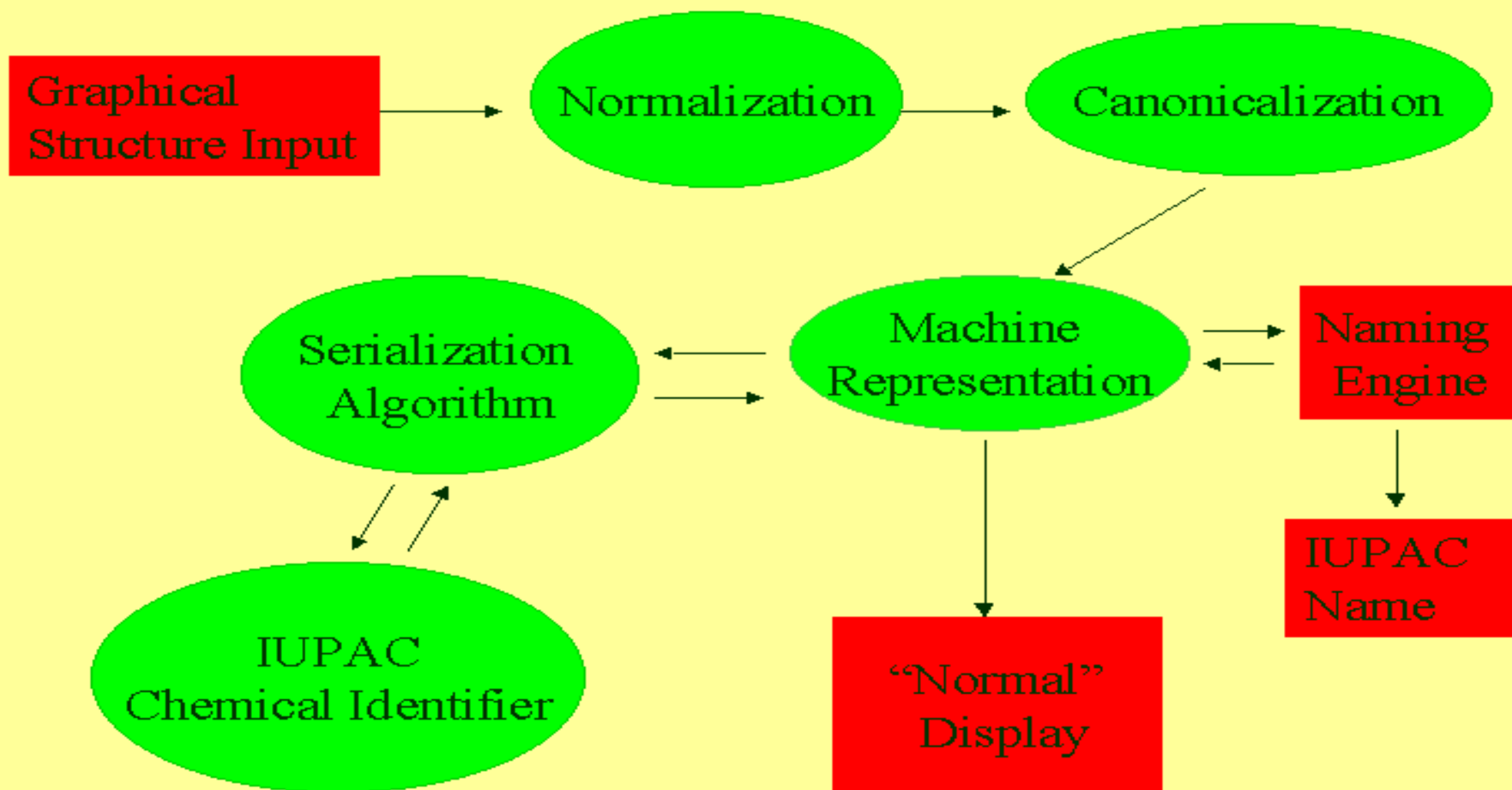
172 SMILES representations

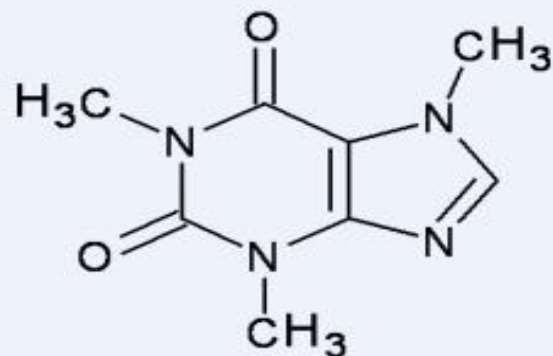


E Pluribus Unum
Out of many, One

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, Bing, etc.) using the InChI (hash) Key.**





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

InChIKey=**RYYVLZVUVIJVGH-UHFFFAOYSA-N**

character indicating the number of protons
(‘N’ means neutral)

flag character for InChI version:
‘A’ for version 1

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

First block (14 letters)

Encodes molecular skeleton
(connectivity)

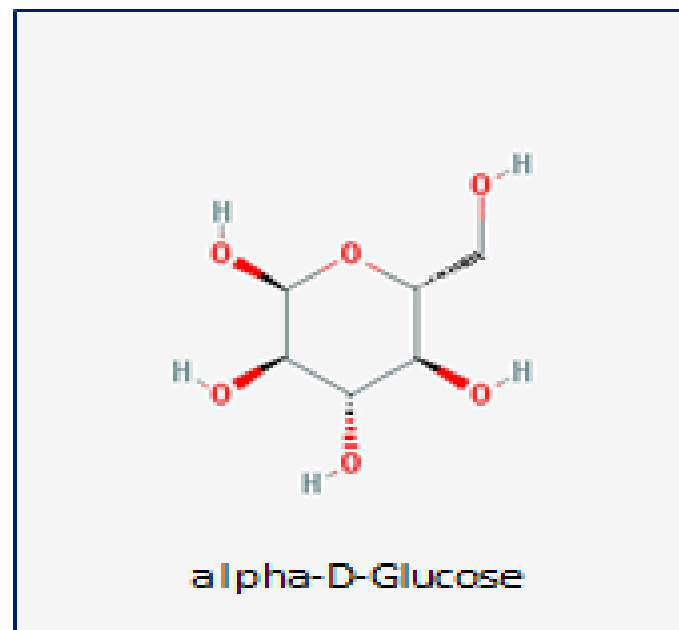
Second block (8 letters)

Encodes stereochemistry and isotopes

InChI is a string

InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m1/s1

Version/Type
 Chemical formula
 Connectivity
 Charge/Proton
 Stereochemical
 Other (e.g., Isotopic)



“layered” line notation

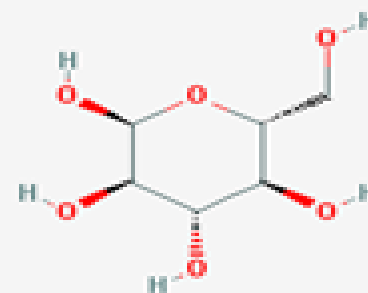
InChIKey is a “hashed” InChI

- Search engine friendly InChI
- May allow for ‘secure’ lookup of a chemical

WQZGKKKJIJFFOK-DVKNGEFBSA-N

Chemical formula
Connectivity
Stereochemical
Other (e.g., Isotopic)
Type
Version
Charge/Proton

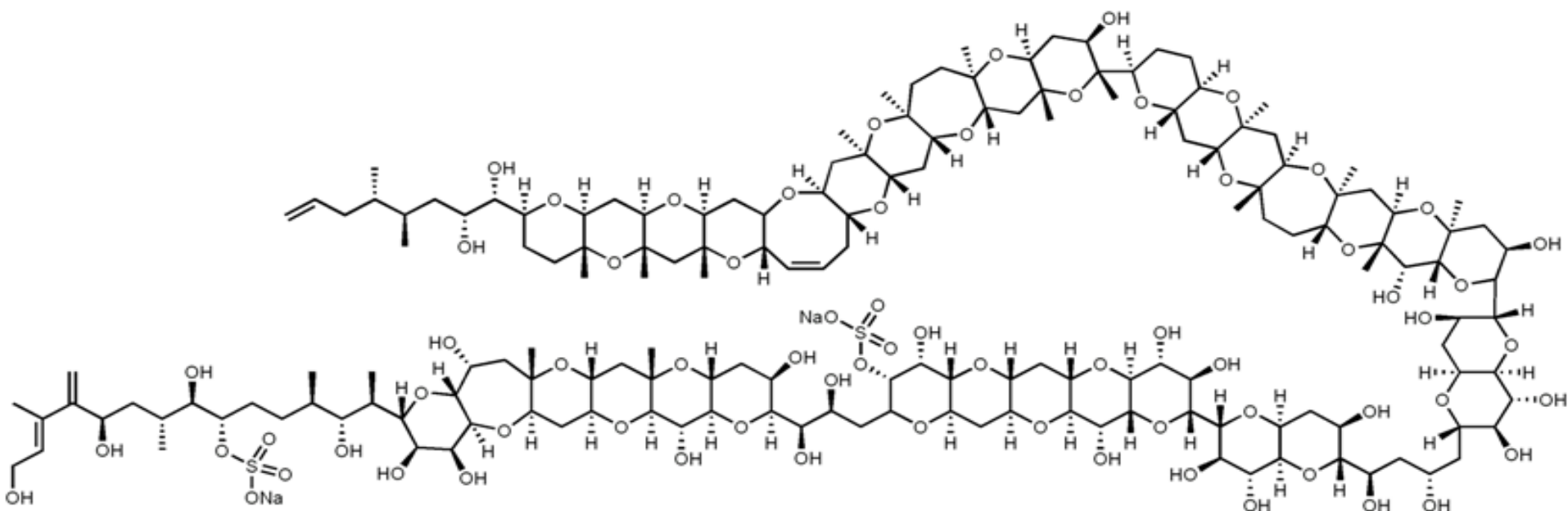
“layered” line notation



alpha-D-Glucose

InChI for Maitotoxin (from Nextmove Software, UK)

InChI=1S/C164H258O68S2.2Na/c1-24-26-65(2)68(5)41-74(168)117(179)85-33-36-152(11)106(203-85)55-109-162(21,231-152)64-161(20)105(210-109)51-89-83(220-161)28-25-27-82-99(199-89)59-157(16)108(202-82)56-107-153(12,230-157)39-38-151(10)112(211-107)61-158(17)111(224-151)54-101(176)163(22,232-158)103-32-31-84-90(204-103)53-110-156(15,219-84)62-113-150(9,223-110)37-34-102-155(14,225-113)63-114-164(23,227-102)147(192)149-159(18,226-114)58-81(175)134(218-149)133-79(173)47-93-136(216-133)120(182)119(181)92(200-93)44-72(166)43-76(170)131-77(171)46-94-137(214-131)122(184)124(186)143(207-94)145-126(188)125(187)144-146(217-145)128(190)139-97(208-144)50-88-87(206-139)49-96-138(205-88)127(189)141(229-234(196,197)198)95(201-96)45-75(169)118(180)132-78(172)48-98-140(215-132)129(191)148-160(19,221-98)60-100-91(209-148)52-104-154(13,222-100)57-80(174)135-142(212-104)123(185)121(183)130(213-135)71(8)115(177)67(4)29-30-86(228-233(193,194)195)116(178)69(6)42-73(167)70(7)66(3)35-40-165;;/h24-25,28,35,65,67-69,71-149,165-192H,1,7,26-27,29-34,36-64H2,2-6,8-23H3,(H,193,194,195)(H,196,197,198);;/q;2*+1/p-2/b28-25-,66-35+;;/t65-,67+,68+,69+,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+,101+,102+,103-,104+,105-,106-,107+,108-,109+,110+,111-,112-,113+,114+,115+,116+,117-,118+,119-,120+,121+,122+,123-,124+,125+,126+,127+,128+,129-,130-,131-,132-,133+,134+,135+,136+,137+,138+,139-,140+,141-,142-,143+,144-,145+,146+,147-,148+,149+,150-,151+,152+,153-,154-,155-,156-,157+,158+,159-,160-,161+,162-,163+,164+;;/m0../s1





What about funding ?

Don't give up - Moses was once
a basket case

**While InChI did not make the top 10
given to Moses, it is #14**

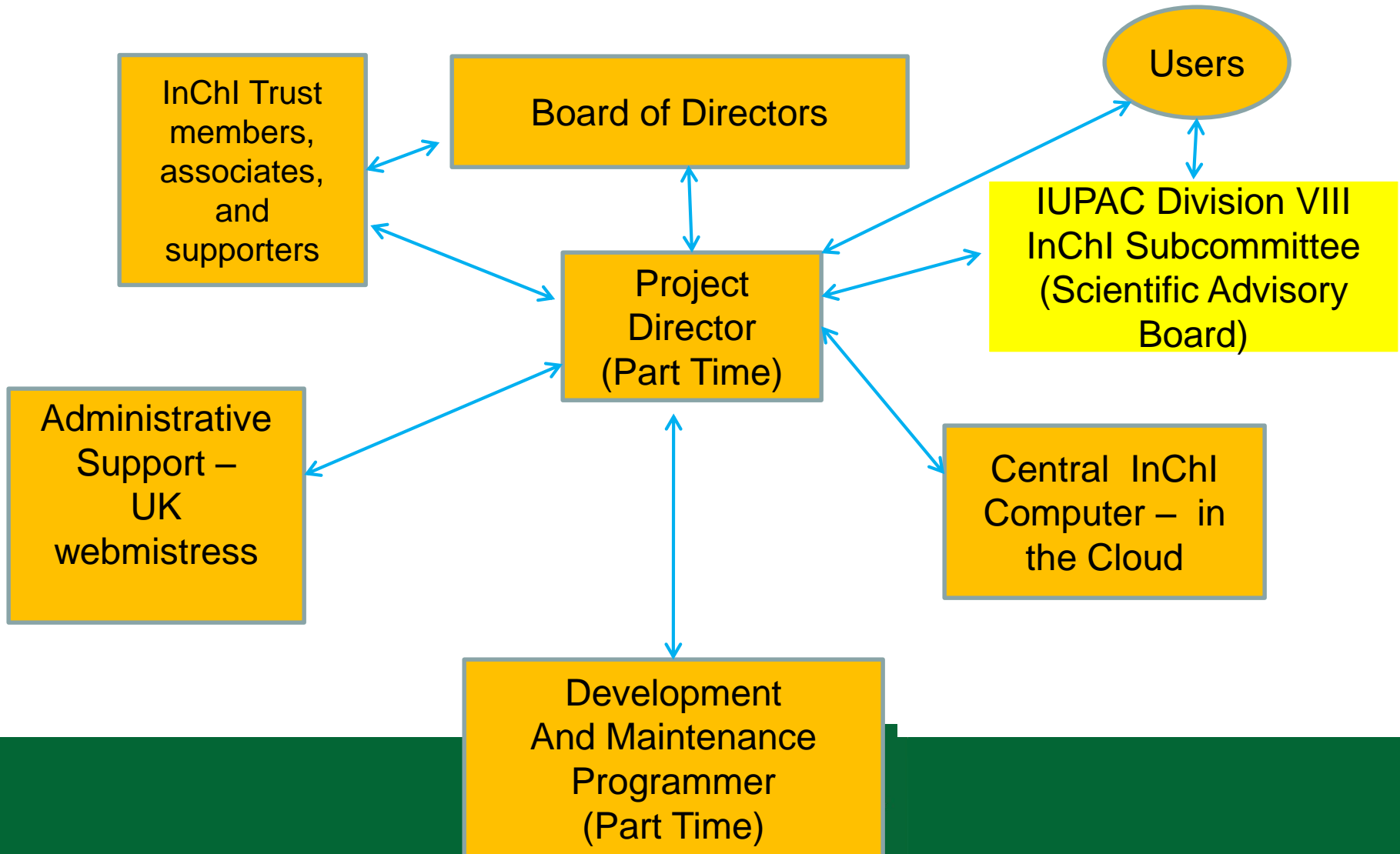
**(Thou shall use InChI for structure
representation.)**

The InChI Trust

The InChI Trust

To function and succeed, InChI had to become personality independent. InChI had to be “institutionalized”. If the work of this project was to be enduring it needed to be 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.

InChI Trust Organization



InChI Staff and Collaborators

The InChI project has had the unusual perfect “good storm” of cooperation and support. It is a truly international project with programming in Moscow, computers in the cloud, incorporated in the UK, and a project director in the USA. Collaborators from over a dozen countries, from academia, Pharma, publishers, and the chemical information industry, have all offered, and continue to offer, senior scientific staff to develop the InChI standard.

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.

Summary

**If you are not part of the
solution; you are part of the
precipitate**

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