InChI & the USPTO

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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 **7/28/2015**

Slides are available at http://www.hellers.com/steve/uspto-7-15.pdf

InChI – The 30,000 foot view

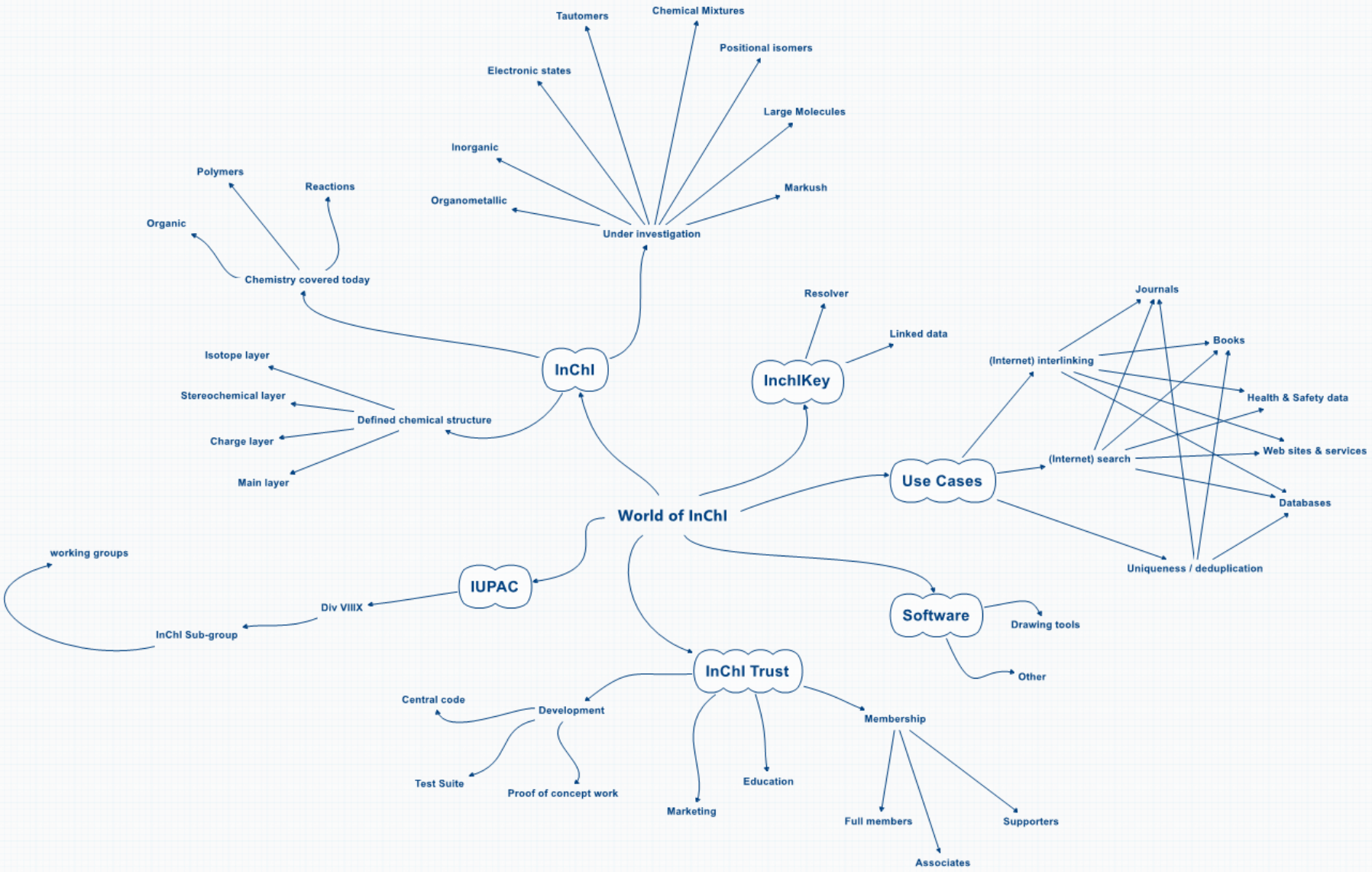
This first talk of the workshop will give the background and history of the InChI project. The remaining talks will provide examples of how InChI is being used.

The goal of these talks is to show the value of InChI as another tool, not an alternative tool, for linking to and finding more information than the USPTO 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)


World of InChI
InChI
Chemistry covered today
Organic
Polymers
Reactions
Under investigation
Tautomers
Chemical Mixtures
Positional isomers
Electronic states
Large Molecules
Inorganic
Organometallic
Markush
Defined chemical structure
Isotope layer
Stereochemical layer
Charge layer
Main layer
InChIKey
Resolver
Linked data
Use Cases
(Internet) interlinking
(Internet) search
Journals
Books
Health & Safety data
Web sites & services
Databases
Uniqueness / deduplication
IUPAC
Div VIIIX
InChI Sub-group
working groups
Software
Drawing tools
Other
InChI Trust
Development
Central code
Test Suite
Proof of concept work
Marketing
Education
Membership
Full members
Associates
Supporters

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 Markush structures due to a lack of funding for an existing approved IUPAC standard and a technical implementation proposal vetted by the InChI project.

InChI will handle Markush. The issue is when, not if, and with whom InChI will work with to implement a Markush 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 USPTO 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 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

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.

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

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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)c2c(=O)n(C)c2=O
c1nc2c(n1C)c(=O)n(C)c(=O)n2C
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(nc1)n(C)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)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)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(c2=O)C)C)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(C)cn2)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(C)c2c(n(C)c(=O)n1C)n(C)cn2
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)c(=O)n(C)c2c(c1=O)n(C)cn2
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(C)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
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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
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(c2c(c1=O)n(cn2)C)C)C
O=c1n(C)c(=O)n(c2c1n(cn2)C)C
n1(c(=O)c2c(ncn2C)n(c1=O)C)C
c1(=O)n(C)c(=O)n(C)c2c1n(cn2)C
O=c1n(C)c(=O)n(c2c1n(cn2)C)C
n1(C)c(=O)n(c2c(n(C)cn2)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(c2c(n(C)cn2)c1=O)C)C
O=c1n(c(=O)n(C)c2c1n(C)cn2)C
n1(C)c2c(n(C)cn2)c(=O)n(C)c1=O
n1(C)c2c(c(=O)n(C)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

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

E Pluribus Unum
Out of many, One

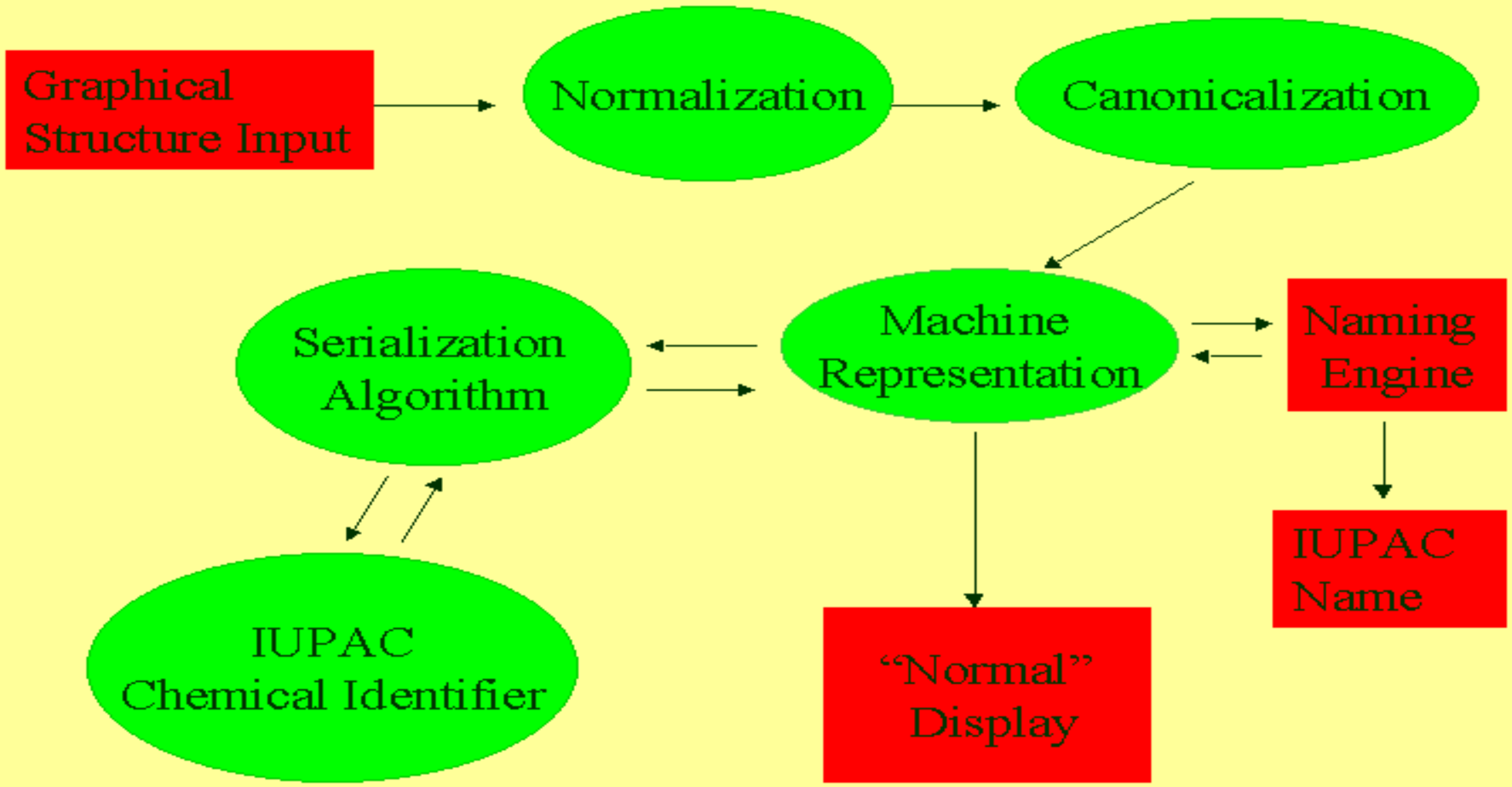
InChI Characteristics

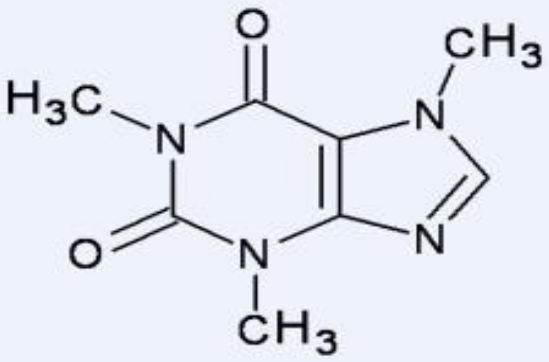
1. Easy to generate (It will use existing software.)

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.


Graphical Structure Input
Normalization
Canonicalization
Serialization Algorithm
Machine Representation
Naming Engine
IUPAC Chemical Identifier
"Normal" Display
IUPAC Name



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

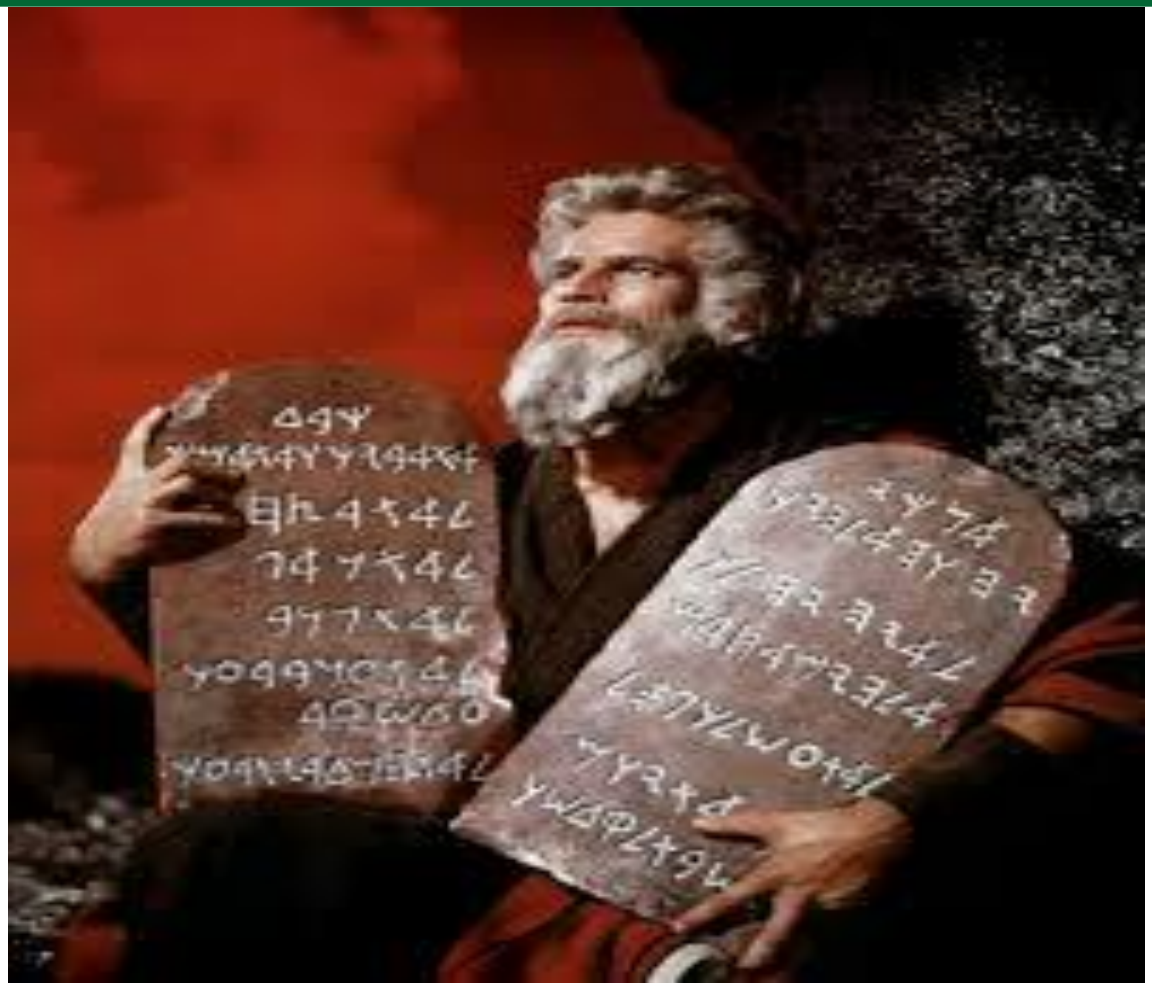
First block (14 letters)

Encodes molecular skeleton (connectivity)

Second block (8 letters)

Encodes stereochemistry and isotopes

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



What about funding ?

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

While InChI did not make the top 10, it is #14

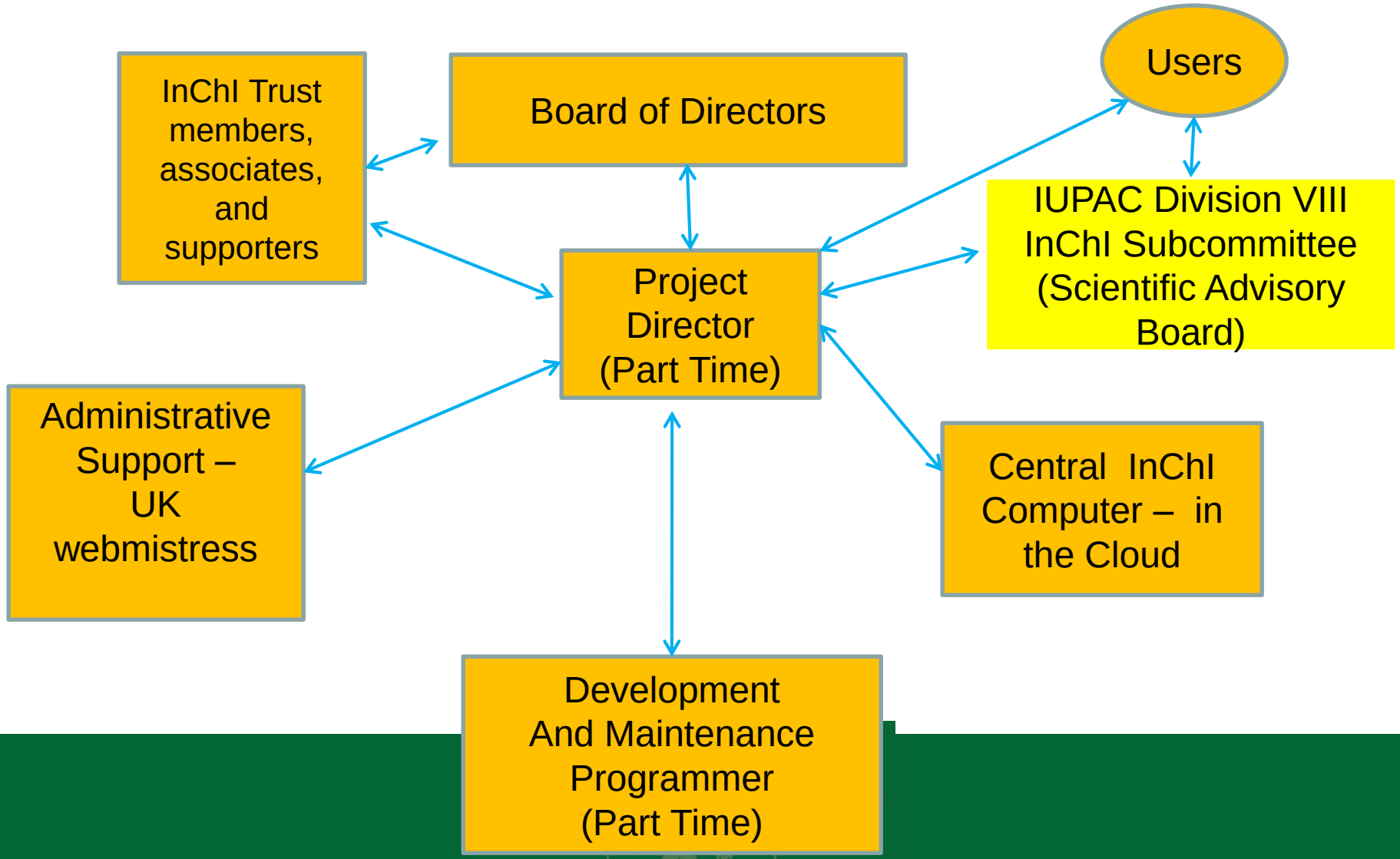
(Thou shall use InChI for structure representation.)

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 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

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, Gary Mallard, 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, Peter Murray-Rust, 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.

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