

InChI Trust Project Director's Newsletter

3 October 2012

Summary:

There continues to be good technical progress with InChI and the InChI Trust in a number of areas. In the non-technical area of support, IUPAC support and new memberships continue to be an issue. The various IUPAC InChI working groups have completed their initial work and/or are continuing to move ahead at a good pace. Publicity for the project is very good and has resulted in considerable increase in the uptake and usage of the InChI algorithm.

Items covered in this report:

Membership/Support
InChI RFP/Contracts
IUPAC InChI subcommittee and working parties/groups
Meetings attended
Talks/ Posters given; Manuscripts written
InChI - ACS Meeting, Philadelphia
InChI Trust Web Site
InChI Brochure
InChI Usage
Technical Issues
Plans for 2012/2013

Membership/Support:

As of October, 2012

Existing Members and Associates: 16

Supporters: 39

Certification Suite purchases: 2 (Novartis & NIH/NCI)

The IUPAC Secretariat continues to provide no support. It is hoped the new Executive Director, who takes office in January 2013 will be in a position to improve the situation.

InChI RFP/Contracts

The contract with Digital Chemistry for the extension of InChI to cover generic/Markush structures is still planned to be funded once the funds are available.



A contract for a few videos to describe and explain InChI was initiated with Martin Freeth. Martin came to NIST in July to film interviews with me, Steve Stein, and Dmitrii Tchekhovskoi. The videos should be ready for release by the end of 2012.

A contract with Digital Chemistry for a new InChI API was finalized in July 2012 and the result is expected to be delivered in October 2012.

IUPAC InChI subcommittee working parties

Resolver - work is now being done at the US National Cancer Institute under Markus Sitzmann

Extension to Polymers – The work on requirements was finished by the working group under Andrey Yerin. Igor Pletnev has started programming this standard.

InChI for Reactions - Guenter Grethe has done a fine job keeping this aspect of InChI proceeding in a timely manner. A progress report from Jonathan Goodman has been completed and sent out to all involved. Jonathan would like graduate student funding to keep working on this since the system/programming is not final or ready for general release. The major part of the programming has been completed and we are now at a point where the working group must test the sample database available on the RInChI website (<http://www-rinchi.ch.cam.ac.uk>) or with their own samples. Testing by the working group members is under way.

Extension to Markush Structures - We continue to wait for the needed financial support before proceeding.

Extension to Electronic States - Don Burgess at NIST has offered to take over, as there is now seems to be interest (i.e., money) at NIST in structure standards. There has been very little progress in the past few months. They may be waiting for the next US Government fiscal year, which starts in October.

InChI for Materials – There is interest at NIST in undertaking this extension. An internal meeting was held at NIST in May 2012. NIST is currently participating in the (poorly named) Materials Genome Initiative (MGI). This effort seeks to create large sets of materials data: something which will be of limited use if people can't reliably identify the materials the data is associated with. NIST believes they will get funding in the next fiscal year which will enable this to move forward.

Extension to Organometallics - A very difficult area, but the working group hopes to have something by the fall.

Extension to Inorganics - Hinnerk Rey from Elsevier/Frankfurt has replaced Nigel Wheatley to head up this working group. He has prepared a draft proposal for IUPAC project funding and will send it in to IUPAC as soon as he is able to get a sufficient number of geographically diverse members

Extension to Biopolymers/Proteins/etc. - Keith Taylor (Accelrys) hopes to have a suggestion late this fall.



Handling of Tautomers - Under the leadership of Marc Nicklaus (US National Cancer Institut) InChI project #2012-023-2-800, "Redesign of Handling of Tautomerism for InChI V2. was approved for funding (\$10,000) jointly by Division VIII and the IUPAC project committee. A report at the AGM by one of the working party members (Wolf-Dietrich Ihlenfeldt) showed serious problems in this area which will take time and effort beyond the working party capabilities to resolve.

Extension to Interlocking Structures (Rotaxanes) - Andrey Yerin will consider starting a project/working group.

Extended Stereochemistry - Evan Bolton is still thinking about what to do in the area of stereogenic centers such as cumulenes.

The revised FAQ that Igor Pletnev rewrote, with some help from Alan McNaught and me, was released in May 2012 (see http://www.inchi-trust.org/fileadmin/user_upload/html/inchifaq/inchi-faq.html).

April - August 2012 activities

Meetings Attended

BioIT World - Boston – April
Pistoia Alliance Annual Conference – Boston – April
BIO – Boston – June (paid by others)
IUPAC – CPEP – July (no cost)
ACS – Philadelphia – August

Talks/Posters Presented

BioIT World - Boston – Poster presentation
ACS – Philadelphia (2 talks)
Pistoia Alliance presentation was, yet again, postponed indefinitely.
(All slides from these talks have been put up on my web site – <http://www.hellers.com/steve/pub-talks/>)

Manuscript

Based on the ACS San Diego InChI symposium two manuscripts have been prepared to be part of the Journal of Chemoinformatics issue on InChI that Tony Williams is organizing.

InChI - ACS Meeting, Philadelphia

To my surprise the two talks at the recent ACS meeting in Philadelphia generated more people coming up and talking with me after my talks as well as the many (3) CINF receptions. Some 50



people were at each of my two talks, which was more than usual. This was quite encouraging, at least to me.

InChI Trust web site

Ulrich Rössler continues to do a very fine and very responsive job! The only issue here is what will happen to the web site when FIZ Chemie disappears, possibly at the end of 2012.

InChI Trust brochure

The new and revised InChI Trust brochure has been completed by Ulrich Rössler and printed by FIZ Chemie and I hand out copies at all meetings I attend.

InChI Usage

For lack of a better a better term, I use InChI Usage to refer to publications and blogs about InChI. Alan McNaught and I have been passing these on to Ulrich Rössler and he has added these to the web site. There have been quite a number of publications using InChI. The numbers continue to grow. Searches on Google (and other search engines) continue to have more hits for InChI strings and InChIKey strings.

Technical Issues

The mechanism to discuss and resolve technical issues continues to work well. Most issues seem to be able to be resolved by email and phone calls, but face-to-face meetings are still very critical as there are some very strongly held opinions that do not get resolved by emails. My regular meetings with NIH (PubChem and NCI) staff have been very useful

Work continues slowly by Igor Pletnev on a full documentation paper on InChI. This should, finally, be completed in late 2012.

Plans for the remainder of 2012 & 2013

For the remainder 2012 my overall plans and goals are as follows:

1. Work to expand the current membership with two basic classes of members (Full and Associate) and add to the number of Supporters. Work to sign up more organizations for the Certification Suite.



2. Continue to attend meetings and give talks on InChI where useful and appropriate. An InChI abstract has been accepted for the GDCh Goslar conference in November. Guenter Grethe has also had an oral presentation accepted at Goslar for the work on InChI for Reactions (RInChI) he is overseeing.
3. Chair, oversee, and coordinate the IUPAC InChI subcommittee activities and working groups. No face-to-face meetings are currently planned for the remainder of 2012
4. Add capabilities to InChI.

Steve Heller

