Status and Future of the IUPAC InChI: Context and Use Cases

InChI & Working Group Reports: Training/Education/Outreach

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Should there be a working group on Training/Education/Outreach?

(Thursday Break-Out Group: 3:00-4:30 PM)

Google: InChI Training

Google

InChI Training

All Videos Images Shopping News More Settings

About 214,000 results (0.47 seconds)

Sacha Inchi Guide - High Protein Superfood - Tiger Fitness

https://content.tigerfitness.com/sacha-inchi-guide-high-protein-superfood/

★★★★★ Rating: 5 - 7 votes

In its raw form, sacha **inchi** is a high protein legume rich in essential fatty acids. ... One ounce (28 grams) of sacha **inchi** offers 13 grams of fat, nearly all of which are polyunsaturated, 5 grams of carbohydrates, all of which ..... Machine **Training** ...

Sacha Inchi Guide – High Protein Superfood

The Truth is:

- Few outside of the Cheminformatics Community are familiar with InChI
- Even within IUPAC many are not familiar
- This is especially true in the chemical education community

InChI Trust WebSite: Key Asset for Training/Education/Outreach

InChI TRUST

Home | About the InChI Trust | About the InChI Standard | Downloads | News | Contact

InChI and InChIKeys for chemical structures

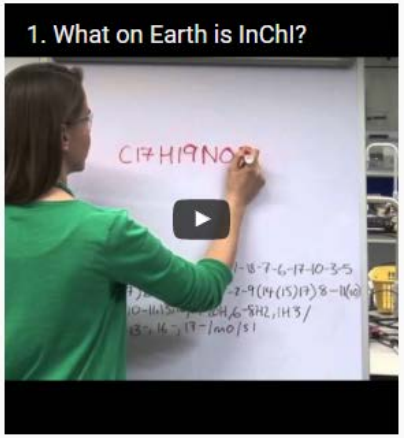
The InChI Trust is a nonprofit charity which works to develop and promote the use of the IUPAC InChI open-source chemical structure representation algorithm.

The InChI with its associated InChIKey was developed as a non-proprietary international standard to represent chemical structures and has just celebrated its tenth anniversary. The Trust aims to develop and improve on the current InChI standard, further enabling the interlinking of chemistry and chemical structures on the web.

Register now for our upcoming "State and Future of the IUPAC InChI" meeting at the NIH 16-18 August 2017 – more details here

What on Earth is InChI?

This video introduces the InChI standard to represent chemical structures.



The Birth of the InChI

This video describes the background to the development of the InChI standard.

The Googlable InChIKey

An InChIKey enables chemical structures to be uniquely identified on the web.

InChI and the Islands

The InChI standard – the International Chemical Identifier – enables the linking of information.

IUPAC Centennial Opportunity for Training/Education/Outreach

IUPAC 100TH ANNIVERSARY TO BE CELEBRATED IN 2019

28 July 2017

Today is the birthday of IUPAC!

Research Triangle Park, NC, USA, July 28, 2017 – The International Union of Pure and Applied Chemistry (IUPAC), the globally-recognized authority on chemical nomenclature and terminology, will celebrate its 100th anniversary on July 28, 2019. The anniversary theme is ***A Common Language for Chemistry***, and while the celebration will recognize the successes of IUPAC's first one hundred years, its purpose is not to solely dwell upon the past, but rather to look to the future of what this international community of chemists, working closely together, can continue to contribute now and into the future in meeting the world's needs through chemical research.

What are the differences between Training/Education/Outreach?

(my shot at this)

Training – Develop understanding of InChI technology and established use scenarios

Education – Develop understanding of how InChI fits into and can impact the practice of science

Outreach – Develop applications of InChI technology to new communities and establish new use scenarios.

InChI TRUST

Training
Web Portal (?)

InChI TRUST

Possible Features:

InChI Primers – repository for technical primers targeting a multiplicity of novice and expert needs

InChI Bibliography – wiki based/crowdsourced

Cheminformatic Education Material – Original material and a links to other sites showing applications of InChI

Education
Two Modes

Traditional– Cheminformatics

- Material like the Cheminformatics OLCC

Non Traditional – CER (Chemical Education Research)

- Add a new paradigm to CER utilizing principles of distributed cognition

InChITRUST

Traditional
Curriculum Integration:

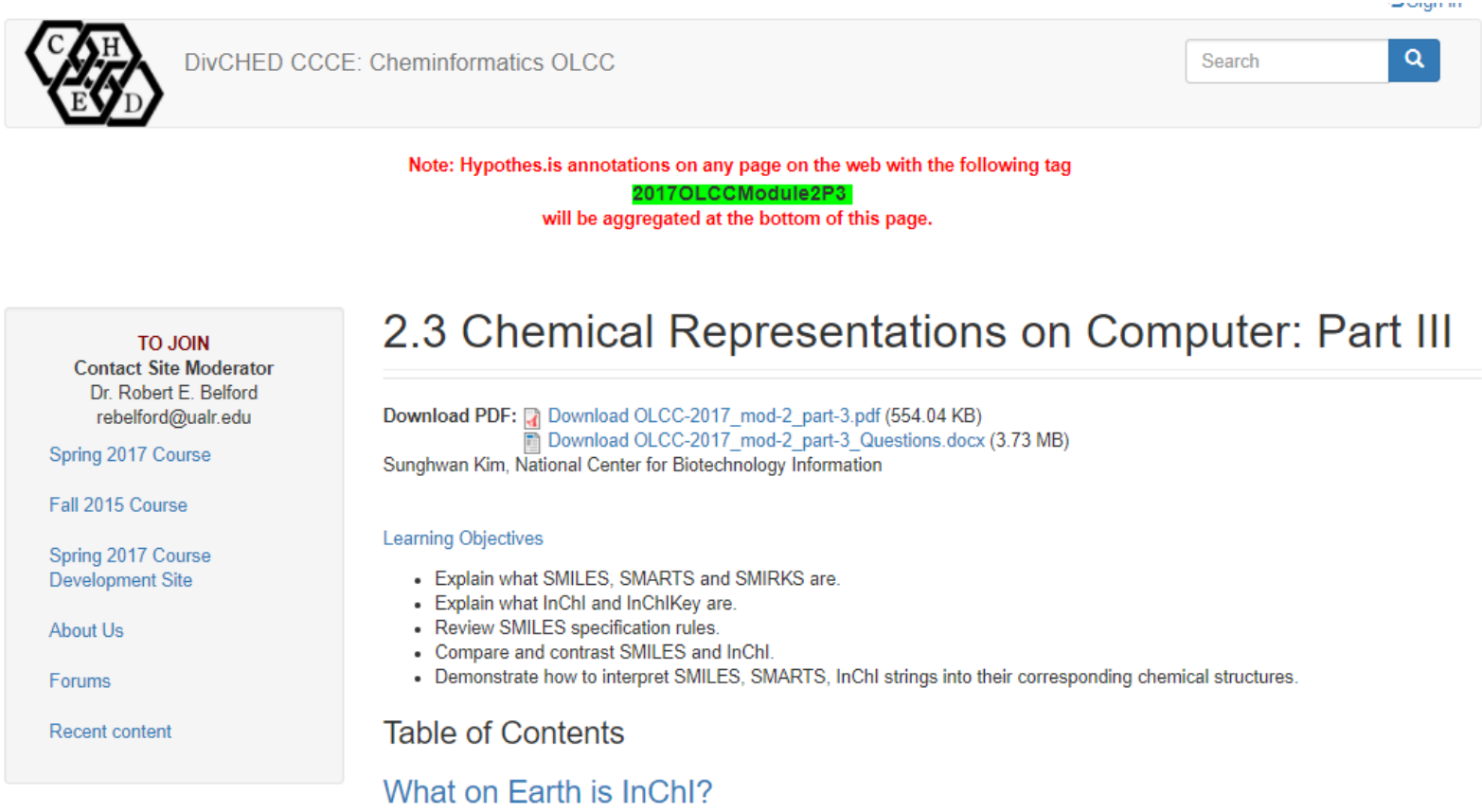
InChITRUST

Quick Overview of Cheminformatics OLCC and LibreText

- Cheminformatics OLCC
  - Intercollegiate course sponsored by ACS CHED CCCE
- Libretext
  - Formerly ChemWiki/STEMWiki hyperlibrary
  - Open access eTextbook generating service

(Both NSF Funded Projects)

Cheminformatics OLCC
Fall 2015 - 4 schools
Spring 2017 – 10 schools



http://olcc.ccce.divched.org/2017OLCCModule2P3

Education: Traditional
LibreText HyperLibrary Integration

Cheminformatics OLCC material was ported to LibreText

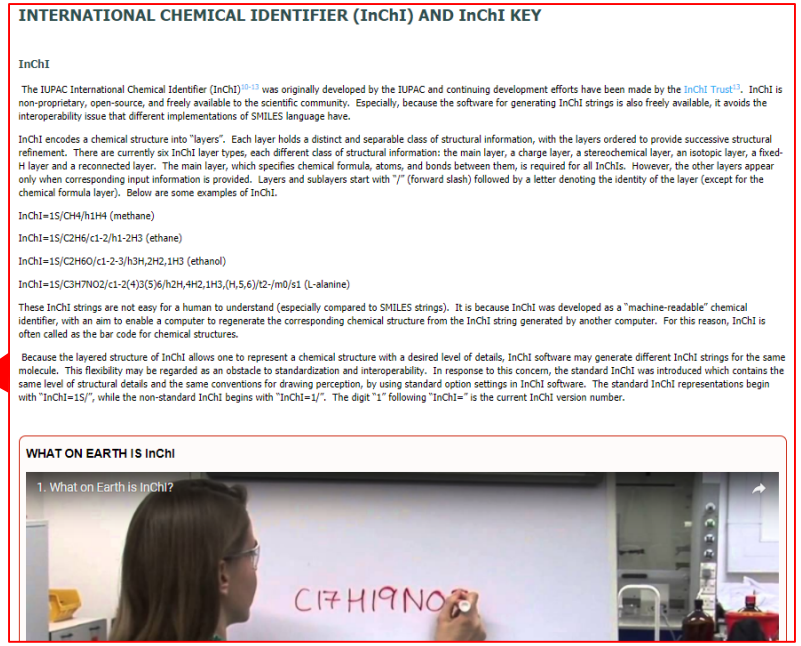
Organic Chemistry Classes at any school using LibreText have access to InChI material from UALR

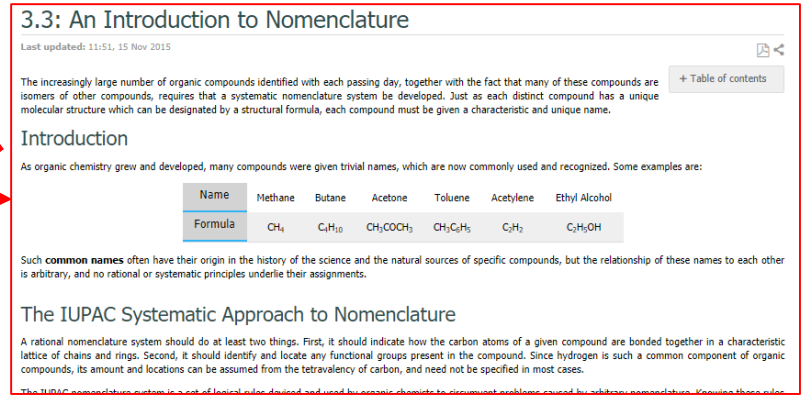
2017 Page Views as of June 20

Chemistry	38,202,891
Biology	1,076,501
Physics	394,677
Geology	59,596
Math	263,490
Statistics	245,862
Medicine*	101,677
Social Sci*	26,943
Engineering*	49,269
Agriculture*	1,251
Humanities*	14,219
Photosciences	114,525

University of Arkansas Little Rock

University of Illinois, Springfield





Cheminformatics OLCC

Fall 2015 - 4 schools

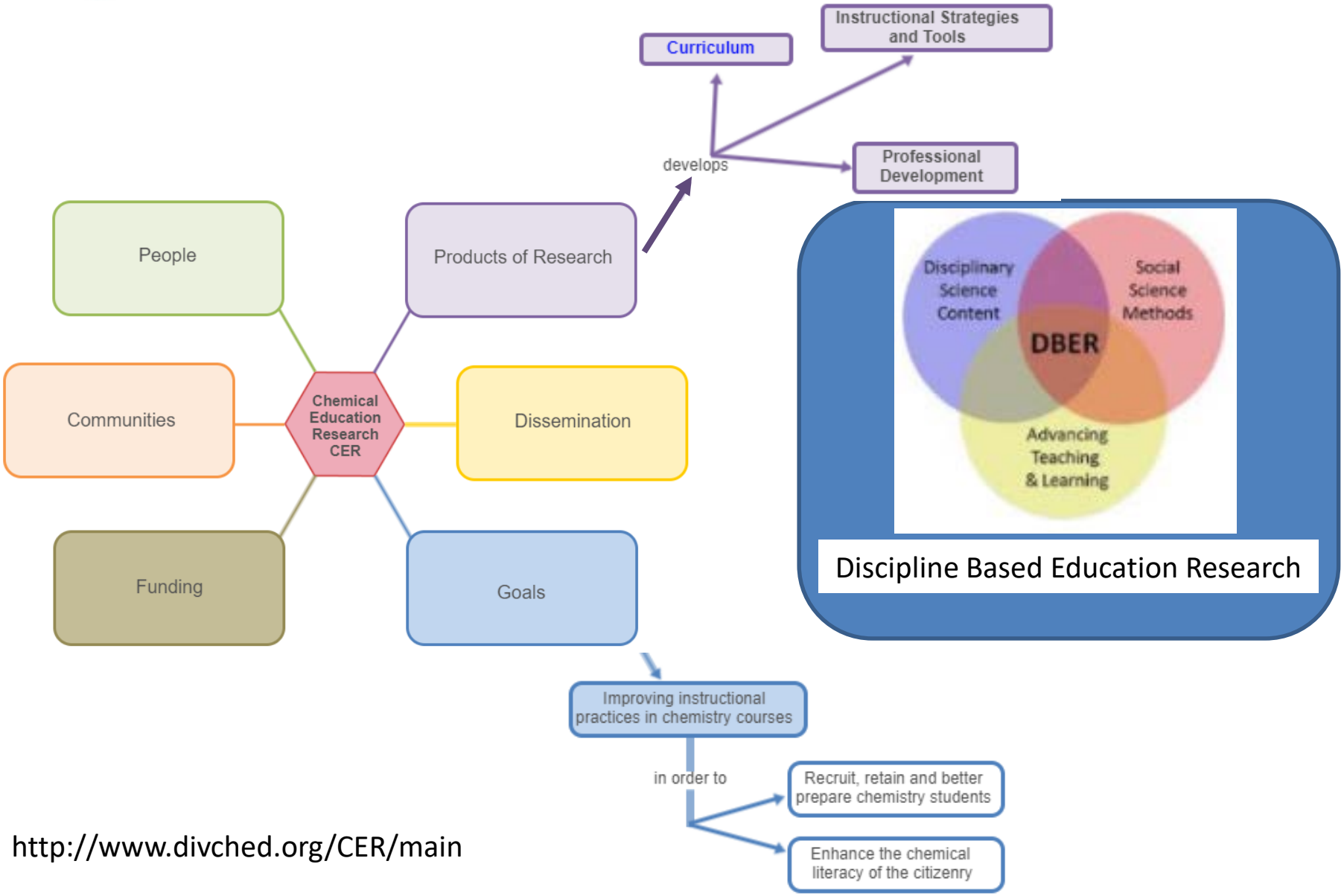
Spring 2017 – 10 schools

Many student projects used InChI and InChI keys

Especially projects with “Smart Spreadsheets”

http://olcc.ccce.divched.org/2017OLCCModule2P3

NonTrational
CER & DBER Education Research:

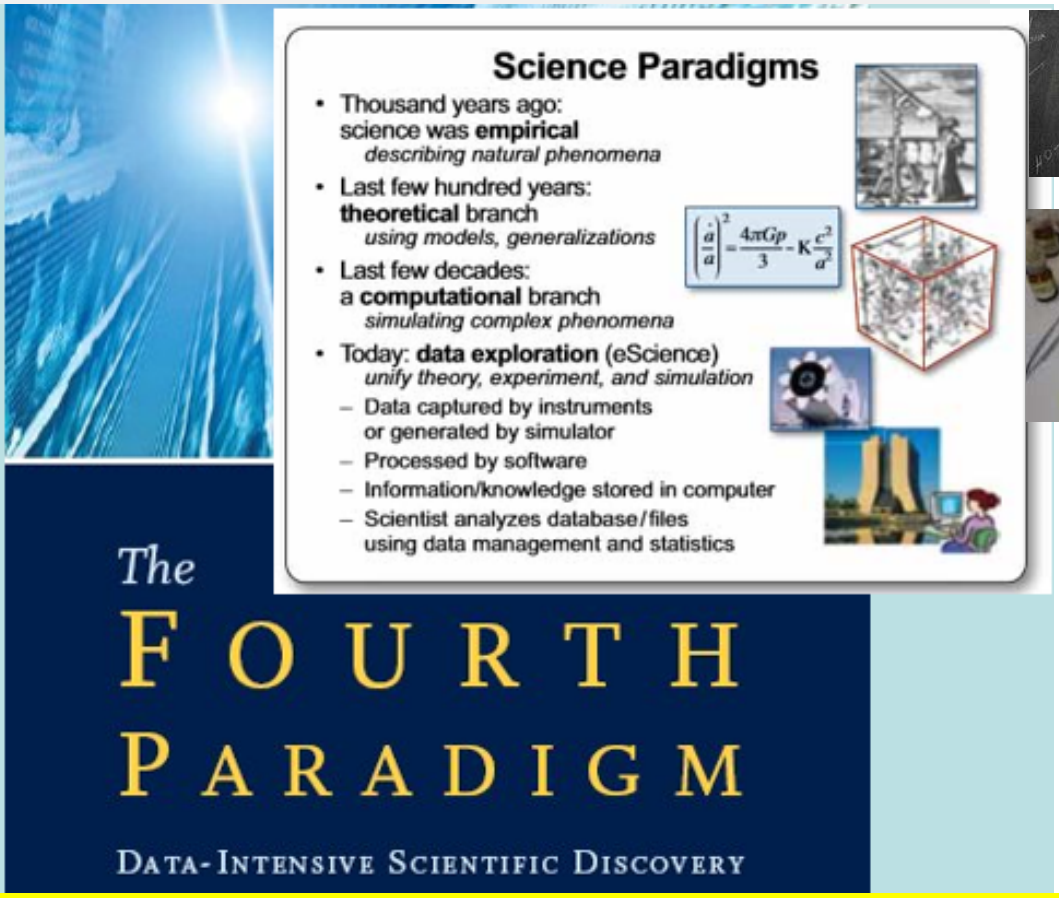


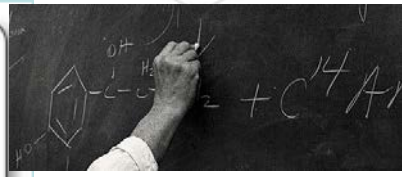
http://www.divched.org/CER/main

Education Research: Cheminformatics and New Paradigms for CER & DBER

(1917)

Youth want to Drive not ride





(2017)

Youth want to use digital tech

Cheminformatics is changing the fundamental
cognitive artifacts
used to represent, manipulate and communicate chemical information.
The Schema educators teach students to solve problems
are based on those artifacts

Outreach
Interacting with other communities

Develop projects that engage other (non-cheminformatic) chemistry communities

- IUPAC CCE (Committee On Chemical Education)
- ACS CHED CCCE (Committee on Computers in Chemical Education)
- CHF (Chemical Heritage Foundation)

Note on Curriculum Integration: and Outreach

They will use cheminformatics technologies for purposes that are different than what they were designed for.

Is that good?

Should understanding that be a part of outreach?

http://olcc.ccce.divched.org/2017OLCCModule2P3

IUPAC Centennial

"A Common Language for Chemistry"

Develop Educational Booklet on:

Evolution of Chemical Nomenclature: From [?Chemicographs?] to InChI

Opportunity for Training/Education/Outreach

Could Involve

- Chemical Heritage Foundation
- IUPAC CCE
- ACS CINF/CHED/HIST
- ACS CHED CCCE