Introduction to the World of Chemical Data—an OnLine College Course (OLCC) on Cheminformatics

In today's emerging world of big data and interconnected science it is critical for tomorrow's chemists to develop skills in the handling of publically available chemical data. You are invited to participate in the Spring 2017 Cheminformatics OLCC, an international multi-campus collaborative taught course that also trains faculty in the latest cheminformatics techniques.

OLCCs (OnLine Chemistry Courses) date back to 1996, and are really hybrid courses where online guest lecturers interact with students and faculty from multiple campuses, enabling schools and faculty to offer courses on topics they would not normally be able to offer. To date 16 schools are involved with offering the 2017 course and we are seeking more schools internationally. Each school has a residential faculty facilitator (instructor of credit) with the course being offered from 1-3 credit hours. Schools offering it as a 1 credit course are running it as an independent study/undergraduate research course with the instructor using it as an opportunity for faculty advancement, while those at 3 credit hours are using it as part of the faculty member's assigned teaching load. This course is built upon the Fall 2015 Cheminformatics OLCC material, which is publically available through LibreTexts (formerly ChemWiki*), but will focus on open access chemical compound datasets.

Overview of Cheminformatics OLCC:

- Course is conducted using blended learning involving online guest lecturers and resident faculty facilitators
- Students and faculty interact with experts in the field of cheminformatics.
- Students will interact with staff scientists at public compound databases like PubChem.
- No programming skills are required to participate.
- Students will gain experience in basic programming and accessing public chemical databases programmatically.
- Student projects provide opportunities to collaborate across multiple institutions, both academic and nonacademic

Students will:

1. Gain an introductory understanding of finding, evaluating and representing chemical information.
   a. Finding chemical information: Automating database access (use of IUPAC InChI).
   b. Evaluating chemical information: Extracting chemical information using simple programming techniques.
   c. Representing chemical information: Programmatically exchanging different chemical representations for purposes of analysis and visualization.
2. Gain experience using spreadsheets and scripting to answer questions in cheminformatics.

All material in this course is open access and will be archived on both the course website, and in Libretexts (formerly the ChemWiki). Schools outside of the US are welcome to participate and interested parties should contact Bob Belford, rebelford@ualr.edu.

*** http://chem.libretexts.org/ search "UALR 4399"**

Chemical Identifier

16-18 August 2017, Bethesda, Maryland, USA

The IUPAC International Chemical Identifier, InChI, has recently celebrated its tenth anniversary, and, building on the past and ongoing work by its working groups, a three-day meeting will be held next year on 16-18 August 2017 (Wednesday to Friday) on the main campus of National Institutes of Health (NIH) in Bethesda, MD. The meeting will bring together the current InChI community and working groups that define the current state of the IUPAC InChI project, together with other interested stakeholders. The aim is to discuss what is needed for the chemical, biomedical, materials, and related academic and industry communities for proper and useful structure standard representation of both small and large molecules, and the future direction and activities of IUPAC InChI development will be a major goal of the meeting.

If you wish to be notified further about the meeting as planning progresses, please sign up for the InChI Trust newsletter at www.inchi-trust.org

We welcome suggestions for the meeting agenda and also offers of assistance in planning the meeting.

Please contact Steve Heller, the project director, at steve@inchi-trust.org www.inchi-trust.org

See Project Place p. 24 for the latest InChI project; see more at iupac.org/body/802