Project Place

InChl Open Education Resource

The InChI Open Education Resource (OER) (https://www.inchi-trust.org/oer/) is designed to provide educators and other interested parties with resources, training material, and information related to InChI. Currently, the OER contains over 100 materials collected from various sources and provides users with search, filtering, and sorting functionalities to locate specific records. New relevant materials can be suggested by anyone, allowing the scientific community to share and find InChI-related resources.

A (open access) paper published online 3 Jan 2024 in *Chemistry Teacher International* (https://doi.org/10.1515/cti-2023-0009) describes the InChI Open Education Resource (OER).

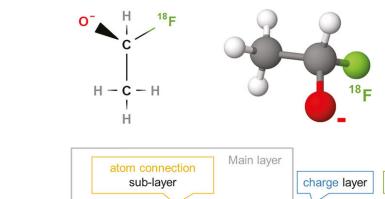
The paper shows how to use the InChI OER tag taxonomy to filter content, and demonstrates two resources within the InChI OER; the ChemNames2LCSS Google Sheet and the InChILayersExplorer, an Excel spreadsheet that breaks an InChI into its layers. While the InChI OER is of value to a broader chemistry community, this paper seeks to reach out to chemical educators and provide them with an understanding of InChI and its role in the practice of science.

For more information and comment, contact Task Group Chair Robert E. Belford <rebelford@ualr.edu> | https://iupac.org/project/2018-012-3-024

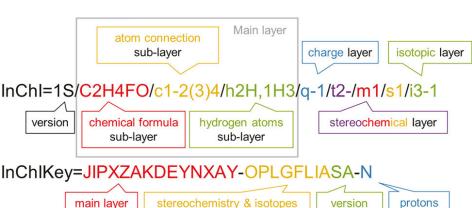
The Gender Gap in Chemistry— Building on the ISC Gender Gap Project

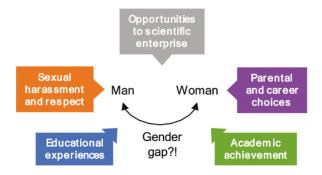
"Gender Gap in Chemistry, Still?!", one outcome of IUPAC project 2020-016-3-020 is published in the *Journal of Chemical Education* and co-authored by Hsiu-Yi Chao, John J. H. Lin, Mark Cesa, and Mei-Hung Chiu; https://doi.org/10.1021/acs.jchemed.2c00650 (7 Feb 2024)

The purpose of this study is to investigate differences between women and men in chemistry, as reflected in their responses to a global gender gap survey. The survey was conducted in 2018; responses from 1343 valid participants across the globe were collected and analyzed. The main results show that first, women were more likely to list their parents and themselves as important influences in their university studies than men. This result was consistent regardless of the Human Development Index (HDI, an index developed by the United Nations assessing the development of a country) and employment sectors. Also, men students reported more positive relationships and support from their advisors or supervisors than women. More women than men indicated that they had personally encountered sexual harassment at school or work. Also, in general, more men than women indicated that they had never experienced discrimination in the assessment or evaluation of their achievement across different HDI regions and in different employment sectors. Men



Layers for the standard InChI and InChIKey of (1*R*)-1-(18F) fluoroethanolate. Note: each layer or sublayer is separated by a forward slash.





reported having more research resources than women. More women than men indicated that their careers had influenced their decisions about their children, marriage, or long-term partnership across high and low HDI regions and employment sectors. Finally, women submitted fewer journal articles than men in the past five years, and this gender difference was also seen in respondents from both high and low HDI regions and working in industry. In contrast, by employment sector, the gender differences were relatively small.

For more information and comment, contact Task Group Chair Mark C. Cesa or Mei-Hung Chiu <mhchiu@ntnu.edu.tw>https://iupac.org/project/2020-016-3-020

Medicinal Chemistry in Drug Discovery & Development, India

A new project of the Chemistry and Human Health Division supports the objective of the Medicinal Chemistry/Drug Discovery & Development India (MCADDI), which is to build and optimize a basic drug discovery & development course for industrial and academic scientists, including medicinal chemists, in India and other South Asian countries. The success of the 2019 program, partly supported by a IUPAC grant, and the feedback from the Industry and Academic groups, post COVID break of 4 years, strongly encourages the task group to continue our theme of applied chemistry education in relation to drug design and development. Biocon Academy (Bangalore, India) has generously agreed to host this event again in 2024 and will provide the access to their facility for the faculty and attendees. This 5-day course will broaden the focus of the program compared to the 2019 Course by adding new lectures on the use of special chemistry topics such as Heterocyclic and Fluorine Chemistry in Drug Discovery, and adding a lecture on antibody-drug conjugate (ADC) discovery and development.

The first part session of the course will be focused on the fundamentals of drug discovery and the second part will be focused on the application of new technologies in the drug discovery and development process. The 2024 program will dedicate a full day session to the discovery and development of biologic drugs, including antibodies, antibody-drug conjugates and therapeutic proteins. The increase in medicinal chemistry employment in Indian and southeast Asian pharmaceutical companies, and in Contract Research Organizations (CROs) collaborating with US and European companies, has created a vital need for chemists to acquire state of the art knowledge of medicinal chemistry and other closely related disciplines.

The performance and value of the MCADDI courses (2013, 2015, 2017, 2019) has been assessed by the participants and faculty, and has received positive feedback from both industrial and academic scientist in India. The 2024 course will also be assessed to determine whether to continue in the same format, or evolve the course further in order to meet the needs of Indian and Southeast Asian medicinal chemists. The desired outcome will be to enroll a new and broader set of drug discovery scientists from industry and academia. The number of participants would be about 100-120 from academia and industry, similar to the attendance in 2019, and the goal is to provide participants with a strong introduction to the fundamentals and practice of medicinal chemistry in drug discovery, including the use of tools such as computer-assisted drug design (CADD) and automated synthesis. The task group is planning to actively seek the participation of scientists from other South Asian countries such as Singapore, Malaysia, South Africa, etc.

For more information and comment, contact Task Group Chair Neel Balu Balasubramanian or William J. Greenlee https://iupac.org/project/2023-033-2-700

Advanced Technologies for Carbon Sequestration and Capture

This new project, building on the insights of the 'Harmonizing Carbon Sequestration Measurement' project (2022-010-2-600), aims to evaluate the efficacy of innovative carbon sequestration technologies. Originating from identified knowledge gaps in the previous project, it seeks to address issues on CO_2 emissions understanding, consistent accounting systems, and the necessity for novel mitigation measures.