

Teaching InChI to Chemistry Students

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Challenges for InChI teaching

Instructor's perspective

Student's perspective

Target audience

Lack of awareness of and interest in

Implementation in curricula

IT literacy

Assessment/ exercise

Practical application/ relevancy

Teaching InChI to develop Information literacy competency

Information Literacy Standards and Guidelines

- ALA/ACRL/STS Task Force on Information Literacy for Science and Technology. 2006. "Information Literacy Standards for Science and Technology." *American Library Association*.
- American Chemical Society, Committee on Professional Training. 2015. Undergraduate Professional Education in Chemistry: ACS Guidelines and Evaluation Procedures for Bachelor's Degree Programs.
- Commission on Accreditation in Clinical Chemistry (COMACC).
- Information Competencies for Chemistry Undergraduates: the Elements of Information Literacy. 2012. *Special Libraries Association, Chemistry Division and American Chemical Society, Division of Chemical Information*.

Chemical Identifiers

- Trade name
- Systematic name
- Registry numbers and database identifiers
- Line notations (SMILES, InChI)

- Chemical naming
- Communicating chemical structures on computer
- Database searches
 - Text search
 - Structure search
 - Identifier search

Learning Objectives

- Review chemical identifiers used to represent molecules
- Understand the InChI and InChI Key
- Explain InChI Layers
- Compare and contrast SMILES and InChI
- Interpret SMILES and InChI strings into their corresponding chemical structures

Exercises/ Assignments

InChI and InChI Key

- Generate an InChI for Ibuprofen
- What compound is the InChI Key "WTDRDQBEARUVNC-ZCFIWIBFSA-N" for?

InChI Layers

- What is the second layers of InChI for 1,1-dibromocyclopropane?
- What information is described in third layer of this InChI?

Database search

- Search "InChI=1S/C₃H₄Br₂/c₄-3(5)1-2-3/h1-2H₂" in
PubChem
ChemSpider
NIST

Resources/ Textbooks

InChI OER

InChI OER. Retrieved August 16, 2019, from InChI Trust website: <https://www.inchi-trust.org/oer/>

Course on LibreTexts

UALR 4399/5399: ChemInformatics

Fall 2015: Belford

[https://chem.libretexts.org/Courses/University_of_Arkansas_Little_Rock/ChemInformatics_\(2015\)%3A_Chem_4399%2F%2F5399/Text](https://chem.libretexts.org/Courses/University_of_Arkansas_Little_Rock/ChemInformatics_(2015)%3A_Chem_4399%2F%2F5399/Text)

Wild, D. (2012). *Introducing cheminformatics: An intensive electronic self-learning guide for new practitioners*. Raleigh, N.C.: Lulu.

References

- Chemical Information Sources—Wikibooks, open books for an open world. Retrieved August 16, 2019, from https://en.wikibooks.org/wiki/Chemical_Information_Sources
- InChI OER. Retrieved August 16, 2019, from InChI Trust website: <https://www.inchi-trust.org/oer/>
- 5 Chemical Identifiers—Chemistry LibreTexts. Retrieved August 16, 2019, from [https://chem.libretexts.org/Courses/University_of_Arkansas_Little_Rock/ChemInformatics_\(2015\)%3A_Chem_4399%2F%2F5399/Text/5_Chemical_Identifiers](https://chem.libretexts.org/Courses/University_of_Arkansas_Little_Rock/ChemInformatics_(2015)%3A_Chem_4399%2F%2F5399/Text/5_Chemical_Identifiers)