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Identifying International Chemical Identifier (InChI) Enhancements— QR Codes and Industry Applications

Seeking feedback on a chemical barcode

Do you wish you could link easily from physical samples to chemical property and safety information? Ready access to chemical information is critical for every wet lab, from experimental planning to clean-up and responding to potential emergencies. The IUPAC International Chemical Identifier (InChI) is a text string that encodes chemical structure and provides a means to search and link chemical information across databases locally and in the cloud. A version of the InChI can be included in a QR code to be printed on chemical samples and solution bottles, in lab notebooks, and on posters. The QR code can be read with a number of free apps on a mobile device and link directly to databases with further chemical information.
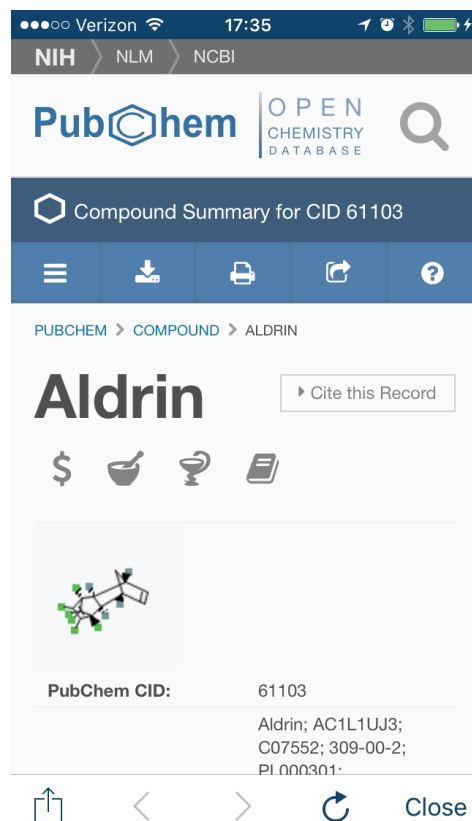
IUPAC project 2015-019-2-800 is consulting with industry and academic representatives and has identified chemical inventory and health and safety applications as being key applications for QR code versions of the InChI. A prototype QR code using InChI was developed as a proof-of-concept in the PubChem database, a public resource provided by the US National Center for Biotechnology Information in the National Library of Medicine. PubChem compiles chemical property information from several authoritative sources of chemical health and safety data, including several US agencies (NIOSH, OSHA) and national/international authorities on GHS chemical hazard classifications from EU, Japan, and Australia. The provenance of these sources is meticulously recorded and displayed with the associated data.

The QR code pictured below links to the PubChem record for Aldrin (a banned insecticide) via a hash version or abbreviated form of the InChI called an InChIKey.

Encoded link:
https://pubchem.ncbi.
nlm.nih.gov/compound/
QBYJBZPUGVGKQQ-
VFBQXPTHSA-N

Any InChIKey among the circa 90 million compound records in the PubChem database may be substituted in the link to retrieve these records. Try scanning the

PubChem record for Aldrin, a banned insecticide

code and let us know your thoughts on using this technology in chemical inventory control, the provision of health and safety data, or other laboratory work. A further workshop is being scheduled in Europe in February 2017.

For more information and comments, contact Task Group Chair Richard Hartshorn <richard.hartshorn@canterbury.ac.nz>, or Member Leah Rae McEwen <lrm1@cornell.edu>.
www.iupac.org/project/2015-019-2-800

Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups 14-16 Elements

The objective of this two-year project is to develop a non-ambiguous terminology for interactions formed by chalcogens, pnictogens, and tetrels, namely the elements of Groups 16, 15, and 14, respectively. Group 16-14 elements can form attractive interactions with