Understanding Human and Environmental Hazards: An activity for undergraduate chemistry students

An activity prepared by Beyond Benign as part of the Green Chemistry in Higher Education program: A workshop for EPA Region 2 Colleges and Universities

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Introduction:

Understanding what makes a molecule hazardous to the environment or toxic to humans is a key piece to green chemistry design. However, what do we mean when we use the terms "hazardous" or "toxic"? There are many toxicological and environmental endpoints that determine whether or not a molecule will have human and environmental impact. This activity will help students to understand more about the various endpoints and how to assess whether or not a molecule poses human and environmental risks.

This activity is a result of an EPA Region 2 Source Reduction grant[1] titled *Green Chemistry in Higher Education: A Workshop for Region 2 Colleges and Universities*. The Green Chemistry in Higher Education workshop was carried out at Siena College on July 18-21, 2013. 29 faculty members participated from 20 different institutions in New York and New Jersey. The workshop consisted of three main focus areas: green chemistry case studies for lecture and course work, green chemistry laboratory exercises, and toxicology and environmental impact. This activity focuses on the third aspect of the workshop, toxicology and environmental impact.

In this activity, students will perform a hazard evaluation of a chemical using the Quick Chemical Assessment Tool (QCAT). They will research each of the toxicological and environmental endpoints and then assign a grade to the chemical. The assessment will allow them to understand more about the different toxicological and environmental endpoints and help them to assess hazards associated with chemicals.

[1] **Disclaimer: Although the information in this document has been funded wholly or in part by the United States Environmental Protection Agency under assistance agreement X9-96296312 to Beyond Benign, it has not gone through the Agency's publications review process and, therefore, may not necessarily reflect the views of the Agency and no official endorsement should be inferred.**

The Quick Chemical Assessment Tool (QCAT):

The QCAT is an assessment tool used to evaluate the hazards associated with chemicals. The tool was developed by the Washington State Department of Ecology[2] and is a simplified version of Clean Production Action's Green Screen®.[3]

This tool allows for the quick comparison of chemicals and their alternatives. An overview of QCAT is provided, along with a how-to guide for generating a QCAT report for a new chemical More information about the QCAT can be found on the Washington State Department of Ecology's website.[2]

How-to evaluate a chemical using QCAT and the Hazard Evaluation Template:

Step 1: Download the *Hazard Evaluation Template* excel file. Use this file to gather data for each of the 9 endpoints within QCAT. The Hazard Evaluation Template provides links for where to best locate the data for each of the endpoints. An extended list of databases can be found in the WA State Department of Ecology's QCAT user guide: http://www.ecy.wa.gov/programs/hwtr/chemalternatives/QCAT.html. More information about each of the 9 endpoints is provided within this document.

Step 2: Use the Chemical Ranking Criteria Quick Reference, which can be found on the Hazard Evaluation Template to assign a score for each of the endpoints (vH, H, M, L, vL). If no data, or limited data is found for an endpoint, then list that endpoint as "DG" for data gap.

Step 3: Assign an Initial Grade for the chemical using the guidelines in the supporting documents, or on the second tab of the Hazard Evaluation Template.

Step 4: Assign a Final Grade for the chemical using the guidelines in the supporting documents, or on the second tab of the Hazard Evaluation Template. Be sure to follow the steps on how to assign the Final Grade if data gaps exist.

[2] The Quick Chemical Assessment Tool, State of Washington Department of Ecology [http://www.ecy.wa.gov/programs/hwtr/chemalternatives/QCAT.html]

[3] Green Screen, Clean Production Action [http://www.greenscreenchemicals.org/]

Understanding hazard endpoints:

The QCAT has 9 toxicological endpoints that are classified as Human Health Hazards, Environmental Hazards and Fate endpoints. Each of the 9 are described further below.

Human Health Hazards:

Carcinogenicity (from AltTox.org): "The term *carcinogen* denotes a chemical substance or a mixture of chemical substances which induce cancer or increase its incidence" (UNECE, 2004, p. 167). An alternate definition is that carcinogenic substances are ones that "induce tumors (benign or malignant), increase their incidence or malignancy, or shorten the time of tumor occurrence when they are inhaled, injected, dermally applied, or ingested" (Maurici, et al., 2005, p. 177).

The International Agency for Research on Cancer (IARC) evaluates chemicals according to their carcinogenic risk and classifies them based on their carcinogenicity.[4] The state of California provides a list of chemical substances that are known to cause cancer in their CA Prop 65 List.[5]

Mutagenicity/Genotoxicity: Genotoxicity is defined as the ability of a chemical to damage the genetic information within a cell, causing mutations, which may lead to cancer. Mutagenicity is defined as the ability of a chemical to cause mutation in an organism as a result of the changing of genetic information.

Reproductive Toxicity: Chemical substances that interfere with normal reproduction have reproductive toxicity. The adverse effects can include effects on sexual function and fertility in males and females, and developmental toxicity in offspring.

Developmental Toxicity: Developmental toxicity is the structural or functional alteration, reversible or irreversible, which interferes with homeostasis, normal growth, differentiation, development or behavior of a developing embryo, fetus or child, which can be caused by chemical substances.

Endocrine Disruption: Endocrine disruptors are chemicals that can interfere with the endocrine (or hormone) system. The chemicals can cause numerous effects in humans, including birth defects, cancerous tumors, and other developmental disorders, as well as behavioral and learning disorders. Endocrine disruptors can cause these negative effects at very low doses.

The Endocrine Disruption Exchange, Inc. (TEDX) is an organization that is focused on the human health and environmental problems caused by low-dose and ambient exposure to chemicals that interfere with development and function (endocrine disruptors). They provide a list of potential endocrine disruptors.[6]

[4] International Agency for Research on Cancer, World Health Organization [http://www.iarc.fr/, Accessed December 2014].
[5] California Prop 65 List [http://oehha.ca.gov/prop65/prop65_list/files/P65single013114.pdf, Accessed November 2014].
[6] TEDX List of Potential Endocrine Disruptors [http://endocrinedisruption.org/endocrine-disruption/tedx-list-of-potential-endocrine-disruptors/overview, Accessed December 2014].

Acute Mammalian Toxicity: Acute toxicity is the adverse effects of a substance from either a single exposure, or from multiple exposures in a short period of time. Most of the data for acute toxicity is derived from animal testing, where animals are exposed to varying doses of a chemical for a period of time and the number of organisms that result in a specific endpoint, such as death, are counted in order to determine the toxicity.

The most common measurement for acute toxicity is LD50, which is the lethal dose by which 50% of the population is killed, or LC50, which is the lethal concentration by which 50% of the population is killed. These doses are measured in animals and translated to human exposure, despite some differences in humans and animals.

Environmental Hazards:

Acute Aquatic Toxicity: Acute aquatic toxicity is the adverse effects on an aquatic organism of a substance from a single exposure or from multiple exposures in a short period of time. Acute aquatic toxicity is measured on fish species, algae and crustaceans to determine the substance's toxicity. The measurements for these tests are typically LC50 or EC50, which is the effective concentration at which 50% of the population has the adverse effect.

Fate:

Persistence: Chemicals that persist in the environment and resist degradation have more of an opportunity to interact with organisms to trigger an adverse effect. Persistence is measured in how well (or not) a chemical breaks down in the water, soil, sediment and air.

Bioaccumulation: Bioaccumulation occurs when a substances is taken up at a higher rate than it can be removed from an organism. Many times this can be due to the chemical being persistent and resisting degradation. Bioaccumulation can result in a high concentration of toxic substances in organisms and the environment.

Bioaccumulation is measured through a Bioconcentration Factor (BCF) or the octanol:water partition coefficient (K_{OW}). The K_{OW} is a measure of the ratio of a substance in octanol as compared to water, indicating whether a substance will bioaccumulate in fatty tissues. The BCF is the ratio of the chemical concentration in an organism in relation to the concentration in water.

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Download this activity and other case studies at the following link: http://www.greenchemistrycommitment.org/resources/case-studies/