**Lesson Plan: Lecture 24**

**Designing Future Products with Reduced Toxicity**

**Description**

This lecture continues to explore different approaches to hazard minimization by changing molecular design. After several practical examples and a case study, students will learn about current methods that scientists use to assess chemical toxicity on a large scale. In vivo and In vitro studies are discussed.

**Prior to Lecture**

Required Readings:

* Voutchkova, A. M., Osimitz, T. G., Anastas, P. T.; “Toward a Comprehensive Molecular Design Framework for Reduced Hazard*” Chem. Rev*, 2010, *110* (10), 5845-5882. doi: 10.1021/cr9003105

<https://pubs.acs.org/doi/abs/10.1021/cr9003105>

* National Academies Press “A Framework to Guide Selection of Chemical Alternatives”, 2014, Chapter 13.

**Topics to Cover in Lecture**

* Approaches to hazard minimization through design
* Case study: Codexis
* Qsars - Quantitative Structure Activity Relationship
* Nexus of chemistry and toxicology
* Sources of high throughput data

**Class Exercise**

Module 5 Glutathione as a Tool for Testing Gene Function (optional)

Scientists use many novel molecular techniques with genes since they can provide a more complete view on the development of diseases.  Methods such as gene silencing, gene knockout, and gene overexpression allow researchers to study different detoxification pathways at the cellular level. This exercise describes the difference between gene silencing, gene knockout and overexpression and uses gluthatione overexpression as an example of genetic modification.

Module 6 Crossroads of Computational Chemistry and Toxicology (optional)

There are thousands of chemicals and only a fraction have been evaluated for specific classes of toxicity (carcinogenicity, genotoxicity, developmental toxicity, etc). It is not possible to test all the chemicals with *in vitro* and *in vivo* assays. Computational methods, such as the *in silico* method of testing (and predicting toxicology before development), is the newest way by which to ensure that toxicology is considered in molecular and product design and that potential toxicological impacts are known. This exercise explains the difference between in vitro and in vivo testing and introduces in silico as an alternative to biological studies.

Module 7 Using ProTox (optional)

The advent of computational and/or predictive modeling has given scientists an important tool for researching potentially harmful chemicals.  This has allowed scientists ranging from drug designers to material chemists to perform molecular pre-screening of thousands of chemicals to determine potential compatibilities to chemicals with already known structures. This exercise will allow students to explore tools which are available to test the toxicity.

**Homework**

Toxicology