The Basics of Toxicology for Green Molecular Design

Introduction
Green chemistry seeks to promote the adoption of safer more efficient chemicals, products and processes. In order to design inherently safer chemicals it is important to understand the basic principles that dictate toxicity. This 1 unit class will introduce the basic tools and paradigms found in toxicology with a focus on ways to design safer chemicals and processes.

Learning Goals
1. Understand the basic principles and modes of action that dictate molecular toxicology.
2. Be able to effectively use tools and metrics to evaluate and compare the hazard profile of chemical substances.
3. Understand and identify structure/function relationships with respect to chemical properties, biological activity, and environmental fate.
4. Be able to understand and evaluate the results of common toxicology assays.

Intended Audience
Graduate students and advanced undergraduates in the College of Chemistry, College of Engineering, College of Natural Resources, and the School of Public Health.

Prerequisites
Graduate standing, or undergraduates with instructor approval. Organic chemistry or equivalent knowledge.

Course Textbooks
Required: none
Recommended:
1) *Mechanistic Toxicology: The Molecular Basis of How Chemical Disrupt Biological Targets* by Urs A. Boelsterli.
Affiliated Faculty and Staff
Chris Vulpe, Professor of Nutritional Science and Toxicology
Martin Mulvihill, Executive Director of the BCGC

Student Assignments

(1) Class Participation: You will be expected to attend class and participate in class discussion. There will be regular course reading and occasional chemical modeling questions to be addressed. (50% of the course grade)

(2) Bio-Based feedstock evaluation project: In teams of 3-5, you will Characterize the relative safety/risk associated with emerging bio-based feedstock as compared to their petroleum based counterparts (50% of the course grade)

Course Calendar

<table>
<thead>
<tr>
<th>Class</th>
<th>Date</th>
<th>Topic</th>
<th>Program and resources introduced</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>March 12</td>
<td>How is toxicity measured and where you find Toxicity data?</td>
<td>ToxCast</td>
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<tr>
<td>2</td>
<td>March 19</td>
<td>Where will the chemicals end up in the Environment? Will they degrade?</td>
<td>PBT Profiler, UM-BBD, ChemSpider, EPI-Suite</td>
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<tr>
<td>3</td>
<td>April 2</td>
<td>How can you predict toxicity? Structural alerts and QSAR introduction</td>
<td>ToxPredict</td>
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<td>4</td>
<td>April 9</td>
<td>How do QSARs work? How could they be improved?</td>
<td>ToxPredict</td>
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<td>5</td>
<td>April 16</td>
<td>How do chemicals move through the body? ADME-T</td>
<td>SMARTcyp, ADME parameters</td>
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<td>6</td>
<td>April 23</td>
<td>Can we just test all of the chemicals?</td>
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<td>7</td>
<td>April 30</td>
<td>Can you differentiate between chemical options based on the tools introduced over the last six weeks?</td>
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