Resources and tools for integrating toxicology concepts in to chemistry programs

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ACS Green Chemistry & Engineering Conference

June 20, 2018, Portland OR

Higher Education: Opportunities

- Valued by industry
  - Environmental, economic and social benefits
- The transformative power of green chemistry principles and practice
- Valued by students
- Better prepares students post-graduation
- Removing hazards from laboratories
  - Making the laboratory **safer**
- Doing chemistry right the first time

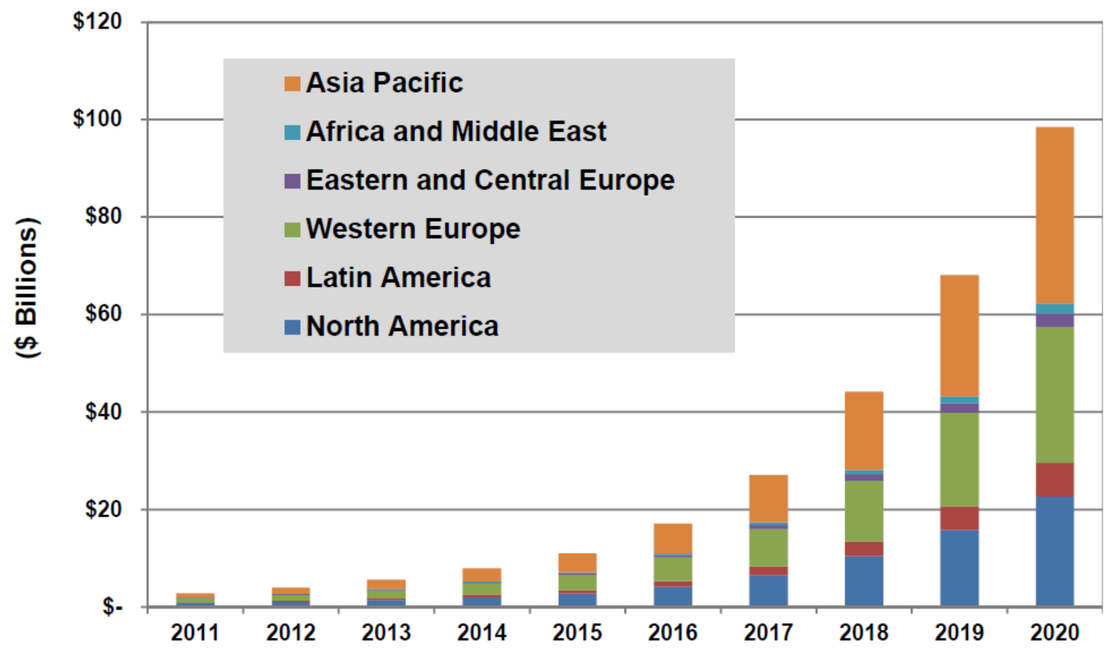
beyondbenign
green chemistry education

Grand Valley State University
Department of Chemistry

GVSU Green Chemistry

Green Chemistry: Valued by Industry

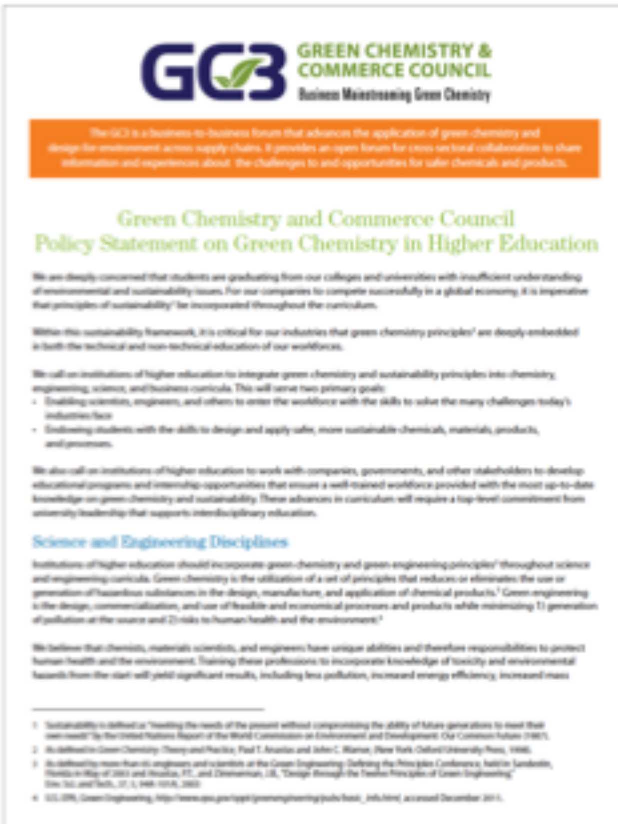
Chart 1.1 Green Chemical Market by Region, World Markets: 2011-2020



(Source: Pike Research)

Navigant Research, Green Chemicals Will Save Industry $65.5 Billion by 2020, http://www.navigantresearch.com/newsroom/green-chemicals-will-save-industry-65-5-billion-by-2020 [Accessed September 2017].

Green Chemistry: Valued by Industry



http://www.greenchemistryandcommerce.org/projects/education

http://www.sigmaaldrich.com/chemistry/greener-alternatives.html

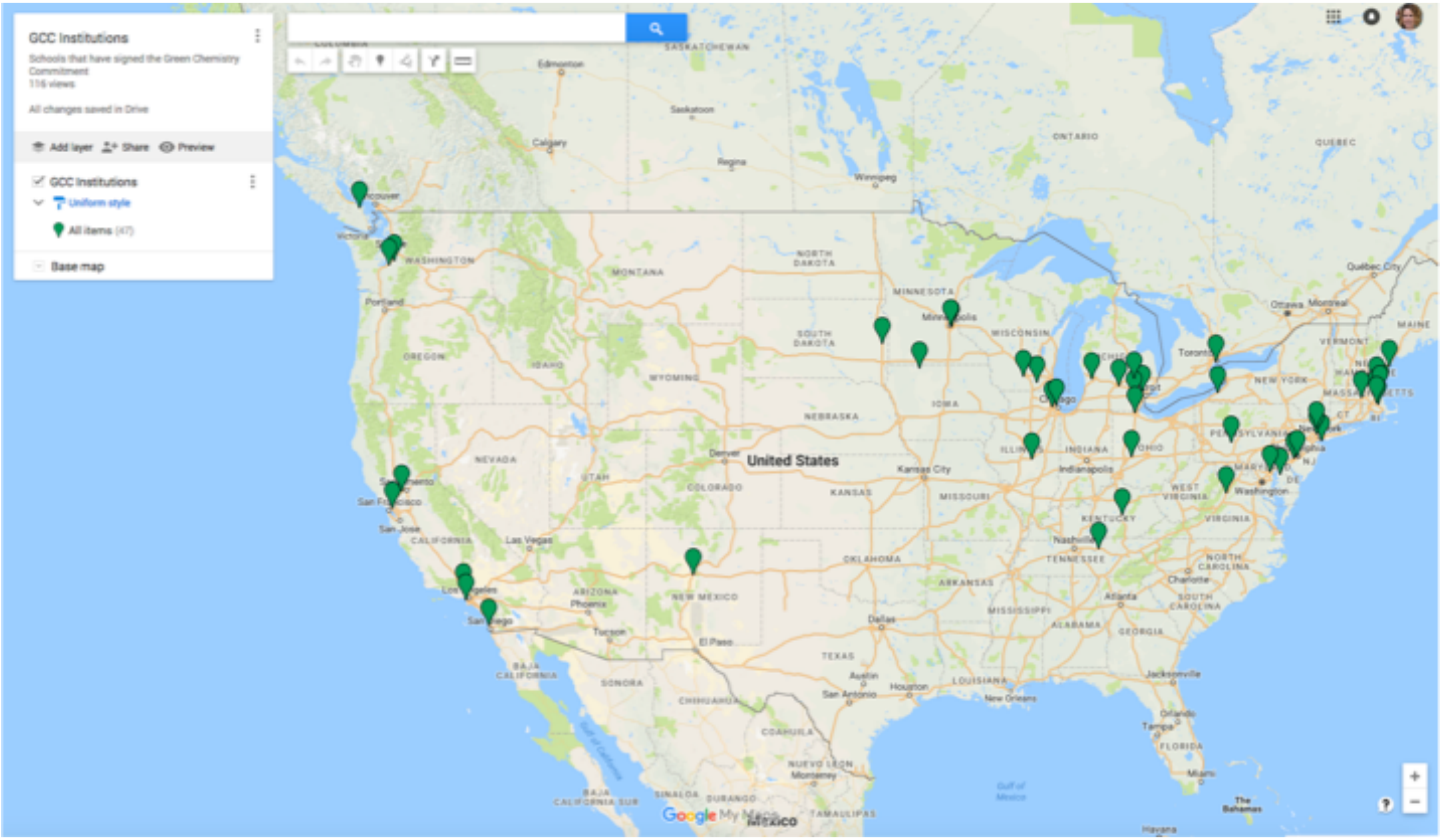
Green Chemistry Commitment

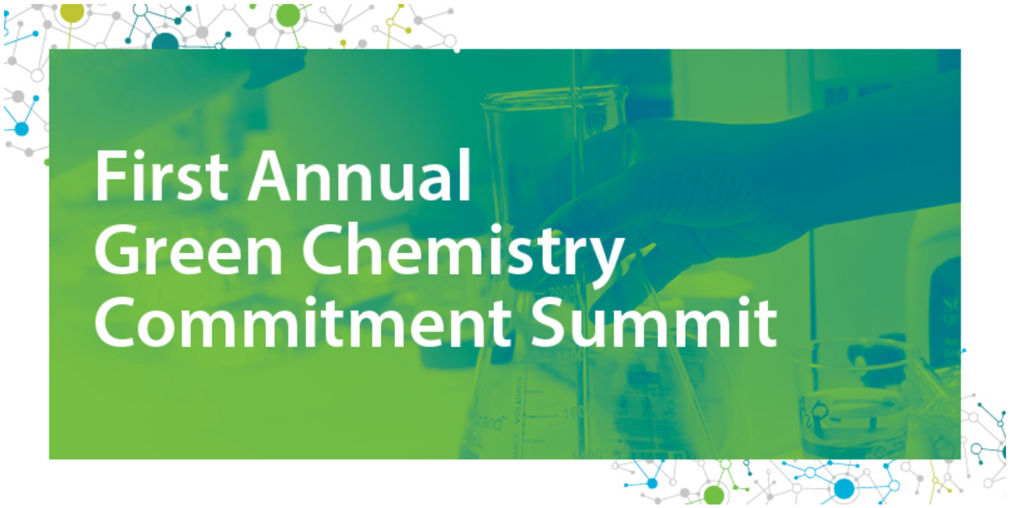
Green Chemistry Student Learning Objectives

Signing institutions agree that upon graduation, all chemistry majors should have proficiency in the following essential **green chemistry competencies**:

- **Theory:** Have a working knowledge of the twelve principles of Green Chemistry
- **Toxicology**: Have an understanding of the principles of toxicology, the molecular mechanisms of how chemicals affect human health and the environment, and the resources to identify and assess molecular hazards
- **Laboratory Skills**: Possess the ability to assess chemical products and processes and design greener alternatives when appropriate
- **Application**: Be prepared to serve society in their professional capacity as scientists and professionals through the articulation, evaluation and employment of methods and chemicals that are benign for human health and the environment

http://www.beyondbenign.org/he-green-chemistry-commitment/


GCC Institutions
Schools that have signed the Green Chemistry Commitment
116 views
All changes saved in Drive
Add layer
Share
Preview
GCC Institutions
Uniform style
All items (47)
Base map
United States



Where: University of Notre Dame

When: July 29, 2018, 9am – 1pm (includes lunch)

Who: Current and prospective signing institutions; Green Chemistry community members

The agenda will feature interactive discussions in 5 key areas:

1) Integrating Toxicology into Chemistry Courses
2) Green Chemistry Courses and Programs
3) Green Chemistry Integration in Undergraduate Teaching Labs
4) Green Chemistry Undergraduate Research
5) Green Chemistry K-12 and Community Outreach

Including a discussion on the new ACS Green Chemistry CPT Supplement

https://www.eventbrite.com/e/green-chemistry-commitment-summit-bcce-2018-tickets-44768604100

Opinion poll: Which is the most difficult to achieve?

Green Chemistry Commitment

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http://www.beyondbenign.org/he-green-chemistry-commitment/

Why is *Teaching Tox in Chem programs* the most difficult among the goals of GCC?

- **Toxicology**: Have an understanding of the principles of toxicology, the molecular mechanisms of how chemicals affect human health and the environment, and the resources to identify and assess molecular hazards

- Lack of expertise/knowledge
- Make the changes sustainable
- Keep up-to-date with the newest trends in the field

Despite the barriers, Toxicology is being considered and tested in chemistry programs across the country

GCC: General Trends

- Organic chemistry laboratory is the first place of focus
- Green chemistry degrees and programs
  - University of Toledo, School of Green Chemistry & Engineering
  - Grand Valley State University, GC undergraduate certificate program
  - University of Michigan, Flint – new undergraduate (BS) degree program (First of it's kind!!)
- Toxicology is being considered and tested in programs across the country

  Wittenberg University, South Dakota State University, UC Berkeley, Simmons College, St. Catherine's University, Grand Valley State Univ., and more
- More resources needed for adoption across all disciplines of chemistry

Growing demand for more resources!

http://www.beyondbenign.org/he-green-chemistry-commitment/

Models for integrating toxicology*

- Simmons College, Mechanistic Toxicology (John Warner, Amy Cannon)
- South Dakota State University, Chemical Toxicology (Doug Raynie)
- Wittenberg University, Integrating Toxicology through Lab Safety (Dave Finster)

*Amy S. Cannon, David Finster, Douglas Raynie & John C. Warner (2017) **Models for integrating toxicology concepts into chemistry courses and programs**, Green Chemistry Letters and Reviews, 10:4, 436-443, https://doi.org/10.1080/17518253.2017.1391880

Models: Simmons College

CHEM 342, Mechanistic Toxicology
Offered Fall 2014, Spring 2016, Fall 2017

Combination of lectures and guest speakers:

- Mary Butow, Beyond the SDS, TURI University of Massachusetts Lowell
- Laura Vandenberg, Low-dose effects and endocrine disruption, University of Massachusetts Amherst
- Dick Clapp, Boston University, Molly Jacobs University of Massachusetts Lowell – Epidemiology
- Jessica Tischler, Monique Wilhelm, University of Michigan, Flint – Flint Water Crisis

Topics include:

- Green Chemistry
- Biochemistry Review (optional)
- History and Introduction of Toxicology
- Principles of Toxicology
- Understanding hazard endpoints
- Toxicokinetics and Toxicodynamics
- Endocrine Disruption and Low Dose Effects
- Epidemiology
- Ozone Depletion, Climate Change and Energy
- Design for Biodegradability: Persistence and Bioaccumulation
- Predictive Tools for Reduced Molecular Hazard
- Understanding Structure-Activity Relationships

*Amy S. Cannon, David Finster, Douglas Raynie & John C. Warner (2017) **Models for integrating toxicology concepts into chemistry courses and programs**, Green Chemistry Letters and Reviews, 10:4, 436-443, https://doi.org/10.1080/17518253.2017.1391880

Models: South Dakota State University

Upper division Chemical Toxicology course, combined with introduction to toxicology in organic courses:

- Toxicodynamics, toxicokinetics
- Environmental toxicology
- Mechanistic toxicology

Learning objectives:

Students would know (a) elementary toxicology principles, vocabulary, and methodologies and (b) resources to identify chemical hazards

3-pronged approach:

- During classroom lectures the principles of toxicology were introduced
- A 2-week laboratory exercise reinforced lectures, introduced bioassays and toxicity testing
- A survey measured potential changes in student attitudes toward topics of concern
  - Increase in concern over chemical safety
  - Increased awareness of chemical hazards
  - More knowledgeable on how to avoid or minimize chemical exposure potential

*Amy S. Cannon, David Finster, Douglas Raynie & John C. Warner (2017) **Models for integrating toxicology concepts into chemistry courses and programs**, Green Chemistry Letters and Reviews, 10:4, 436-443, https://doi.org/10.1080/17518253.2017.1391880

Models: Wittenberg University

From: Hill, R. H.; Finster, D. C. *Laboratory Safety for Chemistry Students,* 2nd ed.; John Wiley & Sons: Hoboken, NJ, 2016

Introductory	Intermediate	Advanced	Topic
3.1.1			Routes of Exposure to Hazards
3.1.3			Finding Hazard Information: Material Safety Data Sheets, Safety Data Sheets, and the GHS
4.1.1			Concepts in Toxicology
4.1.2			Measuring Toxicity
4.1.3			Acute Toxicity
	6.2.2		Understanding Occupational Exposure Limits (OEL)
6.1.2			Managing Risk – Making Decisions about Safety
	4.2.1		Chronic Toxicity
		4.3.1	Carcinogens
		4.3.2	Biological Hazards and Bloodborne Pathogens
		1.3.3	Laws and Regulations Pertaining to Safety
		4.3.3	Hazards of Nanomaterials

- Concepts are introduced in General and Organic Chemistry, advanced courses & seminar program

*Amy S. Cannon, David Finster, Douglas Raynie & John C. Warner (2017) **Models for integrating toxicology concepts into chemistry courses and programs**, Green Chemistry Letters and Reviews, 10:4, 436-443, https://doi.org/10.1080/17518253.2017.1391880

Models: & partnership

Challenges:	**Opportunities**:
• Lack of expertise/knowledge	bring experts to the classroom
• Make the changes sustainable	refine, and continuously improve teaching materials; collect; reuse
• Keep up-to-date with the newest trends in the field	back to the experts; never stop learning, networking, attending meetings, read literature, etc..

Manuscript in preparation

Traverse City
Michigan
Mt Pleasant
Midland
Saginaw
Muskegon
Grand Rapids
Flint
Kentwood
Lansing
Troy
Warren
Livonia
Kalamazoo
Jackson
Ann Arbor
Detroit
Portage
Elkhart
Toledo

Models: Academic-Industry partnership
GVSU DOW

- **Who**: GVSU Chemistry Department and Dow Toxicology and Environment Research and Consulting (TERC) team.

- **What**: prepare and deliver innovative teaching materials in a modern course format; provide fundamental principles of toxicology along with contemporary advances in the field; utilize experienced professionals in delivering information directly to students.

- **How**: actively engage students in learning and applying the principles of toxicology through the lens of green chemistry.

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Department of Chemistry

GVSU Green Chemistry

Manuscript in preparation

DOW

Models: Academic-Industry partnership
GVSU DOW

- A ***multidisciplinary*** overview of the toxic effects of chemicals on human health and environment, public policies, and the development of less hazardous alternatives through chemical design.

- The course focuses on assessments, mechanisms, properties, health effects, and strategies to reduce risk and exposure in everyday life across diverse societal groups.

Grand Valley State University Department of Chemistry

GVSU Green Chemistry

Manuscript in preparation

DOW

Models: Academic-Industry partnership

GVSU DOW

Dalila Kovacs
Rick Rediske

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Sue Marty

Grand Valley State University
Department of Chemistry

GVSU Green Chemistry

Manuscript in preparation

DOW

Models: Academic-Industry partnership GVSU DOW

GVSU

- pedagogy & methodology
- teaching experience
- familiarity with learning management system

Dow-TERC*

- expertise in toxicology
- experience in toxicology training
- training materials

Manuscript in preparation

Models: Academic-Industry partnership GVSU DOW

- **Students**
  - biomedical science
  - biology
  - chemistry
  - allied health sciences
  - nursing
  - industrial hygiene
  - environmental studies
  - others

- **Desired outcome**: familiarity with **tools** and **scientific evidence** necessary to identify :
  - hazardous materials
  - means to reduce health impacts
  - possible design changes for sustainable chemicals and consumer products

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Department of Chemistry

GVSU Green Chemistry

Manuscript in preparation

DOW

DOW guest speaker	Topic presented
Dan Wilson	Introduce Dow: Toxicology in TERC; The future of Toxicology
Robert Ellis-Hutchings	Hazard *vs.* Risk
Bryce Landenberger	Overview of REACH: Session on using ECCHA REACH
Sue Marty	Toxicokinetics: Absorption, Distribution, Metabolism and Elimination
Joe Chai	Environmental Fate and Transport of Chemicals; QSAR
Matt Le Baron	Genetic Toxicology and Carcinogenesis
Kathy Coady	Environmental Toxicology & Ecotoxicity; Future toward Environmental Safety Assessments
Bethany Hannas	Developmental and Reproductive Toxicology (DART)
Bryce Landenberger	Risk assessment: A primer Modeling Tools for Exposure/Risk Assessment
Elke Jansen; Landenberger	ConsExpo- A sample tool for exposure assessment
E. Jansen; Linda McFadden	Introduction to ECETOC TRA
Dan Wilson	Overview of Computational Toxicology
Raja Settivari	Biological Profiling: Designing safer personal care products using alternative models
Shawn Hunter	Product Safety Across the Life Cycle
Scott Arnold*	Metals toxicants
Joanna Klapacz	Pharmaceutical and Food Applications; the case of Propylene Glycol

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DEPARTMENT OF CHEMISTRY

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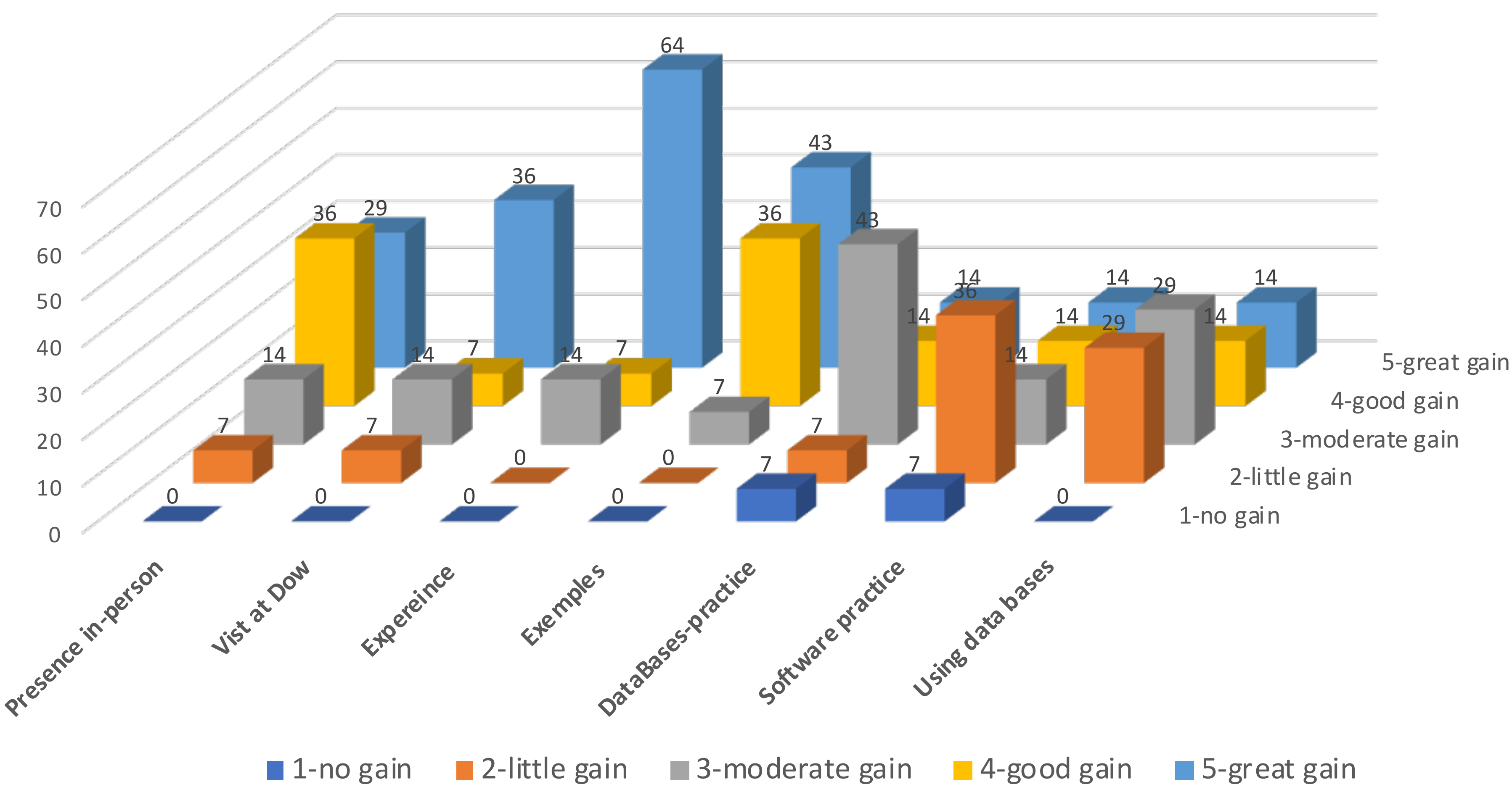
Experts in the classroom: students' perceived effect on thier own learning



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Students' own perception on what SKILLS they gained by taking this class

"I feel like the biggest skill I gained is my ability to talk about issues in toxicology. I'm now more equip to discuss and understand chemicals and how they affect health and environments."

"I found the case studies and journal critiques to be very helpful in applying what was learned in lecture to form my own opinions on the toxicity of various compounds."

"I have gained skills in analyzing chemical properties to understand toxicity. I also learned how to look for articles on chemicals of concern."

"Using chemical/physical properties to gain insight to the toxicity of a chemical."

Manuscript in preparation

Students' own perception on what SKILLS they gained by taking this class

"Understanding different things that need to be considered in order to evaluate the toxicity of a chemical (hazard and risk)."

"Became more aware of the resources available through databases."

"I have gained skills in analyzing chemical properties to understand toxicity. I also learned how to look for articles on chemicals of concern."

"How to use Microsoft Excel"

"I know how to use several modeling tools"

"Using chemical/physical properties to gain insight to the toxicity of a chemical."

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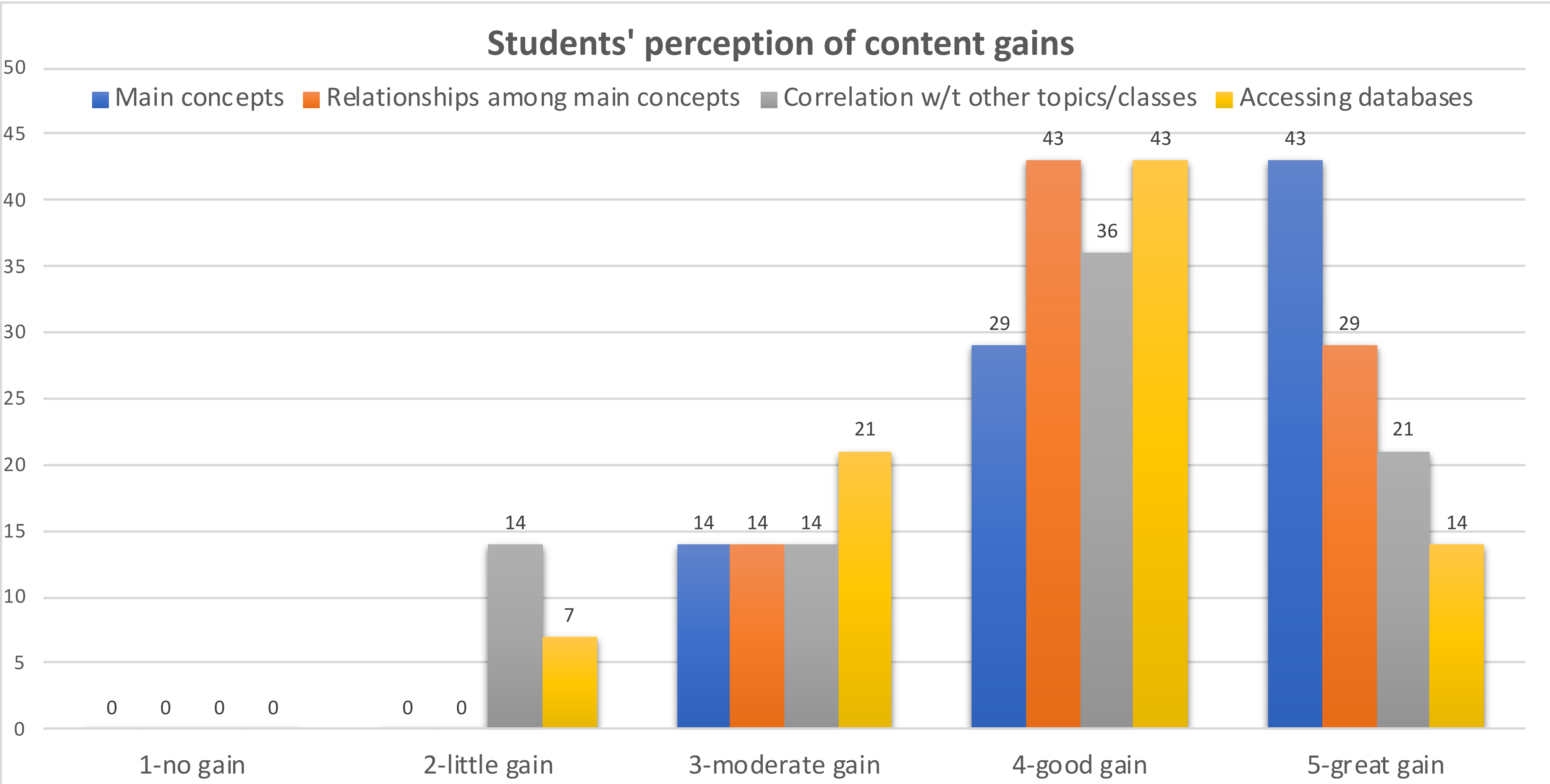


Manuscript in preparation

Students' thoughts at the end of the course

- The enthusiasm and how personal the Dow speakers were made learning about your work even that more interesting
- Being able to learn about individual areas of toxicological research from people who work in the field was very cool, and completely unlike any other classroom experience I've ever had.
- I felt very fortunate to have the opportunity to learn about toxicology from the professionals who work in the field every day.
- I feel like I have a much better knowledge of toxicology now and I am better prepared to make smart choices both as a consumer, and as a future scientist

A discussion: Part 1!

Use the post-it notes to identify 1 of each:

Successes: (Yellow post-it) Something you are doing now, or can do now within your courses/research/activity

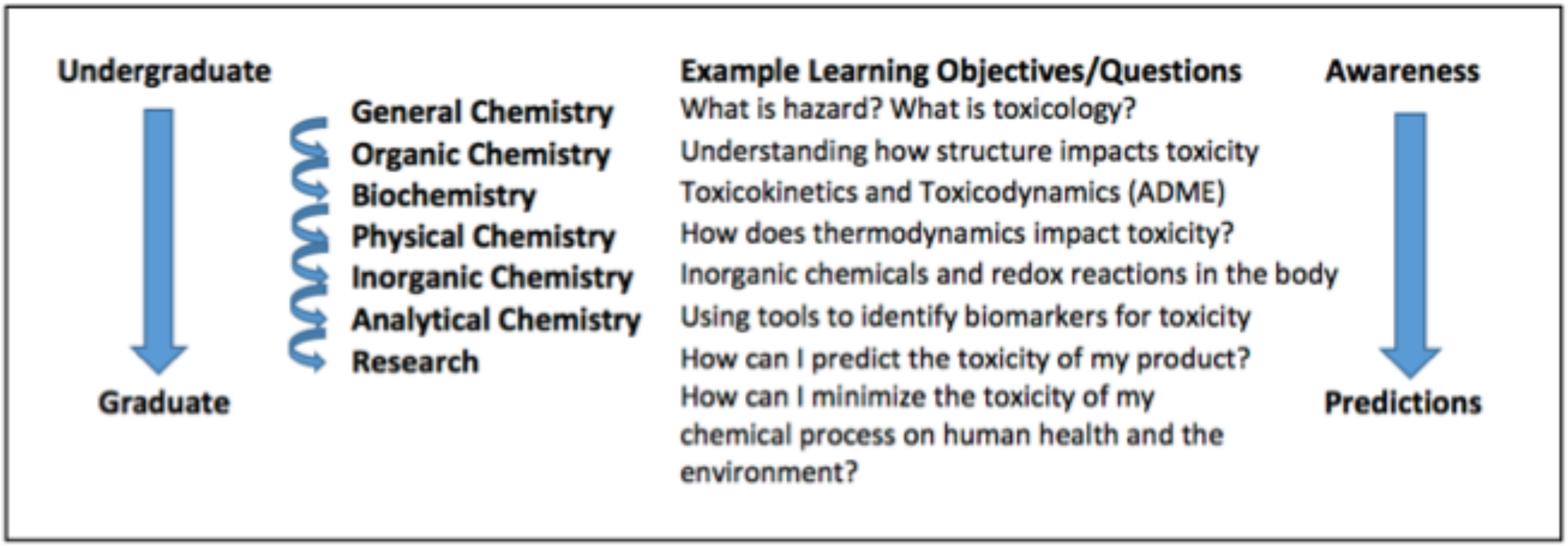
Challenges: (Pink post-it) What are your biggest barriers/challenges? Or, what do you need help with?

Toxicology Working Group

- Addressing the knowledge gap of toxicology and understanding molecular hazards in the chemistry curriculum
- Comprised of Green Chemistry Commitment signers & outside stakeholders
- Collaborate with industry experts
- Generate open-access curricula and case studies linked to chemistry concepts
- Organize Symposia and Workshops
    - Green Chemistry & Engineering Conference, June 18 – 20, 2017
    - BCCE, Toxicology Workshop July 30, 2018 AM

http://www.beyondbenign.org/he-toxicology-for-chemists/

Toxicology Working Group



http://www.beyondbenign.org/he-toxicology-for-chemists/

ACS Anchoring Concepts

- ACS: Anchoring Concept maps
  - General, Organic, Inorganic and Physical Chem.

- ACS GCI working with ACS Exams institute to link concept maps to green chemistry (and toxicology)

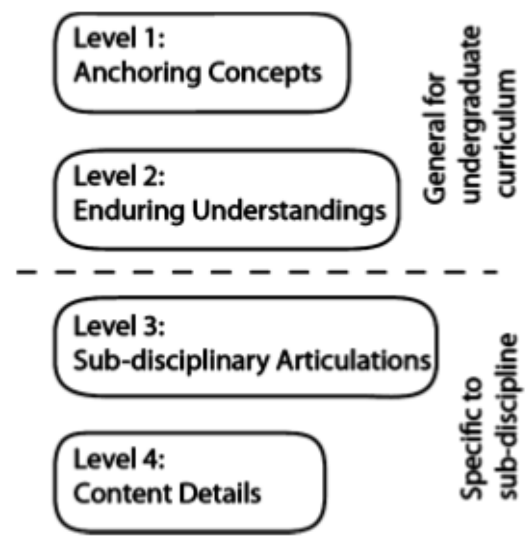


Figure 1. Levels of the ACCM depicting the consistency of the top two levels and the specialization of levels 3 and 4.

Holme, T., Raker, J., Murphy, K., J. Chem. Ed., 2013, 90, 1443-1445

Holme, T., Luxford, C., Murphy, K., J. Chem. Ed., 2015, 92(6), 115-116

Marek, K., Raker, J., Holme, T., Murphy, K., J. Chem. Ed., 2018, 95(2), 233-237

Holme, T., Reed, J., Raker, J., Murphy, K., J. Chem. Ed., 2018, 95(2), 238-241

ACS CPT Green Chemistry Supplement

- ACS CPT guidelines
  - Green Chemistry in the Curriculum – Approved March 2018!!
  - Conceptual topics (4), along with illustrative examples for general, analytical, biochem, inorganic, organic & physical

Conceptual Topics (2 of the 4 are listed):

- The best approach to developing new chemical products and syntheses:
  - Is guided by the principles of green chemistry and life cycle thinking in order to minimize harm.
  - Employs ***molecular design for reduced hazards*** to the environment, health, and safety. It is a fundamental responsibility of chemists to design and synthesize safer chemicals.
  - Analyzes impacts throughout the lifecycle, from feedstock to end of final life using appropriate metrics.
  - Uses available knowledge and ***computational tools to design for function in concert with predicting hazards and environmental fate***.
- Relationships between ***molecular structure and predicted properties*** such as metabolism, rates of chemical or biodegradation, and fate in the environment can be used for rational design of chemicals with reduced negative impact.

https://www.acs.org/content/dam/acsorg/about/governance/committees/training/acsapproved/degreeprogram/green-chemistry-in-the-curriculum-supplement.pdf

T O X / O R G O	EXPOSURE; routes of transport across membranes; Risk assessment	REACTIVE TOXICITY; higher reactivity-> higher hazard; MoA; AOP	Bio- & chemical transformations; METABOLISM; metabolites, AOP and MoA	DEGRADATION Accumulation Persistence; DESIGN for (i)Degradation (ii) toxicity
BONDING: (i)intermolecular forces (ii)chemical bonding	physical properties: MW, Polarity, solubility, pKa-skin irritation (benzyl alcohol), pH, Kow, etc: 4A2a; 4A3a, b-observable properties; 4B1-hydrophilicity&size; 4D&4E-solvents	2A1-HOMO-LUMO gap; 3.2.a-acid strength; pH: EtOH. Fetal& embrionic pH vs mothernal pH.	Biodegradation vs. persistence; 2A1-ex HFC; abiotic fate & transport	physical properties; volatility-ex HFC; solublity-2A1; quaternary carbons, Lipinski's rules; design for degradation DfD
Structure vs. Function/Activity CHEMICAL REACTIVITY Acid-base rxns Equilibrium	3A1-physical properties; 3B2-molecular shape-chirality; 3E2-Chemical rxns: regio & stereo selectivity /specificity	E, Nu, R; SAR; QSAR; ECOSAR ; 5A1-4; 5D1-4; 5G1-2; structural alerts (Matt Slide); 3F1-functional groups & allosters; 3G1a-periodic trends& steric effects-allosters; ex-EAS; rxn to carbonyls; 5Bc-SN2@allyl & benzyl-mustard gas	MoA/MIE and KE; metabolism, metabolites metanbolones effect =, +, -; carcinogenicity, teratogenicity, endocrine disruptors, neorotoxicity; byproduct of metabolism and their toxicity; 3B2a-thalidomide	ex: PFAS/PFOS; pesticides; laundry detergents
RXN MECHANISMS: kinetics & thermodynamics; intermediates; equilibrium	abiotic fate and transport	toxi/pharmaco-kinetics; 7A1-fast&slow rxn (Rates for liver metabolism of MeOH EtOH), pKa/pH-intemediats, MoA, KE; 7B-reactive species; 7E1-silicons (Sue); mechanistic studies via isotop lableing	AOP; cellular sites for reactions; MIE & KEs; 7B-Electrophilic rxns; 7E1-Michael additions; Endocrine disruptors-dioctylsulfosuccinate(deep WaterHorizon cleaning); SN1&SN2;	design for toxicity: insecticides, pesticides, drugs (ex antibiotics)

Anchoring Toxicology Concepts to Organic Chemistry

Case studies:

- **Relationship Between pKa and Skin Irritation**
- **Design for Biodegradability**
  - Design Rules
  - Electrophilic Aromatic Substitution
  - Alkanes: nomenclature and isomers
- **Bond strength and persistence**
- **Chirality**
- **Electrophilic-Nucleophilic Reactions**

https://www.beyondbenign.org/cur-he-toxicology/

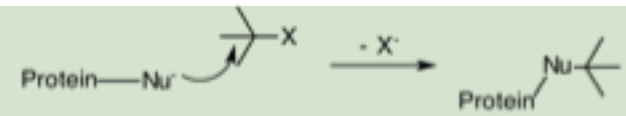
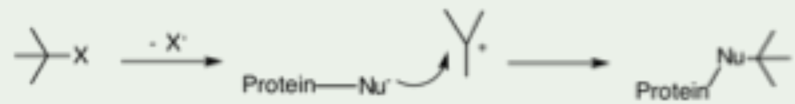
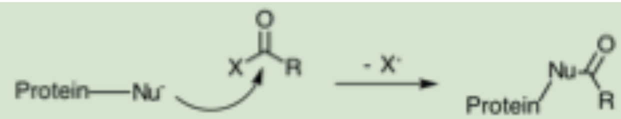
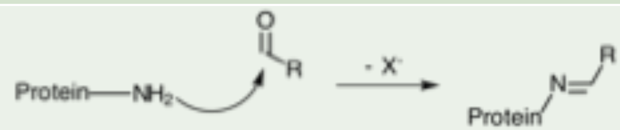
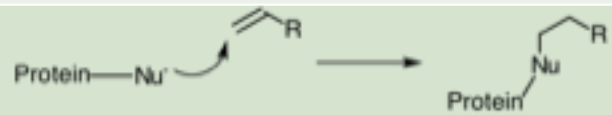
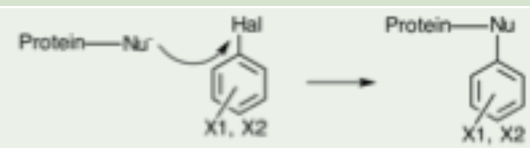
Electrophilic-Nucleophilic Reactions

Organic Chemistry Concepts:

- Electrophiles and Nucleophiles
- Reactions (SN1, SN2, Acylation, Michael Addition, Schiff Base Formation, SNAr)

Toxicology Concepts:

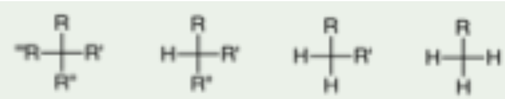
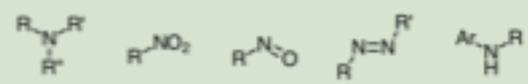
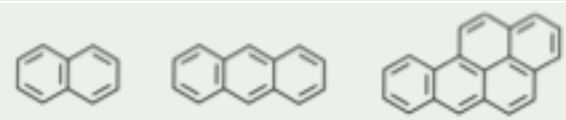
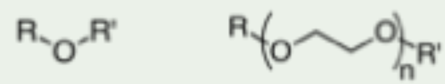
- DNA and protein binding
- Toxicological reaction mechanisms

Mechanism	Protein Binding Reaction
SN2	
SN1	
Acylation	
Schiff Base Formation	
Michael Addition	
SNAr	 X = electron withdrawing groups (NO2, CN, etc.)

Measurement and Estimation of Electrophilic Reactivity for Predictive Toxicity, Cronin, M.T.D., et. al., Chem. Reviews, 2011, 111, 2562-2596.

https://www.beyondbenign.org/lessons/electrophilic-reactions/

Design for Biodegradability

Feature	Structure
Halogens: Especially chlorine and fluorine and if more than 3 in a molecule	R–X
Chain branching if extensive: Quaternary C's are problematic	
Tertiary amine, nitro, nitroso, azo, and arylamino groups	
Polycyclic aromatic residues	
Heterocyclic residues	
Aliphatic ether bonds (except in ethoxylates)	

https://www.beyondbenign.org/lessons/design-for-biodegradability/

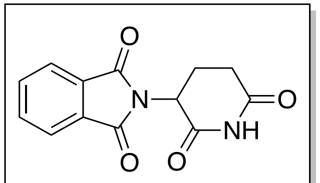
Chirality

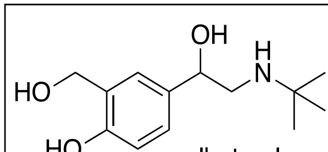
Organic Chemistry Concepts:

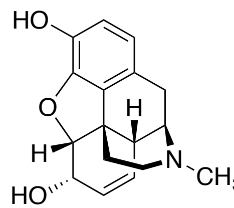
- Chirality
  - Identify chiral center
  - How many stereoisomers?

Toxicology Concepts:

- Structure and function







Toxicity: a dash or a wedge?

Recommended readings: section 4.2.1.1, page 5851* about the toxicokinetics and toxicodynamics of Thalidomide's R and S enantiomers. List the differences between the two enantiomers in their toxicity and efficacy.

S. Biros & D. Kovacs , Grand Valley State University

*Voutchkova, Adelina M.; Osimitz, Thomas G.; Anastas, Paul T. "Toward a Comprehensive Molecular Design Framework for Reduced Hazard" *Chem. Rev.* **2010**, *110*, 5845-5882.

https://www.beyondbenign.org/lessons/chirality/

Textbooks:

- Essentials of Toxicology: The Basic Science of Poisons- Casarett & Doull’s
- Mechanistic Toxicology - Urs A. Boelsterli, CRC Press
- Toxicological Chemistry and Biochemistry - Stanley Manahan (CRC Press, 2003)
- and more!

Additional resources

- MoDRN resources: https://modrn.yale.edu/
  - Open access curriculum resources
  - Youtube videos by Yale (Dr. Paul Anastas) on green chemistry/toxicology
- NIH ToxTutor: https://toxtutor.nlm.nih.gov/
  - Self-paced open access tutorial on toxicokinetics, toxicodynamics and introductory toxicology concepts
- Toxicity testing in the 21st century: A vision and strategy,

The National Academy of Sciences. Engineering , Medicine. https://www.nap.edu/download/11970

- Coursera course: **Toxicology for the Twenty-First Century/Coursera, Johns Hopkins** **https://www.coursera.org/learn/toxicology-21/lecture/KOsqI/toxicology-for-the-twenty-first-century**

Additional resources, cont.

- TOX21: A New Way to Evaluate Chemical Safety and assess risk

https://youtu.be/vKhn1HRXgn8

- Predictive toxicology: Chemical Categories and Read-Across

Category formation, grouping and read across methods are broadly applicable in toxicological assessments and may be used to fill data gaps for chemical safety assessment and regulatory decisions: A strategy for structuring and reporting a read-across prediction of toxicity q T.W. Schultz, P. Amcoff, E. Berggren, F. Gautier, M. Klaric, D.J. Knight, C. Mahony, M. Schwarz, A. White, M.T.D. Cronin Regulatory Toxicology and Pharmacology 72 (2015) 586–601

JRC report - EUR 22941 EN (October 2007)

https://eurl-ecvam.jrc.ec.europa.eu/laboratories-research/predictive toxicology/background/chemical-categories-and-read-across

A discussion: Part 2!

1) Any additional ideas? Add any ideas for successes (or soon to be successes) and challenges!
2) Make a match – can you match a challenge/barrier with a success?

Successes: (Yellow post-it) Something you are doing now, or can do now within your courses/research

Challenges: (Pink post-it) What are your biggest barriers/challenges? Or, what do you need help with?

Thank you!!

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Dalila's notes June 12

- 1 min/slide = 31min. Is it realistic? Probably—if more time left, better!
- 9 min for activity & conversation. Maybe 3min at the mid point and the rest 5-6 min, at the end. Could we 'bribe' somebody (Saskia, for example or Pam) to give a point about what she/her organization could do? Anybody else who might be wiling to "stir' the conversation?
- I am debating the sticky notes…are we going to have white board?

If the room is not conducive to interaction, if people have to move along a row of chairs, it might be difficult.

Goal:
The four stages of competence

http://www.gordontraining.com/free-workplace-articles/learning-a-new-skill-is-easier-said-than-done/

	Level	You…
1	Unconscious incompetence	don't know what you don't know
2	Conscious incompetence	realize you don't have adequate knowledge
3	Conscious competence	are able to function safely and effectively
4	Unconscious competence	are very knowledgeable and experienced regarding the subject at hand

The goal of this course in teaching introductory toxicology is to ***bring all students from level 1 to level 2*** *and* aim for the majority of them to reach level 3, conscious competency.

Course design
sustainable and ***adaptive***

We are currently at:

- submission of course approval
- designing the course materials
- advertising to students

Experiment-→ Winter 2018