MS Program in Environmental and Green Chemistry at GWU

Prof. Jakub Kostal

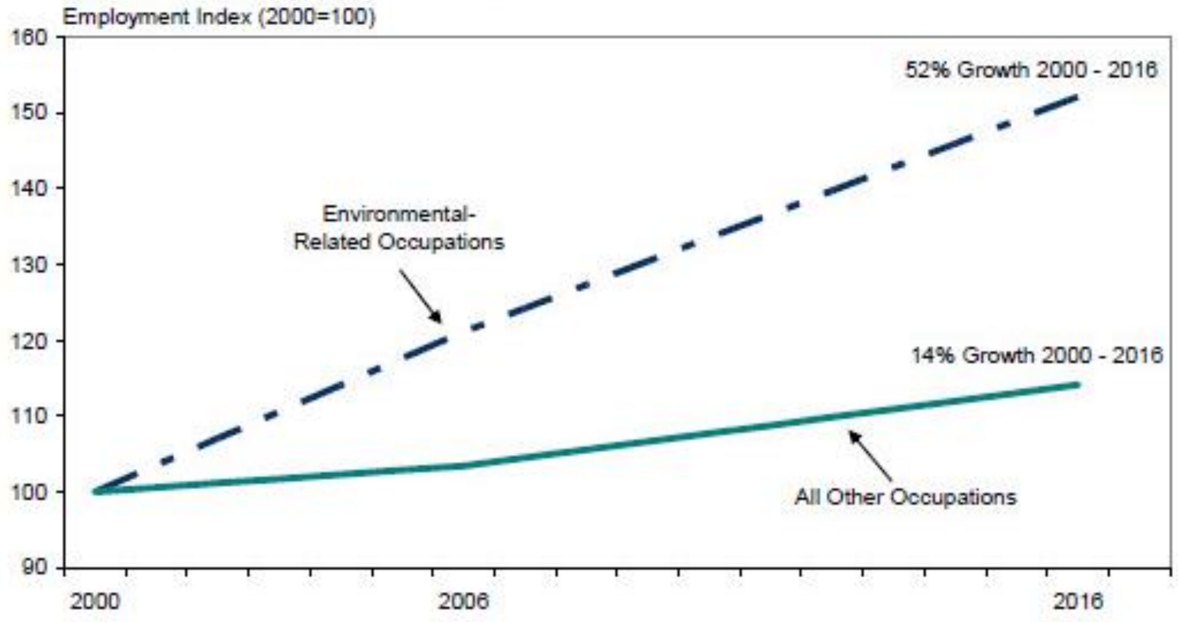
April 26, 2016 2 – 3 PM EDT

The Green Chemistry Education Webinar Series

The Green Chemistry Commitment
TRANSFORMING CHEMISTRY EDUCATION

Assessing the need

- Sustainability and 'Green' Jobs are a growing industry



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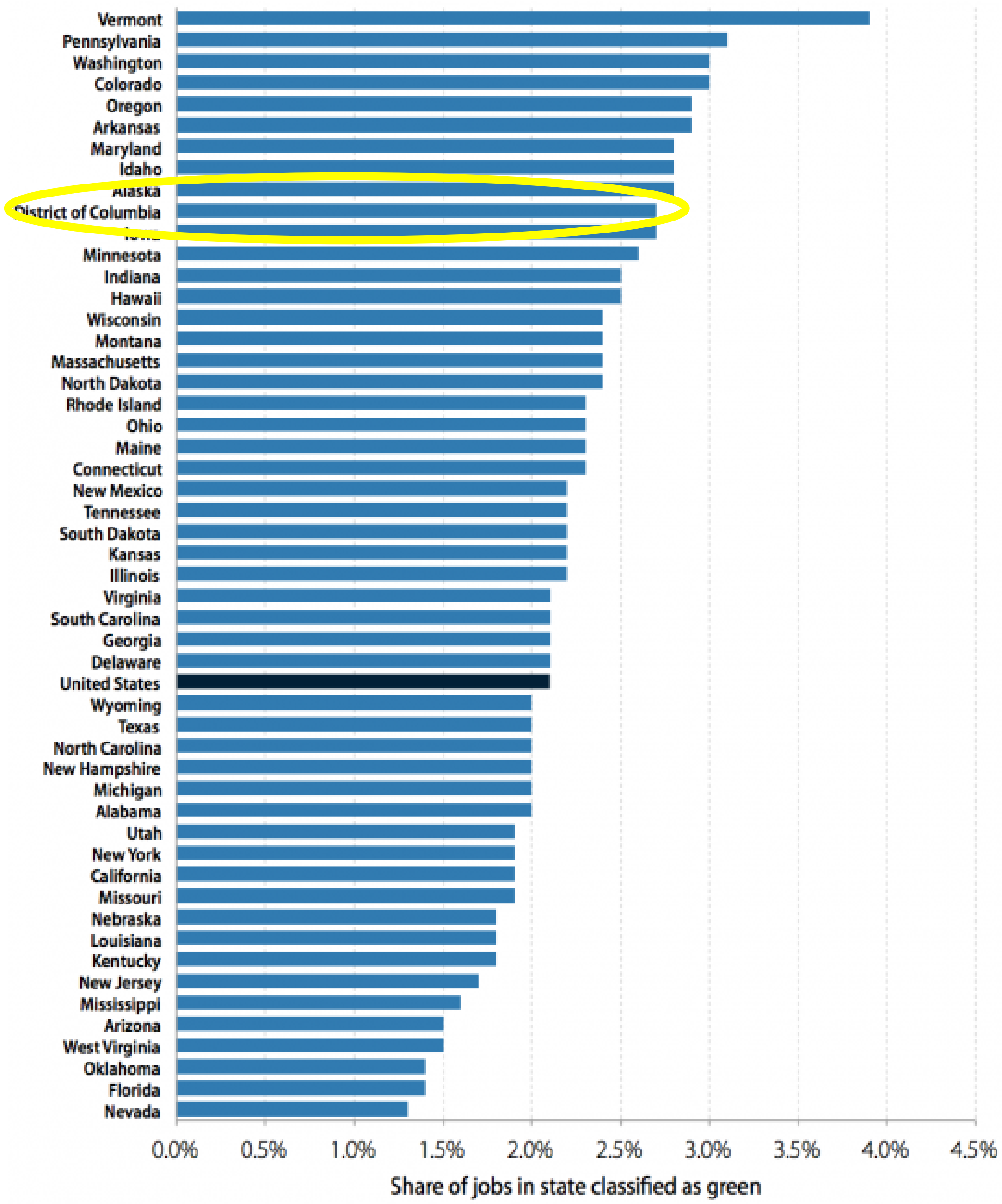

Program description

- 30-credit hour MS program
- 5 core focus areas: energy, environmental analytical chemistry, air/water chemistry, green chemistry processing and green toxicology
- Interdisciplinary, in close collaboration with:

  GWU School of Public Health, School of Public Policy and Administration and School of Engineering and Applied Sciences
- Highly customizable curriculum to suit personal needs and goals
- Housed by Chemistry department

Core courses: 1. Energy and the Environment

- Fundamentals of energy conversion
- Fossil fuel, hydrogen, nuclear and renewable resources systems
- Fuel reforming, hydrogen and synthetic fuel production, fuel cells and batteries, combustion of fossil and bio-derived fuels, hybrids, catalysis, supercritical and combined cycles, photovoltaics, etc.
- Energy storage and transmission
- Source utilization and fuel life cycle analysis

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2. Environmental analytical chemistry

- Advanced modern analytical methodology
- Analytical instrumentation, remote measurements, trace atmospheric constituents, uncertainty analysis, pollutants in air/water/soil and biota, heavy metals and radionuclides
- Emphasis on priority pollutants according to US regulatory agencies

3. Environmental chemistry of water, air and soil

- Behavior, movement and impact of chemicals in air, water and soil
- Chemistry of environmentally important cycles

→ Human factors: acid raid, sewage treatment, ozone destruction, climate change, air pollution and euthrophication

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4. Green chemistry processing

- Design principles for greener technologies
- Challenges and trade-offs in shifting production toward renewable technologies
- Social and technical factors affecting adoption of ‘greener’ solutions
- Focus on real-world case studies

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5. Green Toxicology

- Basic tools and paradigms of predictive toxicology

  medicinal chemistry principles
  computational chemistry/biology methods

  QSARs, expert systems, read-across

  spectroscopic tools
- Focus on strategies for safer chemical design

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Capstone project

- A group-based project in partnership with an external partner/client or a participating Chemistry Department faculty member.

External partners/clients for capstone projects
Government agencies: e.g. EPA, DoE, FDA, NIH, NIEHS;
NGOs: e.g. Environmental Defense Fund; Environmental Working Group; Natural Resources, Advancing Green Chemistry, Clean Production Action, BizNGO, Lowell Center for Sustainable Production;
Private sector organizations: e.g. Seventh Generation, Dow, DuPont, ToxServices, SciVera
Industry groups/ roundtables: e.g. GC3 Council, American Chemical Society, Institute for Green Chemistry
Academic partners: e.g. Berkeley Center for Green Chemistry, Yale Center for Green Chemistry, GreenCentre Canada.

CHEM 6283
Chemical Toxicology and Rational Design of Safer Chemicals
Spring 2017

- Class materials:

  Chasing Molecules: Poisonous Products, Human Health, and the Promise of Green Chemistry, E. Grossman (2011)

  Mechanistic Toxicology: The Molecular Basis of How Chemicals Disrupt Biological Targets, Second Edition, Urs A. Boelsterli (2007)

  Cradle to Cradle: Remaking the Way We Make Things, M. Braungart (2002)

  Voutchkova, A. M.; Boethling, R. and Anastas, P. (Editors). <u>Designing Safer Chemicals</u>, Volume 9 of Handbook of Green Chemistry Series. Wiley-VCH 2012.

  Cronin, M. T. D. and Madden, J. C. (Editors). <u>In silico Toxicology.</u> <u>Principles and Applications.</u> RSC Publishing 2010

Learning Objectives

- Understand toxicological impact of the chemical industry in a historical context
- Use toxicological data for hazard assessment
- Use mechanistic toxicology to identify relevant structural features in chemicals and link them to biological effects
- Understand the tenets of risk assessment (hazard vs. exposure) and life-cycle analysis
- Use computational tools and metrics to evaluate and compare hazard profiles
- Design chemicals that are 'safe' with respect to several toxic endpoints

Course description:

1. **Chemical industry and case studies of chemicals of concern**
    a. BPA
    b. Phthalates
    c. Flame retardants

2. **Mechanistic toxicology: Modes of action of chemical classes**
    a. Connecting reactivity *in chimico* and *in vivo* with focus on electrophilic chemicals
    b. Alkanes, alkenes, alkynes
    c. Epoxides
    d. Benzene
    e. Polyaromatic hydrocarbons
    f. Polybrominated aromatics

3. **Toxicology for chemists**
    a. General principles: dose response curves, statistical methods
    b. Mechanistic toxicology – toxicokinetics and toxicodynamics
    c. Toxicogenomics
    d. Absorption, Distribution, Metabolism and Excretion
    e. Ecotoxicology

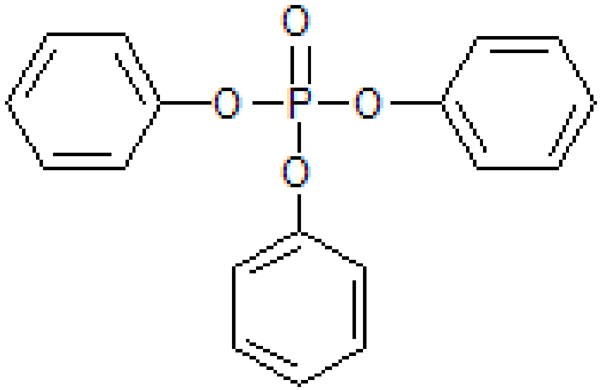
4. **Types of toxicological data**
    a. Overview of types of toxicological testing - models, tools, terminology and limitation
    b. Acute vs chronic
    c. Endpoints
        i. *In vivo assays – fish*
        ii. *In vivo assays – small mammals*
            *Assay-t*ox models - (including what is an assay)
    a. Data sources and data quality
    b. Overview of non-animal testing - what is an assay?
    c. In vitro methods
    d. High throughput screening
    e. TOXCAST and other data sources

5. **Risk Assessments vs Alternatives Assessment**
    a. Hazard vs exposure
    b. What is a risk assessment?
    c. Steps in carrying out a risk assessment
    d. Overview of an AA and its components
    e. Define a chemical hazard assessment
    f. Data gaps exist for existing chemicals

6. **Modeling and Predicting Toxicity**
    a. Quantitative Structure Activity (Toxicity) Relationships
    b. Statistical methods used in QSAR and QSTR analyses
    c. Computational methods used to predict toxicity
    d. Automated Rule Induction Systems
    e. Knowledge-Based Expert Systems
    f. Rea-across approaches
7. **Regulation and Policy**
    a. EPA and TOSCA, EU and REACH
    b. Pesticides
    c. Chemicals in food and cosmetics

8. **Global Hazards**
    a. Review of atmospheric chemistry: aerosols, greenhouse gases, climate change
    b. Introduction to aquatic chemistry
    c. Terrestrial environmental concerns
        i. Persistence
        ii. Soil pollution
9. **Chemicals in water**
    a. Organic chemicals and pharmaceuticals in municipal water and environment
    b. Biodegradation of pharmaceuticals
    c. Catalytic systems for degradation of organics
    d. Alternative methods for extraction: reverse osmosis
10. **“Green” nanotechnology**
    a. Modes of action of nanoparticles
    b. Evidence of toxicity
    c. Designing a safer nanoparticle
11. **Principles for designing safer chemicals**
    a. Design guidelines for minimizing bioavailability
    b. Design guidelines for minimizing mutagenicity
    c. Design guidelines for minimizing aquatic toxicity
12. **Designing for biodegradability**
    a. Biodegradation by functional group
    b. Design guidelines
    c. Cradle to cradle

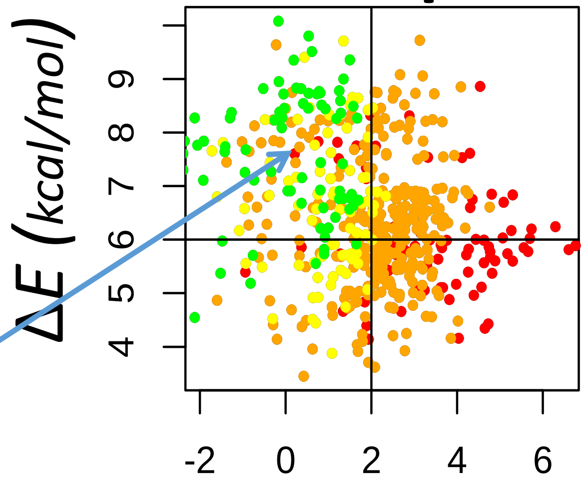
Case Study



LC50 (Fathead minnow, 96hr): 0.87 mg/L

Design guidelines for aq. tox.

Fathead minnow
LC_{50}, 96-h assay
U.S. E.P.A.
555 chemicals



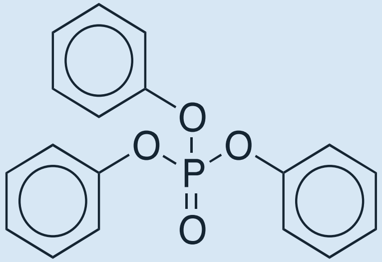
“safer chemical space”: log$D_{o/w}$ <1.7, Δ*E*>6 eV

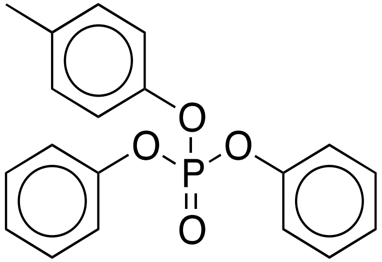
<1 mg/L < 0.0067 mmol/L	1–100 mg/L 0.0067 - 1.49 mmol/L
100–500 mg/L 1.49-3.32 mmol/L	> 500 mg/L >3.32 mmol/L

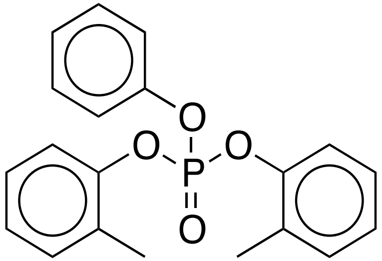
Safer chemical design guidelines:
ΔE = 6.62 eV and logD = 5.09 → not SAFE to aquatic species

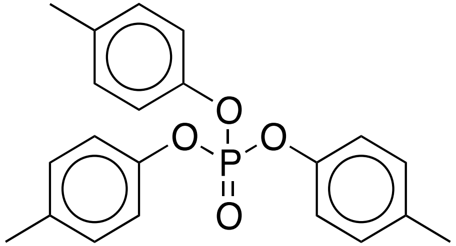
Suitable alternatives?

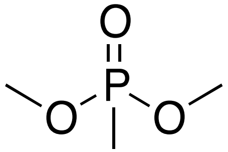
TPP:

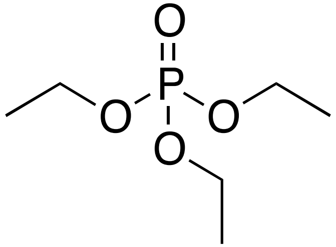


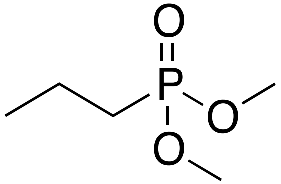


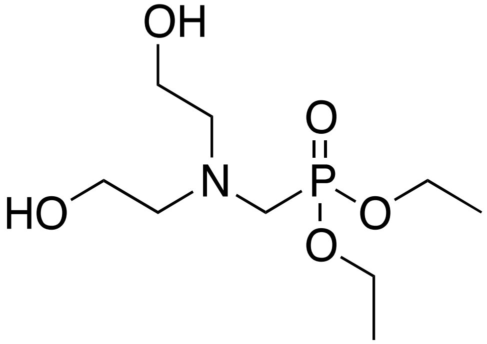






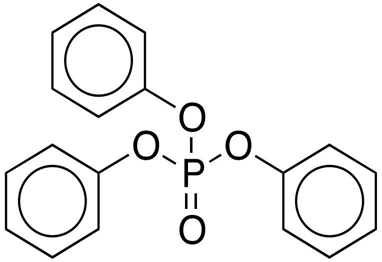




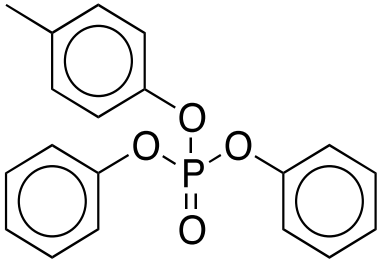


Suitable alternatives with similar functionality?

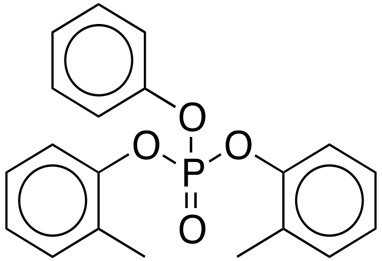
TPP:



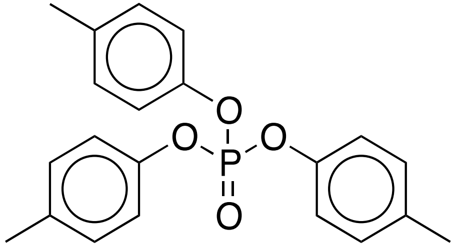
ΔE = 6.6 eV, logD = 5.1



ΔE = 6.4 eV, logD = 5.6

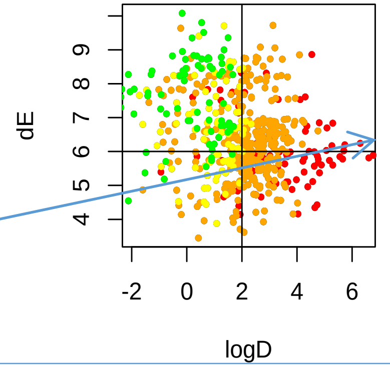


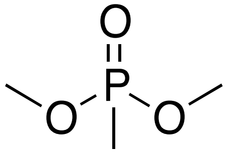
ΔE = 6.5 eV, logD = 6.1



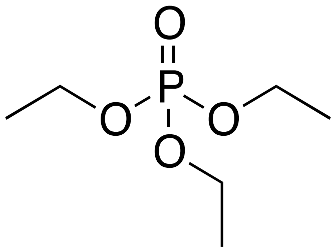
LC50: 0.25 (High tox)

ΔE = 6.4 eV, logD = 6.6



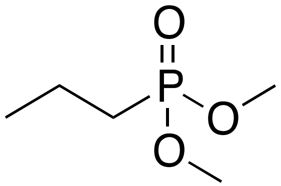


ΔE = 8.6 eV, logD = -0.11

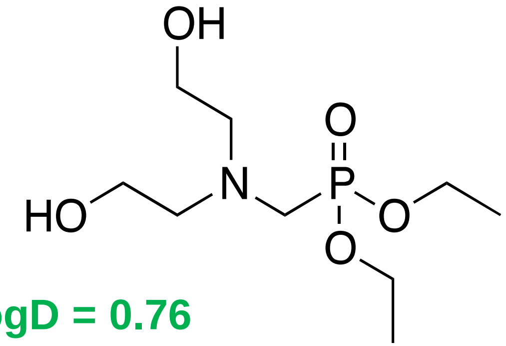


ΔE = 8.8 eV, logD = 1.2

LC50: 350 (low/no tox)

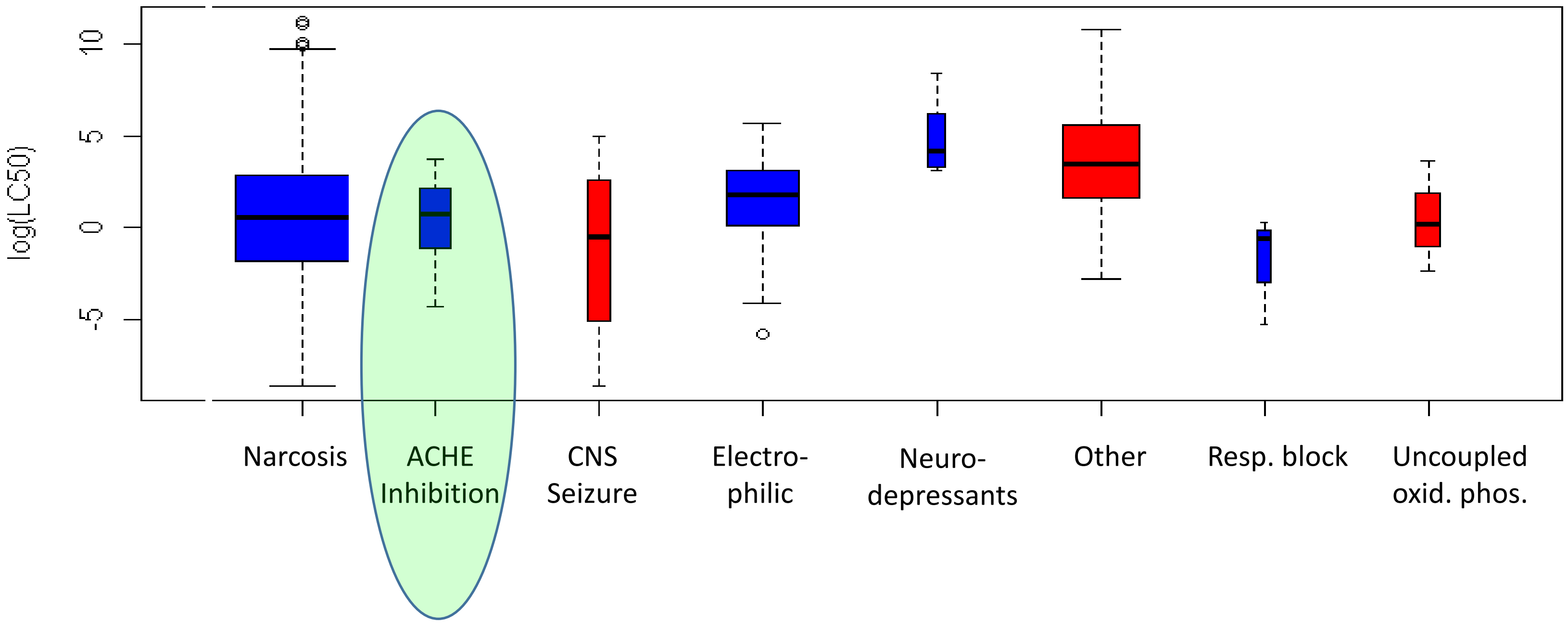


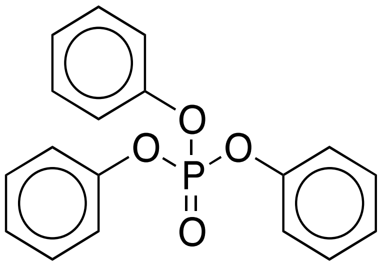
ΔE = 8.5 eV, logD = 0.76



ΔE = 8.5 eV, logD = -0.52

Designing safer OP compounds for specific endpoints:





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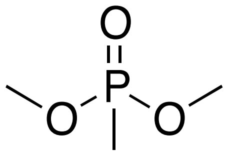
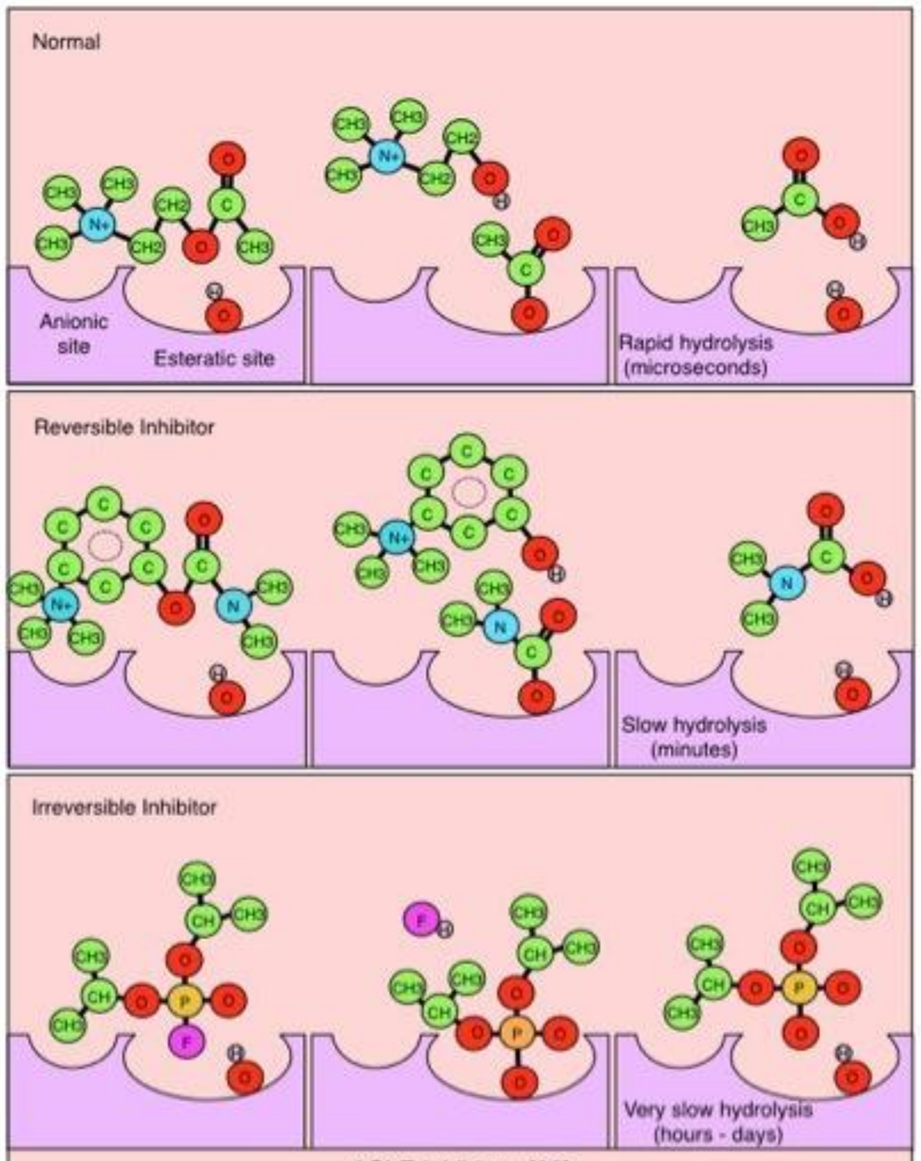
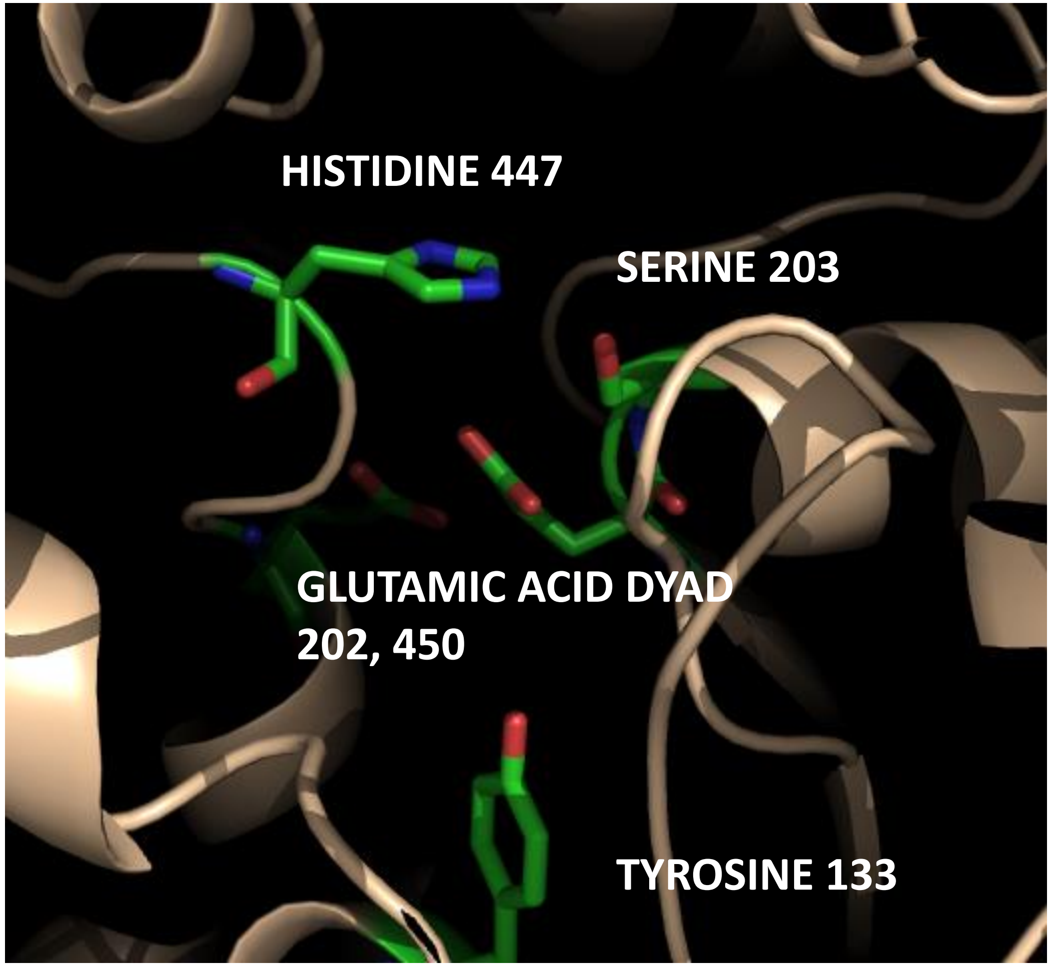


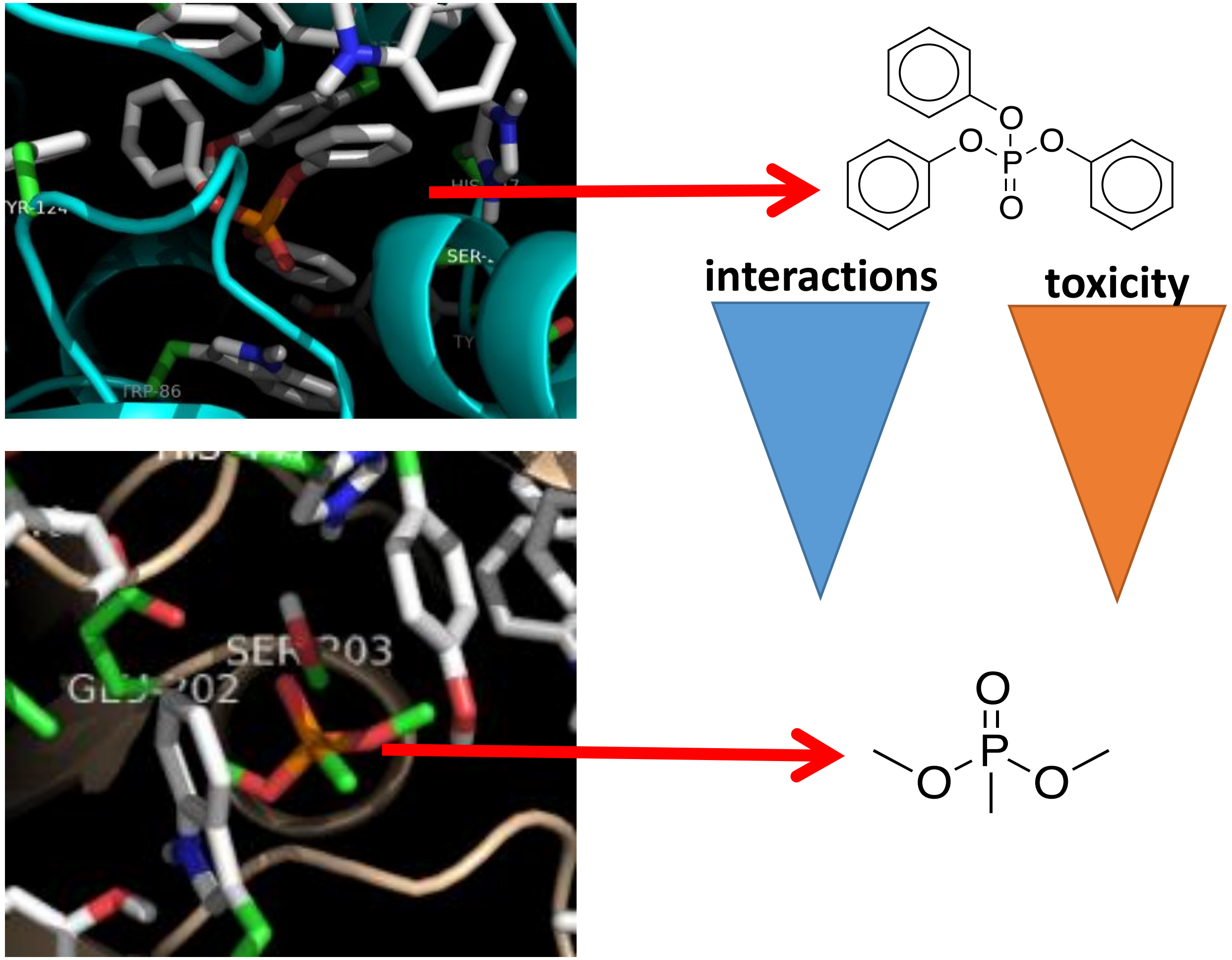


AChE Inhibitors [22]

http://en.wikipedia.org/wiki/Acetylcholinesterase

Active site of AChE: Binding affinity of OPs





Admission requirements

- GRE scores
- bachelor's degree in science or engineering (GPA of 3.0 or above)

At minimum, candidates must have completed:

- Two semesters of general chemistry
- Two semesters of organic or inorganic chemistry
- One semester of quantitative and/or instrumental analysis (recommended)

Supporting Documents Required:

- Official transcripts from all post-secondary institutions attended
- 2 letters of recommendation
- Resume/CV
- Personal Statement

For International students

- Minimum TOEFL scores: 85
- Minimum IELTS score: 6.5

Contact Info

Department website (application link):
https://chemistry.columbian.gwu.edu/ms-environmental-and-green-chemistry

(Application deadline April 1 – Fall semester, October 15 – Spring semester)

Financial Aid:
https://chemistry.columbian.gwu.edu/graduate-student-admissions-and-financial-aid

Further inquiries:
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Michael King (chair), mking@gwu.edu