Welcome to the CLU-IN Internet Seminar

Improved Process for Identifying, Prioritizing and Addressing Emerging Pollutants

Sponsored by: Superfund Research Program

Delivered: March 25, 2010, 2:00 PM - 3:30 PM, EDT (18:00-19:30 GMT)

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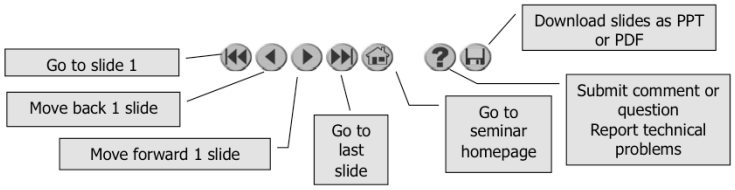
Housekeeping

- Please mute your phone lines, Do NOT put this call on hold
- Q&A
- Turn off any pop-up blockers
- Move through slides using # links on left or buttons



- This event is being recorded
- Archives accessed for free **http://cluin.org/live/archive/**

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Although I'm sure that some of you have these rules memorized from previous CLU-IN events, let's run through them quickly for our new participants.

Please mute your phone lines during the seminar to minimize disruption and background noise. If you do not have a mute button, press *6 to mute #6 to unmute your lines at anytime. Also, please do NOT put this call on hold as this may bring delightful, but unwanted background music over the lines and interupt the seminar.

You should note that throughout the seminar, we will ask for your feedback. You do not need to wait for Q&A breaks to ask questions or provide comments. To submit comments/questions and report technical problems, please use the ? Icon at the top of your screen. You can move forward/backward in the slides by using the single arrow buttons (left moves back 1 slide, right moves advances 1 slide). The double arrowed buttons will take you to 1st and last slides respectively. You may also advance to any slide using the numbered links that appear on the left side of your screen. The button with a house icon will take you back to main seminar page which displays our agenda, speaker information, links to the slides and additional resources. Lastly, the button with a computer disc can be used to download and save today's presentation materials.

With that, please move to slide 3.

Seminar & Workshop Motivation

- Future versus legacy sites
- Proactive versus remediative
- Specific contaminants of concern
- Tools for measurements and judgments
- Initiate an on-going process

Expertise and Input

David Sedlak*
Derek Muir *
Deb Swackhamer *
Eric Weber *
Mort Barlaz
Heather Henry

Bob Arnold
Lee Ferguson
Jennifer Field
Ed Furlong
John Giesy
Rolf Halden
Tala Henry
Ron Hites
Keri Hornbuckle
Phil Howard *
Dick Luthy
Anita Meyer
Eduardo Saez
Fred vom Saal
Chris Vulpe
Mark Wiesner

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SRP Superfund Research Program
NIEHS National Institute of Environmental Health Sciences

What makes a Superfund Site?

Superfund Site: an uncontrolled or abandoned place where hazardous waste is located, possibly affecting local ecosystems and people.

Hazard Ranking System (HRS)

- Release or likelihood of release of hazardous substances
- Characteristics of waste (e.g., toxicity, quantity)
- People or sensitive targets may be affected by release
  - groundwater migration
  - surface water migration
  - soil exposure
  - air migration

Potential for New Sites from New Chemicals

- ~87,000 chemicals in North American commerce
- ~12,000 registered pharmaceuticals and pesticides
- Only 275 compounds appear on CERCLA priority list

Likely Characteristics of "New" Superfund-Relevant Chemicals

- High Production Volume
  - surrogate assuming no specific use data
- Persistence
- Bioavailability
- Toxic
  - poses risk to human population or ecosystem
- Potential Exposure from (Waste) 'Point' Source

Getting There From Here

- Attributes
  - High/medium production volume
  - Persistence and Bioaccumulation (P&B)
  - Predictive & Computational Toxicology
  - Ecotoxicology

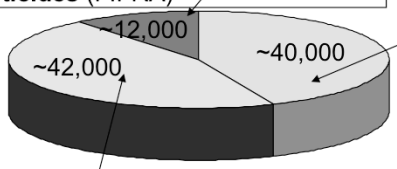
Decreasing data and tools

- Serendipity and Curiosity
- On-going Evaluation & Brain Trusts

HPV and MPV Chemicals

(> 4.5 tonne/yr USA, > 100 kg/yr Canada)

Pharmaceuticals & cosmetics (Food, Drug & Cosmetic Act)
Pesticides (FIFRA)



Polymers
- High molecular weight >>1000 Daltons
- Residuals and byproducts often not well characterized

Industrial chemicals (TSCA/CEPA)
- Individual organic chemicals, organometallics, UVCBs under TSCA and CEPA
- ~21,000 substances since 1976 or 700 new substances per year under TSCA
- Molecular weight generally <1000 and >50 Daltons (99% are organics)

Not included:
- Minor use products (<4.5t/y)
- Degradation products
- Byproducts/impurities
- Isomers/congeners

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Credit: D. Muir & P. Howard

Production Volume + P & B

1. Develop list from known HPV and MPV chemicals (i.e. USEPA TSCA IUR; Canada DSL; EINECS)
2. Use Quantitative Structure-Property Relationships (QSPRs)
3. Use scientific judgment to identify additional chemicals

Credit: D. Muir & P. Howard

QSPRs Based Selection (from 22,263)

QSPR Predicted Characteristics	No.	Notes
Predicted BCF: >1000 **Atmospheric Oxidation: >1 day, and Log K_{aw} >-5 and <-1**	105	Using EPIsuite. Mainly chemicals with predicted bioaccumulation and persistence

Prioritization of Low-Medium Production Volume based on Scientific Judgment

1. Bioaccumulation/biomagnification potential including in air-breathers – log K_{ow}, log K_{oa}
2. Persistence – molecular structures associated with slow biodegradation; adjacent halogens, cyclics, perfluorinated, cyclic siloxanes
3. Quantity in use and potential for emissions (i.e., open use or as an additive vs. as a chemical intermediate)

Further prioritization by scientific judgment	505	Out of about 11400 substances listed as LPV or MPV on TSCA IUR
Total	610	**62% halogenated** **8% siloxanes**

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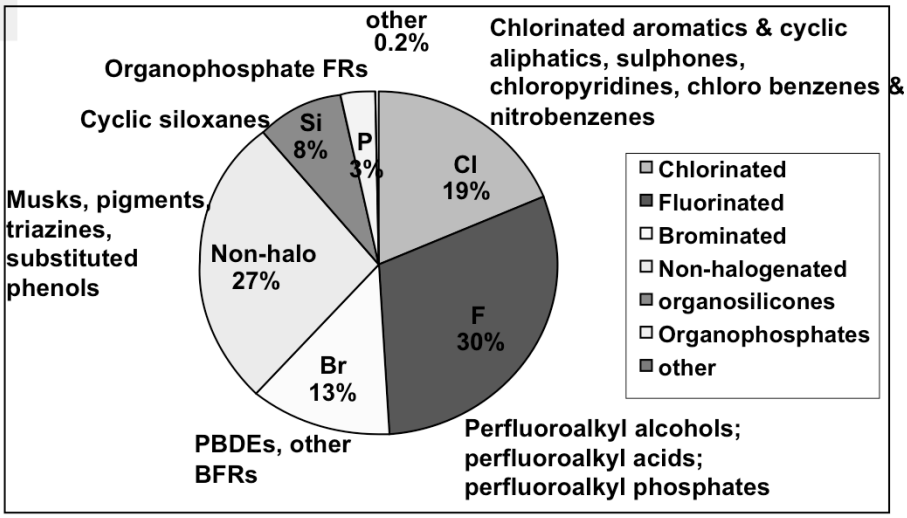
Credit: D. Muir & P. Howard

Classes of 610 Identified Priority Chemicals



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Credit: D. Muir & P. Howard

Limitations of Muir/Howard Screening Approach

- Degradation and byproducts not fully assessed
- Chemicals *within* imported products (e.g., DBDPE) not captured
- Predicted toxicity not used for prioritization
  - QSPR/QSAR model "domains" were often exceeded e.g. ECOSAR, Oncologic
- Information on uses and releases is unknown or limited
- P & B screening may not be appropriate for some important chemicals
  - Polymers – some w/ halo moieties
  - Impurities in non-P & B chemicals

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Credit: D. Muir & P. Howard

Computational Toxicology

- **Computational chemistry**: physical-chemical mathematical modeling at the molecular level
- **Molecular Biology**: application of a wide range of technologies such as genomics, proteomics, and metabolomics
- **Computational Biology:** development of molecular biology data bases and analysis of the data
- **Systems Biology:** application of mathematical modeling and reasoning to the understanding of biological systems

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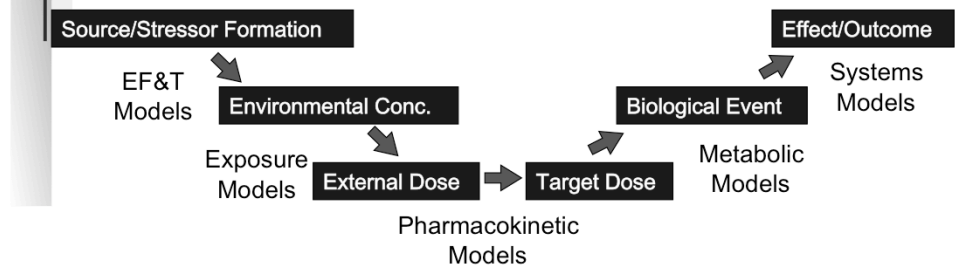
Credit: E. Weber

Source to Outcome Continuum



Primary Goal: To improve the linkages in the

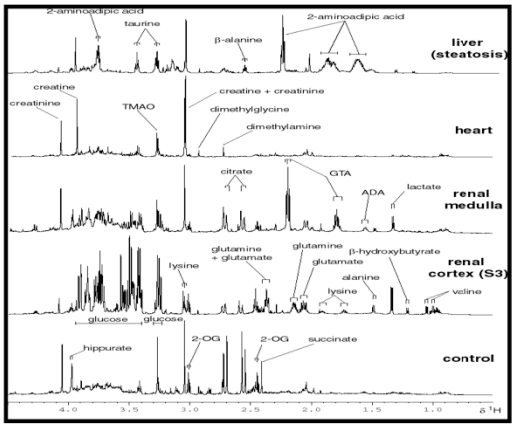
Source-to-Outcome Continuum

Uncertainty and Challenge Increases Roughly from Left to Right

Credit: E. Weber

Metabolomics

NMR Spectra of Urine Samples from Mice Treated with Tissue-Specific Toxins



Lindon, et al., 2002

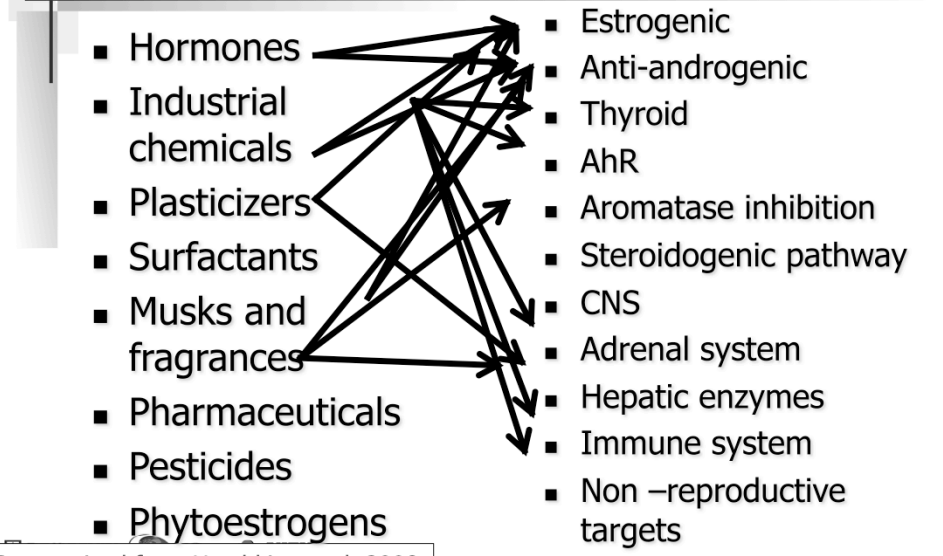
Changes in *endogenous* metabolites are specific for the toxicity site and pathway
These metabolic profiles can be used:

1) **to define toxicity pathways**
2) **as indicators of exposure (for reconstruction)**
3) **to link varying exposure scenarios (magnitude, timing, duration) to likelihood of risk**
4) **to evaluate the impact of exposure to multiple stressors (i.e., mixtures)**
5) **and much more!**

Credit: E. Weber

Ecotoxicology

Perhaps the Biggest Challenge

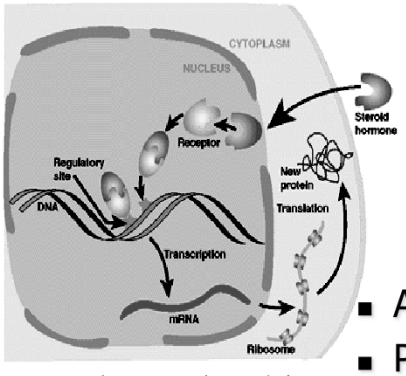


Summarized from Hotchkiss et al. 2008

Credit: D. Swackhamer

Hormone-Receptor Response

Glands direct hormone production → **Hormones bind to receptor** → **Up-regulate or down-regulate genes** → **mRNA transcription** → **Protein production or alteration**



www.ehormone.tulane.edu/

- Affects any part of cascade
- Possible non-linear dose responses

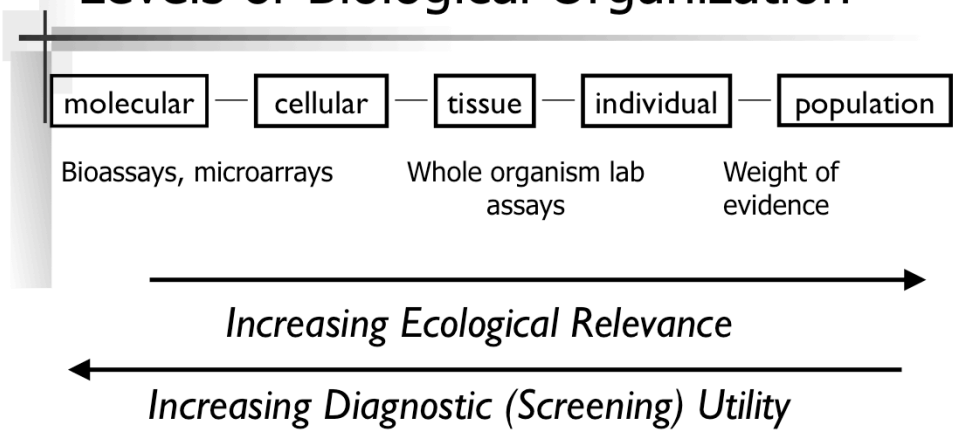
Credit: D. Swackhamer

Confounding Issues

- Any part of cascade can be affected
- Non-linear dose responses possible
- Different doses can lead to different effects
- Different species have different sensitivities and different effects to same exposures
- Different points in life cycle of same species have different sensitivities and different effects to exposure
- Exposure during development can lead to adult disease
- Some effects are transgenerational

Credit: D. Swackhamer

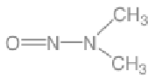
Levels of Biological Organization



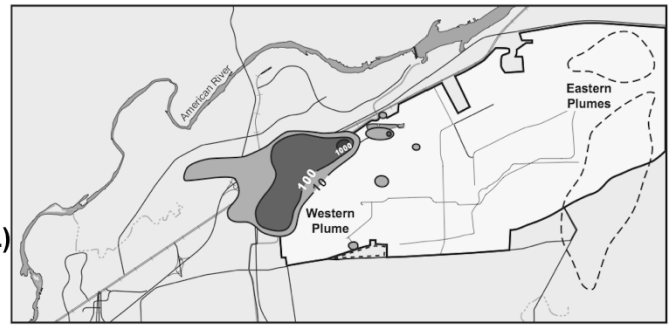
adapted from Miracle and Ankley 2005

Credit: D. Swackhamer

Serendipity and Curiosity



Aerojet Superfund Site: Sacramento, CA



Allowable conc'n
0.6 ng/L (10^{-6} risk)
10 ng/L (CA NL)

History:

- **-rocket testing site (1950-1990)**
- **-1980s: remediation for solvents (NDMA < 1,000 ng/L)**
- **-late 1990s: new analytical method (GC/CI/MS/MS)**
- **-ongoing remediation for NDMA and perchlorate**

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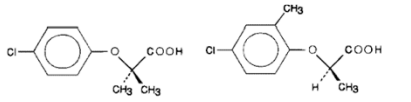
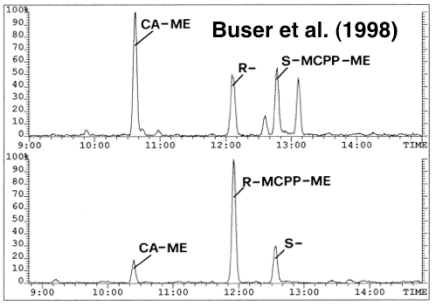
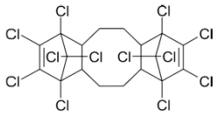
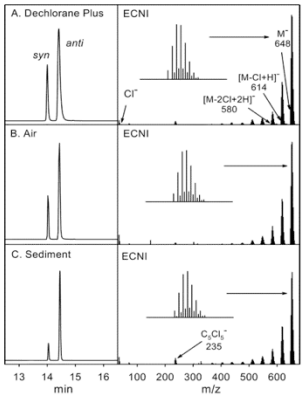
Credit: D. Sedlak

Mystery Peaks









Hoh et al. (2006)

Credit: D. Sedlak

Potential Sites of Accumulation

Note: allowable concentration in drinking water
PFOA: 0.04-0.5 μg/L
PFOS: 0.3 μg/L

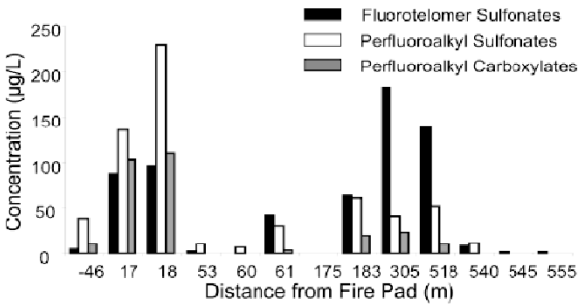


FIGURE 5. Distance vs concentration plot for fluorosurfactants at Wurtsmith AFB.

Schultz et al. (2004)

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Credit: D. Sedlak

Critical Components: Serendipity and Curiosity

- **Development of new analytical methods and monitoring are rarely research priorities.**
- **There are many new tools for investigating mystery peaks.**
- **Algorithms based on HPV chemicals will not capture all important problems.**
- **Bioassay-directed fractionation and other effects-driven tools are promising, but only if coupled to identification of compounds.**

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Credit: D. Sedlak

Focus on Research Gaps

- **Detection and Quantification**
  - End-of-life fate of CECs
  - Bioassay directed methods
- **Environmental Fate and Transport**
  - Transformation processes and products
  - Fate and transport models
- **Health and Risk Assessment**
  - Unconventional responses and impacts
  - Bioaccumulation models
- **Site Identification and Remediation**
  - Epidemiologically and ecologically focused geospatial analysis
  - Remedial technologies

Focus on Potential Accumulation Sites

Traditional sites with new focii (CECs)

- High density food production sites
- Landfills and landfill leachate disposal sites
- Biosolids disposal sites

New sites

- E-waste recycling
- Energy production and recovery processes
- Nanomaterial manufacturing sites
- Fire suppression training sites

Recommendations and Conclusions

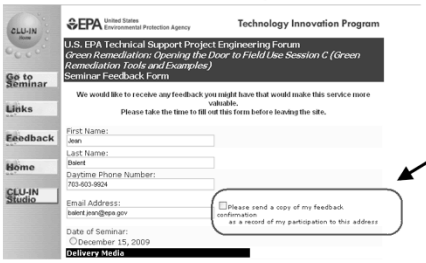
- Clearly a need to expand Superfund scope to hazardous waste site relevant CECs
- Dynamic, evolving list of priority CECs and sites of accumulation will be critical
- Persistence, points of concentration, and toxicity are limiting attributes, while bioaccumulation and production volume are indicators
- Algorithms and expert judgement must be augmented by curiosity, serendipity and analytic development
- New metrics of success will be needed

Thanks

Questions and Comments?

Resources & Feedback

- To view a complete list of resources for this seminar, please visit the **Additional Resources**
- Please complete the **Feedback Form** to help ensure events like this are offered in the future
- Link to "Improving Collaborations" Survey



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