Laboratory use cases for chemical safety information

Ralph Stuart, Leah McEwen, Evan Bolton

8:30am - 8:45am Wed, Aug 24
Room 112A - Pennsylvania Convention Center

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August, 2016

Increasing Concerns about Lab Safety

The Research Lab

2011

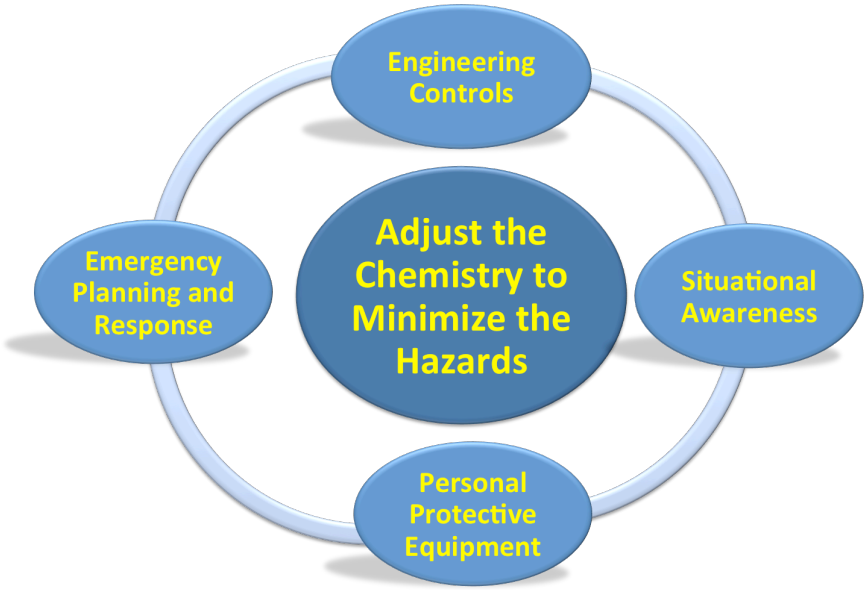
The Teaching Lab

2014

Chemical Safety requires a *System* rather than a *Solution*

Successfully managing chemical hazards in complex setting involves organizing five basic protection strategies into a **resilient management system**.

The Safety System is held together by a group's **Safety Culture**



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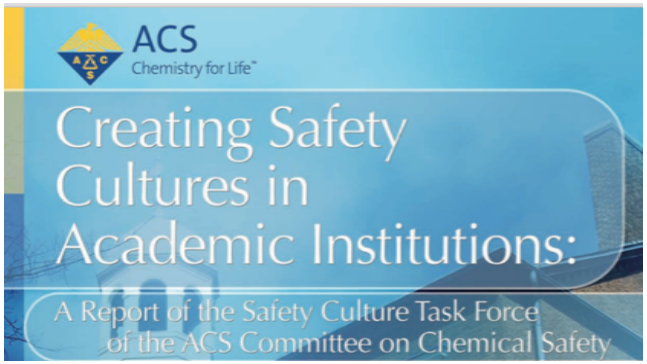
So Attention Turns to Lab Safety Culture

Lab safety culture is continuing to evolve under scrutiny from government, professional and scientific organizations.



American Chemical Society, 2012

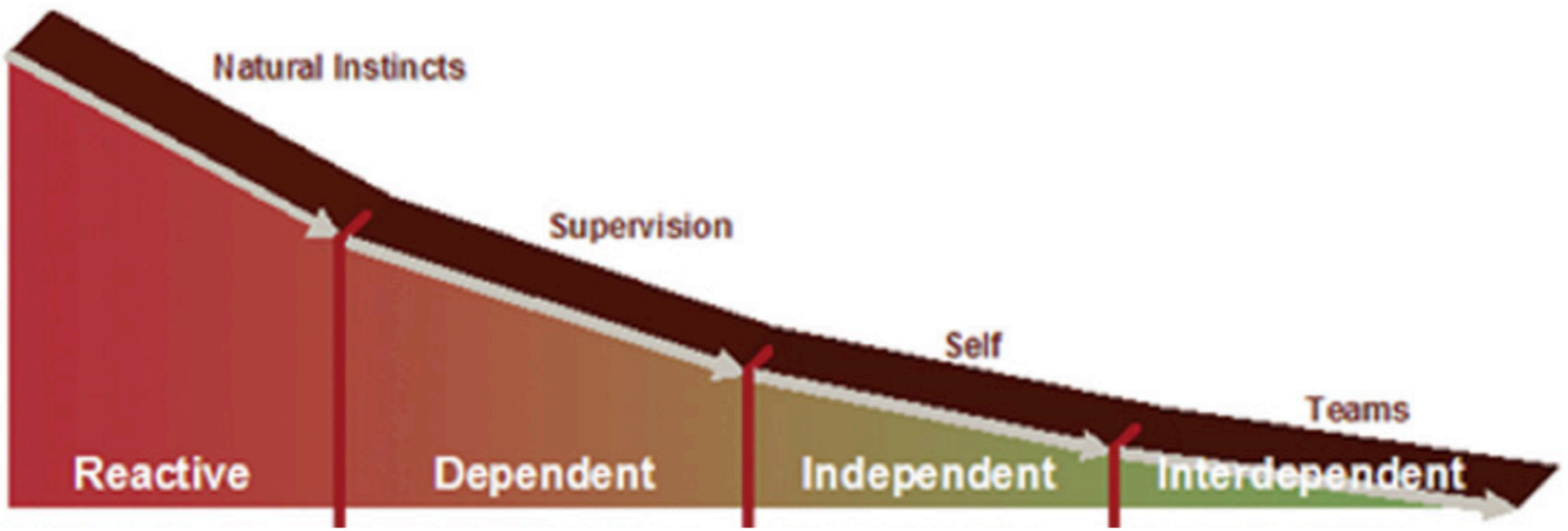
National Academy of Sciences, 2014

Assoc of Public and Land Grant Universities 2016

Safety Information Tools and Safety Culture

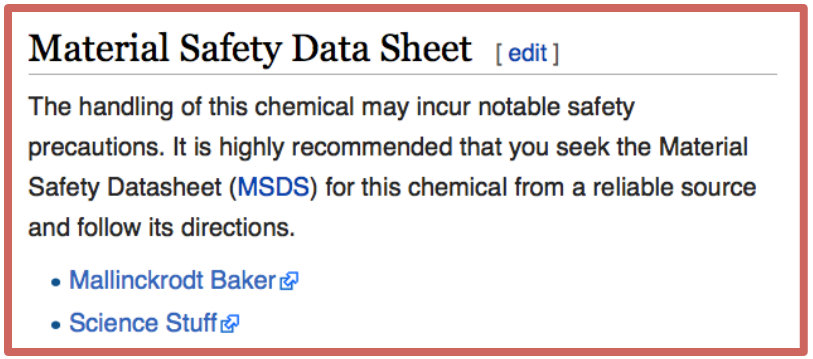
Prevailing Types of Safety Information

Raw Safety Data + Common Sense	Rules and Oversight	SOPs	Risk Assessment and Communication

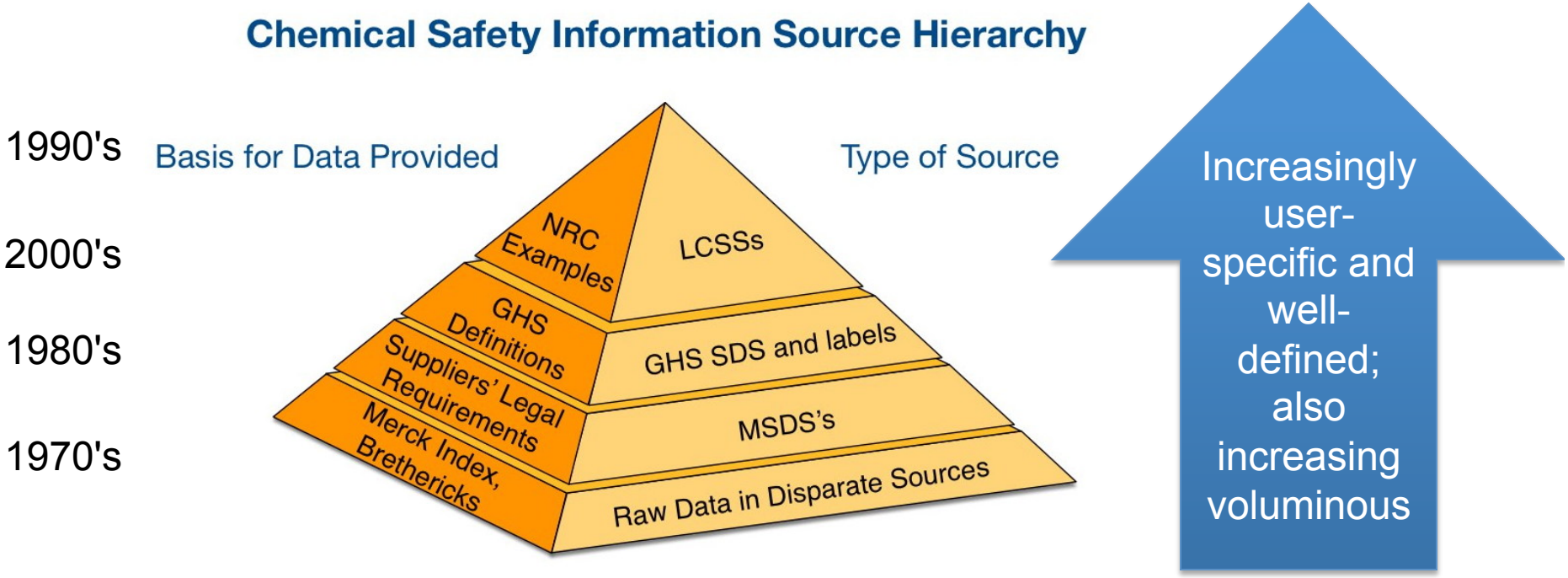


The Current Chemical Safety Info-scape

- **Is caveat emptor**: Chemistry textbooks, laboratory manuals and J Chem Ed articles generally say "be careful, see the MSDS".
- For example, Wikipedia provides links to MSDS sources with no sense of **why that source** was selected and **linkrot** abounds
- Resources are **stakeholder-specific**, e.g. CAS numbers are a standard tool in the hazmat world, but a big problem in the research world



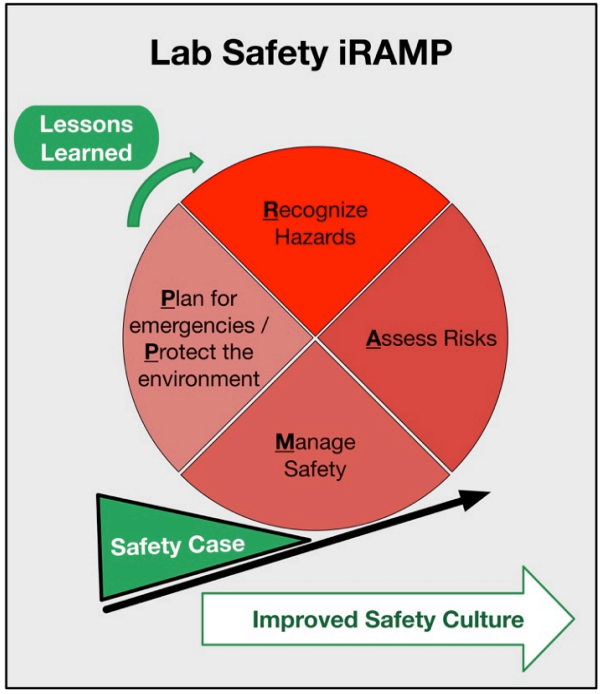
The Evolution of Chemical Safety Information



Moving to the Process: The RAMP approach to Building a Lab Safety System

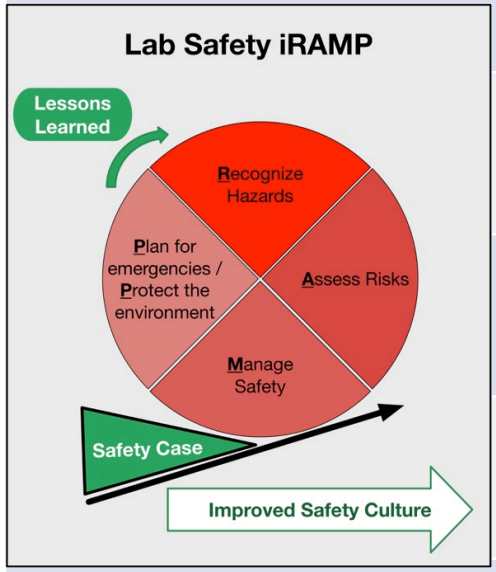
Developing a Chemical Safety system involves addressing six elements:

1. EHS Culture
2. Hazard Identification
3. Risk Assessment
4. Managing Safety
5. Planning for Emergencies
6. Protecting the Environment



From Stuart and McEwen. 2016

Connecting to the Educational Mission: Risk Assessment is a Research Process

The RAMP model of Chemical Safety	Association of College and Research Libraries Information Literacy Skills
Safety culture	**Scope** the Inquiry
	**Collect** Data  **Evaluate** the **Apply** Data t Make Decisi
Plan, Protect *Share Lessons Learned*	**Document** the Process and Outcome

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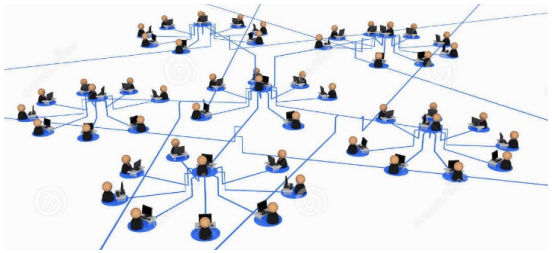
The Situation Moving Forward

- The emerging web favors:
  - Sites designed as a **nodes in the network** rather than Sources of Truth
  - **Contextual Usability** (use of the information beyond the screen)
  - Open source **peer curation**, building on the examples of e-mail lists and Wikipedia



There are Many Different Needs for this Information

Academic Stakeholders

Institutions:
Research
Funding
Regulatory

~ **Students**
Researchers

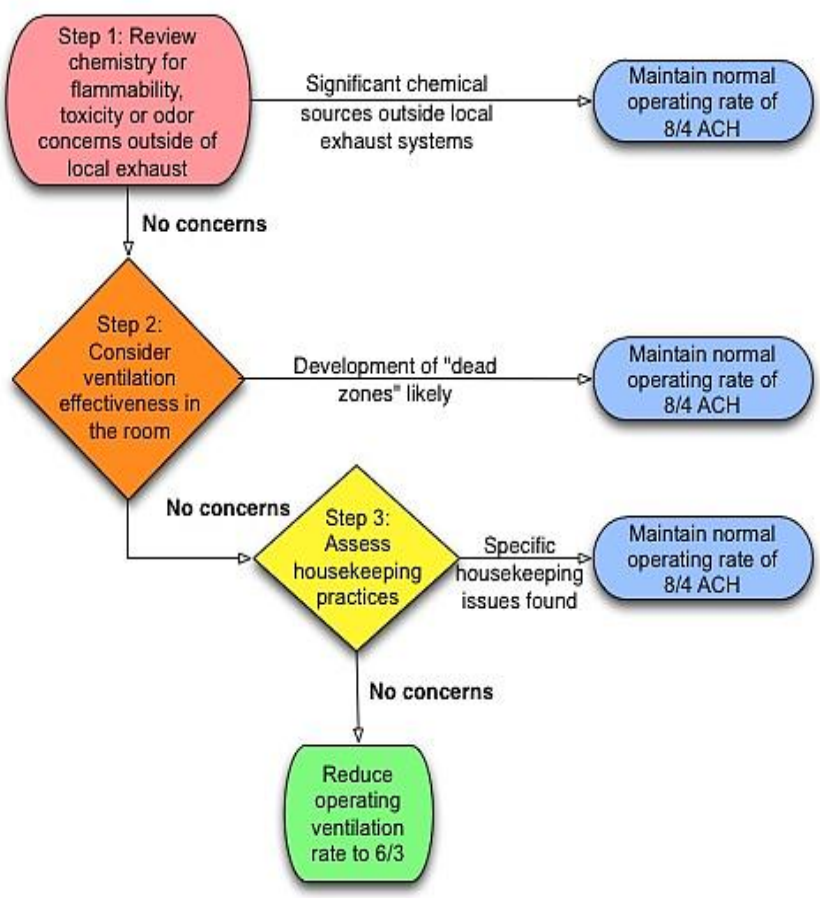
~ **Faculty**
Departments

~ **Safety Officers**
Librarians

http://www.betterlivingwithreiki.com

Safety Office Use Cases

- Inventory systems (consolidated data stream)
- Control Banding (safety planning)
- Incident analysis
- Reactivity classification
- Research tool for safety system studies



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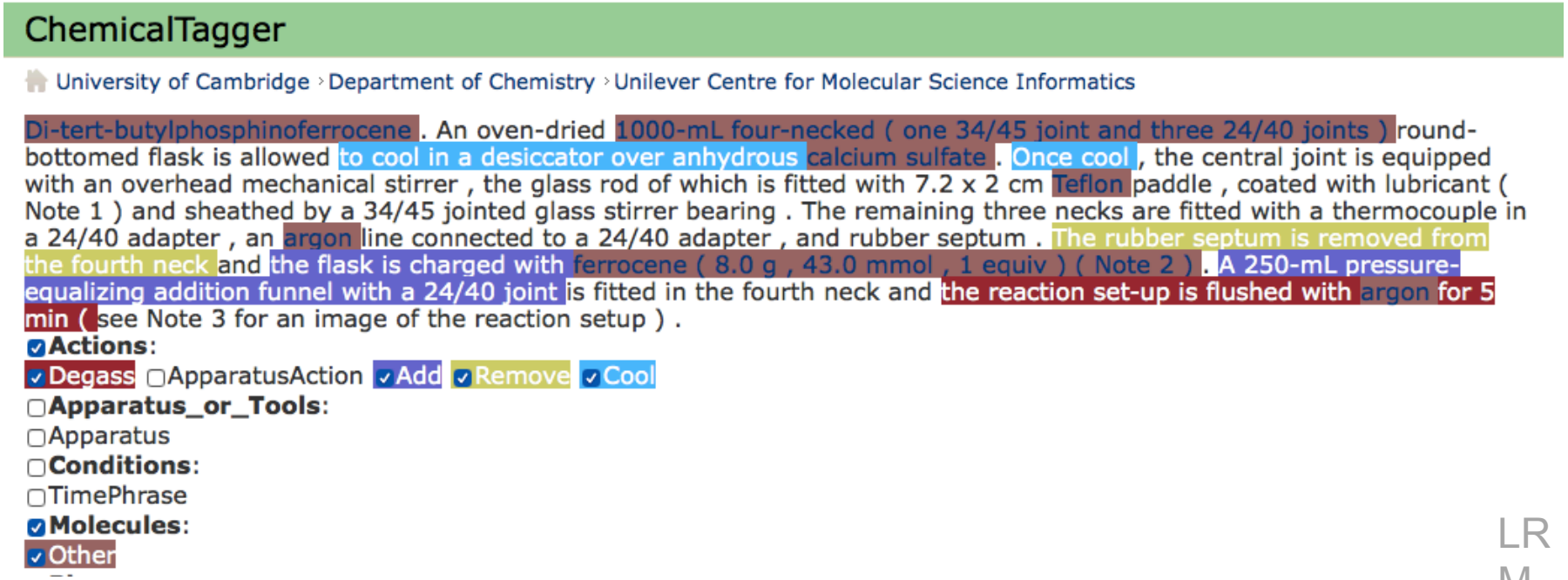
Chemistry Educator Use Cases

- Chemical profiling for lab safety curriculum (download LCSSs for chemical lists)
- Teaching information literacy in RAMP process (searching for information and comparing data sources)
- Analyzing procedures for chemical, equipment and process hazards



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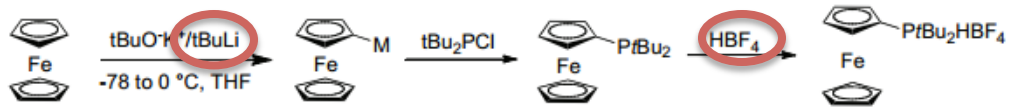
Researcher Use Cases

- Experimental planning
- Capturing lab risk assessments and any lessons learned
- Publication of safety notes as part of Supplemental Information
- Use of safety info tools and documentation promotes safe research group culture



Caution! tert-Butylithium is extremely pyrophoric and must not be allowed to come into contact with the atmosphere. This reagent should only be handled by individuals trained in its proper and safe use. It is recommended that transfers be carried out by using a 20-mL or smaller glass syringe filled to no more than 2/3 capacity or by cannula. For a discussion of procedures for handling air-sensitive reagents, see Aldrich Technical Bulletin AL-134.

Org. Synth. **2013**, *90*, 316-326
Published on the Web 6/10/2013

Need for Targeted Information:

- Identification of reagents, products
- Reactivity and associated hazard analysis
- Associated exposure control information
- Alternative reagents or reaction pathways
- Iterative over repeated experiments

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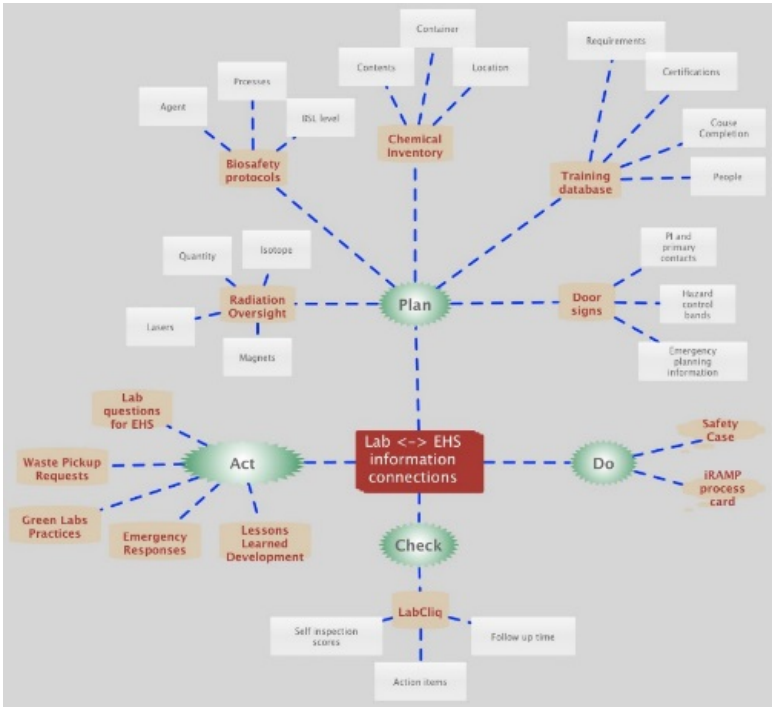
Today's Goal:
Map the iRAMP Landscape

- **Identify Pain Points**
  - Ontology
  - Safety community annotation process
  - Operational implementation
- **Identify Power Points**
  - The GHS
  - PubChem LCSS
  - Educational use cases
- **Assess emerging opportunities**
  - ChemTagger
  - Deepwebaccess Chemical Safety browser
  - ACS resources: Hazard Assessment web site, Safety Education Guidelines



Next Steps

- **Hackathon 2017 Needs:**
  - Stakeholders
  - Experts
  - Projects

References

1. *PubChem Laboratory Chemical Safety Summary,* Kim et al. Fall 2015 ACS CHED CCCE Newsletter http://confchem.ccce.divched.org/2015FallCCCENLP3
2. *The Safety "Use Case": Co-Developing Chemical Information Management and Laboratory Safety Skills,* Stuart and McEwen, Journal of Chemical Education http://pubs.acs.org/doi/abs/10.1021/acs.jchemed.5b00511
3. *Meeting the Google Expectation for Chemical Safety Information: Chemical Risk Assessment in Academic Research and Teaching*, Chemistry International, McEwen and Stuart http://www.degruyter.com/view/j/ci.2015.37.issue-5-6/ci-2015-0505/ci-2015-0505.xml?format=INT

Surveying the academic laboratory population: Project updates from the iRAMP collaboration

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Connecting to the Educational Mission

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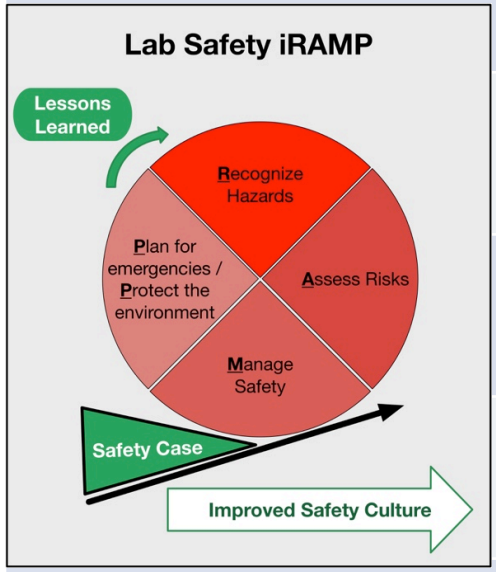	**Collect** Data **Evaluate** the **Apply** Data t Make Decisi
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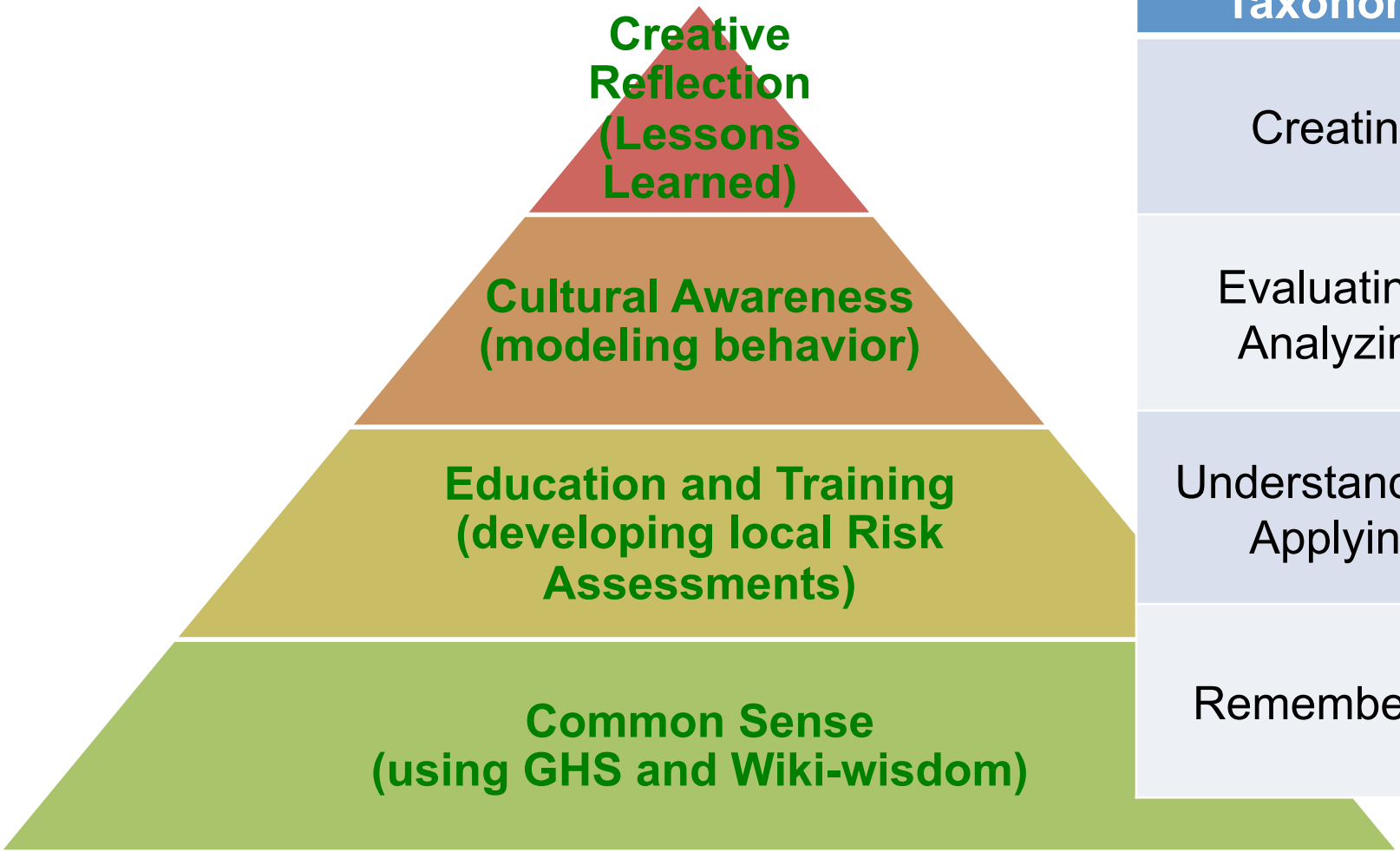
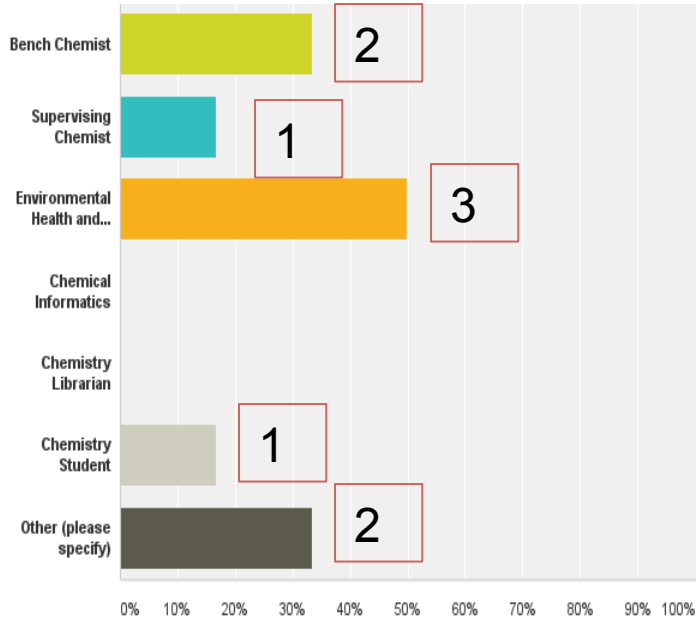
Lab Safety Education supports Critical Thinking

Prudent Practices involve 4 elements:



Bloom's Taxonomy
Creating
Evaluating / Analyzing
Understanding / Applying
Remembering

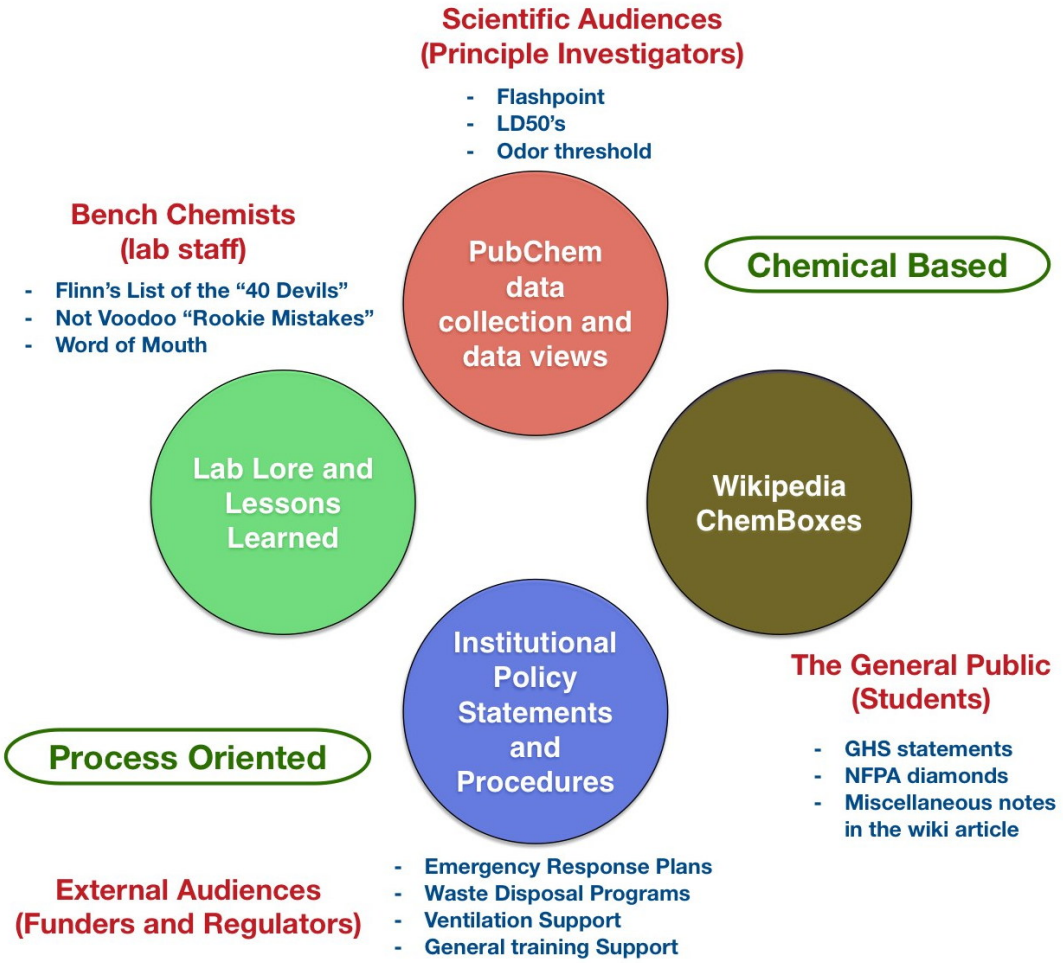
Usability Study 1: Comparing SDSs, Wikipedia and PubChem



Which of these sources would you go to first?

Preferred Source	Sigma Aldrich SDS	Wikipedia Chembox	Prudent Practices LCSS	PubChem LCSS	Full PubChem Record	Other Source	Total
What is the most important hazard associated with this chemical?	**50.00%** 3	**0.00%** 0	**0.00%** 0	**50.00%** 3	**0.00%** 0	**0.00%** 0	6
What other hazards associated with this chemical should be considered?	**50.00%** 3	**0.00%** 0	**0.00%** 0	**33.33%** 2	**16.67%** 1	**0.00%** 0	6
What hazard control recommendations should apply to this use of Chemical X?	**33.33%** 2	**0.00%** 0	**0.00%** 0	**50.00%** 3	**0.00%** 0	**16.67%** 1	6
Would you need to review safety information for other chemicals to make a complete risk assessment for a chemical process after reviewing this source?	**20.00%** 1	**0.00%** 0	**20.00%** 1	**20.00%** 1	**0.00%** 0	**40.00%** 2	5

Usability Study 2: Investigating Public Chemical Safety Information

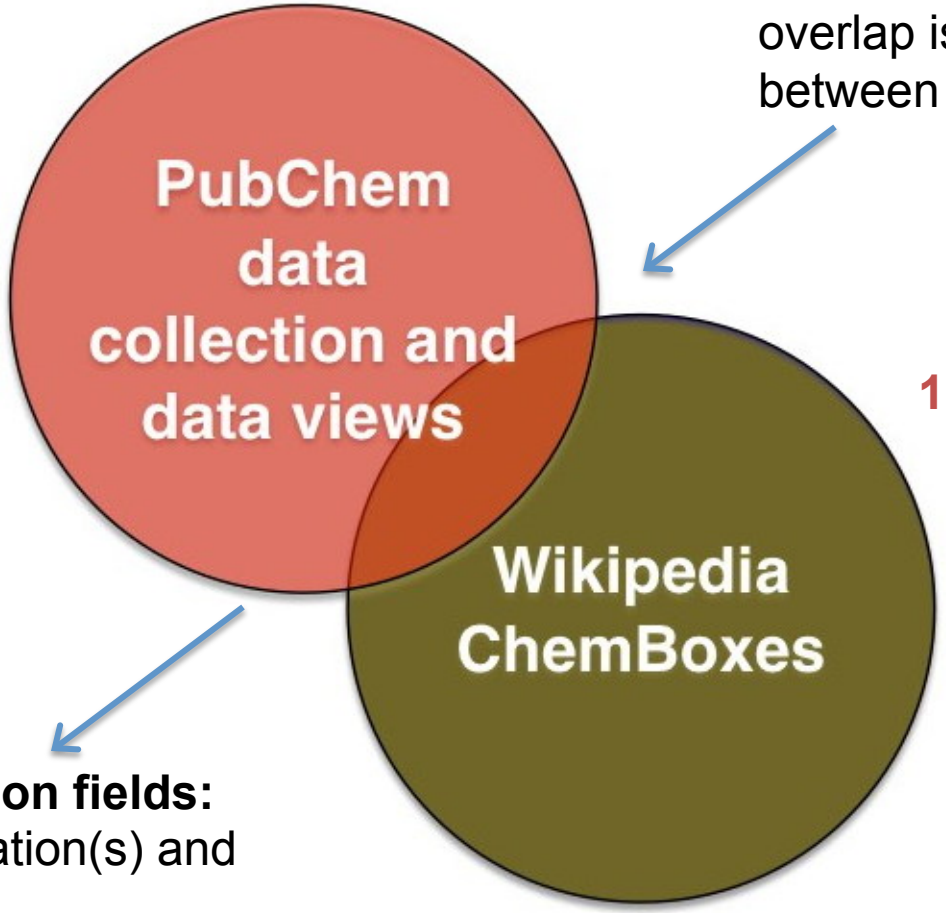


Looking for Structure in the Electronic Data

- How large is the PubChem chem safety information universe?
- How high quality is it (including consistency & provenance information)?

Millions of chemicals; 3500 with GHS info

How much overlap is there between the two?



10,000 Chemboxes

- How large is the Wikipedia chem safety information universe?
- How high quality is it?

Key safety information fields:

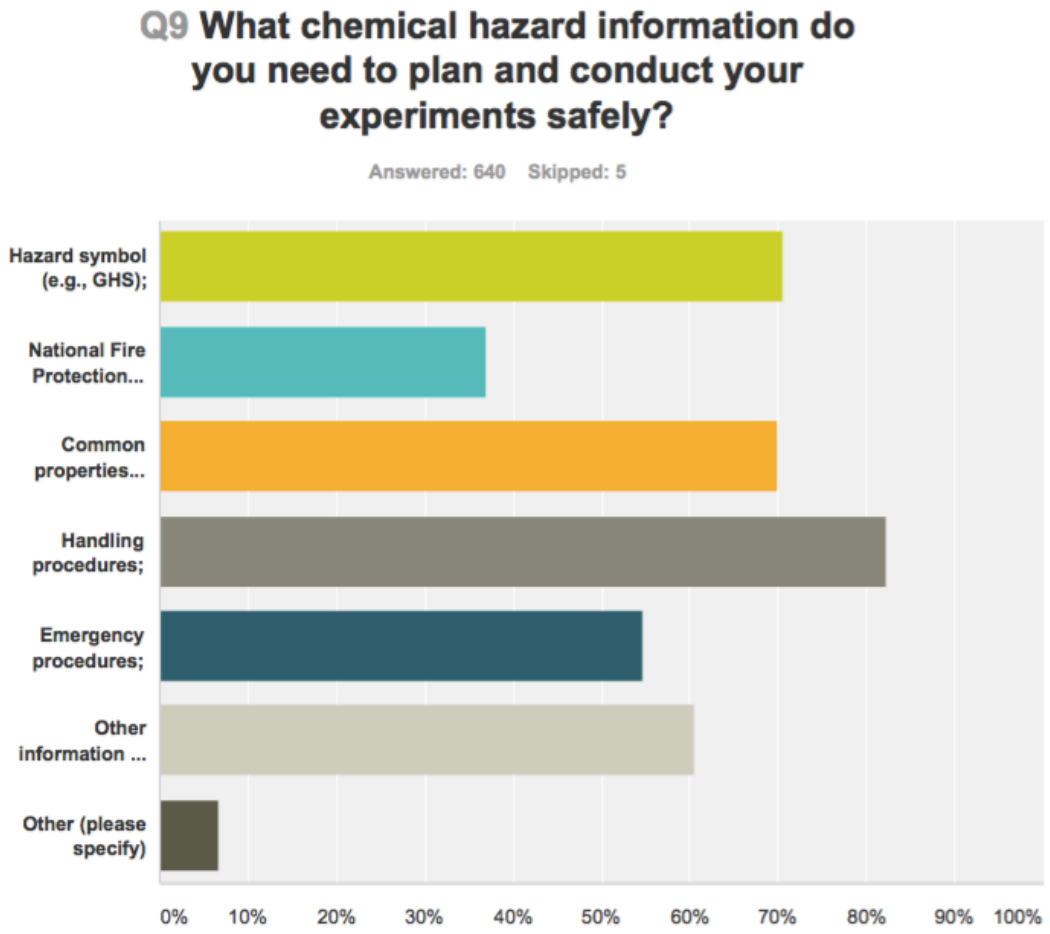
- GHS class designation(s) and signal word
- NFPA diamond information

The Results

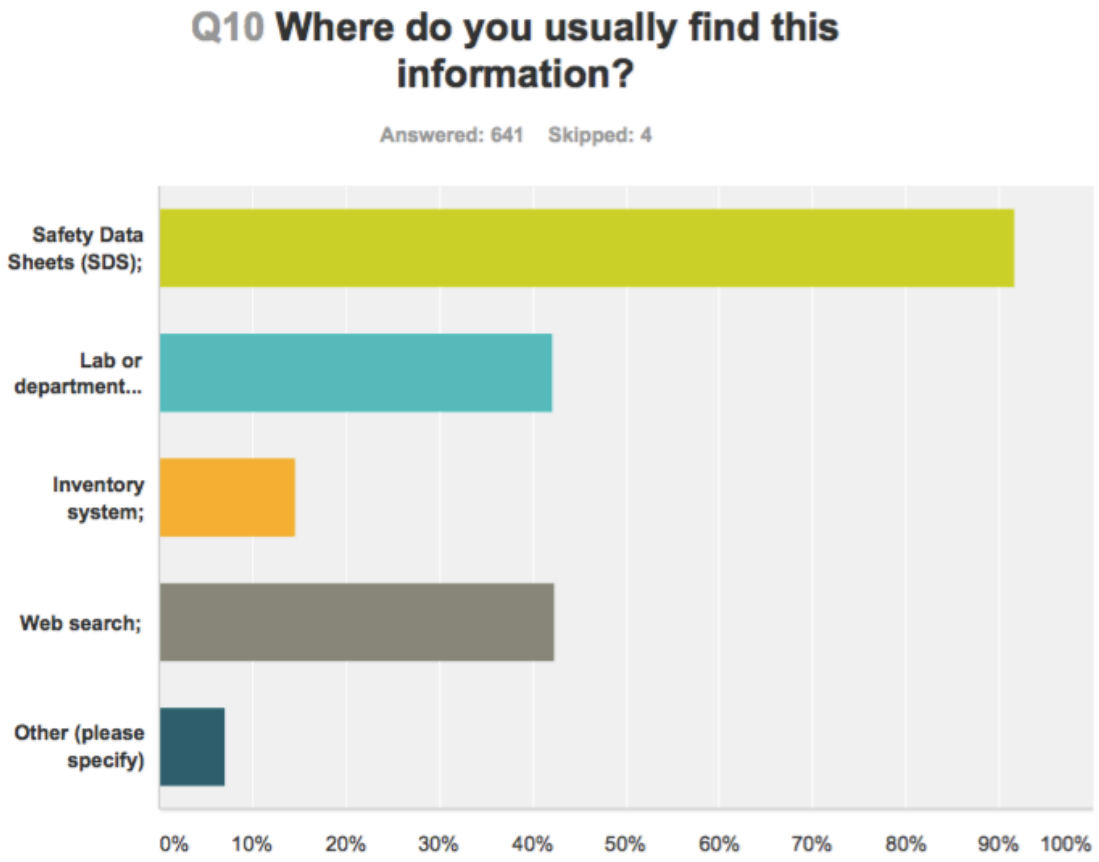
- PubChem has an LCSS view for about 5000 chemicals; Wikipedia has Chemboxes for about 10,000 chemicals
- Of those in the PubChem LCSS collection, about 30% have a ChemBox entry in Wikipedia
- 4% of the Wikipedia collection has GHS information; 12% of the Wikipedia collection has NFPA diamond information

	Not in Wikipedia	In Wikipedia	GHS Hazard Statement	NFPA 704	Total
n	2441	1038	157	431	3486
%	70.02%	29.78%	4.50%	12.36%	

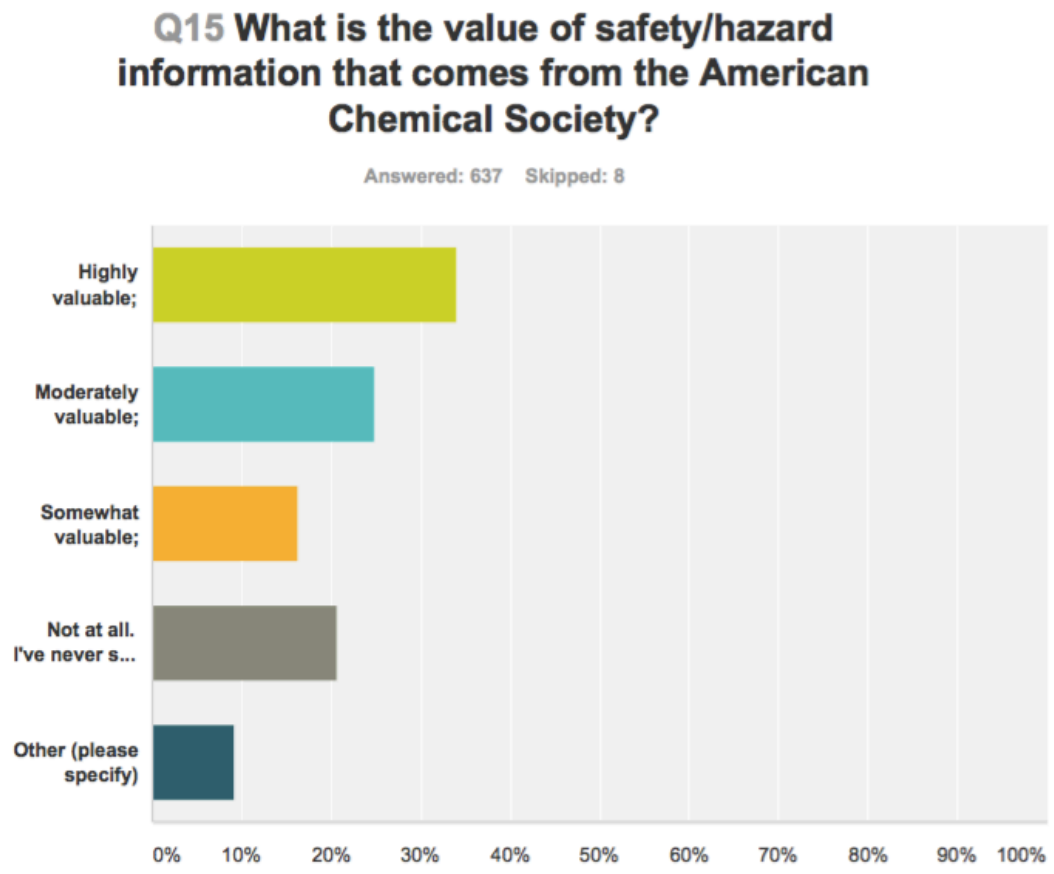
Users Study 1:
Chemist's Safety Information Needs



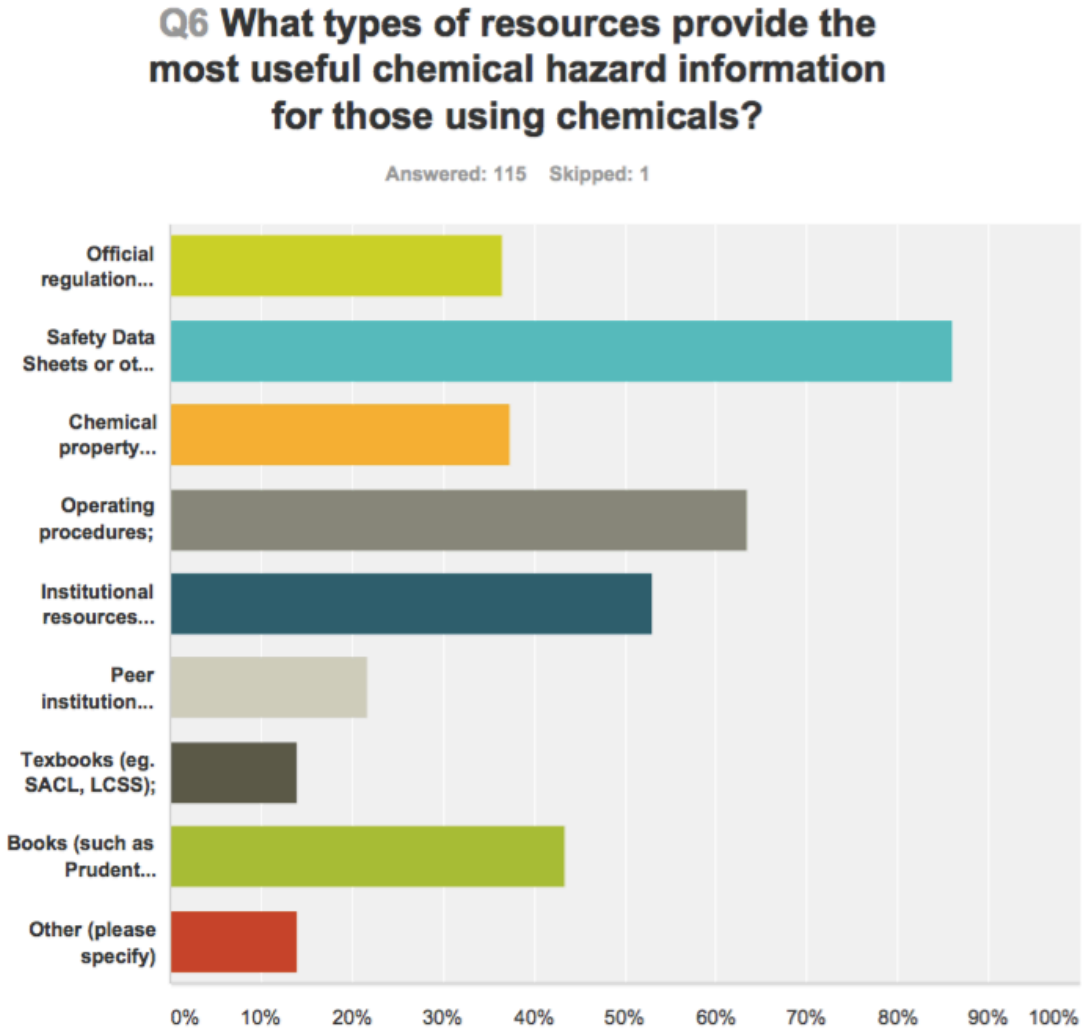
Users Study 1:
Chemist's Safety Information Sources



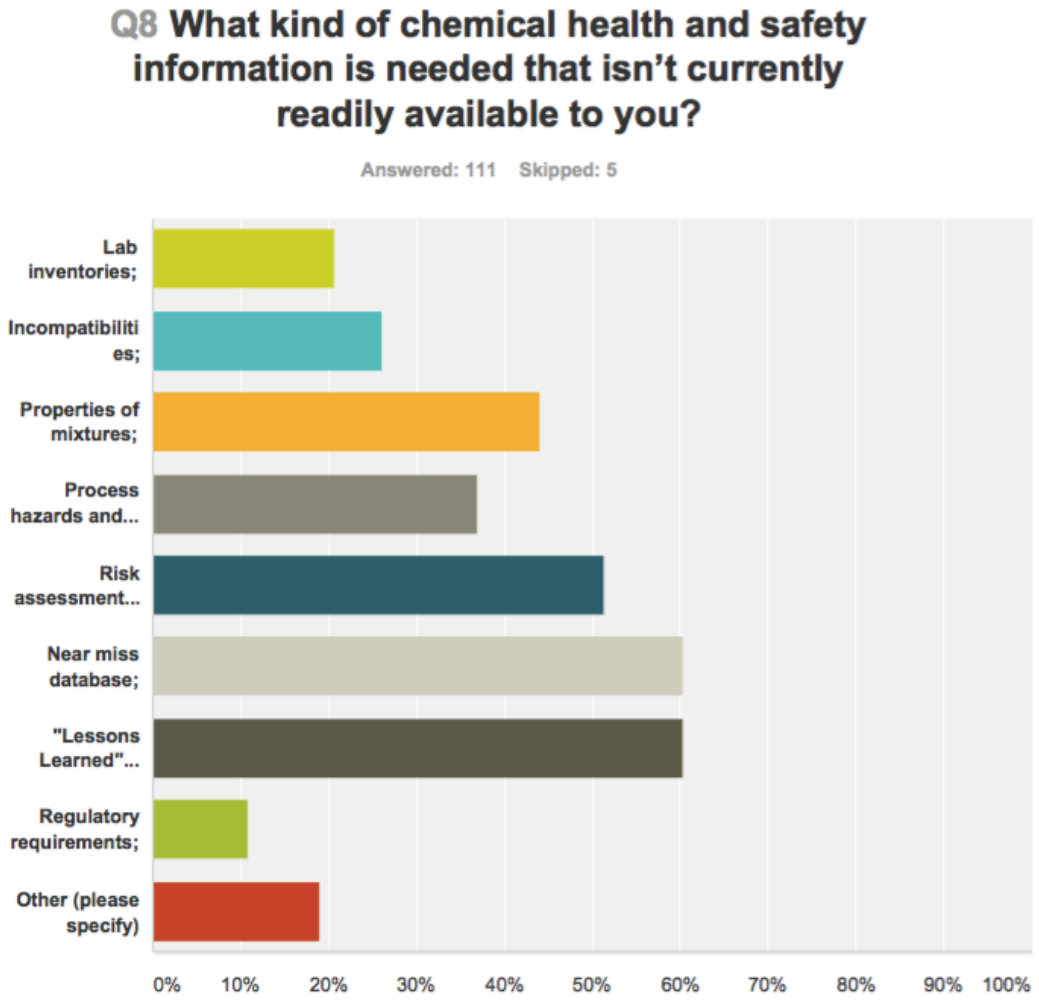
Users Study 1:
Chemist's Value of ACS Info



Users Study 2: Safety Community's Value of Information Sources



Users Study 2:
Safety Community's Missing Information



Moving Forward

- Focus groups this fall with a focus on high school teachers and new chemists
- Formal survey in the spring of the larger chemistry community

iRAMP Goals

- **iRAMP vision:** Capture the imagination of the academic chemistry community by presenting an inspirational vision of the chemical safety and chemical informatics
- **iRAMP mission:** Support a flexibly structured **ecosystem** of data, workflow tools and domain expertise mapped to the **essential commonalities** of the use case and content, connected by **good information management practices**

iRAMP System Diagram

Chemistry InfoSystem Diagram

Mapping the pain points and the Powerpoint in the chemical infoscape