



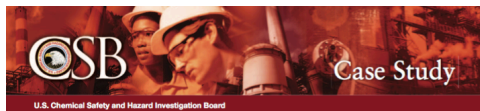
# Laboratory use cases for chemical safety information

**Ralph Stuart, Leah McEwen, Evan Bolton**

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

# Increasing Concerns about Lab Safety

## The Research Lab



Texas Tech University  
Laboratory Explosion  
No. 2010-06A-TX

- ISSUES**
- Laboratory safety management for physical hazards
  - Hazard evaluation of experimental work in research laboratories
  - Organizational accountability and oversight of safety



2011

## The Teaching Lab



October 2014

### Key Lessons for Preventing Incidents from Flammable Chemicals in Educational Demonstrations

Eliminating Flash Fire Hazards by Substituting or Minimizing the use of Flammable Chemicals and Performing an Effective Hazard Review Will Prevent Injuries

**Key Lessons Summarized:**

- Due to flash fire hazards and the potential for serious injuries, do not use bulk containers of flammable chemicals in educational demonstrations when small quantities are sufficient
- Employers should implement strict safety controls when demonstrations necessitate handling hazardous chemicals — including written procedures, effective training, and the required use of appropriate personal protective equipment for all participants
- Conduct a comprehensive hazard review prior to performing any educational demonstration
- Provide a safety barrier between the demonstration and the audience



CSB - Key Lessons for Preventing Incidents from Flammable Chemicals in Educational Demonstrations

2014

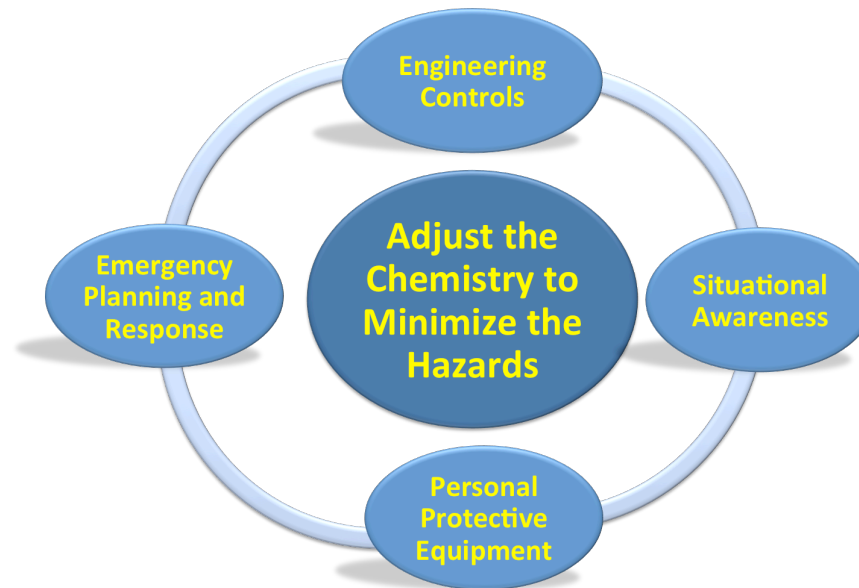


# Chemical Safety requires a System rather than a Solution

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

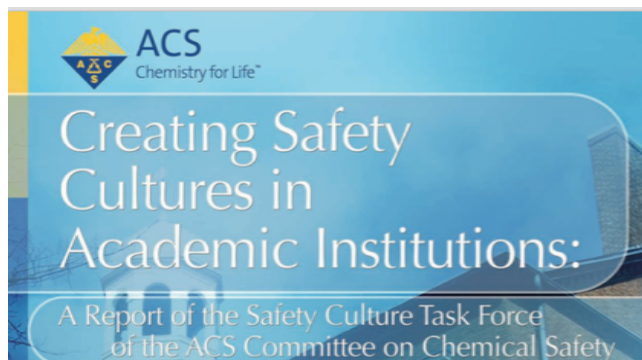
The Safety System is held together by a group's **Safety Culture**



# So Attention Turns to Lab Safety Culture

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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

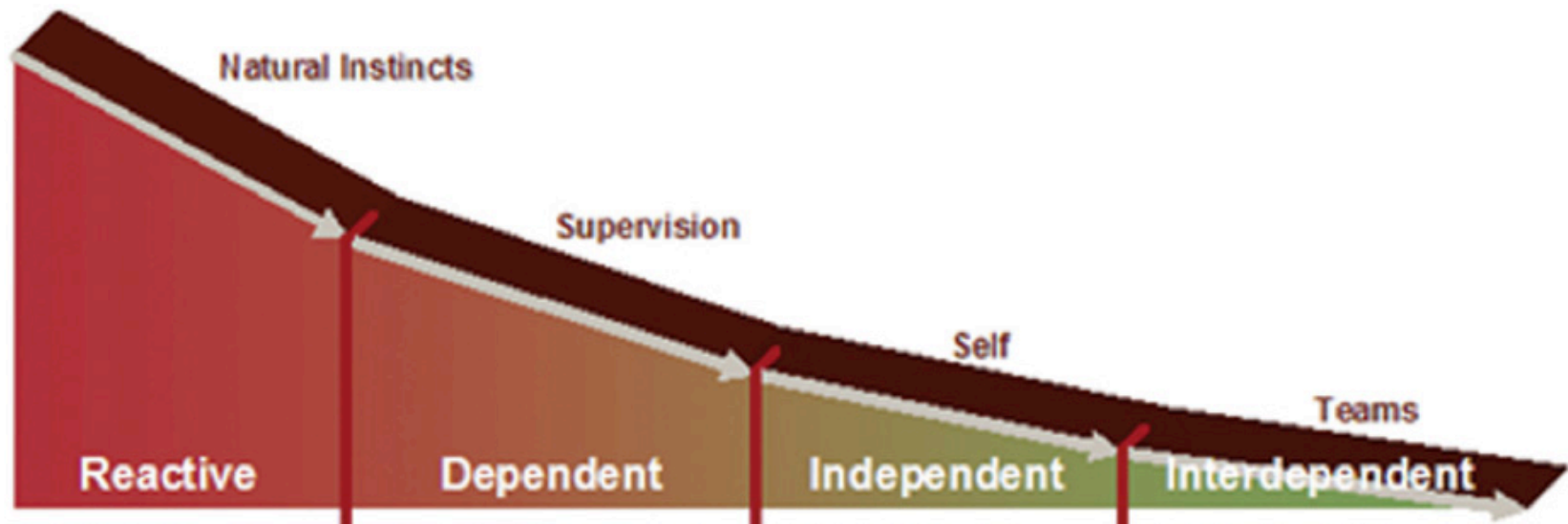
Prevailing Types of Safety Information

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

## Material Safety Data Sheet [\[ edit \]](#)

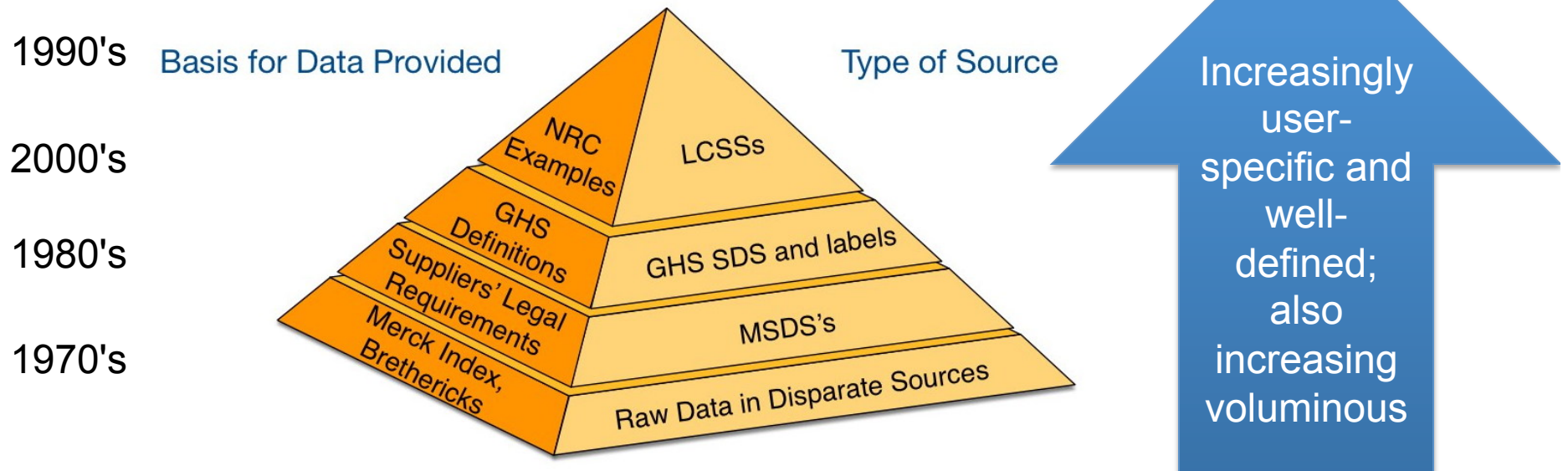
The handling of this chemical may incur notable safety precautions. It is highly recommended that you seek the Material Safety Datasheet ([MSDS](#)) for this chemical from a reliable source and follow its directions.

- [Mallinckrodt Baker](#)
- [Science Stuff](#)



# The Evolution of Chemical Safety Information

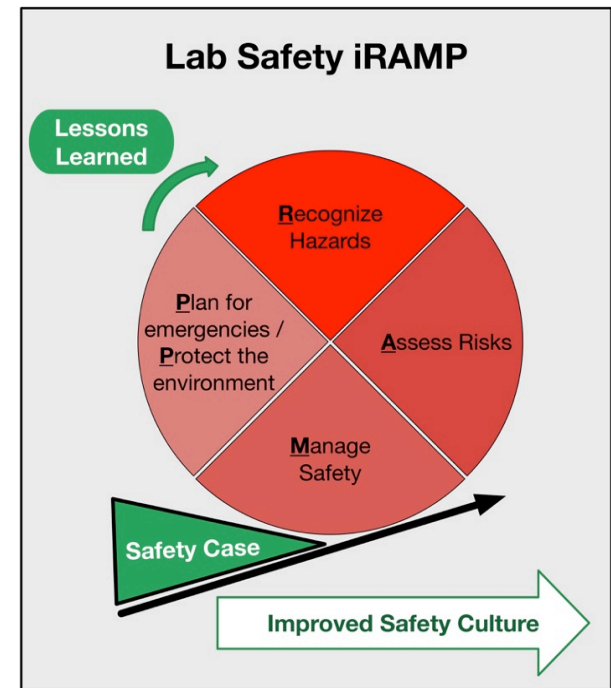
## Chemical Safety Information Source Hierarchy



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

Developing a Chemical Safety system involves addressing six elements:

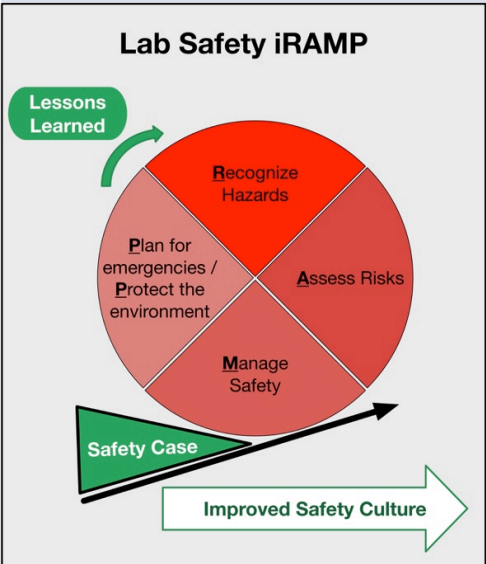

1. EHS Culture
2. Hazard Identification
3. Risk Assessment
4. Managing Safety
5. Planning for Emergencies
6. Protecting the Environment



From Stuart and  
McEwen. 2016



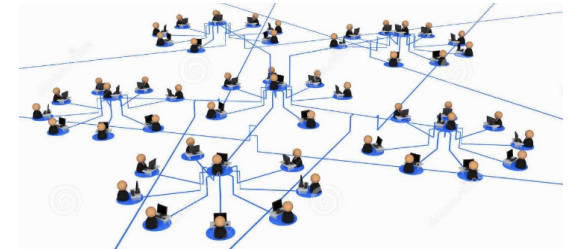
# Connecting to the Educational Mission: Risk Assessment is a Research Process

The RAMP model of Chemical Safety	Association of College and Research Libraries Information Literacy Skills
<p><i>Safety culture</i></p>	<p><b>Scope</b> the Inquiry</p>
	<p><b>Collect Data</b></p> 
<p><b>Evaluate the</b></p>	<p><b>Apply Data to Make Decisions</b></p>
<p><i>Plan, Protect</i> <i>Share Lessons Learned</i></p>	<p><b>Document</b> the Process and Outcome</p>

# The Situation Moving Forward

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- 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

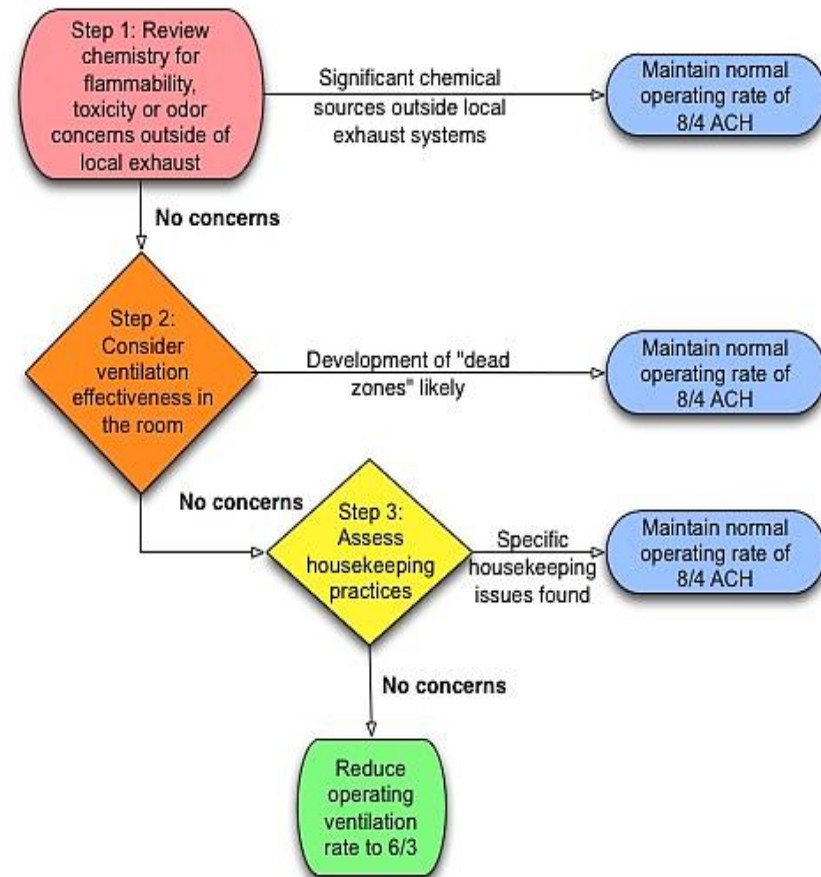
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## Academic Stakeholders



# Safety Office Use Cases

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



# 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

## ChemicalTagger

University of Cambridge > Department of Chemistry > Unilever Centre for Molecular Science Informatics

Di-tert-butylphosphinoferrocene . An oven-dried 1000-mL four-necked ( one 34/45 joint and three 24/40 joints ) round-bottomed flask is allowed to cool in a desiccator over anhydrous calcium sulfate . Once cool , the central joint is equipped with an overhead mechanical stirrer , the glass rod of which is fitted with 7.2 x 2 cm Teflon paddle , coated with lubricant ( Note 1 ) and sheathed by a 34/45 jointed glass stirrer bearing . The remaining three necks are fitted with a thermocouple in a 24/40 adapter , an argon line connected to a 24/40 adapter , and rubber septum . The rubber septum is removed from the fourth neck and the flask is charged with ferrocene ( 8.0 g , 43.0 mmol , 1 equiv ) ( Note 2 ) . A 250-mL pressure-equalizing addition funnel with a 24/40 joint is fitted in the fourth neck and the reaction set-up is flushed with argon for 5 min ( see Note 3 for an image of the reaction setup ) .

### Actions:

Degass  ApparatusAction  Add  Remove  Cool

### Apparatus\_or\_Tools:

Apparatus

### Conditions:

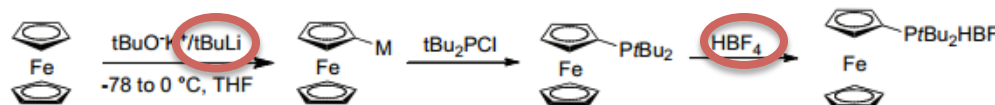
TimePhrase

### Molecules:

Other

# 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-Butyllithium 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.*

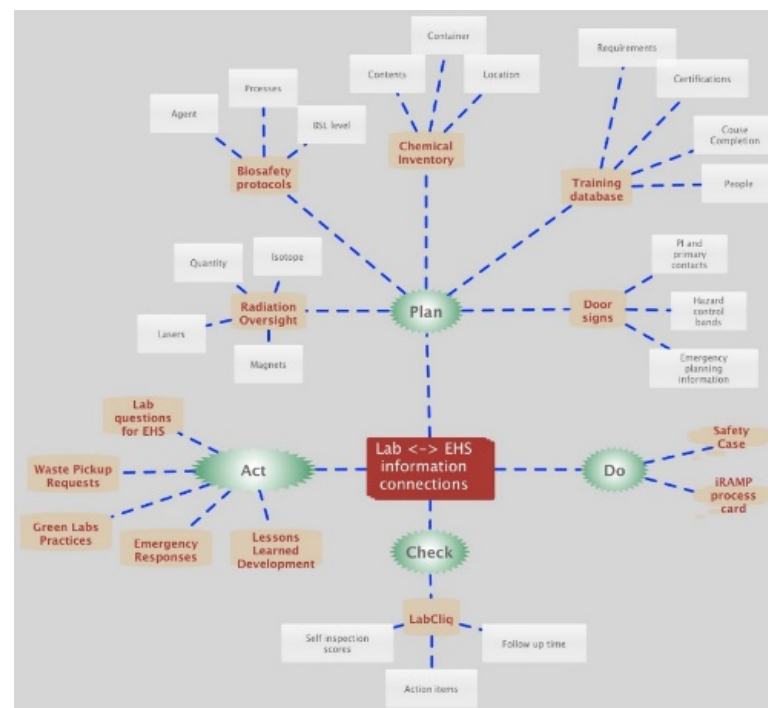
*Org. Synth.* **2013**, *90*, 316-326  
Published on the Web 6/10/2013  
© 2013 Organic Syntheses, Inc.

## 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

# 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

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



# References

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1. *PubChem Laboratory Chemical Safety Summary*, Kim et al. Fall 2015 ACS CHED CCCE Newsletter  
<http://confchem.ccce.divched.org/2015FallCCCEENLP3>
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**

**Leah McEwen, Ralph Stuart**

11:30am - 11:45am Wed, Aug 24  
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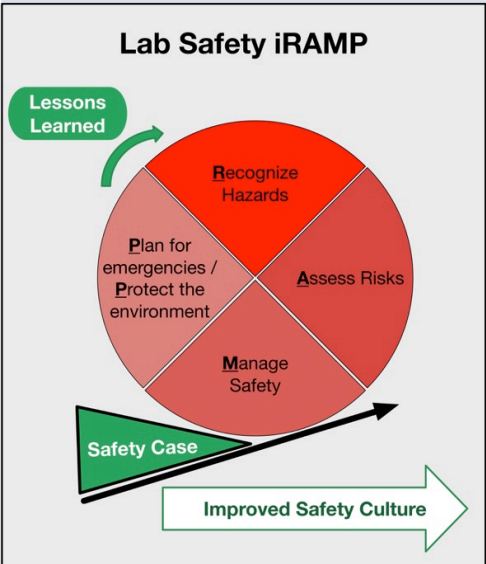
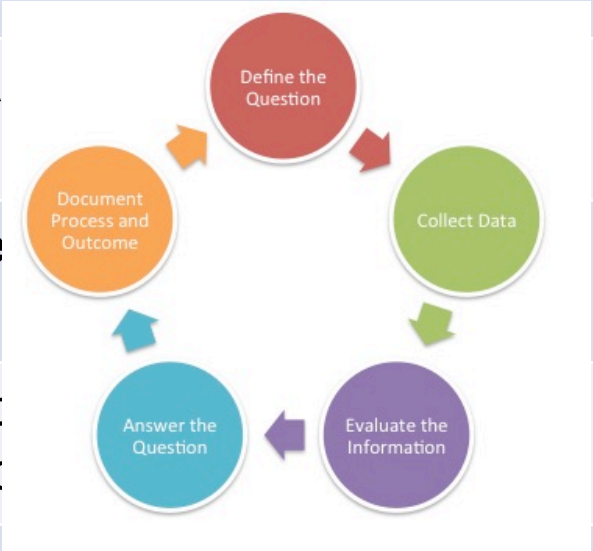


**Keene**  
STATE COLLEGE

Wisdom to make a difference.

**August, 2016**

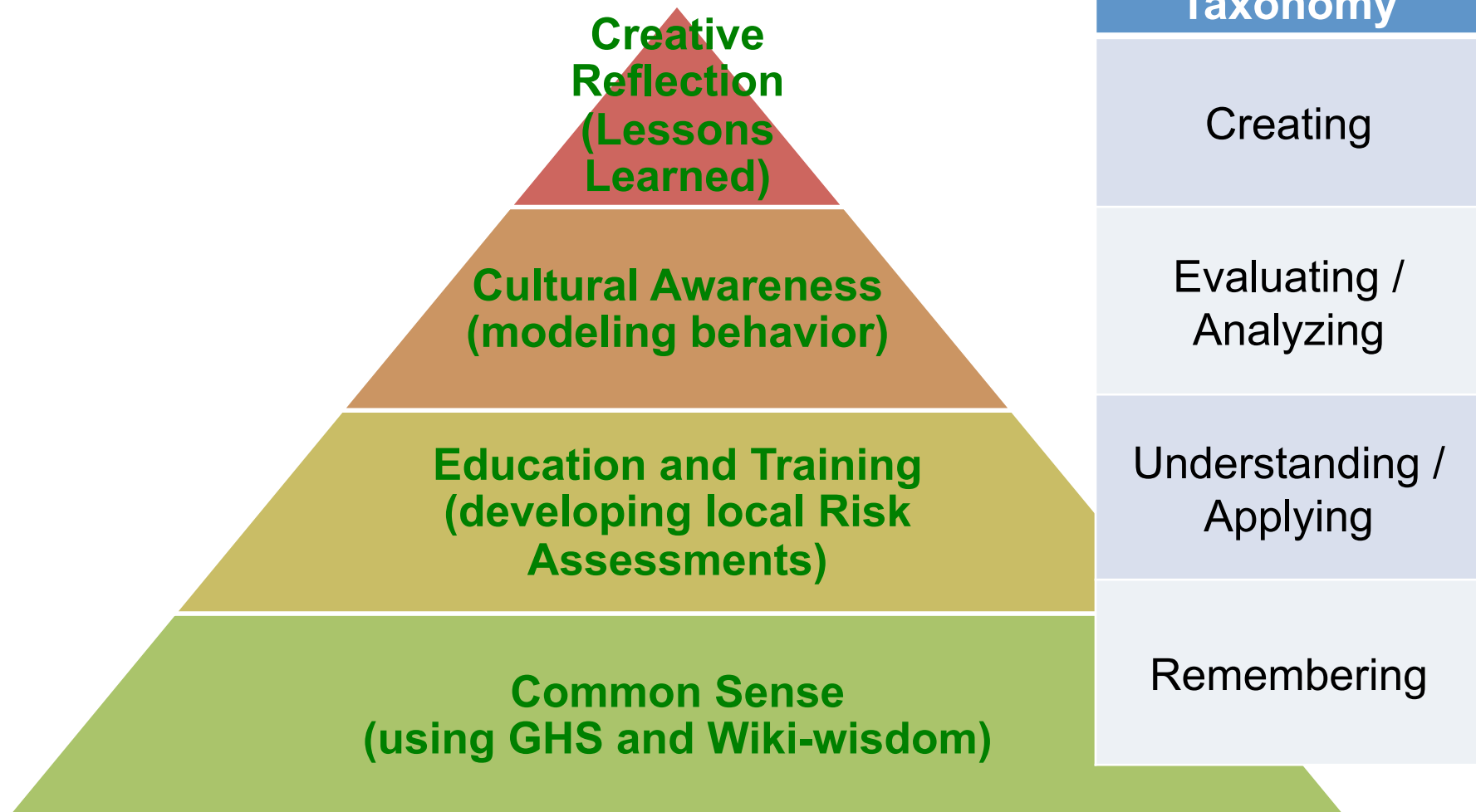
# Connecting to the Educational Mission

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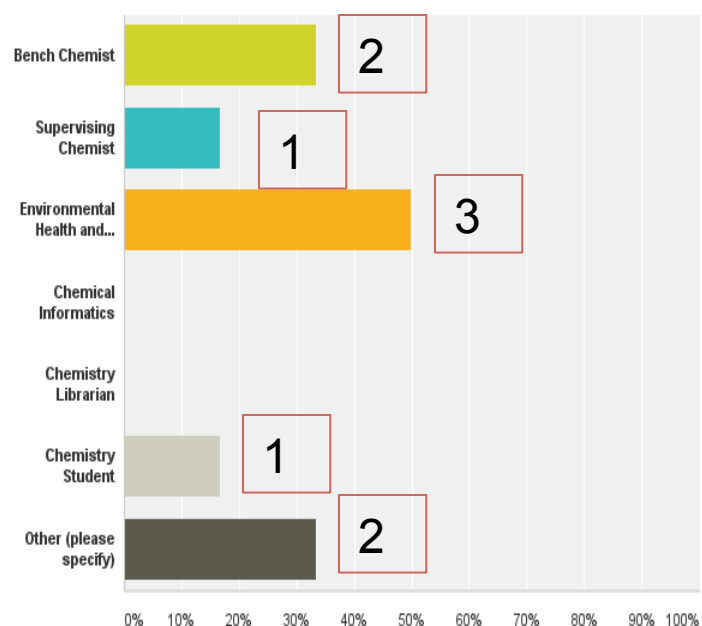
# Lab Safety Education supports Critical Thinking

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Prudent Practices  
involve 4 elements:



# Usability Study 1: Comparing SDSs, Wikipedia and PubChem

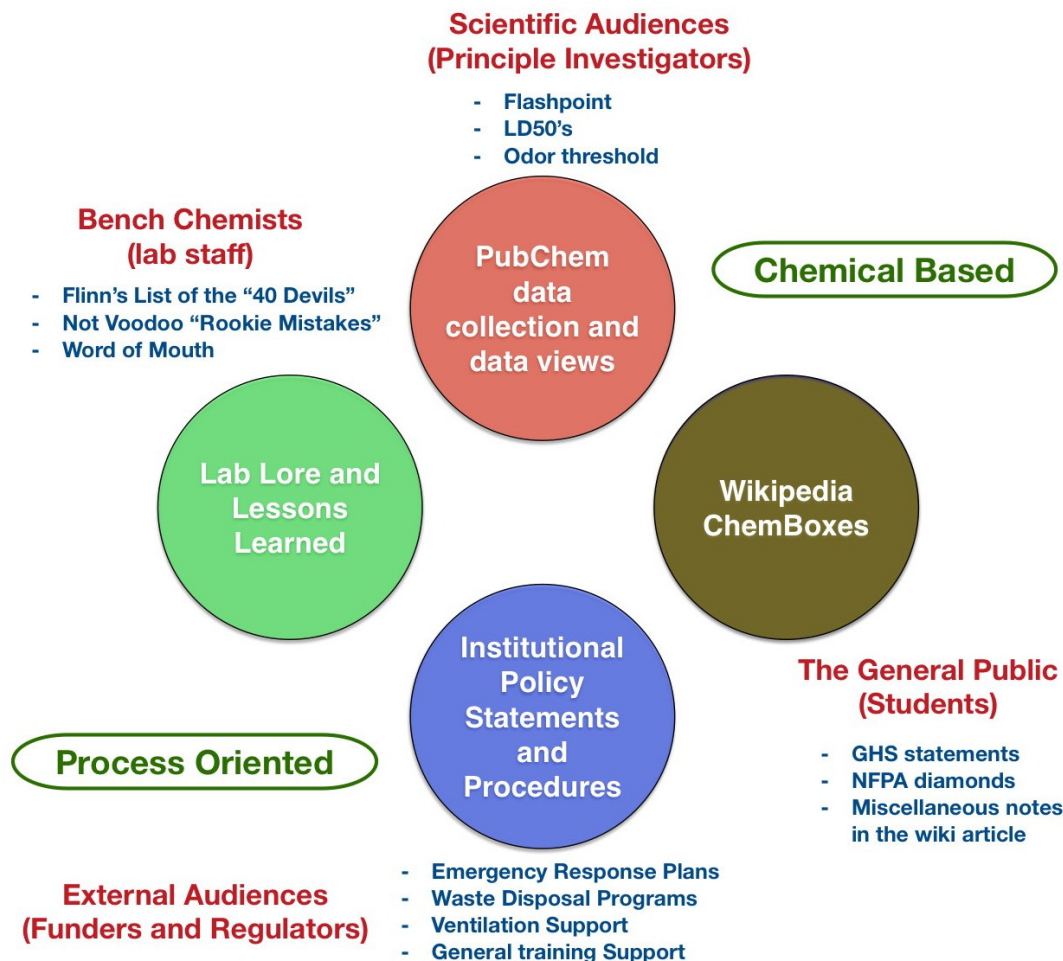


Which of these sources would you go to first?

	Preferred Source						Total
	Sigma Aldrich SDS	Wikipedia Chembox	Prudent Practices LCSS	PubChem LCSS	Full PubChem Record	Other Source	
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

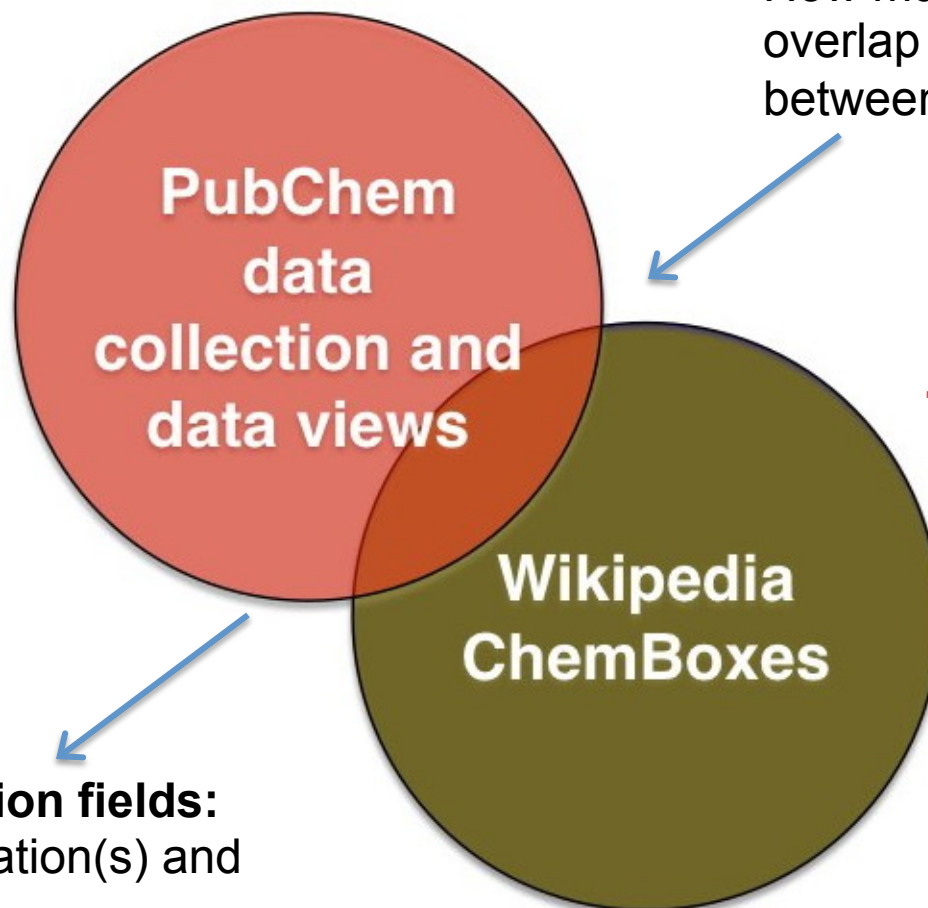
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# Looking for Structure in the Electronic Data

- 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

## Key safety information fields:

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

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

# The Results

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- 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%	

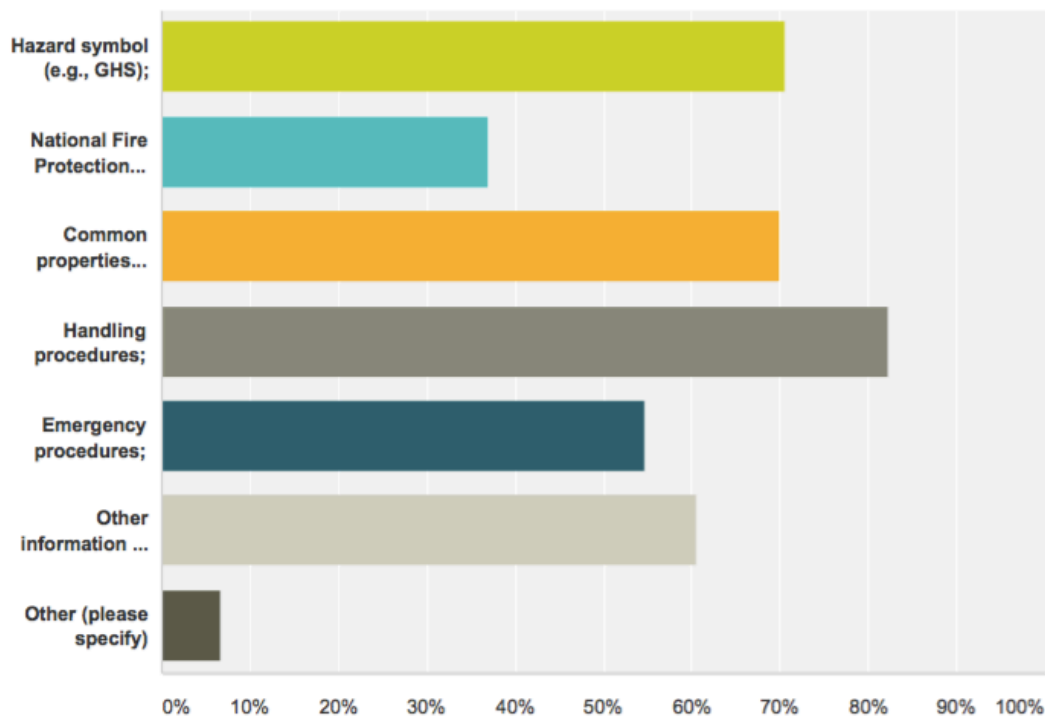


# Users Study 1: Chemist's Safety Information Needs

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**Q9 What chemical hazard information do you need to plan and conduct your experiments safely?**

Answered: 640 Skipped: 5

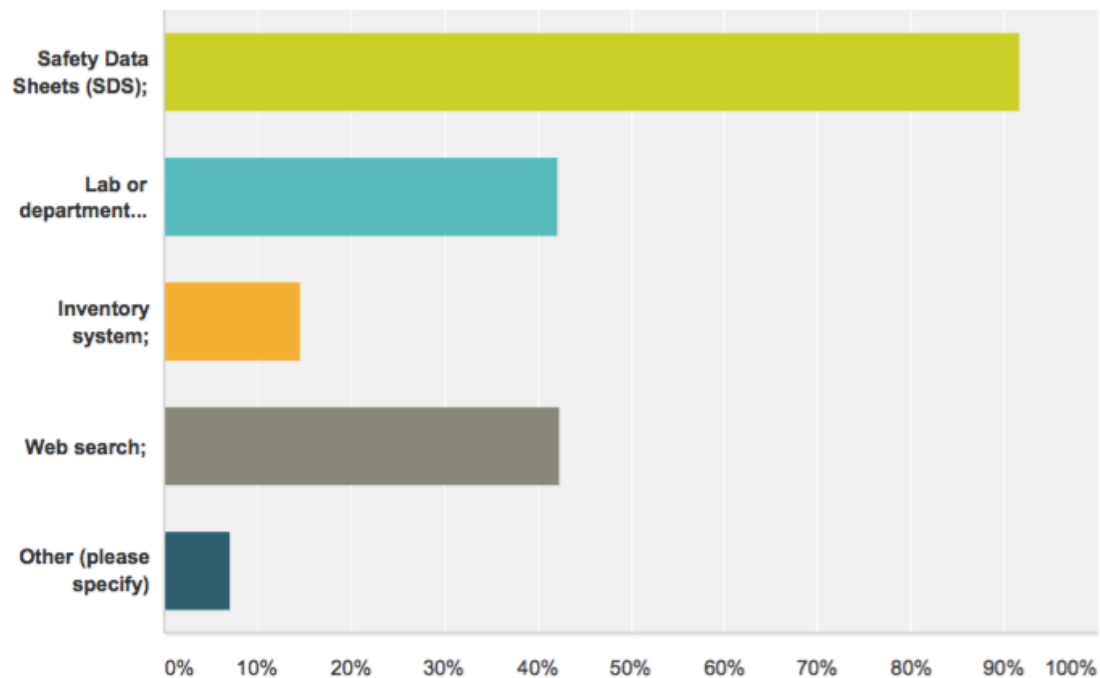


# Users Study 1: Chemist's Safety Information Sources

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## Q10 Where do you usually find this information?

Answered: 641 Skipped: 4

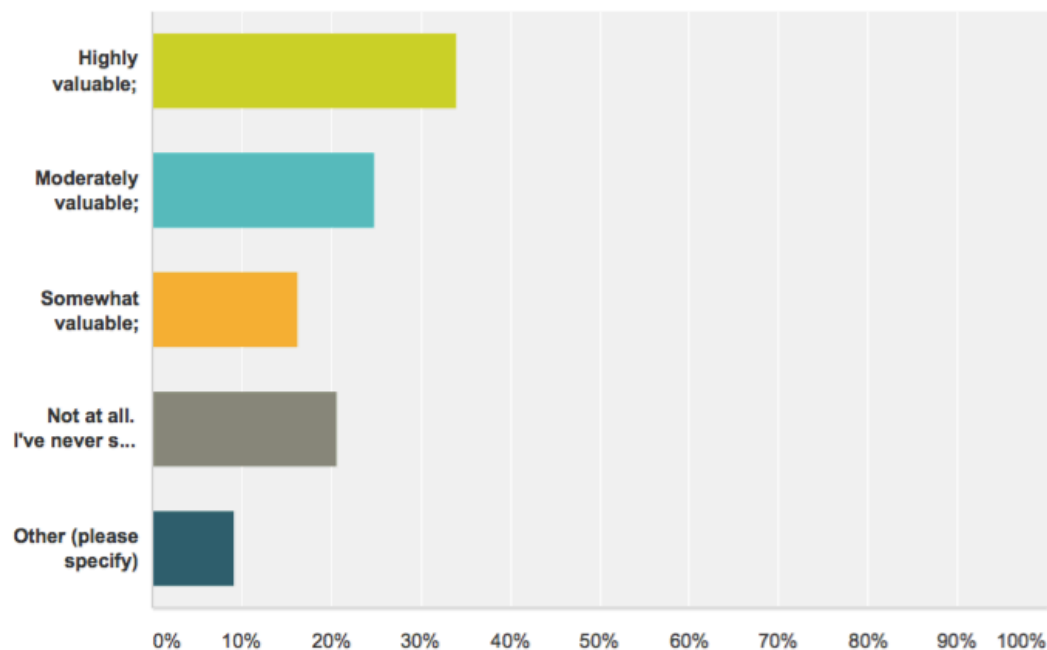


# Users Study 1: Chemist's Value of ACS Info

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## Q15 What is the value of safety/hazard information that comes from the American Chemical Society?

Answered: 637 Skipped: 8

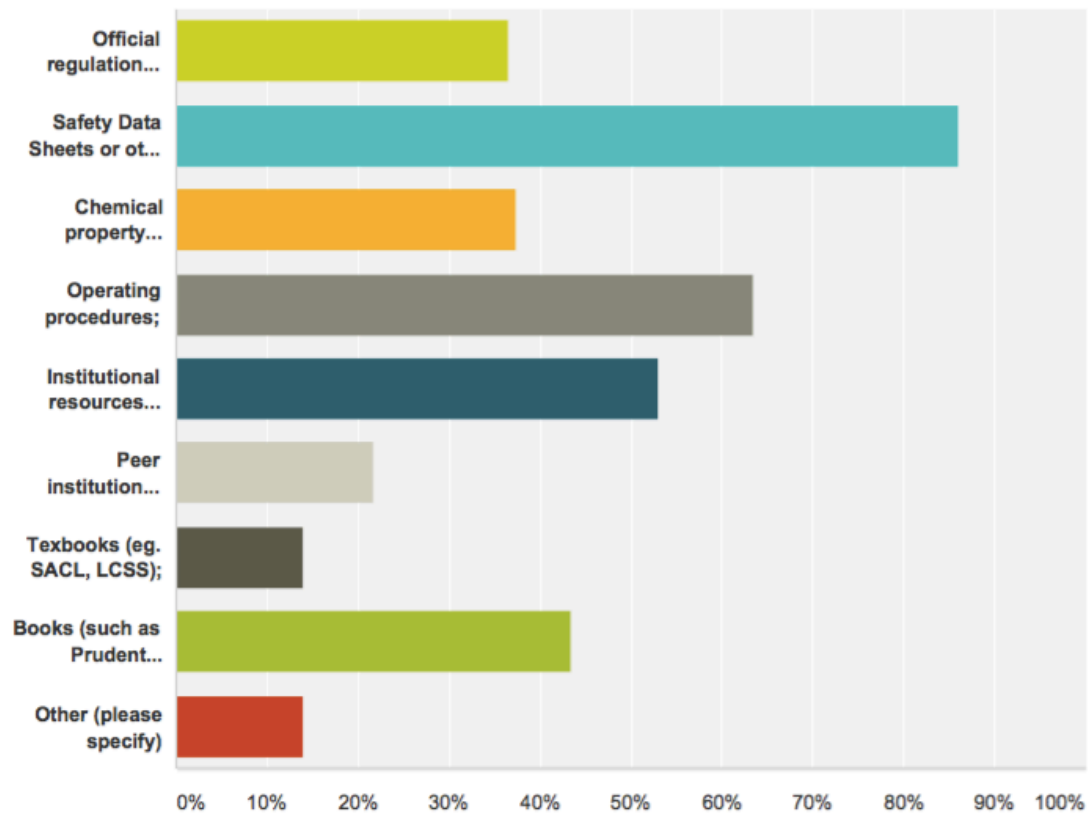


# Users Study 2: Safety Community's Value of Information Sources

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**Q6 What types of resources provide the most useful chemical hazard information for those using chemicals?**

Answered: 115 Skipped: 1

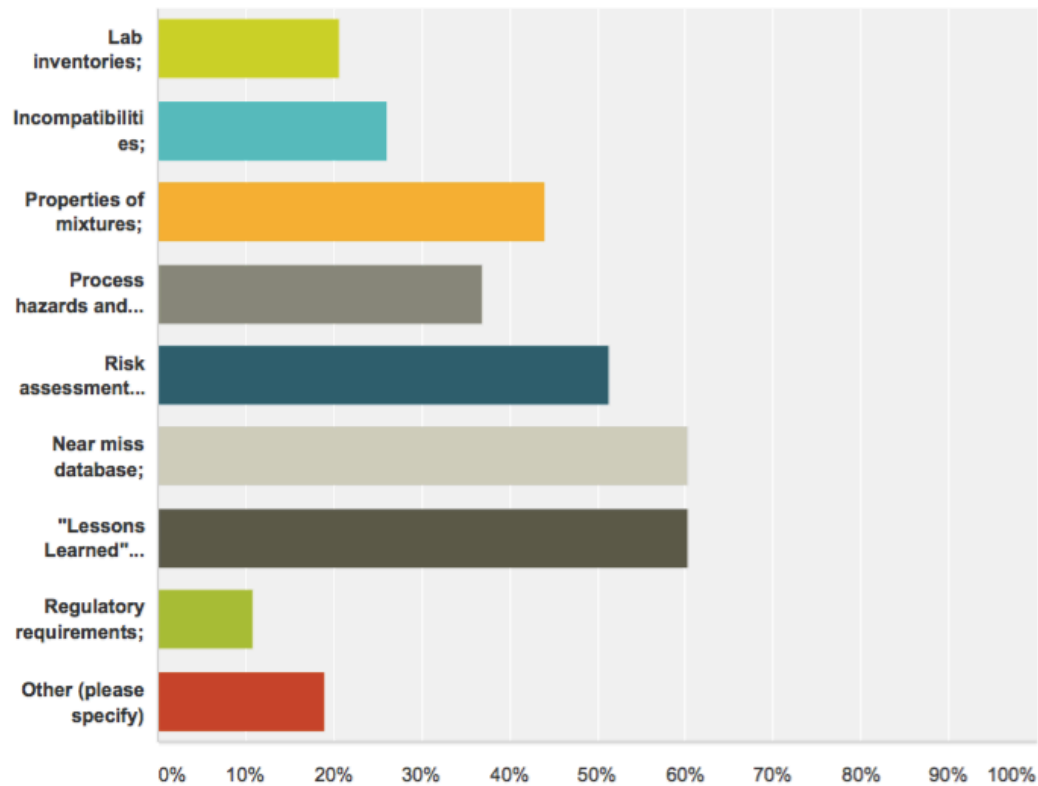


# Users Study 2: Safety Community's Missing Information

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**Q8 What kind of chemical health and safety information is needed that isn't currently readily available to you?**

Answered: 111 Skipped: 5



# Moving Forward

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- 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

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- **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*

### External Inputs:

- Funding
- Truet
- Definition of disciplines
- Etics
- Teamwork

### External Outputs:

- Public Perception
- Recruitment
- Technologies
- Problem solving
- Policies

