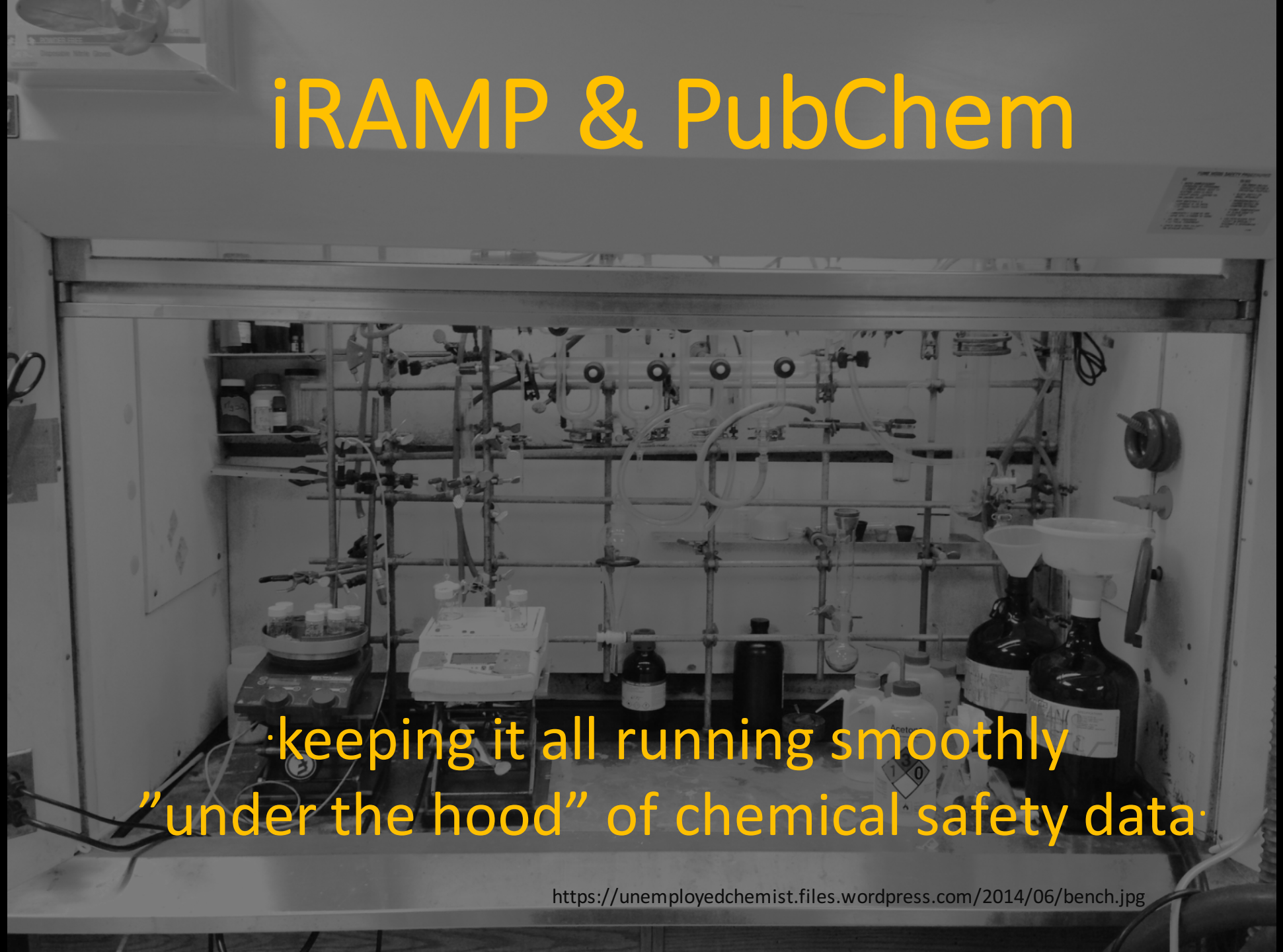
iRAMP & PubChem: Of the People, For the People

Leah McEwen, August 18, 2106

2016 Herman Skolnik Award Symposium

Honoring Drs. Bryant & Bolton

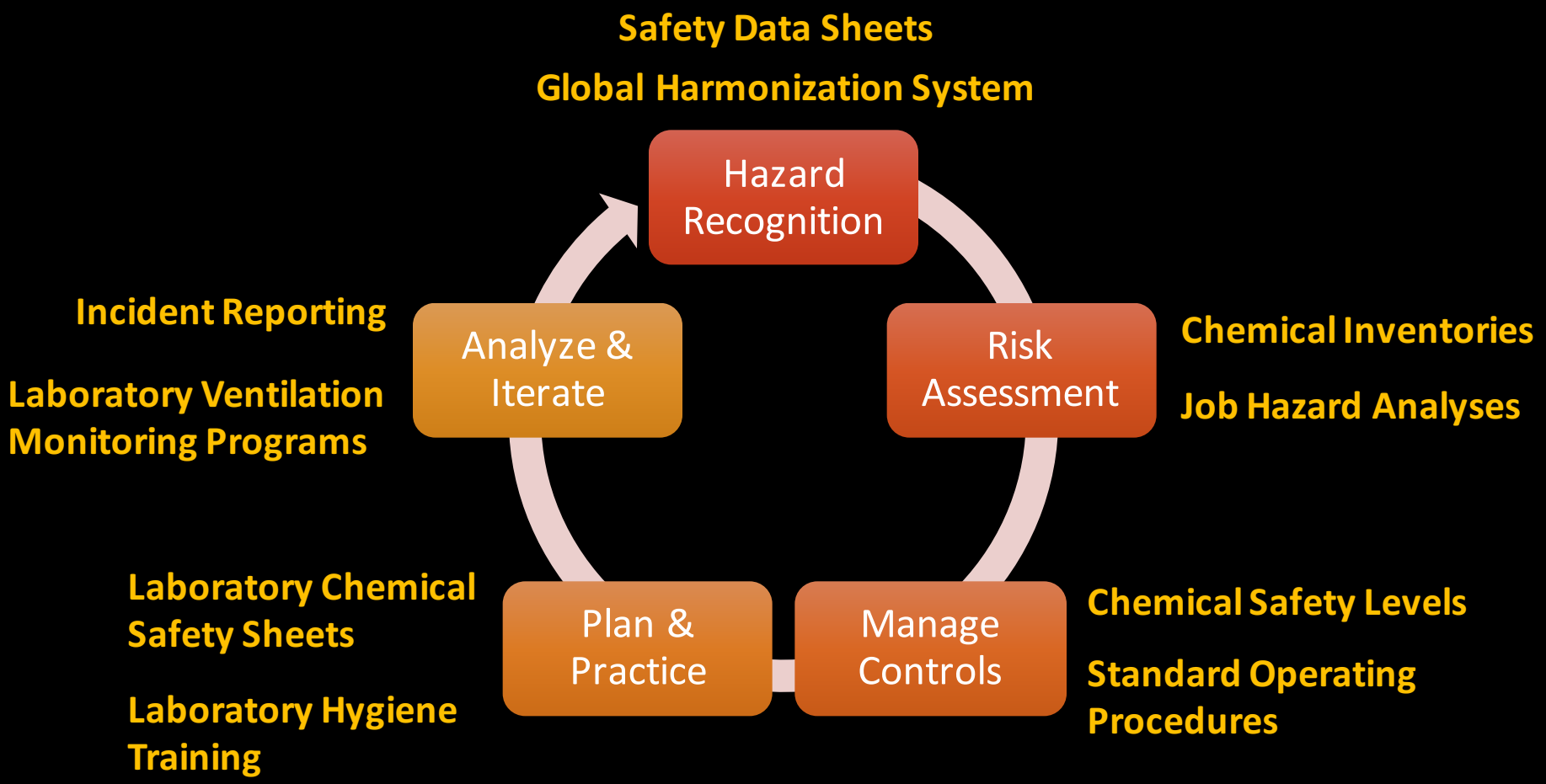
iRAMP & PubChem



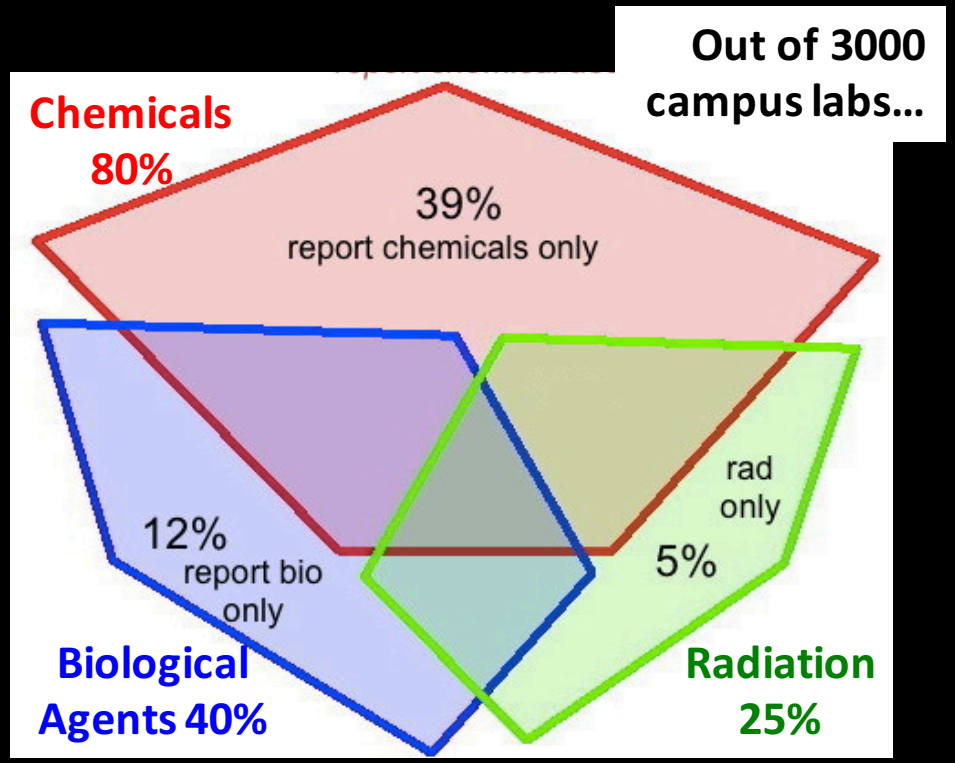
·keeping it all running smoothly
”under the hood” of chemical safety data·

https://unemployedchemist.files.wordpress.com/2014/06/bench.jpg

Chemical Safety Decision Cycle



Research Lab Environment is Complex



Information Environment is Complex

ChemID*plus:* A TOXNET DATABASE

Biological Safety Data Sheets

NIOSH Pocket Guide to Chemical Hazards

http://www.csb.gov/

Pathogen Safety Data Sheets and Risk Assessment

SDS Search and Product Safety Center

SIRI MSDS Index

International Chemical Safety Cards (ICSC)

https://www.dol.gov/

SDS and Chemical Information from Manufacturers

http://www.sigmaaldrich.com/

TOXLINE: A TOXNET DATABASE

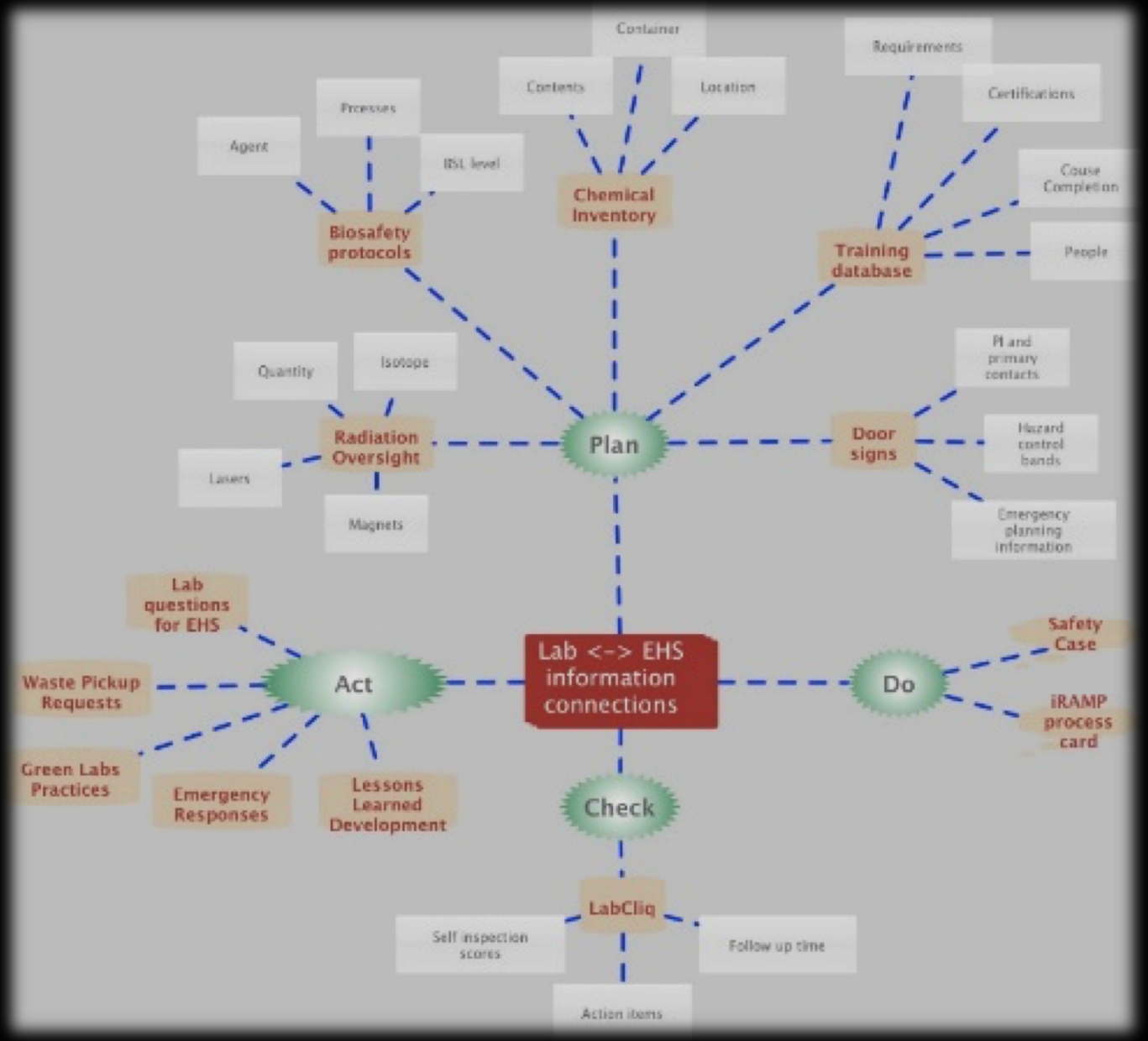
CHEMINDEX ***FREE on the WEB!***

Right to Know Hazardous Substance Fact Sheets

Who can we help?

- Research chemists
- Chemical educators
- **Chemical safety professionals**

➢Target all these groups and *multiply* impact



Questions Safety Professionals Need to Ask

1. What specific chemical and physical hazards are associated with a lab process?
2. What means (including elimination and substitution) are available to reduce or eliminate the hazard(s)?
3. Does this process require the use of engineering controls such as a fume hood, shields, etc.?
4. What PPE is appropriate?
5. What appropriate clean up and disposal protocols are required?
6. What are possible emergencies and procedures to plan for them?

ACS CCS Safety Advisory Panel, 2016

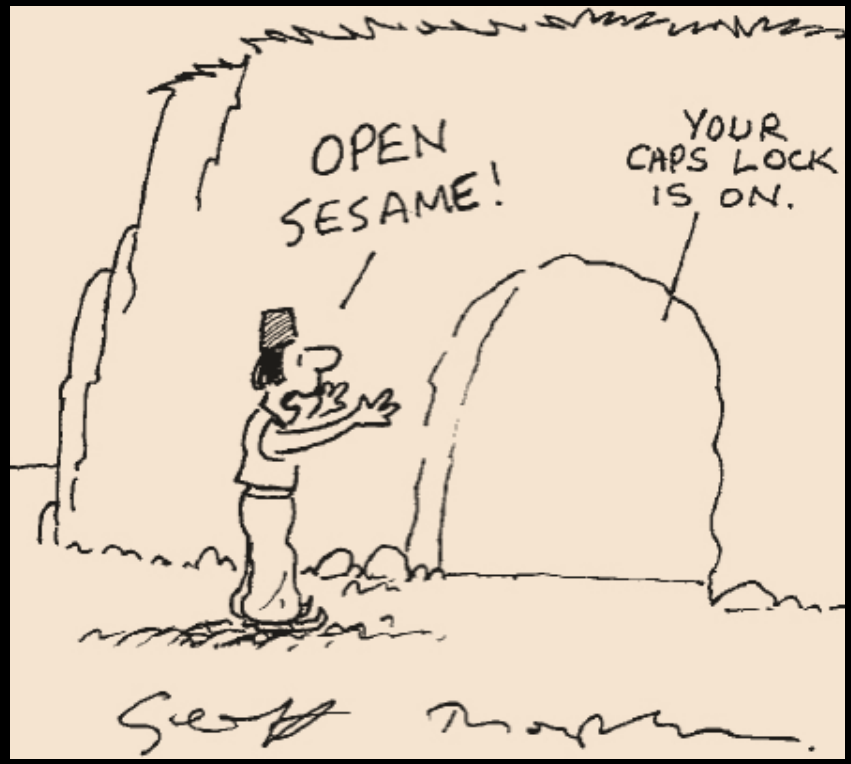
Data Supporting Chemical Risk Assessment

- Chemical Identifiers
- Physical description
- Physical Properties
- Toxicity data
- Exposure limits
- Exposure indicators
- Routes of exposure
- Target organs
- Symptoms
- First aid
- Flammability and explosivity
- Reactivity and compatibility
- Storage and handling
- Cleanup and disposal
- Emergency guidance
- Chemical replacements

Prudent Practices, National Research Council, 2011

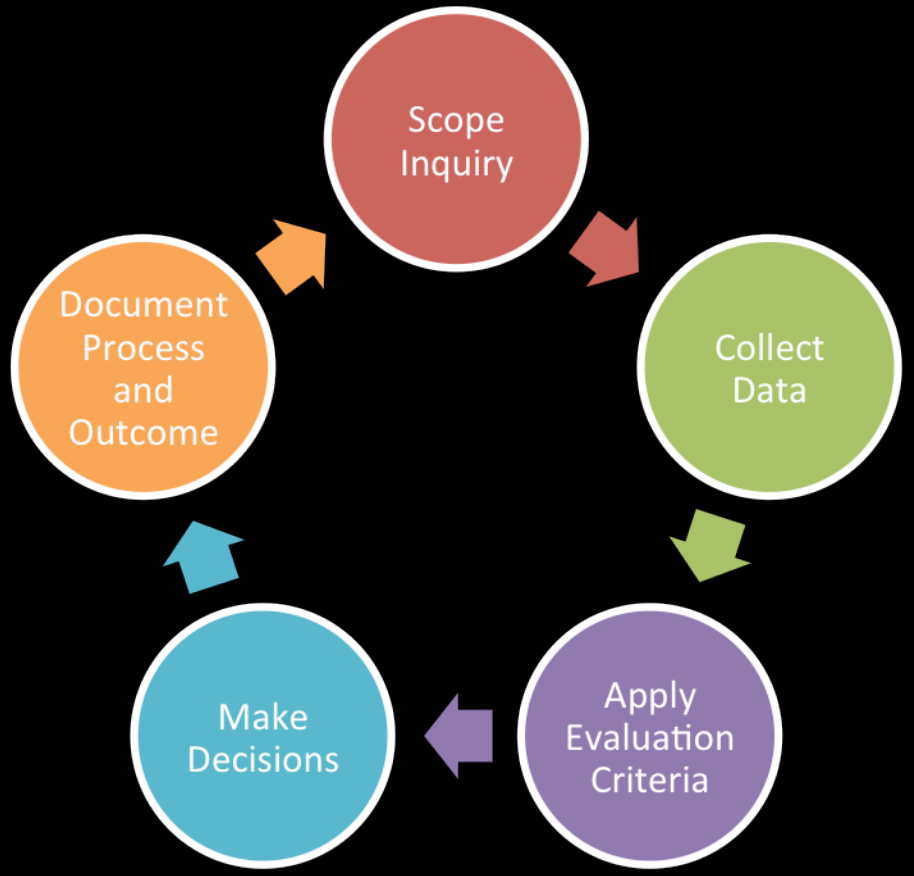
Challenges for the Information Community

- Many chemicals lack critical data
- Broad diversity of substance forms that impact chemical reactivity
- Data scattered across many sources
- Variability of reporting standards
- Most data not readily machine accessible



www.spectator.co.uk

Responsive Librarian to the Rescue!



ACRL Literacy Framework, 2015

KEEP CALM AND SPIN STRAW INTO GOLD

Chemical Safety View in PubChem

NAME

SYNONYMS [synonyms]		**CAS#**	**Formula**
[top header, 3.3]		[top header, 3.2.1]	[top header]
PHYSICAL PROPERTIES [experimental properties]			
Odor: [4.2.3, 4.219]		**Appearance:**	[top header, 4.2.1]
Water Solubility: [4.2.8]		**Vapor Density:**	[4.2.10]
Flash Point: [4.2.7]		**Vapor Pressure:**	[4.2.11]
Autoignition: [4.2.13]		**bp/mp:**	[4.2.5]/ [4.2.6]
TOXICITY [toxicological information]		**EXPOSURE LIMITS [safety and hazard properties]**	
LD_{50} oral ( )	[10.1.8]	**TLV-TWA (ACGIH)**	[9.2.18], [9.2.26]
LC_{50}inhal. ( )	[10.1.8]	**STEL (ACGIH)**	[9.2.26]
LD_{50} skin ( )	[10.1.8]	**PEL (OSHA)**	[9.2.5]
HEALTH AND SYMPTOMS [hazard identification] [toxicological information]			
General	[9.1.2-10/12], [10.1.2]		
Skin	[9.1.7,12]		
Eyes	[9.1.9,12]		
Ingestion	[9.1.10,12]		
Inhalation	[9.1.8,12]		
FIRST AID [first aid measures]			
Skin	[9.3.1,5]		
Eyes	[9.3.1,6]		
Ingestion	[9.3.1,7]		
Inhalation	[9.3.1,4]		
FLAMMABILITY & EXPLOSIVITY [safety and hazard properties],[fire fighting measures],[first aid measures]			
[9.2.9] NFPA rating (flammability) = [9.2.13]; LEL = [9.2.1]; UEL = [9.2.2] [9.4], [9.3.2,3], [9.2.16]			
REACTIVITY & INCOMPATIBILITY [reactivities and incompatibilities],[properties - chemical dangers]			
[9.8], [9.2.17]			
STORAGE & HANDLING [exposure control and personal protection],[handling and storage],[accidental release - other preventative measures]			
[9.7], [9.6], [9.5.4]			
CLEANUP & DISPOSAL [accidental release measures],[handling - nonfire spill response]			
[9.5], [9.6.1]			
ADDITIONAL CONSIDERATIONS			

NRC Form

Data contents in PubChem
Laboratory Chemical Safety Summary (LCSS)

- As of October 30, 2015
- Abbreviations in brackets indicate data sources.

GHS Classification [CLP, ICSC]
Synonyms [PC]
Identifiers
PubChem CID [PC]
CAS [DRGBNK, EPA-CDR, ICSC, NIOSH, OSHA]
InChI [PC]
InChI Key [PC]
Physical Properties
Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]
Odor [HSDB]
Boiling Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Melting Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Flash Point [HSDB, ICSC, NIOSH, OSHA]
Solubility [CAMEO, DRGBNK, HSDB, ICSC, NCI, NIOSH]
Density [CAMEO, HSDB, ICSC, NIOSH, OSHA]
Vapor Density [CAMEO, HSDB, ICSC, OSHA]
Vapor Pressure [CAMEO, HSDB, ICSC, NIOSH, OSHA]
Auto-Ignition [HSDB, ICSC]
Decomposition [HSDB, ICSC]
Corrosivity [HSDB]
Odor Threshold [HSDB]
Toxicity Data
Toxicity Summary [DRGBNK, HSDB]
Human Toxicity Values [HSDB]
Non-Human Toxicity Values [HSDB]
Exposure Limits
Immediately Dangerous to Life or Health Concentration [NIOSH, OSHA]
Recommended Exposure Limit (REL) [NIOSH, OSHA]
Permissible Exposure Limit (PEL) [NIOSH, OSHA]
REL-Time-Weighted Average Concentration (REL-TWAC) [OSHA]
REL-Short-Term Exposure Limit (REL-STEL) [OSHA]
REL-Ceiling (REL-C) [OSHA]
PEL-Time-Weighted Average Concentration (PEL-TWAC) [OSHA]
PEL-Short-Term Exposure Limit (PEL-STEL) [OSHA]
PEL-Ceiling (PEL-C) [OSHA]
Threshold Limit Values [HSDB]
Occupational Exposure Limits [ICSC]
Effects of Short Term Exposure [ICSC]
Effects of Long Term Exposure [ICSC]
Explosive Limits and Potential [HSDB, ICSC]
Radiation Limits and Potential [HSDB]
Acceptable Daily Intakes [HSDB]
Allowable Tolerances [HSDB]

Data Source Abbreviations
- ATSDR = CDC ATSDR Toxic Substance Portal
- CAMEO = NOAA CAMEO Chemicals
- CLP = Regulation (EC) No 12 1272/2008
- DRGBNK = DrugBank
- EPA-AT = EPA Air Toxics
- EPA-CDR = EPA Chemical Data Report

NIH › NLM › NCBI

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

LCSS Laboratory Chemical Safety Summary for CID 180 | Download | Print | Share | Help

PUBCHEM › COMPOUND › ACETONE › LCSS

Read about the LCSS project

Acetone

Cite this Record

PubChem CID:	180
Chemical Names:	Acetone; 2-propanone; Propanone; Dimethyl ketone; Methyl ketone; 67-64-1
Molecular Formula:	C_3H_6O or CH_3-CO-CH_3 or $(CH_3)_2CO$
Molecular Weight:	58.07914 g/mol

Contents

1 GHS Classification
2 Identifiers
3 Physical Properties
4 Toxicity Data
5 Exposure Limits
6 Health and Symptoms
7 First Aid
8 Flammability and Explosivity
9 Stability and Reactivity
10 Storage and Handling
11 Cleanup and Disposal
12 Information Sources

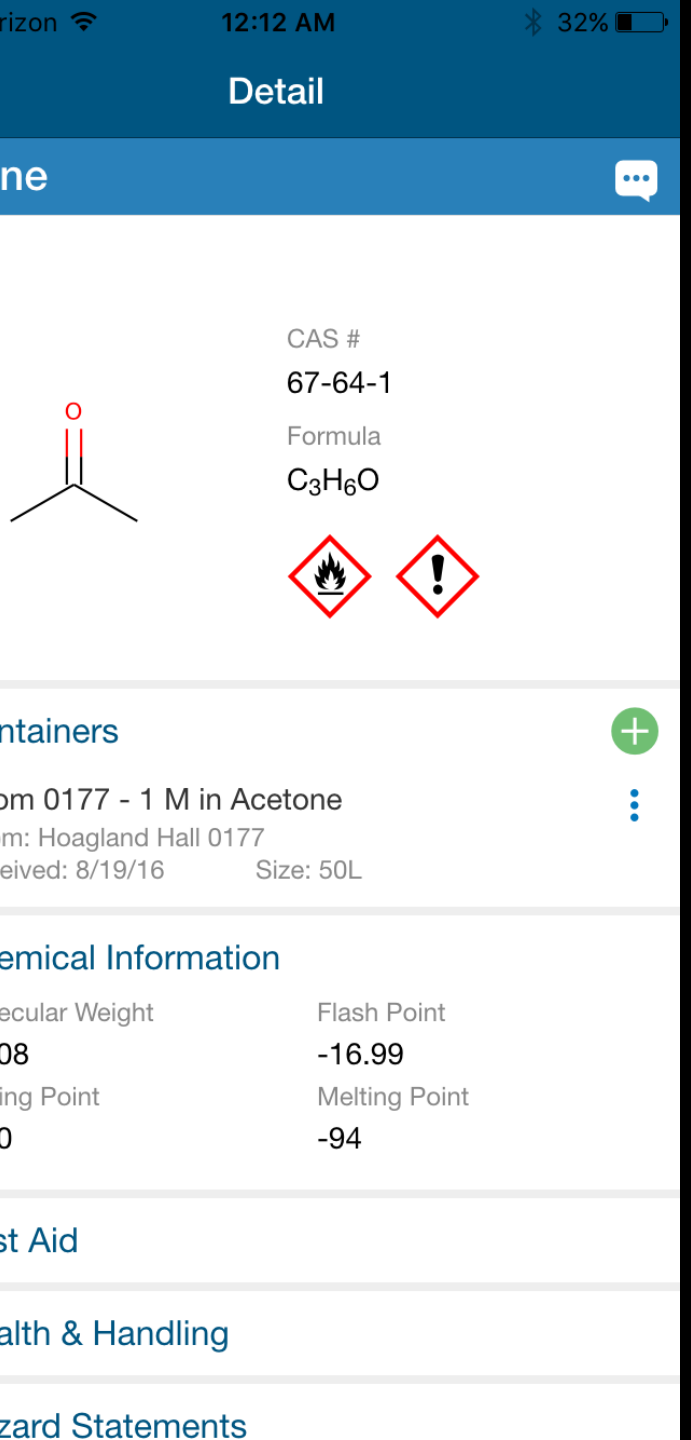
1 GHS Classification

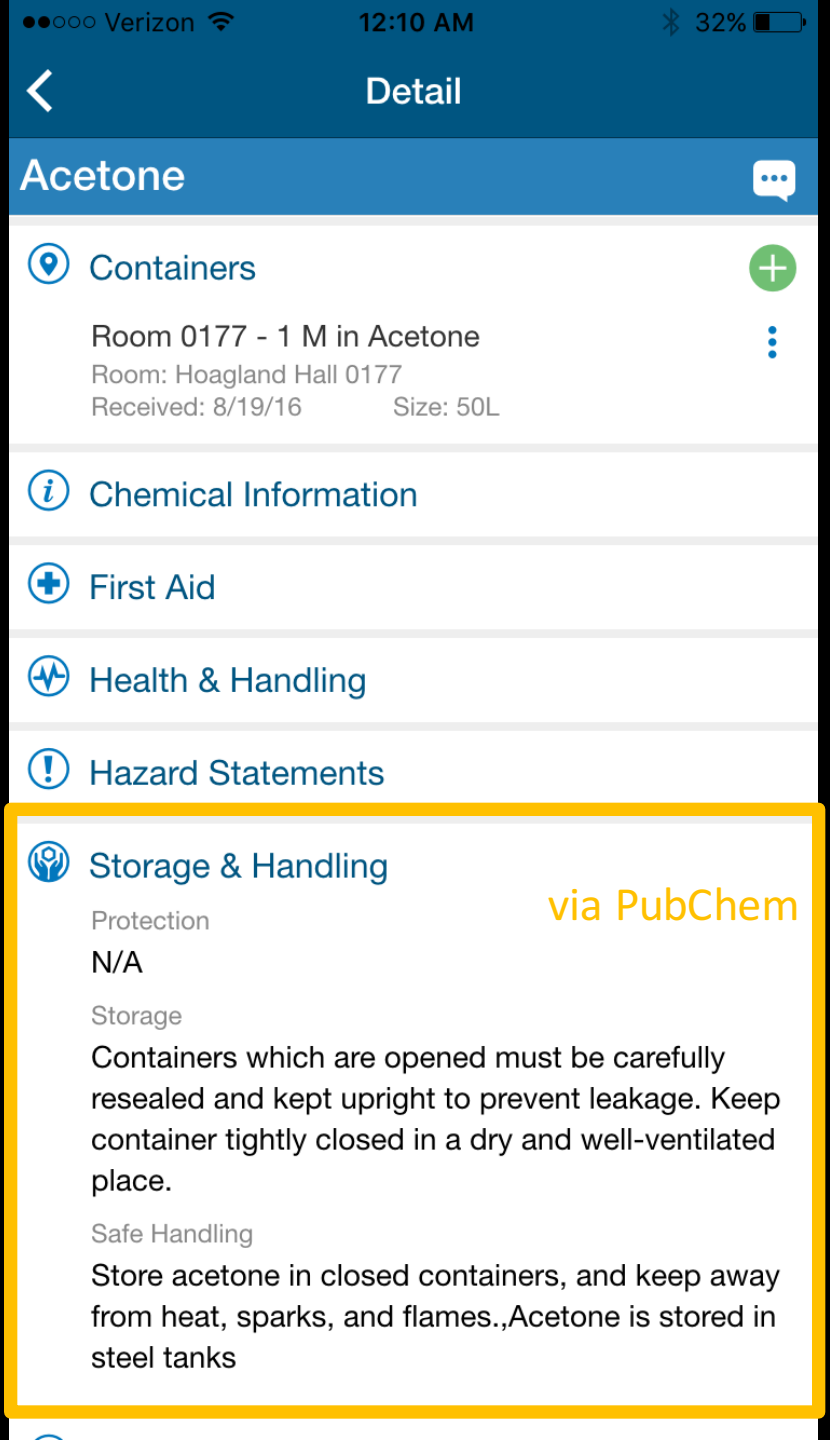
Signal: Danger
GHS Hazard Statements
H225: Highly Flammable liquid and vapor [Danger Flammable liquids - Category 2]
H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation - Category 2A]
H336: May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects - Category 3]
Precautionary Statements
P210: Keep away from heat, hot surface, sparks, open flames and other ignition sources. - No smoking.
P233: Keep container tightly closed.
P240: Ground/bond container and receiving equipment.

Use Case

UC Chemicals – Pilot

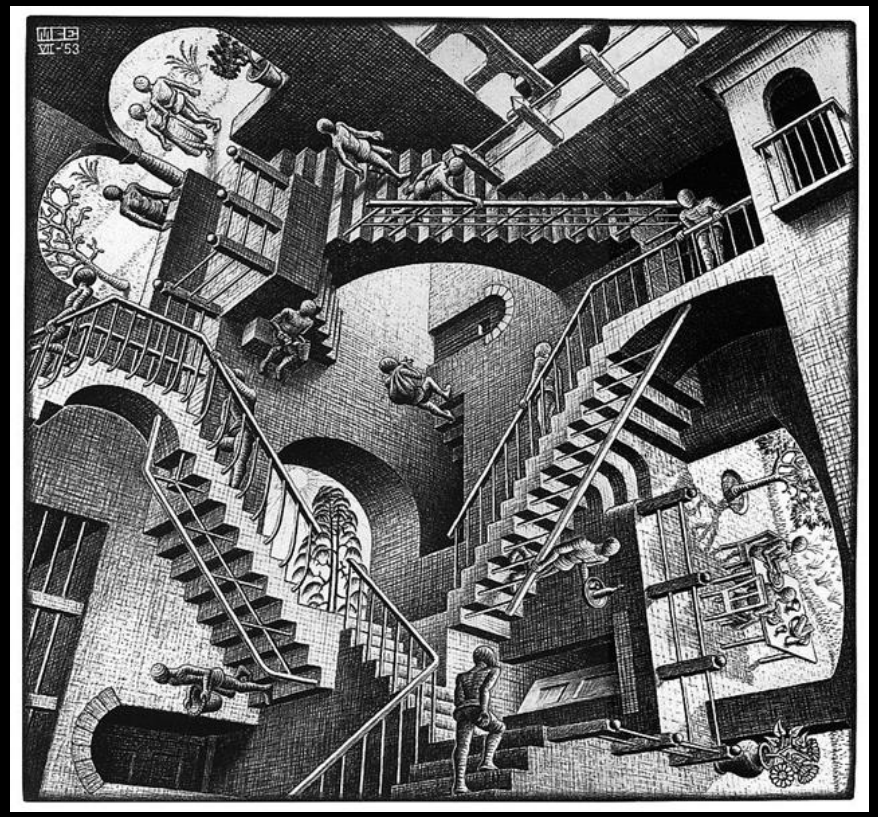
University of California chemical inventory mobile mgmt. tool





Key Gaps

1. Resolvable identifiers for mixtures
2. Associating GHS with supporting data – “Lipinski 5” indicator profile for hazard
3. Mapping chemical concepts to process conditions
4. Mapping procedures to chemical, equipment and process hazards
5. Empirical data from incidents



iRAMP

"flexibly structured ecosystem of data, workflow tools and domain expertise mapped to the essential commonalities of the use cases and content, connected by good information management practices" [3]

PubChem

enabling re-use of data in applied contexts

--

open data, open mission, open process

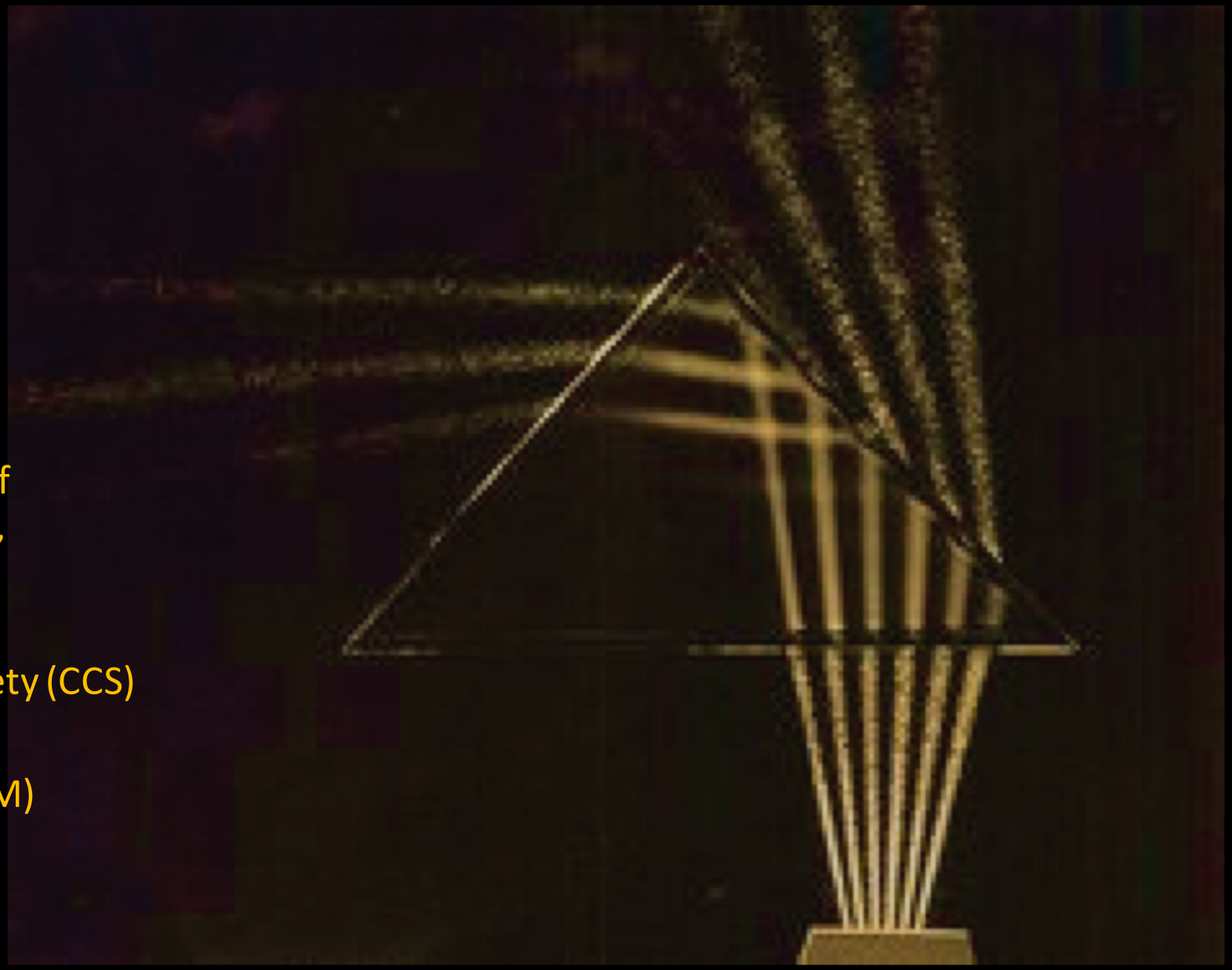
open collaboration

--

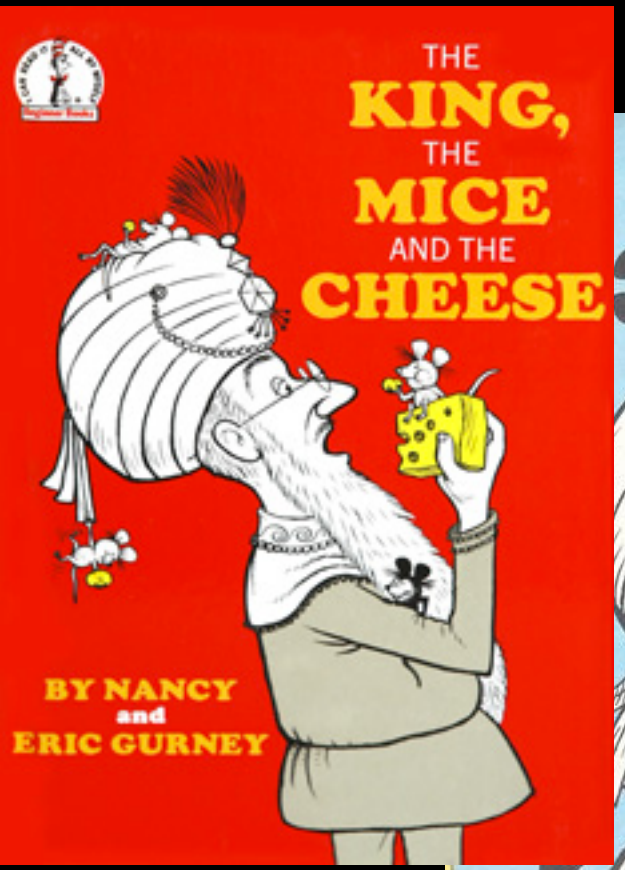
public good

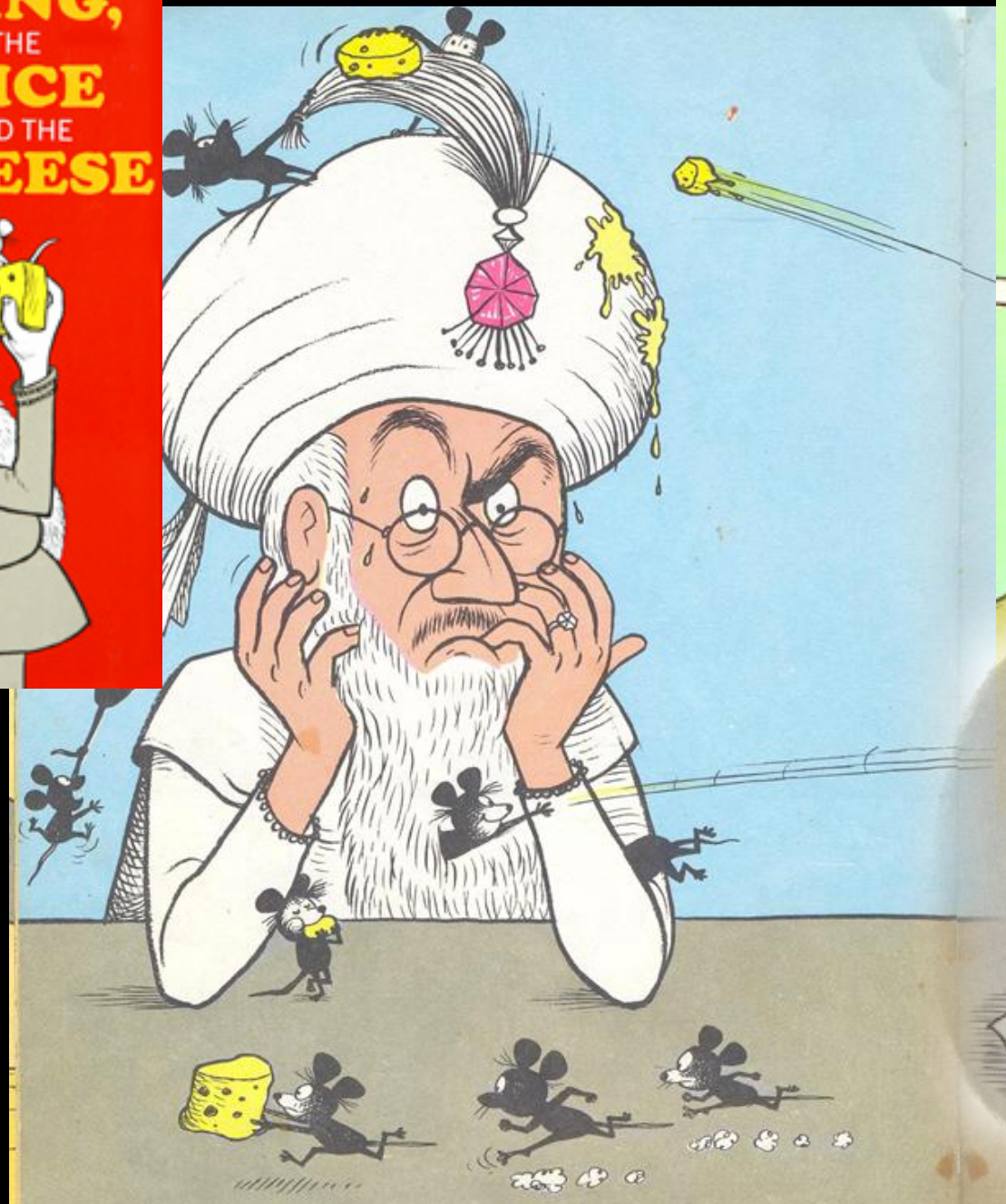
Building an ecosystem,
of the people, by the people, for the people…

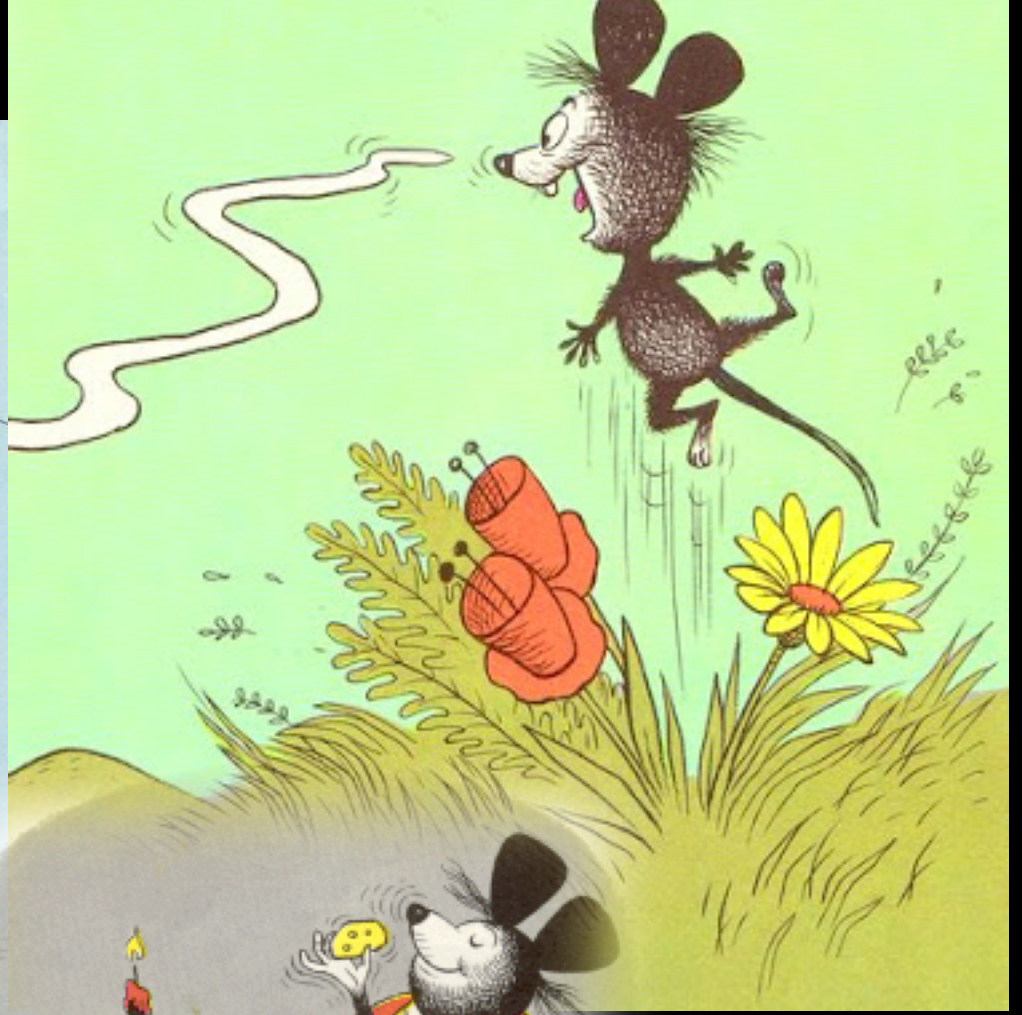
Where do we want to go?



- American Chemical Society (ACS) Professional Member Divisions of Chemical Health & Safety (CHAS), Chemical Information (CINF), Chemical Education (CHED)
- ACS Committee on Chemical Safety (CCS) Safety Advisory Panel (SAP)
- National Library of Medicine (NLM) PubChem Team
- University of California, Office of the President (UCOP)


THE
KING,
THE
MICE
AND THE
CHEESE
BY NANCY
and
ERIC GURNEY





Thank you, Evan and Steve,

for your sanguine and determined efforts towards improving quality of life!

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://dx.doi.org/10.1515/ci-2015-0505
4. More information about the project can be found at https://pubchem.ncbi.nlm.nih.gov/lcss/ and http://www.irampp.org