

Chemical Management Applications for the University of California

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Outline

2

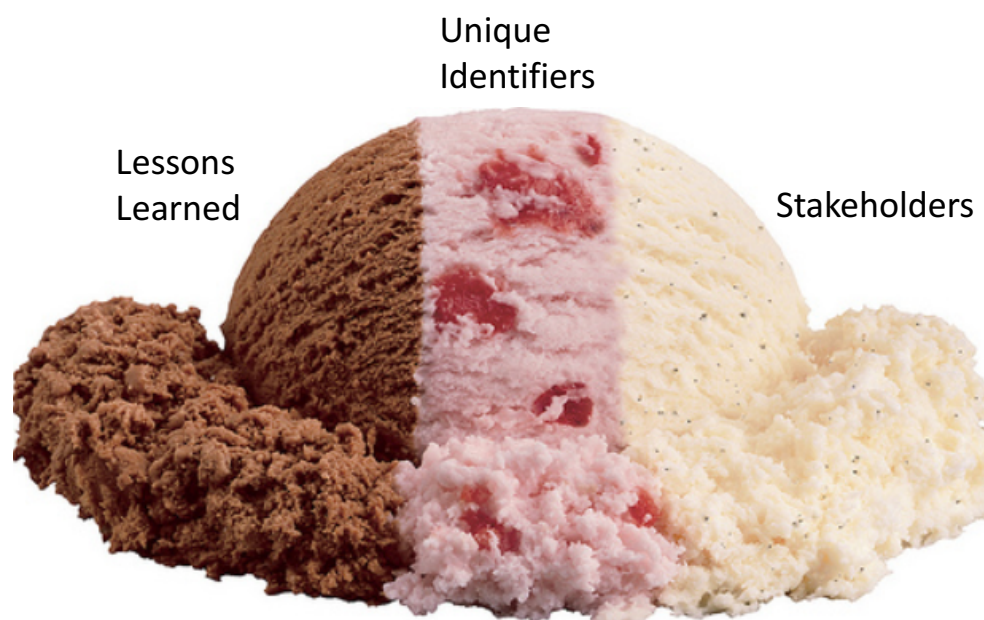
- Overview of the UC Chemical Management Solution

- ❑ Stakeholders

- Data Challenges

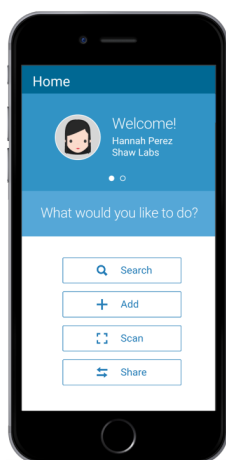
- ❑ Unique Identifiers

- Lessons Learned



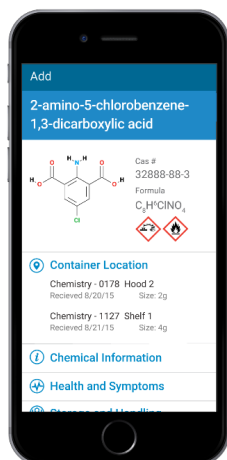
Example Researcher Workflow

- To quickly add a chemical container to an inventory



Step 1

Launch the app



Step 2

Find the chemical



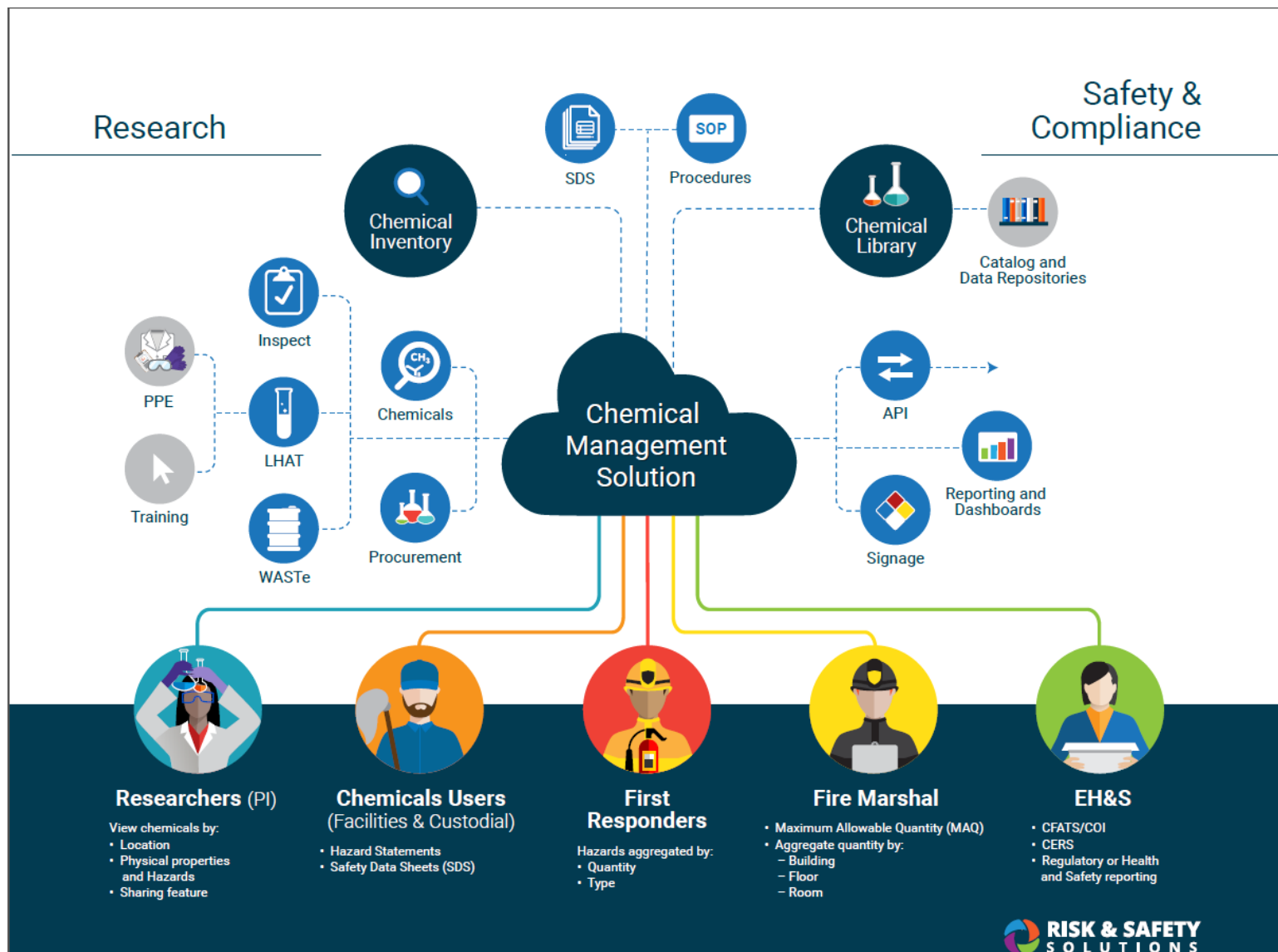
Step 3

Add a barcode sticker



Step 4

Scan it



Stakeholder: Researchers

- Who: Undergraduate, Graduate Researchers at 10 University of California Campuses, Medical Centers
- Use: Locations, Quantities, Physical Properties and Hazards, Chemical Reagent Sharing
- Interface: Edit and Maintain (Inventory) Data



Stakeholder: Chemicals User

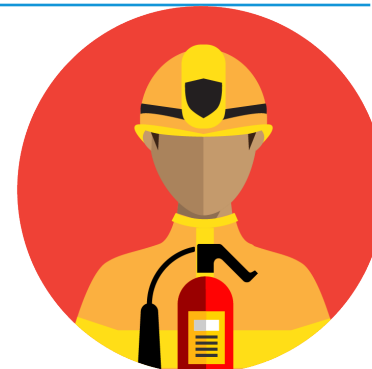
- Who: Facilities, Fleet Services, Theater shop, etc.
- Use: Hazard information (Safety Data Sheets)
- Interface: Edit and Maintain (Inventory) Data



Stakeholder: First Responders

7

- Who: Emergency Service Providers
- Use: Aggregate of Acute Hazards in a Room
- Interface: View Only



Fire Marshal

8

- Who: Campus Fire Marshals, Fire Prevention
- Use: Compliance Reports: Maximum Allowable Quantity (MAQ)
Aggregate by Control Area (Building, Floor, Room)
- Interface: View Only (Inventory)



Safety Professional

9

- Who: Campus Health and Safety
- Use: Compliance reports, Business Intelligence, Carcinogens
- Interface: View and Edit Inventory (Campus Dependent)



Data Challenges: Unique Identifiers

Unique Identifier: Name

ws: 151 Spec - Columns: 2 Properties Flow Variables

S Chemical	Count*...
1,4-tert-butyllithium	1
1,5-n-butyllithium	1
1.6m n-butyl lithium in hexane	1
3-n-butyllithium	2
4-n-butyllithium	1
butyl lithium	4
butyl lithium (sec-butyl lithium)	1
butyl lithium 2.5m	1
butyllithium solution	1
butyllithium solution, 2.5m in hexanes	1
butyllithium	33
butyllithium (2.5 m in hexanes)	6
butyllithium 1.6 m in hexanes	4
butyllithium 2.5 m in hexanes	1
butyllithium 2.5m in hexane, n-	1
butyllithium 2.5m sol in hexanes	1
butyllithium in cyclohexane	1
butyllithium in hexane	1
butyllithium in hexanes	1

Ex) Butyl Lithium nomenclature across the University of California Inventory

-443 “Unique” Names

-Removing capitalization: 151

= ~60 Total Materials

Unique Identifier: CAS

6

Ex) Diisobutyl aluminum hydride solution

Peroxide former

☐ 214981 1.0 M in THF

☐ 214949 1.0 M in cyclohexane

OSHA
specifically
regulated
carcinogen

☐ 214973 1.0 M in methylene chloride

☐ 214965 1.0 M in heptane

☐ 256846 1.0 M in heptane

☐ 190306 1.0 M in hexanes

☐ 256870 1.0 M in toluene

Item Number: Diisobutylaluminum hydride, 1M solution in toluene

Item Number: Diisobutylaluminum hydride, 1M solution in hexane

Item Number: Diisobutylaluminum hydride, 1M solution in toluene, packaged under Argon





Item Number: Diisobutylaluminum hydride, 25% w/w in hexane

Item Number: Diisobutylaluminum hydride, 25% w/w in hexane, packaged under Argon in

Item Number: Diisobutylaluminum hydride, 1M solution in hexane, packaged under Argon

Unique Identifier: Group by Hazard Assessment?

<input type="checkbox"/> 216763	contains inhibitor, 30 wt. % in H ₂ O, ACS reagent
<input type="checkbox"/> 316989	contains potassium stannate as inhibitor, 30-32 wt. % in water, semiconductor grade, 99.999% trace metals basis
<input type="checkbox"/> H3410	contains inhibitor, 30 wt. % in H ₂ O, meets USP testing specifications
<input type="checkbox"/> 16911	for ultratrace analysis
<input type="checkbox"/> 95321	≥30%, for trace analysis
<input type="checkbox"/> 516813	50 wt. % in H ₂ O, stabilized
<input type="checkbox"/> 349887	contains 35 wt. % inhibitor (H ₂ O)
<input type="checkbox"/> H1009	30 % (w/w) in H ₂ O, contains stabilizer
<input type="checkbox"/> 323381	contains ~200 ppm acetanilide as stabilizer, 3 wt. % in H ₂ O
<input type="checkbox"/> 95294	tested according to Ph.Eur.
<input type="checkbox"/> 40287	, ≥30%
<input type="checkbox"/> 40307	≥30%
<input type="checkbox"/> 95299	purum p.a., ≥35% (RT)
<input type="checkbox"/> 18304	meets analytical specification of Ph. Nord., 34.5-36.5%
<input type="checkbox"/> 88597	3%, for microbiology
<input type="checkbox"/> 31642	30% (w/w),

Color	% H ₂ O ₂
	3-30%
	30%
	30-35%<
	50%

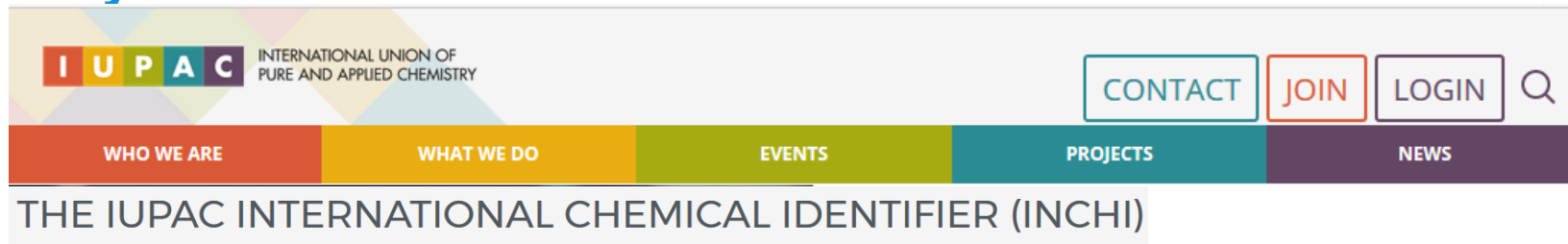
External structures:

Chemical Facilities Anti
Terrorism Standards (**CFATS**):
2 divisions (≤35%)

Occupational Safety and Health
Administration (**OSHA**): 3
divisions (≤20%; 21-60%; >61%)

International Fire Code (**IFC**)
Appendix E: 4 divisions (8-27.5%;
27.5-52%; 59-91%, >91%)

Unique Identifier: Why InChI for Mixtures



- Most (all) substances are mixtures *in practice*
- Many use cases for documenting mixtures of substances
 - Inventories
 - Catalogs
 - Tracking (including during experiments, across literature)
 - Other reporting
- Lack of existing systematic notation
- Machine readable chemical composition useful in these large systems

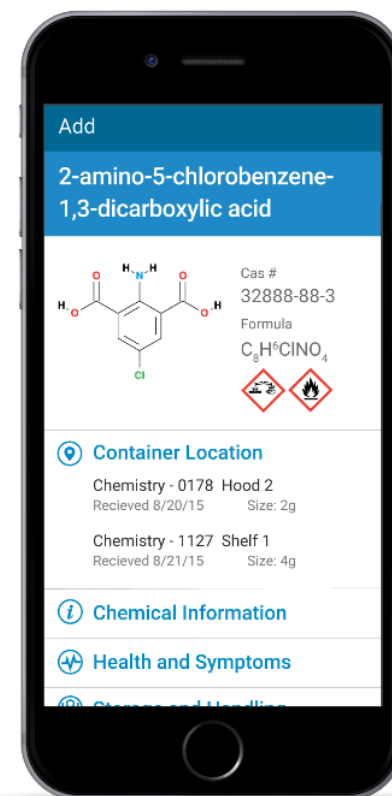
Lessons Learned

Lesson Learned: (Step 2) Find the Chemical

- Expectation: You know what my container is.
- Vs.
- Reality: 1000s of vendors, numerous products
- User Question: How do I find the right entry?
- -Unique Identifiers Displayed to User vs Space
- -Purchasing?

- Rows: 1201 Spec - Columns: 2

(...) vendor	Unique count...
[Gibco]	22
[Thermo]	25
[Fluka]	26
[Gelest]	26
[Pierce]	26
[Clontech]	31
[ACROS]	33
[Ambion]	33
[Bio-Rad]	38
[Difco]	41
[ALFA_AESAR]	42
[Thermo Scientific]	46
[Invitrogen]	51
[IDT]	52
[BD]	56
[Qiagen]	77



Lessons Learned: Ease of Utility

- Free Entry vs Picklist

Free Entry

Comments

Picklist

Type

Choose a Type

- Choose a Type
- Above Ground Tank
- Ampule
- Bag
- Box
- Can
- Carboy
- Cryogenic Dewar
- Cylinder
- Fiber Drum
- Glass Bottle
- Other
- Plastic Bottle
- Plastic/Non-metallic Drum
- Steel Drum
- Tank Inside Room
- Underground Tank

Lessons Learned: Ontologies

- Mapping of External Database Unique Identifiers to Internal Structures
ex.) BoilingPoint – Boiling point, BP, Boiling Point, Boilpoint, etc.
- How/What Should be Grouped



Can of Paint



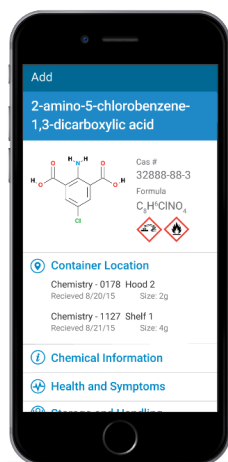
Color



Vendor?

Practicality

- Ease of Access
- High turnover items
- Lab supplies



Mobile

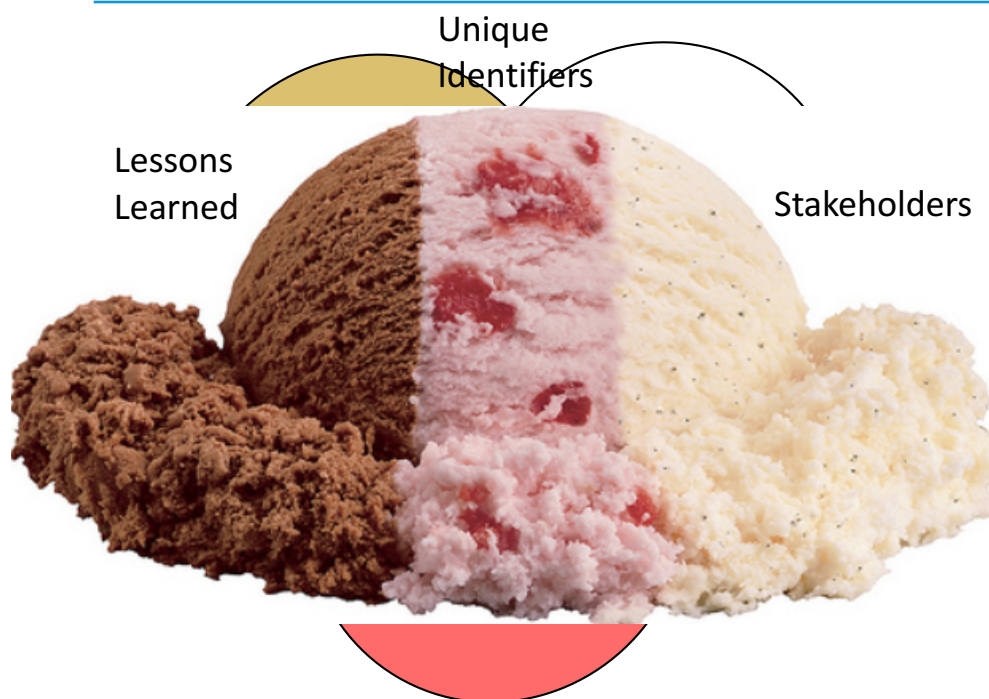


Solvent



Culture Tubes/ Lab Supplies

Summary



External Collaborators

- American Chemical Society
 - Division of Chemical Health and Safety
 - Division of Chemical Information
- Cornell University
- International Union of Pure and Applied Chemistry/ International Chemical Identifier (IUPAC-InChI)
- Keene State
- Millipore-Sigma
- National Institute of Health ([PubChem](#))
- SciQuest
- ThermoFisher Scientific
- U.S. Environmental Protection Agency ([CompTox](#))

Questions?

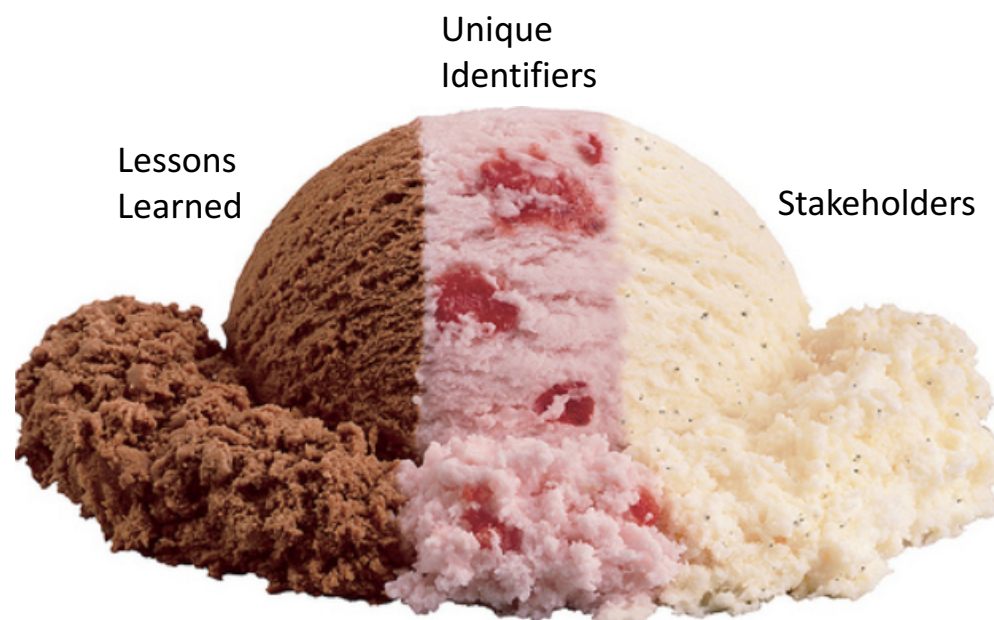
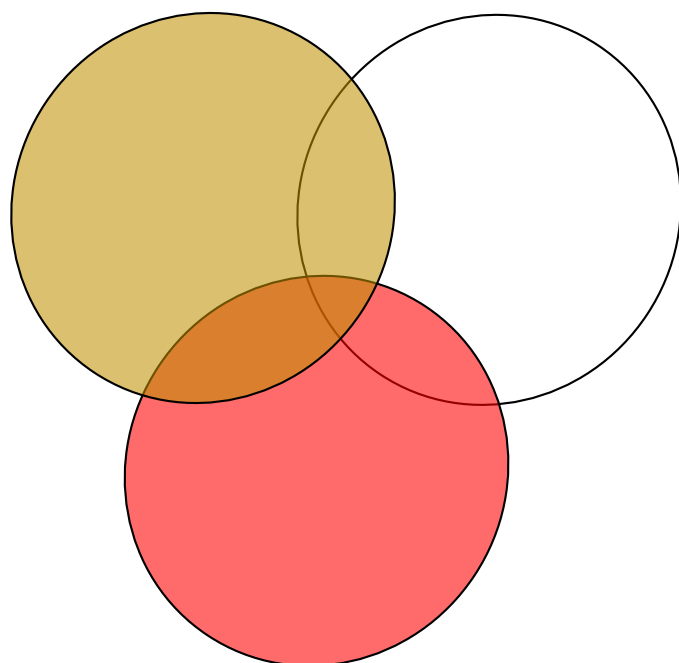
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Stakeholders

Lessons Learned

- Find and Add to my Inventory
- Ease of Utility vs Accuracy
- Ontologies?
- Practicality

- Multiple/One record? (searching is a struggle) (aggregation/disaggregation and affects on search results)

Search add

multiple

- High turnover containers (barcoding an area)
- Information displayed to help identify container (Helping users filter search results down to what they have)