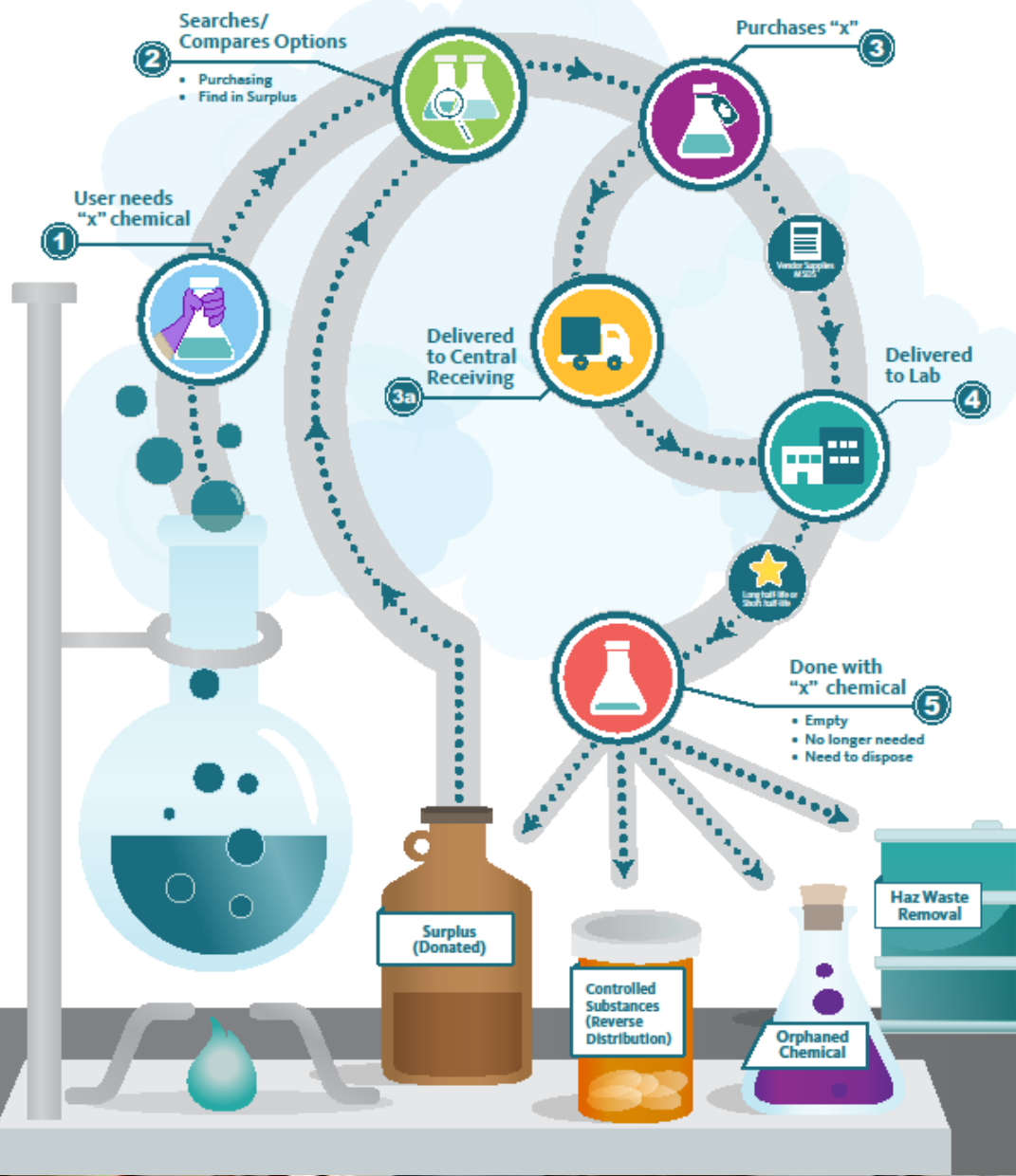


CHEMICAL LIFE CYCLE



UC Chemicals: An overview of growing challenges

Chris Jakober, Russell Vernon, Phillip Painter

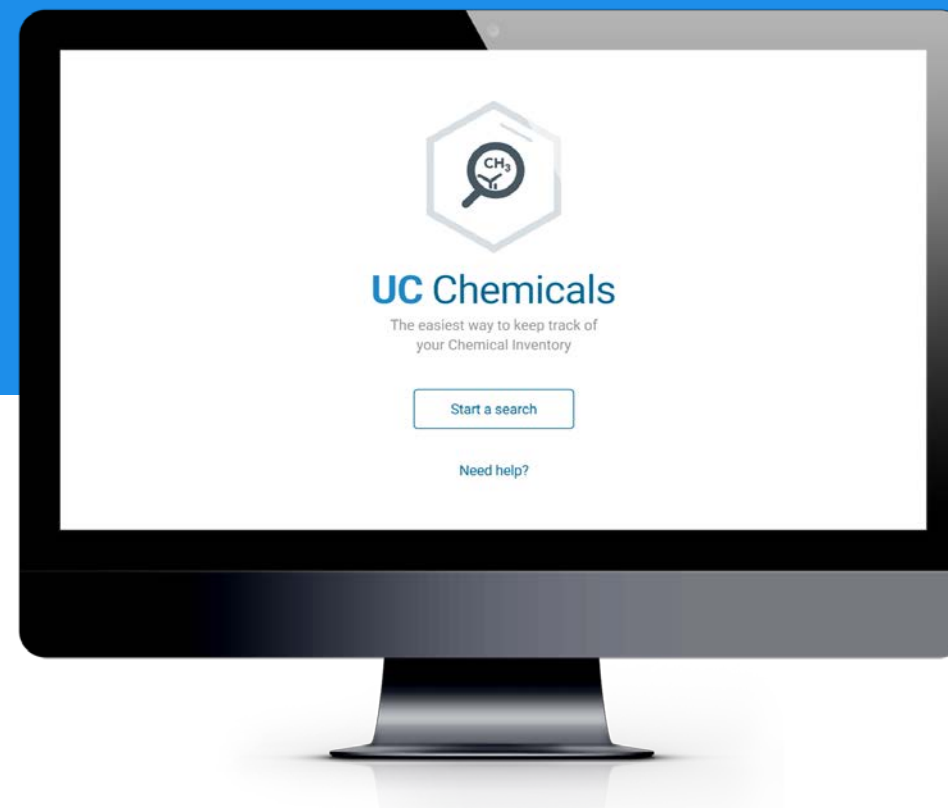
Philadelphia ACS 8/24/16

UC Chemicals: Two Complementary Platforms



Mobile

- Provides access when and where needed
- Leverages device OS barcode scanner

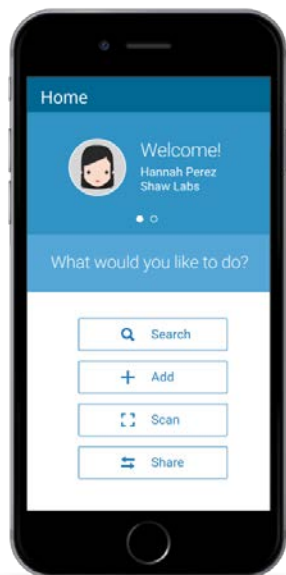


Desktop

- Intuitive Web-application for desktop users
- Quickly reconcile physical inventory w/ a hand held scanner
- Search chemicals by sub-structure

Just 4 steps

- 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

Done!

Data Challenges

- Cross indexing chemicals difficult without unique nomenclature
- Ex) CAS #

3864 matches found for 64-17-5 ☰ ☰ Sort By Relevance ▾

Ethanol

6 Product Results | Match Criteria: Product Name, CAS Number, Description Properties ▮



CH3CH2OH
Synonym: Ethyl alcohol
Linear Formula: CH3CH2OH | Molecular Weight: 46.07 | CAS Number: 64-17-5

<input type="checkbox"/>	32205 absolute, reag. ISO, reag. Ph. Eur., ≥99.8% (GC), liquid (clear, colorless) (Sigma-Aldrich)	◇ SDS		pricing ▾
<input type="checkbox"/>	34923 absolute, ≥99.8% (GC) (Sigma-Aldrich)	◇ SDS		pricing ▾
<input type="checkbox"/>	34852 absolute, for HPLC, ≥99.8% (Sigma-Aldrich)	◇ SDS		pricing ▾

Data Challenges



- Finding and integrating reliable data
- Ex) Formaldehyde from PubChem

4.2.4 Boiling Point  	
-19.5 deg C <i>Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-278</i>	▶ from HSDB
-19.1 °C <i>PhysProp</i>	▶ from DrugBank
-20°C	▶ from ILO-ICSC
98°C	▶ from ILO-ICSC

- Reliable data sources for the 20+ million available commercial consumer chemicals
- Ex) Simple Green SDS

Section 3: COMPOSITION/INFORMATION ON INGREDIENTS

<u>Ingredient</u>	<u>CAS Number</u>	<u>Percent Range</u>
Water	7732-18-5	> 84.8%*
Ethoxylated Alcohol	68439-46-3	< 5%*
Sodium Citrate	68-04-2	< 5%*
Tetrasodium <i>N,N</i> -bis(carboxymethyl)-L-glutamate	51981-21-6	< 1%*
Sodium Carbonate	497-19-8	< 1%*
Citric Acid	77-92-9	< 1%*
Isothiazolinone mixture	55965-84-9	< 0.2%*
Fragrance	Proprietary Mixture	< 1%*
Colorant	Proprietary Mixture	< 1%*

**specific percentages of composition are being withheld as a trade secret*

Data Challenges



- Different physical properties from different manufacturers
- Ex) Peracetic acid

Peragen Systems, LLC.

aq-PAA™ Aqueous Peracetic Acid, Revision June 15, 2009

pH	N.E.
Vapor pressure	approximately 50 mm Hg at 42 deg C
Vapor density (air = 1):	0.79
Boiling point:	105 - 110 deg C at 760 mm Hg (decomposes at temperature >55 deg C)
Melting point	N.E.
Solubility in water:	Completely soluble and miscible.
Specific gravity (H ₂ O = 1):	1.04
SADT	Passed at >50 deg C (49 CFR 173.21, UN Method 28)

Millipore-Sigma

PHYSICAL AND CHEMICAL PROPERTIES

Information on basic physical and chemical properties

a) Appearance	Form: liquid Colour: colourless
b) Odour	pungent
c) Odour Threshold	No data available
d) pH	< 1.0
e) Melting point/freezing point	Melting point/range: -44 °C (-47 °F)
f) Initial boiling point and boiling range	107 °C (225 °F) at 1,013 hPa (760 mmHg)
g) Flash point	56 °C (133 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	27 hPa (20 mmHg) at 25 °C (77 °F)
l) Vapour density	No data available
m) Relative density	1.13 g/cm ³ at 25 °C (77 °F)

Data Challenges



- What models are acceptable for Toxicological classification?
- Ex) Hydrogen Peroxide 30%

Toxicity to Animals:

Acute oral toxicity (LD₅₀): 6667 mg/kg (Mouse) (Calculated value for the mixture) Acute dermal toxicity (LD₅₀): 6667 mg/kg (pig) (Calculated value for the mixture).

SECTION 11 — TOXICOLOGICAL INFORMATION

Acute effects: Corrosive to all body tissues.

Chronic effects: Dermatitis.

Target organs: N.A.

ORL-HUMAN LD₅₀: 1429 mg/kg

IHL-RAT LC₅₀: 2000 mg/m³

SKN-RAT LD₅₀: 3000 mg/kg

- Different values within the same animal model

LC50 Rat inhalation 1462 ppm/4 hr (2.63 mg/L)

[ITI. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 237] **PEER REVIEWED**

- Ex) Ethylene Oxide

LC50 Rat inhalation 1.44 mg/L/4hr

[European Chemicals Bureau; IUCLID Dataset, Ethylene Oxide (CAS # 75-21-8) p. 44 (2000 CD-ROM edition). Available from, as of July 9, 2008: <http://esis.jrc.ec.europa.eu/> **PEER REVIEWED**

LC50 Rat inhalation 0.9 mg/L/1 hr

[European Chemicals Bureau; IUCLID Dataset, Ethylene Oxide (CAS # 75-21-8) p. 45 (2000 CD-ROM edition). Available from, as of July 9, 2008: <http://esis.jrc.ec.europa.eu/> **PEER REVIEWED**

Data Challenges



- Hazards only captured in precautionary statements
- Ex) Bromine

SDS from Millipore-Sigma

Hazard statement(s)

H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H330	Fatal if inhaled.
H400	Very toxic to aquatic life.

10.5 Incompatible materials

Reducing agents. Alkali metals, Powdered metals, Aluminum, Stainless steel, Iron, Copper, Organic will attack some types of plastics, rubber, and coatings, Aldehydes, Ketones, arsenic powder, Aminophenols, Alcohol, reacts violently with: Ammonia, Azides, Ozone

CFC Appendix

E102.1.7 Oxidizers. Examples include:

1. Gases: oxygen, ozone, oxides of nitrogen, fluorine and chlorine (reaction with flammables is similar to that of oxygen).
2. Liquids: bromine, hydrogen peroxide, nitric acid, perchloric acid, sulfuric acid.
3. Solids: chlorates, chromates, chromic acid, iodine, nitrates, nitrites, perchlorates, peroxides.

Data Challenges



Global Harmonized Standard (GHS) can be more descriptive than California Fire Code (CFC)

Material Classification	Class	2013 CFC Definition	UN Definition
Oxidizer		3 Causes severe increase in burning rate of combustible materials it comes into contact with	<p>Oxidizing liquid Category 2: Any chemical which in 1:1 mixture, by mass, of chemical and cellulose tested, shows a mean pressure rise time \leq the mean pressure rise of a 1:1 mixture, by mass, of 40% aqueous sodium chlorate solution and solution; and does not meet Category 1 criteria</p> <p>Oxidizing solid Category 2: Any chemical which in the 4:1 ratio or 1:1 sample-to-cellulose ratio (by mass) tested, exhibits a mean burning time \leq a burning time of a 2:3 mixture by mass of potassium bromate and cellulose and does not meet criteria for Category 1.</p>
Oxidizer		2 Causes moderate increase in burning rate of combustible materials it comes into contact with	<p>Oxidizing solid, Oxidizing liquid,</p> <p>Oxidizing liquid Category 3: Any chemical in 1:1 mixture by mass of chemical and cellulose shows a mean pressure rise time of a 1:1 mixture by mass of 65% aqueous nitric acid and cellulose; and does not meet the criteria for Categories 1 and 2.</p> <p>Oxidizing solid Category 3: Any chemical which, in 4:1 or 1:1 sample-to-cellulose ratio (by mass) tested shows a mean burning time \leq mean burning time of a 3:7 mixture by mass of potassium bromate and cellulose and does not meet the criteria for Categories 1 and 2.</p>

- Different regulatory structures have different classification criteria
- Ex) Water-reactive

Material Classification	Class	2013 CFC Definition	UN Definition
Water-reactive		3 React explosively with water without requiring heat or confinement	Chemicals which in contact with water, emit flammable gases, Category 1: Reacts vigorously with water at ambient temperatures and usually has the gas produced ignite spontaneously, or reacts readily with water at ambient temperatures such that rate of evolution of flammable gas is ≥ 10 L/kg of chemical over any 1 min.
Water-reactive		2 React violently with water or can boil water. Produce flammable, toxic, or hazardous gases , or evolve enough heat to autoignite or ignite combustibles upon exposure to water or moisture	Chemicals which in contact with water, emit flammable gases, Category 2: Reacts readily with water at ambient temperatures such that the maximum rate of evolution of flammable gas is ≥ 20 L/kg of chemical per hour, and does not meet criteria for Category 1.

Challenges



- Chemicals can be shipped with a stabilizer modifying their reactivity.
 - Ex) Peracetic acid is classified as an Unstable Reactive 3
- Used as example of Class 4 material in the CFC

California Fire Code (CFC)

E102.1.10 Unstable (reactive) materials. Examples include:

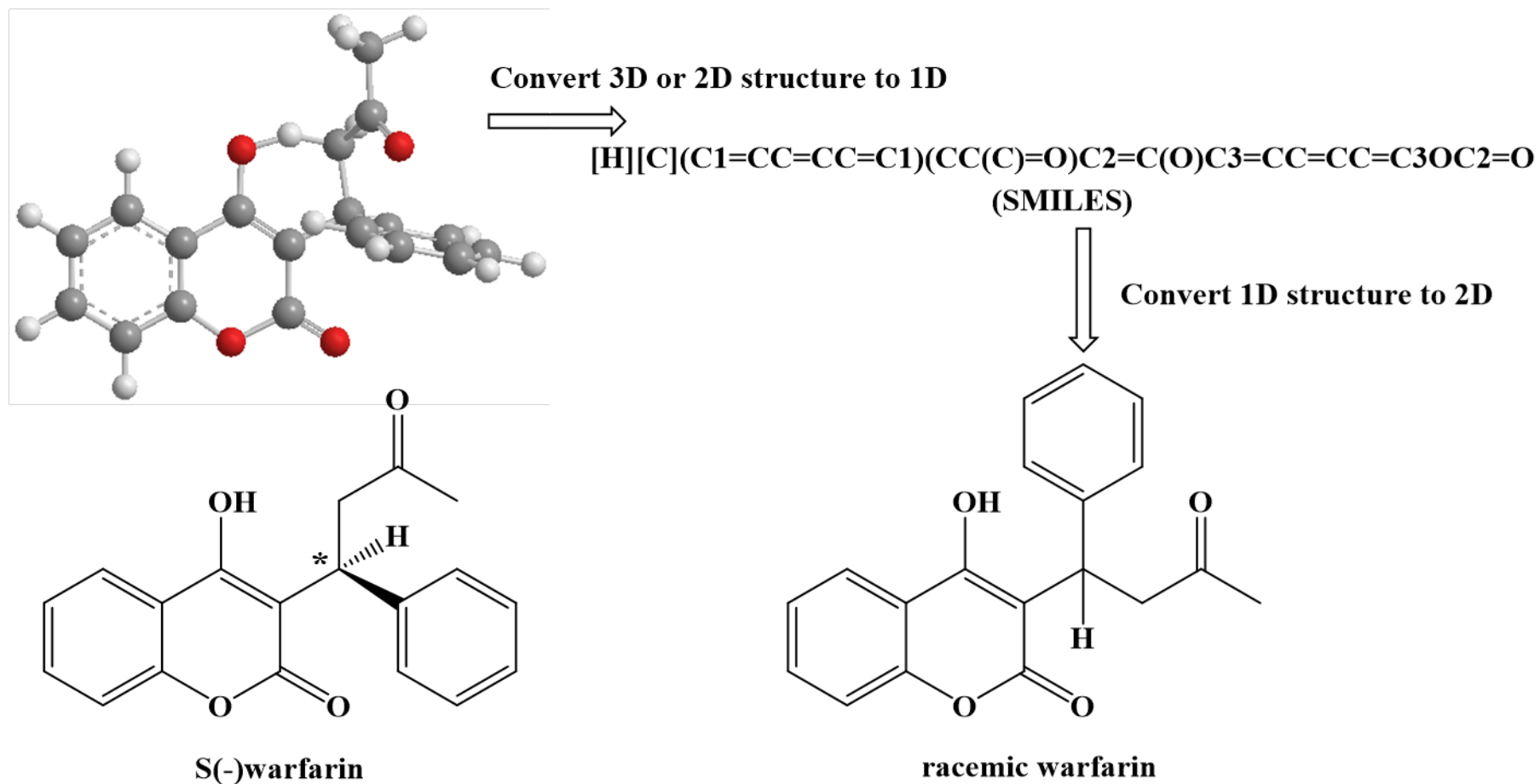
Class 4: acetyl peroxide, dibutyl peroxide, dinitrobenzene, ethyl nitrate, peroxyacetic acid and picric acid (dry) trinitrobenzene.

Class 3: hydrogen peroxide (greater than 52 percent), hydroxylamine, nitromethane, paranitroaniline, perchloric acid and tetrafluoroethylene monomer.

Class 2: acrolein, acrylic acid, hydrazine, methacrylic acid, sodium perchlorate, styrene and vinyl acetate.

Class 1: acetic acid, hydrogen peroxide 35 percent to 52 percent, paraldehyde and tetrahydrofuran.

- Maintaining stereochemical information of molecules in a digital format.
- Ex) (S)-Warfarin





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website <http://www.ucop.edu/enterprise-risk-management/resources/centers-of-excellence/chemical-informatics.html>

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