UNIVERSITY OF Southampton

Health and Safety on the Semantic Web

Automated Completion of COSHH Risk Assessment Forms

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RSC CICAG Meeting

21st October 2014, Burlington House

Outline

- Background
- Problem Statement
- Method
- Results
- Discussion
- Conclusion

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GHS

- = Globally Harmonized System of Classification and Labelling of Chemicals
- International standard, created by the UN
- Aims to supersede the various standards currently used in different countries, providing a new *lingua franca*

GHS (cont.)

- Classification elements:
  - Hazard classes
  - Hazard categories
  - Notes
- Labelling elements:
  - Hazard pictograms
  - Signal words
  - Hazard and precautionary statements

http://www.orosha.org/resource-newsletter/2013/06-2013/image/chemical-x-medium.jpg

CLP Regulation (EC) No 1272/2008

- = Classification, Labelling and Packaging
- Aligns older EU systems with GHS, e.g., Dangerous Substances Directive 67/548/EEC
- Came into force in January 2009
- Mandatory from June 2015

COSHH

- = Control and Substances Hazardous to Health Regulations 2002 (UK statutory instrument)
- Requires employers to protect their employees from the effects of exposure to hazardous chemical substances

COSHH ASSESSMENT FORM

Record No.

SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD
Water	liquid	1000ml	None
Dextrose	Solid	<20 g	possible irritation to eyes and skin
Caffeine	Solid (tea)	<1 g	Harmful if swallowed, induce vomiting.
Milk	liquid	<100ml	No particular hazards

NATURE OF PROCESS

liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink

Is there a less hazardous substance? No
If so, why not use it?

CONTROL MEASURES REQUIRED No specific measure required
(Local exhaust ventilation, personal protection, etc.)

c/o SmartTea

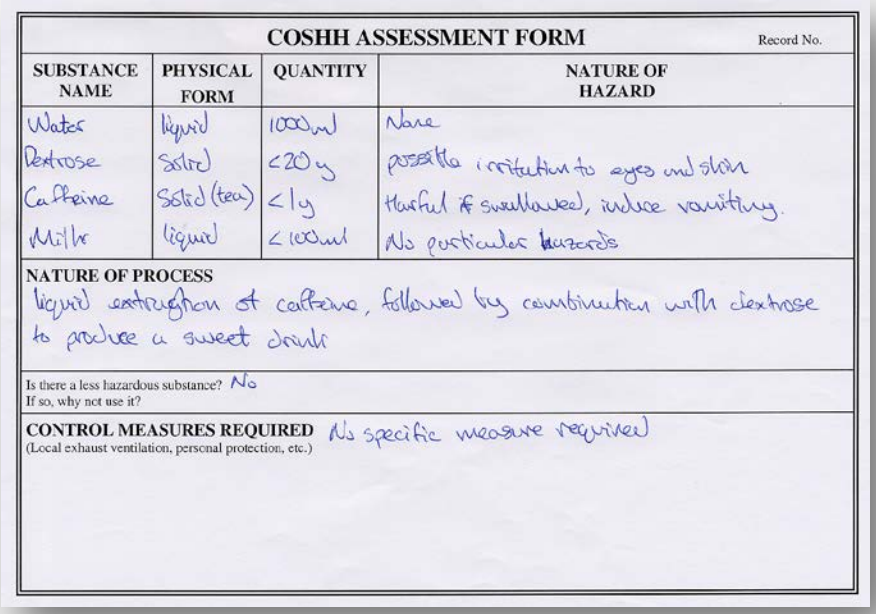
COSHH Risk Assessment

0. Describe scientific experiment

1. Enumerate chemical substances

2. Discover health and safety information

3. Interpolate template



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Problem Statement

- For humans, performing COSHH risk assessment has two key drawbacks:
  1. Reduced working time
  2. Inherent danger

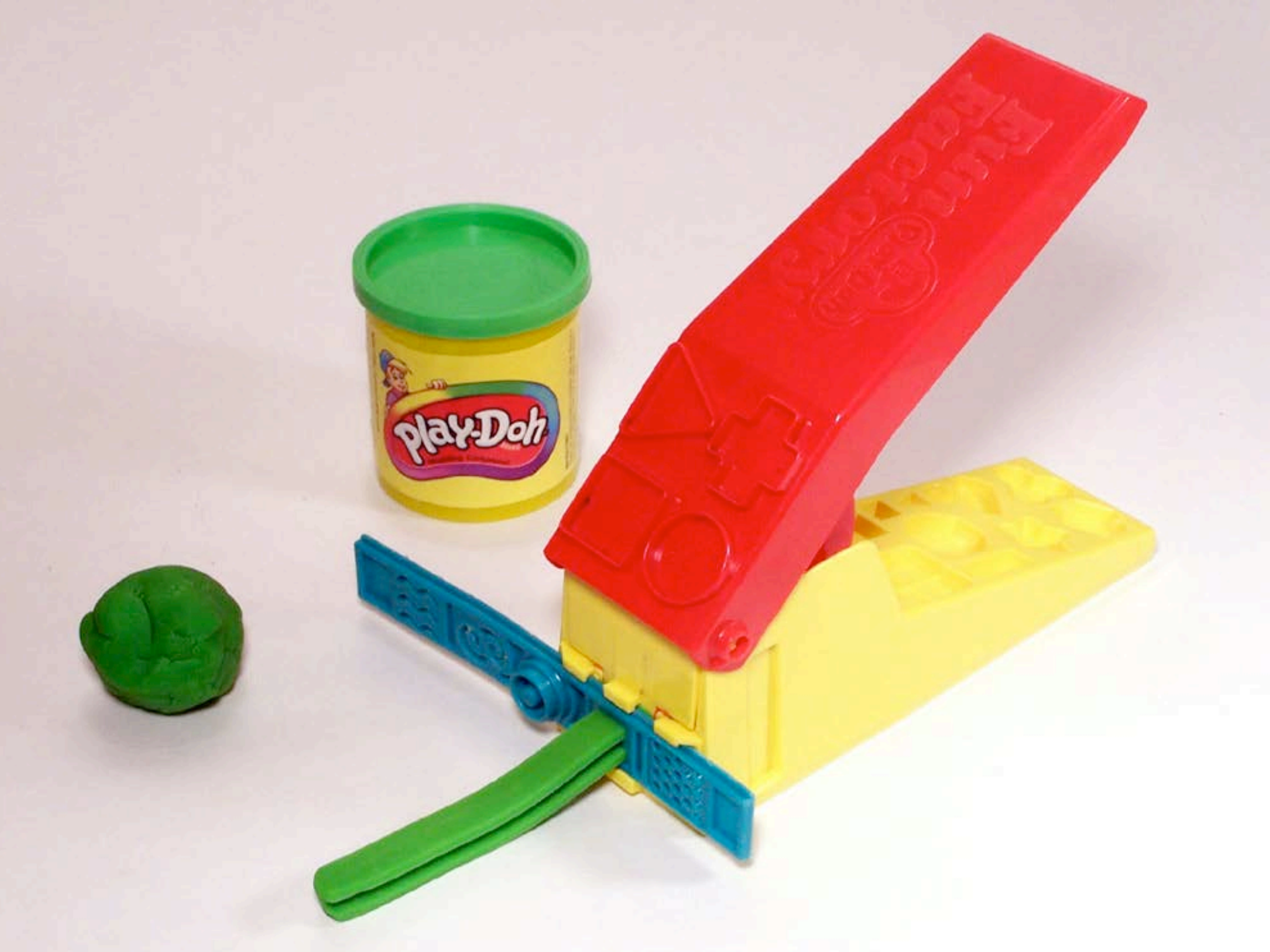
COSHH Risk Assessment Hazards

0. Incorrect description of scientific experiment

1. Incorrect enumeration of chemical substances
2. Incorrect health and safety information
3. Transcription errors

Problem Statement (cont.)

- An incorrect COSHH risk assessment is a potential source of danger, i.e., a hazard
- Using automation, the associated risk can be managed, e.g.,
  - Input
    - Description of scientific experiment
    - Template
  - Output
    - Interpolated template


Play-Doh

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Method

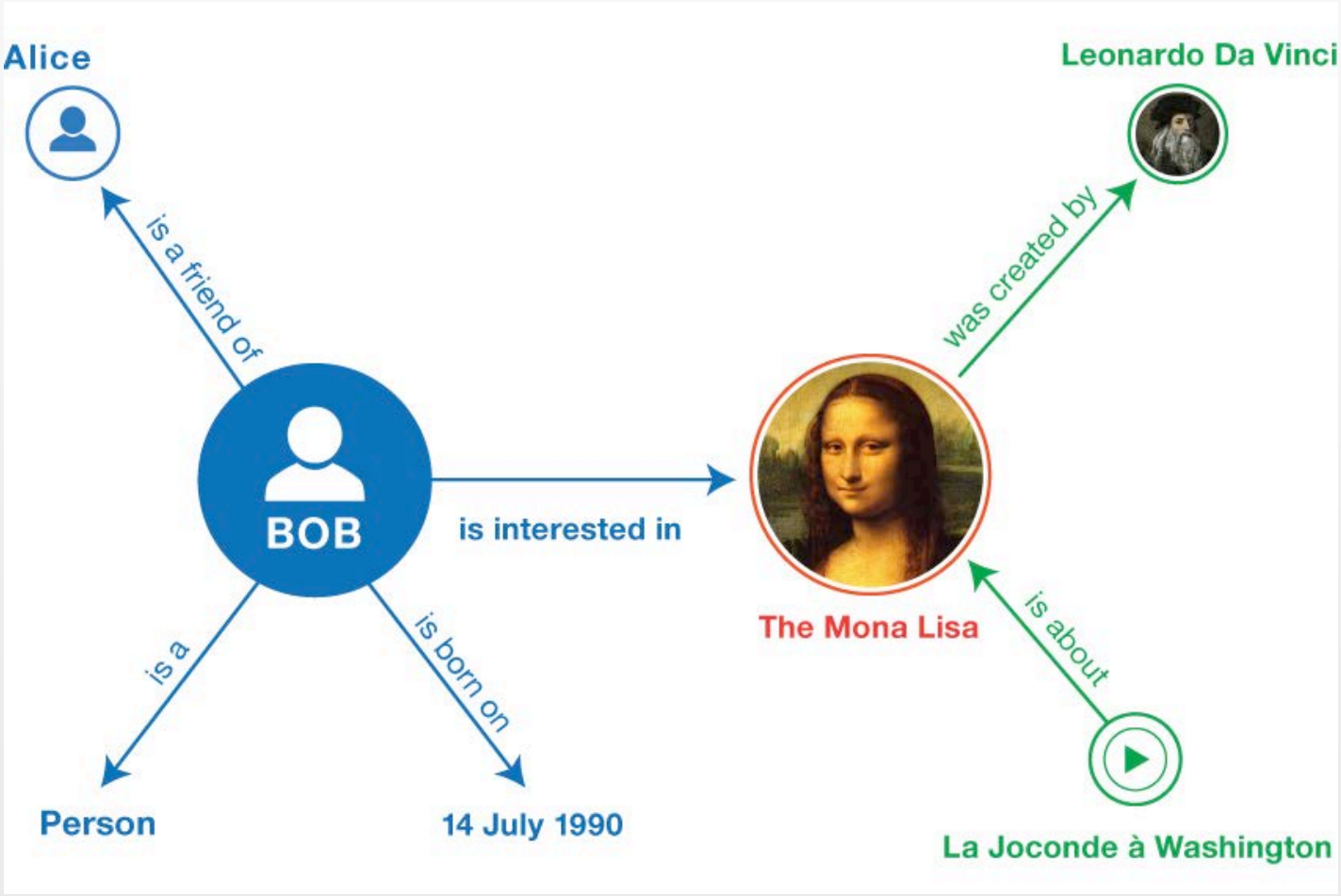
- Identify/generate required information resources:
  - Formalisation of CLP Regulation
  - Database of classified* chemical substances
  - Templates
- Implement Web application

* As specified by CLP Regulation

RDF

- = Resource Description Framework
- Family of W3C specifications for modelling information as Web resources
- Used in knowledge management systems
- Core data model is based upon making “subject—predicate—object” statements

RDF (cont.)

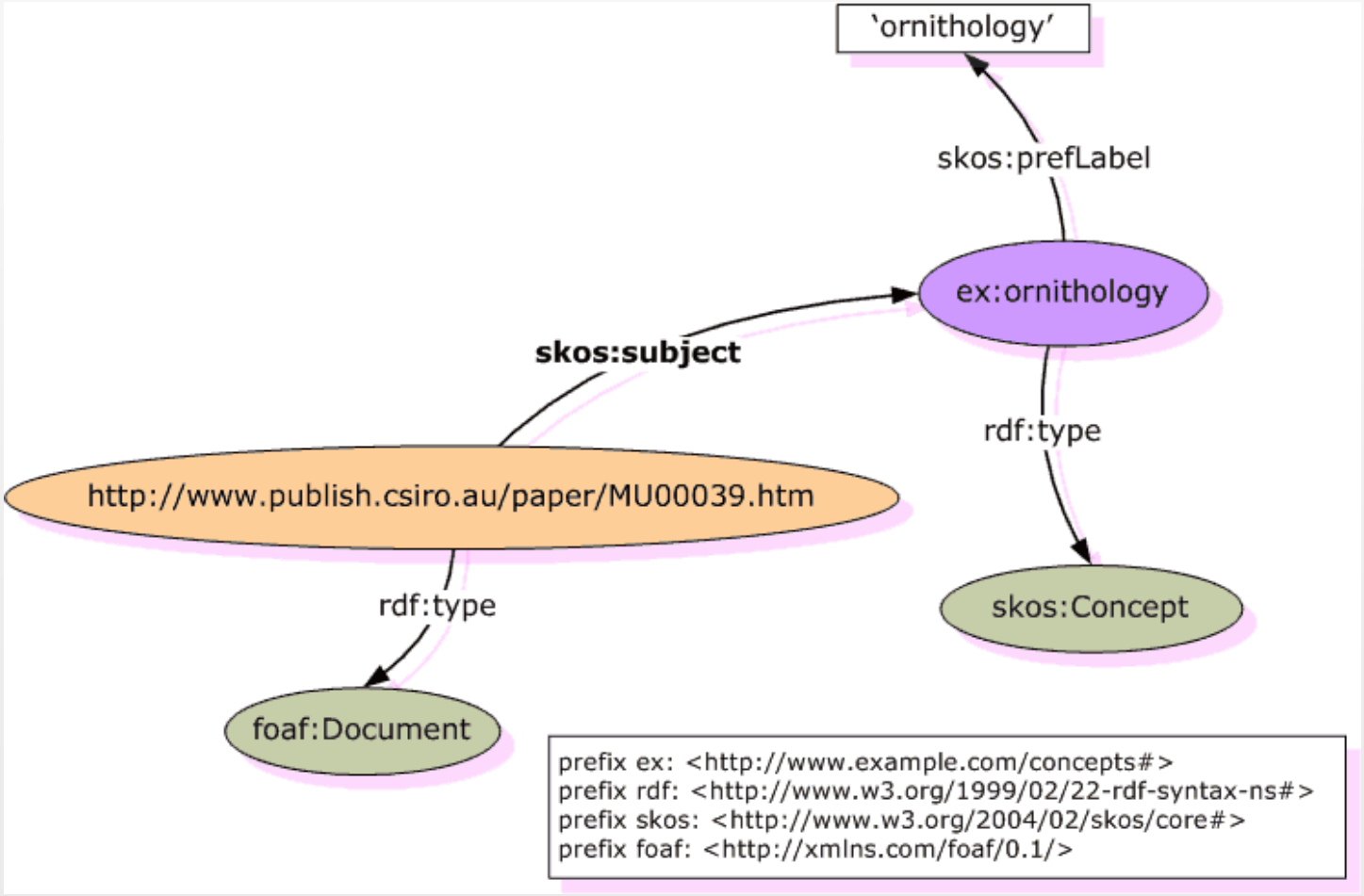


http://www.w3.org/TR/rdf11-primer/example-graph.jpg

SKOS

- = Simple Knowledge Organisation System
- W3C recommendation for representation of controlled vocabularies
- Built upon RDF and RDF Schema

SKOS (cont.)



http://www.w3.org/TR/2005/WD-swbp-skos-core-guide-20051102/img/ex-sub.png

Method (cont.)

- Use RDF, RDF Schema and SKOS
- Transfer definitions verbatim*
- Automate* extraction and enrichment of classifications

* Facilitates curation of provenance information

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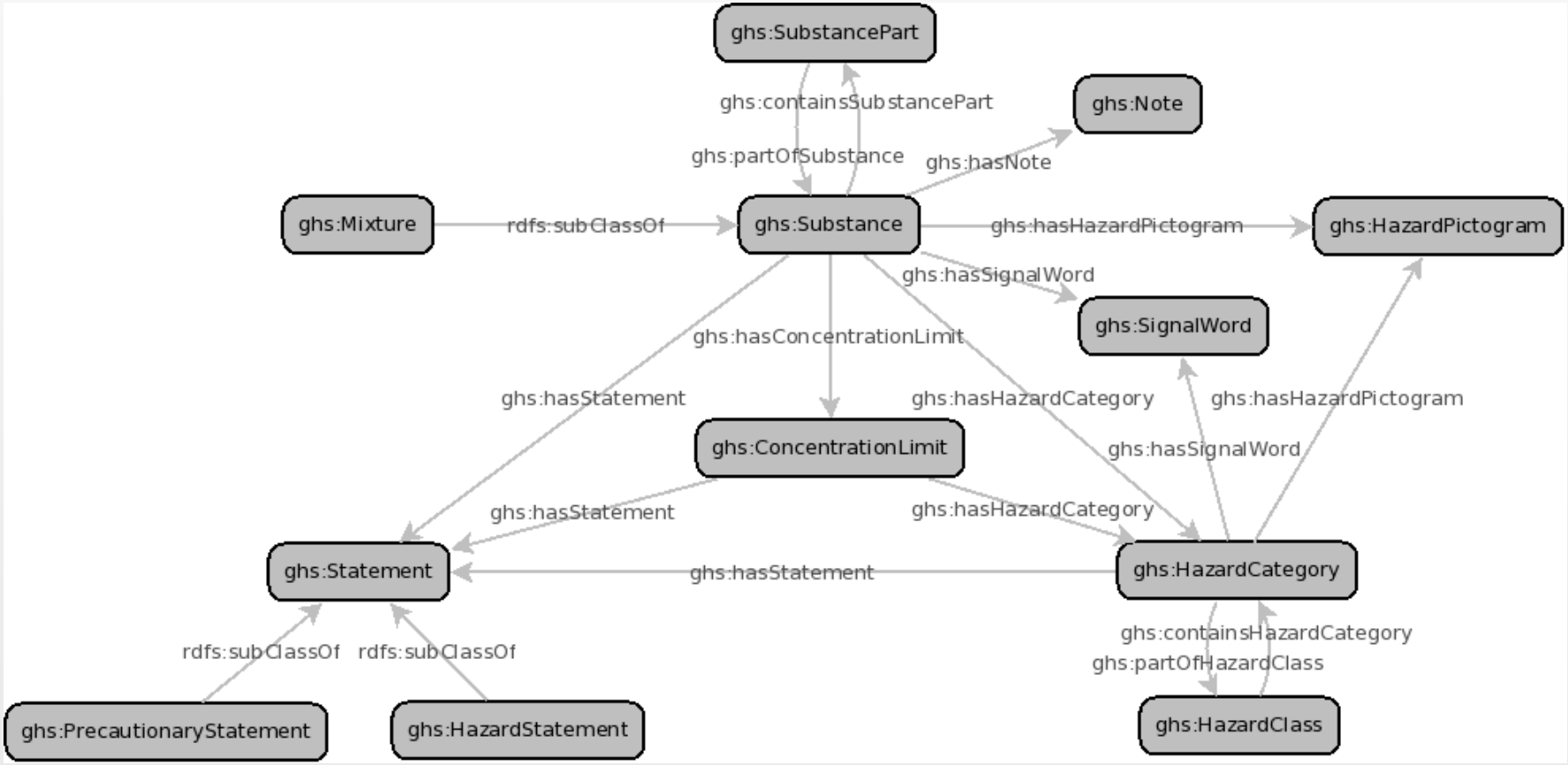
Results

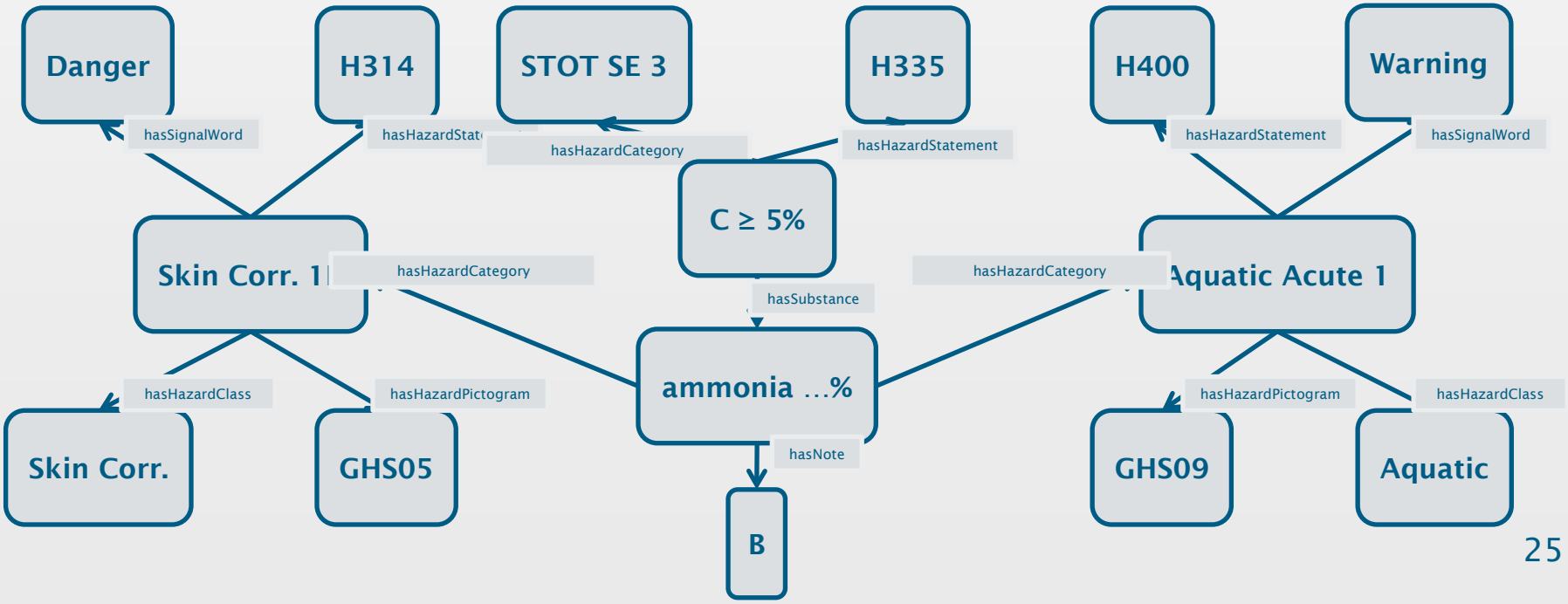
- Machine-accessible representation of GHS/CLP Regulation
  - Definitions (annexes I—V)
  - Classified chemical substances (annex VI)
- Dataset available at: http://bit.ly/1fvDO5u

RDF Schema for GHS/CLP Regulation



RDF for EC (No) 007-001-01-2

Index No	International Chemical Identification	EC No	CAS No	Classification		Labelling			Specific Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement Code(s)	Pictogram, Signal Word Code(s)	Hazard statement Code(s)	Suppl. Hazard statement Code(s)		
007-001-01-2	ammonia ....%	215-647-6	1336-21-6	Skin Corr. 1B Aquatic Acute 1	H314 H400	GHS05 GHS09 Dgr	H314 H400		STOT SE 3; H335: C ≥ 5 %	B



Results (cont.)

- The dataset is interesting, but not practical
- It only contains ~3000 classifications

Observation

- Many researchers procure their chemical substances from specialist suppliers

12540 FLUKA

Benzene

analytical standard

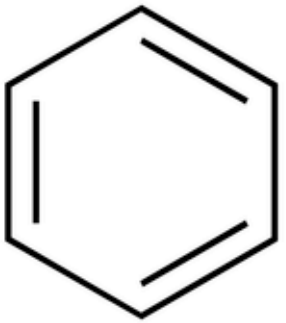
◇ DOWNLOAD MSDS (PDF)

CAS Number 71-43-2 | Empirical Formula (Hill Notation) C_6H_6 | Molecular Weight 78.11

Beilstein Registry Number 969212 | EC Number 200-753-7 | MDL number MFCD00003009

PubChem Substance ID 24847664

POPULAR DOCUMENTS: FTNMR (PDF)



Purchase | Safety & Documentation | Peer-Reviewed Papers 50

Documents

Bulk Quote-Order Product
MSDS

Certificate of Analysis

Enter Lot No.

FT-IR Raman
FT-NMR
Pressure-Temperature Nomograph
Similar Products
Structure Search

Safety Information

Symbol	GHS08 GHS02, GHS07, GHS08
Signal word	Danger
Hazard statements	H225-H304-H315-H319-H340-H350-H372
Precautionary statements	P201-P210-P301 + P310-P305 + P351 + P338-P308 + P313-P331
Personal Protective Equipment	Eyeshields, Faceshields, full-face respirator (US), Gloves, multi-purpose combination respirator cartridge (US), type ABEK (EN14387) respirator filter
Hazard Codes (Europe)	F,T
Risk Statements (Europe)	45-46-11-36/38-48/23/24/25-65

Excerpt of RDF for <fluka/12540>

```
@base <http://www.sigmaaldrich.com/catalog/product/> .
@prefix chemaxiomprop: <http://www.polymerinformatics.com/ChemAxiom/ChemAxiomProp.owl#> .
@prefix chemdomain: <http://www.polymerinformatics.com/ChemAxiom/ChemDomain.owl#> .
@prefix ghs: <http://xmlns.com/ghs/0.1/> .
@prefix sial: <http://www.sigmaaldrich.com/ns#> .

<fluka/12540> a chemdomain:NamedChemicalSpecies;
   chemdomain:hasIdentifier [ a sial:ChemicalNumber;
     chemdomain:hasValue "042802"],
     [ a chemdomain:Name;
     chemdomain:hasValue "Benzene"],
     [ a chemdomain:CASNumber;
     chemdomain:hasValue "71-43-2"],
     [ a chemdomain:SMILES;
     chemdomain:hasValue "c1ccccc1"],
     [ a chemdomain:MolecularFormula;
     chemdomain:hasValue "C6H6"];
   ghs:hasHazardCategory <http://id.unece.org/ghs/hazard_categories/Flam_Liq_2>,
     <http://id.unece.org/ghs/hazard_categories/SPEC_RE_1>,
     <http://id.unece.org/ghs/hazard_categories/Skin_Irrit_2>,
     <http://id.unece.org/ghs/hazard_categories/Carc_1A>,
     <http://id.unece.org/ghs/hazard_categories/Asp_Tox_1>,
     <http://id.unece.org/ghs/hazard_categories/Eye_Irrit_2>,
     <http://id.unece.org/ghs/hazard_categories/Muta_1B> .
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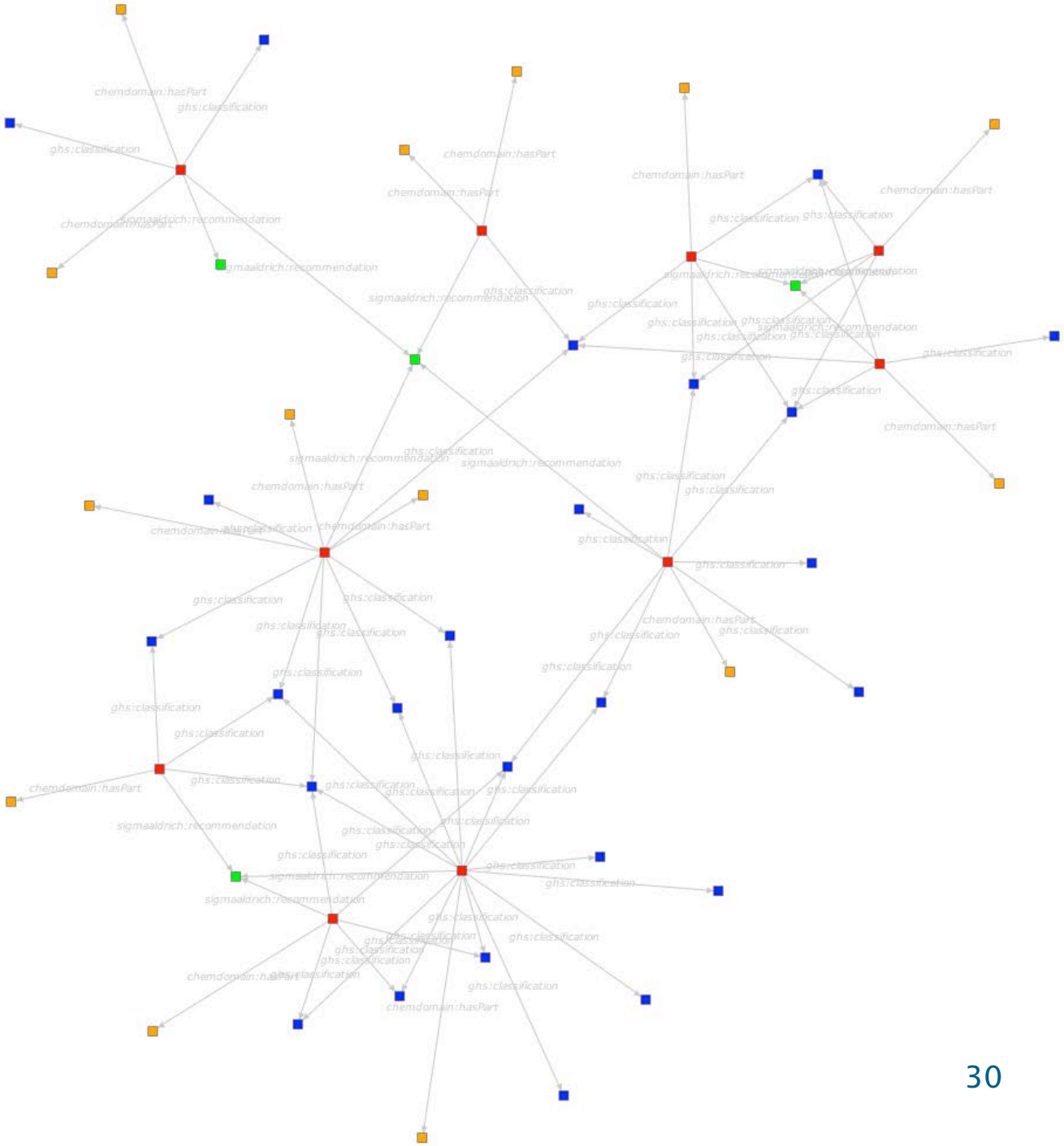


Red square = Chemical substance

Orange square = Mixture part

Green square = PPE product, e.g., gloves

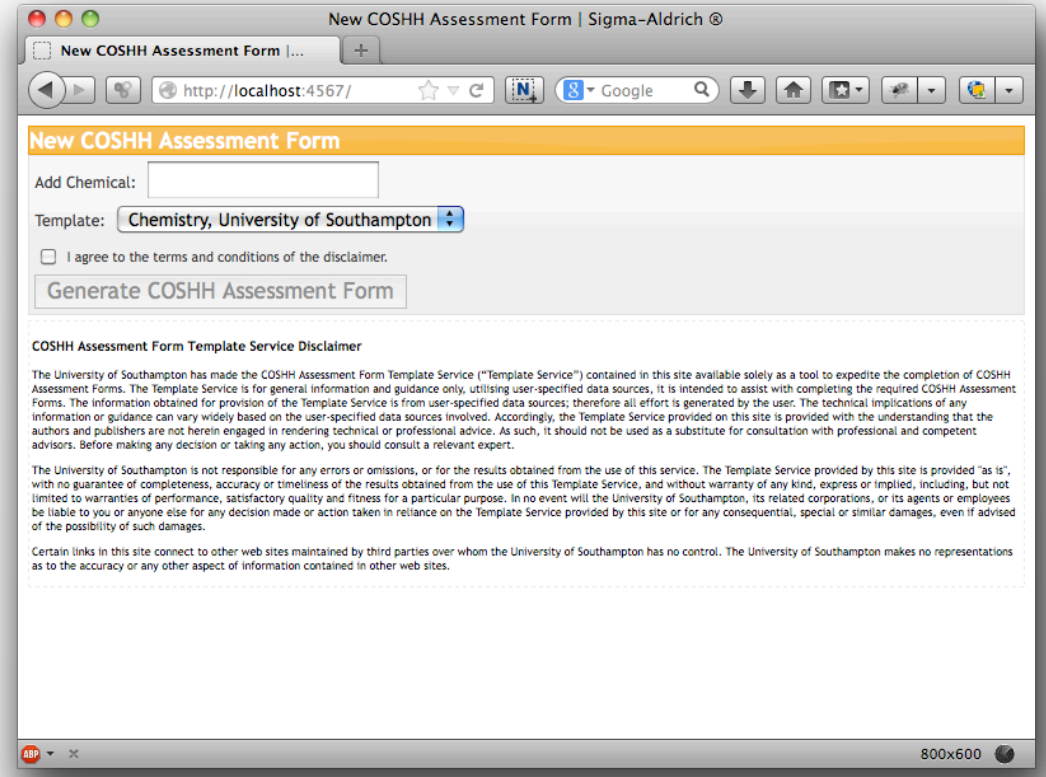
Blue square = GHS hazard category

Web Application Protocol

1. Load Web application
2. Describe scientific experiment
3. Select template
4. Accept terms and conditions
5. Receive interpolated template

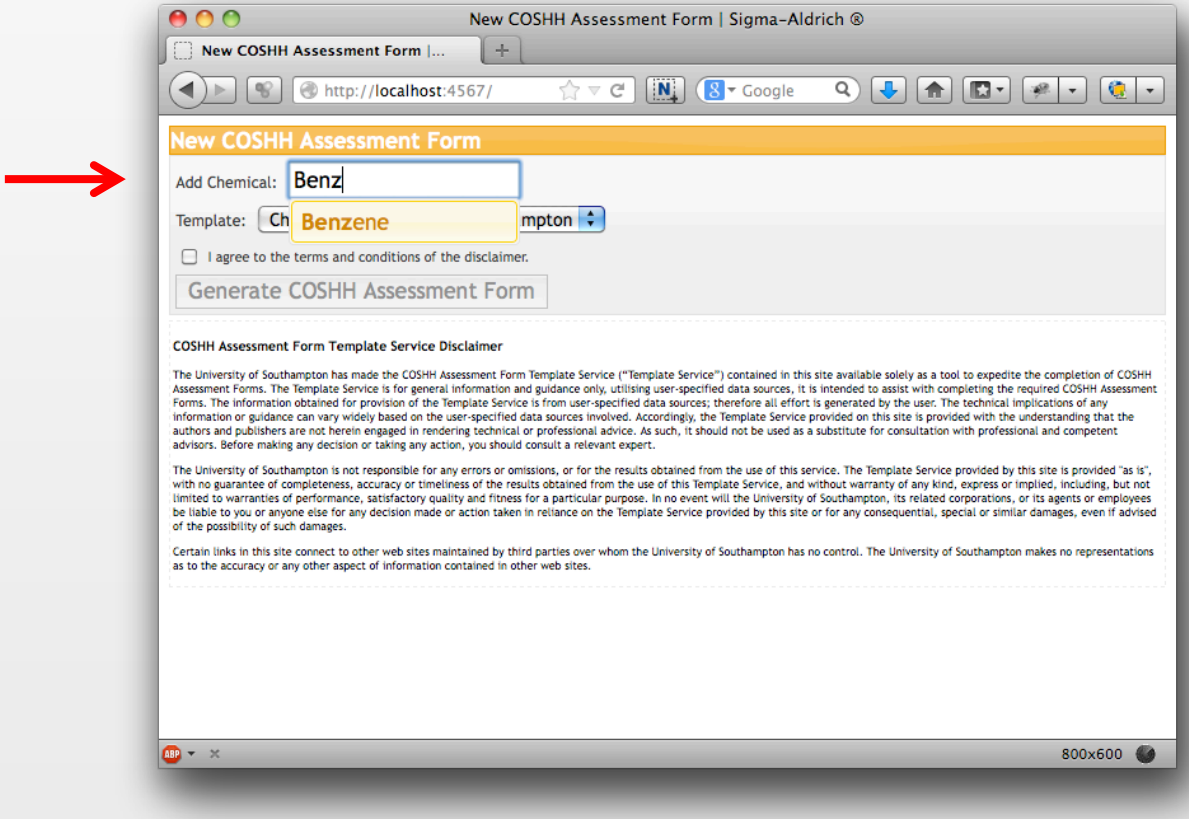
1) Load Web Application

"Generate" button is disabled



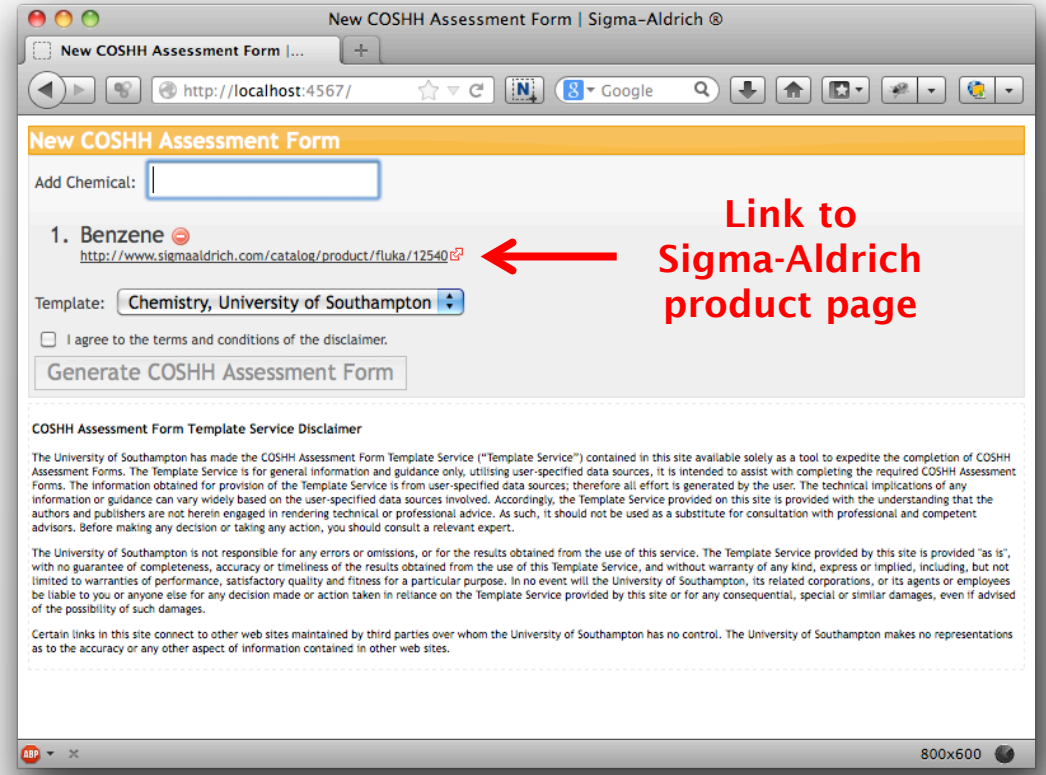
2) Describe Scientific Experiment

Dynamic search with auto-completion



2) Describe Scientific Experiment

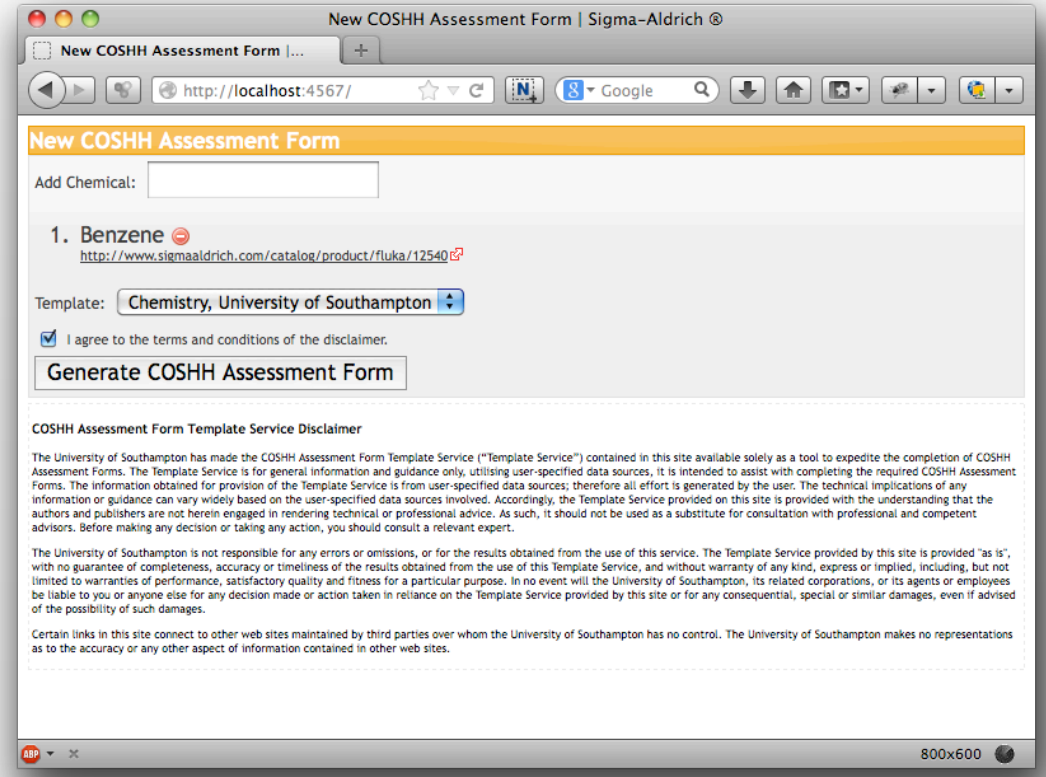
Selected product is added to list



Link to Sigma-Aldrich product page

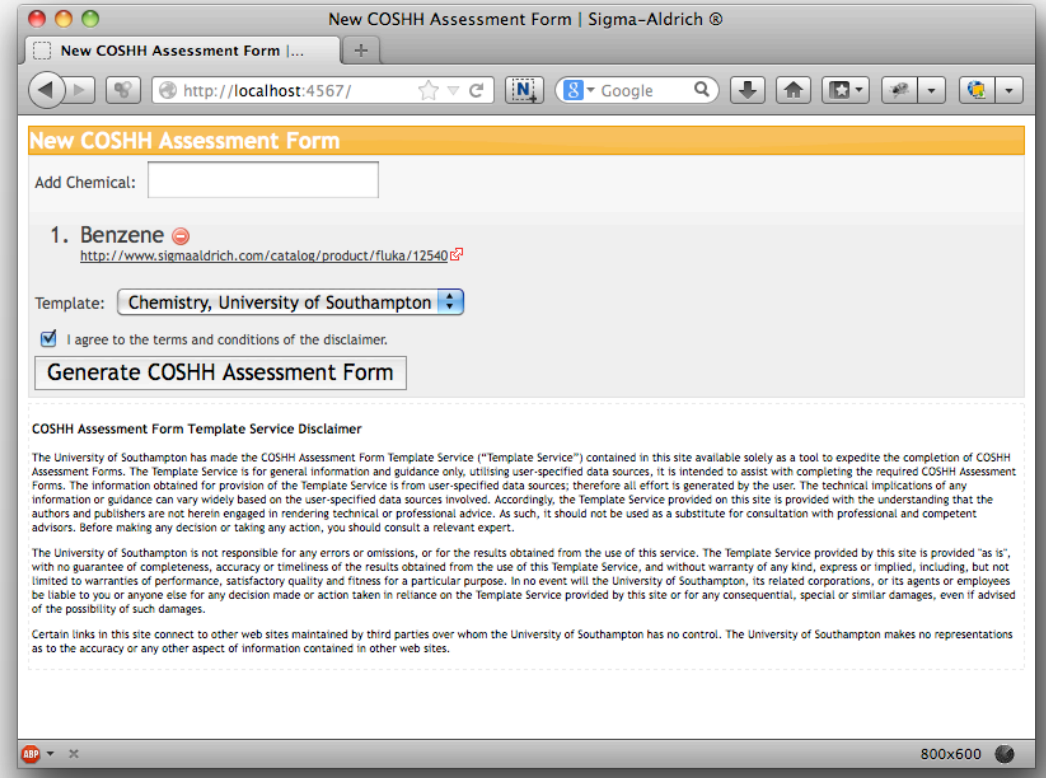
3) Select Template

List of Templates

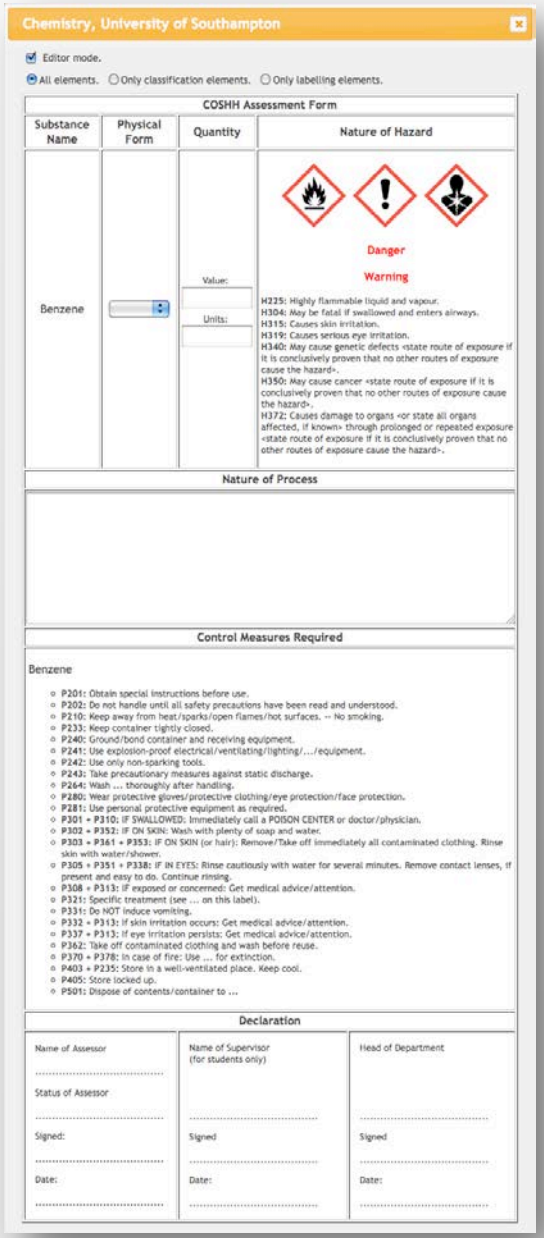


4) Accept Terms and Conditions

"Generate" button is enabled



Editable text fields for "Physical Form" and "Quantity"



One row per product

Editable text area for "Nature of Process"

The University requires that assessment forms are printed and signed

Toggle visibility of classification and labelling elements

Integration with purchasing platform

Web Application Limitations

- Descriptions of scientific experiments are just sets of “Chemical substance—Phase—Quantity” triples
- To enable more detailed analysis, we need richer descriptions

This plan describes **3 activities**, **2 entities**, and **3 usages**.

- Initialize [edit] [destroy]
  - New Usage
  - *Generates:* **Acetaldehyde** puriss. p.a., anhydrous, >=99.5% (GC) [destroy]
  - *Generates:* **Benzene** analytical standard [destroy]
  - New Entity
- Mix [edit] [destroy]
  - *Uses:* Initialize → **Acetaldehyde** puriss. p.a., anhydrous, >=99.5% (GC) (Role: Primary Target) [edit] [destroy]
  - *Uses:* Initialize → **Benzene** analytical standard (Role: Secondary Target) [edit] [destroy]
  - New Usage
  - New Entity
- Non-Linear Activity [edit] [destroy]
  - *Uses:* Initialize → **Acetaldehyde** puriss. p.a., anhydrous, >=99.5% (GC) [edit] [destroy]
  - New Usage
  - New Entity
- New Activity

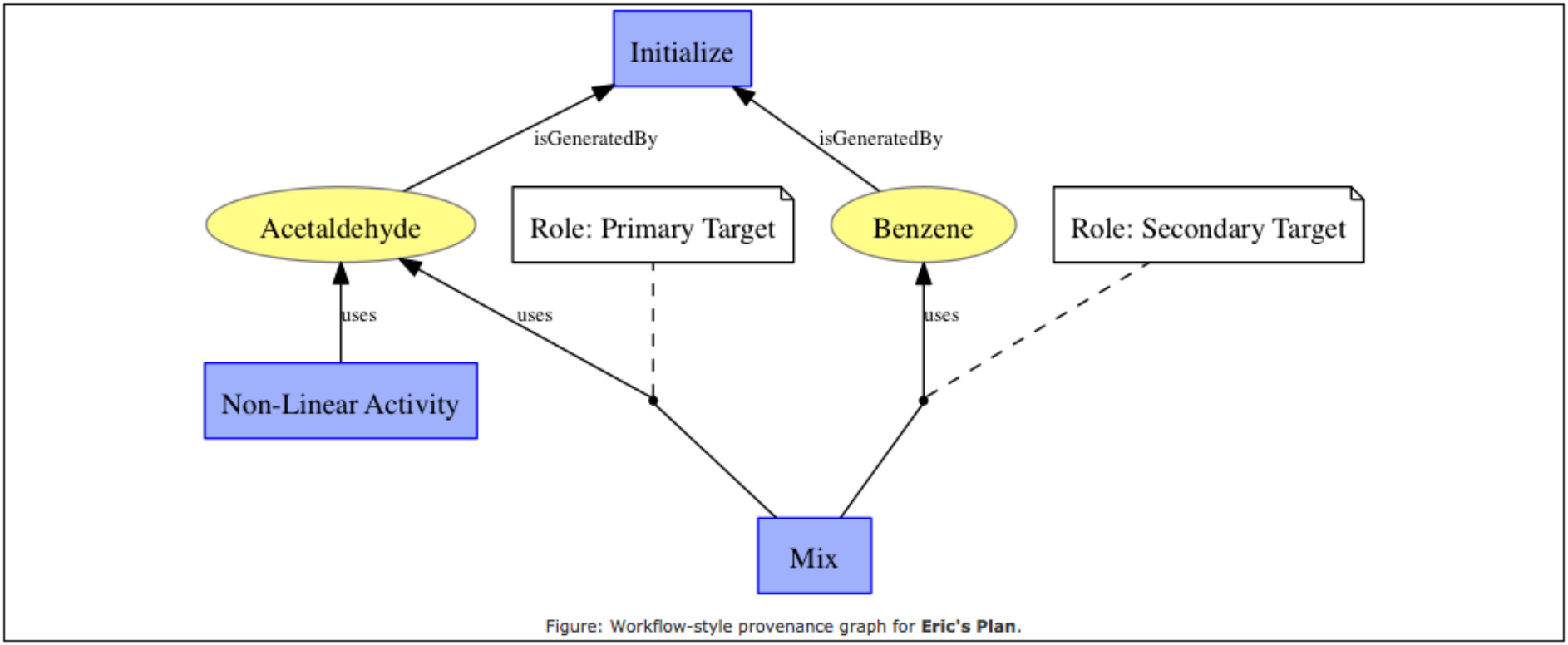
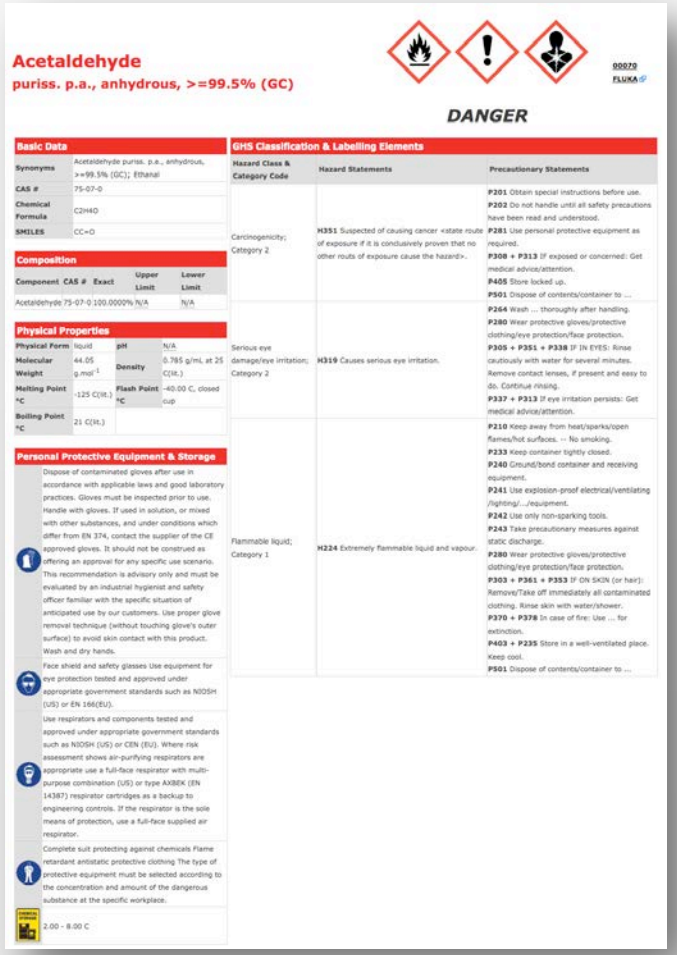


Figure: Workflow-style provenance graph for **Eric's Plan**.

Sigma-Aldrich One Page Safety Data Sheets (“One Pagers”)



Acetaldehyde

puriss. p.a., anhydrous, >=99.5% (GC)

00070
FLUKA

DANGER

Basic Data

Synonyms	Acetaldehyde puriss. p.a., anhydrous, >=99.5% (GC); Ethanal
CAS #	75-07-0
Chemical Formula	C2H4O
SMILES	CC=O

Composition

Component	CAS #	Exact	Upper Limit	Lower Limit
Acetaldehyde	75-07-0	100.0000%	N/A	N/A

Physical Properties

Physical Form	liquid	pH	N/A
Molecular Weight	44.05 g.mol^{-1}	Density	0.785 g/mL at 25 C(lit.)
Melting Point °C	-125 C(lit.)	Flash Point °C	-40.00 C, closed cup
Boiling Point °C	21 C(lit.)		

Personal Protective Equipment & Storage

Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Gloves must be inspected prior to use. Handle with gloves. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. It should not be construed as offering an approval for any specific use scenario. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Wash and dry hands.

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

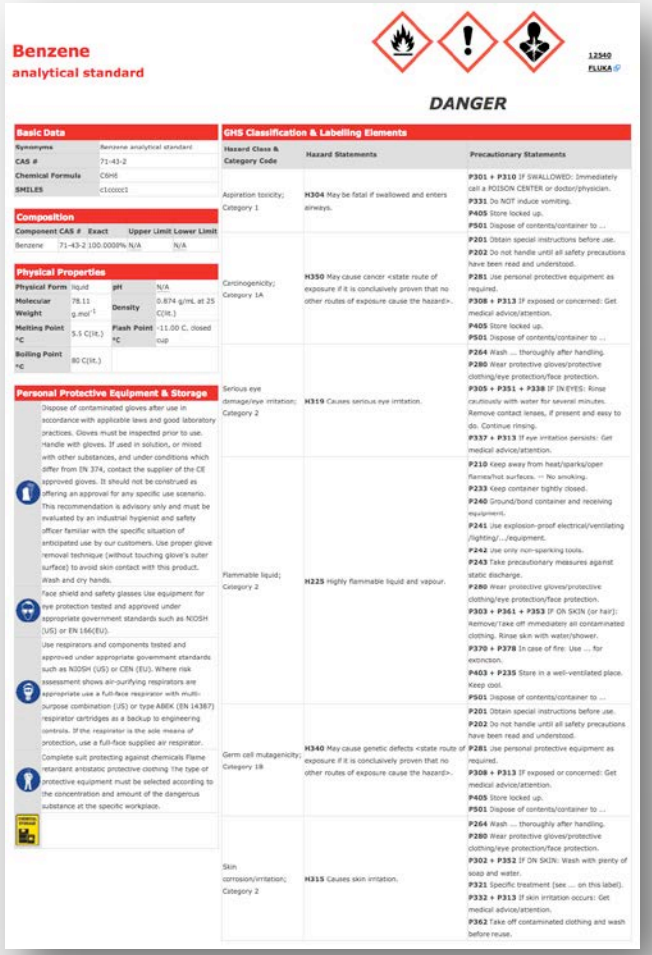
Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.

Complete suit protecting against chemicals Flame retardant antistatic protective clothing The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

2.00 - 8.00 C

GHS Classification & Labelling Elements

Hazard Class & Category Code	Hazard Statements	Precautionary Statements
Carcinogenicity; Category 2	**H351** Suspected of causing cancer <state route of exposure if it is conclusively proven that no other routs of exposure cause the hazard>.	**P201** Obtain special instructions before use. **P202** Do not handle until all safety precautions have been read and understood. **P281** Use personal protective equipment as required. **P308 + P313** IF exposed or concerned: Get medical advice/attention. **P405** Store locked up. **P501** Dispose of contents/container to ...
Serious eye damage/eye irritation; Category 2	**H319** Causes serious eye irritation.	**P264** Wash ... thoroughly after handling. **P280** Wear protective gloves/protective clothing/eye protection/face protection. **P305 + P351 + P338** IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. **P337 + P313** If eye irritation persists: Get medical advice/attention.
Flammable liquid; Category 1	**H224** Extremely flammable liquid and vapour.	**P210** Keep away from heat/sparks/open flames/hot surfaces. -- No smoking. **P233** Keep container tightly closed. **P240** Ground/bond container and receiving equipment. **P241** Use explosion-proof electrical/ventilating /lighting/.../equipment. **P242** Use only non-sparking tools. **P243** Take precautionary measures against static discharge. **P280** Wear protective gloves/protective clothing/eye protection/face protection. **P303 + P361 + P353** IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower. **P370 + P378** In case of fire: Use ... for extinction. **P403 + P235** Store in a well-ventilated place. Keep cool. **P501** Dispose of contents/container to ...



Benzene

analytical standard

12340
FLUKA

DANGER

Basic Data

Synonyms	Benzene analytical standard
CAS #	71-43-2
Chemical Formula	C6H6
SMILES	c1ccccc1

Composition

Component	CAS #	Exact	Upper Limit	Lower Limit
Benzene	71-43-2	100.0000%	N/A	N/A

Physical Properties

Physical Form	liquid	pH	N/A
Molecular Weight	78.11 g.mol^{-1}	Density	0.874 g/mL at 25 C(lit.)
Melting Point °C	5.5 C(lit.)	Flash Point °C	-11.00 C, closed cup
Boiling Point °C	80 C(lit.)		

Personal Protective Equipment & Storage

Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Gloves must be inspected prior to use. Handle with gloves. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. It should not be construed as offering an approval for any specific use scenario. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Wash and dry hands.

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.

Complete suit protecting against chemicals Flame retardant antistatic protective clothing The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

GHS Classification & Labelling Elements

Hazard Class & Category Code	Hazard Statements	Precautionary Statements
Aspiration toxicity; Category 1	**H304** May be fatal if swallowed and enters airways.	**P301 + P310** IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. **P331** Do NOT induce vomiting. **P405** Store locked up. **P501** Dispose of contents/container to ...
Carcinogenicity; Category 1A	**H350** May cause cancer <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>.	**P201** Obtain special instructions before use. **P202** Do not handle until all safety precautions have been read and understood. **P281** Use personal protective equipment as required. **P308 + P313** IF exposed or concerned: Get medical advice/attention. **P405** Store locked up. **P501** Dispose of contents/container to ...
Serious eye damage/eye irritation; Category 2	**H319** Causes serious eye irritation.	**P264** Wash ... thoroughly after handling. **P280** Wear protective gloves/protective clothing/eye protection/face protection. **P305 + P351 + P338** IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. **P337 + P313** If eye irritation persists: Get medical advice/attention.
Flammable liquid; Category 2	**H225** Highly flammable liquid and vapour.	**P210** Keep away from heat/sparks/open flames/hot surfaces. -- No smoking. **P233** Keep container tightly closed. **P240** Ground/bond container and receiving equipment. **P241** Use explosion-proof electrical/ventilating /lighting/.../equipment. **P242** Use only non-sparking tools. **P243** Take precautionary measures against static discharge. **P280** Wear protective gloves/protective clothing/eye protection/face protection. **P303 + P361 + P353** IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower. **P370 + P378** In case of fire: Use ... for extinction. **P403 + P235** Store in a well-ventilated place. Keep cool. **P501** Dispose of contents/container to ...
Germ cell mutagenicity; Category 1B	**H340** May cause genetic defects <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>.	**P201** Obtain special instructions before use. **P202** Do not handle until all safety precautions have been read and understood. **P281** Use personal protective equipment as required. **P308 + P313** IF exposed or concerned: Get medical advice/attention. **P405** Store locked up. **P501** Dispose of contents/container to ...
Skin corrosion/irritation; Category 2	**H315** Causes skin irritation.	**P264** Wash ... thoroughly after handling. **P280** Wear protective gloves/protective clothing/eye protection/face protection. **P302 + P352** IF ON SKIN: Wash with plenty of soap and water. **P321** Specific treatment (see ... on this label). **P332 + P313** If skin irritation occurs: Get medical advice/attention. **P362** Take off contaminated clothing and wash before reuse.

Sigma-Aldrich “Quick Order Form”

★ = Recommended Product

Select	Product Number	Description	Quantity	Your Price	Item Total
☑	FLUKA 00070	Acetaldehyde puriss. p.a., anhydrous, >=99.5% (GC)	1	*Not Calculated*	*Not Calculated*
☐	ALDRICH Z677647	★ Butoject gloves	0	*Not Calculated*	*Not Calculated*
☑	FLUKA 12540	Benzene analytical standard	1	*Not Calculated*	*Not Calculated*
☐	ALDRICH Z677698	★ Vitoject gloves	0	*Not Calculated*	*Not Calculated*

Add Selected Items to Shopping Cart

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- Background
- Problem Statement
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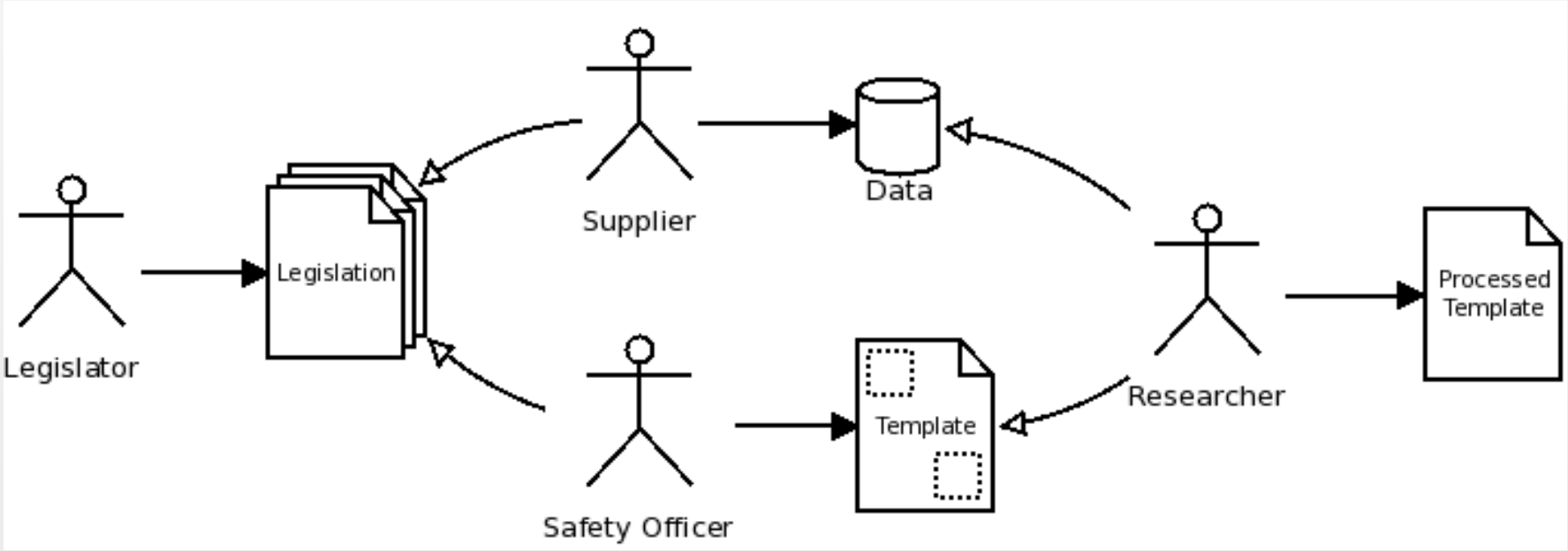
Data Stakeholders



Data Stakeholders (cont.)

- Bidirectional data exchange
- Forwards
  - Suppliers and safety officers consume the legislation
  - Researchers consume chemical information and templates
- Backwards
  - Legislators, suppliers and safety officers gather usage statistics

The Wrong Question

- Who has legal liability when users act upon the correct answer to an incorrect question?
  - USER Can I drink this poison?
  - SYSTEM Yes
  - USER Is it safe to drink this poison?
  - SYSTEM No

Issues with GHS/CLP Regulation

- Does not identify hazards associated with presence of strong magnetic fields
- Identifies hazards of reagents and products of chemical reactions, but not kinetics
- Labelling elements do not have requirement levels
- *et al*

GHS Statements

- Statements are fragments of text that describe the *"nature of"* and *"recommended measure(s) to minimise or prevent adverse effects resulting from exposure to"* hazardous chemical substances
- Statements are either atomic or compound

P301+330+331

“P301: IF SWALLOWED:”

+

“P330: Rinse mouth”

+

“P331: Do NOT induce vomiting”

=

“P301+330+331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting”

P301+330+331 (cont.)

- The notation suggests that there is a binary statement composition operator
- However, this is not the case
- There is a statement composition operator *per se*, but it is variadic and partial
- Hence, new compound statements cannot be derived

Algebraic GHS Statements

- Translate phrases into controlled natural language, and then into expressions of terms and logical operators
- Terms constitute a controlled vocabulary

Controlled P301+330+331

"P301: If you swallow the substance then …"

+

"P330: You rinse mouth"

+

"P331: Not you induce vomiting"

=

"P301+330+331: If you swallow the substance then you rinse mouth and not you induce vomiting"

Algebraic P301+330+331

P301 = λx. “swallow the substance” $\Rightarrow x$

P330 = “rinse mouth”

P331 = ¬“induce vomiting”

P301+330+331 = P301 (P330 $\wedge$ P331)

Outline

- Background
- Problem Statement
- Method
- Results
- Discussion
- Conclusion

Conclusion

- Given formalisation of legislation, automated completion of COSHH risk assessment forms is trivial
- Legal mitigations, such as disclaimers and curation of provenance information, are vital
- Linchpin is availability of accurate and trustworthy chemical information
- Despite the success of GHS/CLP Regulation, there still exist many opportunities for enhancement

Thank You For Listening

- Questions?

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IUPAC Green Book