

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.osha.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)	<1g	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? <i>No</i> If so, why not use it?			
CONTROL MEASURES REQUIRED <i>No specific measure required</i> (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

COSHH ASSESSMENT FORM				Record No.
SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD	
Water	liquid	1000ml	None	
Dextrose	Solids	<20g	possible irritation to eyes and skin	
Caffeine	Solids (tea)	<1g	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? <i>No</i> If so, why not use it?				
CONTROL MEASURES REQUIRED (Local exhaust ventilation, personal protection, etc.) <i>No specific measure required</i>				

c/o SmartTea

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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



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Method

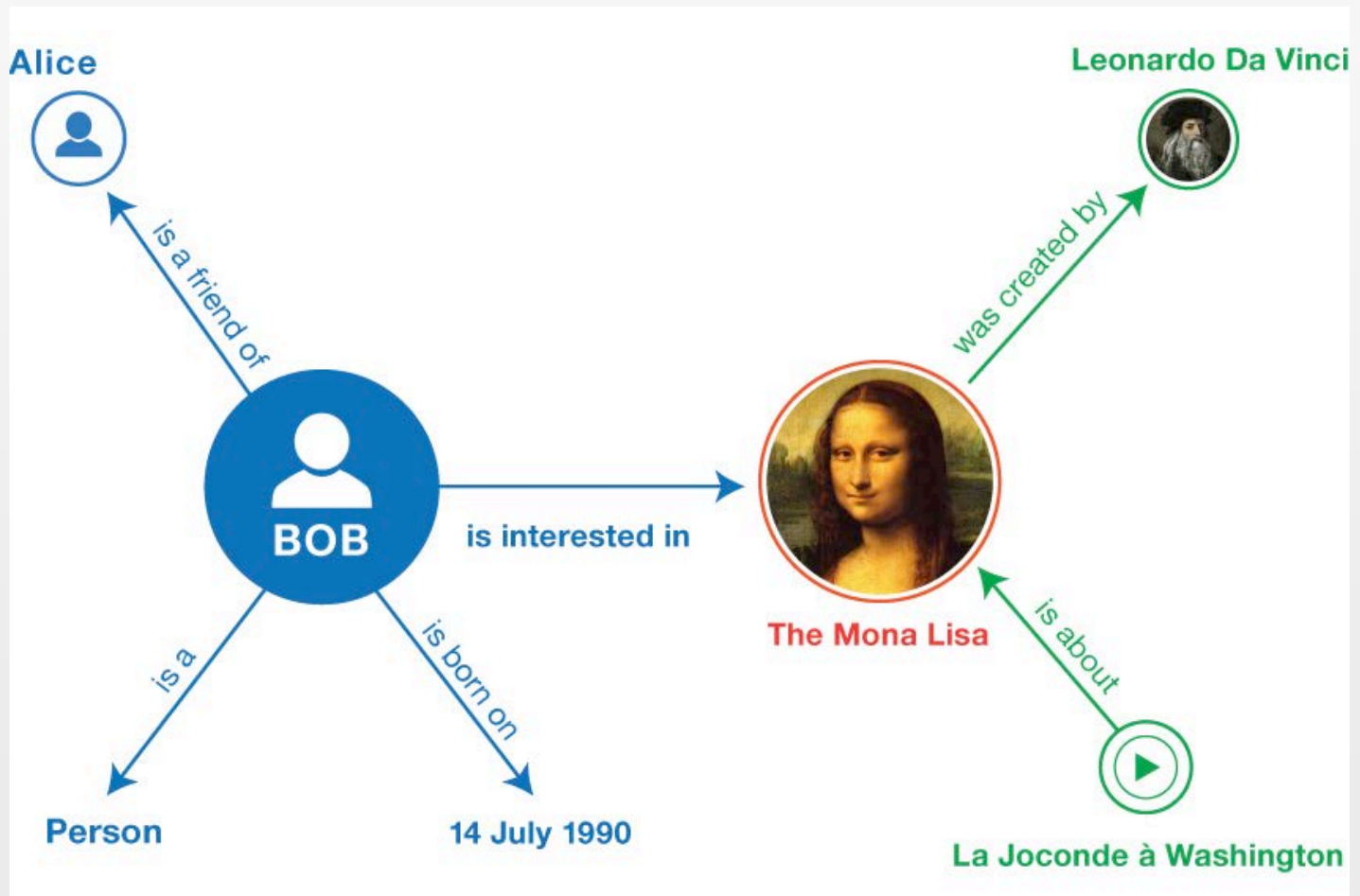
- Identify/generate required information resources:
 - Formalisation of CLP Regulation
 - Database of classified* chemical substances
 - Templates
- Implement Web application

* 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.)

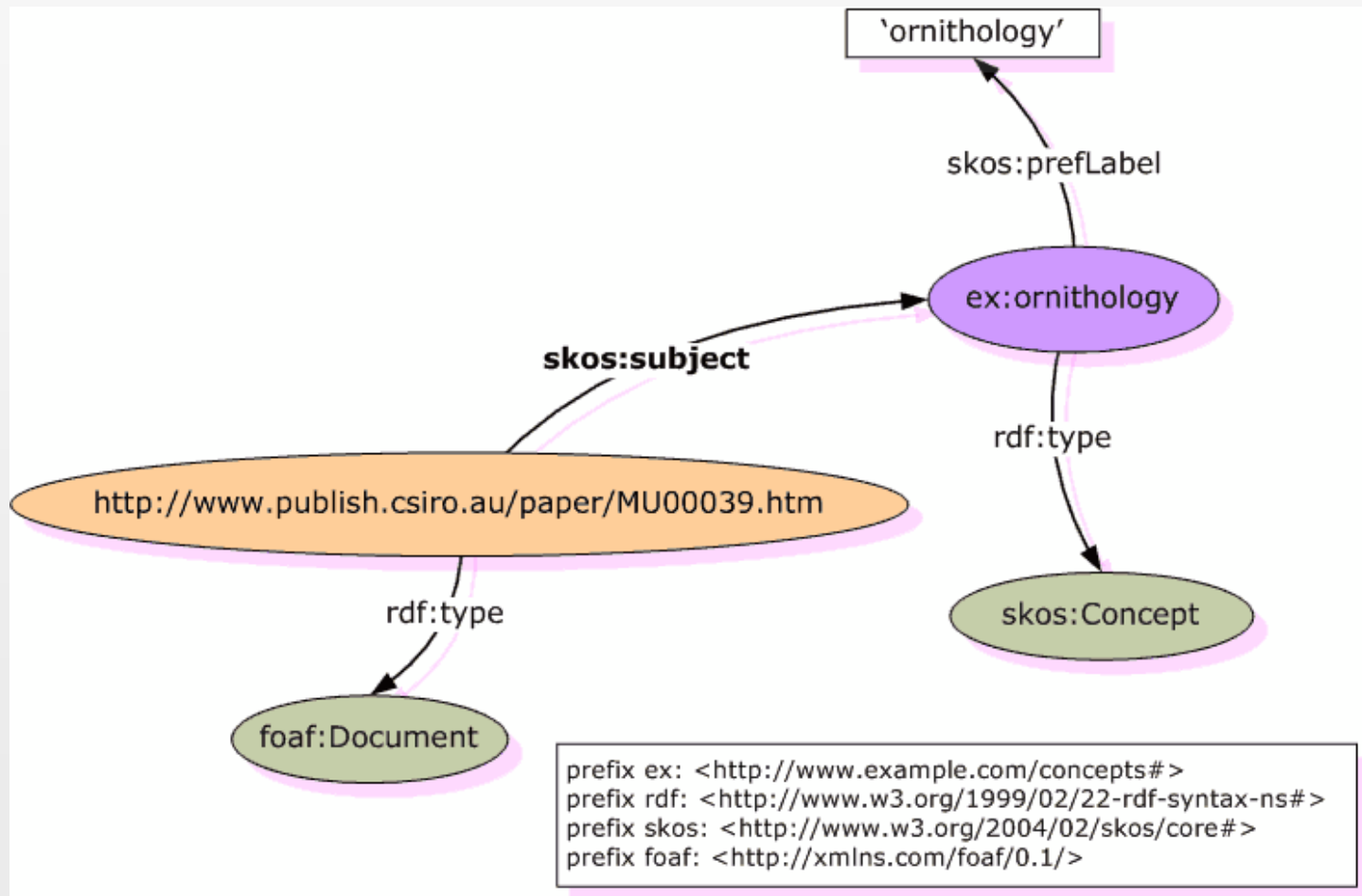


<http://www.w3.org/TR/rdf11-primer/example-graph.jpg>

SKOS

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

SKOS (cont.)



Method (cont.)

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

^{*} Facilitates curation of provenance information

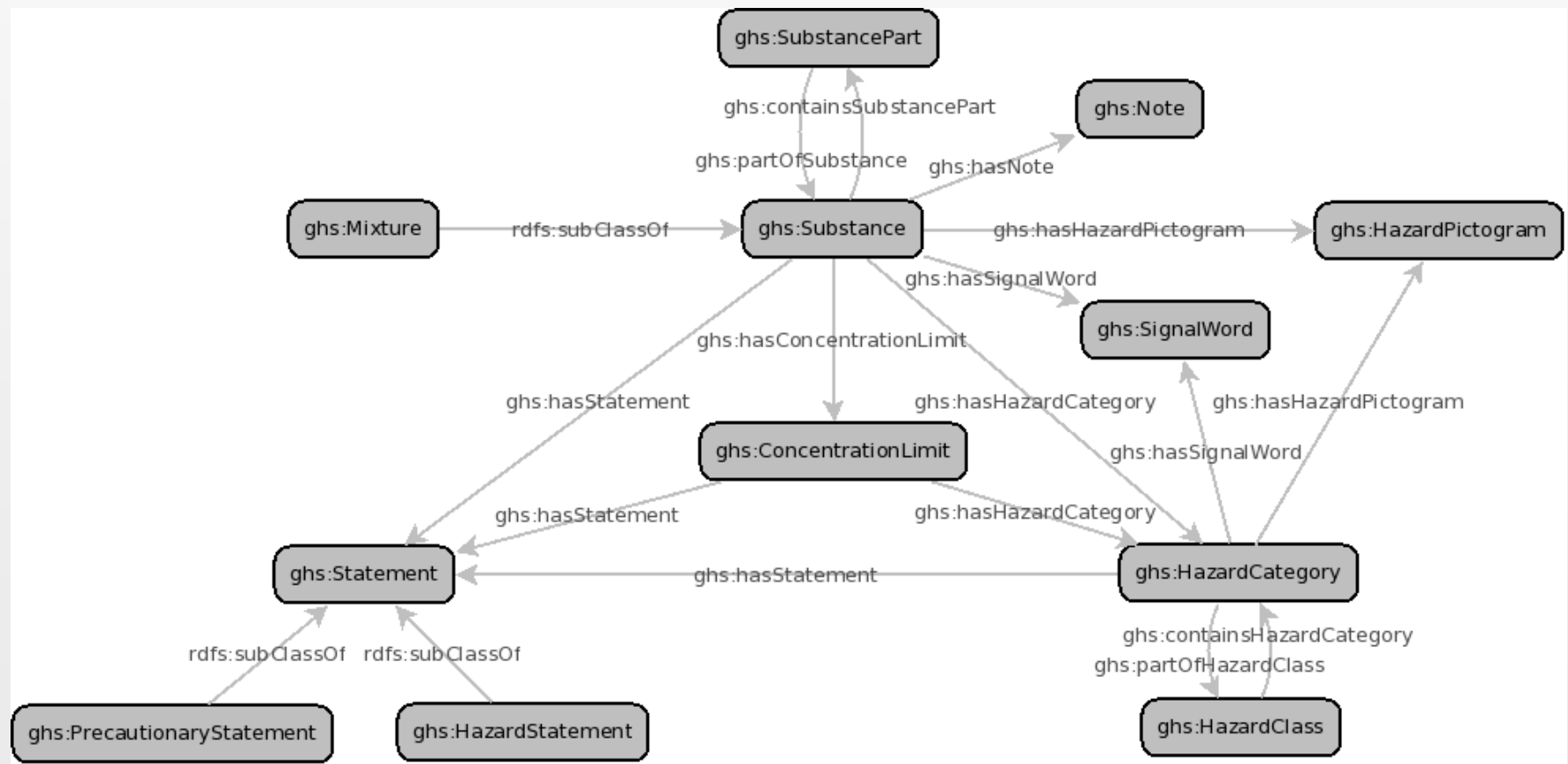
Outline

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Results

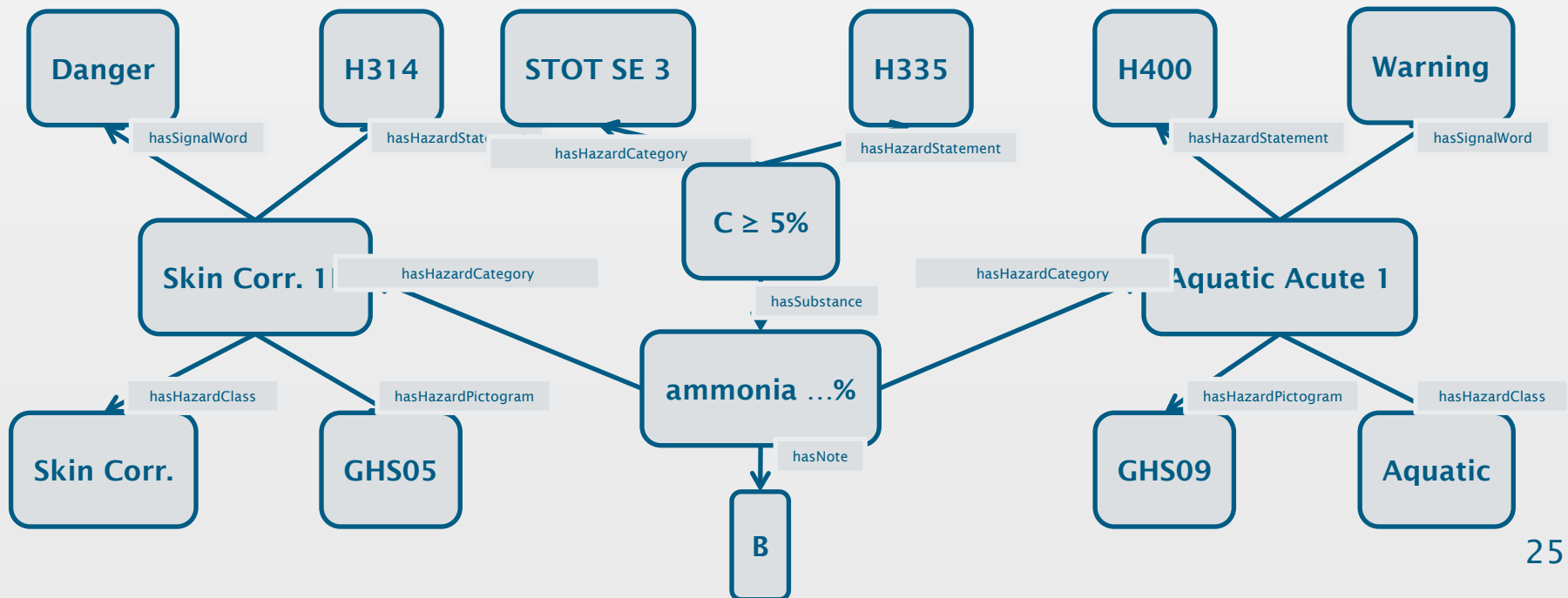
- Machine-accessible representation of GHS/CLP Regulation
 - Definitions (annexes I—V)
 - Classified chemical substances (annex VI)
- Dataset available at: <http://bit.ly/1fvDO5u>

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

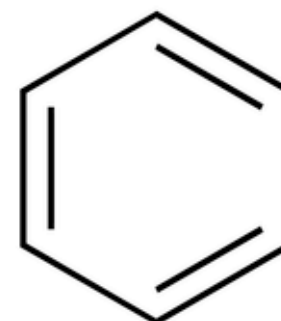
analytical standard

[DOWNLOAD MSDS \(PDF\)](#)

CAS Number **71-43-2** | Empirical Formula (Hill Notation) **C₆H₆** | Molecular Weight **78.11**

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

PubChem Substance ID **24847664**

POPULAR DOCUMENTS: [FTNMR \(PDF\)](#)

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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#> .
```

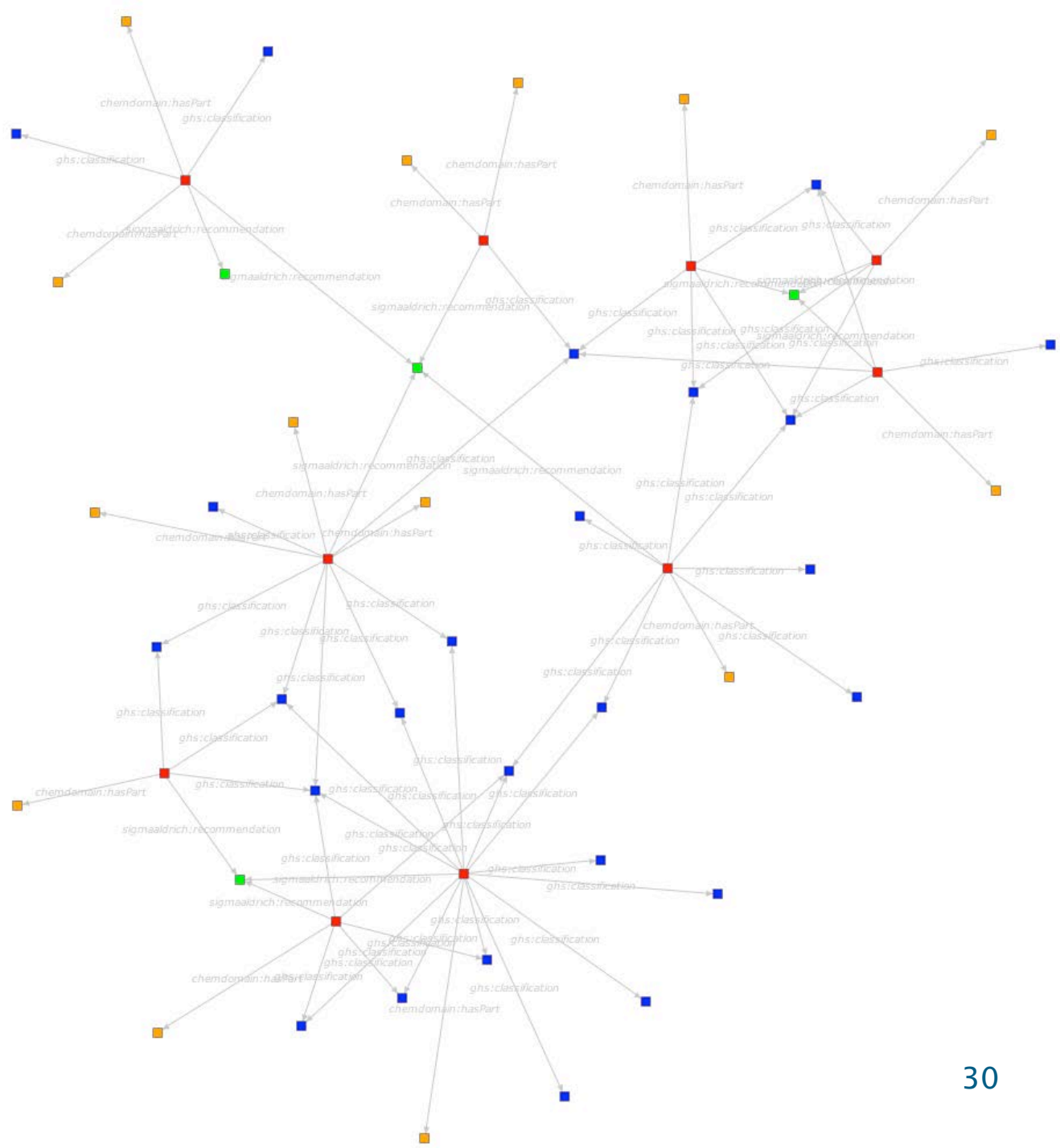
```
<fluka/12540> a chemdomain:NamedChemicalSpecies;
  chemdomain:hasIdentifier [ a sial:ChemicalNumber;
    chemdomain:hasValue "042802"],
  [ a chemdomain:Name;
    chemdomain:hasValue "Benzene"],
  [ a chemdomain:CASNumber;
    chemdomain:hasValue "71-43-2"],
  [ a chemdomain:SMILES;
    chemdomain:hasValue "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> .
```

Red square = Chemical substance

Orange square = Mixture part

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

Blue square = GHS hazard category

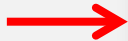


Web Application Protocol

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**



New COSHH Assessment Form | Sigma-Aldrich ©

New COSHH Assessment Form | ...

http://localhost:4567/

New COSHH Assessment Form

Add Chemical:

Template: Chemistry, University of Southampton

☐ I agree to the terms and conditions of the disclaimer.

Generate COSHH Assessment Form

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800x600

2) Describe Scientific Experiment

Dynamic
search
with auto-
completion



New COSHH Assessment Form | Sigma-Aldrich ©

New COSHH Assessment Form | ...

http://localhost:4567/

New COSHH Assessment Form

Add Chemical: Benz

Template: Ch Benzene mpton

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800x600

2) Describe Scientific Experiment

Selected product is added to list




New COSHH Assessment Form | Sigma-Aldrich ©

New COSHH Assessment Form | ...

http://localhost:4567/

New COSHH Assessment Form

Add Chemical:

1. Benzene 
<http://www.sigmaaldrich.com/catalog/product/fluka/12540>

Template:

☐ I agree to the terms and conditions of the disclaimer.

Generate COSHH Assessment Form

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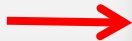
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800x600

Link to
Sigma-Aldrich
product page

3) Select Template

List of
Templates



New COSHH Assessment Form | Sigma-Aldrich ©

New COSHH Assessment Form | ...

http://localhost:4567/

New COSHH Assessment Form

Add Chemical:

1. Benzene

<http://www.sigmaaldrich.com/catalog/product/fluka/12540>

Template:

☒ I agree to the terms and conditions of the disclaimer.

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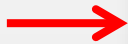
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800x600

4) Accept Terms and Conditions

“Generate”
button is
enabled

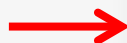


The screenshot shows a web browser window titled "New COSHH Assessment Form | Sigma-Aldrich". The address bar shows "http://localhost:4567/". The page has an orange header with the title "New COSHH Assessment Form". Below the header, there is a form with the following elements:

- "Add Chemical:" followed by a text input field.
- "1. Benzene" with a red minus icon and a link to "http://www.sigmaaldrich.com/catalog/product/fluka/12540".
- "Template:" followed by a dropdown menu showing "Chemistry, University of Southampton".
- A checked checkbox with the text "I agree to the terms and conditions of the disclaimer."
- A button labeled "Generate COSHH Assessment Form".

Below the form, there is a section titled "COSHH Assessment Form Template Service Disclaimer" containing two paragraphs of text. The first paragraph states that the University of Southampton has made the Template Service available as a tool to expedite the completion of COSHH Assessment Forms. The second paragraph states that the University of Southampton is not responsible for any errors or omissions, or for the results obtained from the use of this service. The disclaimer is followed by a dashed line.

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



Chemistry, University of Southampton

Editor mode.
☒ All elements. ☐ Only classification elements. ☐ Only labelling elements.

COSHH Assessment Form

Substance Name	Physical Form	Quantity	Nature of Hazard
Benzene	Value: <input type="text"/> Units: <input type="text"/>		 Danger Warning H225: Highly flammable liquid and vapour. H304: May be fatal if swallowed and enters airways. H315: Causes skin irritation. H319: Causes serious eye irritation. H340: May cause genetic defects -state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard- H350: May cause cancer -state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard- H372: Causes damage to organs -or state all organs affected, if known- through prolonged or repeated exposure -state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard- H373: Causes damage to organs -or state all organs affected, if known- through prolonged or repeated exposure -state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard-

Nature of Process

Control Measures Required

Benzene

- P201: Obtain special instructions before use.
- P202: Do not handle until all safety precautions have been read and understood.
- 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.
- P264: Wash ... thoroughly after handling.
- P280: Wear protective gloves/protective clothing/eye protection/face protection.
- P281: Use personal protective equipment as required.
- P301 + P310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
- P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
- P303 + P361 + P353: IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.
- P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P308 + P313: IF exposed or concerned: Get medical advice/attention.
- P312: Specific treatment (see ... on this label).
- P331: Do NOT induce vomiting.
- P332 + P313: If skin irritation occurs: Get medical advice/attention.
- P337 + P313: If eye irritation persists: Get medical advice/attention.
- P362: Take off contaminated clothing and wash before reuse.
- P370 + P378: In case of fire: Use ... for extinction.
- P403 + P235: Store in a well-ventilated place. Keep cool.
- P405: Store locked up.
- P501: Dispose of contents/container to ...

Declaration

Name of Assessor	Name of Supervisor (for students only)	Head of Department
.....
Status of Assessor		
Signed:	Signed	Signed
Date:	Date:	Date:

Toggle
visibility of
classification
and labelling
elements



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☒ All elements. ☐ Only classification elements. ☐ Only labelling elements.

SIGMA-ALDRICH®

Benzene

<http://www.sigmaaldrich.com/catalog/product/fluka/12540>

Symbols	   <div>GHS02 GHS07</div> <div>GHS08</div>
Signal word	<div>Danger</div> <div>Warning</div>
Hazard statements	H225 H304 H315 H319 H340 H350 H372
Precautionary statements	P201 P202 P210 P233 P240 P241 P242 P243 P264 P280 P281 P301 + P310 P302 + P352 P303 + P361 + P353 P305 + P351 + P338 P308 + P313 P321 P331 P332 + P313 P337 + P313 P362 P370 + P378 P403 + P235 P405 P501

 ADD TO CART

>



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

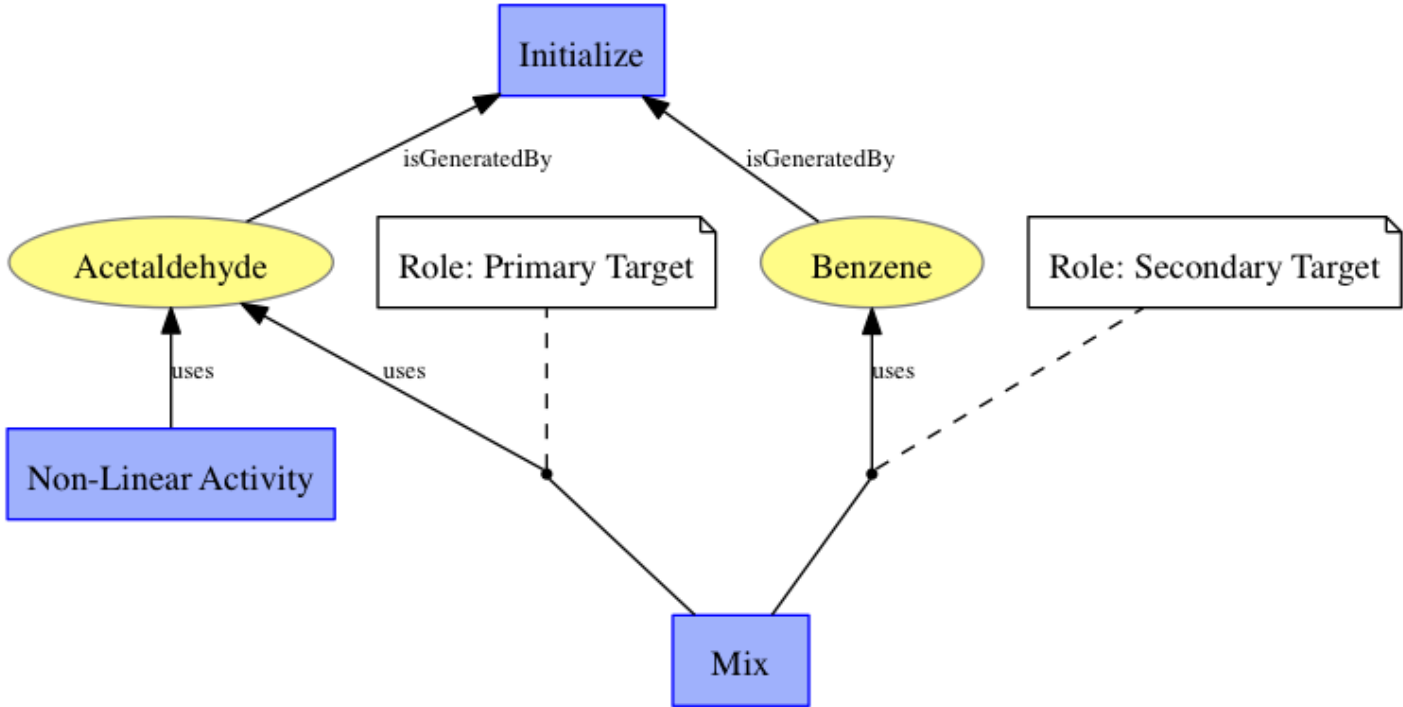


Figure: Workflow-style provenance graph for **Eric's Plan**.

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

<div> <div>Acetaldehyde</div> <div>puriss. p.a., anhydrous, >=99.5% (GC)</div> </div>			<div> <div> <div></div> <div></div> <div></div> </div> <div>008070 FLUKA</div> </div>				
<div>DANGER</div>							
<div>Basic Data</div>			<div>GHS Classification & Labelling Elements</div>				
Synonyms	Acetaldehyde puriss. p.a., anhydrous, >=99.5% (GC); Ethanal		Hazard Class & Category Code	Hazard Statements	Precautionary Statements		
CAS #	75-07-0		Carcinogenicity; Category 2	H351 Suspected of causing cancer «state of exposure if it is conclusively proven that no other risks 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.		
Chemical Formula	CH ₃ CHO				P308 + P313 If exposed or concerned: Get medical advice/attention. P405 Store locked up.		
SMILES	CC=O				P501 Dispose of contents/container to ...		
<div>Composition</div>							
Component CAS #	Exact	Upper Limit					
Acetaldehyde	75-07-0	100.0000% N/A					
<div>Physical Properties</div>							
Physical Form	Liquid	pH					
Molecular Weight	44.05 g/mol	Density					
Boiling Point °C	-125 C(95.1 °F)	Flash Point °C					
Boiling Point °C	21 C(69.8 °F)						
<div>Personal Protective Equipment & Storage</div>							
<div> <div> <div>Disposal 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 your customers. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Wash and dry hands.</div> <div> <div>Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 186(CE).</div> <div> <div>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.</div> <div> <div>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.</div> </div> </div> </div> </div></div>			<div>Flammable liquid; Category 1</div>	<div>H224 Extremely flammable liquid and vapour.</div>	<div> P210 Keep away from heat/sparks/open flames/hot surfaces. – No smoking. P232 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 (in case of) contact (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 ... </div>		
<div>2.00 - 8.00 C</div>							

Benzene

analytical standard

12340
FLUKA®

DANGER

Basic Data			GHS Classification & Labelling Elements			
Synonyms	Benzene, analytical standard		Hazard Class	Precautionary Statements		
CAS #	71-43-2		Category Code			
Chemical Formula	C ₆ H ₆					
SMILES	c1ccccc1					
Composition						
Compliant CAS #s: Exact: Upper Limit Lower Limit						
Benzene 71-43-2 100.000%/N/A N/A						
Physical Properties						
Physical Form	liquid	pH	N/A			
Molecular Weight	78.13	Density	0.874 g/mL @ 25 °C (lit.)			
Boiling Point	80.1 °C	Flash Point	-11.00 °C, closed cup			
Melting Point	5.5 °C (lit.)					
Boiling Point	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 solid, or mixed with other substances, and under conditions which differ from the SDS, 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 1861(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-purifier 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 chemical flame (including protective protection) for the type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.						
Skin contamination/irritation: Category 2						
Serious eye irritation/eye irritation: Category 2						
Flammable liquid: Category 2						
Germ cell mutagenicity: Category 1B						
Skin corrosion/irritation: Category 2						
H304 May be fatal if swallowed and enters airways.						
H305 May cause cancer - irritate route of exposure if it is conclusively proven that no other routes of exposure cause the hazard(s).						
H310 Causes serious eye irritation.						
H315 Highly flammable liquid and vapour.						
H330 May cause genetic defects - irritate route of exposure if it is conclusively proven that no other routes of exposure cause the hazard(s).						
H331 Causes skin irritation.						
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. P313 Do NOT induce vomiting. P303 Store locked up. P501 Dispose of contents/container to ...						
P302 Obtain special instructions before use. P303 Store locked up. P501 Dispose of contents/container to ...						
P264 Wash ... thoroughly after handling. P273 Do not get inside clothing. P280 Wear protective gloves/protective clothing/eye protection/face protection. P301 + P311 IF SWALLOWED: Rinse mouth cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P313 IF SWALLOWED: IF you are irritated/present: Get medical advice/attention.						
P210 Keep away from heat/spark/open flame/hot surfaces. -- No smoking. P223 Keep container tightly closed. P240 Ground/bond container and receiving equipment. P241 Use explosion-proof electrical/lighting/... equipment. P242 Use only non-sparking tools. P243 Take precautionary measures against static discharge. P273 Wear protective gloves/protective clothing/eye protection/face protection. P301 + P311 IF SWALLOWED: Rinse mouth cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P313 IF SWALLOWED: IF you are irritated/present: Get medical advice/attention.						
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Sigma-Aldrich “Quick Order Form”

★ = Recommended Product

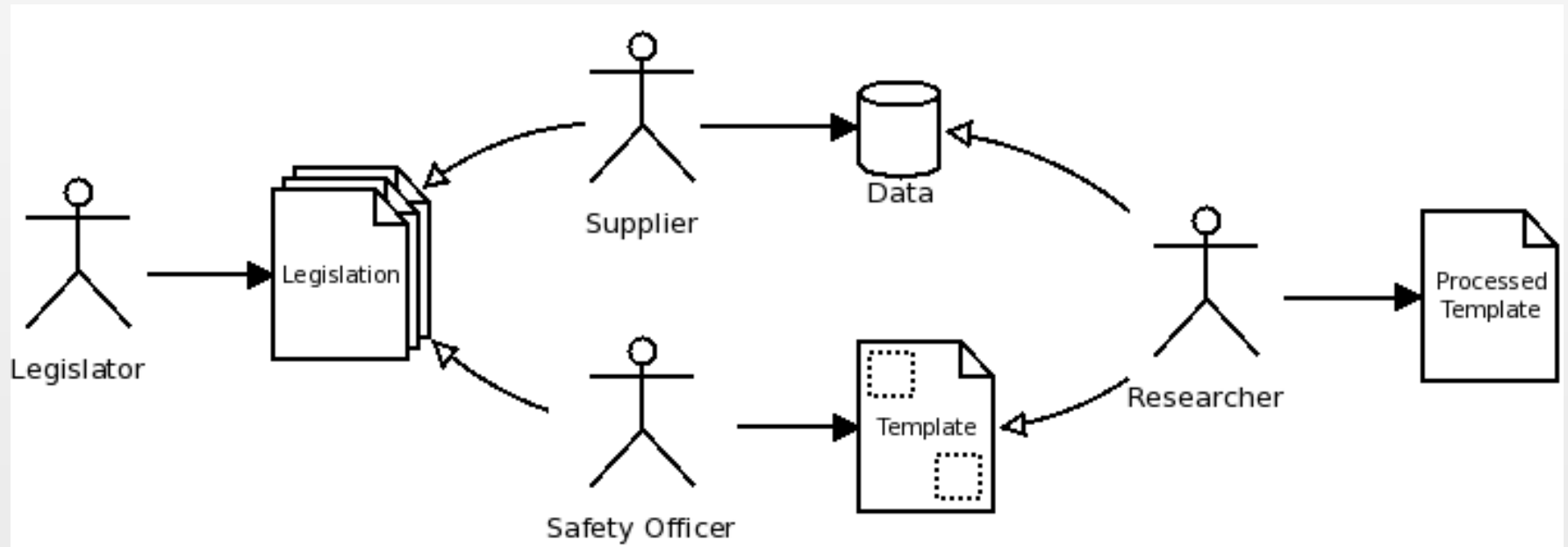
Select	Product Number	Description	Quantity	Your Price	Item Total
<input checked="" type="checkbox"/>	FLUKA 00070	Acetaldehyde puriss. p.a., anhydrous, >=99.5% (GC)	<input type="text" value="1"/>	Not Calculated	Not Calculated
<input type="checkbox"/>	ALDRICH Z677647	★ Butoject gloves	<input type="text" value="0"/>	Not Calculated	Not Calculated
<input checked="" type="checkbox"/>	FLUKA 12540	Benzene analytical standard	<input type="text" value="1"/>	Not Calculated	Not Calculated
<input type="checkbox"/>	ALDRICH Z677698	★ Vitoject gloves	<input type="text" value="0"/>	Not Calculated	Not Calculated

Add Selected Items to Shopping Cart

Outline

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

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 = \neg “induce vomiting”

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

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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?

Acknowledgements

- University of Southampton
 - Jeremy Frey, David Kinnison
- Sigma-Aldrich
 - Bo Jin, Jane Murray, Tom Pieper, Judith Pruss

IUPAC Green Book

