



# Reaction Incident Information

Engaging the community in collecting and sharing safety learnings

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# Safety must be a priority

## Safety is hard

- When things go wrong, we tend to blame the individual
- In reality systemic, process weaknesses contribute to failure
- What is obvious to you may not be to others
- Just because nothing bad happened does not mean it was safe

## To cultivate safety culture

- Focus on prevention
- Examine systems and processes
- All levels must be involved
- **Reward sharing**
- **Promote institutional knowledge retention**



# The Drivers for the Chemical Safety Library (CSL)

- Accidents and near-misses happen every day
- Prevention depends on knowledge of what has happened before
- Our colleagues are often our best teachers
- No one wants to get hurt in the lab
- Difficult to find real-life insights
- Data is scattered in silos
- Lessons learned are often forgotten
- Even reported incidents are not readily discoverable



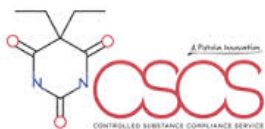
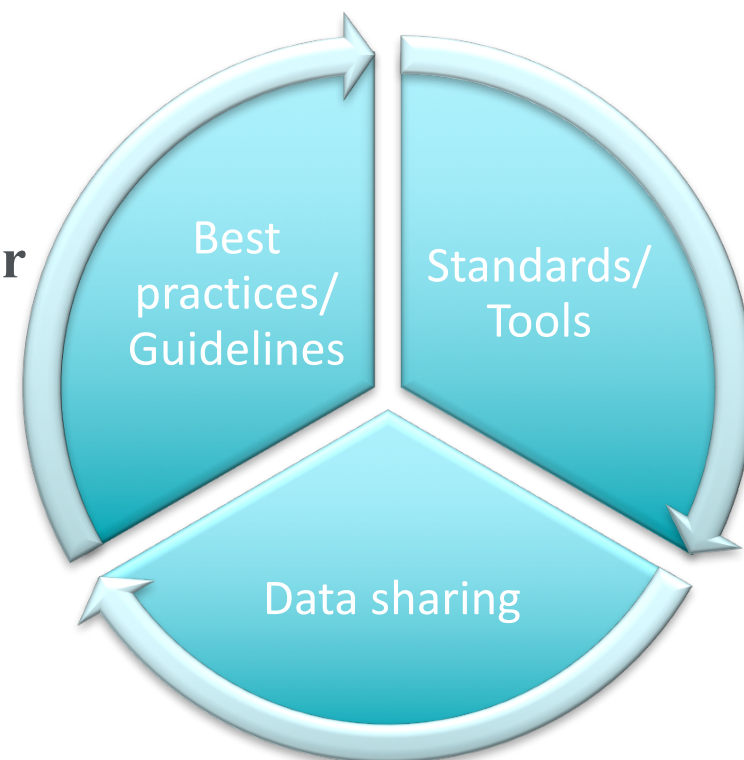
# The Drivers for the Chemical Safety Library

- Accidents and near-misses happen every day
- Prevalence of known hazards
- Our industry is siloed
- No one wants to get hurt in the lab
- Difficult to find real-life examples of incidents
- Information is often shared in silos
- Many incidents are preventable
- Many incidents are preventable

**Ideal opportunity for  
cross-industry  
collaboration and  
cooperation**

# The Pistoia Alliance: Who we are & what we do

- A global, **not-for-profit 501(c)(6)** alliance of life science companies, technology vendors, publishers, and academic groups.
- Dedicated to **improving life sciences R&D** innovation and effectiveness through **pre-competitive collaborative projects and other activities**
- Offer a proven framework for **open innovation & collaboration**

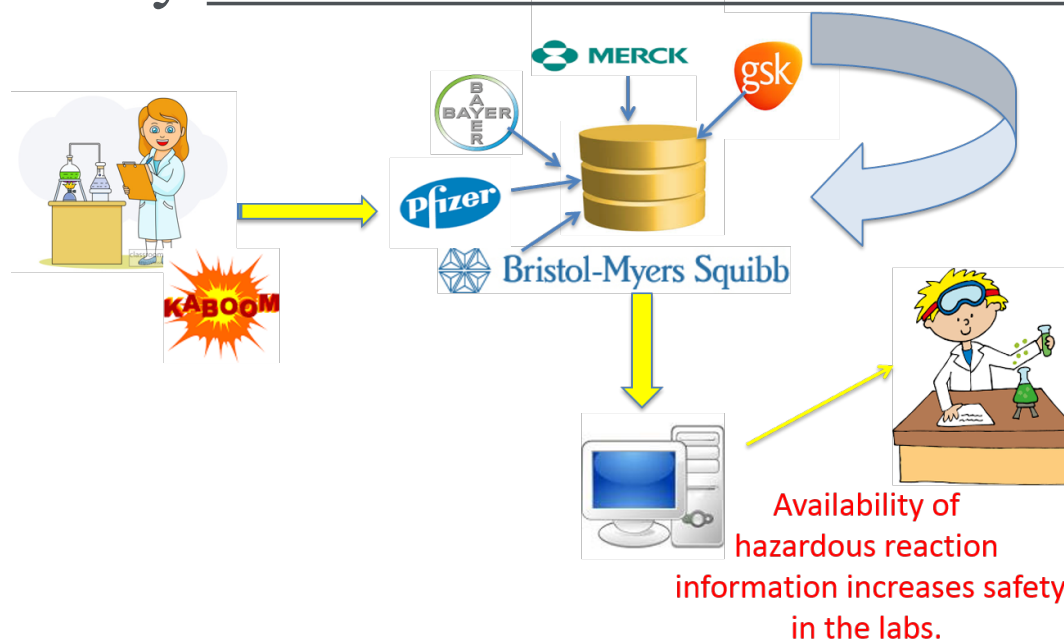






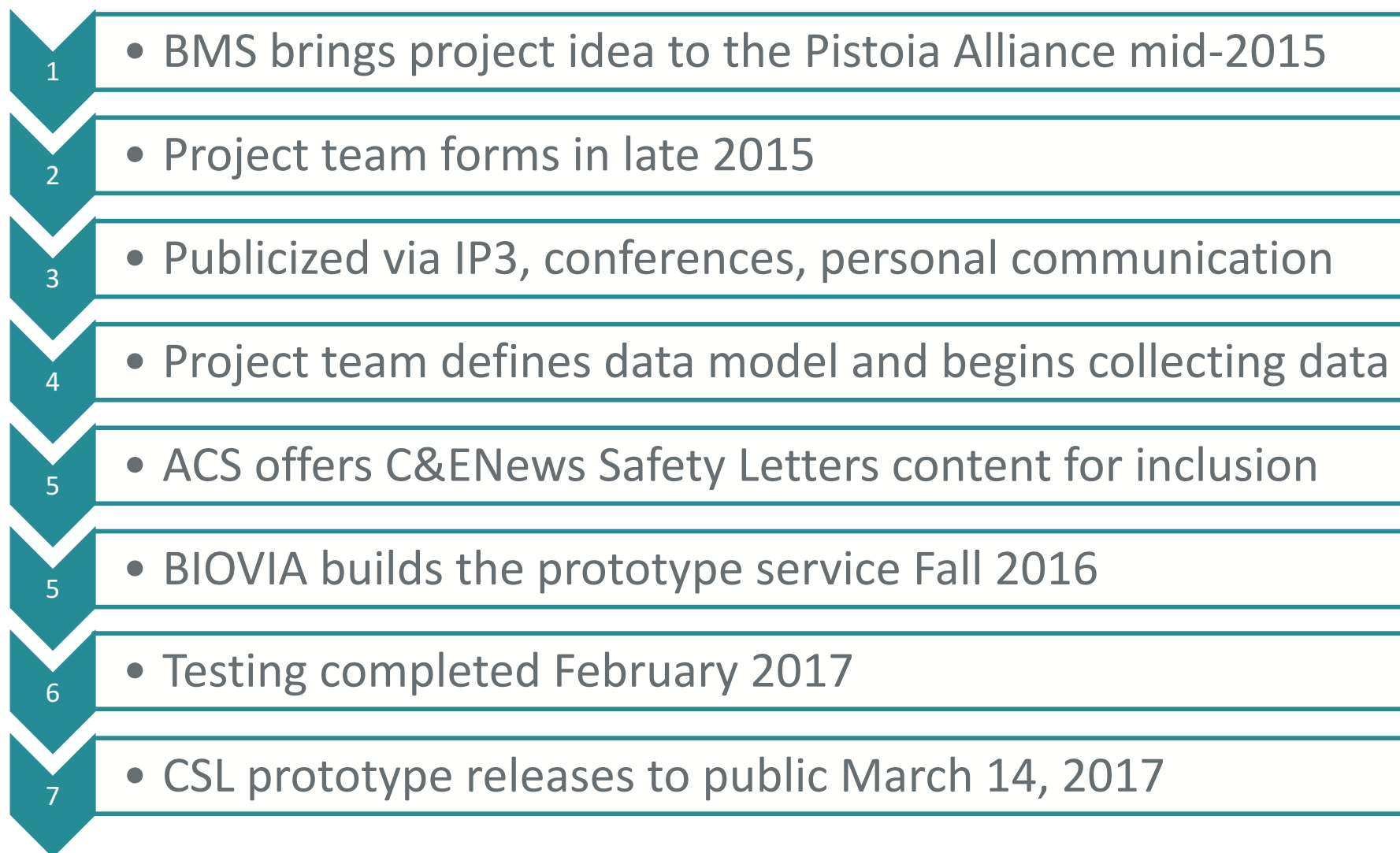
# Chemical Safety Library: goal & value proposition

The Pistoia Alliance *Chemical Safety Library* project will capture and share previously inaccessible reaction incident information.



Making this data available to the chemical community at large will allow organizations to learn and avoid reaction incidents experienced by the wider community, enhancing overall laboratory safety.

# Project progression



# What resources are used today?

- Various substance-based reference sources
- Material Safety Data Sheets (MSDS)
- Scientific literature
- Personal knowledge and experience
- Laboratory Chemical Safety Summaries (LCSS)
  - <https://pubchem.ncbi.nlm.nih.gov/lcss/>
  - Collaboration between PubChem and [ACS-CHAS](#), [ACS-CINF](#) and the [ACS-CCS](#)

Source Name	Total
Bretherick's	13
MSDS *	6
Employee Knowledge	5
SciFinder	4
ACS + Journals	2
Sax's Dangerous properties	2
Vendor SDS *	2
CAMEO	1
Chemwatch SDS *	1
Google	1



# What resources are used today?

- Various substance-based reference sources
- Mat (MS)
- Sci
- Pers exp
- Lab Sum
  - <http://www.fda.gov/ocss/>
  - Collaboration between PubChem and [ACS-CHAS](#), [ACS-CINF](#) and the [ACS-CCS](#)

Reagent/substance  
safety data sources  
abound

Not so for reactions

	Total
	13
	6
	5
	4
	2
erties	2
	2
	1
	1
Google	1

# Creating the prototype service

- **Requirements**

- Build simple service to validate premise: community is willing to share incident info
- Make sure data is movable and reusable
- Implement features that simplify curation and oversight
- Leverage existing reagent info during data entry process

- **Execution**

- Based on BIOVIA CISPro
- Takes 3 minutes to enter an incident
- Has basic search capability for incidents by reagent
- Full set of data available as csv (by reagent)
- Registration required
- Sigma Aldrich reagent data preloaded to simplify user data entry

# CSL prototype

<http://www.pistoiaalliance.org/projects/chemical-safety-library/>



*Lowering Barriers to R&D Innovation*

Home

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 Register

 Download user training material

 Access the CSL tool

The Pistoia Alliance Chemical Safety Library project is dedicated to **sharing previously inaccessible hazardous reaction information** in the interest of **increased laboratory and personal safety across the chemical industries**. Previously, this information may only have been available within the company where the incident occurred. The Pistoia Alliance have now developed a data submission tool to capture, store and search such hazardous reaction information. You can input events to warn others, and you can check individual incidents or download the entire data set to use within your own systems.


By building a rich data source of hazardous reaction information through this tool, and making it easily accessible we can all improve safety for those scientist carrying out experiments in the lab.

## Top Tips

- ✓ Supported browsers: Internet Explorer, Chrome, Safari (make sure your browser is set to allow pop-ups)
- ✓ When submitting a reaction you must set Reporter to your name by searching for and selecting it
- ✓ When submitting a reaction you must create the reaction first, save it, and then on the next screen add the reagents
- ✓ After adding reagents to return to the Home screen, if clicking the Home button





# The CSL prototype


 All ▾ Begins ▾  Search ▾


Home | Preferences ▾ | Help ▾ | Logout

Select a View

  
[Submit Reaction to the Pistoia Alliance Chemical Safety Library](#)

  
[Search Approved Reactions by Reagent](#)

  
[My Submitted Reactions](#)

  
[Pistoia Alliance Chemical Safety Library Data Download](#)

# The CSL prototype: adding an incident

Submit Reaction to the Pistoia Alliance Chemical Safety Library

**Reporter\***  Search

**Source\***

**Reaction Class**  Search

**Functional Group**

**GHS Category**

- ALDEHYDE
- Aryl methyl
- Aryl methyl ketone
- AZIDE
- Heteroaryl chloride
- HeteroAryl Methyl
- NITRO
- ☐ Corrosive to Metals
- ☐ Explosive
- ☐ Flammable
- ☐ Gas Emitter
- ☐ Gas Under Pressure
- ☐ Genotoxic
- ☐ Harmful
- ☐ Organic Peroxide
- ☐ Oxidizer
- ☐ Pyrophoric
- ☐ Reproductive Toxin
- ☐ Self-Reactive
- ☐ Sensitizer
- ☐ Toxic
- ☐ Water Reactive

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**Scale with unit**

**DOI Link** Text   
URL body

**Warning Message\***

**Additional Information**

# The CSL prototype: new reaction added

BIOVIA CISPro

All ▾ Begins ▾ Search ▾ Home | Admin ▾ | Preferences ▾ | Help ▾ | Logout

Add ▾ | More ▾

CSL Reactions

Expand All

- CSL00002 oxidation
- CSL00003 oxidation
- CSL00004 Nitration
- CSL00005
- CSL00006 Substitution
- CSL00007 Deprotonation
- CSL00008 BOCN3 formation
- CSL00009
- CSL00010 Cycloaddition
- CSL00011 Friedel Crafts
- CSL00012 NITRO
- CSL00013
- CSL00014
- CSL00015
- CSL00016 ALDEHYDE
- CSL00017
- CSL00018
- CSL00019
- CSL00020 AZIDE
- CSL00021 oxidation
- CSL00022
- CSL00023 Bromination Aryl methyl ketone
- CSL00024

CSL00002 oxidation

Edit Options ▾

CSL No CSL00002

Reaction Class oxidation

Functional Group

Reaction Approval History

Add ▾ | More ▾

Incident Reagents

Disable Paging

Reagent	CAS No	MFCID	InChI
DMSO	67-68-5		
perchloric acid	7601-90-3		

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Source Internal

GHS Category Explosive

Scale with unit 1 gram

DOI Link

Warning Message mixture can result in explosion

Date Created 2/10/2017

Date Modified 2/13/2017

Reporter

Organization



# The CSL prototype: all data available for download

CSL Data Download									
Disable Paging									
CSL No	Reaction Class	Functional Group	Reagent Name	CAS No	MFCID	GHS Category	SMILES	INCHI	Warning Message
CSL00002	oxidation		DMSO	67-68-5		Explosive			mixture can result in explosion
CSL00002	oxidation		perchloric acid	7601-90-3		Explosive			mixture can result in explosion
CSL00003	oxidation		sodium percarbonate	15680-89-4		Explosive			can form explosive acetone peroxide compound
CSL00003	oxidation		ACETONE	67-64-1		Explosive			can form explosive acetone peroxide compound
CSL00004	Nitration		NITRIC ACID	52583-42-3, 7697-...	MFCID00011349	Explosive	O[N+](=O)[O-]	InChI=1S/HNO3/c2-...	Can explode and/or have large exotherm. Use
CSL00004	Nitration		Ac2O			Explosive			Can explode and/or have large exotherm. Use
CSL00005			THF						Can polymerize, large exotherm. Avoid combin
CSL00005			Triflic anhydride						Can polymerize, large exotherm. Avoid combin
CSL00006	Substitution		DICHLOROMETHANE	75-09-2	MFCID0000881	Explosive	ClCCl	InChI=1S/CH2Cl2/c2...	Formation of diazidomethane which can explo
CSL00006	Substitution		SODIUM AZIDE	26628-22-8	MFCID00003536	Explosive	[Na]N=[N+]=[N-]	InChI=1S/N3.Na/c1-...	Formation of diazidomethane which can explo
CSL00007	Deprotonation		SODIUM HYDRIDE	7646-69-7	MFCID00003471				Thermal runaway reaction already at tempera
CSL00007	Deprotonation		DMF						Thermal runaway reaction already at tempera
CSL00008	BOCN3 formation		HNO2			Explosive			Explosion during workup when half of the solv
CSL00008	BOCN3 formation		BOCNHNH2			Explosive			Explosion during workup when half of the solv
CSL00009			ACETONE	67-64-1		Explosive			Formation of acetone peroxides possible. Try
CSL00009			H2O2			Explosive			Formation of acetone peroxides possible. Try
CSL00010	Cycloaddition		BF3			Explosive			Combinations of TMSN3 and Lewis acids can d
CSL00010	Cycloaddition		TMSN3			Explosive			Combinations of TMSN3 and Lewis acids can d
CSL00011	Friedel Crafts		AlCl3						Explosive decomposition > 120Å°C observed c
CSL00011	Friedel Crafts		NITROBENZENE	98-95-3	MFCID00007043		[O-][N+](=O)c1ccccc1	InChI=1S/C6H5NO2...	Explosive decomposition > 120Å°C observed c
CSL00012		NITRO	2-ETHYLHEXYLAMINE	104-75-6	MFCID00008148	Explosive	CCCCC(CC)CN	InChI=1S/C8H19N/c...	Warning - This combination can cause a run-a
CSL00012		NITRO	1-CHLORO-2-NITRO...	88-73-3	MFCID00007061	Explosive	[O-][N+](=O)c1ccccc1Cl	InChI=1S/C6H4ClNO...	Warning - This combination can cause a run-a


# Administrators monitor new incident inputs

**DS BIOVIA CISPro** All Begins Search

Select a View Add More

**Reactions Pending Review**

Disable Paging

CSL No	GHS Category	Scale with unit	Warning Message	Additional Informat	Date Created	Review Status
 CSL00028	Gas Emitter	1:1 mole	A significant am...		3/23/2017	Pending

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# The CSL prototype launch

The screenshot shows the c&en Chemical & Engineering News website. The header includes the c&en logo and navigation links: Home, Magazine, News, Departments, Collections, and Blogs. Below the header, there's a search bar and a navigation bar. The main content area features a large article titled "Database of hazardous reactions launched" with a sub-headline "Tool allows scientists to submit and search for safety information not publicly cataloged elsewhere" by Jyllian Kemsley. The article text mentions a nonprofit group releasing a database tool for sharing hazardous chemical reaction information, called the Chemical Safety Library. An inset image shows a screenshot of the database interface with fields for chemical name, CAS No., and reaction details.

<http://cen.acs.org/articles/95/i12/Database-hazardous-reactions-launched.html>

The screenshot shows the Chemistry World website. The header includes the Chemistry World logo and navigation links: HOME, NEWS, OPINION, MATTER, ENERGY, EARTH, LIFE, CULTURE, CAREERS, PODCASTS, WEBINARS, and LONG READS. Below the header, there's a search bar and a navigation bar. The main content area features a large article titled "New database highlights cumulative chemical dangers" by Rebecca Trager, dated 20 March 2017. The article text mentions a collaborative effort offering information on hazardous chemical reactions and allows users to add their own incident reports. It also mentions a collaborative and publicly available database of previously inaccessible hazardous chemical reactions has been launched by the Pistoia Alliance, a not for profit group based in Boston, US.

<https://www.chemistryworld.com/news/new-database-highlights-cumulative-chemical-dangers/3006996.article>

- 300 accounts requested within 36 hrs
- Last week: over 500 requested
- April 2: over 600 accounts requested

## Prototype next steps

- Validate the premise: **community is interested**
- Validate the premise: **community ready to share**
- Validate the data model: We are **capturing the right data**
- Establish the effort needed to maintain the system
- Look for **long term partner** to sustain the effort
- Hackathons/competitions to leverage the data and enhance offering



# We need your help

- **Enter your incidents, near misses, literature-backed events**
- **Get your colleagues involved**



- What barriers do you see to general participation?
- Would you submit an entry?

# Acknowledgements

## CSL Funding Members

Bayer	Merck Co
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## Steering Committee

David Nirschl BMS - Project Champion  
Mark Manfredi BMS - Project Lead  
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Beth Fisher	Merck
Sudhir Hande	AZ
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## Community of Interest

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Rob Brown  
Nathan Watson  
Ron Gantt  
David Christenson  
Marc Rounsaville  
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Jon Patterson  
Roger Sayle  
Tim Dudgeon  
Ralph Stuart



If you want to go fast,  
*go alone.*

If you want to go far,  
*go together.*

- African Proverb -





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