

CHEMICAL SAFETY LIBRARY (CSL)

A great journey with innovation, collaboration, and education

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CAS

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The Pistoia Alliance CSL project: An inspiration from BMS story

Trifluoroacetoxyborohydride

Original synthesis described in United States Patent 4,835,278

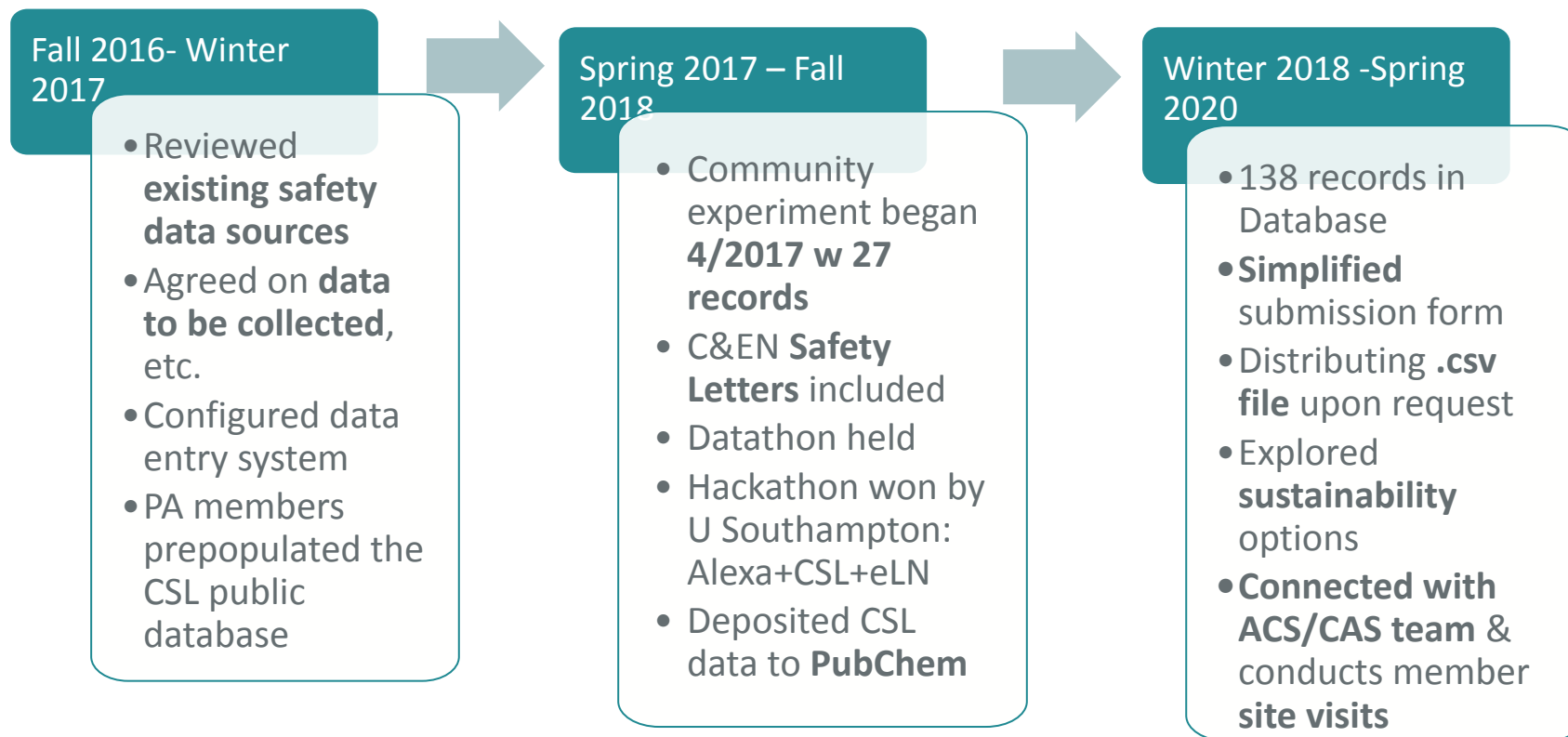


- Exothermic reaction
- Byproduct: hydrogen gas
- Powder dissolves rapidly, reaction not controlled, will consistently catch fire
- Lesson: Must use pelletized NaBH_4 , dissolution controls reaction rate

* *Ensuring That Lessons Learned Are Not Forgotten, Leveraging ELN to Transform the Safety Paradigm*, Mark Manfredi (BMS), ACS Fall 2016 – CHAS Division talk

Early innovation journey: Ideation and prototyping

Driven by Pistoia Alliance and its partners



Test, learn and adjust CSL through partnering with CAS

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CAS Makes Commitment to Enhance Laboratory Safety by Partnering with the Pistoia Alliance for Chemical Safety Library

New agreement will leverage CAS information management capabilities to grow critical safety resource pioneered by the Pistoia Alliance for the chemical community

Columbus, OH, and Boston, MA June 23, 2020 - CAS, a division of the American Chemical Society specializing in scientific information solutions, and the Pistoia Alliance, a global, not-for-profit members' organization that works to lower barriers to innovation in life sciences R&D, announced today the signing of an agreement under which CAS

Home > Resources > Press Releases

> Launch of Pistoia Alliance Chemical Safety Library powered by CAS platform facilitates information sharing

Launch of Pistoia Alliance Chemical Safety Library powered by CAS platform facilitates information sharing between scientists to improve laboratory safety

New open access search platform simplifies access to critical crowd-sourced reaction hazard information to reduce repeat incidents.

Columbus, OH and Boston, MA – (October 19th, 2020) – [CAS](#), a division of the American Chemical Society specializing in scientific

Team Work,
Innovation,
Creativity,
Individual
Commitment

**Build-A-Thon to
deliver the CSL**

Proactively promoted CSL and lab safety through marketing efforts, social media, and strategic alliances

Included in ACS Safety Portfolio

Published blogs to raise awareness of CSL

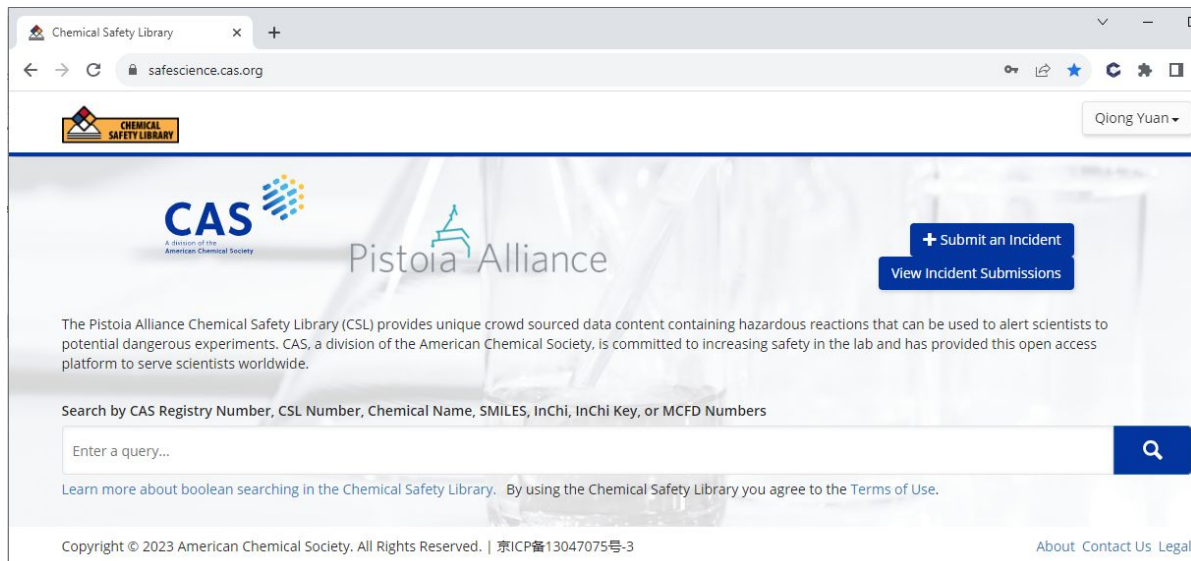
Applied for ACS CHAS grant to develop CSL in the box



Signed MOU with CSHEMA as Strategic Alliance Partner in August 2021, attended its annual meeting in July 2022 and safety week in 2023



CSL (safescience.cas.org) page views and usage metrics



Users by Country



COUNTRY	USERS
United States	1.9K
Japan	994
Germany	993
China	267
United Kingdom	55
Mexico	44
India	30

Users 4.6K
New users 1.6K



A total of
~147K page views
~22K unique users
~ 550 registered users
~ 10 new submissions

Connected with Purdue Data Mine to leverage AI for content extraction

Educated data science students lab safety and chemical information resources

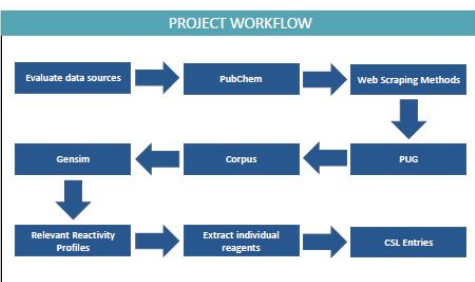
PURDUE UNIVERSITY The Data Mine | **Chemical Safety Library** | **Pistoia Alliance** | **CAS** A Division of the American Chemical Society

Christian Durbin, EunGyun Lee, Nicole Lu, Joel Kuriakose, Sophie Zhou

INTRODUCTION

- Pistoia Alliance and CAS: Not-for-profit organizations committed on obtaining crowd sourced data to promote safety in laboratories
- Pistoia's CSL: An open access platform developed by CAS that provides hazardous reaction information to alert scientists of dangerous reactions
- Goal: Expand the CSL by identifying new hazardous 2+ reagent reactions
- Method: Develop model to find most reactive chemicals to enter into CSL database

PROJECT WORKFLOW



RESEARCH METHODOLOGY 1: GENSIM

Created a corpus with reactivity profiles of a list of compounds from PubChem

Used Gensim to create a frequency list of select key words including:

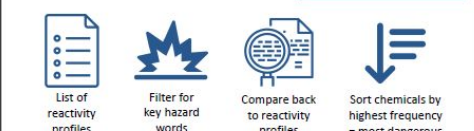
- Explosive, flammable, combustible, accidental, hazard

Used to determine which compounds are the most dangerous by comparing how often these key words are shown in profiles

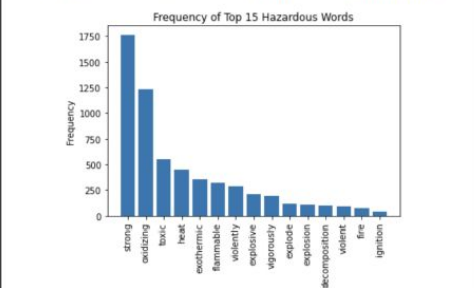
PubChem

Why Reactivity Profiles?

- Existence of the structured Reactivity Profile indicates of a hazardous reaction
- Contains all necessary information to file incident report



Frequency of Top 15 Hazardous Words



9.2 Reactivity Profile

Mixing acetic acid in equal molar portions with any of the following substances in a closed container caused the temperature and pressure to increase: 2-aminocrotonic acid, chlorosulfonic acid, ethylene diamine, ethylenimine (NFA 1919), acetic acid or acetic anhydride can **explode** with nitric acid if not kept cold. Potassium hydroxide residue in a catalyst pot reacted **violently** when acetic acid was added (MCA Case History 303, 1963). During the production of terephthalic acid, m-xylene is oxidized in the presence of acetic acid. During these processes, **detonating** mixtures may be produced. Addition of a small amount of water may largely eliminate the risk of **explosion**. (NFA 4934, 1961 p. 7). Acetaldehyde was put in drums previously pickled with acetic acid. The acid caused the acetaldehyde to polymerize and the drums got hot and vented (MCA Case History 1764, 1971). A mixture of ammonium nitrate and acetic acid **explodes** when warmed, especially if concentrated (Jen-Schroeter 1938, p. 322). Several laboratory **explosions** have been reported using acetic acid and phosphorus trichloride to form acetyl chloride. Poor heat control probably caused the formation of phosphine (J. Am. Chem. Soc. 60:488, 1938). Acetic acid forms **explosion** mixtures with p-xylene and air (Skauer, 81, 1970. Chem. Prom. 46(10):747-750).

METHODOLOGY 2: REACTIVITY PROFILE EXTRACTION

- Web-scraped PubChem using the PUG-VIEW API to request information such as the reactivity profile and IUPAC name for a particular compound
- Split reactivity profile into sentences and extracted compounds, shown as embedded links, to form reactant groups along with the specific compound
- Filtered out sentences not containing hazard words to create warning messages for the reactant group

Reactant 1: hydrogen
Reactant 2: 1-aminopropan-2-ol
Warning Message: Flammable gaseous hydrogen is generated by amines in combination with strong reducing agents, such as hydrides.

Reactant 1: hydrazine hydrate
Reactant 2: 1-cis-2,3-dichloroethane
Warning Message: The mixture of this compound with hydrazine hydrate caused a violent reaction.

Reactant 1: ammonia
Reactant 2: 1,2-dichloroethane
Warning Message: Liquid ammonia and ethylene dichloride can cause an explosion when mixed, nfp 491m, 1991.

- Tf-idf model to sort reactivity profiles by highest frequency of hazard words
- Compares individual reactivity profile to pre-determined list of words
- Determines most dangerous compounds and reactions to add to CSL first

Chemical Name	Similarity Score
Acetyl Chloride	0.62683517
Isopropylamine	0.6027288
Bromoform	0.55904955
Ethyl Chloride	0.5437039

CONCLUSION

- Successfully built up models to extract reactivity information from PubChem
- Sorted through the corpus using dangerous word frequencies
- Formed an organized list of 2+ reagent reactions with warning messages that can be manually inputted into the CSL
- Next steps:
 - Running key word searches on different data sources
 - Automation of incident report filing
 - Include reactions of 3+ reagents

ACKNOWLEDGEMENTS & REFERENCES

Special thanks to:

- Pistoia Alliance Advisors: Gabrielle Whittick, Qiong Yuan, Mark Manfredi, Grace Baysinger, Thomas Vickery, Ralph Stuart, Jian (Jeff) Zhang
- Data Mine Mentors: Rachel Pfeifer, Ryan Altman, Nick Rosenorn, Nick Lenfestey, Mark Ward, Maggie Betz, and Data Mine Staff

References:
[PubChem](#) | [Gensim](#) | [PUG](#) | [Cameo Chemicals](#)

EXAMPLE SUBMISSION / ENTRIES TO CSL

Incident Report Form

Reagent(s)

BROMINE
CAS RN: 7726-95-6
MPCD: MFC00001896
SMILES: BrBr
InChI: InChI=1S/Br2(c1-1
InChI Key: GD1B9J2TBHREO-UHFFFAOYSA-N

SULFURIC ACID
CAS RN: 7664-93-9
MPCD: MFC00064589
SMILES: OS(=O)(=O)O
InChI: InChI=1S/O=S(=O)(O)O
InChI Key: QAOQWNCQDCNURD-UHFFFAOYSA-N

SODIUM BROMIDE
CAS RN: 59217-43-0, 7647-15-6
MPCD: MFC00003475
SMILES: [Na+].[Br-]
InChI: InChI=1S/[Na+].[Br-]1/2-1
InChI Key: [BTNAGRQKSI-UHFFFAOYSA-M

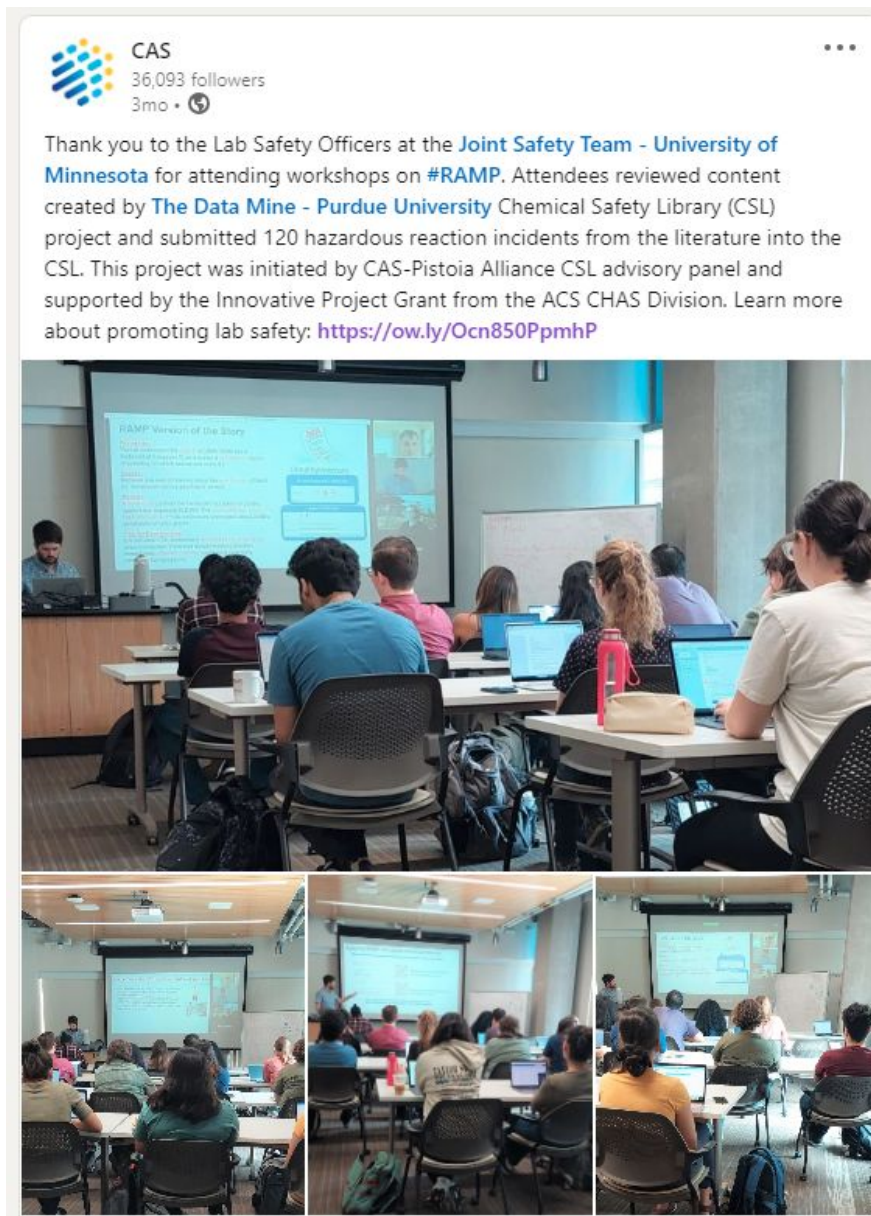
- 2023 spring semester
- 5 students + 1TA
- CSL advisors one hour/week

Developed ~1,000 ranked hazards information from PubChem through data mining algorithm

The Data Mine Corporate Partners Symposium 2023

Conducted workshops with University of Minnesota Lab Safety Officers (LSOs) and validated 120 records from Purdue work

- 17 LSOs/graduate students
- 2-day, 4-hour workshops
- Refreshed on RAMP
- Learned about using AI for chemical safety
- Met with industry experts
- Reviewed content created by Purdue
- Submitted 120 records to CSL



CSL-CAS Advisory Panel review and guide CSL development

- Chair Elected: **Mark Manfredi**, Senior Manager of BMS (retired in April)
- Current Advisors:
 - **Grace Baysinger**, Chemistry and Chemical Engineering Librarian at Stanford; ACS CINF
 - **George Athens**, R&D EH&S and Learning Director, Dow
 - **Christopher Kolodziej**, Chemical Hygiene Officer at UCLA, CSHEMA
 - **Thomas Vickery**, Senior Engineer, Process Research and Development, Merck
 - **Meghan Lafferty**, Chemistry, Chemical Engineering & Materials Sciences Librarian, University of Minnesota
 - **Ralph Stuart**, Chemical Hygiene Officer at Keene State College, ACS CHAS (retired)
 - **Chengjian Zhu**, Dean of the School of Chemistry and Chemical Engineering, Nanjing University, China
 - **Gabrielle Whittick**, Director of GMW Consulting, Pistoia Alliance
 - **Qiong Yuan**, Director of Innovation, CAS



We deeply appreciate the support and contributions of Executive Leaders **Kathy Gibson** (head of CAS Innovation), **Becky Upton** (President of Pistoia Alliance) and former Chair **Carmen Nitsche** (General Manager of CCDC) and former Advisors: **Alison Frontier** (University of Rochester) and **Ramesh Durvasula** (Lilly Research Labs).



Scale up and adoption: Your attention and support is needed

Calling all experts and volunteers

- Be an educator: Cite this resource to lab workers for their awareness
- Be a contributor: Submit an incident record to CSL from your reading, experience, and learning
- Be a collaborator: Share your resources to help us improve CSL
- Be a champion in your organization for CSL: Promote CSL and download database for internal use
- Be an advisor: Attend our monthly meeting and provide input/feedback

Our congratulations to Pistoia Alliance for this great initiative!



CSL will become part of the CAS Innovation portfolio in 2Q/2024 since we value safety!

Contact Dr. Qiong Yuan at qyuan@cas.org for opportunities to work together on CSL!