

# Ensuring That Lessons Learned Are Not Forgotten

## *Leveraging ELN to Transform the Safety Paradigm*

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Research Informatics  
& Automation

# IDENTIFYING AND EVALUATING HAZARDS IN RESEARCH LABORATORIES

GUIDELINES DEVELOPED BY THE HAZARDS IDENTIFICATION AND EVALUATION TASK FORCE OF THE AMERICAN CHEMICAL SOCIETY'S COMMITTEE ON CHEMICAL SAFETY



# C&EN

CHEMICAL & ENGINEERING NEWS

## MINIMIZING LAB HAZARDS

**ACS MEETING NEWS:** ACS guidelines are directed at small-scale research lab activities

**I**N THE WAKE of several serious accidents in research laboratories across the U.S., the American Chemical Society has issued new guidelines in a 132-page report titled "Identifying and Evaluating Hazards in Research Laboratories." The document was developed by the ACS Committee on Chemical Safety and made publicly available online on Sept. 4 (<http://cenm.ag/hazard>).

Hazard analysis is "a core process that's necessary

<http://cen.acs.org/content/dam/cen/static/pdfs/ACSHazardAnalysis20130904.pdf>

 Bristol-Myers Squibb

# Agenda

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**Case Study**

**People or Process ?**

**IT Requirements**

**New Directions**

**Pistoia Alliance Project**

# Sodium Trifluoroacetoxyborohydride

*United States Patent 4,835,278*

## EXAMPLE 3

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A suspension of sodium trifluoroacetoxyborohydride (ca. 1 mMole, freshly prepared from trifluoroacetic acid and sodium borohydride in tetrahydrofuran, 0.5 ml) was

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added dropwise at 0° to a stirred solution of intermediate 2 (0.50 g) and cerium trichloride heptahydrate (0.38 g) in dichloromethane (1 ml) and methanol (4 ml). The temperature of the reaction mixture was kept at 0° during the addition. The mixture was stirred at 0° for 10 minutes and worked up according to System A. Analy-

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sis of the product by h.p.l.c. revealed that the title compound had been obtained in a ratio of the 3- $\beta$  and 11- $\alpha$  epimers of 97.1:2.9.

# Sodium Trifluoroacetoxyborohydride

**SIGMA-ALDRICH**®

## Material Safety Data Sheet

Version 4.2

Revision Date 01/17/2012

Print Date 09/17/2012

### 10. STABILITY AND REACTIVITY

#### Chemical stability

Stable under recommended storage conditions.

#### Possibility of hazardous reactions

Reacts violently with water.

#### Conditions to avoid

Exposure to moisture.

#### Materials to avoid

Oxidizing agents, Chemically active metals, acids, Reacts violently with water.

#### Hazardous decomposition products

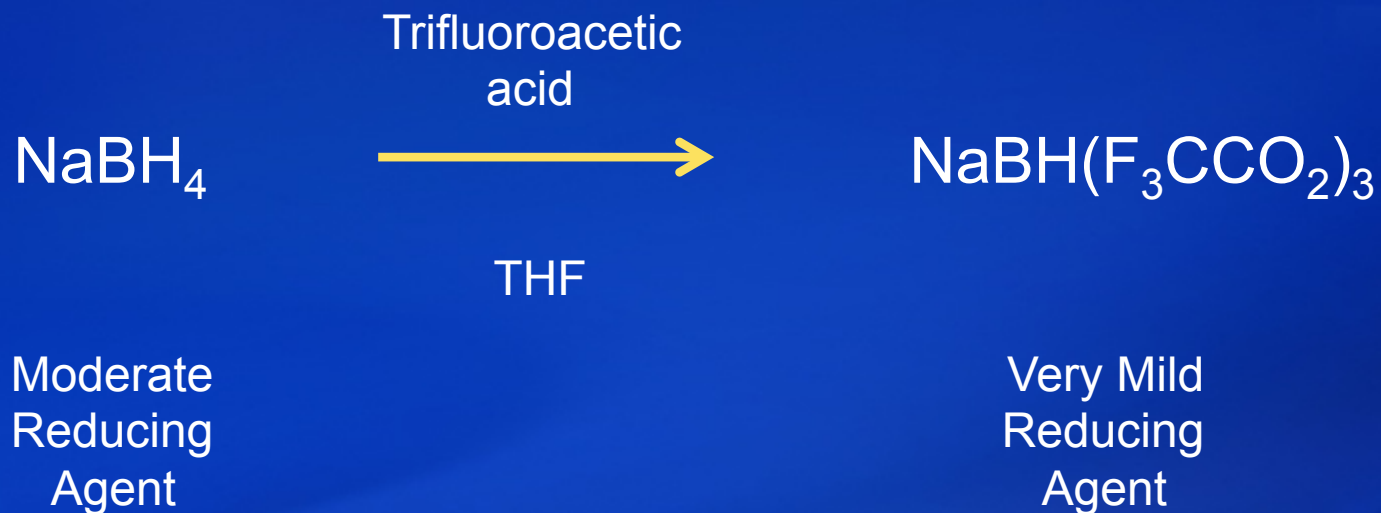
Hazardous decomposition products formed under fire conditions. - Nature of decomposition products not known.

Other decomposition products - no data available

Sodium borohydride

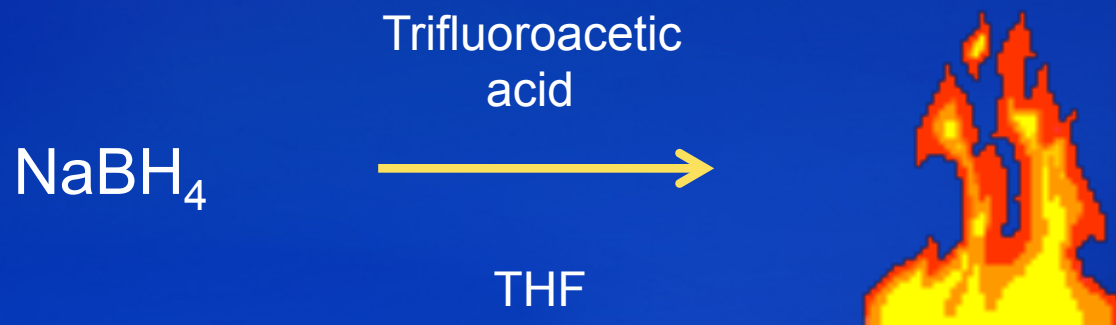
# Sodium Trifluoroacetoxymborohydride

United States Patent 4,835,278

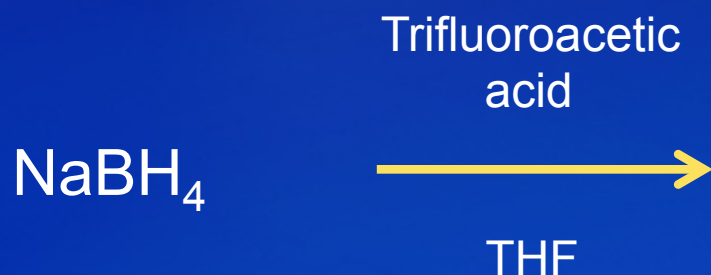


# Sodium Trifluoroacetoxyborohydride

United States Patent 4,835,278



# Sodium Trifluoroacetoxyborohydride



**Exothermic Reaction**

**Byproduct: hydrogen gas**

**Powder dissolves rapidly, reaction not controlled, will consistently catch fire**

**Lesson: Must use pelletized  $\text{NaBH}_4$ , dissolution controls reaction rate**



# Sodium Trifluoroacetoxymethylborohydride

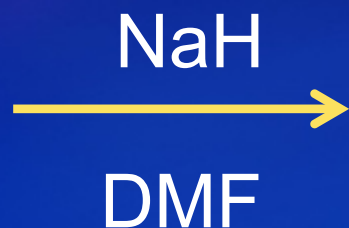
Reaction Issue  
First Identified

Same Incident  
Occurred



Communicated  
at Department  
Safety Briefing

# Other Lessons Requiring Re-Learning



Above ambient temperature can decompose violently



Exceptionally cell penetrable  
Causes acid burns well in excess of acid strength



Quench requires vigorous stirring for > 15 min with ice, violent exotherm likely

# Challenge – How to Ensure Lessons are Learned by Everyone?

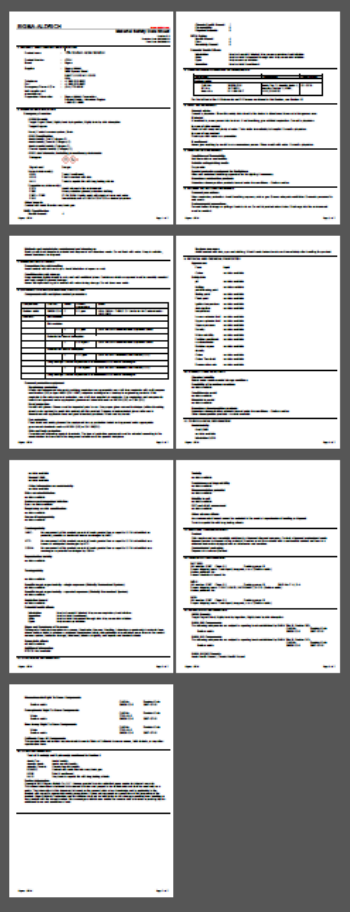


Dilbert, 3/26/2006



**Is the Problem the Chemist or the Process?**

# The Three Factors: INFO, Time, Vehicle



← **Material Safety Data Sheet**

**vs.**

**Actionable Information**



**Reagent: SODIUM AZIDE**

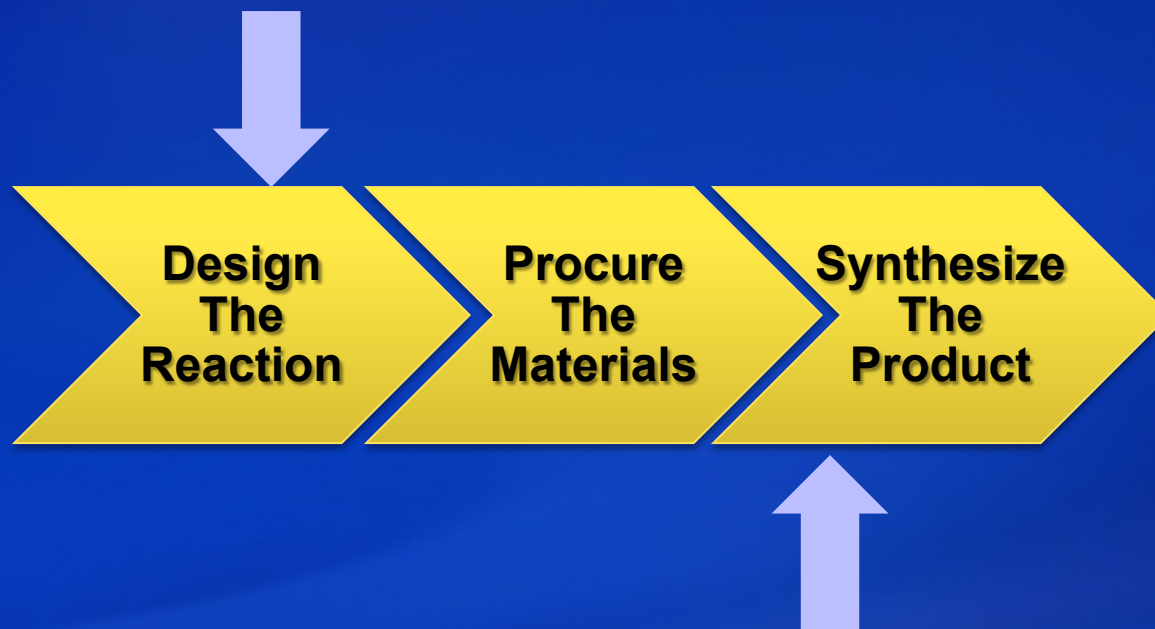
**Warning:**

Reagent Safety Warning for [SODIUM AZIDE]

Warning - Sodium azide is explosive and recently resulted in serious injuries in a chemistry lab at the University of Florida. Please use care when handling this reagent. The MSDS and a presentation on explosive hazards can be found on the Research Chemistry Safety SharePoint site:

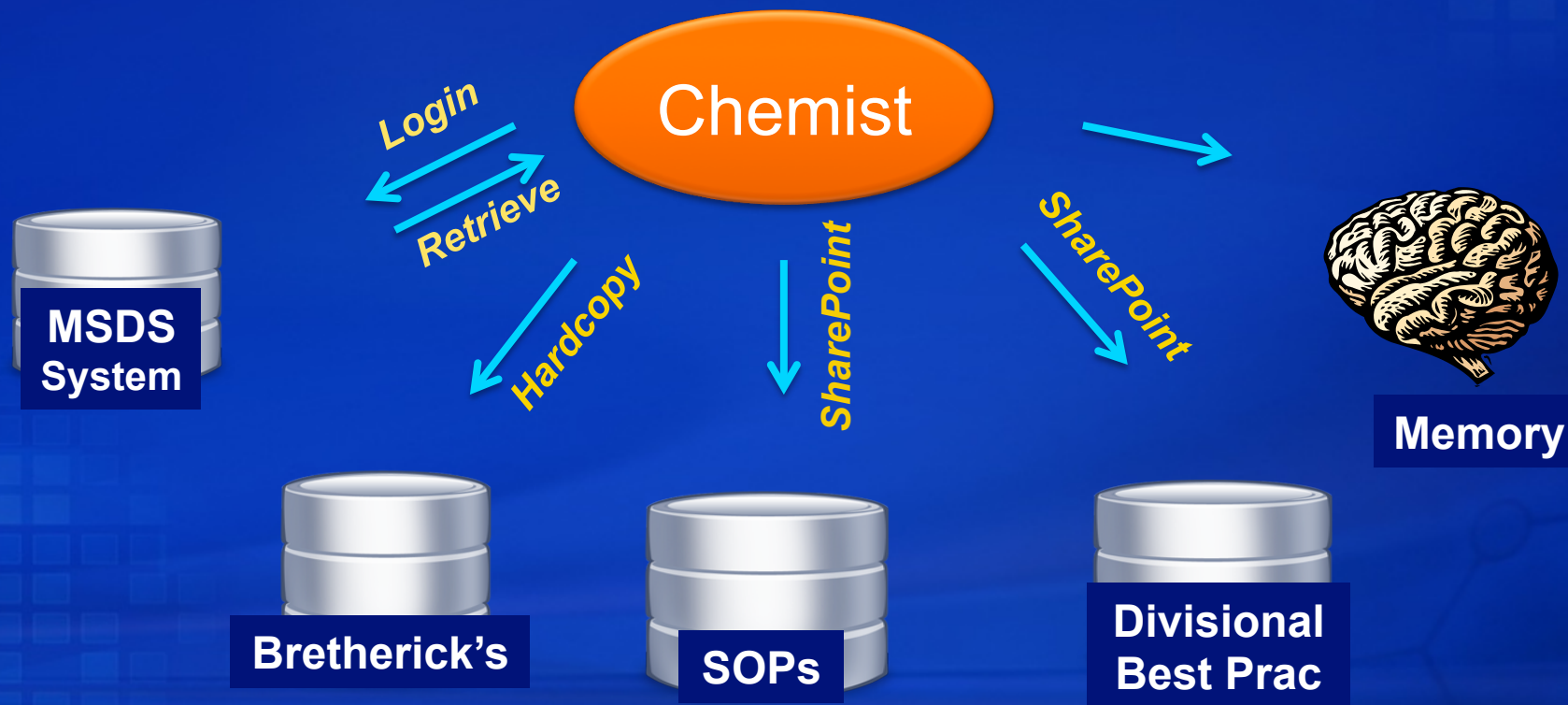
# The Three Factors: Info, **TIME**, Vehicle

When does chemist **FETCH** safety info?



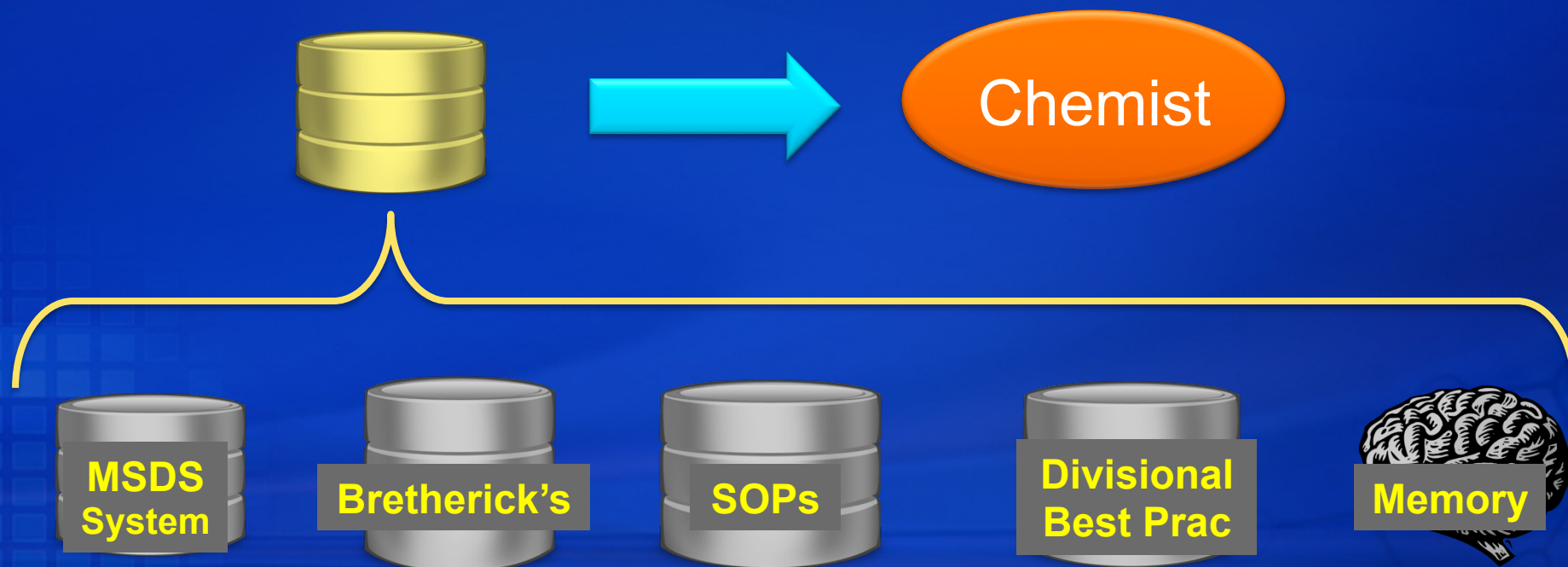
When does chemist **NEED** safety info?

# The Three Factors: Info, Time, **VEHICLE**



# The Three Factors: Info, Time, **VEHICLE**

From a **FRAGMENTED PULL** to a **UNIFIED PUSH**



# Business Requirements

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## INFO, TIME, VEHICLE

- **Centralizing the lessons (i.e., business rules)**
- **Turning “offline pull” into “timely PUSH”**
- **High Specificity, Low False Warnings**
- **Simplify the process for CURATING the Rules**
- **Monitoring & alert mechanism for Safety Committee**



# Electronic Lab Notebooks

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1. Reagent calculator function drives consistent use for all reactions
2. The last IT interaction before chemist runs the experiment in the lab
3. ELN can be customized to deliver event-driven or data-driven triggers/messages



# Curating the Rules – SharePoint

Editable by Safety Committee

Tool for importing rules into ELN database



The screenshot shows a SharePoint site interface. At the top, there is a header for 'Policies and Procedures' with the subtitle 'Team Collaboration Site - Powered by SharePoint'. Below this, a breadcrumb trail reads 'Research Chemistry Safety > Policies and Procedures > ELN Safety Triggers'. The main content area is titled 'ELN Safety Triggers' and contains a table with one entry: 'Chemistry Safety Triggers new urls'. The table has columns for 'Type' and 'Name'. To the left of the table is a sidebar with 'Site Content' and a list of items including 'Scale Reactions', 'Safety Triggers', 'ous Reagent', 'nations', and 'ous Reagents'. A red border highlights the main content area of the screenshot.

Type	Name
	Chemistry Safety Triggers new urls

# Multiple Trigger Mechanisms

1. Single Hazardous Chemical
2. Hazardous Combinations of Chemicals
3. Large Scale of Reaction

46	MFCD00036119	Phosgene	Please handle ONEP in fume hoods that are well-ventilated. The reagent is quenched and neutralized prior to disposal. phosgene can be found at the link below:
47	MFCD00003536	Sodium Azide	Warning - Sodium azide is explosive and recently resulted
48	MFCD00070838	hydrogen	Warning - Multiple fires have occurred internally resulting f
			Warning - Multiple fires have occurred internally resulting f
49	MFCD00070839	H2	Pd catalysts and flammable solvents. Proper setup and w avoid hydrogenation fires. Please review the hydrogenatio up checklist available at the link below:
			Warning - Multiple fires have occurred internally resulting f
50	MFCD00064599	palladium(II) hydroxide	Pd catalysts and flammable solvents. Proper setup and w avoid hydrogenation fires. Please review the hydrogenatio up checklist available at the link below:
51	MFCD00064600	Pearlman'sCatalyst	Warning - Multiple fires have occurred internally resulting f
52	MFCD00011184	platinum(IV) oxide	Warning - Multiple fires have occurred internally resulting f
53	MFCD03457879	Pd/C	Warning - Multiple fires have occurred internally resulting f
54	MFCD00167392	Raney Ni	Warning - Multiple fires have occurred internally resulting f
55			
56			

# Excel → SharePoint → ELN

**Reagent Safety Warning**

Reagent: SODIUM AZIDE

**Warning:**

Reagent Safety Warning for [SODIUM AZIDE]

Warning - Sodium azide is explosive and recently resulted in serious injuries in a chemistry lab at the University of Florida. Please use care when handling this reagent. The MSDS and a presentation on explosive hazards can be found on the Research Chemistry Safety SharePoint site:

Click Accept if you understand and will follow procedures, Click Cancel if you have entered the value by mistake.

**Policies and Procedures Link:**

<http://teams.bms.com/sites/chemsafety/policiesprocedures/hazrgnt/Forms/AllItems.aspx>

Accept Cancel

**Predecessors & Successors**

Error

Add... Quick Add SODIUM AZIDE

**Reactants, Solvents & Products**

Reactant
1 (S,E)-4-(2-(3-(3-chloro-2-fluoro-6-(1H-tetrazol-1-yl)phenyl)acryloyl
2

Solvent	Ratio	Volume

Product	BMS#-form-lot	MF

**Preparation**

Arial 8

- AutoText Definitions
  - Test Procedure
- Reaction
  - Fill
  - Fill 2
  - Fill 3
  - Add
  - Add 2
  - Dilute
  - Dilute 2
- Workup
  - Wash
  - Backextract

# Monitoring & Alerting for EHS/Safety Group

## Reagent Safety Warning for [SODIUM AZIDE]: lil 96107-054

ELN ChemSafety [ELN\_ChemSafety@bms.com]

Sent: Wed 10/3/2012 4:43 PM

To: [Redacted], [Redacted], [Redacted], [Redacted], [Redacted], [Redacted]

Reagent Safety Warning

User: lil

Experiment: 96107-054

Owner: lil

Reactant(s): SODIUM AZIDE

Warning Message: Warning - Sodium azide is explosive and recently resulted in serious injuries in a chemistry lab at the University of Florida. Please use care when handling this reagent. The MSDS and a presentation on explosive hazards can be found on the Research Chemistry Safety SharePoint site:

SOP Link:

<http://teams.bms.com/teams/chemsafety/policiesprocedures/hazrgnt/Forms/AllItems.aspx>

User Accepted: True

# Technical Implementation

## Chemistry Safety section

- Safety log table: stores the chemistry safety warning logs, and a section listener that prevents users from deleting/renaming the section.

## User collection listeners

- Has been added to enable adding the Chemistry Safety section to it at run time.

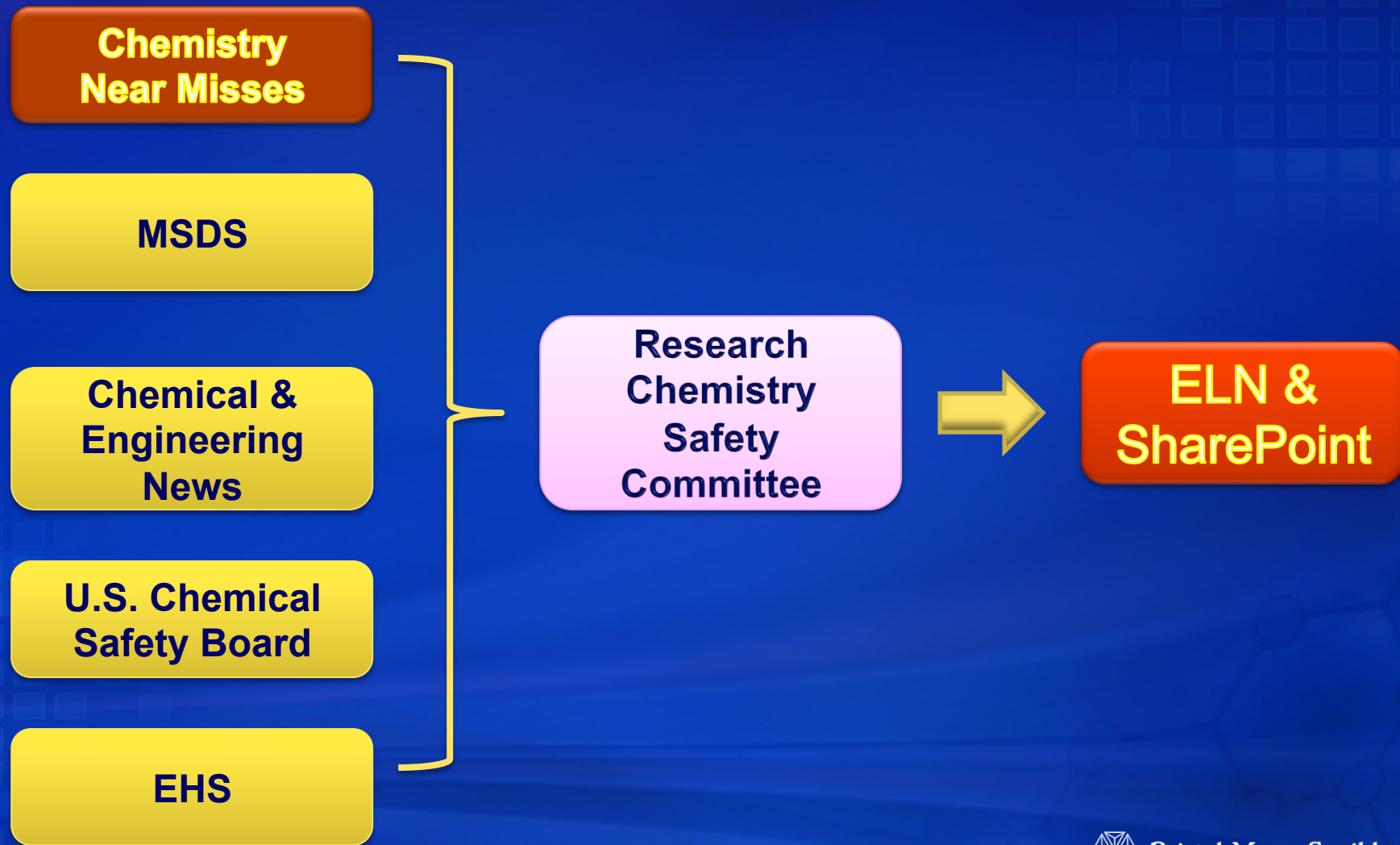
## Chemistry Experiment collection listener

- Captures the Collection Saving event, and performs chemistry safety check if necessary.

## Reaction section listener

- One section listener has been created on the Reaction section to accomplish two things. First, to capture the Show event of the reactant table to get the original list of reactants, and second, to capture the SectionAdding event to display the general chemistry safety warning before the reaction section being added.

# New Data Flow



# The Impact

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- ✓ **Large Scale Reaction Notifications Up 300%**
- ✓ **No incidents or near misses for the documented rules**



# BioITWorld Best Practices 2012



## Bio-IT World Announces Winners of 2012 Best Practices Awards

By Bio-IT World Staff

**April 25, 2012** | BOSTON—Bio-IT World announced the winners of its eighth Best Practices Awards competition this morning in a plenary session at the 2012 Bio-IT World Conference & Expo in Boston.

Grand Prize winners from five life sciences awards categories included entries from three big pharma companies—Merck, Pfizer, and Merck KGaA (Germany)—and two genomics organizations, BGI Shenzhen and the University of Utah/Omicia.

In addition, the Judges' Prize was awarded to Bristol-Myer Squibb, while the Editors' Choice Award was given to Elizabeth Worthey & her colleagues at the Medical College of Wisconsin for the Carpe Novo clinical genome analysis platform.

"We extend our sincere congratulations to the winners of this year's Bio-IT World Best Practices Awards competition" said Kevin Davies, editor of Bio-IT World. "Our select judges enjoyed evaluating the dozens of excellent entries received this year, and believe that the contest has

<http://www.bio-itworld.com/2012/04/25/bio-it-world-announces-winners-2012-best-practices-awards.html>

# Roadmap: BMS Safety Data Flow

Multiple Sources for Collecting Rules

Multiple Destinations for Rules Enforcement



# Industry-wide Collaboration?

Pre-competitive Collaboration for the benefit of the community



# Chemical Safety Library Project

<https://main.qmarkets.org/live/pistoia/node/1365>

- Currently Fundraising
- Project kick-off in Fall
- New participants
  - Team participants
  - Expert advisors
  - Contributors of data
- [Carmen.Nitsche@pistoiaalliance.org](mailto:Carmen.Nitsche@pistoiaalliance.org)



# THANK YOU

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