Finding Chemical Safety Information
(Post-Workshop Version, revised 2023-07-21)

Also see: https://guides.library.stanford.edu/lab-safety

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UMN RAMP REFRESHER AND CSL BUILDING WORKSHOP, JUNE 27-28, 2023

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Introduction

FINDING CHEMICAL SAFETY INFORMATION

Safety Statement *Science of Synthesis*

Warning! Read carefully the following: Although this reference work has been written by experts, the user must be advised that the handling of chemicals, microorganisms, and chemical apparatus carries potentially life-threatening risks. For example, serious dangers could occur through quantities being incorrectly given. The authors took the utmost care that the quantities and experimental details described herein reflected the current state of the art of science when the work was published. However, the authors, editors, and publishers take no responsibility as to the correctness of the content. Further, scientific knowledge is constantly changing. As new information becomes available, the user must consult it. Although the authors, publishers, and editors took great care in publishing this work, it is possible that typographical errors exist, including errors in the formulas given herein. Therefore, **it is imperative that and the responsibility of every user to carefully check whether quantities, experimental details, or other information given herein are correct based on the user's own understanding as a scientist.** Scale-up of experimental procedures published in **Science of Synthesis** carries additional risks. In cases of doubt, the user is strongly advised to seek the opinion of an expert in the field, the publishers, the editors, or the authors. When using the information described herein, the user is ultimately responsible for his or her own actions, as well as the actions of subordinates and assistants, and the consequences arising therefrom.

Safety Statement in *Science of Synthesis*

Although authors, editors, publishers, take great care in publishing a work, incorrect quantities or typographical errors may occur.

Scientific knowledge is constantly changing. As new information becomes available, a user must consult it.

Scale-up of experimental procedures carries additional risks.

Warning statements based on a prescribed list of reagents used in a reaction are embedded in the full text of *SoS*.

- Chemical Substances
  - Name
  - CAS Registry Number
  - Structure
  - Class of substance
- Physical Properties
  - Experimental
  - Predicted
- Reactions
  - Experimental
  - Predicted

- Comments & Caveats:
  - Properties vary by physical state (liquid, solid, gas) and by concentration levels
  - Experimental methods are usually the most detailed in journal articles
  - Confirm information by using > 1 source
  - Unknowns: it is possible to search for unknowns using physical appearance (e.g., color), properties, and keywords.

Common Ways to Search for Chemical Safety Information

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
CAS Common Chemistry	Includes basic data on ~500,000 commonly used and regulated substances.	Find substance identifiers & basic compound properties.	Annually	Open access /API	CAS
PubChem	A "21st century handbook" w/ data from over 925 data sources covering more than 115 million chemicals.	Laboratory Chemical Safety Summary Datasheets and reactivity information from government hazmat sources.	Daily	Open access / API	NLM/NIH
CAMEO Chemicals	Covers 9,000 hazardous chemicals. Identifies reactions and precautions for pairs of chemicals at commercial scale.	Reactivity alerts, hazmat profile plus emergency response guidance.	Annually	Open access	NOAA/EPA
Pistoia Alliance Chemical Safety Library	Catalogs hazardous reactions to alert scientists to potentially dangerous experiments.	Laboratory scale reaction incidents reported by users or from the literature.	Crowd-sourced	Open access	CAS/Pistoia Alliance
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
Organic Syntheses	Provides detailed, reliable, and carefully checked procedures for the synthesis of organic compounds. Reproducibility is checked Editorial Board members.	Beginning August 2017, the first Note in every article is devoted to addressing safety aspects of the procedures described in the article.	1 Volume/Year. Includes Pre-Pub articles	Open Access	Organic Syntheses, Inc.
Science of Synthesis	Expert reviews of best synthetic methods for organic & organometallic compounds.	Safety warnings are highlighted the full text description of a method.	3-4 Times/Year plus Pre-Pub articles	Subscription / API	Thieme
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Reaxys	Core database (includes Beilstein, Gmelin, Chem Patents) w/ content going back to 1771. Reactions for organic, organometallic, and inorganic compounds.	Identification, reactions, and properties data plus "Laboratory Use and Handling" in "Other Data."	Weekly	Subscription	Elsevier
Dimensions	Multidisciplinary database for articles, preprints, conference proceedings, & books.	Ability to do a full-text search for finding safety info such as methods.	Daily	Open access (Publications)	Digital Science

Summary of Sources Covered in UMN Workshop

“Foundational” - Chemical Safety Information Databases

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
CAS Common Chemistry	Includes basic data on ~500,000 commonly used and regulated substances.	Find substance identifiers & basic compound properties	Annually	Open access /API	CAS
PubChem	A “21st century handbook” w/ data from over 925 data sources covering more than 115 million chemicals.	Laboratory Chemical Safety Summary Datasheets and reactivity information from government hazmat sources	Daily	Open access / API	NLM/NIH
CAMEO Chemicals	Covers 9,000 hazardous chemicals. Identifies reactions and precautions for pairs of chemicals at commercial scale.	Reactivity alerts, hazmat profile plus emergency response guidance	Annually	Open access	NOAA/EPA
Pistoia Alliance Chemical Safety Library (CSL)	Catalogs hazardous reactions to alert scientists to potentially dangerous experiments.	Laboratory scale reaction incidents reported by users or from the literature	Crowd-sourced	Open access	CAS/Pistoia Alliance

a relatively new and developing foundational resource

Advanced Undergraduate - Chemical Safety Information Databases

CAS Common Chemistry, PubChem, & CAMEO Chemicals plus

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
Organic Syntheses	Provides detailed, reliable, and carefully checked procedures for the synthesis of organic compounds. Reproducibility is checked by an Editorial Board member.	Beginning August 2017, the first Note in every article is devoted to addressing the safety aspects of the procedures described in the article.	1 Volume/Year. Includes Pre-Pub articles	Open Access	Organic Syntheses, Inc.
E-EROS (Encyclopedia of Reagents for Organic Synthesis	Gives detailed information on more than 5,250 reagents and catalysts	Handling, Storage, and Precautions: (storage lifetime under certain conditions, dry box, etc.; incompatibilities with solvents and other reagents; emphasizes personal safety) [in Abstract]	Up to 200 new or updated articles added annually	Subscription, Open access to abstracts	Wiley
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Not Voodoo X	Collect of Lessons Learned and lab mishaps with a "vote up" mechanism to indicate similar experiences	Data related to undergraduate organic chemistry research	As needed	Publicly available	Univ of Rochester

Research & Specialty Labs - Chemical Safety Information Databases

Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
E-EROS (Encyclopedia of Reagents for Organic Synthesis	Gives detailed information on more than 5,250 reagents and catalysts	Handling, Storage, and Precautions: (storage lifetime under certain conditions, dry box, etc.; incompatibilities with solvents and other reagents; emphasizes personal safety) [in Abstract]	Up to 200 new or updated articles added annually	Subscription, Open access to abstracts	Wiley
Science of Synthesis	Expert reviews of best synthetic methods for organic & organometallic compounds.	Safety warnings are highlighted the full text description of a method.	3-4 Times/Year plus Pre-Pub articles	Subscription / API	Thieme
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Reaxys	Core database (includes Beilstein, Gmelin, Chem Patents) w/ content going back to 1771. Reactions for organic, organometallic, and inorganic compounds.	Identification, reactions, and properties data plus “Laboratory Use and Handling” in “Other Data.”	Weekly	Subscription	Elsevier
Dimensions	Multidisciplinary database for articles, preprints, conference proceedings, & books.	Ability to do a full-text search for finding safety info such as methods.	Daily	Open access (Publications)	Digital Science

EH&S Professionals – Chemical Safety Information Databases

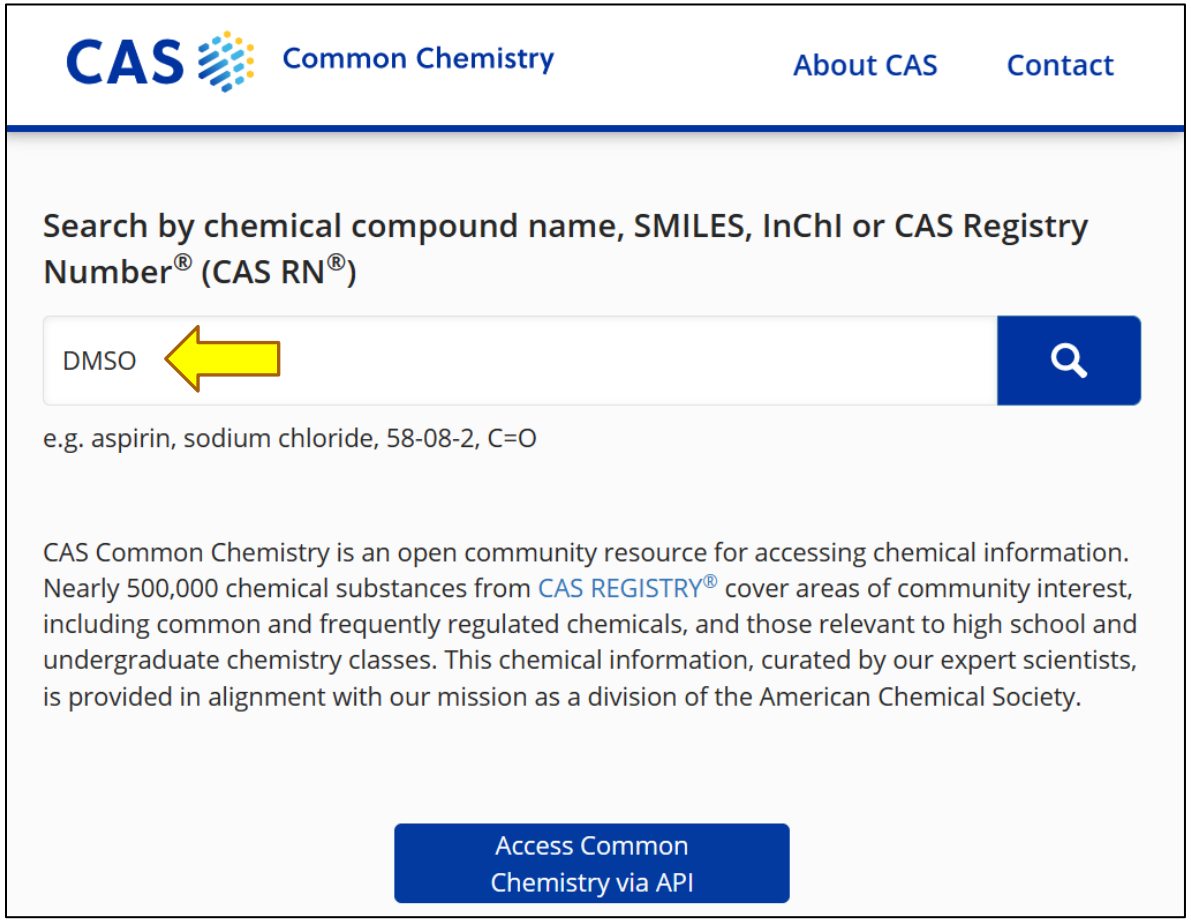
Database Name	Description	Focus for Safety	Update Frequency	Access	Owner
Knovel	Has ~12,000 sci-tech handbooks plus interactive & visualization tools.	Full-text and tables to chemical safety handbooks.	1-3 Months	Subscription	Elsevier
CCOHS – Academic Support Program	Collection of environmental and occupational health and safety databases, selected and priced specifically for the academic community.	Includes access to SDS, CHEMINFO, RTECS, OSH References, Toxicology, plus more. CHEMpendium, a supplemental product, offers cross-database search capabilities.	Monthly	Subscription	Canadian Centre for Occupational Health and Safety
E-EROS (Encyclopedia of Reagents for Organic Synthesis	Gives detailed information on more than 5,250 reagents and catalysts	Handling, Storage, and Precautions: (storage lifetime under certain conditions, dry box, etc.; incompatibilities with solvents and other reagents; emphasizes personal safety) [in Abstract]	Up to 200 new or updated articles added annually	Subscription, Open access to abstracts	Wiley
SciFinder-n	Comprehensive database in chemistry and chemical engineering. Reactions for organic & organometallic compounds.	References, substances, and reactions. Includes properties, safety notes & methods for reactions.	Daily	Subscription	CAS
Dimensions	Multidisciplinary database for articles, preprints, conference proceedings, & books.	Ability to do a full-text search for finding safety info such as methods.	Daily	Open access (Publications)	Digital Science

CAS Common Chemistry

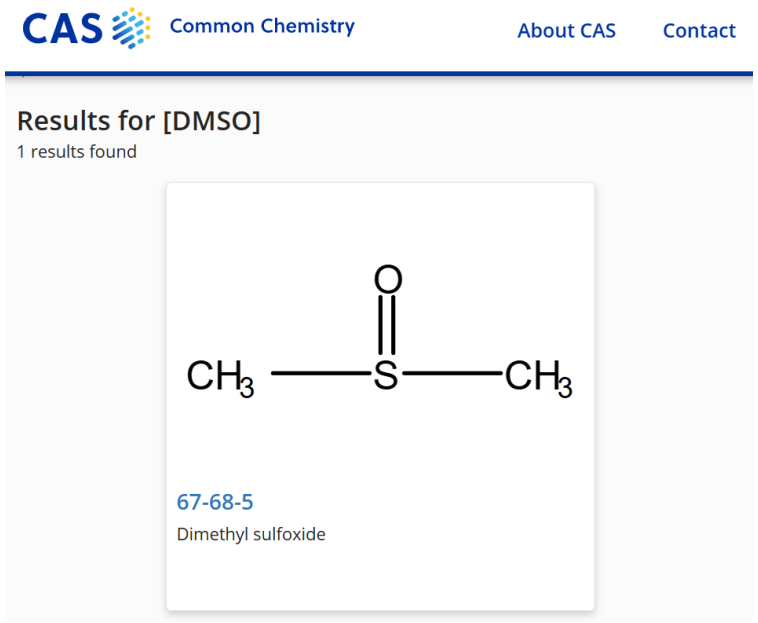
INCLUDES NEARLY 500,000 COMMONLY USED SUBSTANCES

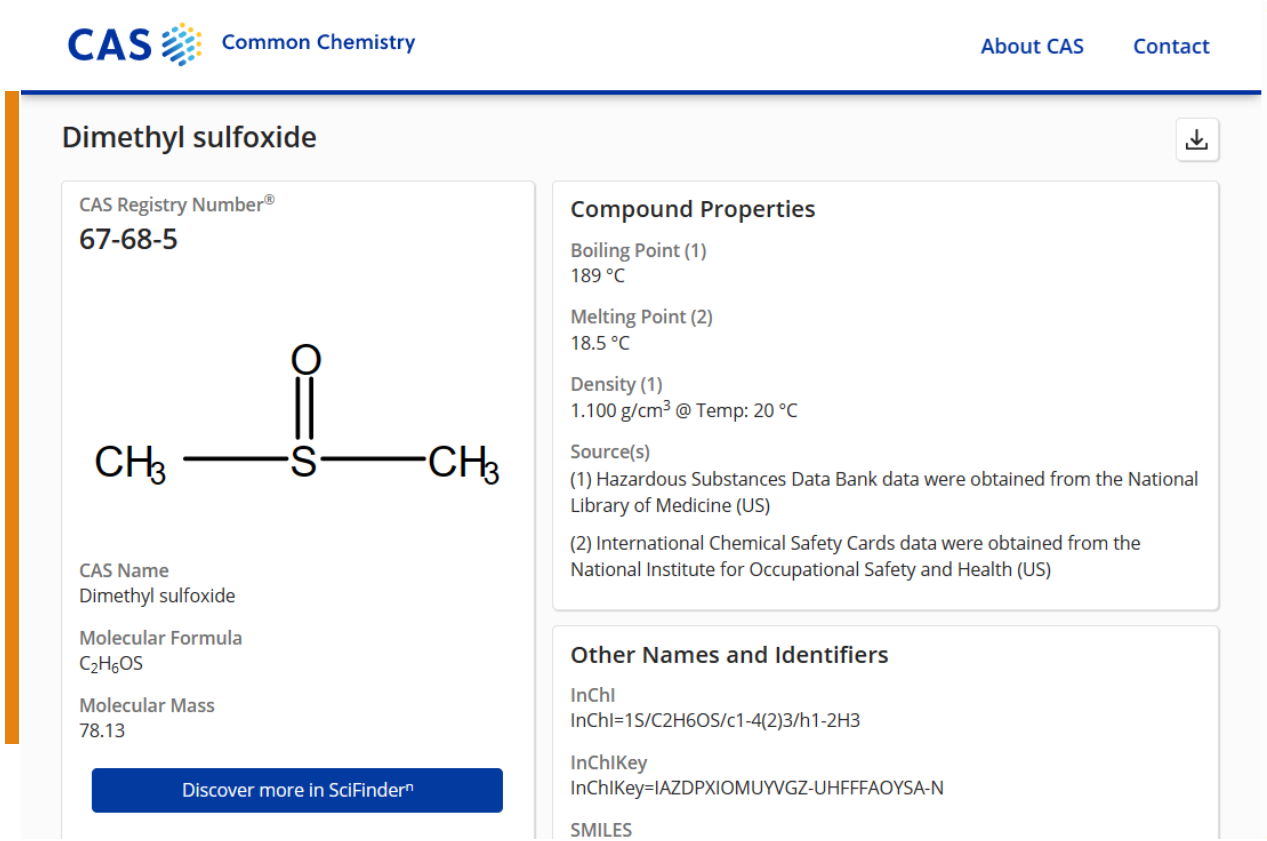
SEARCH BY CHEMICAL NAME, CAS REGISTRY NUMBER

HTTPS://COMMONCHEMISTRY.CAS.ORG/



CAS Common Chemistry





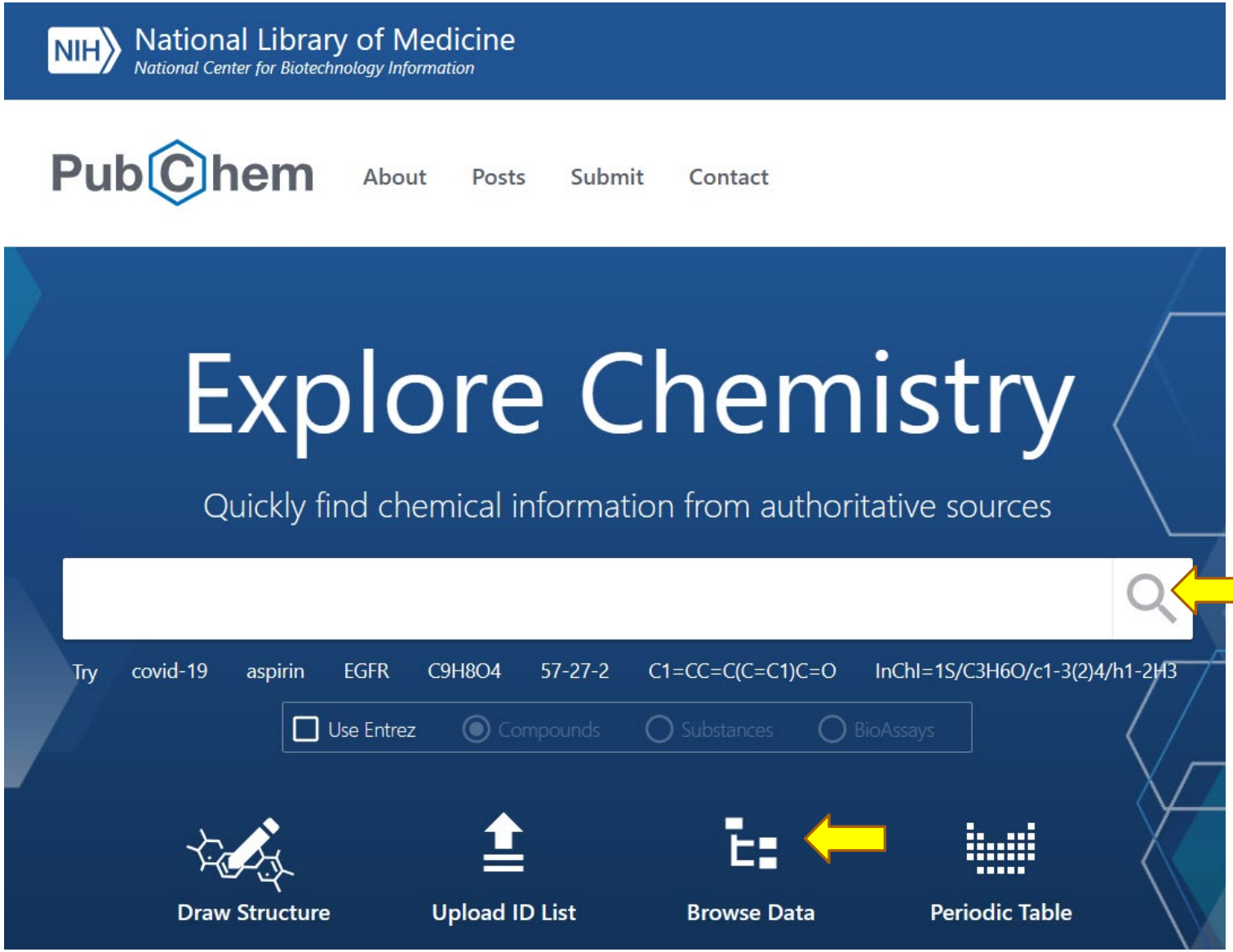
CAS Common Chemistry Search Results for DMSO

PubChem

OVER 900 DATA SOURCES. INCLUDES LABORATORY CHEMICAL SAFETY SUMMARY SHEETS

SEARCH BY COMPOUND NAME, CAS REGISTRY NUMBER, STRUCTURE, SEQUENCE, TAXONOMIC NAME

HTTPS://PUBCHEM.NCBI.NLM.NIH.GOV/

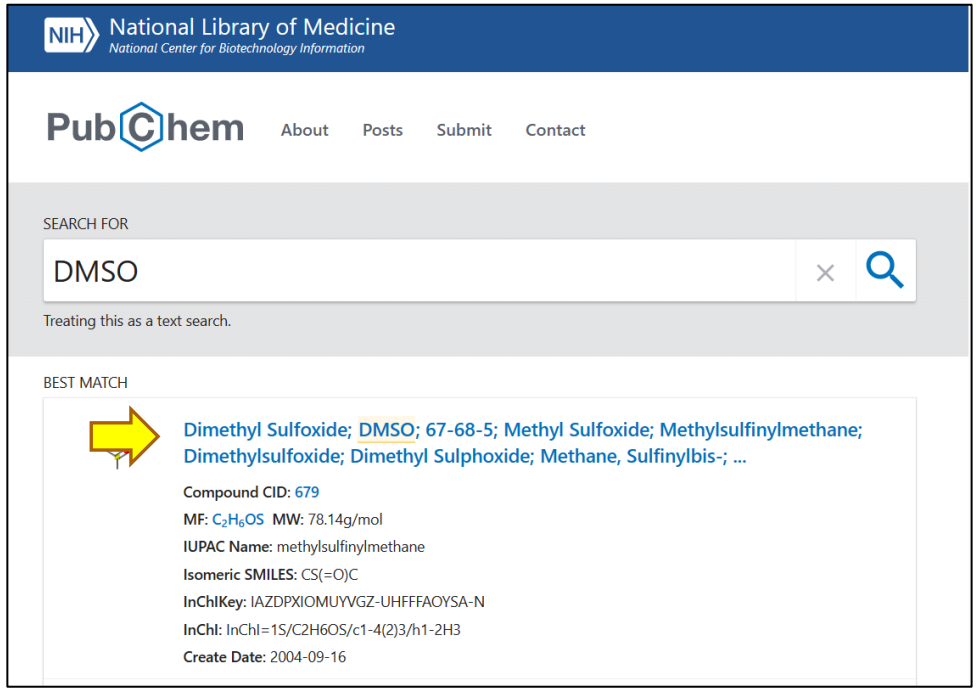


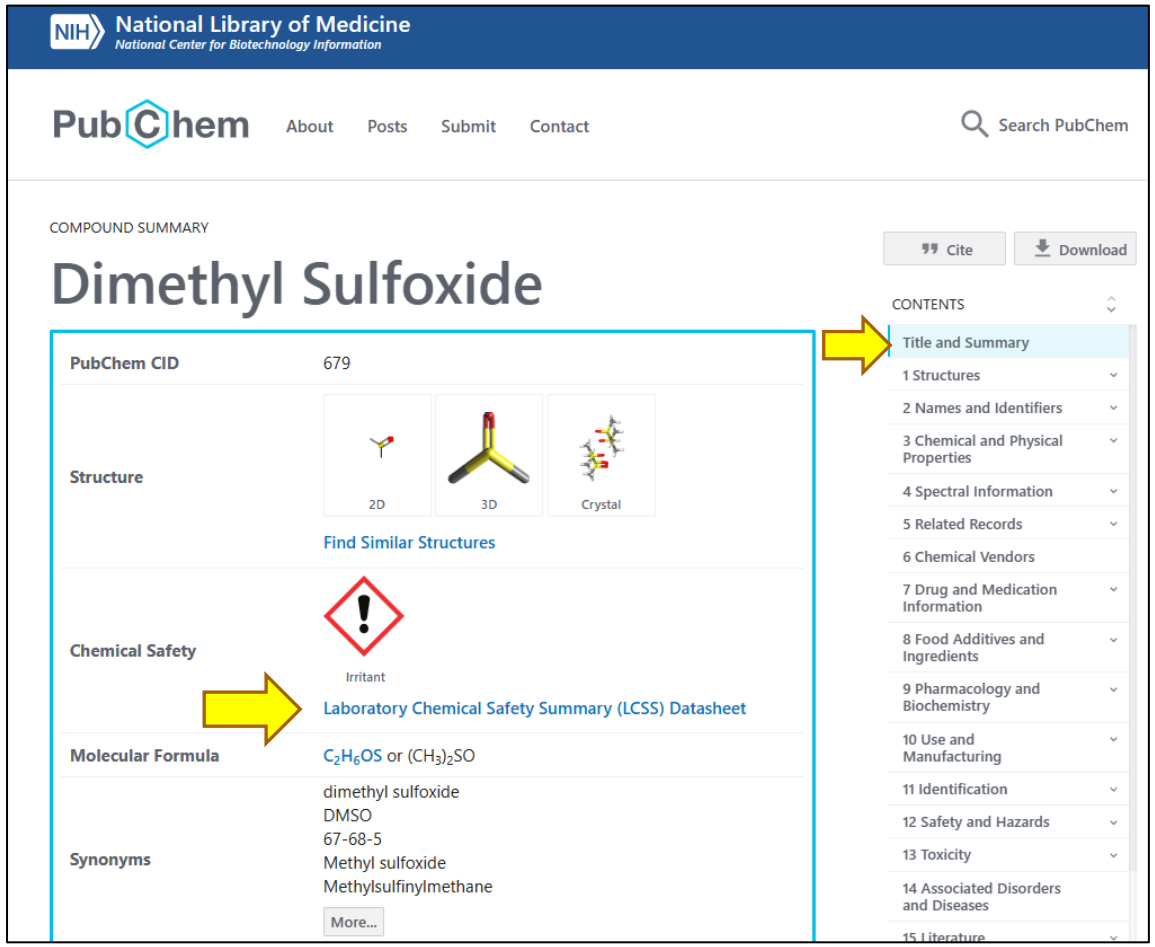
PubChem

Search compounds

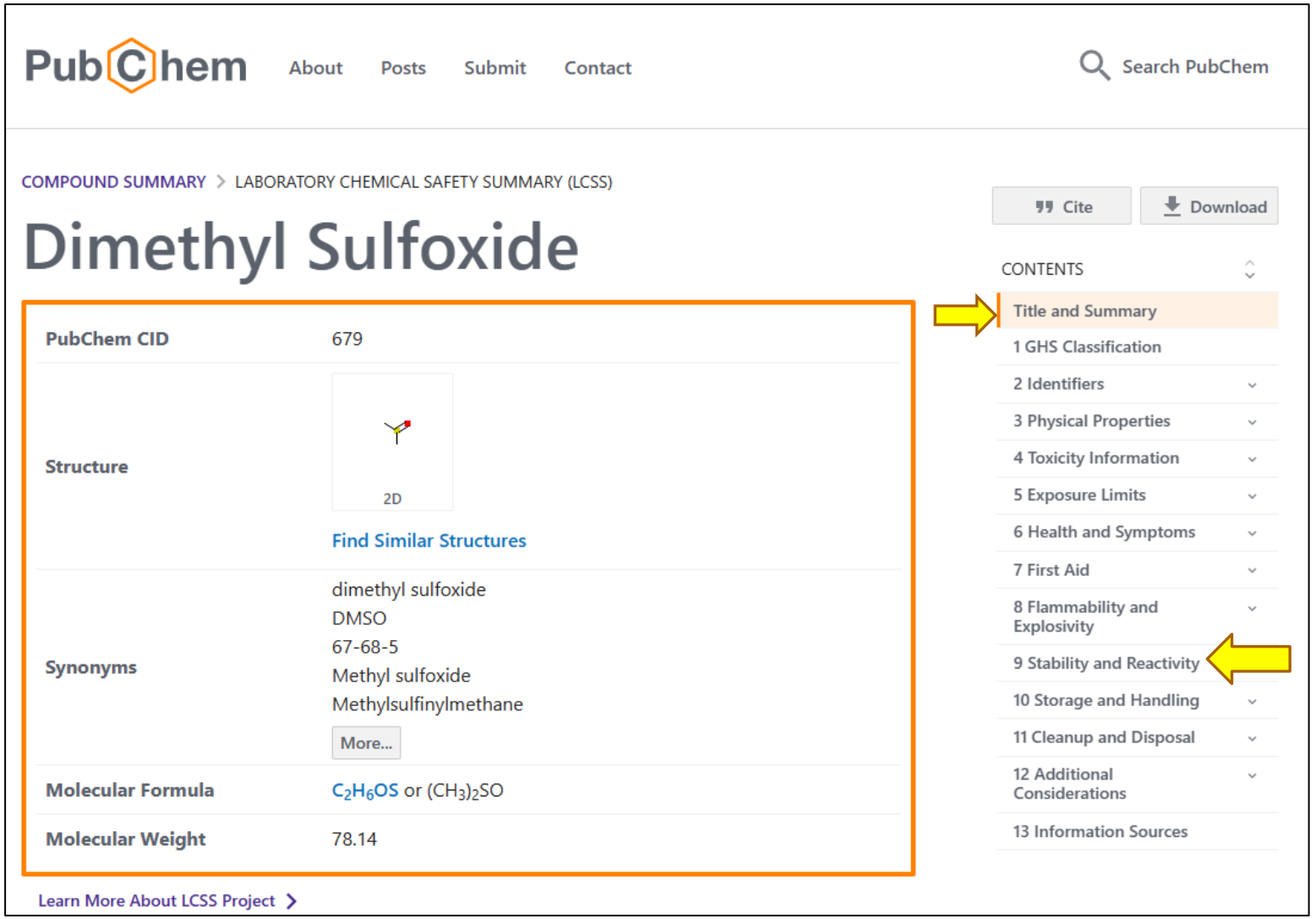
Browse Data to view types of data available (see example below).

Learn more about Data Sources: https://pubchem.ncbi.nlm.nih.gov/docs/data-sources





PubChem Search Results for DMSO



PubChem's Laboratory Chemical Safety Summary (LCSS) for DMSO

PubChem Dimethyl Sulfoxide (Compound)

9 Stability and Reactivity

9.1 Reactivity Profile

DIMETHYL SULFOXIDE decomposes violently on contact with many acyl halides and related compounds such as acetyl chloride, benzenesulfonyl chloride, benzoyl chloride, cyanuric chloride, phosphorus trichloride, phosphorus oxychloride, and thionyl chloride [Chem. Eng. News 35(9):87 (1957)].

▸ CAMEO Chemicals

9.2 Reactivity Alerts

9.2.1 CSL Reaction Information

1 of 5	
CSL No	CSL00002
Reactants/Reagents	DMSO; perchloric acid
Reaction Class	oxidation
GHS Category	Explosive
Reaction Scale	S (up to 1g)
Warning Message	mixture can result in explosion
Source Reference	User-Reported
CSL Status	Approved
Additional Info	Lam et al, JTAC v 85 (2006) I, 25-30
Modified Date	2/27/2018

▸ Pistoia Alliance Chemical Safety Library

▾ CAMEO Chemicals

Source	CAMEO Chemicals
Record Name	DIMETHYL SULFOXIDE
URL	https://cameochemicals.noaa.gov/chemical/8559
Description	CAMEO Chemicals is a chemical database designed for people who are involved in hazardous material incident response and planning. CAMEO Chemicals contains a library with thousands of datasheets containing response-related information and recommendations for hazardous materials that are commonly transported, used, or stored in the United States. CAMEO Chemicals was developed by the National Oceanic and Atmospheric Administration's Office of Response and Restoration in partnership with the Environmental Protection Agency's Office of Emergency Management.
License	CAMEO Chemicals and all other CAMEO products are available at no charge to those organizations and individuals (recipients) responsible for the safe handling of chemicals. However, some of the chemical data itself is subject to the copyright restrictions of the companies or organizations that provided the data. https://cameochemicals.noaa.gov/help/reference/terms_and_conditions.htm?d_f=false

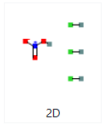
▾ Pistoia Alliance Chemical Safety Library

Source	Pistoia Alliance Chemical Safety Library
Record Name	DMSO; perchloric acid
URL	http://www.pistoiaalliance.org/projects/chemical-safety-library/
Description	The Pistoia Alliance Chemical Safety Library project is dedicated to sharing hazardous reaction safety information across the chemical industries.
License	https://www.cas.org/sites/default/files/documents/chemical-safety-library-terms.pdf

PubChem LCSS for DMSO – Section 9. Stability & Reactivity

PubChem

Aqua regia

PubChem CID	90477010
Structure	 2D
Molecular Formula	$Cl_3H_4NO_3$
Synonyms	AQUA REGIA Nitrohydrochloric acid nitromuriatic acid 8007-56-5 UNII-X3TT5X989E View More...

CONTENTS

PubChem Aqua regia (Compound)

8.1.2 Health Hazards

Excerpt from ERG Guide 157 [Substances - Toxic and/or Corrosive (Non-Combustible / Water-Sensitive)]:

TOXIC; inhalation, ingestion or contact (skin, eyes) with vapors, dusts or substance may cause severe injury, burns or death. Reaction with water or moist air may release toxic, corrosive or flammable gases. Reaction with water may generate much heat that will increase the concentration of fumes in the air. Fire will produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause environmental contamination. (ERG, 2020)

▸ CAMEO Chemicals

8.1.3 Fire Hazards

Excerpt from ERG Guide 157 [Substances - Toxic and/or Corrosive (Non-Combustible / Water-Sensitive)]:

Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes. UN1796, UN1802, UN1826, UN2032, UN3084, UN3085, and, at concentrations above 65%, UN2031 may act as oxidizers. Also consult ERG Guide 140. Vapors may accumulate in confined areas (basement, tanks, hopper/tank cars, etc.). Substance may react with water (some violently), releasing corrosive and/or toxic gases and runoff. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated or if contaminated with water. (ERG, 2020)

▸ CAMEO Chemicals

8.1.4 Hazards Summary

Contains nitrosyl chloride and free chlorine; Corrosive; [Merck Index] A strong oxidizing agent with known catalytic activity; Reacts with air; Causes burns; [CAMEO] Causes burns and severe respiratory tract irritation; Highly toxic by ingestion and inhalation; [University of Oxford MSDS] See Nitric acid and Hydrogen chloride.

Merck Index - O'Neil MJ, Heckelman PE, Dobbelaar PH, Roman KJ (eds). The Merck Index, An Encyclopedia of Chemicals, Drugs, and Biologicals, 15th Ed. Cambridge, UK: The Royal Society of Chemistry, 2013.

▸ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

CAMEO Chemicals

AQUA REGIA

https://cameochemicals.noaa.gov/chemical/4079

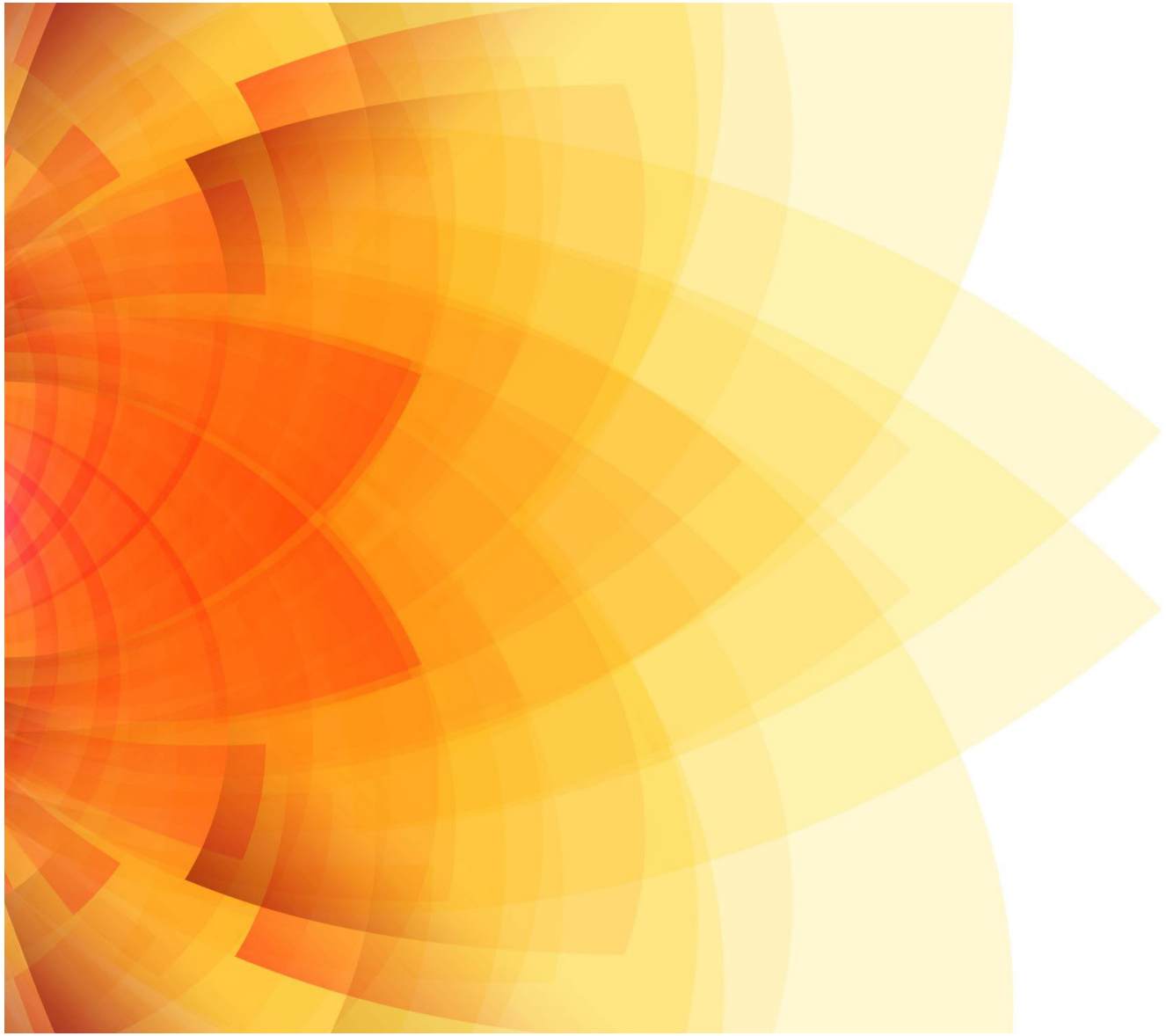
Reactivity Profile

AQUA REGIA is a powerful oxidizing agent and a strong acid. Reacts exothermically with chemical bases (for example: amines and inorganic hydroxides) to form salts and water. Reacts with most metals, including gold and platinum, to dissolve them with generation of toxic and/or flammable gases. Can initiate polymerization in polymerizable organic compounds. Reacts with cyanide salts to generate toxic hydrogen cyanide gas. Generates flammable and/or toxic gases with dithiocarbamates, isocyanates, mercaptans, nitrides, nitriles, sulfides, and weak or strong reducing agents. Additional exothermic gas-generating reactions occur with sulfites, nitrites, thiosulfates (to give H2S and SO3), dithionites (SO2), and carbonates (CO2).

Belongs to the Following Reactive Group(s)

- Acids, Strong Oxidizing

PubChem – No LCSS or GHS Codes / Reactivity Profile in CAMEO



CAMEO Chemicals

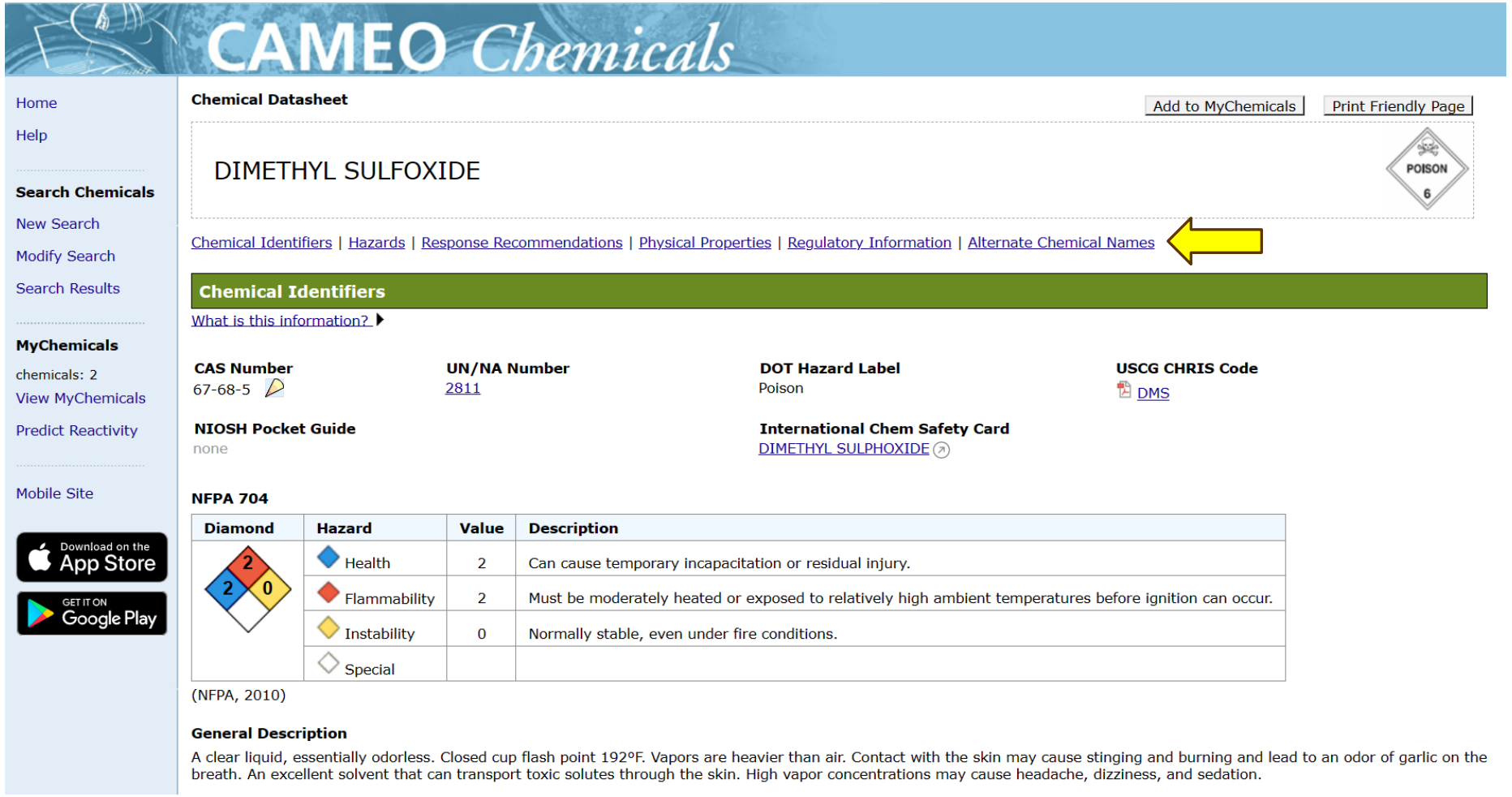
(Computer-Aided Management of Emergency Operations)

FIND RESPONSE INFORMATION FOR 9,000 HAZARDOUS MATERIALS

SEARCH BY NAME, CAS REGISTRY NUMBER, PREDICT REACTIVITY USING MYCHEMICALS

AVAILABLE IN MULTIPLE FORMATS: MOBILE, WEBSITE, DESKTOP SOFTWARE

HTTPS://CAMEOCHEMICALS.NOAA.GOV/



CAMEO Chemicals record for DMSO

Hazards

What is this information?

Reactivity Alerts

none

Air & Water Reactions

Denser than water and miscible in water.

Fire Hazard

Special Hazards of Combustion Products: Sulfur dioxide, formaldehyde, and methyl mercaptan can form (USCG, 1999)

Health Hazard

Slight eye irritation. (USCG, 1999)

Reactivity Profile

DIMETHYL SULFOXIDE decomposes violently on contact with many acyl halides and related compounds such as acetyl chloride, benzenesulfonyl chloride, benzoyl chloride, cyanuric chloride, phosphorus trichloride, phosphorus oxychloride, and thionyl chloride [Chem. Eng. News 35(9):87 (1957)].

Belongs to the Following Reactive Group(s)

- Sulfonates, Phosphonates, and Thiophosphonates, Organic

Potentially Incompatible Absorbents

No information available.

CAMEO Chemicals record for DMSO - Hazards

Response Recommendations

What is this information?

Isolation and Evacuation

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (7

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail car or tank truck is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 me

Firefighting

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

SMALL FIRE: Dry chemical, CO2 or water spray.

LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or water spray. If it can be done safely, move undamaged containers away from the area arour

FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do r
water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away f

Non-Fire Response

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. Do not touch damaged containers or spilled material unless
risk. Prevent entry into waterways, sewers, basements or confined areas. Absorb or cover with dry earth, sand or other non-combustible material and t

Protective Clothing

Butyl rubber gloves, safety goggles. Respiratory filter if airborne sprays or drops are present. (USCG, 1999)

DuPont Tychem® Suit Fabrics

Fabric legend, testing details, and a caution from DuPont

Normalized Breakthrough Times (in Minutes)

Chemical	CAS Number	State	QS	QC	SL	C3	TF	TP	RC	TK	RF
Dimethyl sulfoxide	67-68-5	Liquid				>480	>480	>480	>480	>480	>480

> indicates greater than.

Special Warning from DuPont: Tychem® and Tyvek® fabrics should not be used around heat, flames, sparks or in potentially flammable or explosive e
More Info...

(DuPont, 2022)

CAMEO Chemicals record for DMSO – Response Recommendations

First Aid

EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

Physical Properties

What is this information?

Chemical Formula: C2H6OS

Flash Point: 203°F (NTP, 1992)

Lower Explosive Limit (LEL): 2.6 % (NTP, 1992)

Upper Explosive Limit (UEL): 63 % (NTP, 1992)

Autoignition Temperature: 419°F (USCG, 1999)

Melting Point: 65.3°F (NTP, 1992)

Vapor Pressure: 0.42 mmHg at 68°F (NTP, 1992)

Vapor Density (Relative to Air): 2.71 (NTP, 1992)

Specific Gravity: 1.101 at 68°F (USCG, 1999)

CAMEO Chemicals record for DMSO – Response Recommendations continued and Physical Properties

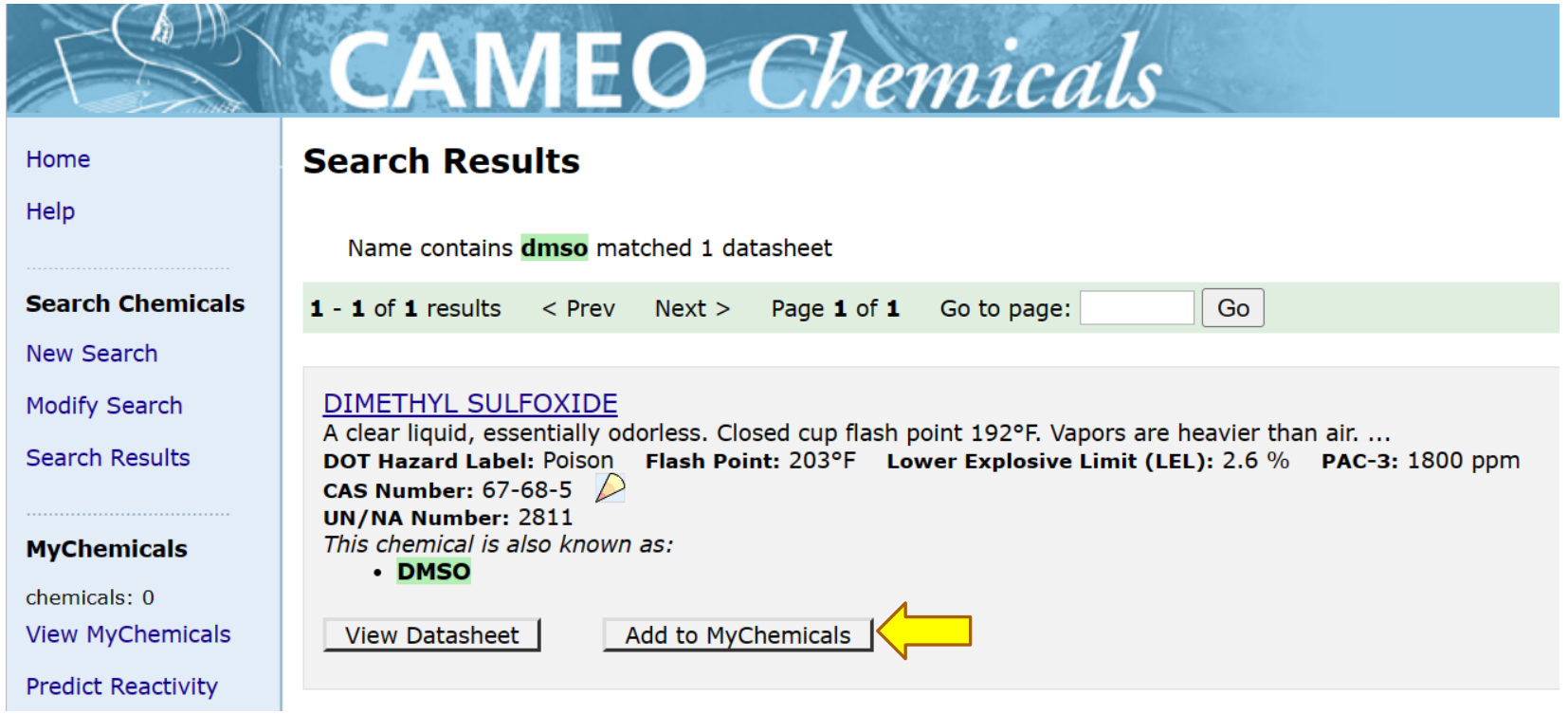
CAMEO Chemicals – Predict Reactivity

Step-by-step instructions:

1. Search substances one at a time.

From Search Results (or from Datasheet), press **Add to My Chemicals**.

Please note: **Advanced search** page lets you search fragments of chemical names, properties, etc.



CAMEO Chemicals – Predict Reactivity

Step-by-step instructions continued:

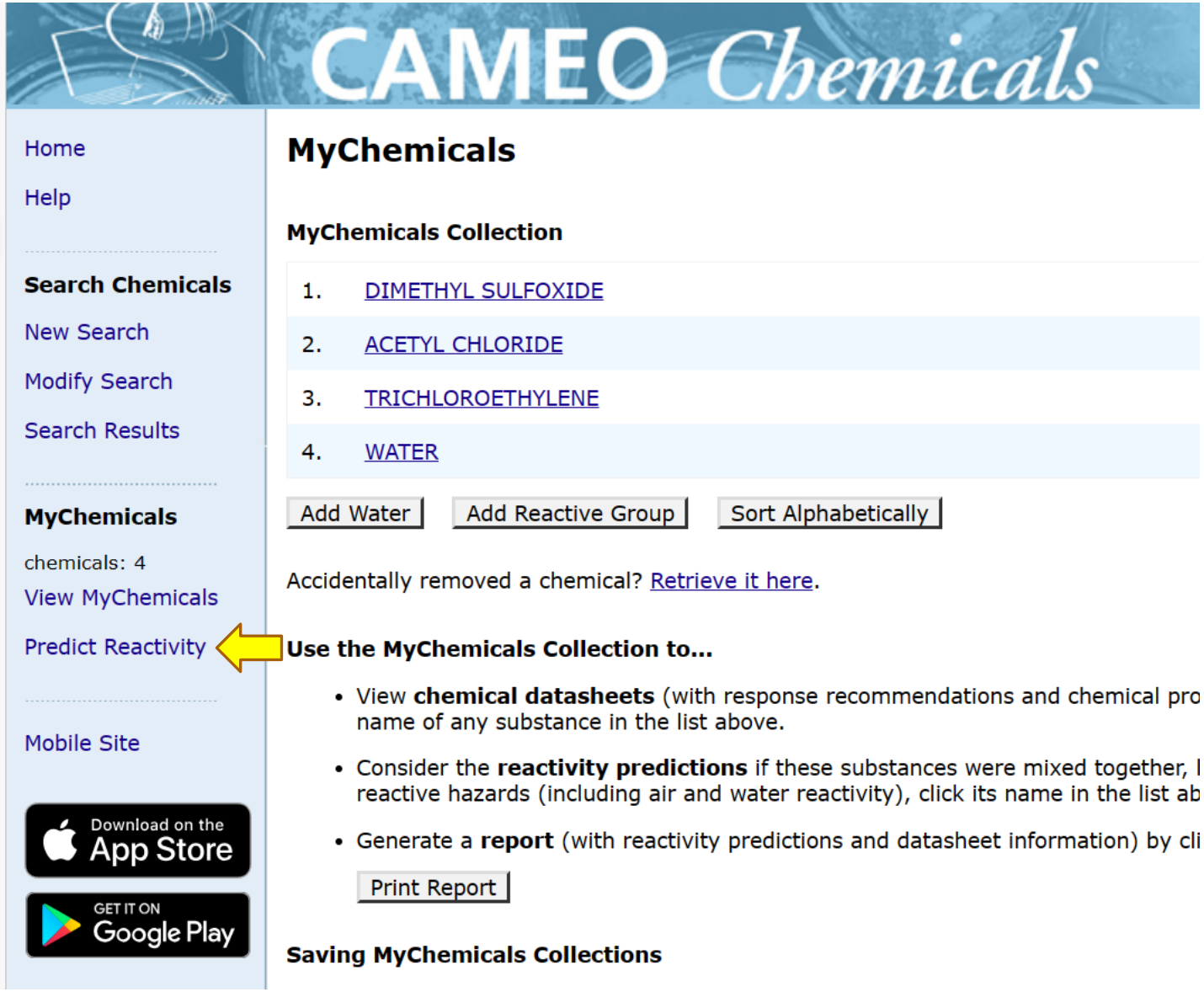
2. After adding substances to **MyChemicals,** click on **Predict Reactivity** on the left side.

Notes:

Reactivity Predictions are based on a PAIR or TWO substances.

Recommend adding no more than 20 compounds to **MyChemicals** to keep size of prediction table from becoming unwieldy.

See HELP for more details.



Compatibility Chart

This chart provides an overview of the reactivity predictions. For more details, click on a cell or scroll down the page.

How do I read this chart?

	DIMETHYL SULFOXIDE		
ACETYL CHLORIDE	**Caution** Generates heat Intense or explosive reaction	ACETYL CHLORIDE	
TRICHLOROETHYLENE	**Compatible**	**Compatible**	TRICHLOROETHYLENE
WATER	**Compatible**	**Incompatible** Corrosive Generates gas Generates heat Intense or explosive reaction Toxic	**Caution** Corrosive Generates gas

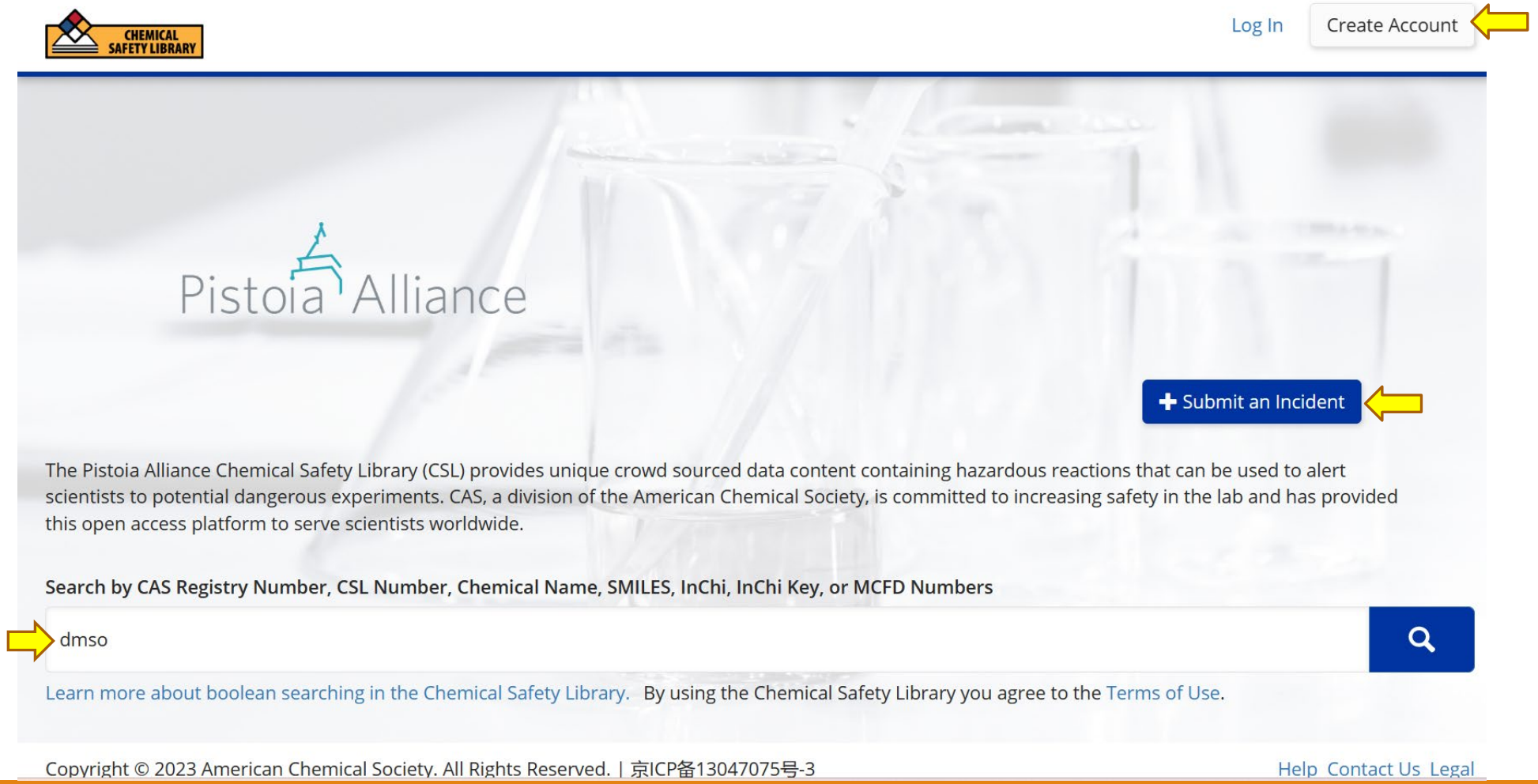
CAMEO Chemicals – Predict Reactivity – Compatibility Chart

Pistoia Alliance Chemical Safety Library (CSL)

CONTAINS LAB SAFETY INCIDENTS REPORTED BY USERS OR REPORTED IN THE LITERATURE

SEARCH BY CHEMICAL NAME OR CAS REGISTRY NUMBER

HTTPS://SAFESCIENCE.CAS.ORG/



Pistoia Alliance Chemical Safety Library (CSL)

CHEMICAL SAFETY LIBRARY

dmso

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Search Results for dmso 2 Results

+ Submit an Incident

	CSL Number	Reagent(s) Name	Warning Message	Source
1	CSL00022	Hydrogen peroxide (7722-84-1) **DMSO** (67-68-5)	Overpressurization Hazard if heated above 150 degrees C	C&EN
2	CSL00002	**DMSO** (67-68-5) perchloric acid (7601-90-3)	mixture can result in explosion	User-Reported

CSL Search Results

Chemical Safety Library
Hazardous Reaction Incident Submission Form

Thank you so much for contributing to the Pistoia Alliance Chemical Safety Library (CSL), a community crowd-sourced collection of hazardous reaction incidents, those "reactions gone wrong in the lab." This important new source allows all of us to learn from the wider-community's experiences.

Your entry (excluding your contact information) will be published to the CSL database, and will be deposited in PubChem (section 12.8.3.1). You can request a copy of the entire database (as a .csv file) from the Chemical Safety Library administrator.

Enter your reaction incident information in the form below. Be as complete as possible. Our curators will enter the data you provide into the CSL database. If they have any questions about your entry, they will be in touch via email.

Hazardous Reaction Incident Submission Form

CSL Hazardous Reaction Incident Submission Form

Name and Institution are NOT displayed in published CSL records. This information is needed for CSL admin reviewers if they have questions and need to contact a submitter.

Required Field*

Company or Institution*

Grace Baysinger

Source*

Literature Citation

Enter a DOI into ZoteroBib - **https://zbib.org/** - to quickly and easily get a citation. Scroll down the page to choose a different style format. The ACS Style Quick Guide - **https://pubs.acs.org/doi/full/10.1021/acsguide.40303** - has examples you can use too.
CAMEO Chemicals sample citation: Diisopropyl peroxydicarbonate. CAMEO Chemicals. NOAA/EPA. https://cameochemicals.noaa.gov/chemical/953 (accessed 2023-06-26). (CAS RN: 105-64-6)

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Example: **https://doi.org/10.1021/jacs.3c03627**

Warning Message*

Please enter as much detail as possible about the incident and what could have been done to prevent it

Warning Message: Reactivity Profile information in CAMEO Chemicals - https://cameochemicals.noaa.gov/ - have reaction incide information. Also see ACS Publications Author Guidelines about Safety Considerations that include recommendations about creating safety caution statements - https://publish.acs.org/publish/author_guidelines?coden=acscii#safety_considerations

CSL Hazardous Reaction Incident Submission Form

Substance (Reactants/Reagents/Solvents/Catalysts) in the reaction involved in this Incident Report*

Substance 1 - Name*

Use Semicolons As A Delimiter

Substance 1 - CAS#

Substance 1 - Role*

Substance 2 - Name*

Use Semicolons As A Delimiter

Substance 2 - CAS#

Substance 2 - Role*

+ Add Another Substance

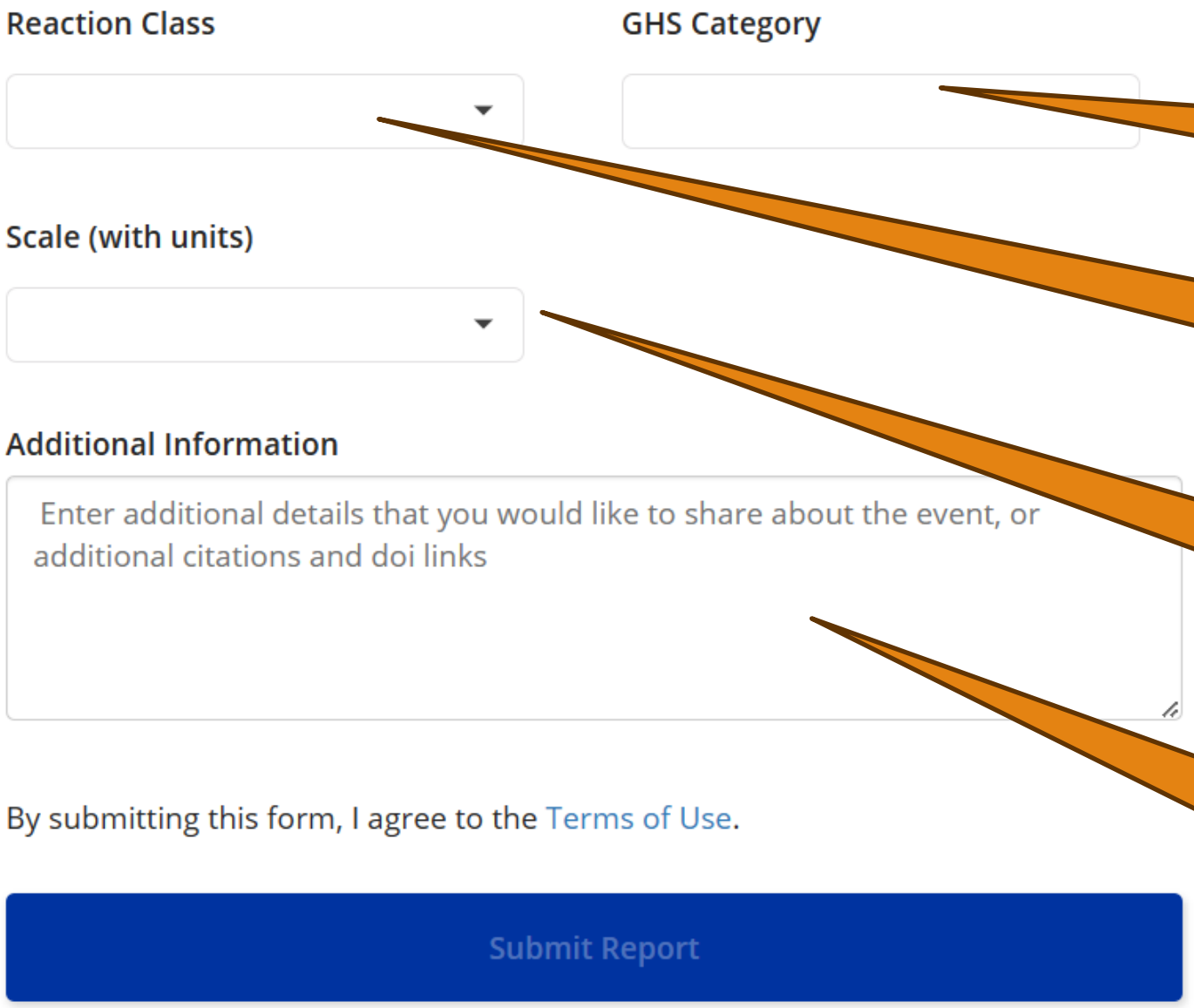
Roles include:
Reactant
Reagent
Solvent
Catalyst
Product
Unknown

Note that incompatibility between two substances is not enough. The two or more substances must be involved in hazardous or potentially hazardous reaction to be accepted into the CSL database.

Possible values for substances include an individual substance name, an element, or a compound class name. While CAS Registry Numbers are available for individual substances and elements, no CAS Registry Numbers are assigned to compound class names.

It is okay to use an acronym for a substance but please also add a chemical substance name too. To locate names, synonyms, and CAS Registry Numbers use CAS Common Chemistry - https://commonchemistry.cas.org/ - or SciFinder.

CSL Hazardous Reaction Incident Submission Form

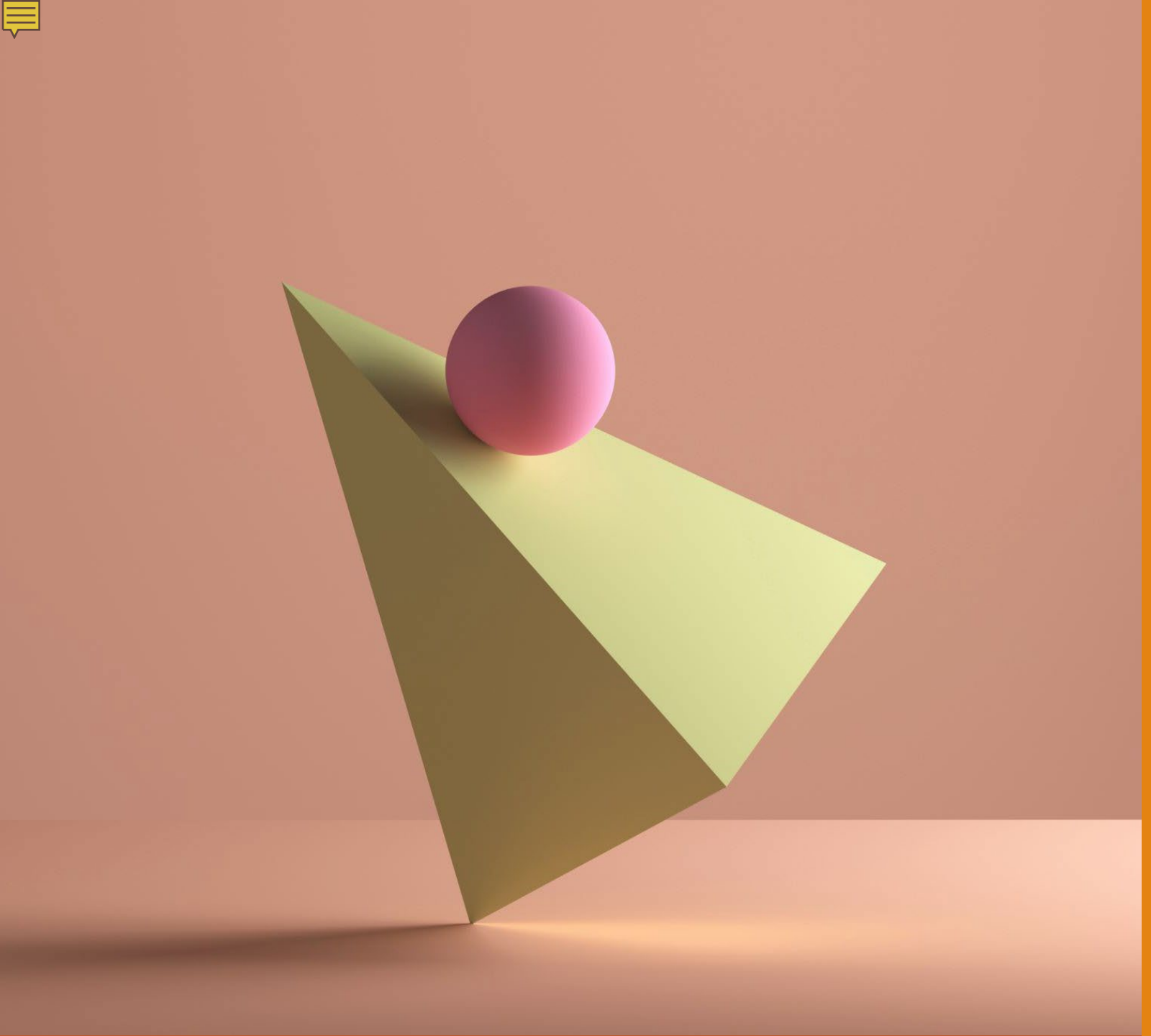


Globally Harmonized System for Classifying Individual Chemical Substances. Can select multiple values that apply to substances involved in the hazardous reaction.

Selected list of reaction classes. Can select multiple values. Last choice is “Other” that allows submitters to add an additional reaction class name.

Scale options include:
Small (up to 1g)
Medium (up to 100g)
Large (>100g)
Not available

Do NOT include health hazards or emergency response recommendations because this information may be incomplete and may become outdated.



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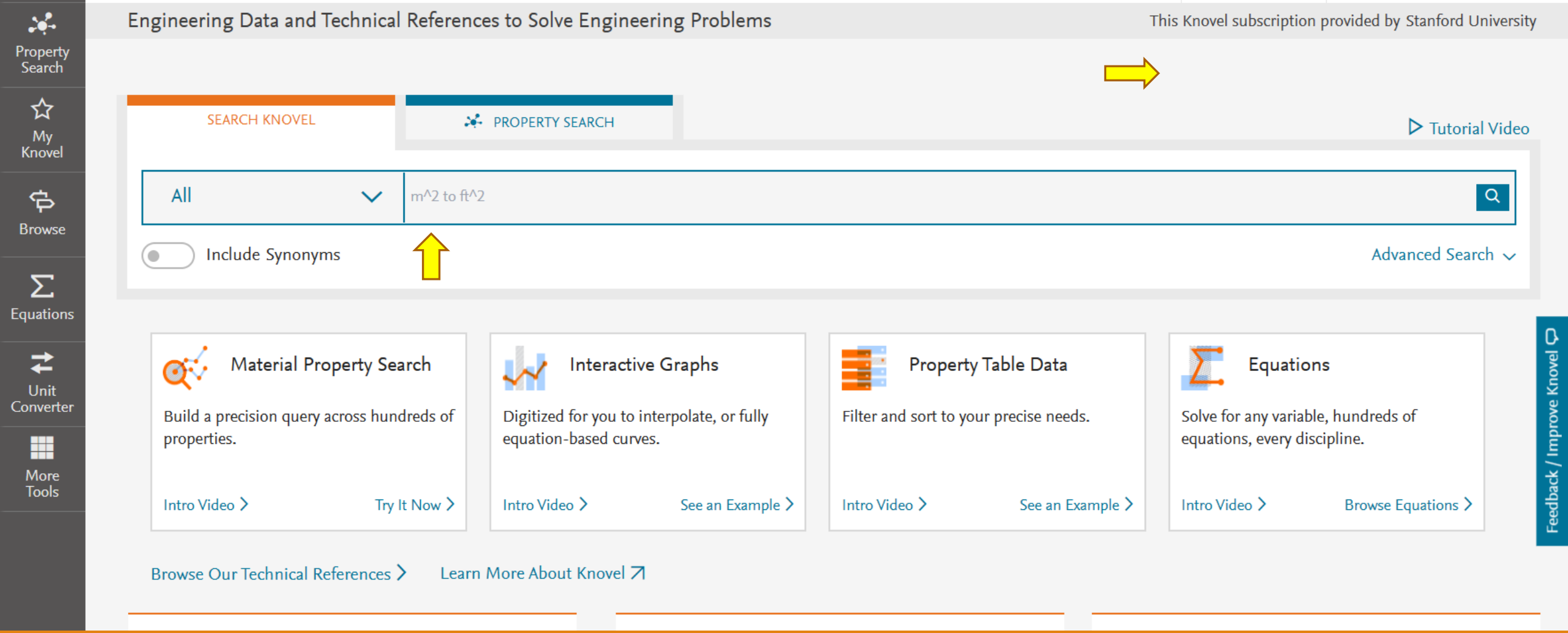
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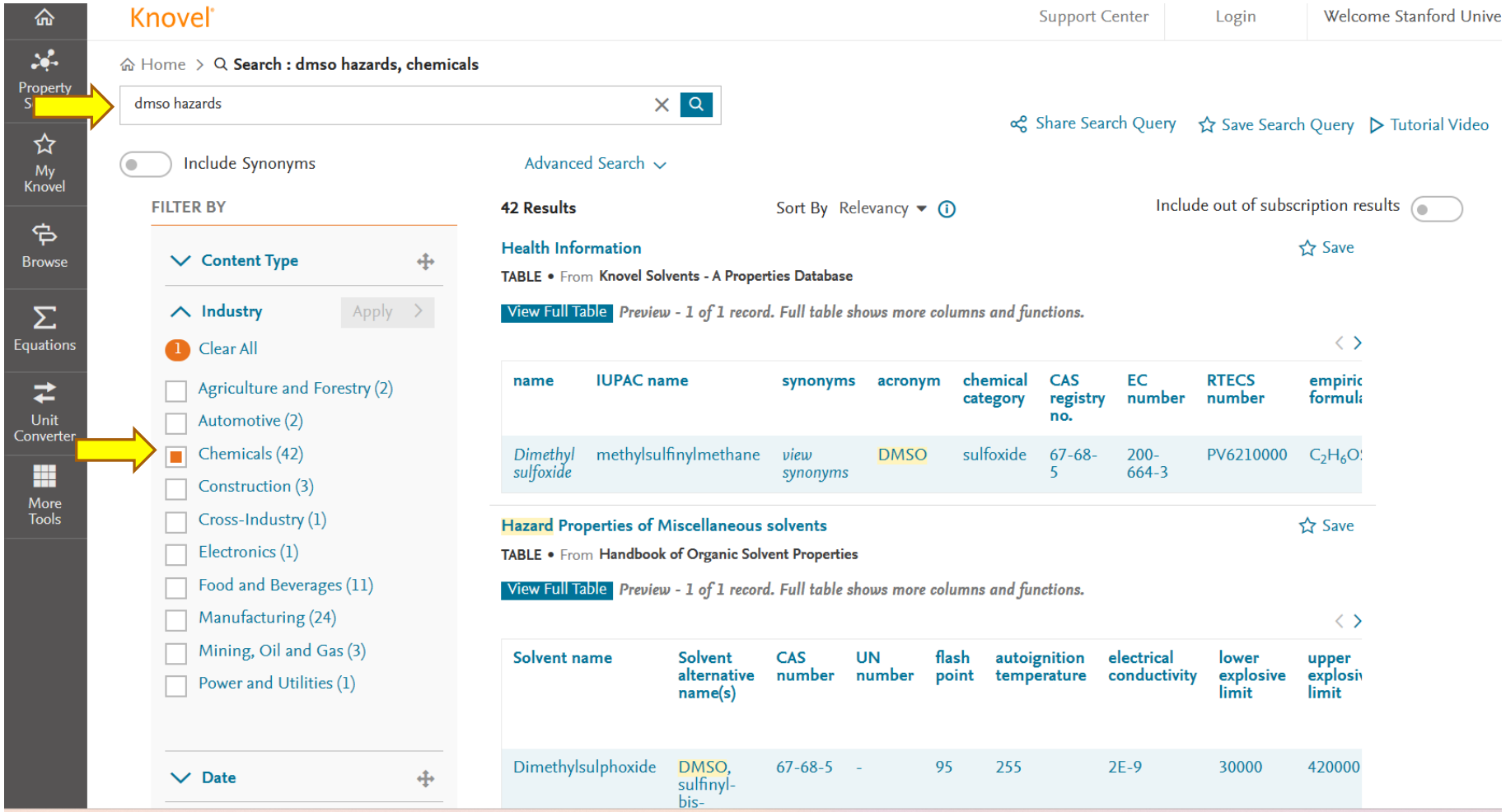
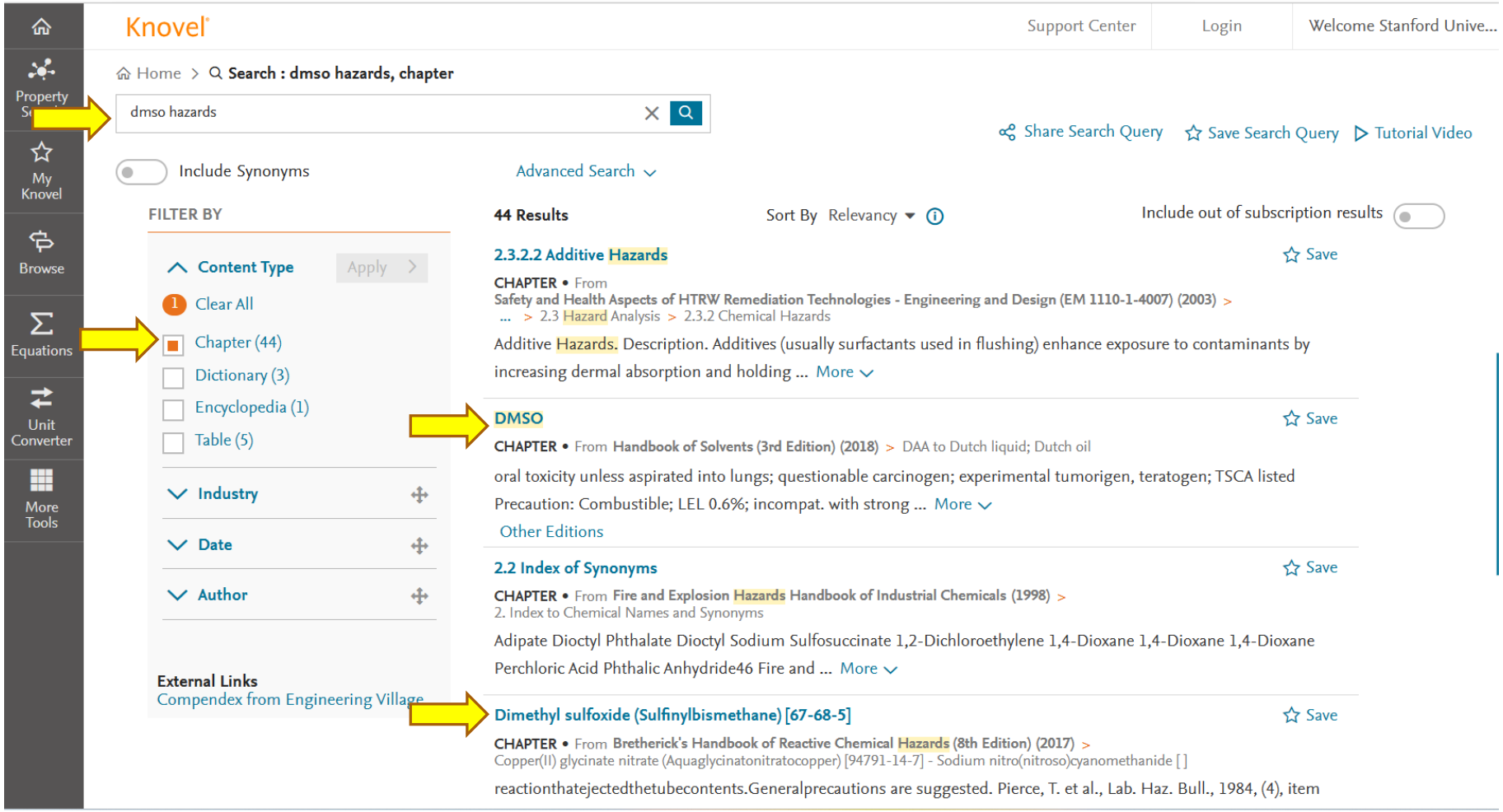


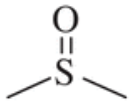
Knovel search results for "DMSO hazards" filtered by Industry = "Chemicals"



Knovel search results for "DMSO hazards" filtered by Content Type = "Chapter"

†0917 Dimethyl sulfoxide (Sulfinylbismethane)

[67-68-5] **C_2H_6OS**



HCS 1980, 435; *RSC Lab. Hazard Data Sheet No. 11*, 1983

Two instances of used DMSO decomposing exothermally while being kept at 150°C prior to recovery by vacuum distillation were investigated. Traces of alkyl bromides lead to a delayed, vigorous, and strongly exothermic reaction (Q = 0.85 kJ/g) at 180°C. Adding zinc oxide as a stabilizer extends the induction period and markedly reduces the exothermicity [1]. ARC examination shows that exothermic decomposition sets in by a radical mechanism at 190°C, just above the b.p., 189°C. The proposed retardants, sodium carbonate and zinc oxide, do not affect the decomposition temperature, and a maximum decomposition pressure of 60 bar was attained (at up to 4 bar/min) at the low sample loading of 18 w/v% in the bomb [2]. The thermolytic degradation of the sulfoxide to give acidic products that catalyze further decomposition was discussed previously [3]. T_{ait24} was determined as 213°C by adiabatic Dewar tests, with an apparent energy of activation of 243 kJ/mol. At elevated temperatures (200°C) DSC shows decomposition to be both faster and more energetic when chloroform or sodium hydroxide is present [4]. A conference paper presents real synthetic situations where the instability of the solvent, often increased by solutes, became a potential safety hazard [5].

Knovel> Bretherick's Handbook of Reactive Chemical Hazards, 8th Edition

1. Brogli, F. *et al., Proc. 3rd Int. Symp. Loss Prev. Safety Prom. Proc. Ind.*, 681–682, Basle, SSCI, 1980
2. Cardillo, P. *et al., Chim. e Ind.* (Milan), 1982, **44**, 231–234
3. Santosusso, T. M. *et al., Tetrahedron Lett.*, 1974, 4255–4258
4. *See* THERMOCHEMISTRY AND EXOTHERMIC DECOMPOSITION (reference 2)
5. Lam. T. T. *et al., J. Therm. Anal. & Calorimetry*, 2006, **85**(1), 25

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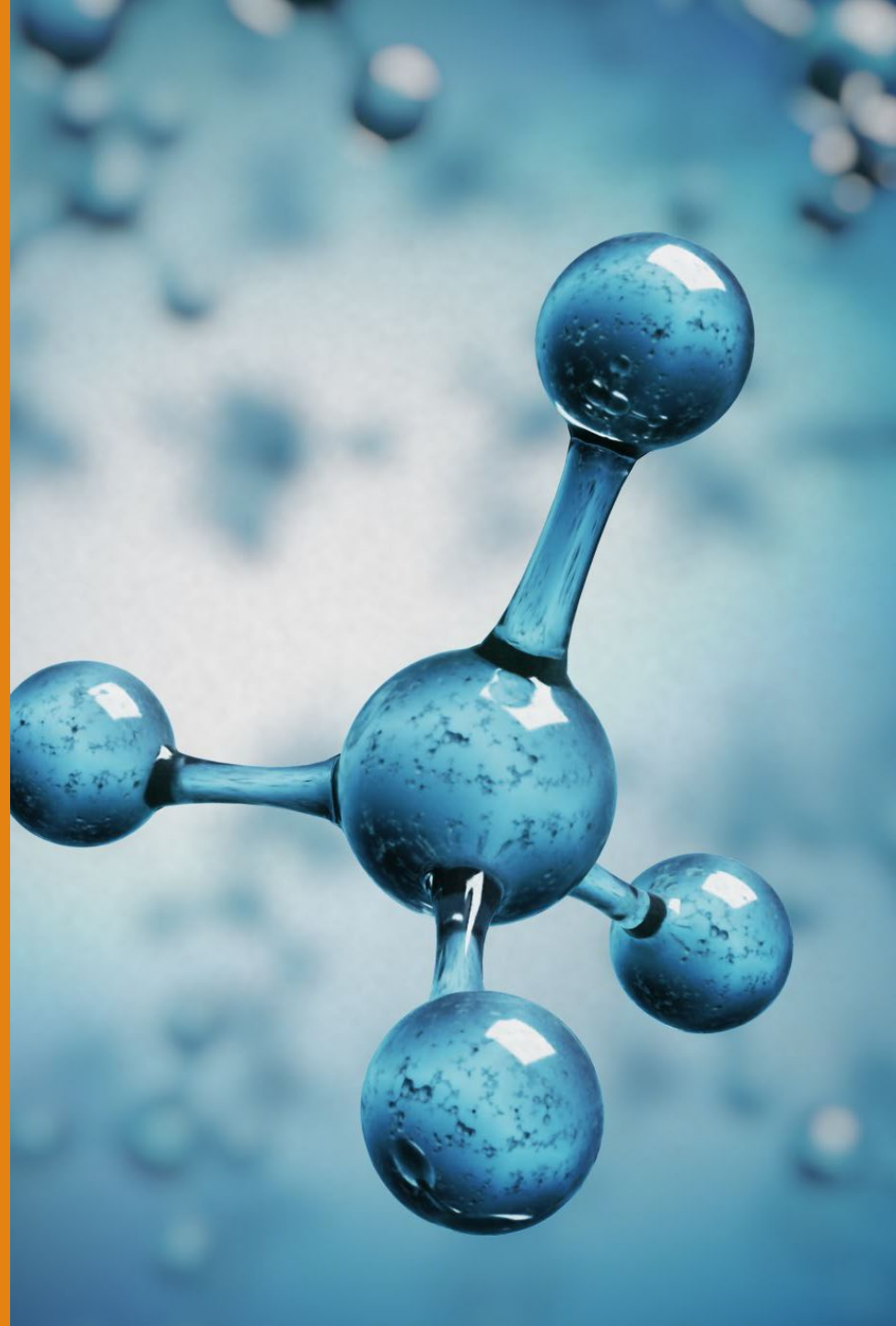

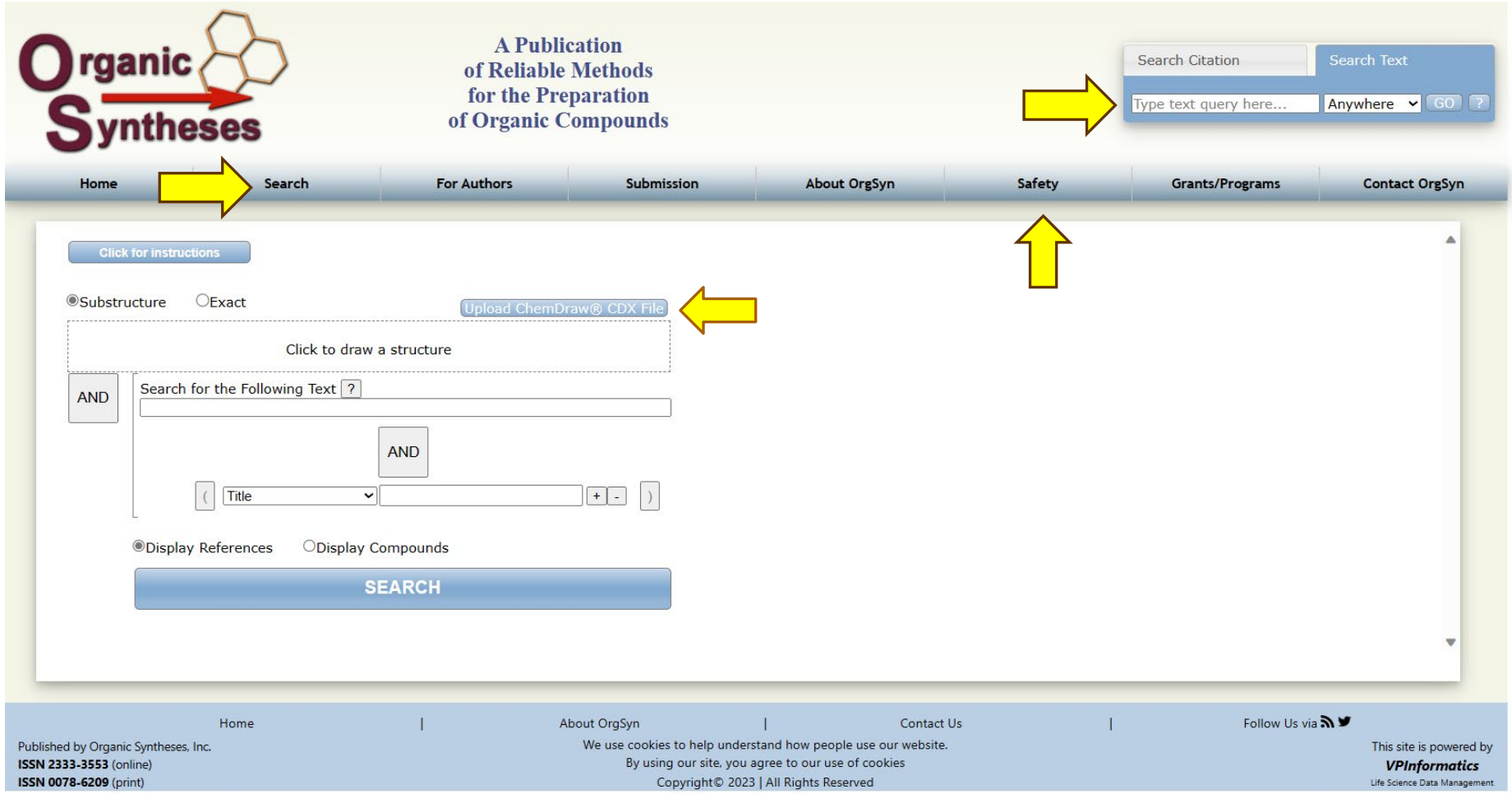

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Effective in August 2017, the first Note in every article is devoted to addressing the safety aspects of the procedures described in the article. The Article Template provides the required wording and format for Note 1, which reminds readers of the importance of carrying out risk assessments and hazard analyses prior to performing all experiments.

Prior to performing each reaction, a thorough hazard analysis and risk assessment should be carried out with regard to each chemical substance and experimental operation on the scale planned and in the context of the laboratory where the procedures will be carried out.”

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Organic Syntheses - Safety

Organic Syntheses – Search Results for DMSO Anywhere in the Text

1

Preparation of MIDA Anhydride and Reaction with Boronic Acids

Peng-Jui Chen, Aidan M. Kelly, Daniel J. Blair, and Martin D. Burke

Org. Synth. **2022**, *99*, 92
DOI: 10.15227/orgsyn.099.0092

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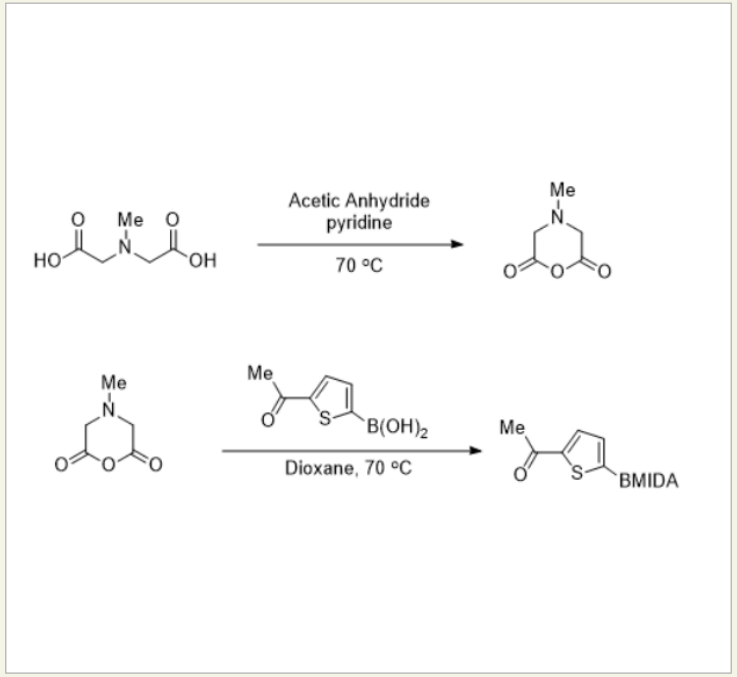
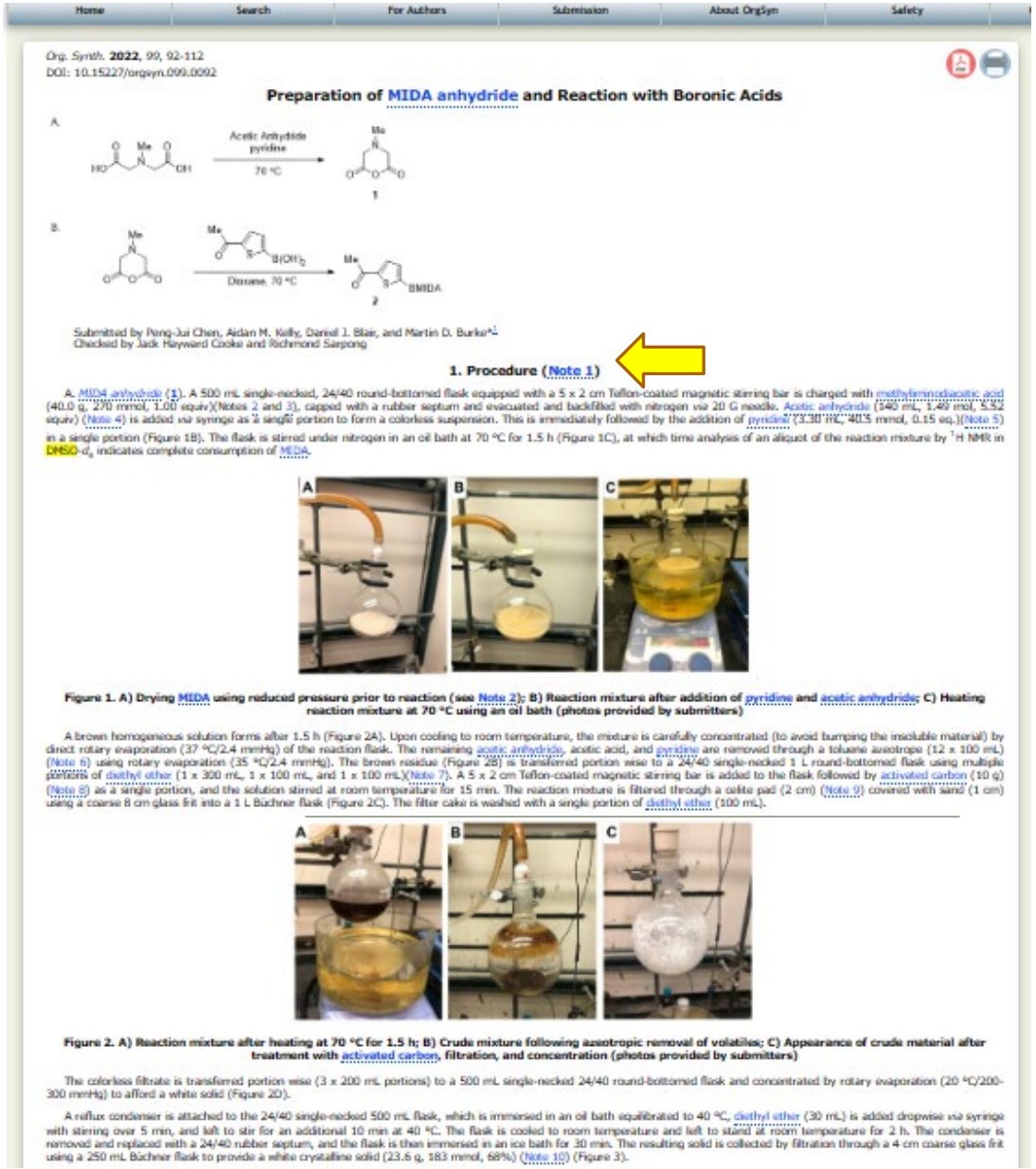


f an aliquot of the reaction mixture by 1H NMR in **dmso**-d6 indicates complete consumption of MIDA. Fig...23.3 g (67%) of 1. mp 42–44 °C; 1H NMR (500 MHz, **dmso**-d6) d: 2.31 (s, 3H), 3.60 (s, 4H); 13C NMR (126 MH....8 g (79%) of 2. mp 225–227 °C; 1H NMR (500 MHz, **dmso**-d6) δ: 2.53 (s, 3H), 2.64 (s, 3H) 4.17 (d, J = 17....



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Org. Synth. **2022**, *99*, 92-112
DOI: 10.15227/orgsyn.099.0092

Preparation of MIDA anhydride and Reaction with Boronic Acids

Submitted by Peng-Jui Chen, Aidan M. Kelly, Daniel J. Blair, and Martin D. Burke*
Checked by Jack Hayward Cooke and Richmond Sarpong

1. Procedure (Note 1)

A. MIDA anhydride (1). A 500 mL single-necked, 24/40 round-bottomed flask equipped with a 5 x 2 cm Teflon-coated magnetic stirring bar is charged with methyliminodiacetic acid (40.0 g, 270 mmol, 1.00 equiv)(Notes 2 and 3), capped with a rubber septum and evacuated and backfilled with nitrogen via 20 G needle. Acetic anhydride (140 mL, 1.49 mol, 5.52 equiv) (Note 4) is added via syringe as a single portion to form a colorless suspension. This is immediately followed by the addition of pyridine (3.30 mL, 40.5 mmol, 0.15 eq.)(Note 5) in a single portion (Figure 1B). The flask is stirred under nitrogen in an oil bath at 70 °C for 1.5 h (Figure 1C), at which time analysis of an aliquot of the reaction mixture by ^{1}H NMR in DMSO-d_6 indicates complete consumption of MIDA.

Figure 1. A) Drying MIDA using reduced pressure prior to reaction (see Note 2); B) Reaction mixture after addition of pyridine and acetic anhydride; C) Heating reaction mixture at 70 °C using an oil bath (photos provided by submitters)

A brown homogeneous solution forms after 1.5 h (Figure 2A). Upon cooling to room temperature, the mixture is carefully concentrated (to avoid bumping the insoluble material) by direct rotary evaporation (37 °C/2.4 mmHg) of the reaction flask. The remaining acetic anhydride, acetic acid, and pyridine are removed through a toluene azeotrope (12 x 100 mL) (Note 6) using rotary evaporation (35 °C/2.4 mmHg). The brown residue (Figure 2B) is transferred portion wise to a 24/40 single-necked 1 L round-bottomed flask using multiple portions of diethyl ether (1 x 300 mL, 1 x 100 mL, and 1 x 100 mL)(Note 7). A 5 x 2 cm Teflon-coated magnetic stirring bar is added to the flask followed by activated carbon (10 g) (Note 8) as a single portion, and the solution stirred at room temperature for 15 min. The reaction mixture is filtered through a celite pad (2 cm) (Note 9) covered with sand (1 cm) using a coarse 8 cm glass frit into a 1 L Büchner flask (Figure 2C). The filter cake is washed with a single portion of diethyl ether (100 mL).

Figure 2. A) Reaction mixture after heating at 70 °C for 1.5 h; B) Crude mixture following azeotropic removal of volatiles; C) Appearance of crude material after treatment with activated carbon, filtration, and concentration (photos provided by submitters)

The colorless filtrate is transferred portion wise (3 x 200 mL portions) to a 500 mL single-necked 24/40 round-bottomed flask and concentrated by rotary evaporation (20 °C/200-300 mmHg) to afford a white solid (Figure 2D).

A reflux condenser is attached to the 24/40 single-necked 500 mL flask, which is immersed in an oil bath equilibrated to 40 °C, diethyl ether (30 mL) is added dropwise via syringe with stirring over 5 min, and left to stir for an additional 10 min at 40 °C. The flask is cooled to room temperature and left to stand at room temperature for 2 h. The condenser is removed and replaced with a 24/40 rubber septum, and the flask is then immersed in an ice bath for 30 min. The resulting solid is collected by filtration through a 4 cm coarse glass frit using a 250 mL Büchner flask to provide a white crystalline solid (23.6 g, 183 mmol, 68%) (Note 10) (Figure 3).

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Print ISBN: 9780471936237 | Online ISBN: 9780470842898 | DOI: 10.1002/047084289X

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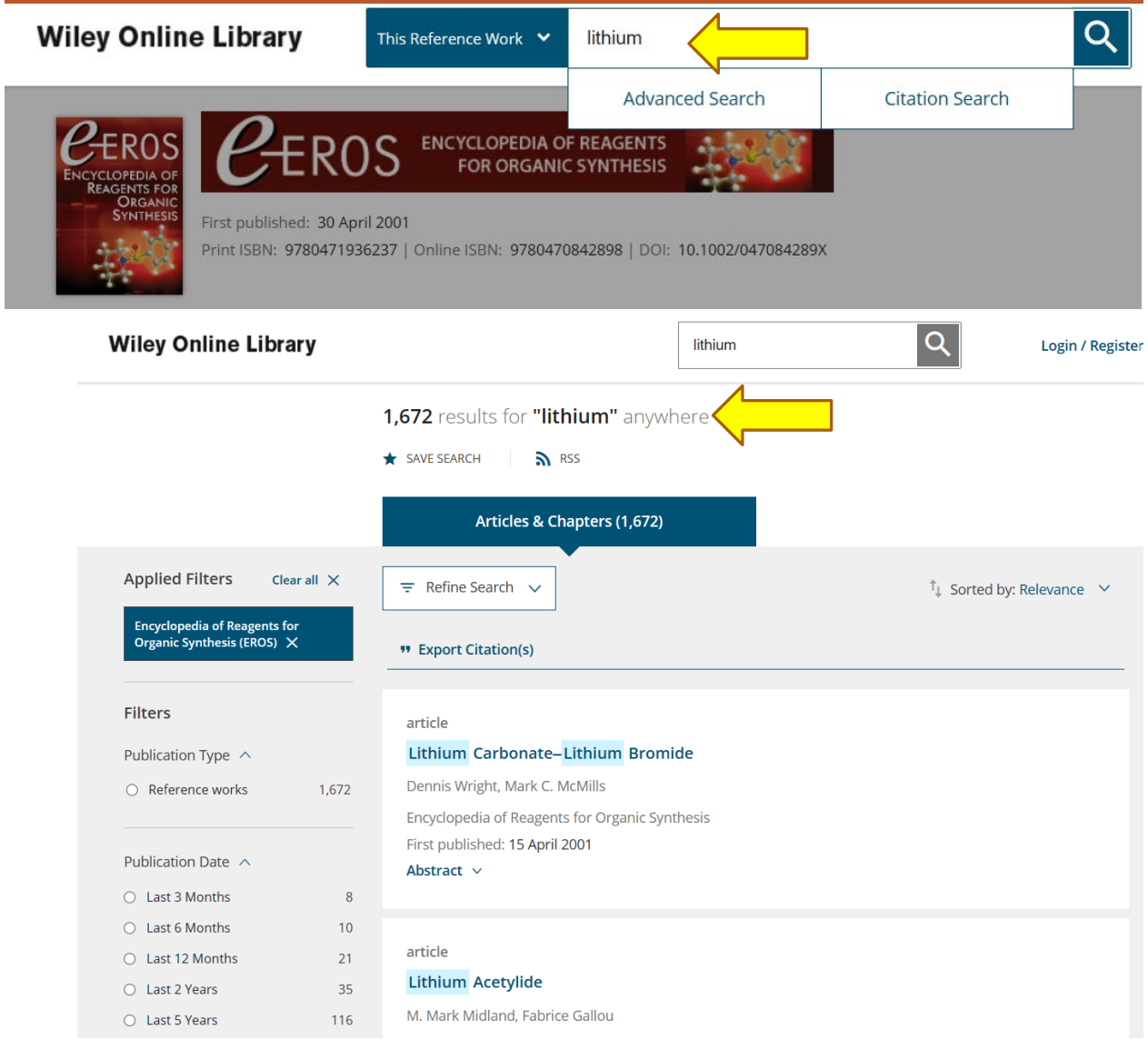

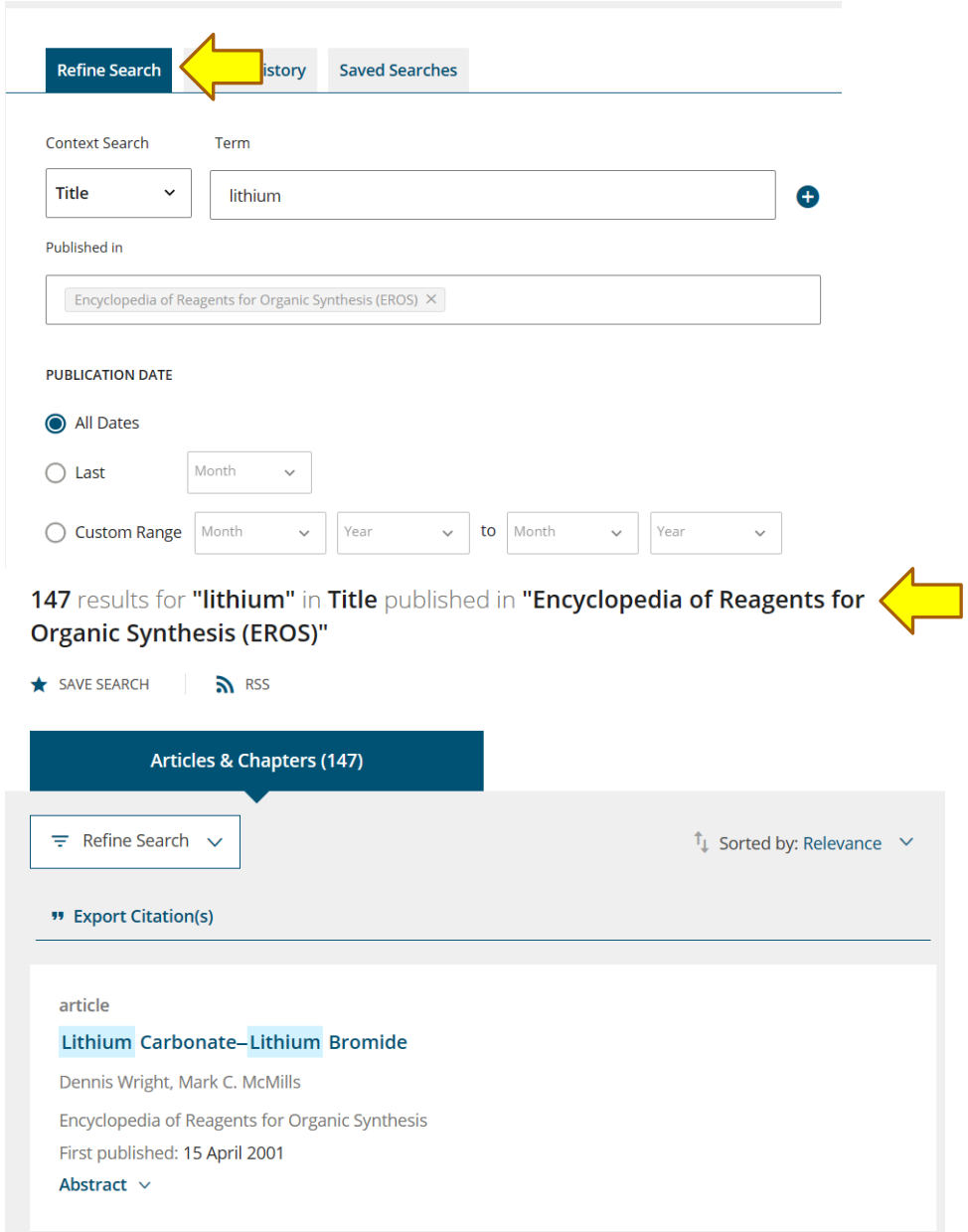

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Lithium Dichloro(1-methylethyl)-magnesate

Paul Knochel, Andrei Gavryushin

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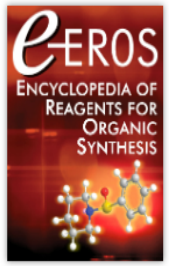

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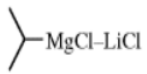

[807329-97-1] $C_3H_7Cl_2LiMg$ (MW 145.24)

InChI = 1S/C3H7.2ClH.Li.Mg/c1-3-2;;;;/h3H,1-2H3;2*1H;;/q;;;;2*+1/p-2

InChIKey = CWTUREABAILGIK-UHFFFAOYSA-L

(reagent used in preparation of various organomagnesium compounds via halogen–magnesium exchange reactions)

Alternate Name: isopropylmagnesium chloride–lithium chloride complex.

Recommended

Lithium Dichloro(2,2,6,6-tetramethylpiperidinato)-zincate

Thomas Klatt, Paul Knochel, Marc Mosrin

Encyclopedia of Reagents for Organic Synthesis (EROS), [1]

1,2,3,4-Tetrahydro-1-(1-methylethyl)-1-silanaphthalene

Marius Mewald, Martin Oestreich

Encyclopedia of Reagents for Organic Synthesis (EROS), [1]

1,3-Dichloro-2-trimethylsiloxy-1-butene

e-EROS Sample content

Lithium Dichloro(1-methylethyl)-magnesite

Subscription required to view the full text.

Physical Data: solution in THF, similar to the solvent.

Solubility: solution in THF miscible with the majority of organic solvents. The neat compound is insoluble in alkanes and soluble in coordinating solvents (ethers, amines, etc.)

Form Supplied in: THF solution (1.1–1.3 M).

Purification: not considered.

Handling, Storage, and Precautions: the solution of the reagent rapidly reacts with oxygen and water and should be stored and handled in an inert atmosphere. Vigorously reacts with water and aqueous solutions, evolving highly flammable gases. Due to its strong dehydrating ability, spills may cause serious damage to the skin and eyes. The commercial solution in THF is a flammable liquid.

Citing Literature

Bibliography

Nobujiro Shimizu

Encyclopedia of Reagents for Organic Synthesis (EROS), [1]

Zinc Trifluoromethanesulfinate

Yoshihiro Ishihara, Ryan Gianatassio, Phil S. Baran

Encyclopedia of Reagents for Organic Synthesis (EROS), [1]

e-EROS Sample content

Lithium Dichloro(1-methylethyl)-magnesite

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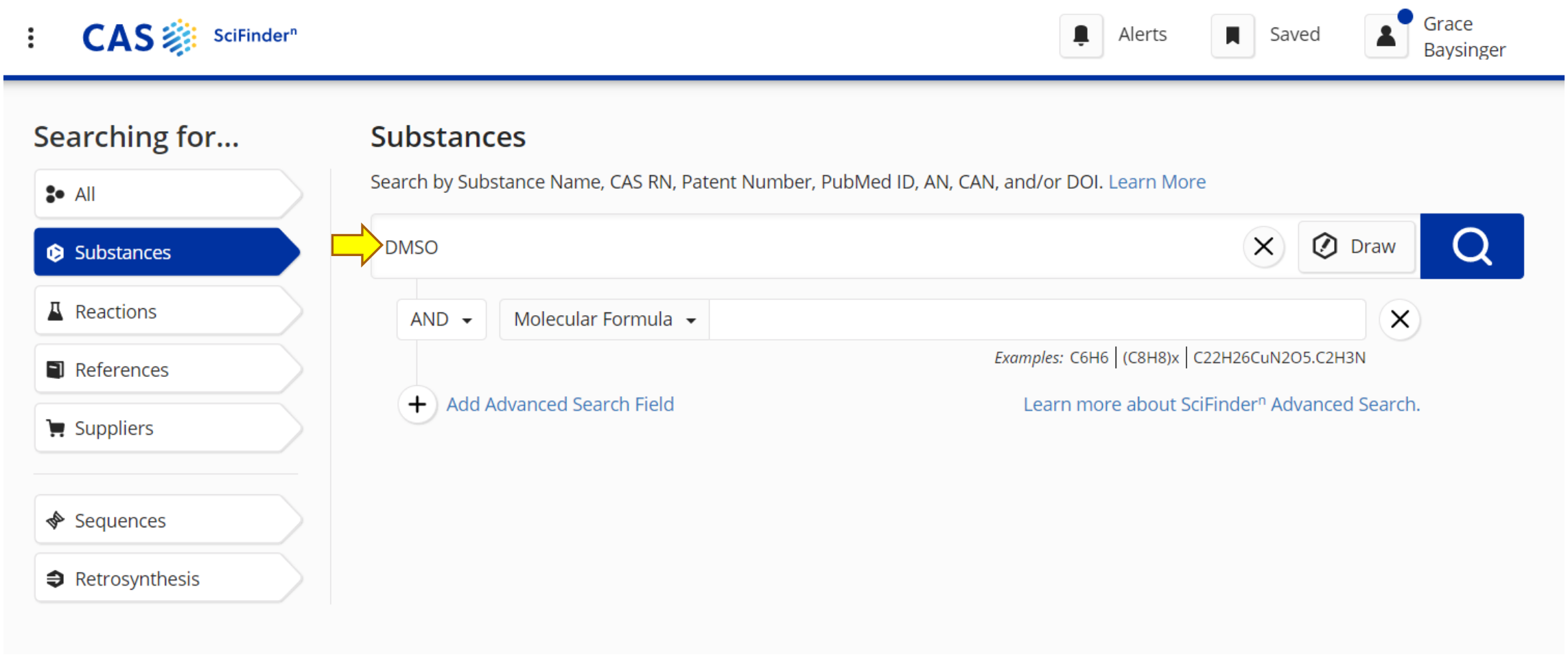
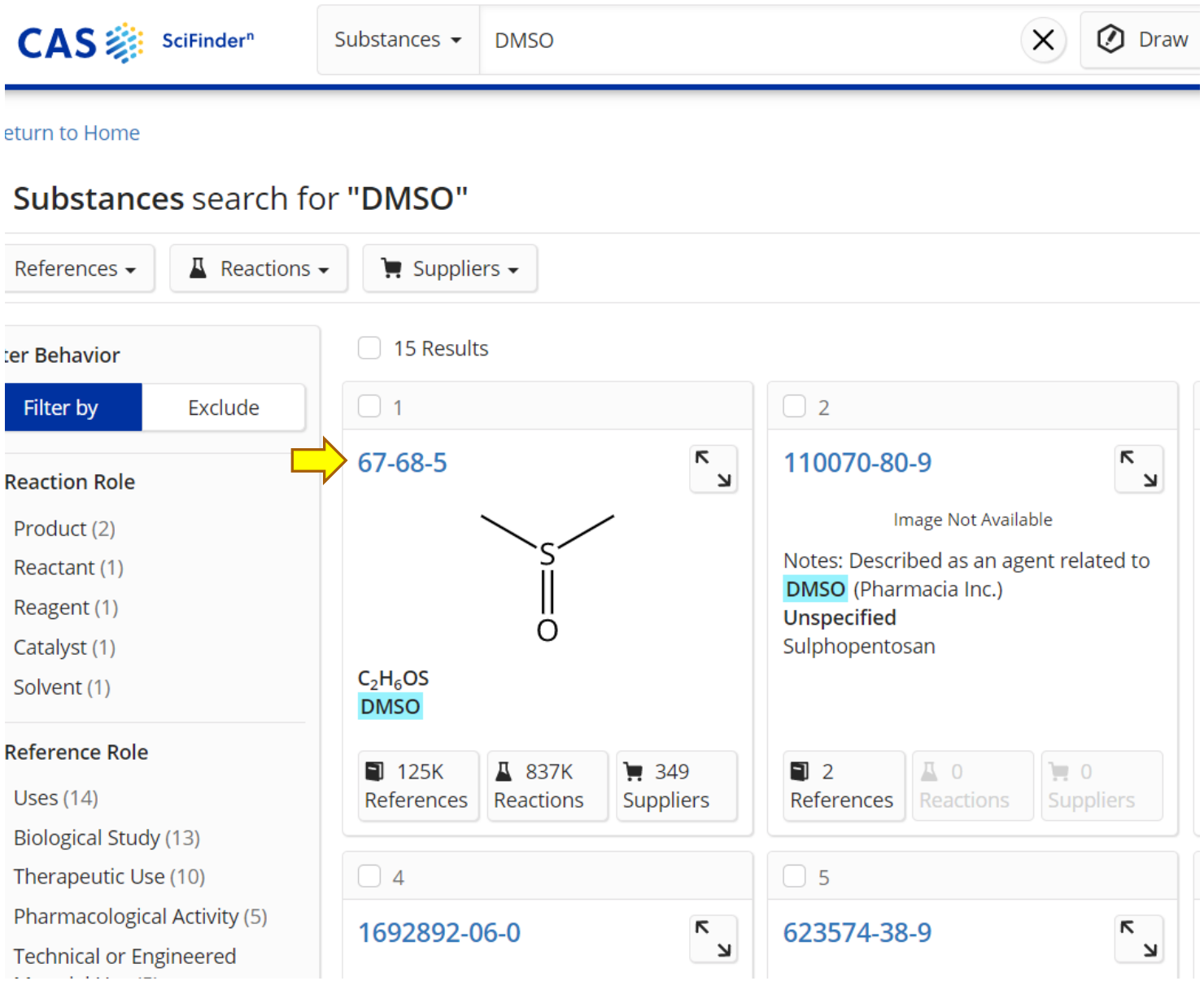


SciFinder-n – Searching for DMSO as a Substance



SciFinder-n – Substance search results for DMSO

CAS SciFinder^n | Substances | DMSO | Draw

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CAS Registry Number: 67-68-5

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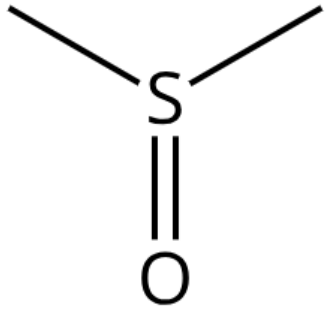


- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Predicted Properties
- Predicted Spectra
- Regulatory Information
- GHS Hazard Statements
- Additional Details

C_2H_6OS

Methane, 1,1'-sulfinylbis- (ACI)

SciFinder-n Substance Details – Includes links to References, Reactions, and Suppliers, plus Other Names & Identifiers, Properties, Spectra, Regulatory Information.

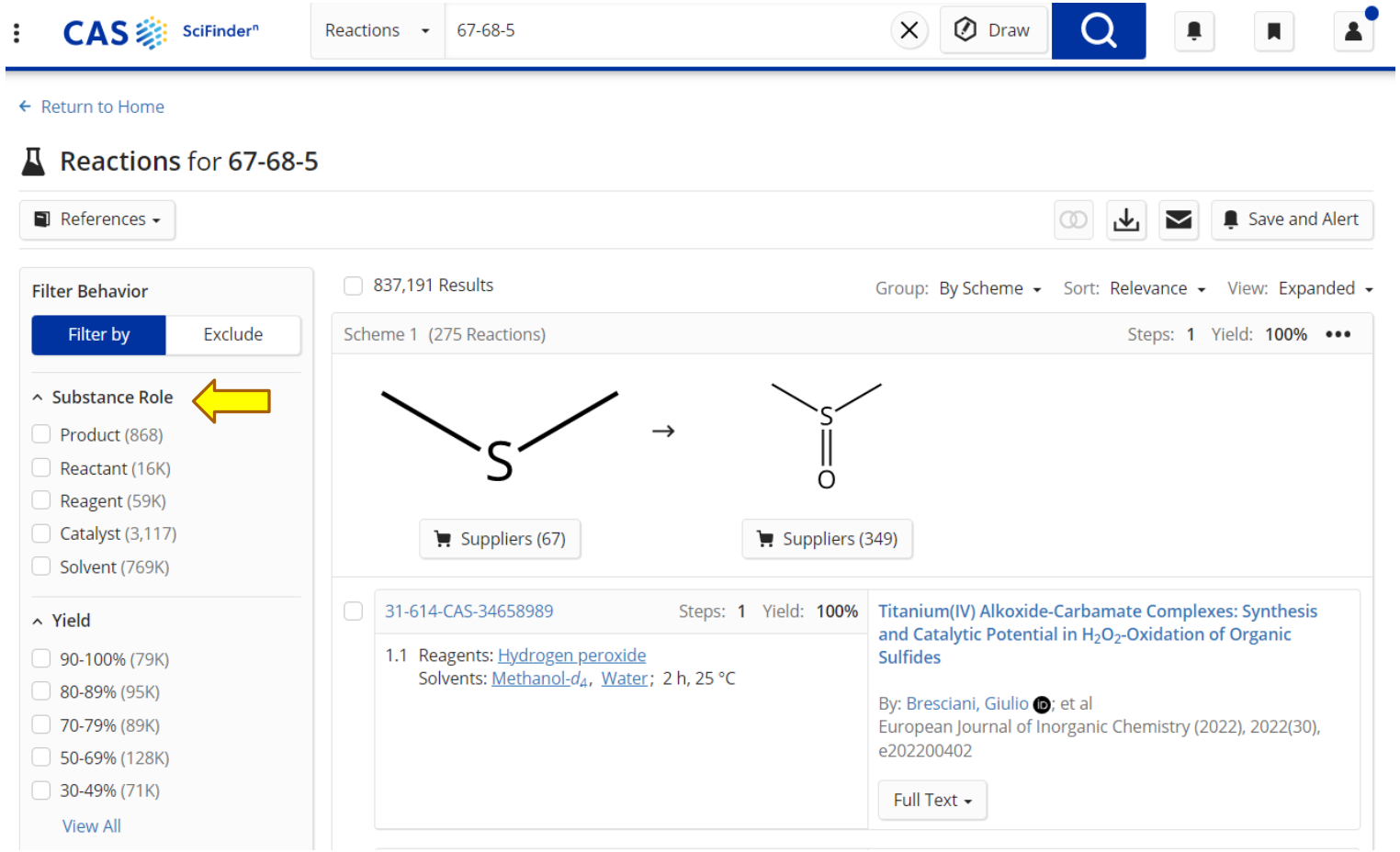
Code, statements, and pictograms from the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) became available in SF-n on June 26, 2023.

CAS SciFinder^{n} Substances DMSO

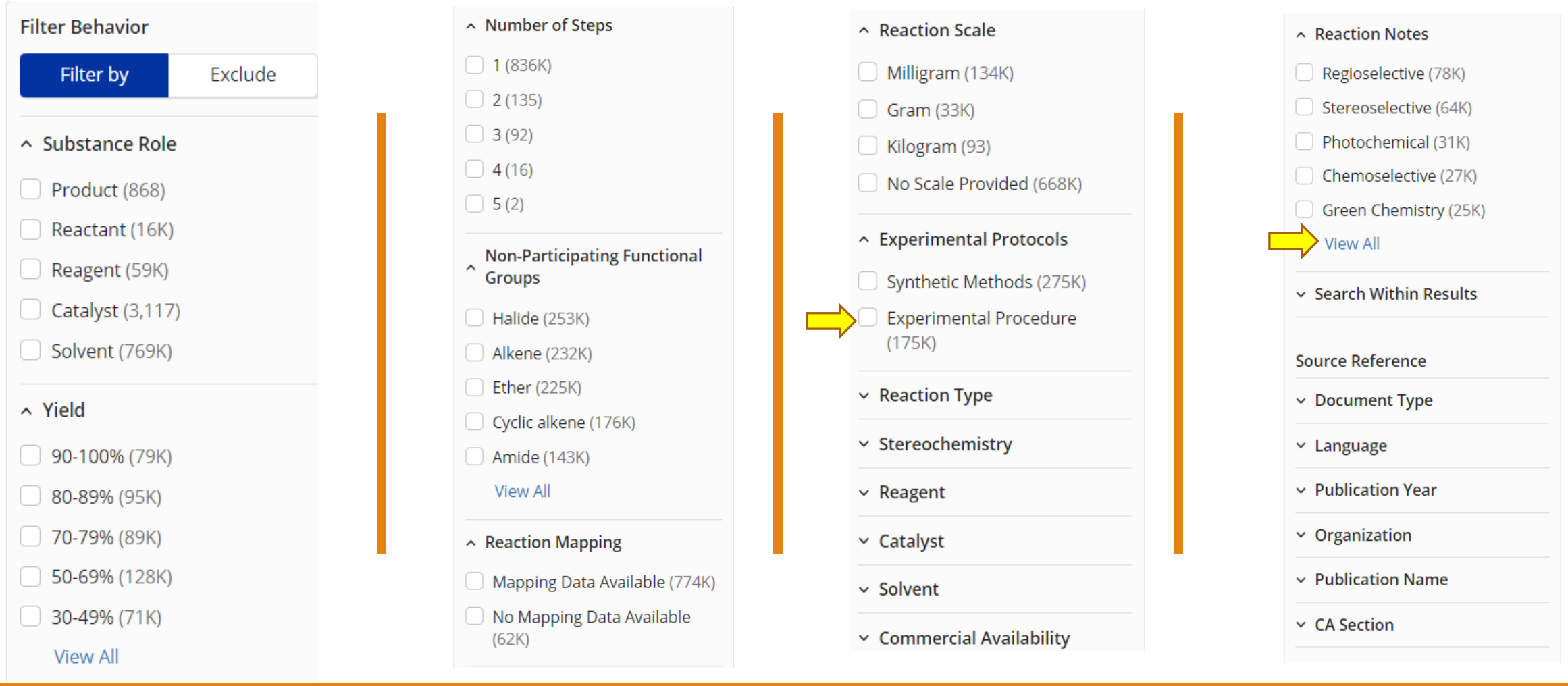
GHS Hazard Statements

Code	Hazard Statement	Source
H432	Toxic to terrestrial vertebrates	Fisher Scientific (Lomb)
H373	May cause damage to organs; through prolonged or repeated exposure	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria, TCI America, Tokyo Chemical Industry Co (Tokyo Kasei Kogyo Co)
H371	May cause damage to organs	Expert Curated, Japan GHS Classifications (Japanese)
H351	Suspected of causing cancer	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria

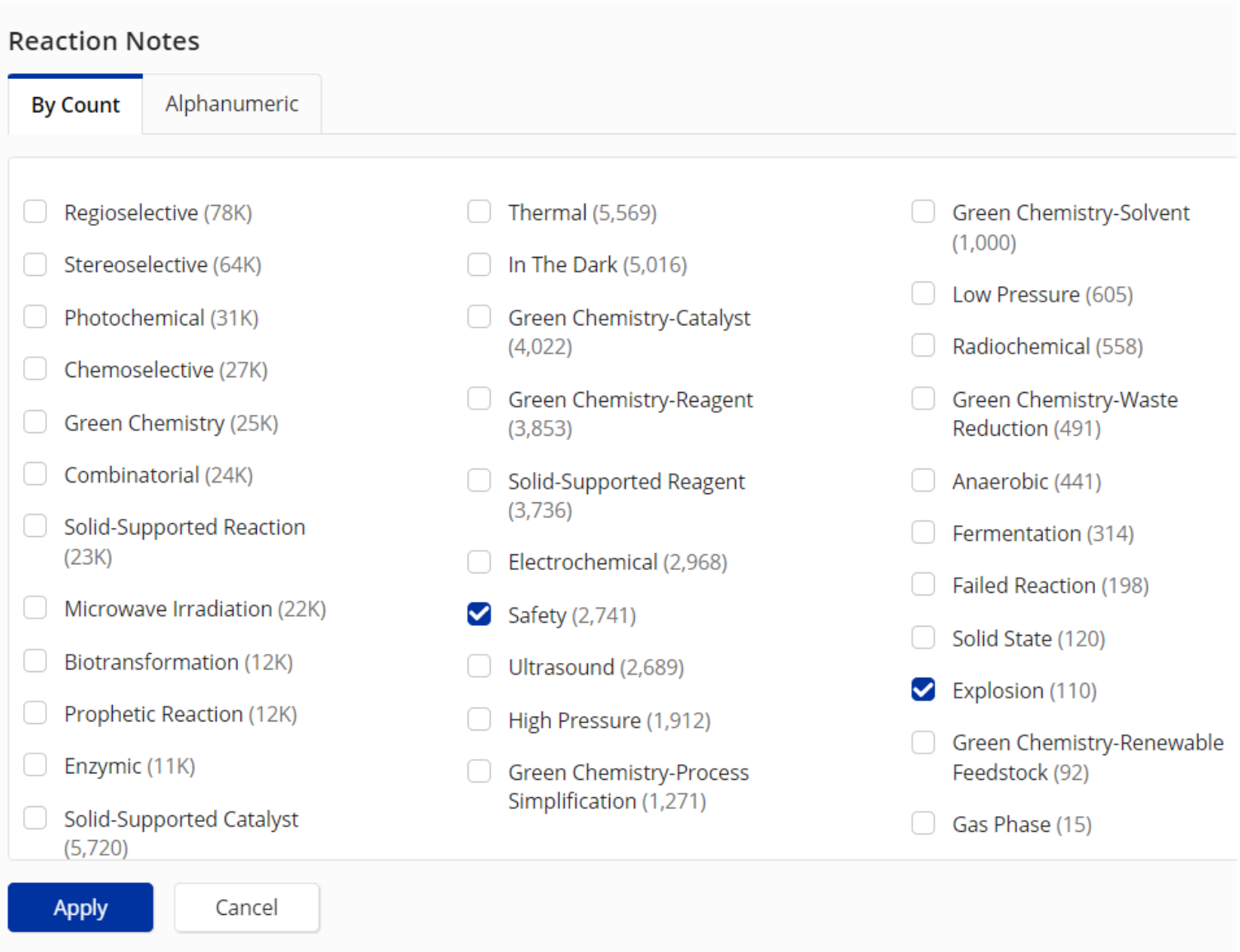
Selected GHS Hazard Statements for DMSO



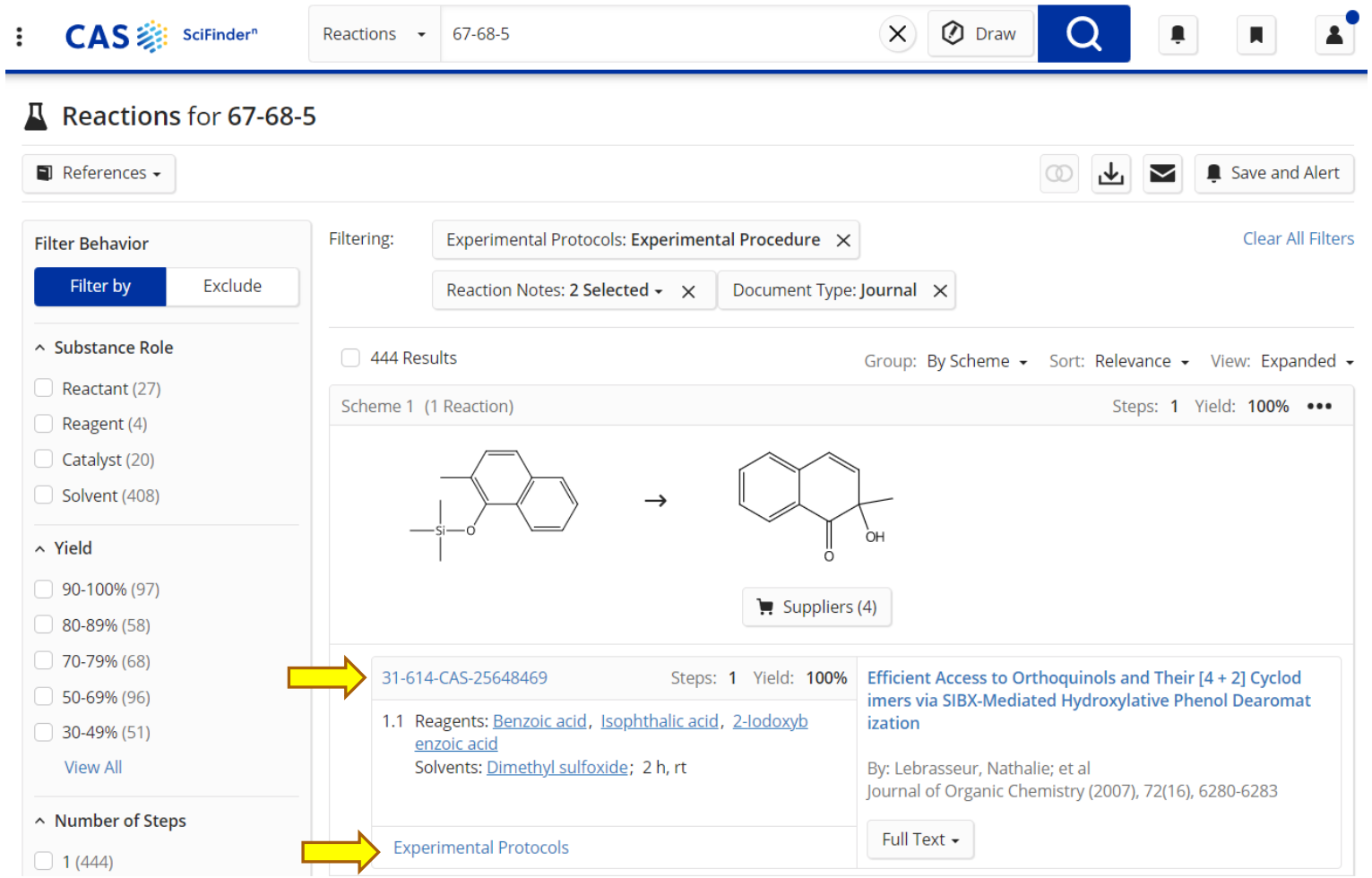
SciFinder-n – Viewing Reactions



SciFinder-n – Options for Filtering Reaction Search Results



SciFinder-n – Reaction Notes



SciFinder-n Search Results – 1st Reaction Scheme

Experimental Protocols

Synthetic Methods | Experimental Procedure

Products	2-Hydroxy-2-methyl-1(2*H*)-naphthalenone, Yield: 100%
Reactants	2-Methyl-1-[(trimethylsilyl)oxy]naphthalene
Reagents	Benzoic acid Isophthalic acid 2-Iodoxybenzoic acid
Solvents	Dimethyl sulfoxide
Procedure	1. Treat the trimethylsilylated 2-methylnaphthol (0.2 mmol) in DMSO (1 mL) with SIBX (255 mg, 0.5 mmol, i.e., 2.5 equivalent of IBX) at room temperature for 2 hours. 2. After 2 hours, dilute the reaction mixture with EtOAc (20 mL). 3. Wash the reaction mixture with saturated aqueous $NaHCO_3$ (3 × 5 mL) and brine (5 mL). 4. Dry the reaction mixture over Na_2SO_4. 5. Filter the reaction mixture. 6. Evaporate the reaction mixture.
Scale	milligram

Characterization Data

2-Hydroxy-2-methyl-1(2*H*)-naphthalenone

State	red oil.

CAS Method Number 3-614-CAS-2488692

Reaction Notes
chemoselective, safety (stabilized IBX used 1st stage)

SciFinder-n – Experimental Protocols > Synthetic Methods & Reaction Notes

Alternative Steps (0)

Experimental Protocols

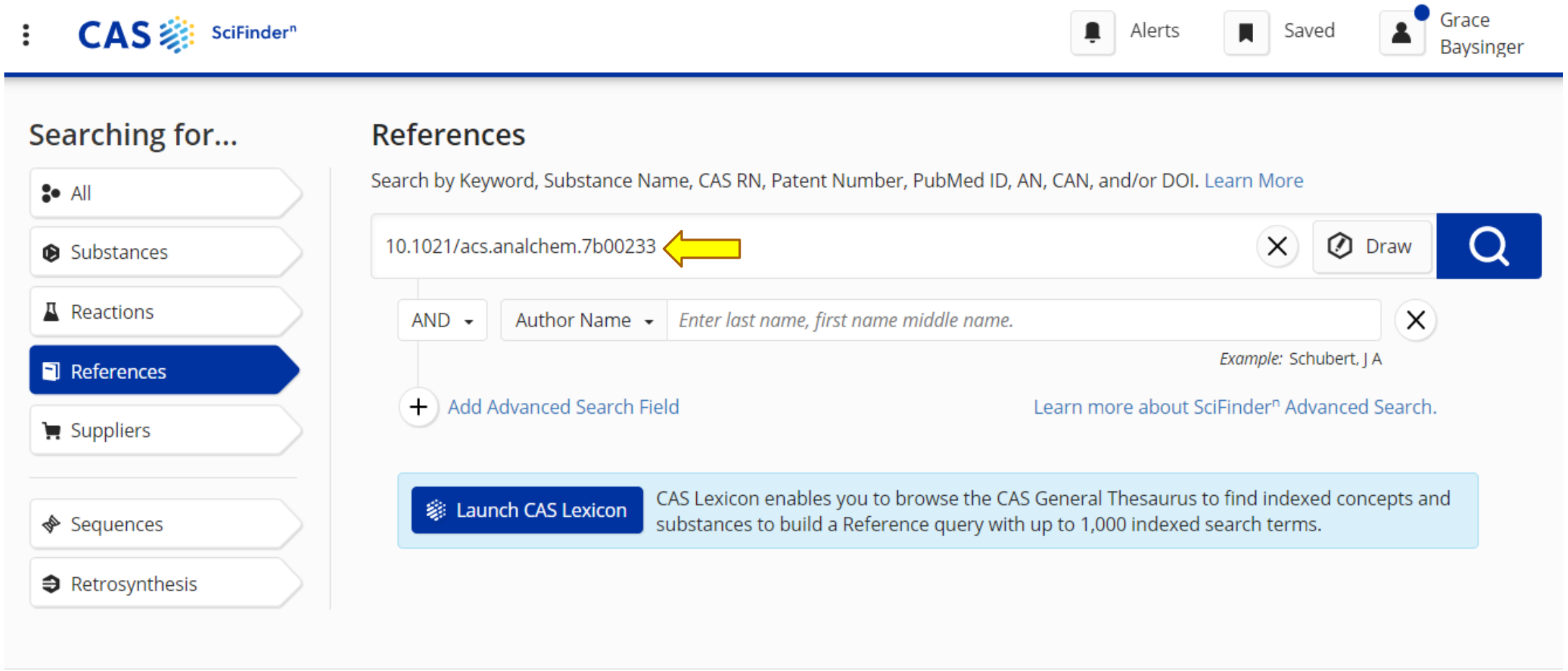
Synthetic Methods | **Experimental Procedure**

JOC The Journal of Organic Chemistry

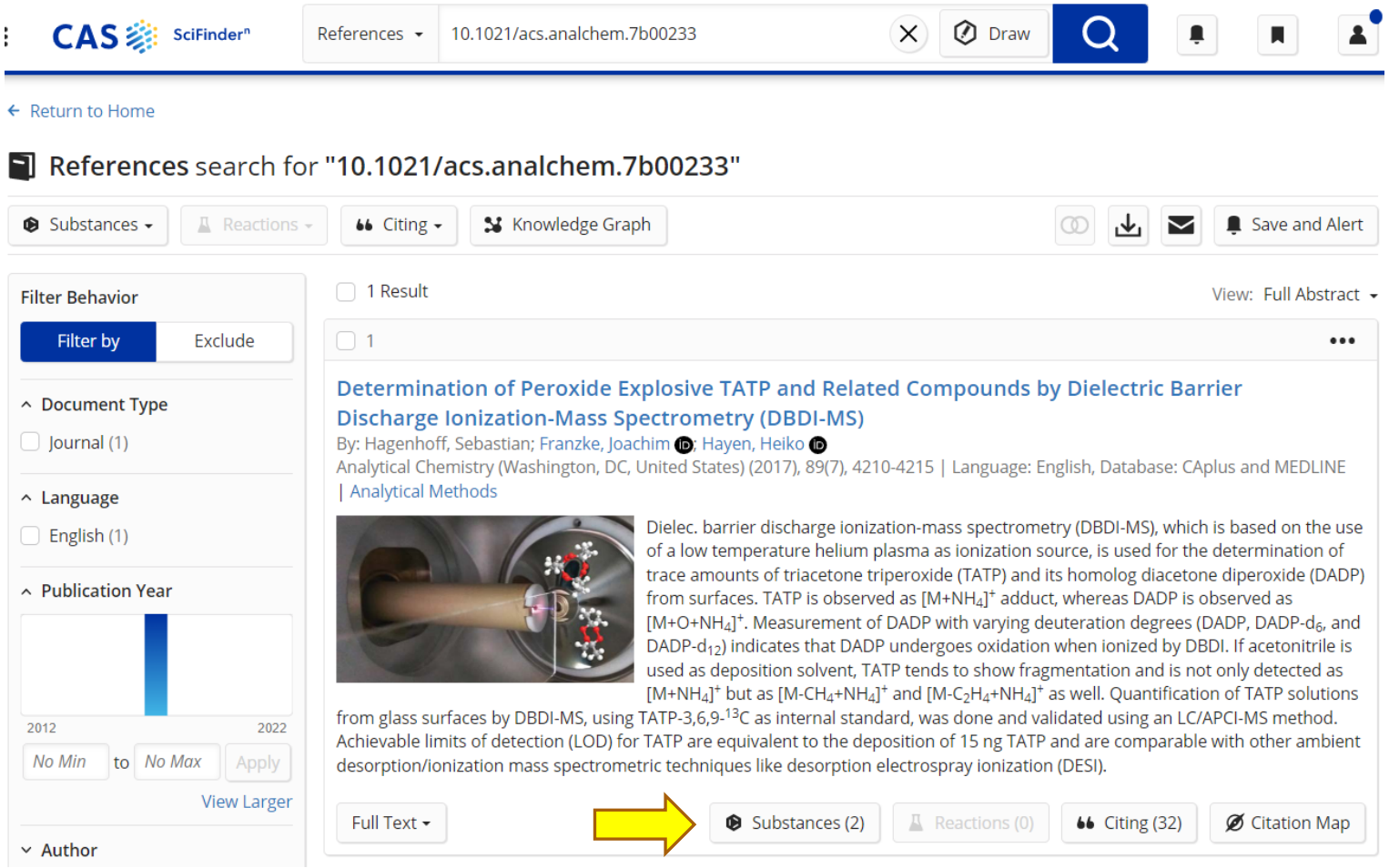
Method B. Treatment of the trimethylsilylated 2-methylnaphthol **11b** (50 mg, 0.2 mmol) in DMSO (1 mL) with SIBX (255 mg, 0.5 mmol, i.e., 2.5 equiv of IBX) was run at room temperature for 2 h, after which time the reaction mixture was diluted with EtOAc (20 mL), washed with saturated aqueous $NaHCO_3$ (3 × 5 mL), and brine (5 mL), dried over Na_2SO_4, filtered and evaporated to furnish orthoquinol **12** (35 mg, 100%) as a red oil.

Reaction Notes
chemoselective, safety (stabilized IBX used 1st stage)

SciFinder-n – Experimental Protocols > Experimental Procedure



SciFinder-n – References Search using DOI (Digital Object Identifier) of Paper



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CAS SciFinder^n References 10.1021/acs.analchem.7b00233 Draw

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Determination of Peroxide Explosive TATP and Related Compounds by Dielectric Barrier Discharge Ionization-Mass Spectrometry (DBDI-MS)

Substances (2) Reactions (0) Citing (32) Citation Map Save

JOURNAL

Source

Analytical Chemistry (Washington, DC, United States)
Volume: 89
Issue: 7
Pages: 4210-4215
Journal; Article
2017
DOI:
10.1021/acs.analchem.7b00233

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ISSN-L: 0003-2700

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AN: 2017:366343
CAN: 166:330172
PubMed ID: 28253619
CAplus and MEDLINE

Company/Organization

By: Hagenhoff, Sebastian; Franzke, Joachim; Hayen, Heiko

Dielec. barrier discharge ionization-mass spectrometry (DBDI-MS), which is based on the use of a low temperature helium plasma as ionization source, is used for the determination of trace amounts of triacetone triperoxide (TATP) and its homolog diacetone diperoxide (DADP) from surfaces. TATP is observed as $[M+NH_4]^+$ adduct, whereas DADP is observed as $[M+O+NH_4]^+$. Measurement of DADP with varying deuteration degrees (DADP, DADP-d_6, and DADP-d_{12}) indicates that DADP undergoes oxidation when ionized by DBDI. If acetonitrile is used as deposition solvent, TATP tends to show fragmentation and is not only detected as $[M+NH_4]^+$ but as $[M-CH_4+NH_4]^+$ and $[M-C_2H_4+NH_4]^+$ as well. Quantification of TATP solutions from glass surfaces by DBDI-MS, using TATP-3,6,9-^{13}C as internal standard, was done and validated using an LC/APCI-MS method. Achievable limits of detection (LOD) for TATP are equivalent to the deposition of 15 ng TATP and are comparable with other ambient desorption/ionization mass spectrometric techniques like desorption electrospray ionization (DESI).

SciFinder-n - Full Display Format

Keywords: peroxide explosive compound dielec barrier discharge ionization mass spectrometry

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Direct Determination of Peroxide Explosives on Polycarbazole/Gold Nanoparticle-Modified Glassy Carbon Sensor Electrodes...
Analytical Chemistry (Washington, DC, United States) (2022), 94(50), 17662-17669 | Language: English, Database: CAplus and MEDLINE

Electrochemical determination of triacetone triperoxide (TATP) using polycarbazole modified glassy carbon electrode
Abstracts of Papers, ACS Spring 2021 (2021), No pp. given | Language: English, Database: CAplus

Determining the vapor pressures of diacetone diperoxide (DADP) and hexamethylene triperoxide diamine (HMTD)
Propellants, Explosives, Pyrotechnics (2009), 34(6), 539-543 | Language: English, Database: CAplus

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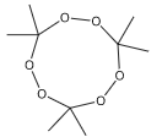
Concepts

Explosives

Substances

Substances (2)

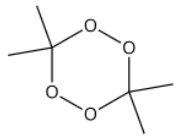
17088-37-8



$C_9H_{18}O_6$
Triacetonetriperoxide

Role: Analyte, Technical or Engineered Material Use, Analytical Study, Uses

1073-91-2



$C_6H_{12}O_4$
Diacetone diperoxide

Role: Analyte, Technical or Engineered Material Use, Analytical Study, Uses

Analytical Methods

Title	CAS Method Number
Analysis of Triacetonetriperoxide by Dielectric spectroscopy	1-121-CAS-276727

SciFinder-n - Full Display Format for Record continued

SciFinder-n: For a more comprehensive search, use multiple search strategies

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Find substances, view references, and then refine by topics to further focus results.

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DATA RELATED TO UNDERGRADUATE ORGANIC CHEMISTRY RESEARCH

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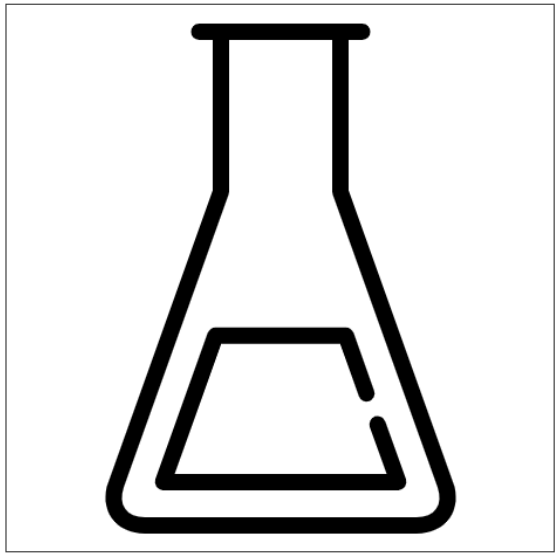
Not Voodoo X.4

Demystifying Synthetic Organic Chemistry since 2004

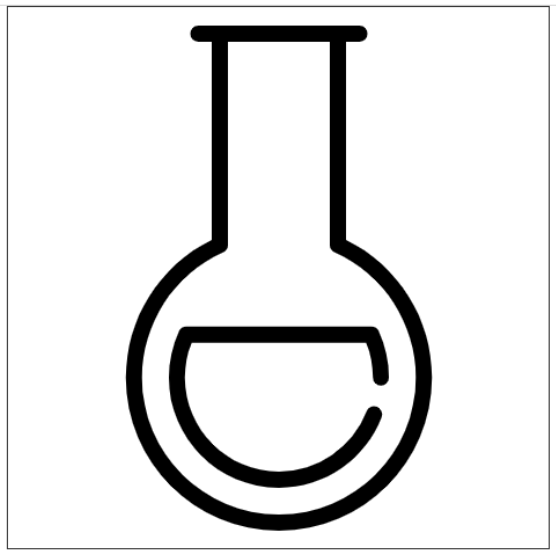
Search...

Magic Formulas	Tips and Tricks	Troubleshooting	How To	Rookie Mistakes
Chemists Weigh In	Chromatography	Reagents and Solvents	Workup	Purification

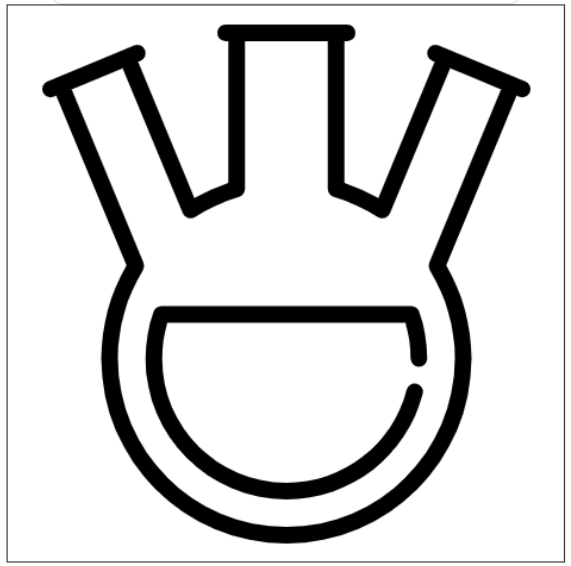
Laboratory Techniques and Methods to Improve Your Experimental Skills



For First-Time Independent Researchers



For Beginning Ph.D. Students



For Advanced Researchers

For First-Time Independent Researchers

- How to Wash Glassware
- How to Run a Reaction
- Flammable Reagents
- Explosive Reagents
- Toxic Reagents
- First Time Through a Procedure
- Leaving the Lab
- How to Stain your TLC plate
- How to Get a High Quality NMR Spectrum
- Stirring
- Weighing
- Drying Methods
- Proverbs

For Beginning Ph.D. Students

- Reagents
- Common Formulas
- Rules of Thumb
- How To...
- How to Run a Reaction
- Troubleshooting an Experiment
- Rookie Mistakes
- Proverbs
- A Day in the Life of Successful Researcher
- 1,2,3... Ph.D.

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- Magic Formulas
- Cooling Bath Mixtures
- Protecting Groups
- Oxidants
- Reagents
- Buy It or Make It?
- Purification
- Workup Tricks: Reagents
- Emulsions

About

Rookie Mistakes:

This collection of pages began with a list of eleven mistakes in September 2004. The idea was that beginning experimentalists might learn from experienced chemists, chemists who have run hundreds of reactions, and made lots of mistakes.

What follows is the collected wisdom of years of shaky chemistry, documented for posterity in the hopes that you, will learn from our mistakes. But we wouldn't bet on it!

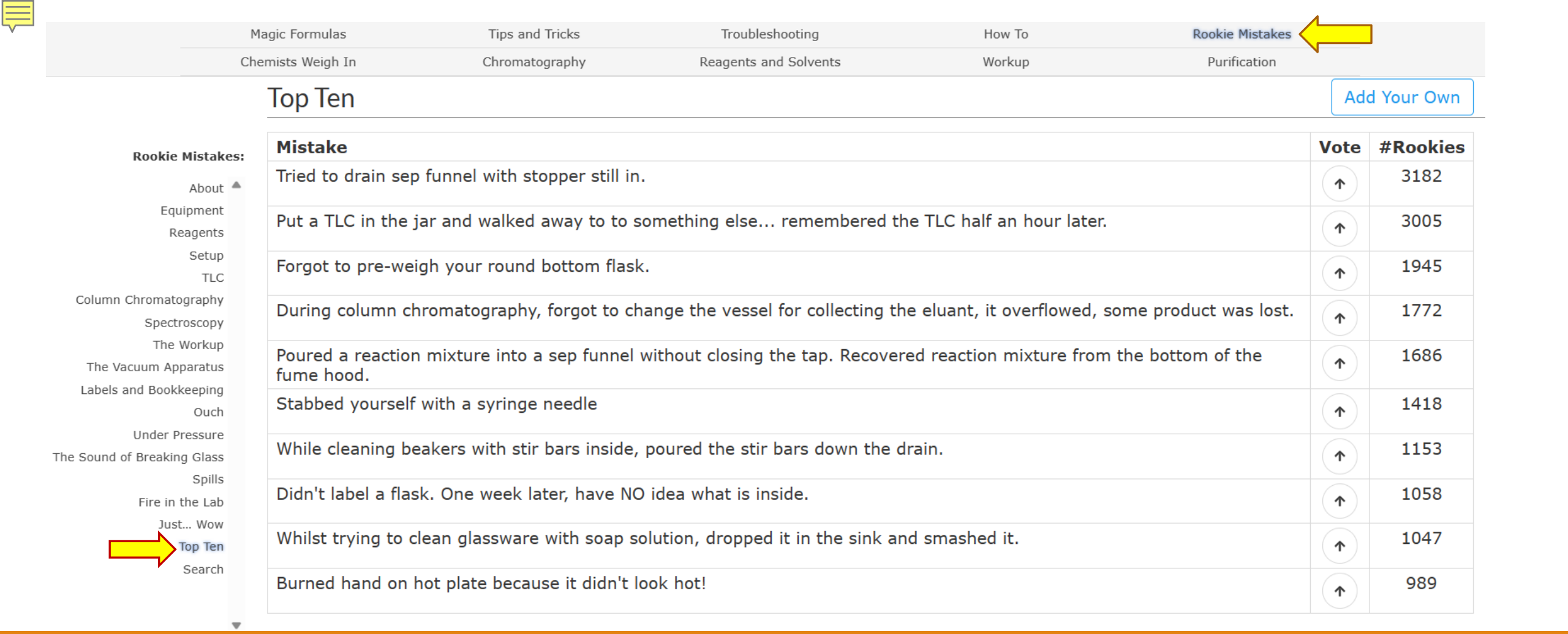
The Rookie Mistakes did not exactly work out that way. What began as an innocent compilation of beginner bungles evolved into an entertaining catalog of honest errors, freak accidents, relatively innocuous events that cascaded in horrific directions, and incidents worthy of a Darwin award. After a few years of this, reading the list involved scrolling through a vast catalog of catastrophe encompassing all the classes of chemical experimentation.

Over time, I learned that "Rookie Mistakes" was appreciated for reasons far beyond its intended role as a guide to help people avoid common pitfalls in the lab. Incredibly, students told me that the list was an unexpected source of solace after a frustrating day in the lab. That's partly because it's funny, but also because you don't feel quite so incompetent after reading about how other people accidently destroyed their experiments.

With these observations in mind, Rookie Mistakes X has some new features:

1. The mistakes are divided into different categories (listed on the lefthand menu), focusing on important aspects of experimentation, or common themes. For rare and mystifying mistakes, take a look at " Just...Wow."
2. You can search the mistakes by keyword , or view the Top Ten most common mistakes.
3. You can use the tab "add your experience" to help us count common mistakes or to add new mistakes (...your bumbling technological distinctiveness will be added to our own...)

Not Voodoo X.4 > Rookie Mistakes



Not Voodoo X.4 > Rookie Mistakes > Top Ten

About Reagents and Solvents

Reagents & Solvents:

Reagents

When you're just starting out in the organic chemistry lab, every experiment involves a new and unfamiliar reagent. You'll have a lot of questions. Should you buy it or should you make it in the lab? If you found a bottle in the lab, should you add it directly to your reaction, or should you purify it first? If you bought a new bottle, how should you store it? Is the reagent especially toxic, or likely to catch fire or explode? Once you've got a handle on these important questions, you'll want to weigh the reagent, and add it to your reaction. Easier said than done, in some instances.

You will also find that you're running reactions in many different solvents, and that each one has unique properties. Each solvent behaves differently when it comes time to isolate your product, and using the wrong technique can lead to serious headaches during workup and purification. Check the list of workup tricks to find methods for:

- Performing aqueous workup when your solvent is polar or miscible with water
- Removing tin, copper and boron byproducts, amines and many other common reagents and solvents
- Removing byproducts generated during aluminum hydride reductions, Wittig reactions, DCC couplings, and *m*-CPBA oxidations.

Ever wonder: which oxidant should I use? Do you want to make LDA or the Jones reagent, or need to titrate n-BuLi? Are you curious about molecular sieves, or exotic solvents?

Aaaand, visit Rookie Mistakes: Reagents for a different perspective on the subject.

Solvents

Chemists use solvents for reactions, column chromatography, and crystallization. For successful experimentation, the properties of various solvents are important to understand. Furthermore, since much of the chemical waste we generate is derived from solvent, the environmental impact of common solvents is a growing concern.

You can find information on relative solvent polarity, solvent properties relevant to chromatography, and a "solvent selection guide" from GSK comparing the toxicity of different solvents.

An article expanding on the GSK solvent selection guide can be found here
For a chart of suggested replacements for undesirable solvents (as used at Pfizer), see this article.

Not Voodoo X.4 > Reagents and Solvents

Should I Buy It or Make It Myself?

Add Your Own

Should you buy or make this reagent?	Total Votes		Vote
(+) or (-) (Ipc)2BOMe for Brown allylations/crotylations	143	65% say make it	Make It! Buy It!
(Pyridine)(Tetrahydroborato)Zinc ([Zn(BH4)2(Py)])	26	65% say make it	Make It! Buy It!
(Trimethylsilyl)diazomethane ((CH3)SiCHN2)	144	90% say buy it	Make It! Buy It!
1 1'-thiocarbonyldiimidazole	39	90% say buy it	Make It! Buy It!
1,1,1,3,3,3-hexachloropropan-2-ol	17	76% say buy it	Make It! Buy It!
1,8-diaminonaphthalene	34	91% say buy it	Make It! Buy It!
1-acetoxybutadiene	21	57% say buy it	Make It! Buy It!
2,4,4,6-Tetrabromo-2,5-cyclohexadienone	8	75% say buy it	Make It! Buy It!
2-iodoxybenzoic acid (IBX)	364	93% say make it	Make It! Buy It!
AD mix alpha and beta	293	88% say buy it	Make It! Buy It!
AIBN (Azobisisobutyronitrile)	103	95% say buy it	Make It! Buy It!
Alkyne Hydration Catalyst	59	93% say buy it	Make It! Buy It!

Not Voodoo X.4 > Reagents and Solvents > Should I Buy It or Make It Myself?

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Full-text resource for methods in synthetic organic chemistry. Organized by Functional Groups plus a reference library of best methods in specialized fields.

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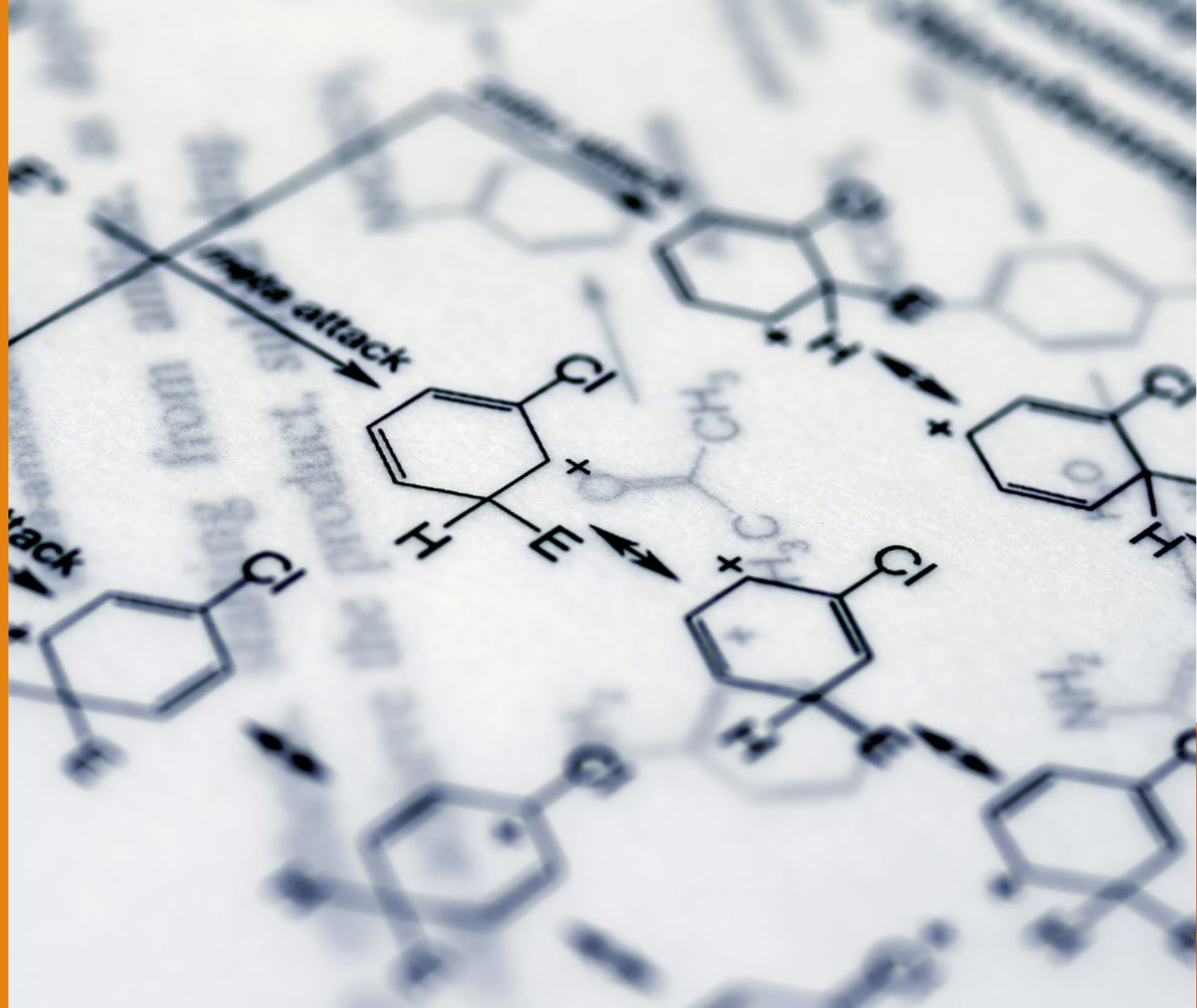

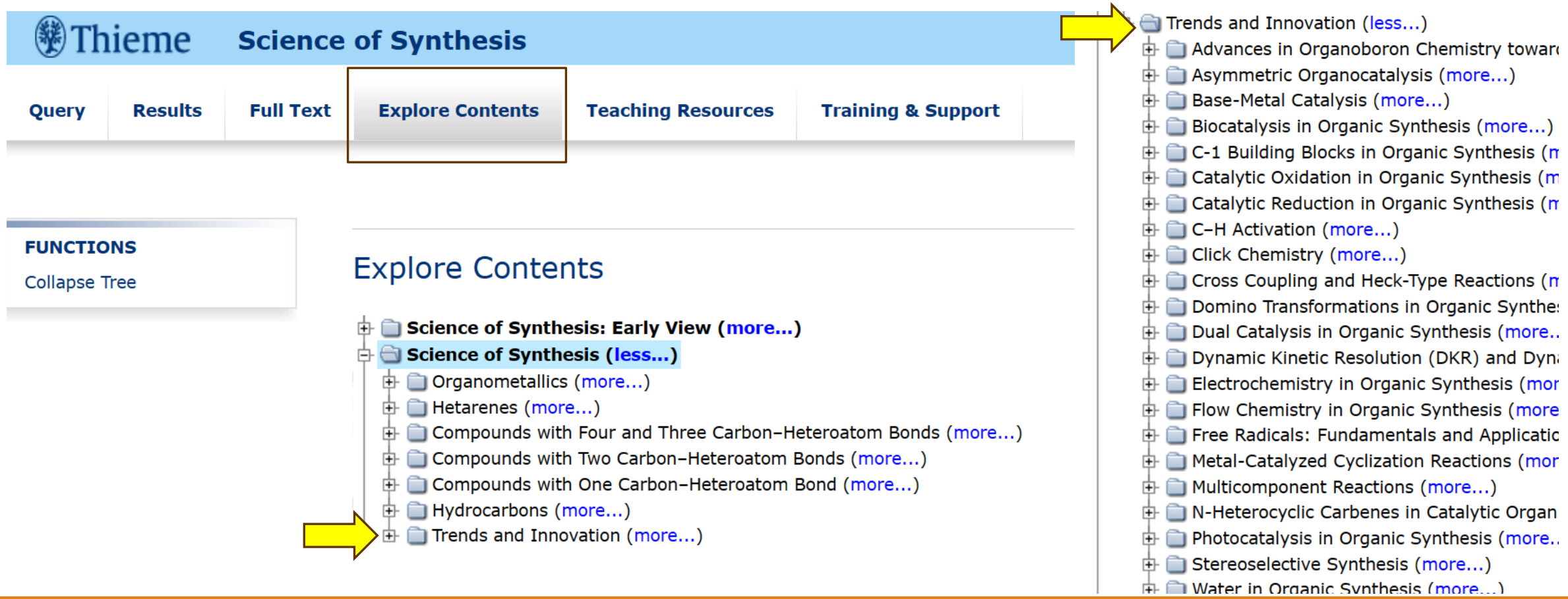

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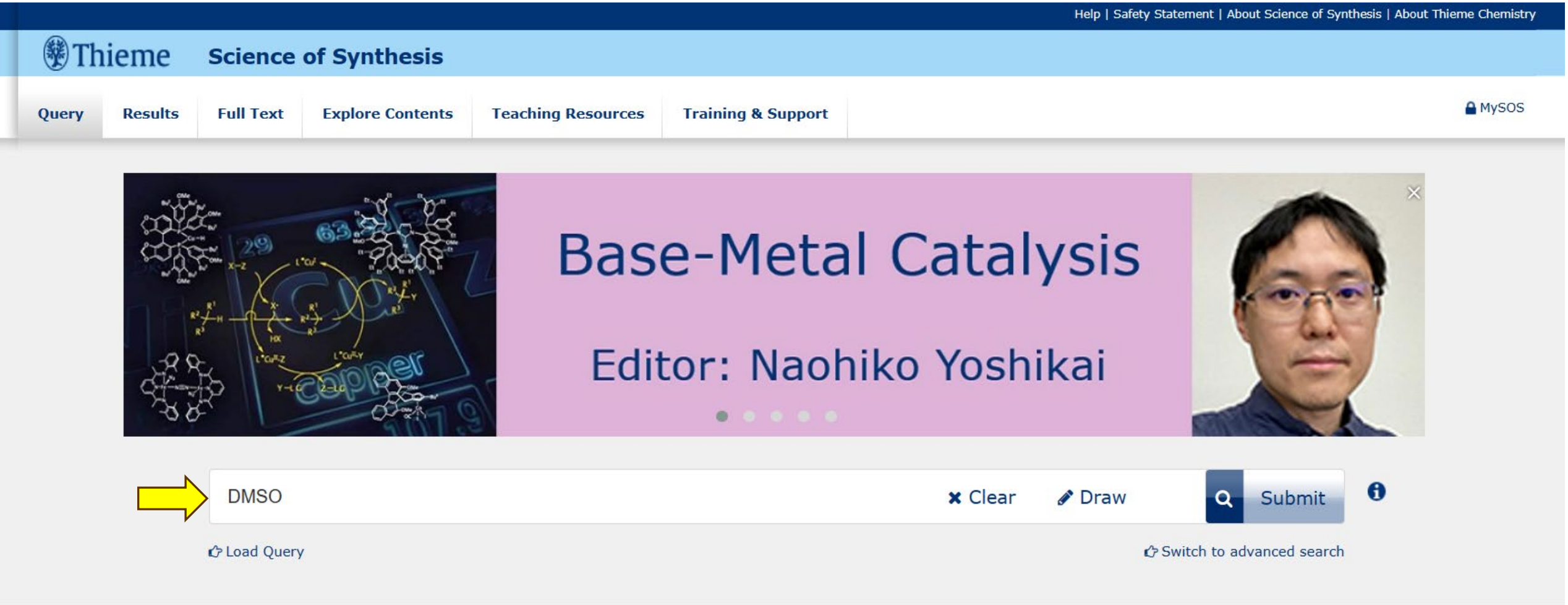

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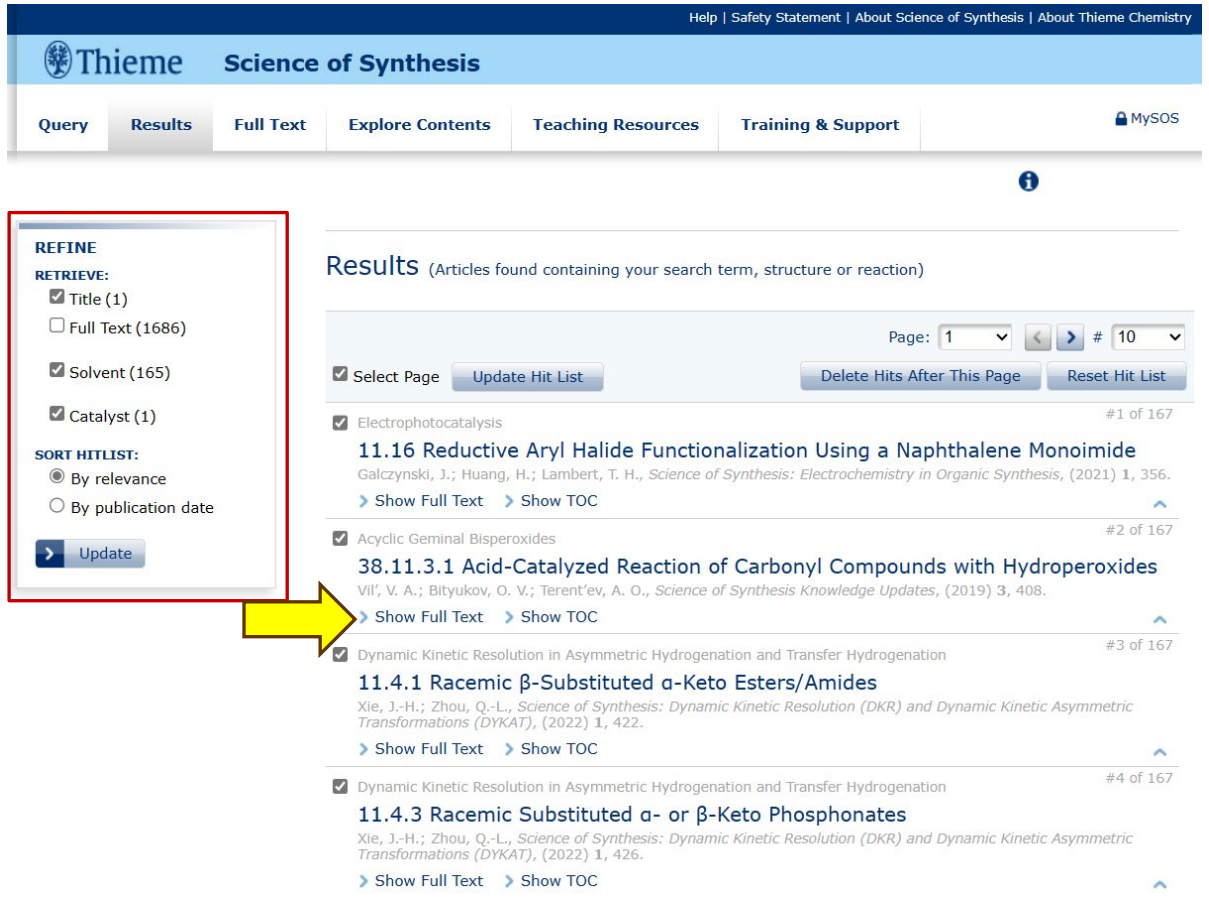

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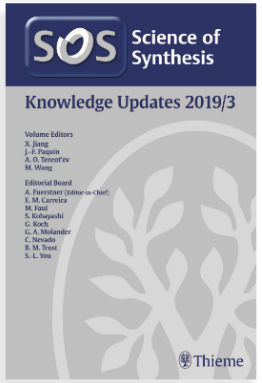


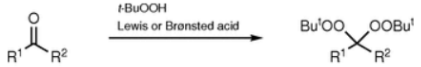
38.11.3.1 Acid-Catalyzed Reaction of Carbonyl Compounds with Hydroperoxides

DOI: 10.1055/sos-SD-138-00067

Vil', V. A.; Bityukov, O. V.; Terent'ev, A. O., *Science of Synthesis Knowledge Updates*, (2019) **3**, 408.

The reaction of carbonyl compounds **62** with *tert*-butyl hydroperoxide provides geminal di-*tert*-butyl peroxides **63** (**Scheme 28**). Synthesis proceeds in the presence of sulfuric, [128–131] hydrochloric, [132–136] perchloric, [133,137–142] 4-toluenesulfonic, [143] and other acids, usually with the use of dehydrators ($CaCl_2$, Na_2SO_4, B_2O_3, etc.) at 0–60°C. Molecular iodine can also be used as catalyst. [92]

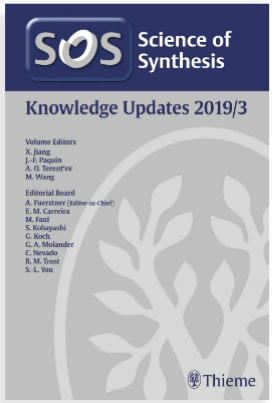
Scheme 28 Acid-Catalyzed Synthesis of Geminal Bisperoxides from Carbonyl Compounds and *tert*-Butyl Hydroperoxide [92,128–143]



62 **63**

R^1	R^2	*t*-BuOOH (Equiv)	Conditions	Yield (%)	Ref
H	Et	2	35% HCl, 0–30°C	76	[132]
H	Pr	2	70% $HClO_4$, 5–7°C, then rt, then 60°C	85	[133]
H	iPr	2	70% $HClO_4$, 5–7°C, then rt, then 60°C	80	[133]
H	2-FC_6H_4	2	35% $HClO_4$, $CaCl_2$, benzene, 0–40°C	85	[137]

NAVIGATION
Hit 2 of 167
Previous / Next



$(CH_2)_5$	*t*-Bu	1.1	40% aq HBF_4, pentane, rt, 2 h	33	[147]

2,2-Bis(*tert*-butylperoxy)-1-phenylpropane (63, R^1 = Bn; R^2 = Me); Typical Procedure by Catalysis with Concentrated Hydrochloric Acid: [136]

In a 50-mL, round-bottomed flask, 1-phenylpropan-2-one (**62**, R^1 = Bn; R^2 = Me; 1 g, 7.46 mmol) was dissolved in hexanes (6 mL) and the soln was cooled to 0°C (ice bath). Ground $CaCl_2$ (500 mg) was added, followed by 70% aq *t*-BuOOH (4 mL, 29.2 mmol) and concd HCl (0.5 mL), making sure the temperature did not exceed 5°C. The resulting mixture was vigorously stirred at 0°C for 4 h. Hexane (30 mL) was added and the phases were separated. The organic phase was then successively washed with 2 M aq NaOH (15 mL) and distilled H_2O (2 × 15 mL), dried (Na_2SO_4), filtered, and concentrated. The resulting clear liquid was purified by flash chromatography (silica gel prewashed with hexane containing 1% Et_3N, hexane) to afford the product as a white solid; yield: 1.85 g (83%).

4-*tert*-Butyl-1,1-bis(*tert*-butylperoxy)cyclohexane [63, R^1,R^2 = $(CH_2)_2CH(t\text{-Bu})(CH_2)_2$]; Typical Procedure by Molecular Iodine Catalysis: [92]

To a soln of I_2 (25.4 mg, 0.1 mmol, 10 mol%) and 60% *t*-BuOOH in decane (0.72 mL, 2 mmol) in MeCN (1 mL) was added 4-*tert*-butylcyclohexanone [**62**, R^1,R^2 = $(CH_2)_2CH(t\text{-Bu})(CH_2)_2$; 154 mg, 1 mmol], and the soln was stirred at 22°C for 24 h. The mixture was concentrated under reduced pressure (ca. 20 Torr), and the product was isolated by column chromatography (silica gel, petroleum ether/Et_2O 95:5); yield: 259 mg (82%).

Geminal Bisperoxides 69; General Procedure by Tetrafluoroboric Acid Catalysis: [146]

⚠ **CAUTION:** *Tetrafluoroboric acid is extremely destructive to the skin, eyes, and respiratory tract.*

50% aq HBF_4 (2–4 mmol) was added to a mixture of the acetal **67** (5 mmol), 70% aq *t*-BuOOH (**68**, R^3 = *t*-Bu; 15–25 mmol), $CaCl_2$ (0.56 g, 5 mmol), and petroleum ether (35 mL). The mixture was stirred at rt until the acetal had been completely converted (20–180 min, TLC monitoring). Petroleum ether (bp 40–70°C; 20 mL) was added, and the organic phase was washed with 5% aq NaOH (30 mL) and H_2O (2 × 20 mL), dried (Na_2SO_4), filtered, and concentrated.

References

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[130] Yasushi, S.; Yasumasa, W.; Hiromi, K.; Tomoyuki, N.; Shuji, S.; Yasuhiko, S., *Bull. Chem. Soc. Jpn.*, (1992) **65**,

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      - Acyclic Geminal Bisperoxides (abstract | pdf)
        - A History of Geminal Bisperoxide Synthesis
        - Geminal Bishydroperoxides (more...)
        - Geminal Bisperoxides (less...)
          - Acid-Catalyzed Reaction of Carbonyl Compounds with Hydroperoxides
          - Trityl Perchlorate Catalyzed Condensation of Aldehydes with *tert*-Butyl Trimethylsilyl Peroxide
          - Synthesis of Geminal Bisperoxides via Alkylation or Acylation of Geminal Bishydroperoxides
          - Silylation of Bishydroperoxides
          - Miscellaneous Methods

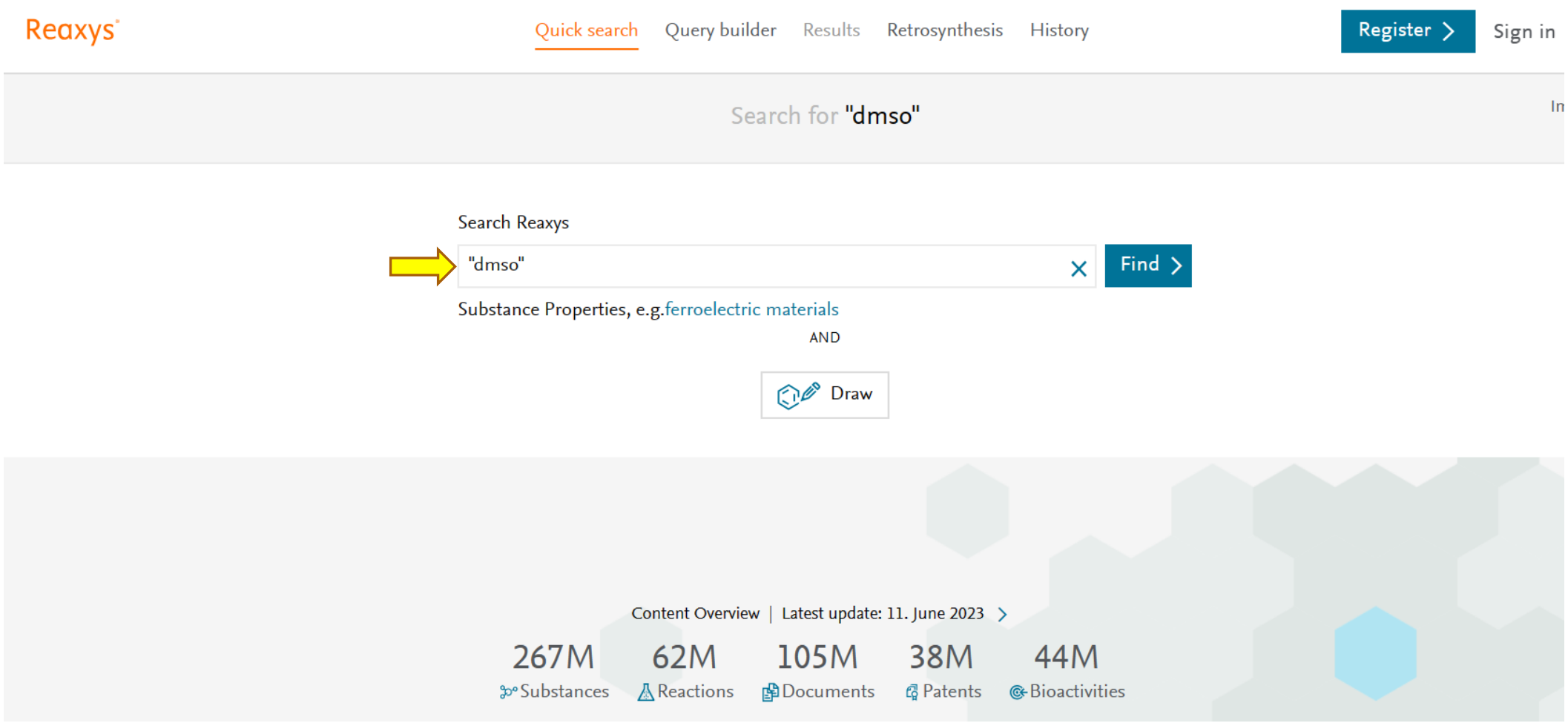
Reaxys

MAJOR RESOURCE THAT CONTAINS SUBSTANCES, REACTIONS (ORGANIC AND INORGANIC), AND PROPERTIES. HAS THE LARGEST COLLECTION OF PROPERTIES DATA.

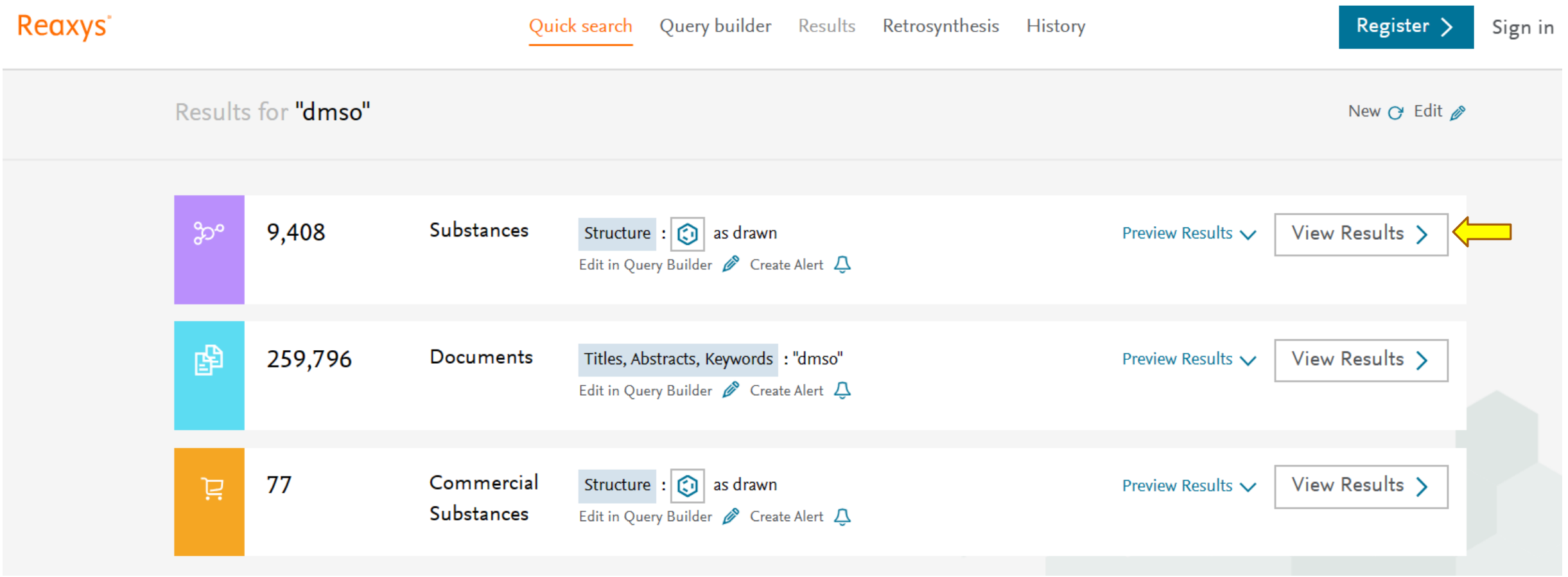
SEARCH OPTIONS INCLUDE SEARCHING BY NAME OR CAS REGISTRY NUMBER, STRUCTURES, REACTIONS, NUMERIC RANGES FOR PROPERTIES, PLUS MORE

ABOUT

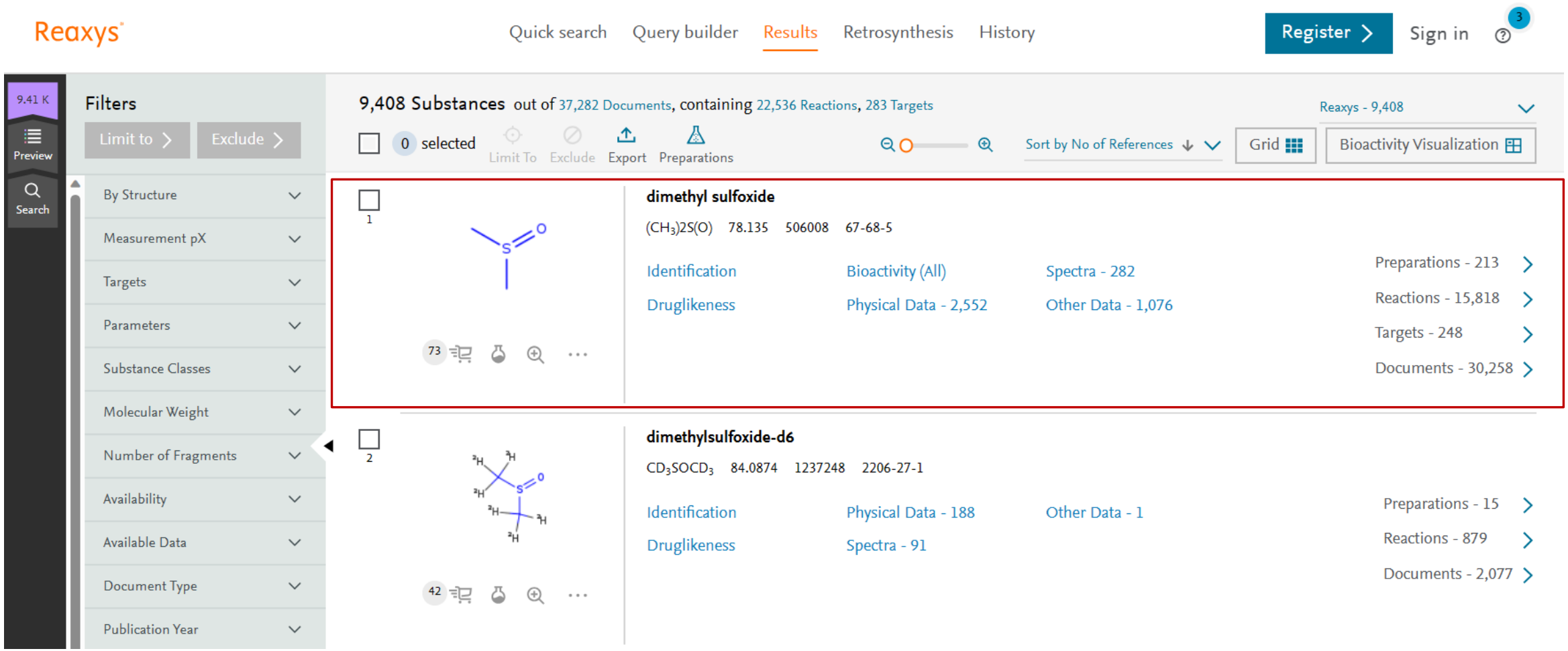
HTTPS://WWW.ELSEVIER.COM/EN-GB/SOLUTIONS/REAXYS



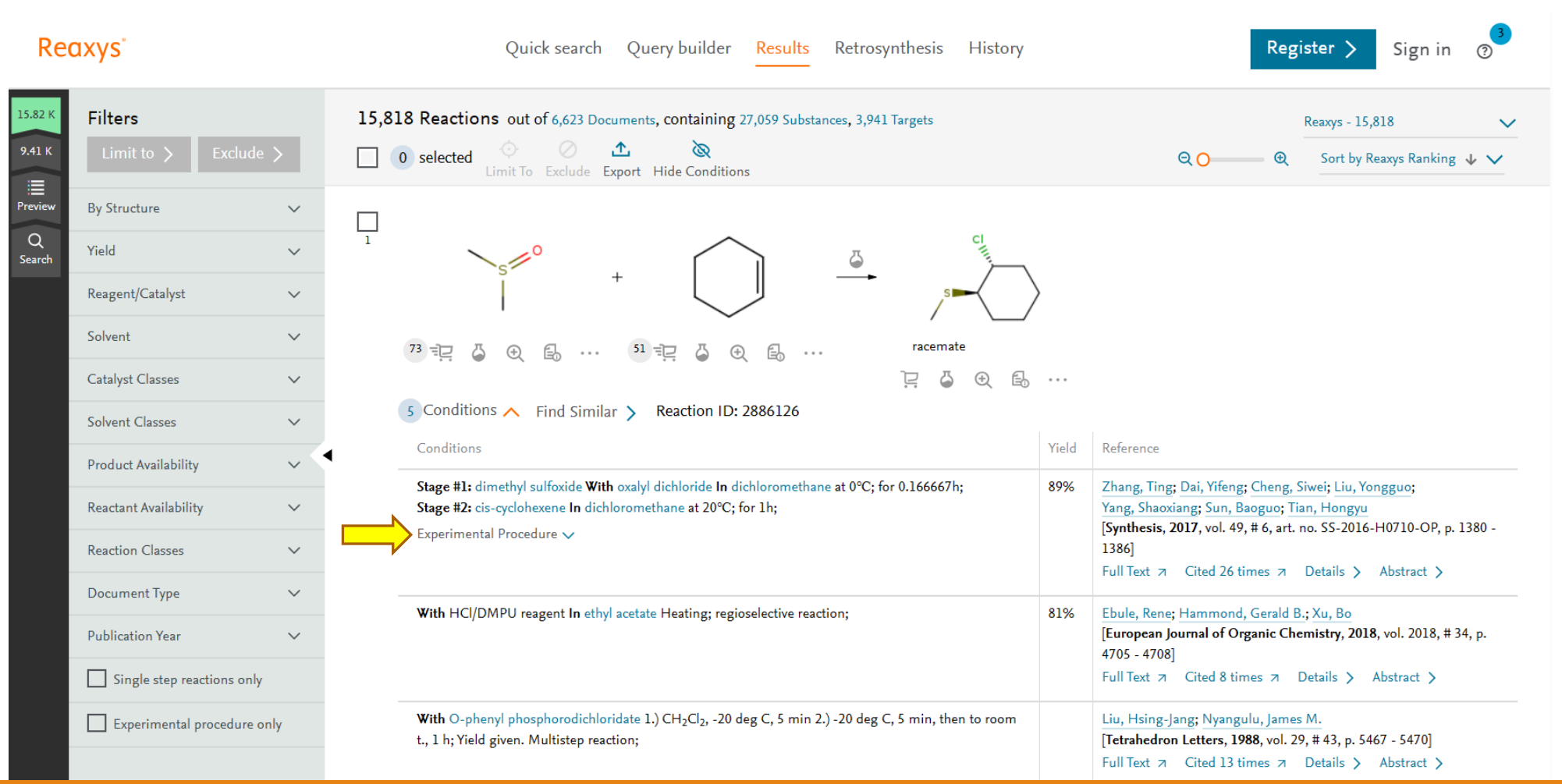
Reaxys Search for DMSO



Reaxys search results – View Substances



Reaxys – Search Results



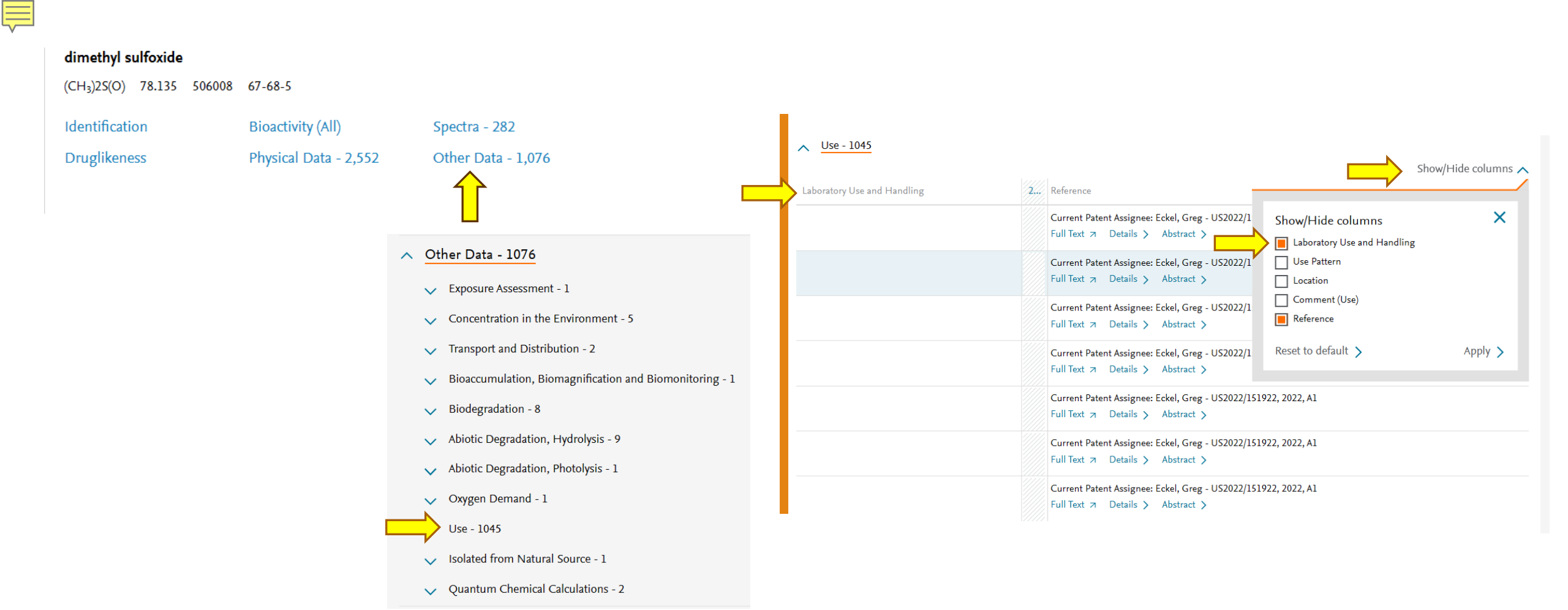
Reaxys Search Results for DMSO – View Reactions

Energy Data (MCS) - 155

Show/Hide columns

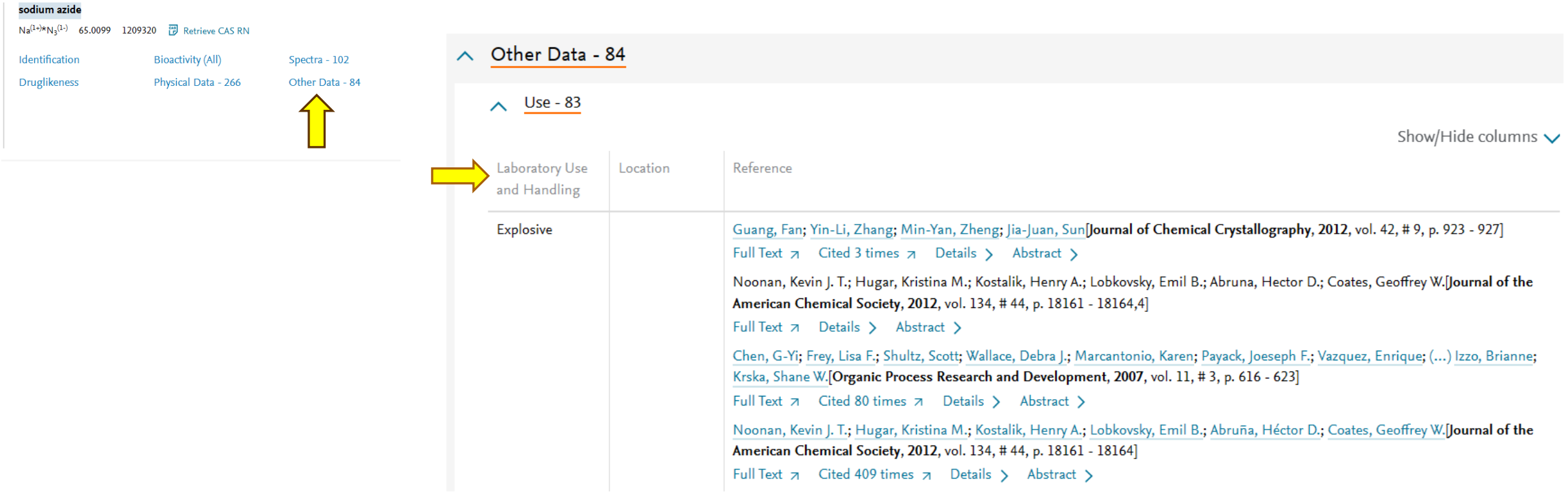
Description (Energy Data (MCS))	Temperature (Energy Data (MCS)), °C	Partner (Energy Data (MCS))	Reference
Heat capacity Cp	19.99 - 39.99	Oxane	Comelli, Fabio; Francesconi, Romolo; Bigi, Adriana; Rubini, Katia[**Journal of Chemical and Engineering Data, 2007**, vol. 52, # 2, p. 639 - 644] Full Text Cited 33 times Details Abstract
Heat capacity Cp	19.99 - 39.99	2-methyltetrahydrofuran	Comelli, Fabio; Francesconi, Romolo; Bigi, Adriana; Rubini, Katia[**Journal of Chemical and Engineering Data, 2007**, vol. 52, # 2, p. 639 - 644] Full Text Cited 33 times Details Abstract
Excess thermochemical parameter	35	carbonic acid dimethyl ester	Comelli, Fabio; Francesconi, Romolo; Bigi, Adriana; Rubini, Katia[**Journal of Chemical and Engineering Data, 2006**, vol. 51, # 2, p. 665 - 670] Full Text Cited 41 times Details Abstract
Excess thermochemical parameter	35	Diethyl carbonate	Comelli, Fabio; Francesconi, Romolo; Bigi, Adriana; Rubini, Katia[**Journal of Chemical and Engineering Data, 2006**, vol. 51, # 2, p. 665 - 670] Full Text Cited 41 times Details Abstract
Excess thermochemical parameter	35	1,2-propylene cyclic carbonate	Comelli, Fabio; Francesconi, Romolo; Bigi, Adriana; Rubini, Katia[**Journal of Chemical and Engineering Data, 2006**, vol. 51, # 2, p. 665 - 670] Full Text Cited 41 times Details Abstract
Excess heat capacity Cp	35	carbonic acid dimethyl ester	Comelli, Fabio; Francesconi, Romolo; Bigi, Adriana; Rubini, Katia[**Journal of Chemical and Engineering Data, 2006**, vol. 51, # 2, p. 665 - 670] Full Text Cited 41 times Details Abstract

Reaxys – Search Results for DMSO – View Physical Data – Energy data



Reaxys Search Results for DMSO – Other Data – Use – Laboratory Use and Handling

Reaxys Search Results for Sodium Azide – Other Data – Use – Laboratory Use and Handling

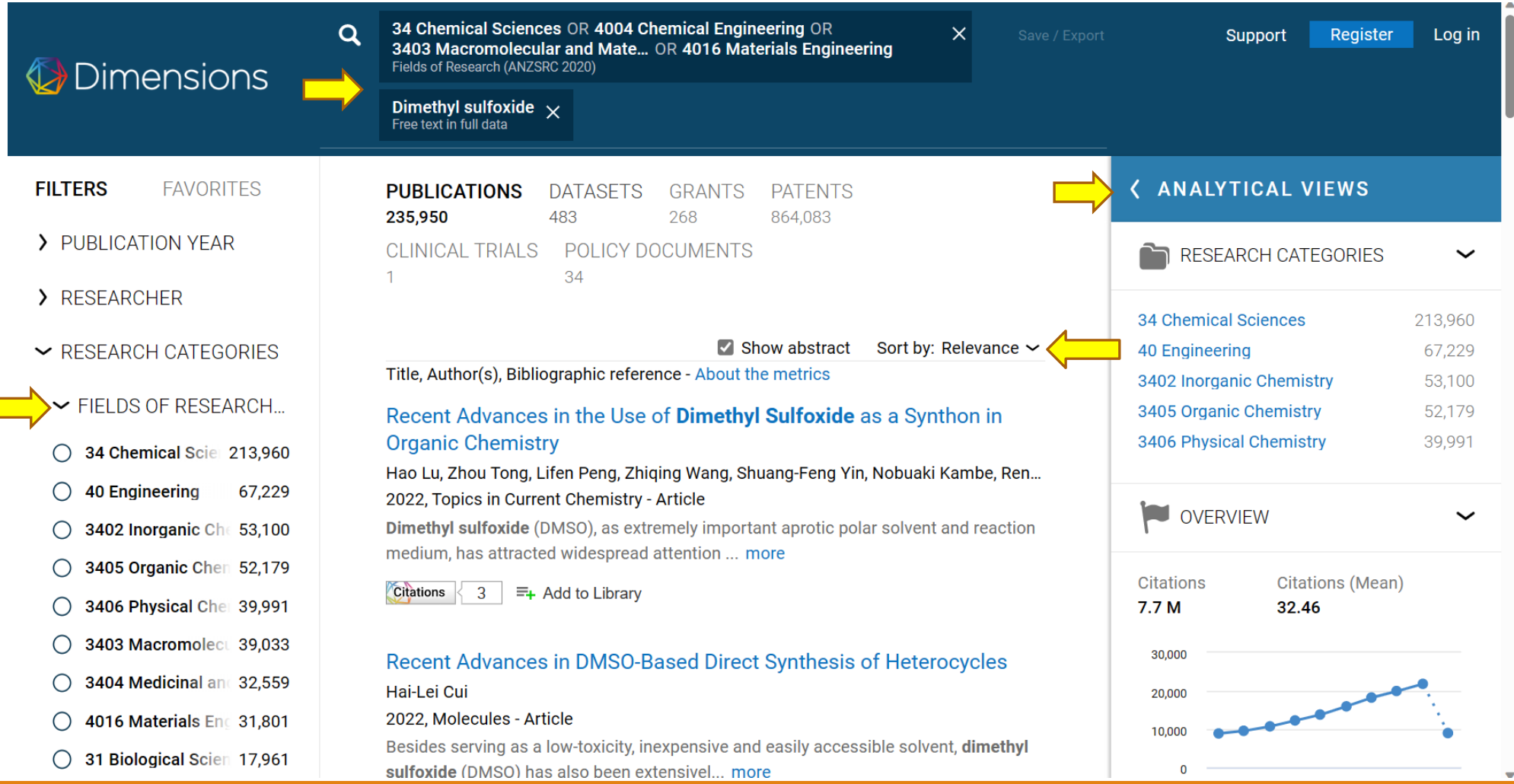


Dimensions

LARGE MULTIDISCIPLINARY DATABASE

SEARCH THE FULL TEXT OF ARTICLES, PREPRINTS, BOOKS, CONFERENCE PROCEEDINGS, AND MORE

HTTPS://APP.DIMENSIONS.AI/DISCOVER/PUBLICATION



Dimensions Search Results (Full Text Search)

Canadian Centre for Occupational Health and Safety - Academic Support Program (CCOHS-ASP)

COLLECTION OF ENVIRONMENTAL AND OCCUPATIONAL HEALTH AND SAFETY DATABASES, SELECTED AND PRICED SPECIFICALLY FOR THE ACADEMIC COMMUNITY

INCLUDES ACCESS TO SDS, CHEMINFO, RTECS, OSH REFERENCES, TOXICOLOGY, PLUS MORE. CHEMPENDIUM, A SUPPLEMENTAL PRODUCT, OFFERS CROSS-DATABASE SEARCH CAPABILITIES.

HTTPS://WWW.CCOHS.CA/PRODUCTS/

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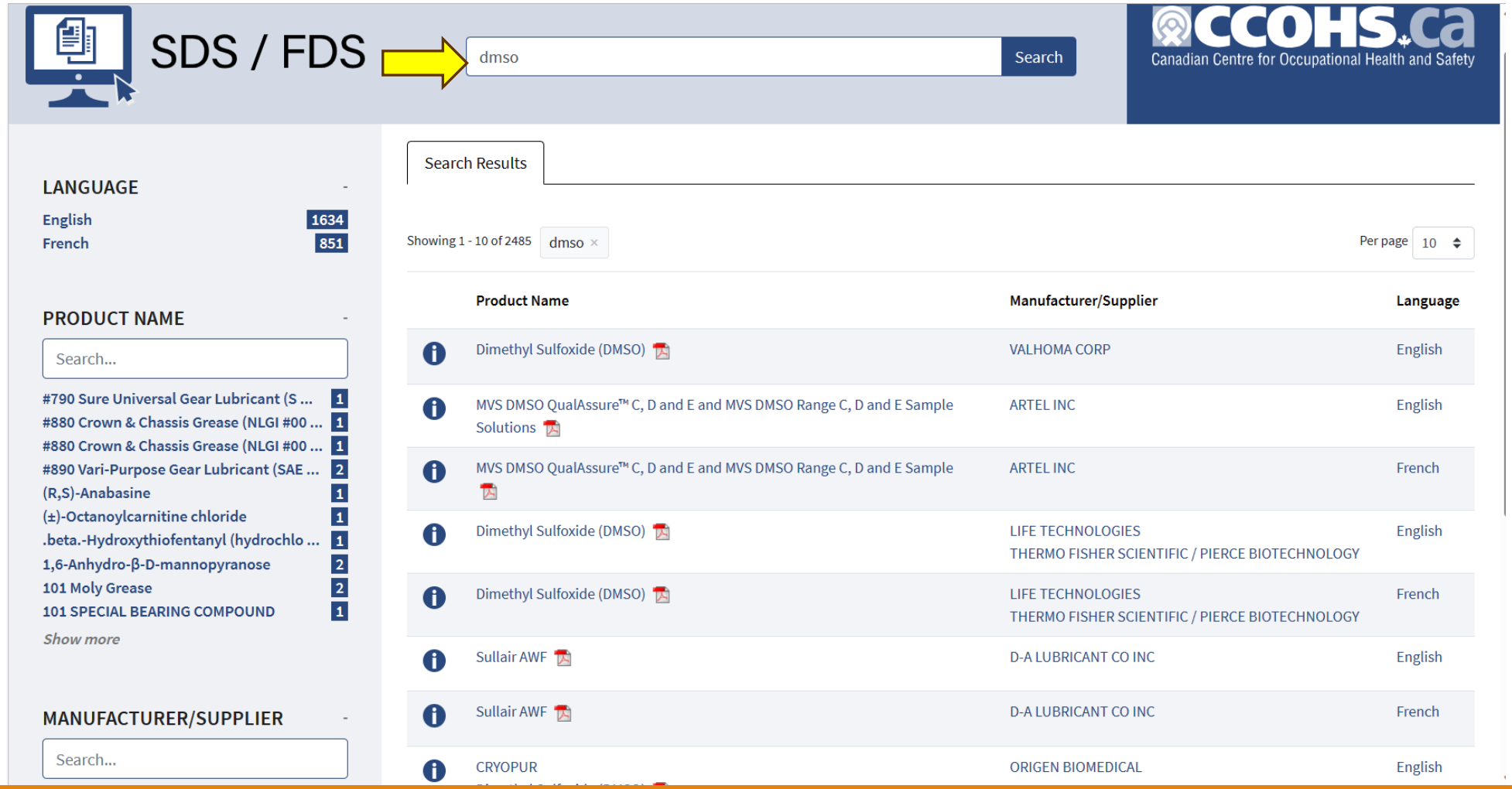
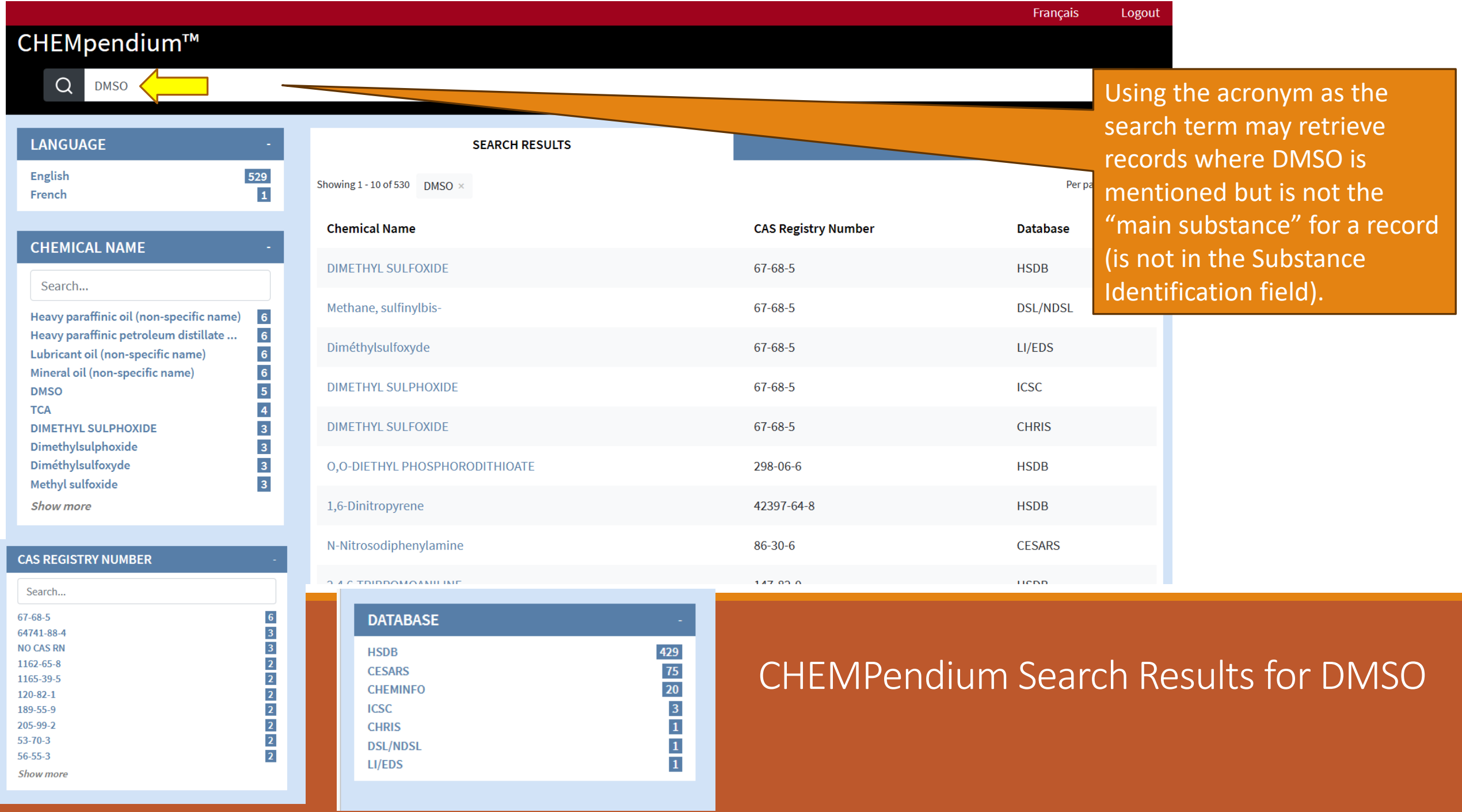
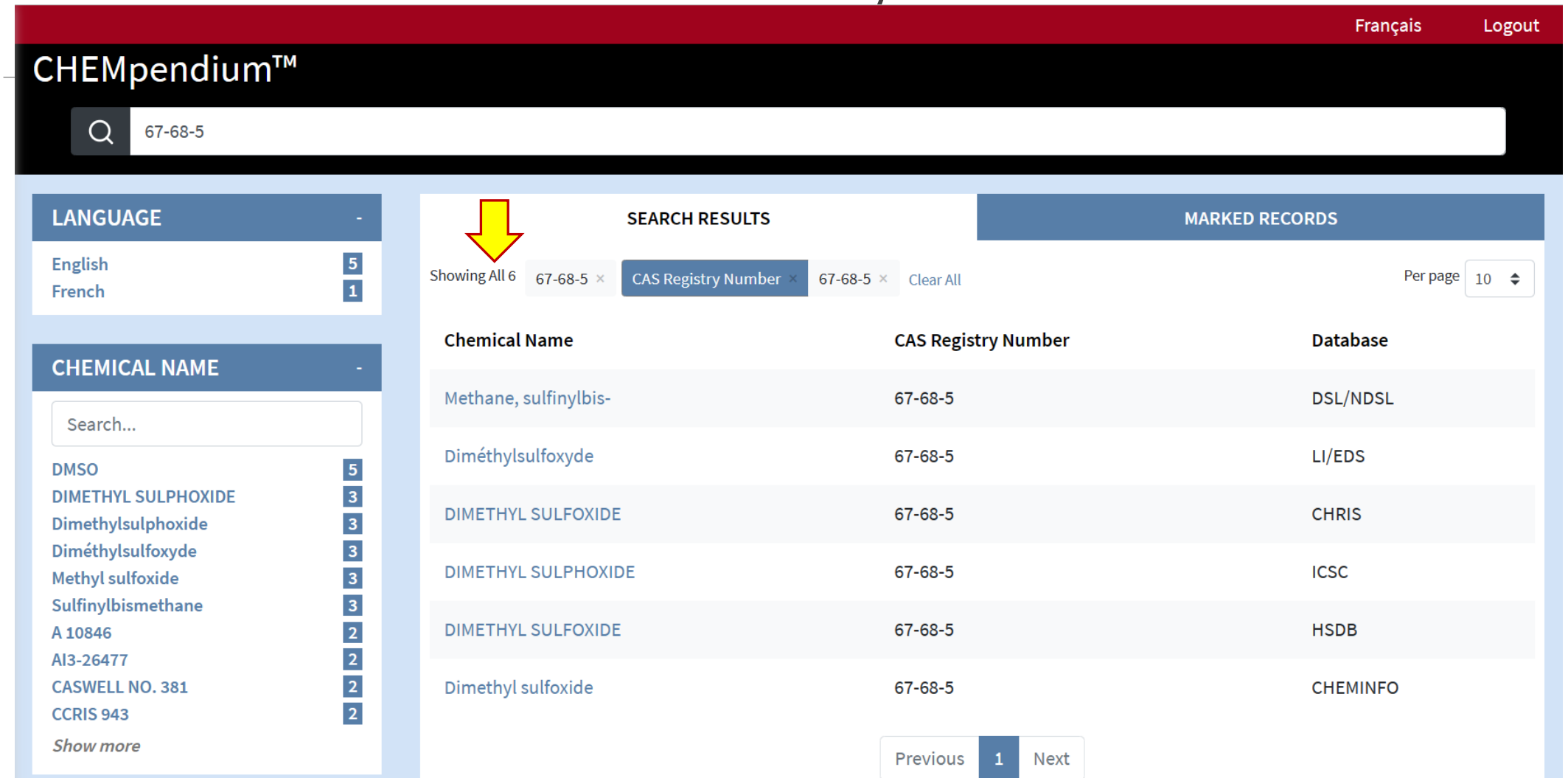


Safety Data Sheets (SDS) Search for DMSO

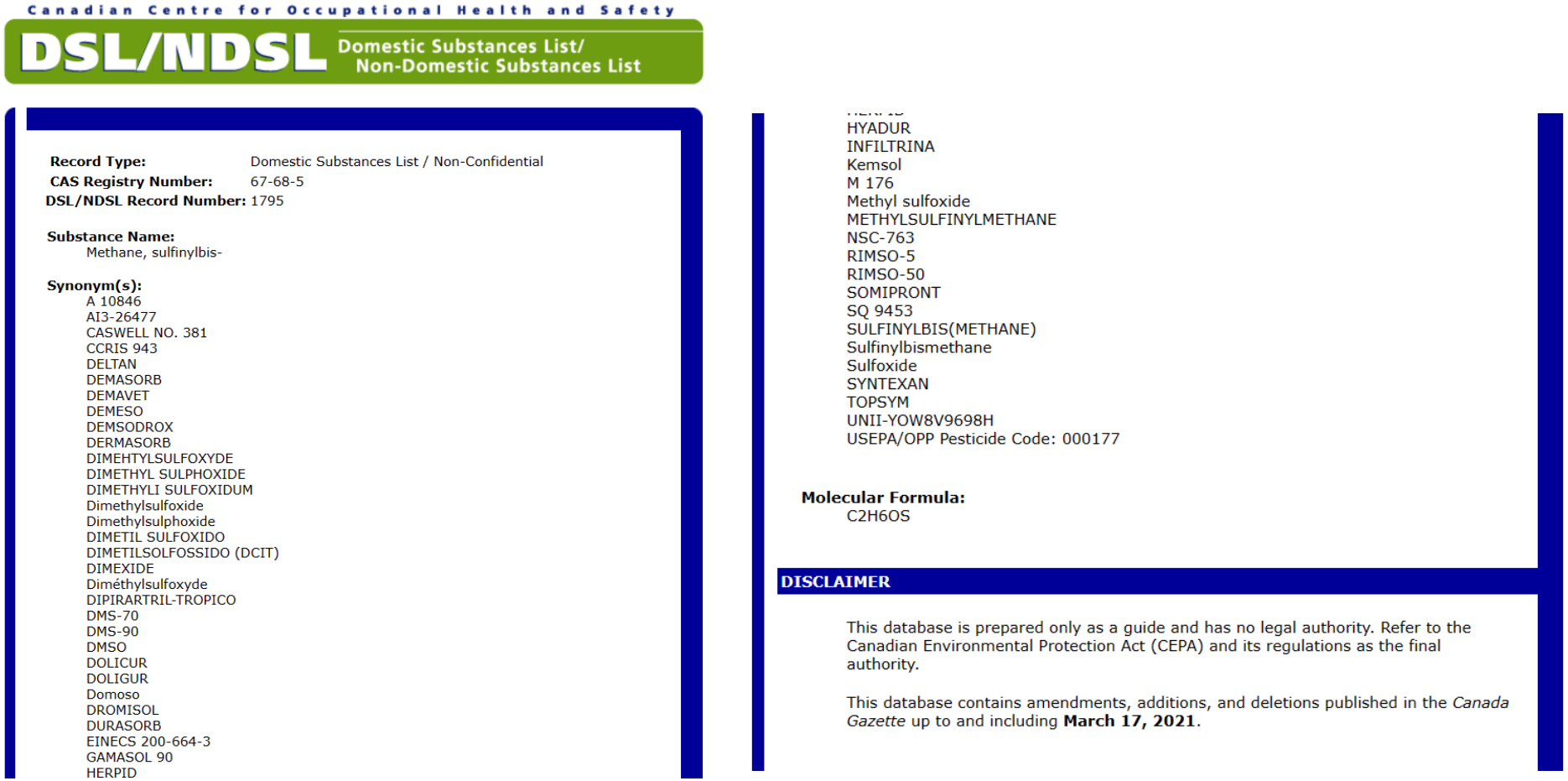


CHEMPendium Search Results for DMSO

CHEMpendium Search Using CAS Registry Number for a Substance is a More Precise Way to Search



DSL/NDSL - Domestic Substances List/Non-Domestic Substances List



Canadian Centre for Occupational Health and Safety

DSL/NDSL Domestic Substances List/ Non-Domestic Substances List

Record Type: Domestic Substances List / Non-Confidential
CAS Registry Number: 67-68-5
DSL/NDSL Record Number: 1795

Substance Name:
Methane, sulfinylbis-

Synonym(s):
A 10846
AI3-26477
CASWELL NO. 381
CCRIS 943
DELTAN
DEMASORB
DEMAVET
DEMESO
DEMSODROX
DERMASORB
DIMEHTYLSULFOXYDE
DIMETHYL SULPHOXIDE
DIMETHYLI SULFOXIDUM
Dimethylsulfoxide
Dimethylsulphoxide
DIMETIL SULFOXIDO
DIMETILSOLFOSSIDO (DCIT)
DIMEXIDE
Diméthylsulfoxyde
DIPIRARTRIL-TROPICO
DMS-70
DMS-90
DMSO
DOLICUR
DOLIGUR
Domoso
DROMISOL
DURASORB
EINECS 200-664-3
GAMASOL 90
HERPID
HYADUR
INFILTRINA
Kemsol
M 176
Methyl sulfoxide
METHYLSULFINYLMETHANE
NSC-763
RIMSO-5
RIMSO-50
SOMIPRONT
SQ 9453
SULFINYLBIS(METHANE)
Sulfinylbismethane
Sulfoxide
SYNTEXAN
TOPSYM
UNII-YOW8V9698H
USEPA/OPP Pesticide Code: 000177

Molecular Formula:
C2H6OS

DISCLAIMER

This database is prepared only as a guide and has no legal authority. Refer to the Canadian Environmental Protection Act (CEPA) and its regulations as the final authority.

This database contains amendments, additions, and deletions published in the *Canada Gazette* up to and including **March 17, 2021**.

CHRIS: Chemical Hazards Response Information System – Excerpts from Record on DMSO

Canadian Centre for Occupational Health and Safety

CHRIS Chemical Hazards Response Information System

Data source: US Coast Guard

OVERVIEW

Record Number 470
CHRIS Code DMS
Chemical Name DIMETHYL SULFOXIDE

Synonym(s)
Methyl Sulfoxide
DMSO

CAS Registry No	67-68-5
Coast Guard Compatibility Class	Not listed.
IMO/UN Designation	Not listed
DOT ID Number	Not listed
NAERG Guide No.	Not listed
Chemical Formula	CH3SOCH3
Standard Industry Trade Classification	51549

Characteristics
Liquid Colorless Mild garlic odor Sinks and mixes with water.

Emergency Actions
Call fire department.
Avoid inhalation.
Avoid contact with liquid.
Notify local health and pollution control agencies.
Protect water intakes.

Fire Hazard/Response
Combustible.
POISONOUS GASES MAY BE PRODUCED IN FIRE.
Wear goggles, self-contained breathing apparatus, and rubber overclothing (including gloves).
Extinguish with water, dry chemical, alcohol foam, or carbon dioxide.

Exposure Hazard/Response
CALL FOR MEDICAL AID.

LIQUID
Irritating to skin and eyes.
Flush affected areas with plenty of water.
IF IN EYES, hold eyelids open and flush with plenty of water.

Water Pollution Hazard/Response
Dangerous to aquatic life in high concentrations.
May be dangerous if it enters water intakes.
Notify local health and wildlife officials.
Notify operators of nearby water intakes.

CORRECTIVE RESPONSE ACTIONS

Dilute and disperse
Stop discharge
Do not burn

WATER POLLUTION

Food Chain Concentration Potential	None
Aquatic Toxicity	33,500 ppm/48 hr/bluegill/TLm/fresh water
Waterfowl Toxicity	Currently not available
Biological Oxygen Demand (BOD)	Currently not available

END OF RECORD

The current database reflects the contents of the CHRIS Manual last published by the U.S. Coast Guard in **June, 1999**.

DIMETHYL SULPHOXIDE

ICSC: 0459
Peer-Review Status: 10.04.2000 Validated

Methyl sulphoxide
DMSO

CAS #: 67-68-5 RTECS #: PV6210000
EINECS #: 200-664-3

Formula: C_2H_6OS / $(CH_3)_2SO$
Molecular mass: 78.1

TYPES OF HAZARD / EXPOSURE	ACUTE HAZARDS / SYMPTOMS	PREVENTION	FIRST AID / FIRE FIGHTING
FIRE	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.	NO open flames.	Use water spray, foam, powder, carbon dioxide.
EXPLOSION	Above 87Â°C explosive vapour/air mixtures may be formed.	Above 87Â°C use a closed system, ventilation and explosion-proof electrical equipment.	In case of fire: keep drums, etc., cool by spraying with water.
EXPOSURE		**PREVENT GENERATION OF MISTS! STRICT HYGIENE!**	
Inhalation	Headache. Nausea.	Use ventilation, local exhaust or breathing protection.	Fresh air, rest.
Skin	MAY BE ABSORBED! Dry skin.	Protective gloves. Protective clothing.	Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .
Eyes	Redness. Blurred vision.	Wear safety spectacles.	First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.
Ingestion	Nausea. Vomiting. Drowsiness.	Do not eat, drink, or smoke during work.	Do NOT induce vomiting. Refer for medical attention .

SPILLAGE DISPOSAL

Personal protection: chemical protection suit and filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

PACKAGING & LABELLING

EC Classification

UN Classification

GHS Classification

EMERGENCY RESPONSE

NFPA Code: H1; F1; R0.

SAFE STORAGE

Separated from strong oxidants. Cool. Keep in the dark. Keep in a well-ventilated room.

IMPORTANT DATA

Physical State; Appearance
COLOURLESS HYGROSCOPIC LIQUID.

Physical dangers
The vapour is heavier than air and may travel along the ground; distant ignition possible.

Chemical dangers
Decomposes on heating and on burning. This produces toxic fumes including sulfur oxides. Reacts violently with strong oxidants such as perchlorates.

Occupational exposure limits
TLV (NOT-ESTABLISHED):.
MAK: 50 ppm, 160 mg/mÂ³; Peak limitation category: I(2); Pregnancy risk group: D; Skin absorption (H); (DFG 2008).

Routes of exposure
The substance can be absorbed into the body by inhalation, through the skin and by ingestion.

Inhalation risk
No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20Â°C.

Effects of short-term exposure
The substance is irritating to the eyes and skin. Exposure to high concentrations could cause lowering of consciousness. May accelerate skin absorption of other materials. See Notes.

Effects of long-term or repeated exposure
Repeated or prolonged contact with skin may cause dermatitis. The substance may have effects on the liver and blood. This may result in impaired functions and lesions of blood cells.

PHYSICAL PROPERTIES

Boiling point: 189Â°C
Melting point: 18.5Â°C
Relative density (water = 1): 1.1
Solubility in water: miscible
Vapour pressure, Pa at 20Â°C: 59.4
Relative vapour density (air = 1): 2.7
Flash point: 87Â°C c.c.
Auto-ignition temperature: 215Â°C
Explosive limits, vol% in air: 2.6-42.0
Octanol/water partition coefficient as log Pow: -1.35 (calculated)

ENVIRONMENTAL DATA

NOTES

Special attention needed when toxic materials present in Dimethyl sulphoxide because of enhanced skin absorption.
Card has been partly updated in October 2005.
See section Occupational Exposure Limits.

CHEMPendium Search Results – HSDB and CESARS

Canadian Centre for Occupational Health and Safety

HSDB® Hazardous Substances Data Bank®

Data source: US National Library of Medicine

Record Contents

Format: All Sections

- Substance Identification
- Description and Warning Properties
- Safety Hazards and Protection
  - Fire and Reactivity
  - Protective Equipment and Controls
  - Shipment, Storage, Cleanup and Disposal
- Health Hazards and Toxic Effects
  - Emergency Treatment
- Metabolism and Pharmacology
  - Pharmacology
- Environmental Fate and Exposure Potential
  - Sources and Concentrations
  - Human Environmental Exposure
- Standards and Regulations
- Monitoring and Analysis Methods
- Manufacturing and Use Information
- Chemical and Physical Properties
- References

Canadian Centre for Occupational Health and Safety

CESARS Chemical Evaluation Search and Retrieval System

Data source: Michigan Department of Environmental Quality and Ontario Ministry of the Environment

Record Contents

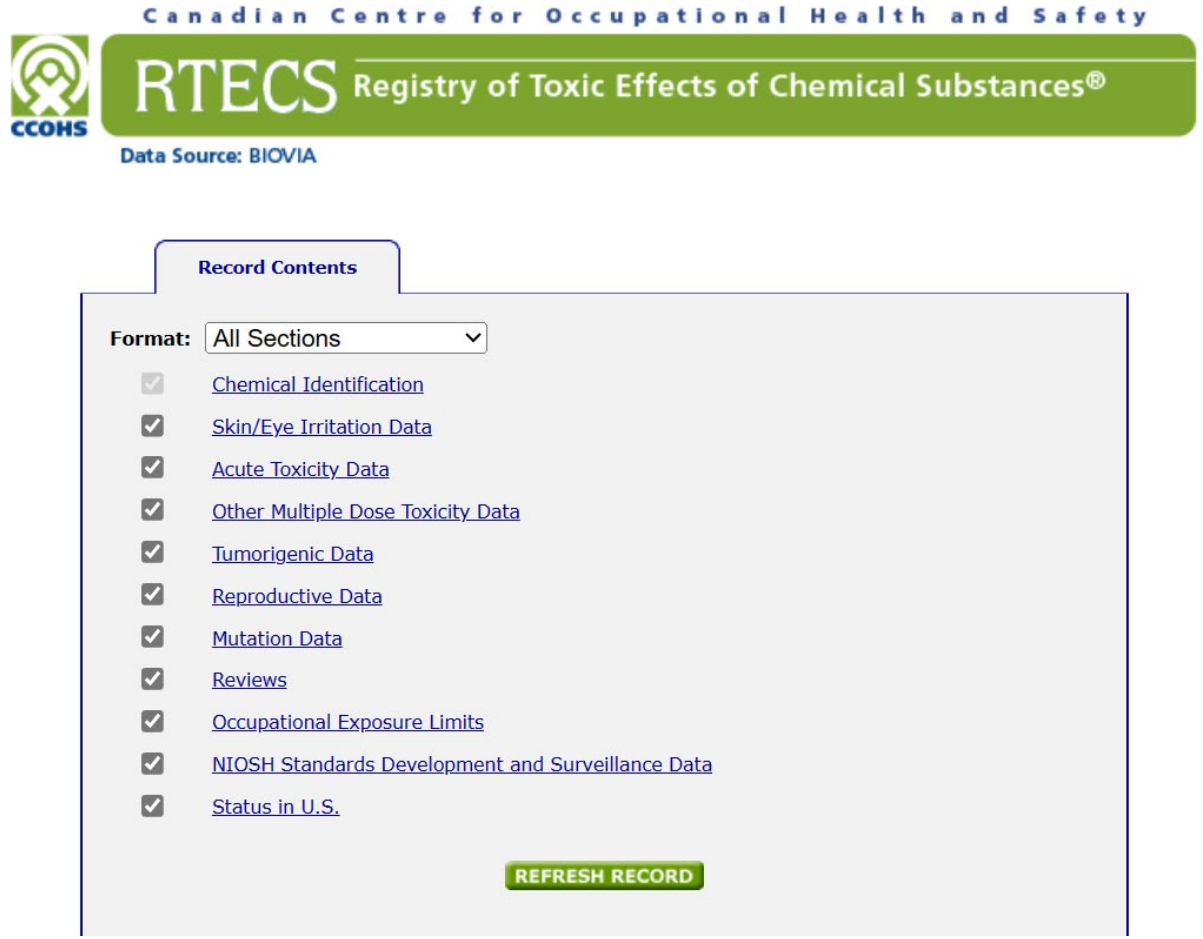
Format: Environment

- Properties
- Manufacture
- Acute Toxicity - Terrestrial Animals
- Acute Toxicity - Humans
- Acute Toxicity - Aquatic Animals
- Chronic Toxicity - Terrestrial Animals
- Chronic Toxicity - Humans
- Chronic Toxicity - Aquatic Animals
- Phytotoxicity
- Carcinogenicity
- Mutagenicity
- Reproductive and Developmental Effects
- Other Adverse Effects
- Pharmacokinetics/Metabolism
- Bioaccumulation/Bioconcentration
- Transport Process
- General Fate Process
- Transformation Processes
- Analysis and Treatment
- References
- Topic Area Summaries

DMSO is not in CESARS so this example is the record contents for **Dimethyl Disulfide** (CAS RN: 624-92-0)

Note: CESARS includes toxicity information for plants, animals, and humans

RTECS – Registry of Toxic Effects of Chemical Substances – Categories of Information Available for Methyl Sulfoxide



DMSO was not in RTECS. This record outline is for **Methyl Sulfoxide**.

RTECS Profile for **Methyl Sulfoxide** > Chemical Identification, Health Hazard > Skin/Eye Irritation Data

CHEMICAL IDENTIFICATION

RTECS Number	PV6210000
Chemical Name	Methyl sulfoxide
CAS Registry Number	67-68-5
Last Updated	202009
Data Items Cited	184
Molecular Formula	C2-H6-O-S
Molecular Weight	78.14
Wiswesser Line Notation	OS1&1
Compound Descriptor	Tumorigen Drug Mutagen Reproductive Effector Human Primary Irritant

Synonyms/Trade Names

* A 10846
* DMS-70
* DMS-90
* DMSO
* Deltan
* Demasorb
* Demavet
* Demeso
* Demsodrox
* Dermasorb
* Dimethyl sulfoxide
* Dimethyl sulphoxide
* Dimexide
* Dipirartril-tropico
* Dolicur
* Domoso
* Dromisol
* Durasorb
* Gamasol 90
* Hyadur
* Infiltrina
* M 176
* Methane, sulfinylbis-

HEALTH HAZARD DATA

SKIN/EYE IRRITATION DATA

Type of Test	Route of Exposure or Administration	Species/Test System	Dose Data	Reaction Severity	Reference
Open irritation test	Administration onto the skin	Rodent - rabbit	10 mg/24H	Mild	AIHAAP American Industrial Hygiene Association Journal. (AIHA, 475 Wolf Ledges Pkwy., Akron, OH 44311) V.19- 1958- Volume(issue)/page/year: 23,95,1962
Standard Draize test	Administration onto the skin	Rodent - rabbit	500 mg/24H	Mild	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague, Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1044,1986
Standard Draize test	Administration into the eye	Rodent - rabbit	100 mg		TXAPA9 Toxicology and Applied Pharmacology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1959- Volume(issue)/page/year: 39,129,1977
Standard Draize test	Administration into the eye	Rodent - rabbit	500 mg/24H	Mild	85JCAE "Prehled Prumyslove Toxikologie; Organicke Latky," Marhold, J., Prague, Czechoslovakia, Avicenum, 1986 Volume(issue)/page/year: -,1044,1986
Standard Draize test	Administration onto the skin	Rodent - rabbit	100 mg	Mild	ENTOX* Encyclopedia of Toxicology: Reference Book, Elsevier, 2005 Volume(issue)/page/year: 51,-,2005
Standard Draize test	Administration into the eye	Rodent - rabbit	100 mg	Mild	ENTOX* Encyclopedia of Toxicology: Reference Book, Elsevier, 2005 Volume(issue)/page/year: 51,-,2005
Standard Draize test	Administration into the eye	Rodent - rabbit	0.1 mL	Mild	HPV212 U.S. Environmental Protection Agency; High Production Volume (HPV) Challenge; Dimethyl sulfoxide.pdf http://www.epa.gov/HPV/pubs/summaries/dimthslf/c14721tc.htm Volume(issue)/page/year: -,-,2003

SEARCH RESULTS

MARK

Showing 1 - 10 of 20 DMSO ×

Chemical Name	CAS Registry Number
Dimethyl sulfoxide	67-68-5
4-tert-Butylbenzoic acid	98-73-7
Dibenzo(a,i)pyrene	189-55-9
Benzo(b)fluoranthene	205-99-2
Dibenz(a,h)anthracene	53-70-3
Benz(a)anthracene	56-55-3
Trichloroacetic acid solid	76-03-9
Trichloroacetic acid solutions	76-03-9

CHEMINFO Search Results for DMSO

CCOHS Chemical Name: Dimethyl sulfoxide

Record Contents

Format: All Sections

- Chemical Identification
- Description
- Hazards Identification
  - Emergency Overview
  - Potential Health Effects
- First Aid Measures
- Fire Fighting Measures
- Accidental Release Measures
- Handling and Storage
- Exposure Controls/Personal Protection
  - Exposure Guidelines
- Physical and Chemical Properties
- Stability and Reactivity
- Toxicological Information
- Ecological Information
- Disposal Considerations
- Transport Information
- Regulatory Information
  - Canadian Workplace Hazardous Materials Information System (WHMIS)
- Other Information

CHEMINFO Profiles are Created by CCOHS

Profile for DMSO

CHEMINFO Profile for DMSO > Chemical Identification & Description

SECTION 1. CHEMICAL IDENTIFICATION

CHEMINFO Record Number: 793
CCOHS Chemical Name: Dimethyl sulfoxide

Synonyms:
Dimethylsulphoxide
Dimethyl sulphoxide
DMSO
Methyl sulfoxide
Sulfinylbismethane
Diméthylsulfoxyde

Chemical Name French: Sulfoxyde de diméthyle
Chemical Name Spanish: Dimetil sulfoxido

CAS Registry Number: 67-68-5
Molecular Formula: C2-H6-0-S

Status of Record:
The CHEMINFO record for this chemical is complete. The full format provides a detailed evaluation of health, fire and reactivity hazards, as well as recommendations on topics such as handling and storage, personal protective equipment, accidental release and first aid.

SECTION 2. DESCRIPTION

Appearance and Odour:
Clear, colourless, odourless liquid.(15,56) Commercial grades have a strong sulfur odour.(13) Strongly hygroscopic (absorbs moisture from the air).(15,56)

Odour Threshold:
Not available

Warning Properties:
Information not available for evaluation.

Composition/Purity:
Dimethyl sulfoxide is available commercially in 99.9% plus purity. The main impurity is water.(58) It has an equilibrium moisture content of 10% with air at 20 deg C.(57)

Uses and Occurrences:
Dimethyl sulfoxide is widely used as a solvent for polymerization and spinning, and other polymerization reactions; for chemical extractions; in chemical analysis and polargraphic studies; for cellulose, cellulose esters and cellulose ethers, and many metal salts; for clean-up; for industrial cleaners and hydraulic fluids; and as a reaction medium for chemical and electrolytic reactions.(56,58,59)
Dimethyl sulfoxide is also used as a pharmaceutical and is used in veterinary medicine, and plant pathology.(14,56,58,59) It was formerly used as a vehicle for the dermal administration of drugs.(14)
Dimethyl sulfoxide occurs naturally in spearmint oil, grains, vegetables, beverages, beer, coffee, milk, and tea. It is a common constituent of ground water, seawater, and rainwater.(58)

CHEMINFO Profile for DMSO > Hazard Identification > Potential Health Effects

SECTION 3. HAZARDS IDENTIFICATION

EMERGENCY OVERVIEW:

Clear, colourless, odourless liquid. Commercial grades have a strong sulfur odour. Strongly hygroscopic. COMBUSTIBLE LIQUID AND VAPOUR. Can decompose at high temperatures forming toxic gases, such as sulfur oxides, organic sulfides, methanethiol, and formaldehyde. Essentially non-toxic following short-term exposure. Significantly enhances the absorption of numerous chemicals and drugs. Increased absorption could lead to increased toxicity.

POTENTIAL HEALTH EFFECTS

Effects of Short-Term (Acute) Exposure

Inhalation:

Dimethyl sulfoxide does not readily form a vapour at room temperature. Therefore, inhalation exposure is unlikely to occur unless it is heated or misted. No human information about the potential harmful effects of inhaled dimethyl sulfoxide was located. The limited animal information available suggests that it is not very harmful by this route of exposure.

Skin Contact:

Dimethyl sulfoxide is a very mild skin irritant, based on animal and limited human information. However, concentrated dimethyl sulfoxide has produced warmth, wheals and flaring (contact urticaria).(1,2,3,4) In a study with 200 volunteers, application of 100% dimethyl sulfoxide provoked definite wheal formation on the forearm, while 90% for 5 minutes did not produce any response in most volunteers.(2) In another study, whealing and flaring were observed following application of 70% dimethyl sulfoxide or greater for 5 minutes. In the same study, prominent whealing was observed following the application of 90% dimethyl sulfoxide for 10 or 60 minutes.(1) Similar results have been obtained in other studies.(3,4) There may be individual susceptibility to wheal formation since people have developed wheals following exposure to concentrations as low as 20%.(3)
Skin absorption may result in a garlic-like breath odour and central nervous system effects such as headache, nausea and dizziness.(4,5)

Eye Contact:

Dimethyl sulfoxide is either not irritating or a very mild eye irritant, based on human and animal information. Application of 2 drops of 50-100% has caused a temporary burning sensation or stinging in volunteers. Concentrations of less than 50% produced no effects.(6) No to mild irritation has been observed in several animal studies.

Ingestion:

Animal toxicity information indicates that the oral toxicity of dimethyl sulfoxide is low. Oral administration is not approved therapeutically for humans, but is occasionally used. Gastrointestinal discomfort is the most common side effect reported.(7) Central nervous system (CNS) effects such as headache, nausea, vomiting and dizziness may be experienced if large doses are ingested. Ingestion is not a common route of occupational exposure.

CHEMINFO Profile for DMSO > Hazard Identification > Effects of Long-Term (Chronic) Exposure

Effects of Long-Term (Chronic) Exposure

Nervous System:

Long-term non-occupational skin application of 80-90% dimethyl sulfoxide has produced central nervous system effects (such as fatigue, nausea, vomiting, sedation, dizziness, and headaches).(5) These effects were also noted following short-term exposures and the authors did not differentiate between the long-term and short-term effects.

Skin:

Repeated or prolonged skin contact has resulted in dermatitis (red, dry, scaly skin) in people treated with dimethyl sulfoxide therapeutically.(4,8) Animal studies also indicate that dimethyl sulfoxide produces severe dermatitis at the site of application.
Dimethyl sulfoxide has also produced warmth, wheals and flaring (contact urticaria) following repeated exposure. This is a temporary reaction, which generally disappears shortly after exposure stops.(80)

Skin Sensitization:

Dimethyl sulfoxide is not a skin sensitizer.
Skin sensitization was not reported in hundreds of volunteers participating in a dimethyl sulfoxide clinical trial. Also in this study, sensitizing capacity was evaluated by applying 90% dimethyl sulfoxide to 25 volunteers using five 48-hour occlusive patches to sites previously inflamed by 10% sodium lauryl sulfate. None of the volunteers showed contact allergy when challenged with 50% dimethyl sulfoxide 2 weeks later.(6) Negative results were also obtained in a maximization test using 23 volunteers.(51) Negative results were also obtained in several animal studies.

Eyes/Vision:

Several sources indicate that research has shown no effects on the eyes or vision in humans following skin application of dimethyl sulfoxide. (9,10,11,12,13,14)

Carcinogenicity:

Dimethyl sulfoxide is not known to be a carcinogen. No human information was located. No conclusions can be drawn based on the limited animal studies available.
Dimethyl sulfoxide may significantly increase the skin absorption of known carcinogens.(15)

The International Agency for Research on Cancer (IARC) has not evaluated the carcinogenicity of this chemical.

The American Conference of Governmental Industrial Hygienists (ACGIH) has no listing for this chemical.

The US National Toxicology Program (NTP) has not listed this chemical in its report on carcinogens.

Teratogenicity and Embryotoxicity:

Dimethyl sulfoxide is not known to cause developmental toxicity. No human information was located. Embryotoxicity or fetotoxicity has been seen in rats and mice exposed orally to doses which also cause maternal toxicity. Other animal studies cannot be evaluated due to poor reporting and/or study design or have not reported teratogenic, embryotoxic, or fetotoxic effects.

Reproductive Toxicity:

Dimethyl sulfoxide is not known to be a reproductive hazard. No human information was located. The limited animal information located has not shown reproductive effects.

Mutagenicity:

Dimethyl sulfoxide is not known to be mutagenic. No human information was located. No studies in live animals using a relevant route of exposure were located. Dimethyl sulfoxide has given mostly negative results in tests using cultured mammalian cells, bacteria, yeast, and fruit flies (Drosophila). It is widely used as a solvent for other chemicals in mutagenicity tests.

CHEMINFO Profile for DMSO > Hazard Identification > Effects of Long-Term (Chronic) Exposure AND First Aid Measures

Toxicologically Synergistic Materials:

Dimethyl sulfoxide has significantly enhanced the absorption of numerous chemicals and drugs in humans, rats, mice, and guinea pigs. Increased absorption could lead to increased toxicity.(1,10,11,19-22) The ability of dimethyl sulfoxide to increase the absorption of other chemicals is its most significant occupational hazard. In animal studies, dimethyl sulfoxide has been shown to protect the liver and kidneys from the injury produced by some drugs and chemicals.

Potential for Accumulation:

Dimethyl sulfoxide is very readily absorbed through the skin and other membranes and is rapidly absorbed into the blood and transported throughout the body. It is metabolized to the volatile dimethyl sulfide, which has a characteristic garlic-like odour, or to dimethyl sulfone.
Unchanged dimethyl sulfoxide is primarily excreted in the urine together with dimethyl sulfone, while some unchanged dimethyl sulfoxide and the volatile dimethyl sulfide are exhaled in the breath.(13,14,15)

SECTION 4. FIRST AID MEASURES

Inhalation:

If symptoms are experienced, remove source of contamination of move victim to fresh air and obtain medical attention.

Skin Contact:

Avoid direct contact. Wear chemical protective clothing, if necessary. As quickly as possible, flush with lukewarm, gently flowing water for at least 5 minutes or until the chemical is removed. Obtain medical advice.
Completely decontaminate clothing, shoes and leather goods before re-use or discard.

Eye Contact:

Avoid direct contact. Wear chemical protective gloves, if necessary. Immediately flush the contaminated eye(s) with lukewarm, gently flowing water for 5 minutes or until the chemical is removed, while holding the eyelid(s) open. Obtain medical advice.

Ingestion:

If irritation or discomfort occur, obtain medical advice immediately.

First Aid Comments:

Consult a doctor and/or the nearest Poison Control Centre for all exposures except minor instances of inhalation or skin contact.
All first aid procedures should be periodically reviewed by a doctor familiar with the material and its conditions of use in the workplace.

Note to Physicians:

DMSO can significantly enhance the absorption of many other chemicals and drugs.

CHEMINFO Profile for DMSO > Firefighting Measures

SECTION 5. FIRE FIGHTING MEASURES

Flash Point:
87 deg C (188.6 deg F) (closed cup) (69)

Lower Flammable (Explosive) Limit (LFL/LEL):
2.6% (60,61)

Upper Flammable (Explosive) Limit (UFL/UEL):
28.5% (62); 42% (60,61)

Autoignition (Ignition) Temperature:
215 deg C (419 deg F) (61,62); also reported as 300-302 deg C (572-575.6 deg F) (58)

Sensitivity to Mechanical Impact:
Probably not sensitive. Stable compound.

Electrical Conductivity:
3 x 10(6) pS/m at 20 deg C (58); 2 x 10(5) pS/m at 25 deg C (57,73)

Flammable Properties:
Combustible liquid. Can form explosive mixtures with air at, or above, 87 deg C. Will not accumulate static charge, since the electrical conductivity is high.(58,57,73)

Specific Hazards Arising from the Chemical:
Carbon monoxide, carbon dioxide, sulfur oxides, and other toxic and irritating gases and vapours may be formed in a fire. Decomposes slowly at, or above, 189 deg C forming methanethiol, formaldehyde, water, bis(methylthio)methane, dimethyl disulfide, dimethyl sulfone, dimethyl sulfide, and other chemicals.(58) Pure dimethyl sulfoxide may decompose violently at 270-355 deg C.(66) Closed containers may rupture violently or explode and suddenly release large amounts of product when exposed to fire or excessive heat for a sufficient period of time.

Suitable Extinguishing Media:
Carbon dioxide, dry chemical powder, appropriate foam, water spray or fog. "Multipurpose " alcohol-resistant foams are recommended for use on water soluble combustible polar liquids, like dimethyl sulfoxide.(61) Foam manufacturers should be consulted for recommendations regarding types of foams and application rates.

Special Protective Precautions for Firefighters:
Evacuate area and fight fire from a safe distance or protected location. Approach fire from upwind to avoid hazardous and toxic decomposition products, such as sulfur oxides. Wear full protective suit if exposure is possible. See Protection of Firefighters.
If possible, isolate materials not yet involved in the fire, and move containers from the fire area if this can be done without risk, and protect personnel. Closed containers may rupture violently when exposed to the heat of a fire. Therefore, fire-exposed containers, tanks or equipment should be cooled by application of hose streams. Application should begin as soon as possible (within the first several minutes) and should concentrate on any unwetted portions of the container. Apply water from the side and from a safe distance until well after the fire is out. Stay away from ends of tanks, involved in the fire, but be aware that flying material from ruptured tanks may travel in any direction. Withdraw immediately in case of rising sound from venting safety device or any discolouration of tank due to fire. Cooling should continue until well after the fire is out. If this is not possible, use unmanned monitor nozzles and immediately evacuate the area.
If a leak or spill has not ignited, use water spray in large quantities to disperse the vapours and to protect personnel attempting to stop a leak. Water spray can be used to flush spills away from ignition sources and to dilute spills to non-flammable mixtures. Dike fire control water for appropriate disposal. Solid streams of water may be ineffective and spread material.
For an advanced or massive fire in a large area, use unmanned hose holder or monitor nozzles; if this is not possible withdraw from fire area and allow fire to burn.
Tanks, drums or other containers should not be approached directly after they have been involved in a fire or heated by exposure, until they have been completely cooled down. After the fire has been extinguished, toxic and irritating atmospheres may be present. Before entering such an area, especially confined areas, check the atmosphere with an appropriate monitoring device.

Protection of Fire Fighters:
The decomposition products of dimethyl sulfoxide are hazardous to health. Firefighters may enter the area if positive pressure self-contained breathing apparatus (NIOSH approved or equivalent) and full Bunker Gear is worn.

CHEMINFO Profile for DMSO > NFPA Hazard Identification, Accidental Release Measures, Handling and Storage

NATIONAL FIRE PROTECTION ASSOCIATION (NFPA) HAZARD IDENTIFICATION

NFPA - Health:	2 - Can cause temporary incapacitation or residual injury under emergency conditions.
NFPA - Flammability:	2 - Must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.
NFPA - Instability:	0 - Normally stable, even under fire conditions.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Spill Precautions:

Restrict access to area until completion of clean-up. Ensure clean-up is conducted by trained personnel only. Wear adequate personal protective equipment. Extinguish or remove all ignition sources.
Notify government occupational and environmental authorities.

Clean-up:

Do not touch spilled material. Prevent material from entering sewers or confined spaces. Stop or reduce leak if safe to do so. Contain spill with earth, sand, or absorbent material which does not react with spilled material.
Remove liquid by pumps or vacuum equipment. Place in suitable, covered, labelled containers.
SMALL SPILLS: Soak up spill with absorbent material which does not react with spilled chemical. Put material in suitable, covered, labelled containers. Flush area with water.
Contaminated absorbent material may pose the same hazards as the spilled product.
LARGE SPILLS: Contact fire and emergency services and supplier for advice.

SECTION 7. HANDLING AND STORAGE

Handling:

This material is a COMBUSTIBLE liquid. Dimethyl sulfoxide significantly enhances the skin absorption of many other chemicals and drugs. Increased absorption could lead to increased toxicity. Before handling, it is very important that engineering controls are operating and that protective equipment requirements and personal hygiene measures are being followed. People working with this chemical should be properly trained regarding its hazards and its safe use.
Maintenance and emergency personnel should be advised of potential hazards.
Avoid all ignition sources. Post "NO-SMOKING" signs. It is good practice to keep all areas where this material is handled clear of other materials which can burn (e.g. cardboard, sawdust).
Avoid generating mists. Avoid heating this material. Prevent the release of vapours or mists into the air. Use the smallest possible amounts in a ventilated area, separate from the storage area.
Never perform any welding, cutting, soldering, drilling or other hot work on an empty vessel, containers or piping until all liquid and vapours have been cleared.
Never return contaminated material to its original container. Do not use with incompatible materials such as oxidizing agents and strong bases. See Incompatibilities - Materials to Avoid section for more information.
Inspect containers for damage or leaks before handling. Cautiously, dispense into sturdy containers made of compatible materials. Whenever possible, use self-closing, portable containers for dispensing small amounts of this material. Never transfer liquid by pressurizing original container with air or inert gas.
Label containers. Avoid damaging containers. Keep containers closed when not in use. Follow handling precautions on Material Safety Data Sheet. Have suitable emergency equipment for fires, spills and leaks readily available. Practice good housekeeping. Maintain handling equipment. Comply with applicable regulations.

CHEMINFO Profile for DMSO > Handling and Storage, Exposure Controls/Personal Protection

Storage:

Store in a cool, ventilated area, out of direct sunlight and away from heat and ignition sources. Keep quantities stored as small as possible.
Store away from incompatible materials, such as oxidizing agents and bases. See Incompatibilities - Materials to Avoid section for more information.
Inspect all incoming containers to make sure they are properly labelled and not damaged. Protect the label and keep it visible. Keep containers tightly closed when not in use. Protect from damage.
Keep empty containers in separate storage area. Empty containers may contain hazardous residues. Keep closed.
Storage area should be clearly identified, clear of obstruction and accessible only to trained and authorized personnel. Keep storage area separate from work areas, elevators, building and room exits or main aisles leading to exits. Keep storage area clear of burnable materials (e.g. old rags, cardboard). Lighted cigarettes, matches, or any other ignition sources should not be allowed around indoor or outdoor storage areas. Post warning signs. Inspect periodically for evidence of corrosion or leaks.
Storage facilities should be made of fire-resistant materials. Have appropriate fire extinguishers and spill clean-up equipment in storage area. Contain spills or leaks by storing in trays made from compatible materials. Keep absorbents for leaks and spills readily available. Provide raised sills or ramps at doorways or create a trench which drains to a safe location. Floors should be sealed to prevent absorption.
Storage tanks should be above ground and surrounded with a dike capable of holding entire contents.
Follow any special instructions for storage on Material Safety Data Sheet. Store this material according to applicable occupational health and safety regulations and fire and building codes.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

NOTE: Exposure to this material can be controlled in many ways. The measures appropriate for a particular worksite depend on how this material is used and on the extent of exposure. This general information can be used to help develop specific control measures. Ensure that control systems are properly designed and maintained. Comply with occupational, environmental, fire, and other applicable regulations.

Engineering Controls:

Engineering control methods to reduce hazardous exposures are preferred. Methods include mechanical ventilation (dilution and local exhaust), process or personnel enclosure, control of process conditions, and process modification (e.g. substitution of a less hazardous material). Administrative controls and personal protective equipment may also be required.
If dimethyl sulfoxide is heated or misted, use a non-sparking, grounded ventilation system separate from other exhaust ventilation systems. Exhaust directly to the outside.
Supply sufficient replacement air to make up for air removed by exhaust systems.

Personal Protective Equipment:

If engineering controls and work practices are not effective in controlling exposure to this material, then wear suitable personal protective equipment including approved respiratory protection. Have appropriate equipment available for use in emergencies such as spills or fire.
If respiratory protection is required, institute a complete respiratory protection program including selection, fit testing, training, maintenance and inspection. Refer to the CSA Standard Z94.4-11 "Selection, Use and Care of Respirators," available from the Canadian Standards Association.

Respiratory Protection Guidelines:

No specific guidelines are available. Contact chemical manufacturer, supplier or appropriate government agencies for advice.

Eye/Face Protection:

No specific requirement but it is good practice to wear chemical safety goggles.

Skin Protection:

Chemical protective gloves, coveralls, boots, and/or other chemical protective clothing.

CHEMINFO Profile for DMSO > Exposure Controls/Personal Protection

Resistance of Materials for Protective Clothing:

Guidelines for dimethyl sulfoxide (68):

RECOMMENDED (resistance to breakthrough longer than 8 hours): Butyl rubber, Viton(R)/Butyl rubber, Barrier(R) - PE/PA/PE, Silver Shield(R) - PE/EVAL/PE, ChemMAX(R) 4, Interceptor(R), Microchem(R) 4000, Trellchem(R) HPS, Trellchem(R) VPS, Tychem(R) CPF3, Tychem(R) BR/LV, Tychem(R) Responder(R) CSM, Tychem(R) TK, Tychem(R) Reflector.

RECOMMENDED (resistance to breakthrough longer than 4 hours): Neoprene rubber.

CAUTION, use for short periods only (resistance to breakthrough within 1 to 4 hours): Nitrile rubber, Viton(R).

NOT RECOMMENDED for use (resistance to breakthrough less than 1 hour and/or poor degradation rating): Natural rubber, Polyvinyl alcohol (PVAL), Polyvinyl chloride (PVC), Tychem(R) F, Tychem(R) Thermopro.

Recommendations are NOT valid for very thin Natural rubber, Neoprene rubber, Nitrile rubber, and PVC gloves (0.3 mm or less). Resistance of specific materials can vary from product to product. Breakthrough times are obtained under conditions of continuous contact, generally at room temperature. Evaluate resistance under conditions of use and maintain clothing carefully.

Personal Hygiene:

Remove contaminated clothing promptly. Discard or launder before rewearing. Inform laundry personnel of contaminant's hazards. Do not eat, drink or smoke in work areas. Wash hands thoroughly after handling this material. Maintain good housekeeping.

EXPOSURE GUIDELINES

THRESHOLD LIMIT VALUES (TLVs®) / AMERICAN CONFERENCE OF GOVERNMENTAL INDUSTRIAL HYGIENISTS (ACGIH®) / 2018

Time-Weighted Average (TLV-TWA): Not established

TLV Comments:

NOTE: In many jurisdictions, exposure limits are similar to the ACGIH TLVs. Since a TLV has not been established for this substance, appropriate government agencies in each jurisdiction should be consulted to determine which regulations apply.

WORKPLACE ENVIRONMENTAL EXPOSURE LEVELS (WEELs®) / AIHA GUIDELINE FOUNDATION/OARS® / 2018

8-Hour Time Weighted Average (WEEL-TWA): 250 ppm

WEEL Comments:

Source: AIHA

PERMISSIBLE EXPOSURE LIMITS (PELs) / US OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION (OSHA)

Time-Weighted Average (PEL-TWA): Not established

CHEMINFO Profile for DMSO > Physical and Chemical Properties, Stability and Reactivity

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Molecular Weight: 78.13

Conversion Factor:
1 ppm = 3.19 mg/m3; 1 mg/m3 = 0.314 ppm at 25 deg C (calculated)

Physical State:	Liquid
Melting Point:	18.5 deg C (65.3 deg F) (56,58)
Boiling Point:	189 deg C (372 deg F) (56,58)
Decomposition Temperature:	270-355 deg C (518-671 deg F) (66)
Relative Density (Specific Gravity):	1.1 at 20 or 25 deg C (water = 1) (57,58,63)
Solubility in Water:	Soluble in all proportions.(13,60,74)
Solubility in Other Liquids:	Soluble in ethanol, acetone, diethyl ether, benzene, and chloroform.(14,75)
Coefficient of Oil/Water Distribution (Partition Coefficient):	Log P(oct) = -1.35 (experimental) (64)
pH Value:	Not available
Viscosity-Dynamic:	2.22 mPa.s (2.22 centipoises) at 20 deg C (57); 1.99 mPa.s (1.99 centipoises) at 25 deg C (14,57); also reported as 2.47 mPa.s (2.47 centipoises) at 20 deg C (63,75)
Viscosity-Kinematic:	2.02 or 2.25 mm2/s (2.02 or 2.25 centistokes) at 20 deg C; 1.82 mm2/s (1.82 centistokes) at 25 deg C (calculated)
Vapour Density:	2.69 (air = 1) (calculated)
Vapour Pressure:	0.056 kPa (0.42 mm Hg) at 20 deg C (74); 0.081 kPa (0.61 mm Hg) at 25 deg C (58,74)
Saturated Vapour Concentration:	553 ppm (0.055%) at 20 deg C; 800 ppm (0.08%) at 25 deg C (calculated)
Evaporation Rate:	Very low; greater than 300 (diethyl ether = 1) (60)

Other Physical Properties:
47.24 at 20 deg C (63); 46.45 at 25 deg C (57)

SECTION 10. STABILITY AND REACTIVITY

Chemical Stability:
Normally stable.

Possibility of Hazardous Reactions:
None known.

Hazardous Polymerization:
Does not occur

Flammable Gases Released Upon Contact with Water:
None reported.

Conditions to Avoid:
Open flames, temperatures above 87 deg C

Incompatible Materials:

NOTE: Chemical reactions that could result in a hazardous situation (e.g. generation of flammable or toxic chemicals, fire or detonation) are listed here. Many of these reactions can be done safely if specific control measures (e.g. cooling of the reaction) are in place. Although not intended to be complete, an overview of important reactions involving common chemicals is provided to assist in the development of safe work practices.

STRONG OXIDIZING AGENTS (e.g. nitric acid, periodic acid or solid potassium permanganate) - react violently, with risk of fire and explosion.(61,66,67)
STRONG ACIDS (e.g. sulfuric acid) or ACID ANHYDRIDES (e.g. trifluoroacetic anhydride) - violent or explosive reaction.(66)
STRONG BASES such as METAL ALKOXIDES (e.g. potassium tert-butoxide or sodium isopropoxide) or ALKALI METALS (e.g. potassium) - can cause ignition or a violent reaction.(66)
ACYL HALIDES (e.g. acetyl chloride, benzenesulfonyl chloride, benzoyl chloride or cyanuric chloride) or NON-METAL HALIDES (e.g. phosphorus trichloride, phosphoryl chloride, tetrachlorosilane, sulfuryl chloride or thionyl chloride), DINITROGEN TETRAOXIDE, CARBONYL DIISOCYANATE, HEXACHLOROCYCLOTRIPHOSPHAZINE or SODIUM HYDRIDE - react violently or explosively, with decomposition of dimethyl sulfoxide.(61,66)
METAL OXOSALTS (e.g. aluminum, chromium, magnesium or sodium perchlorates, or iron(III) nitrate), PERCHLORIC ACID (70%), BORON COMPOUNDS (e.g. diborane) or METHYL BROMIDE - react explosively.(61,66)
IODINE PENTAFLUORIDE, SILVER DIFLUORIDE or PHOSPHORUS(III) OXIDE - react violently.(61,66)
COPPER and TRICHLOROACETIC ACID or SULFUR TRIOXIDE - violent exothermic (gives off heat) reaction.(66)

CHEMINFO Profile for DMSO > Stability and Reactivity, Toxicological Information

Hazardous Decomposition Products:
Decomposes slowly above 189 deg C forming methanethiol, formaldehyde, water, bis(methylthio)methane, dimethyl disulfide, dimethyl sulfone, dimethyl sulfide, sulfur dioxide, and other chemicals.(58,62)

Corrosivity to Metals:
No information was located. Probably not corrosive to metals.

Corrosivity to Non-Metals:
Dimethyl sulfoxide attacks plastics, such as polyvinylidene fluoride (Kynar), chlorinated polyvinyl chloride (CPVC), polyvinyl chloride (PVC), nylon 11 and 89, polyurethane (rigid), thermoset polyesters (bisphenol-A-fumarate, isophthalic acid and general purpose), thermoset vinyl ester and thermoset chlorinated polyester (77,78); elastomers, such as Viton A, styrene butadiene (SBR), nylon 11, polyurethane and flexible polyvinyl chloride (PVC) (77,79); and coatings, such as coal tar epoxy, epoxy polyamide, polyester and vinyls (77). Dimethyl sulfoxide does not attack plastics, such as Teflon and other fluorocarbons, like ethylene chlorotrifluoroethylene (Halar), and ethylene tetrafluoroethylene (Tefzel), polypropylene, nylon 6 and 66, high-density polyethylene (HDPE), polyphenylene oxide (Noryl), and polyethylene sulfide (Ryton) (77,78); and elastomers, such as Chemraz, Kalrez, Teflon and low-density polyethylene (LDPE) (77,79)

Stability and Reactivity Comments:
Dimethyl sulfoxide decomposes slowly in water to dimethyl sulfide, which has a strong sulfur odour, and dimethyl sulfone. The reaction is catalyzed by light.(60)

SECTION 11. TOXICOLOGICAL INFORMATION

LC50 (rat): greater than 5330 mg/m3 (vapour/aerosol mixture) (4-hour exposure; no deaths) (80)

LD50 (oral, rat): 14500 mg/kg (23)
LD50 (oral, guinea pig): greater than 11000 mg/kg (cited as greater than 10 mL/kg) (no deaths) (24)
LD50 (oral, mouse): 7920 mg/kg (25, unconfirmed)

LD50 (dermal, rat): approximately 40000 mg/kg has been reported, but is not considered valid. The animals were immersed in dimethyl sulfoxide solutions for a few seconds. The dose was then estimated based on a comparison of the animal weights before and after dipping.(26)

Eye Irritation:

Dimethyl sulfoxide has produced no to very mild irritation.

In an unpublished study conducted according to the OECD Guideline, application of 0.1 mL of undiluted dimethyl sulfoxide produced very mild irritation, which cleared in 3 days (mean scores at 24, 48 and 72 hours: chemosis: 0.33; redness: 1.13; iris: 0; cornea: 0).(80, unconfirmed) Application of 0.5 mL of 100% dimethyl sulfoxide caused very mild injury in rabbits (graded 2/10).(27) Application of 0.1 mL of 100% was mildly irritating in rabbits according to Draize methods.(28) Application of 0.1 mL of 30, 50, 70, and 90% was non-irritating in rabbits according to Draize methods (mean total scores 0, 0.2, 0.2, and 1.6, respectively).(29) Other studies with rabbits have shown similar results.(19,23,80)

CHEMINFO Profile for DMSO > Toxicological Information > Effects of Short-Term Exposure, Effects of Long-Term (Chronic) Exposure

Skin Irritation:

Dimethyl sulfoxide has produced very mild skin irritation.

In a test conducted according to the OECD guideline, application of pure dimethyl sulfoxide for 4 hours caused very mild irritation in rabbits. The mean scores over 24, 48 and 72 hours for each animal were 0.3, 0.0 and 0.7 for erythema and 0.0, 0.0 and 0.0 for edema. The erythema persisted until day 2 for one animal and until day 3 in another one.(80, unconfirmed) Similar results were obtained in a modified Draize test. (81) Application of 0.01 mL of 100% dimethyl sulfoxide produced very mild injury in rabbits (graded 2/10).(27) Application of an unspecified amount of dimethyl sulfoxide using the Draize test produced only slight redness in rabbits, which faded quickly after removal of the taped patch under which the dimethyl sulfoxide had been applied.(23) Whealing and flaring have been observed in guinea pigs following short-term skin contact. Application of 0.05 mL of 60, 80, or 100% to the earlobe of female guinea pigs resulted in immediate (within 5 minutes) redness and swelling. This effect lasted longer than 3 hours. Ear thickness increased after 1-2 hours. This study was designed to evaluate a model for identifying chemicals that cause non-immunologic contact urticaria (whealing and flaring) (NICU). Dimethyl sulfoxide produced a positive result. (20)

Effects of Short-Term (Acute) Exposure:

Inhalation:

No rats died following a 4 hour exposure to air saturated with dimethyl sulfoxide (approximately 500 ppm at 20 deg C or 800 ppm at 25 deg C).(27) In a study limited by poor design and poor reporting, rats were exposed to 1600 mg/m3 for 4 hours, 2900 mg/m3 for 24 hours, or 2000 mg/m3 for 40 hours, probably as an aerosol. All animals survived. The authors reported pulmonary edema in some of the exposed animals.(23)

Skin Contact:

Reduced body weight and minor blood cell changes (e.g. clotting times and platelet count) were observed in rats following skin application. Rats had 0.1 mL of 50 or 100% dimethyl sulfoxide applied for 14 days. The approximate doses were 550 or 1100 mg/kg, respectively.(31)

Ingestion:

Very high oral doses (1100-40000 mg/kg) have produced signs of central nervous system (CNS) depression (reduced activity and incoordination), congestion, and inflammation of the eyes, increased urination, excessive thirst, and deaths in rats.(20,23,32) In one study, male rats were orally administered 1100 mg/kg (cited as 1.0 mL/kg) of 50 or 100% dimethyl sulfoxide. A reduction in spontaneous motor activity was observed 15 minutes after exposure to 1100 mg/kg (cited as 1 mL/kg 100%),which became more pronounced after 45 and 60 minutes. No effect was noted after exposure to 550 mg/kg (cited as 1 mL/kg of 50% dimethyl sulfoxide in water).(20)

Effects of Long-Term (Chronic) Exposure:

Inhalation:

In an unpublished, OECD-compliant study, rats were exposed to 0.31, 0.96 or 2.8 mg/L for 13 weeks (6 hr/d; 7 d/wk) using a snout-only exposure system. At 2.8 mg/L, treatment related changes were observed in the nasal passages and pharnyx, indicating respiratory tract irritation. There were no remarkable findings upon examination of the eyes, a functional observation battery, hematology, biochemistry, macroscopic pathology or organ weights.(80, unconfirmed) No significant effects were observed in male rats exposed by inhalation to 62.8 ppm (cited as 200 mg/m3) for 30 days.(23) There are insufficient details available to evaluate another inhalation study in which rabbits developed lung, liver, and renal effects following inhalation of up to 50 mL/hour intermittently for 2 months.(10,15)

Skin Contact:

Several studies with mice, rats, guinea pigs, dogs, and monkeys treated dermally with very high doses (3300-33000 mg/kg for 28 days to 87 weeks) have shown no significant systemic effects. Swelling and ulceration of the skin and dermatitis (dry, red scaly skin) at the site of application were observed in some studies.(11,26,33,34) Eye changes were observed in rabbits exposed to high dermal doses. Rabbits were exposed to up to 8800 mg/kg (cited as up to 8 mL/kg) 100% dimethyl sulfoxide or up to 8800 mg/kg (cited as up to 16 mL/kg) 50% dimethyl sulfoxide or water for 90 days. Harmful eye effects were observed in 3-4/4 animals at the high dose for both concentrations.(35)

Ingestion:

Very high oral doses have caused significant eye and vision changes in dogs (5500 mg/kg for 11 months; 3300 or 9900 mg/kg/day for up to 2 years; 2500-40000 mg/kg for 18 weeks) and rabbits (10000 mg/kg for 11 weeks). In some cases, the changes were irreversible.(35,36,37,38,39) In one study, oral administration of 100, 500 or 1000 mg/kg/day to rabbits produced "suggestive" lens changes after 8 weeks.(12) Further details are not available for evaluation. Similar changes in the eyes and vision were not observed in monkeys exposed to up to 9000 mg/kg for 18 months.(33)

Skin Sensitization:

Dimethyl sulfoxide is not a skin sensitizer.
Negative results were obtained in several studies including the Guinea pig maximization test, the Buehler test, the Draize test, the Mouse ear swelling test and a Local lymph node assay.(40,53,80) Dimethyl sulfoxide has been used, or is suggested for use, as a solvent for other chemicals in the mouse local lymph node assay because it is not a skin sensitizer itself.(54)

CHEMINFO Profile for DMSO > Toxicological Information > Effects of Long-Term (Chronic) Exposure

Carcinogenicity:

Only limited animal information was located.
Mice were orally dosed with 330 mg/kg/week in 198 administrations. Tumours were observed in 18/54 surviving mice, a significant increase over controls. Tumour sites included the lungs, liver, kidneys, and lymph nodes.(14) The reviewers indicated that the original article did not contain sufficient detail to make a detailed evaluation and that the study would not have met International Agency for Research on Carcinogens (IARC) standards. In the same study, rats were orally exposed to 3000 mg/kg/week in 243 administrations. Tumours were observed in 17/65 animals after 11.5 months. Breast tumours were observed in 7/34 females. These observations were not significantly different from controls.(14) In tumour initiation/promotion studies, dimethyl sulfoxide either showed ehancement, no effect or inhibition.(14,15,80) Dimethyl sulfoxide may enhance the skin penetration of known carcinogens.(80)

Teratogenicity, Embryotoxicity and/or Fetotoxicity:

The available evidence does not indicate that dimethyl sulfoxide is a developmental toxin. Embryotoxicity or fetotoxicity has only been seen in rats and mice exposed orally to doses that also cause maternal toxicity.
In an unpublished study conducted according to the OECD Guideline, rats were orally exposed to 0, 100, 300, or 1000 mg/kg dimethyl sulfoxide (purity 99.977%) before mating and through mating and, for females, through pregnancy until day 21 post-partum. No significant effects were observed in the offspring.(80, unconfirmed) In an unpublished study conducted according to the OECD Guideline, rabbits were orally exposed to 0, 100, 300 or 1000 mg/kg on days 7 to 28 of pregnancy. Maternal toxicity was observed at 300 mg/kg, and there were no signs of developmental toxicity.(80, unconfirmed) Mice were orally administered 3200 mg/kg on days 5-9 of pregnancy. Maternal toxicity, as evidenced by a reduction in maternal body weight, and embryotoxicity (a significant reduction in the number of implantations) were observed. (41) In a study reported by abstract, rats were given 0, 200, 1000, or 5000 mg/kg/day on days 6-15 of pregnancy. At 5000 mg/kg/day, there was a decrease in maternal body weight gain and food consumption. In the offspring, there was a decreased fetal weight and an increase in delayed ossification. No effects were seen on mothers or offspring at 1000 mg/kg/day. No statistical evaluation was reported. However, the study was reported to be performed according to OECD guidelines.(55) Other studies cannot be evaluated because of factors such as poor study design, lack of reporting on maternal toxicity, high maternal toxicity, and/or lack of statistical analysis.(42,43,44) Other studies have not reported teratogenic, embryotoxic, or fetotoxic effects. (10,42,45)

Reproductive Toxicity:

The limited information available does not indicate that dimethyl sulfoxide is a reproductive toxin.
In an unpublished study conducted according to the OECD Guideline, rats were exposed to 0, 100, 300, or 1000 mg/kg dimethyl sulfoxide (purity 99.977%) orally before mating and through mating and, for females, through pregnancy until day 21 post-partum. No significant reproductive effects were observed.(80, unconfirmed) Daily oral administration of 5000 mg/kg to both male and female rats for 4 days before mating and to females throughout pregnancy failed to interfere with fertility. Rabbits receiving dimethyl sulfoxide orally at a dose of 10000 mg/kg/day were successfully bred and had litters of normal size.(10, unconfirmed) In an unpublished, OECD-compliant study, rats were exposed to 0.31, 0.96 or 2.8 mg/L for 13 weeks (6 hr/d; 7 d/wk) using a snout-only exposure system. There were no effects noted on the estrus cycle or sperm.(80, unpublished)

Mutagenicity:

The available evidence does not indicate that dimethyl sulfoxide is mutagenic. No studies in live animals using a relevant route of exposure were located. Dimethyl sulfoxide has given mostly negative results in tests using cultured mammalian cells, bacteria, yeast, and fruit flies (Drosophila). Dimethyl sulfoxide is widely used as a solvent for other chemicals in mutagenicity tests.
Negative results (micronucleus, dominant lethal) and positive results (chromosome aberrations, DNA damage) have been obtained in tests using live mice and rats exposed by intraperitoneal administration, which is a not a relevant route of exposure. (14,69,80-unconfirmed)
Negative results have been obtained in most tests using cultured mammalian cells, bacteria, and yeast.(14,52,69,80-unconfirmed) Dimethyl sulfoxide is widely used as a solvent for other chemicals in mutagenicity tests. In a few tests high concentrations have given positive results in cultured mammalian cells and bacteria.(46,47,48,49,80) Negative results have been obtained in fruit flies (Drosophila).(14,52,60-unconfirmed)

Toxicological Synergisms:

Dimethyl sulfoxide has been shown to protect the liver and kidneys from injury produced by several drugs and chemicals in studies using animal.(70,71,72)

CHEMINFO Profile for DMSO > Ecological Information, Disposal Considerations, Transport Information

SECTION 12. ECOLOGICAL INFORMATION

NOTE : Inclusion of Ecological Information on a Safety Data Sheet (SDS) is optional under the US Hazard Communication Standard (2012), and the Canadian WHMIS regulations. In other jurisdictions, inclusion of Ecological Information may be a requirement. For specific requirements, contact the relevant regulatory authorities in the jurisdiction where the SDS is intended to be used.

The American National Standard for Hazardous Workplace Chemicals - Hazard Evaluation and Safety Data Sheet and Precautionary Labeling Preparation (ANSI Z400.1/Z129.1-2010) and the Globally Harmonized System for Classification and Labelling of Chemicals (GHS) guidance document provide advice on data that could be included in this section.

Databases in CCOHS's CHEMpendium™ collection which may contain useful Ecological Information include Transport TDG, Transport 49CFR, CESARS, HSDB® (Hazardous Substances Data Bank), and CHRIS (Chemical Hazards Response Information System).

SECTION 13. DISPOSAL CONSIDERATIONS

Review federal, provincial and local government requirements prior to disposal. Store material for disposal as indicated in Storage Conditions. Disposal by controlled incineration or secure landfill may be acceptable.

SECTION 14. TRANSPORT INFORMATION

CANADIAN TRANSPORTATION OF DANGEROUS GOODS (TDG) SHIPPING INFORMATION

This chemical is not specifically listed in the Canadian Transportation of Dangerous Goods Regulations. However, it may be regulated as a part of a chemical family or group Not Otherwise Specified (N.O.S.) (e.g. LIQUID DYES N.O.S.). Consult the regulation.

NOTE: This information incorporates the Transportation of Dangerous Goods Regulations SOR/2001-286, effective October 21, 2015.

US DEPARTMENT OF TRANSPORT (DOT) HAZARDOUS MATERIALS SHIPPING INFORMATION (49 CFR)

This chemical is not specifically listed in the US hazardous materials shipping regulations (49 CFR, Table 172.101). However, it may be regulated as part of a chemical family or group Not Otherwise Specified (N.O.S.) (e.g. mercury-based pesticides). Consult the regulation.

NOTE: This information was taken from the US Code of Federal Regulations Title 49 - Transportation and is effective February 1, 2016.

CHEMINFO Profile for DMSO > Transport Information

SECTION 15. REGULATORY INFORMATION

CANADIAN WORKPLACE HAZARDOUS MATERIALS INFORMATION SYSTEM (WHMIS) 1988

CCOHS WHMIS 1988 Classification:
B3 - Flammable and combustible material - Combustible liquid

WHMIS 1988 Health Effects Criteria Met by this Chemical:
Insufficient information

WHMIS 1988 Ingredient Disclosure List:
Included for disclosure at 1% or greater.

Detailed WHMIS 1988 Classification According to Criteria:

Class A - Compressed Gas:
Does not meet criteria.

Class B - Flammable and Combustible Material:
Meets criteria for "Combustible liquid".
Closed cup flash point: 87 deg C (188.6 deg F).

Class C - Oxidizing Material:
Does not meet criteria.

Class D - Poisonous and Infectious Material. Division 1 - Immediate and Serious Toxic Effects:
Does not meet criteria.

Acute Lethality:
Does not meet criteria.
LC50 (rat): greater than 5330 mg/m3 (vapour/aerosol mixture) (4-hour exposure); LD50 (oral, rat): 14500 mg/kg (an unconfirmed value - LD50 (oral, mouse): 7920 mg/kg has also been reported); no reliable LD50 (dermal) values were located.

Class D - Poisonous and Infectious Material. Division 2 - Other Toxic Effects:
Insufficient information for classification.
See detailed evaluation below.

Chronic Health Effects:
Does not meet criteria.
No significant toxic effects observed in humans or animals.

Carcinogenicity:
Does not meet criteria. Not included in standard reference lists.

Teratogenicity and Embryotoxicity:
Does not meet criteria.
Embryotoxicity or fetotoxicity has been seen in rats and mice exposed orally to doses which also cause maternal toxicity. Other animal studies cannot be evaluated due to poor reporting and/or study design, or have not reported teratogenic, embryotoxic, or fetotoxic effects. No human information was located.

Reproductive Toxicity:
Does not meet criteria.
The limited animal information located has not shown reproductive effects. No human information was located.

Mutagenicity:
Does not meet criteria.
No human information was located. No studies in live animals using a relevant route of exposure were located. Mostly negative results were obtained in in tests using cultured mammalian cells, bacteria, yeast, and fruit flies (Drosophila).

Respiratory Tract Sensitization:
Does not meet criteria.
Not reported as human respiratory sensitizer.

Skin Irritation:
Does not meet criteria.
Very mild skin irritant, based on animal and limited human information.

Eye Irritation:
Does not meet criteria.
Not irritating or a very mild eye irritant, based on human and animal information.

Skin Sensitization:
Does not meet criteria.
Skin sensitization was not observed in human volunteers or in animal tests. Non-immunological whealing and flaring have been observed in animals and humans.

CHEMINFO Profile for DMSO > Transport Information, Other Information – Selected Bibliography

Class E - Corrosive Material:
Does not meet criteria.
Not corrosive to animal skin. Probably not corrosive to carbon steel or aluminum.

Class F - Dangerously Reactive Material:
Does not meet criteria.

EUROPEAN UNION (EU) CLASSIFICATION AND LABELLING INFORMATION

Harmonized classifications derived from Annex VI to the European Union Classification, Labelling and Packaging (CLP) Regulation can be found in the ECHA C&L Inventory. The CLP Regulation is the European Union implementation of the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). For current information, see: http://echa.europa.eu/regulations/clp/cl-inventory

NOTE: The harmonized hazard classifications contained in the C&L Inventory may not necessarily be the same as hazard classifications obtained according to the classification criteria of WHMIS 2015 or the U.S. Hazard Communication Standard 2012.

SECTION 16. OTHER INFORMATION

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Information on chemicals reviewed in the CHEMINFO database is drawn from a number of publicly available sources. A list of general references used to compile CHEMINFO records is available in the database Help.

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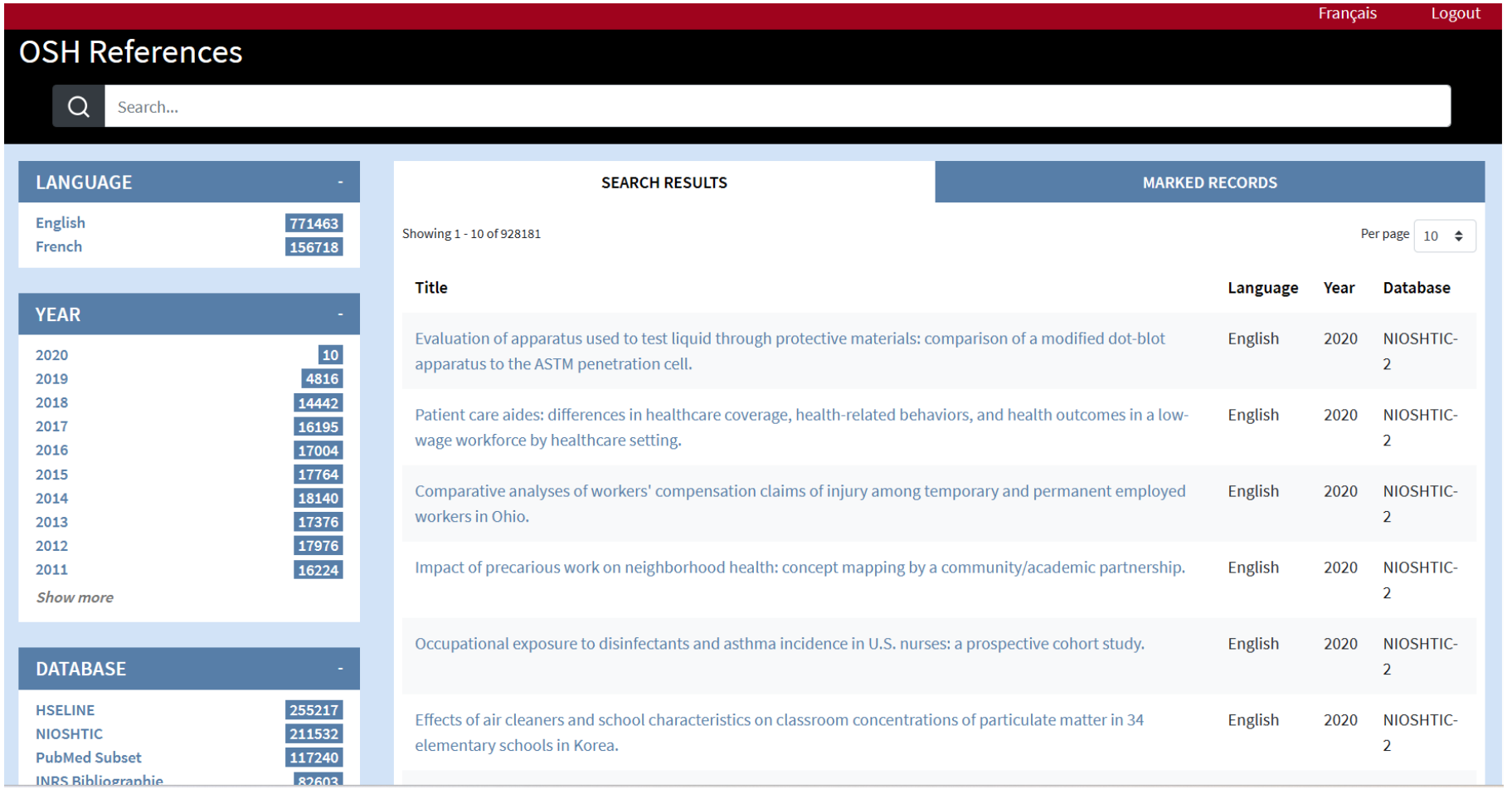

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