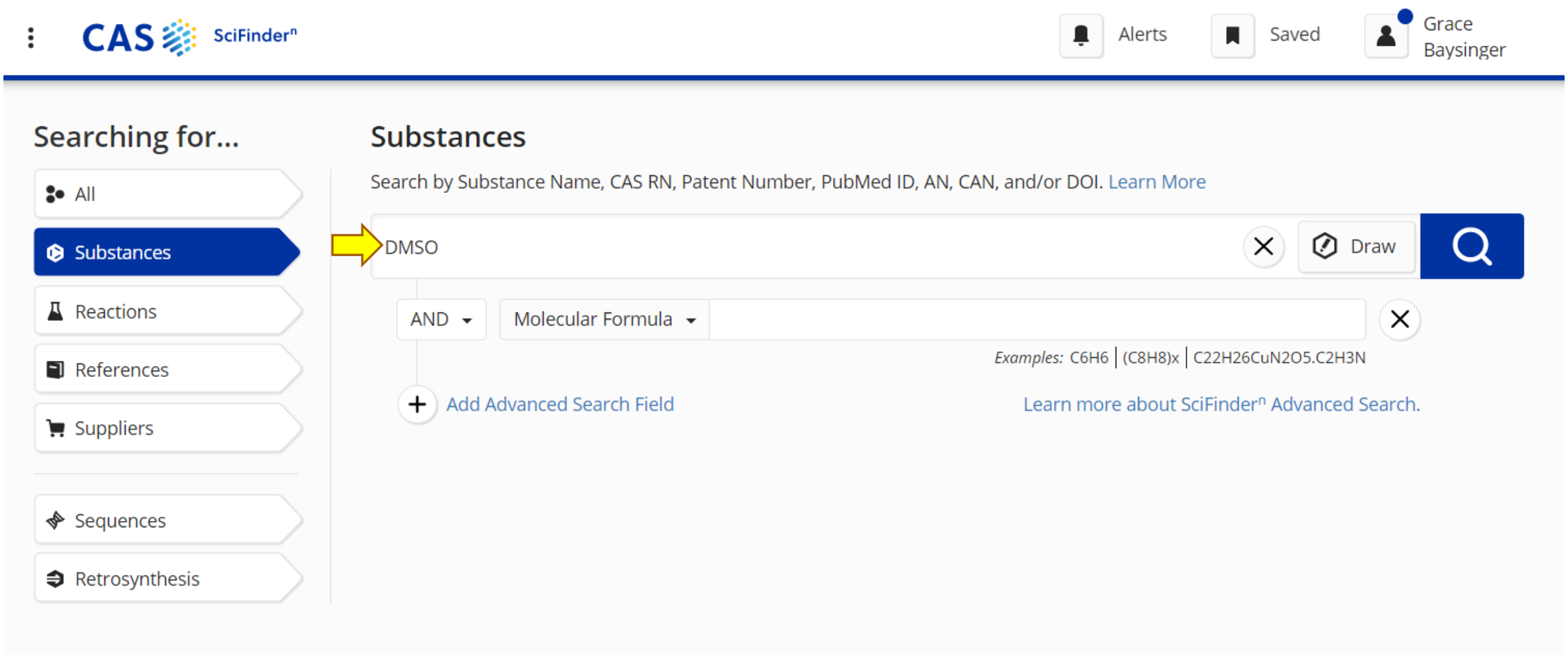
SciFinder-n

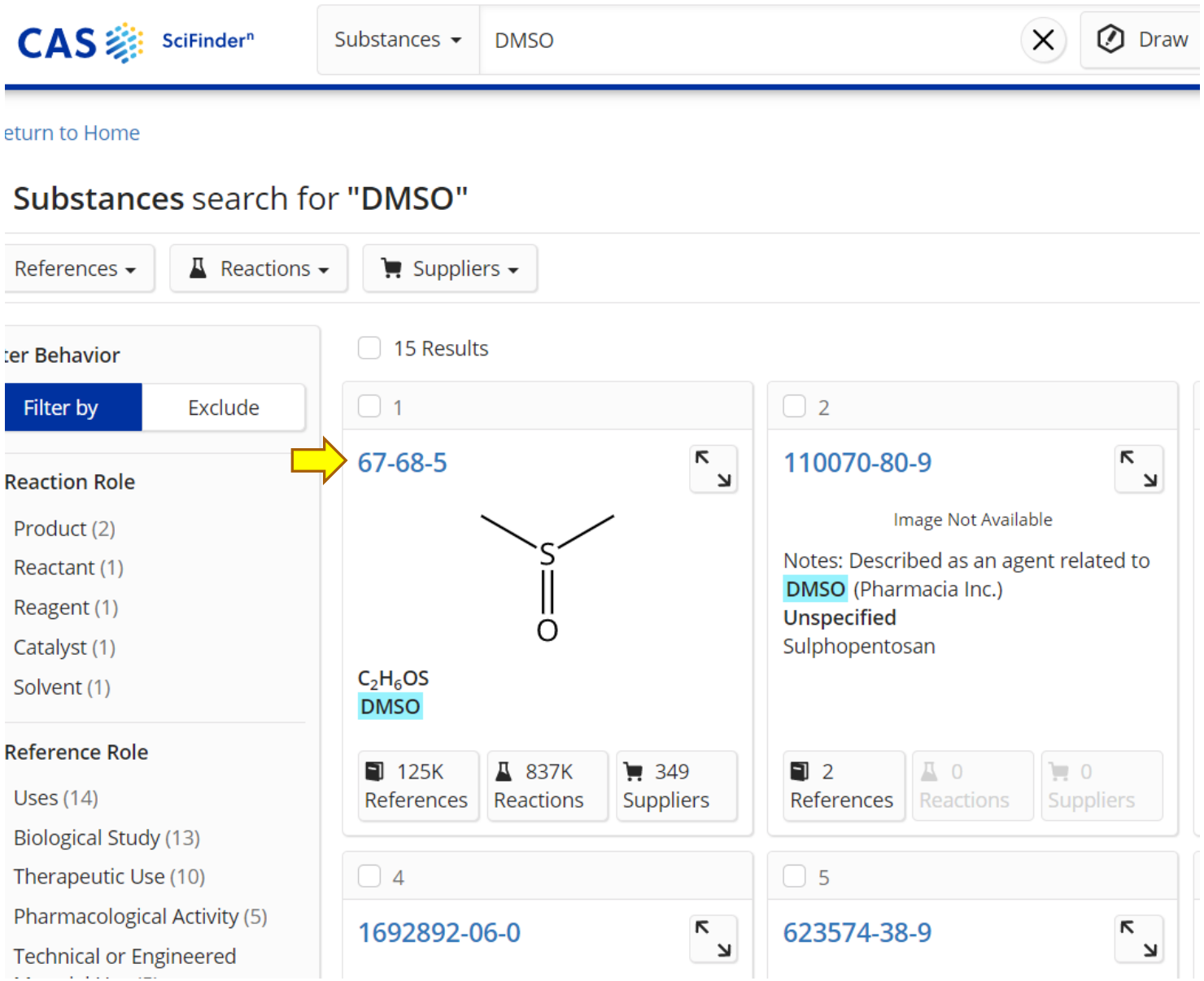
THE MOST COMPREHENSIVE CHEMISTRY AND CHEMICAL ENGINEERING DATABASE

SEARCH BY SUBSTANCES, REACTIONS (ORGANIC), REFERENCES, AND MORE

ABOUT
HTTPS://WWW.CAS.ORG/SOLUTIONS/CAS-SCIFINDER-DISCOVERY-PLATFORM/CAS-SCIFINDER-N



SciFinder-n – Searching for DMSO as a Substance



SciFinder-n – Substance search results for DMSO

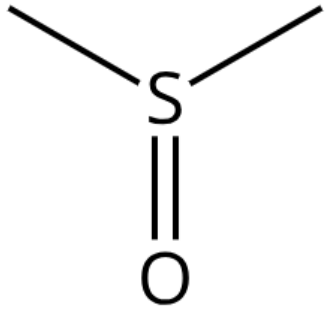
CAS SciFinder^n | Substances | DMSO | Draw

← Return to Results

← Prev (1 of 15) Next →

CAS Registry Number: 67-68-5

References (127K) | Reactions (848K) | Suppliers (352) | Save



- 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.

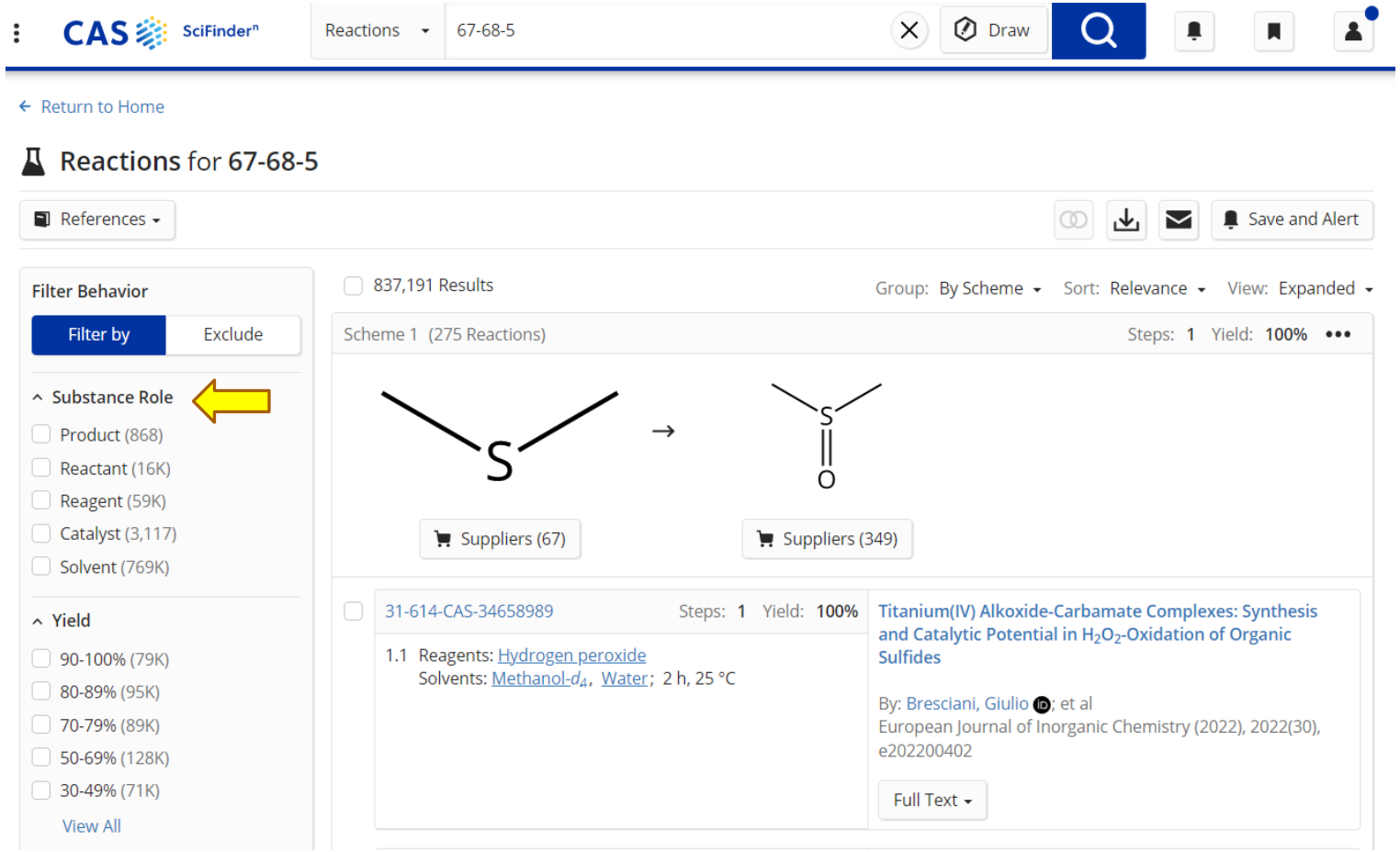
Code, statements, and pictograms from the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) became available in SF-n on June 26, 2023.

CAS SciFinder^{n} Substances DMSO

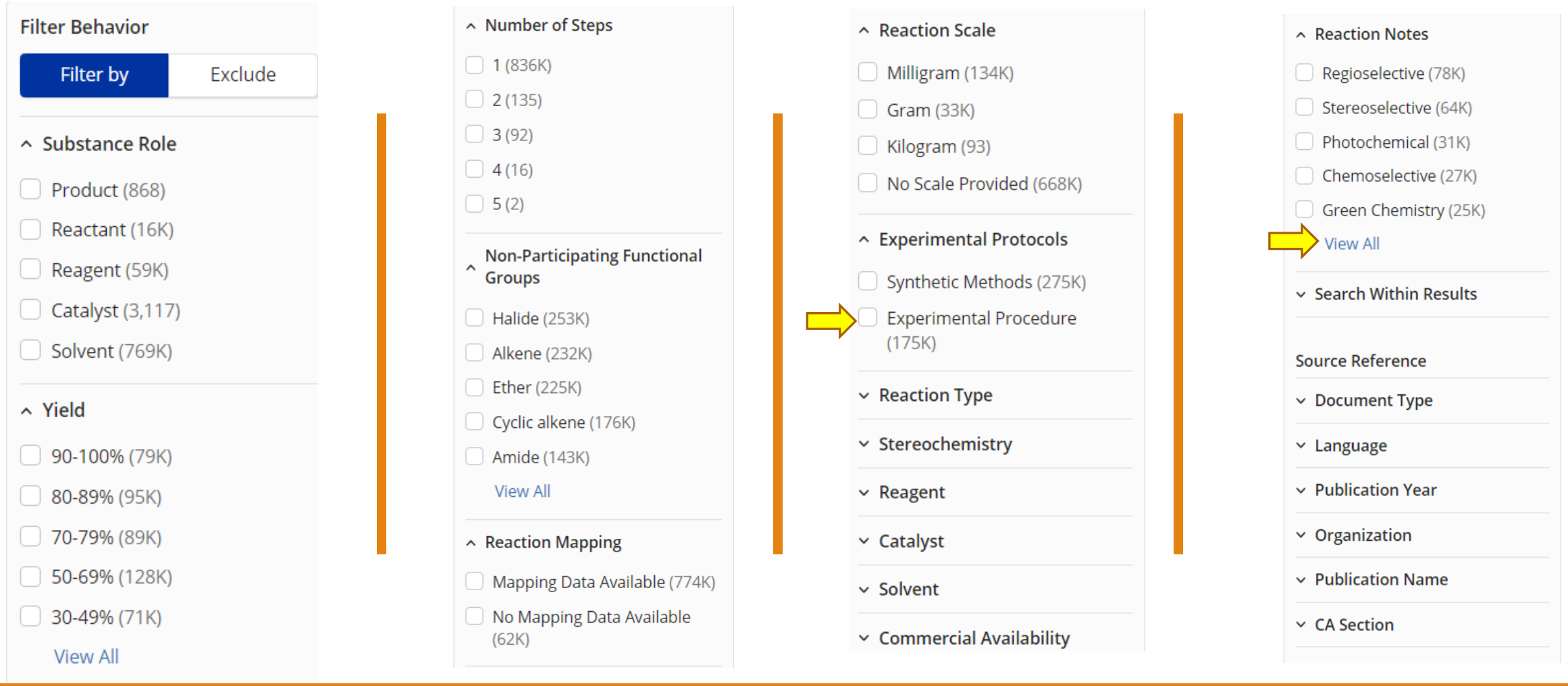
GHS Hazard Statements

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

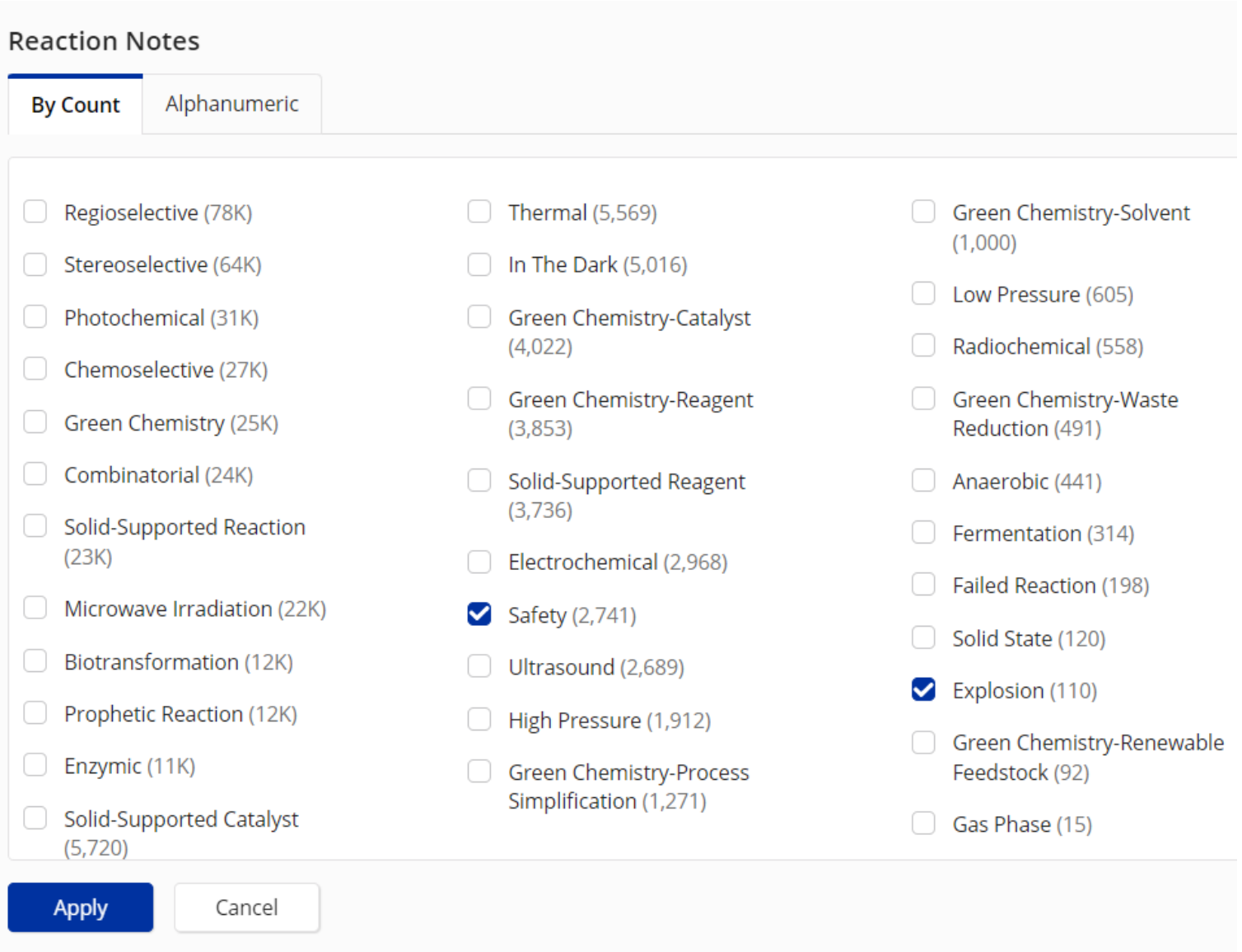
Selected GHS Hazard Statements for DMSO



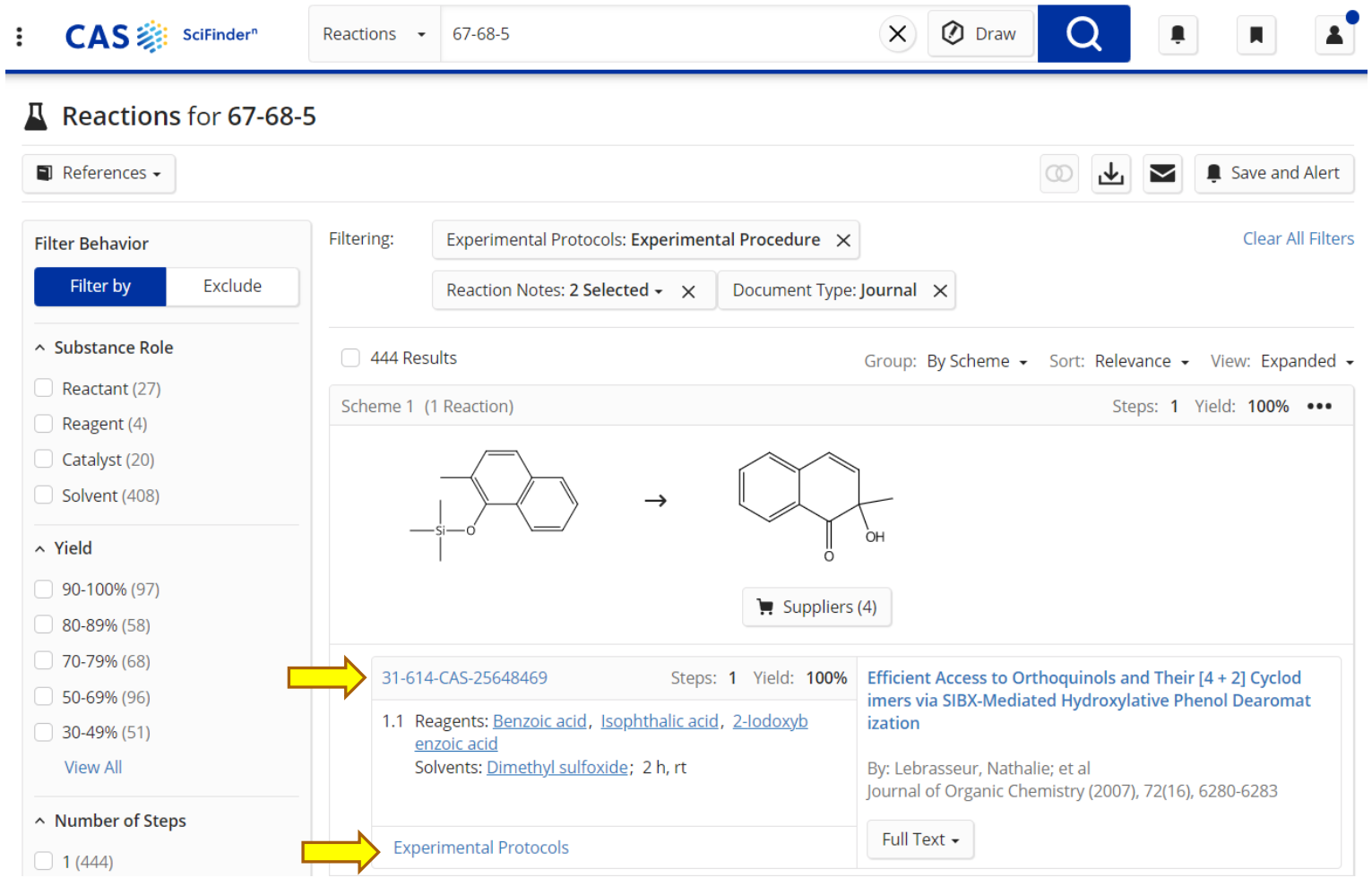
SciFinder-n – Viewing Reactions



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

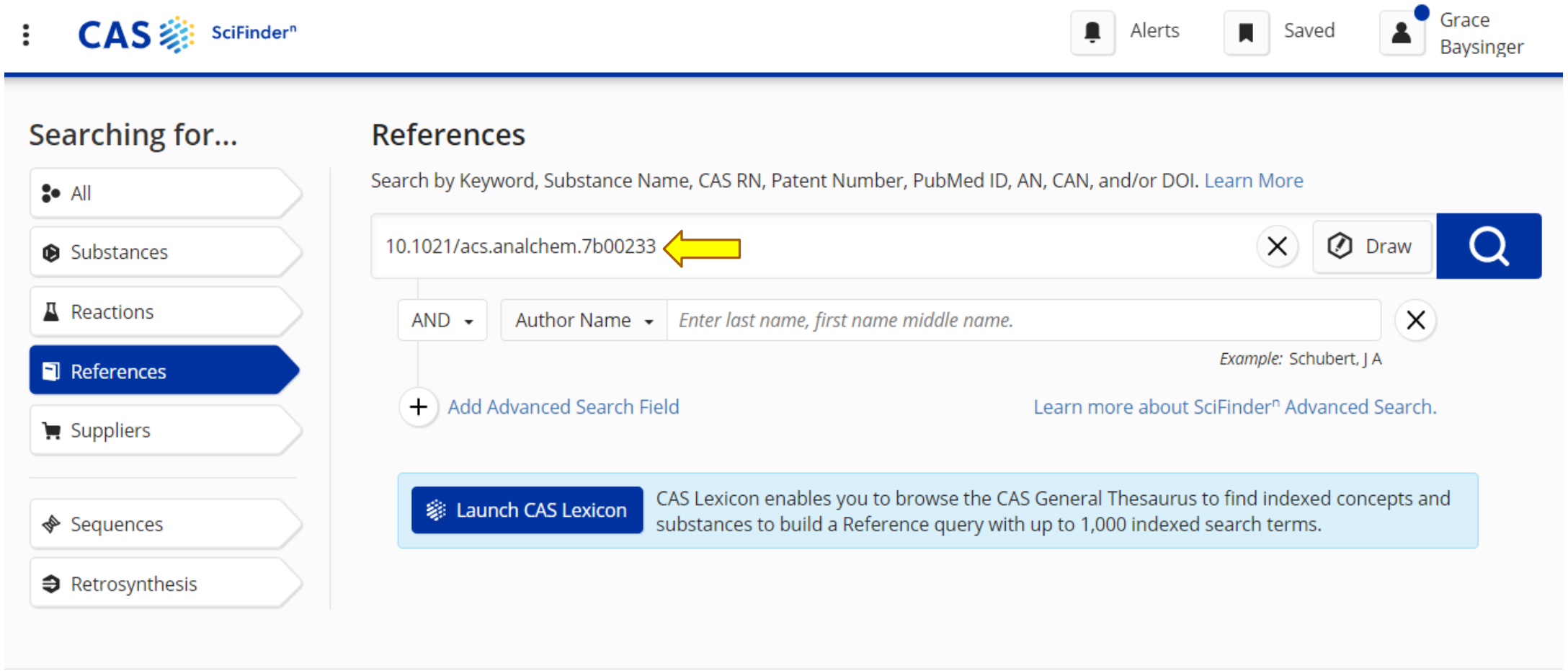
Synthetic Methods | **Experimental Procedure**

JOC The Journal of Organic Chemistry

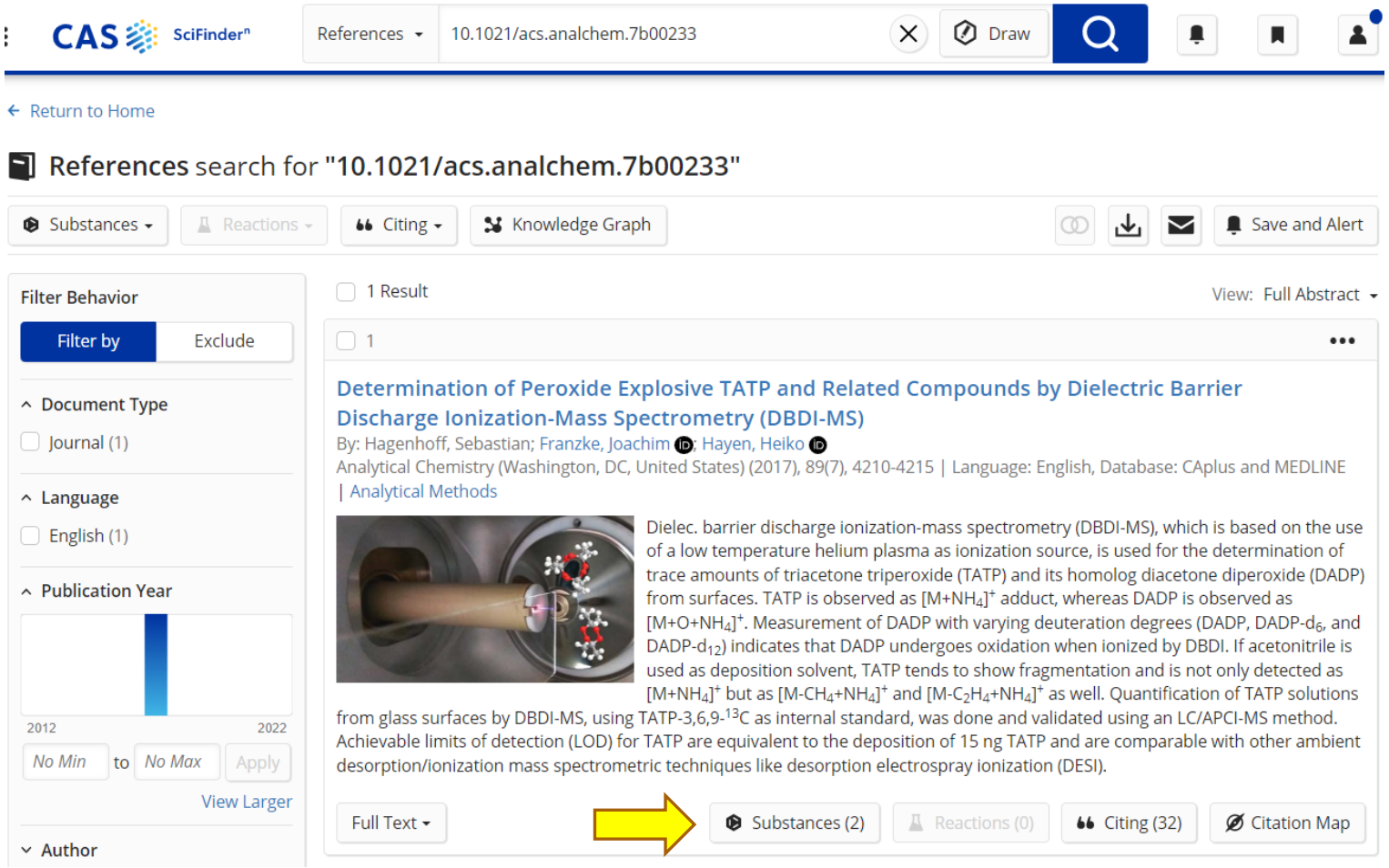
Method B. Treatment of the trimethylsilylated 2-methylnaphthol **11b** (50 mg, 0.2 mmol) in DMSO (1 mL) with SIBX (255 mg, 0.5 mmol, i.e., 2.5 equiv of IBX) was run at room temperature for 2 h, after which time the reaction mixture was diluted with EtOAc (20 mL), washed with saturated aqueous $NaHCO_3$ (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



SciFinder-n Search Results for DOI

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

← Return to Results ← Prev (1 of 1) Next →

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

CODEN: ANCHAM
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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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Similar References NEW

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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

Expand All | Collapse All

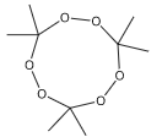
Concepts

Explosives

Substances

Substances (2)

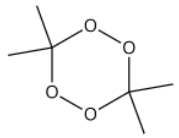
17088-37-8



$C_9H_{18}O_6$
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

Find substances by Name, CAS Registry Number, or chemical structure; find reactions; and then filter or refine results to reactions that have safety notes and/or experimental details.

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

Search by keyword in references to find names, functional groups, or compounds class names mentioned in abstracts or as index terms.

Search the DOI from a relevant article and see how it is indexed in SciFinder-n so that you are more easily able to find other, similar papers.

For SF-n users, start with the CAS Lexicon that includes both controlled subject terms as well as functional groups and classes of compounds.