PubChem's Laboratory Chemical Safety Summary (LCSS)

Sunghwan Kim[1] (kimsungh@ncbi.nlm.nih.gov), Jian Zhang[1], Asta Gindulyte[1], Paul Thiessen[1], Leah McEwen[2], Ralph Stuart[3], Evan E. Bolton[1], Stephen H. Bryant[1]

[1] National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health
[2] Clark Physical Science Library, Cornell University.
[3] Office of Environmental Health & Safety, Keene State College,

❑ Acknowledgements

- **The PubChem Team**

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- **PubChem depositors, users, and collaborators**
- **Funded by the National Library of Medicine**
- **Leah McEwen (Cornell) & Ralph Stuart (Keene State)**

❑ PubChem Presentations at ACS San Diego

- 10 presentations has been given already.
- 3 more presentations will be given tomorrow.
- See the PubChem Blog for a list of PubChem presentations (https://pubchemblog.ncbi.nlm.nih.gov).

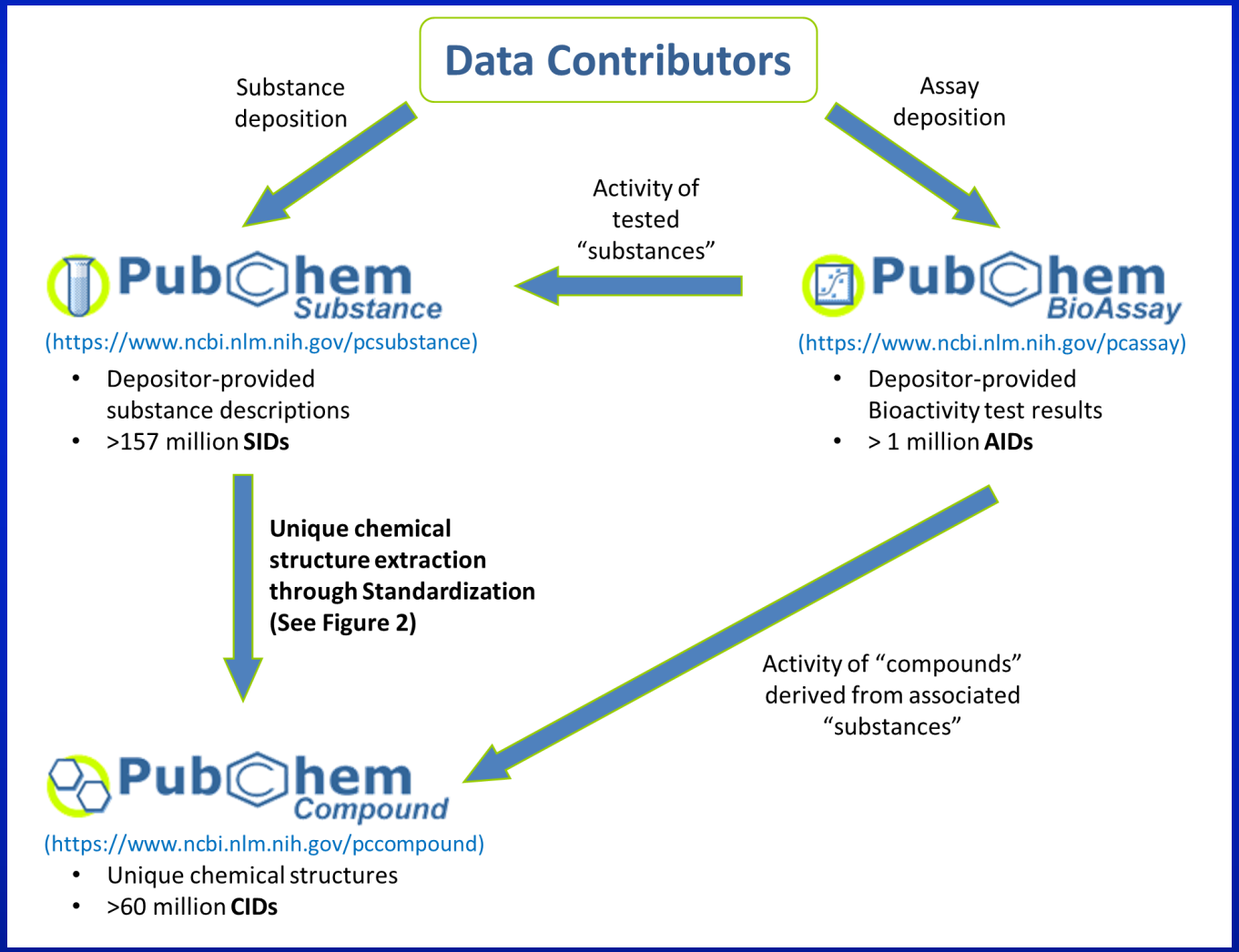
PubChem

(https://pubchem.ncbi.nlm.nih.gov)

❑ PubChem (https://pubchem.ncbi.nlm.nih.gov)

- A "public" repository of information on small molecules and their biological activities, developed and maintained by the U.S. National Institutes of Health (NIH).
- Launched in 2004 as a part of the Molecular Libraries Roadmap initiatives.
- A key resource of chemical information for researchers in the area of cheminformatics, chemical biology, medicinal chemistry, and many others.

❑ PubChem (https://pubchem.ncbi.nlm.nih.gov)

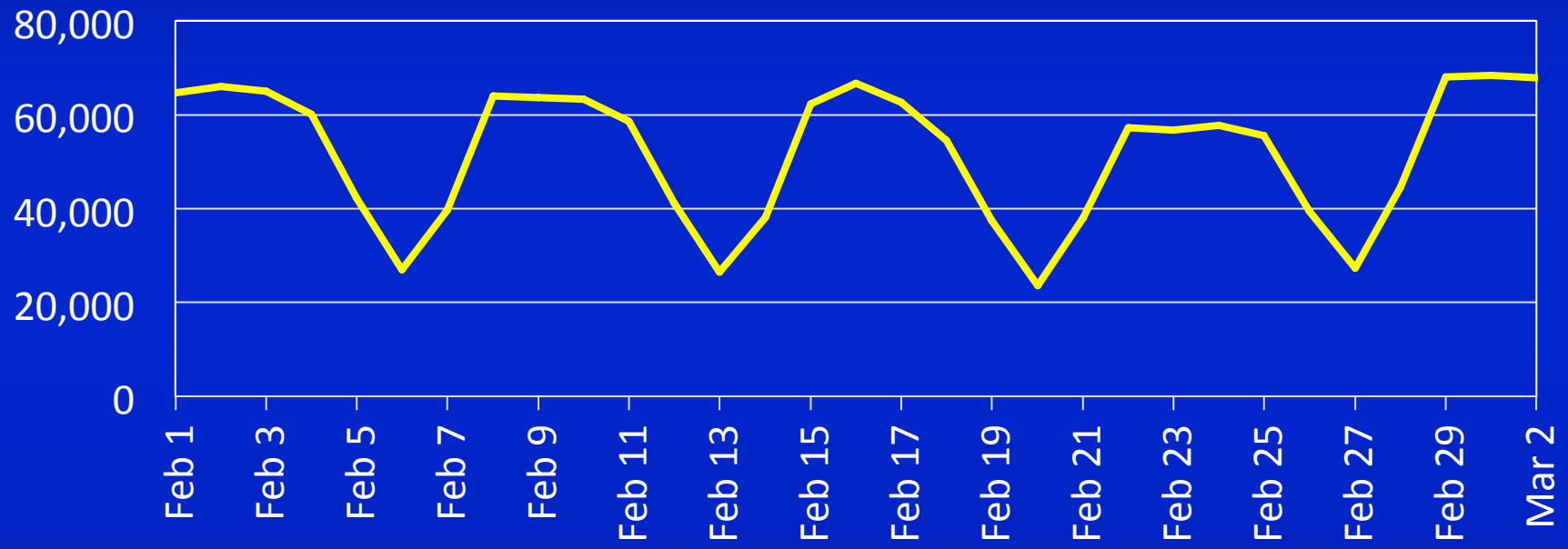


❑ PubChem (http://pubchem.ncbi.nlm.nih.gov)

- PubChem contains:
  - >218 million substance descriptions,
  - >88 million unique chemical structures,
  - >229 million biological test results
  - >1 million biological assays, covering ~10,000 unique protein sequence targets.

(Arguably) the largest corpus of publicly available chemical information from more than 400 data contributors.

❑ Number of PubChem Users

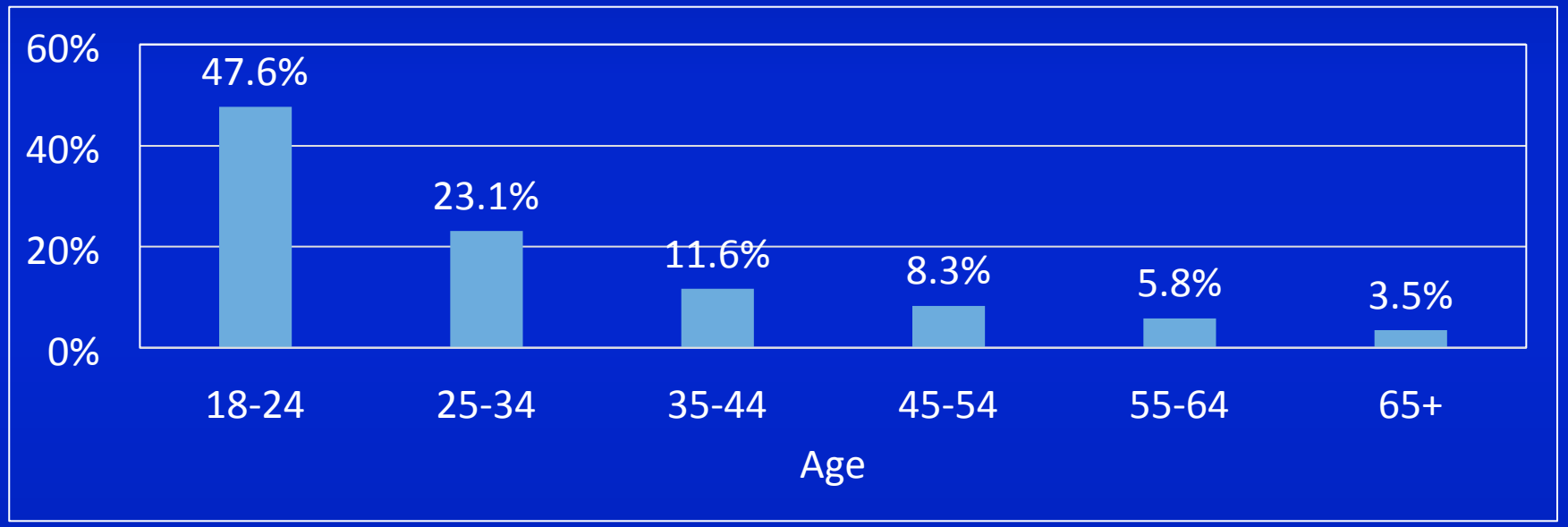


- For the 30-day period (between Feb. 1 – Mar. 2, 2016)
  - Average daily users: **51, 871**
  - Unique users for the past 30 days: **1,201,813**

Source: Google Analytics

Demographics of PubChem Users

among 467,671 users (45.6 % of 1,026,283 Users)



- ~50% of PubChem users are at **age 18-24**
- **They are likely to be students**

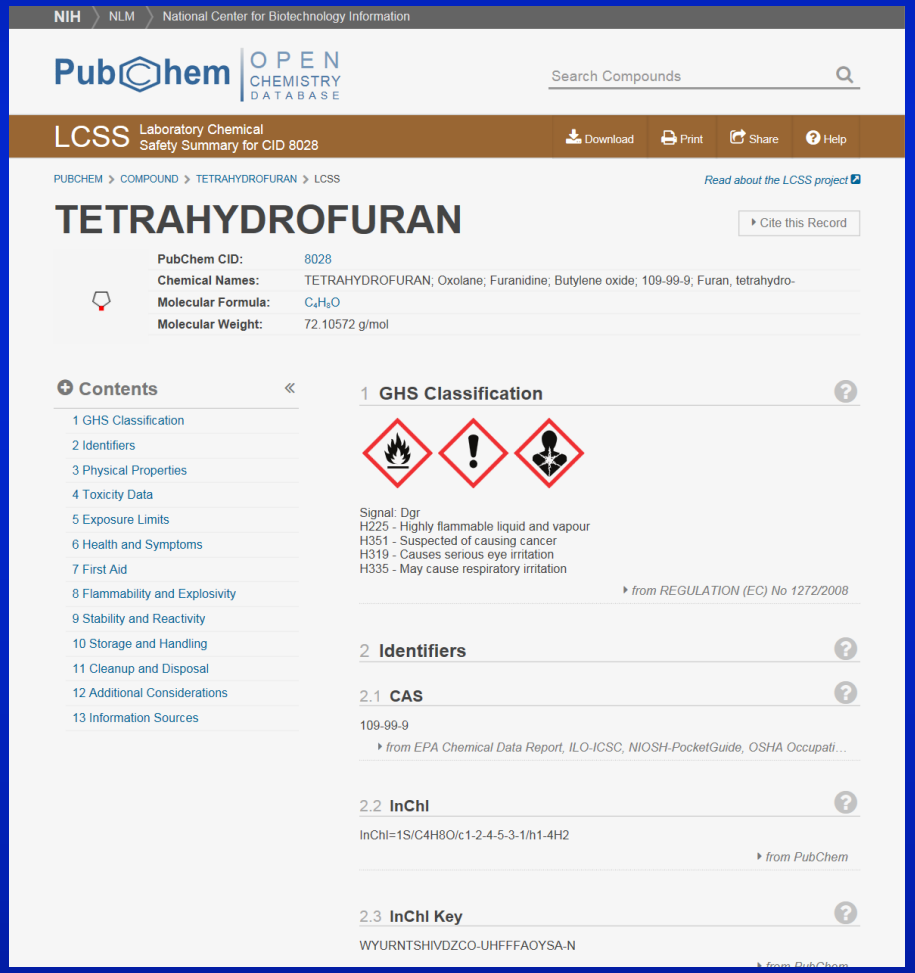
Source: Google Analytics

PubChem Laboratory Chemical Safety Summary (LCSS)

(https://pubchem.ncbi.nlm.nih.gov/lcss)

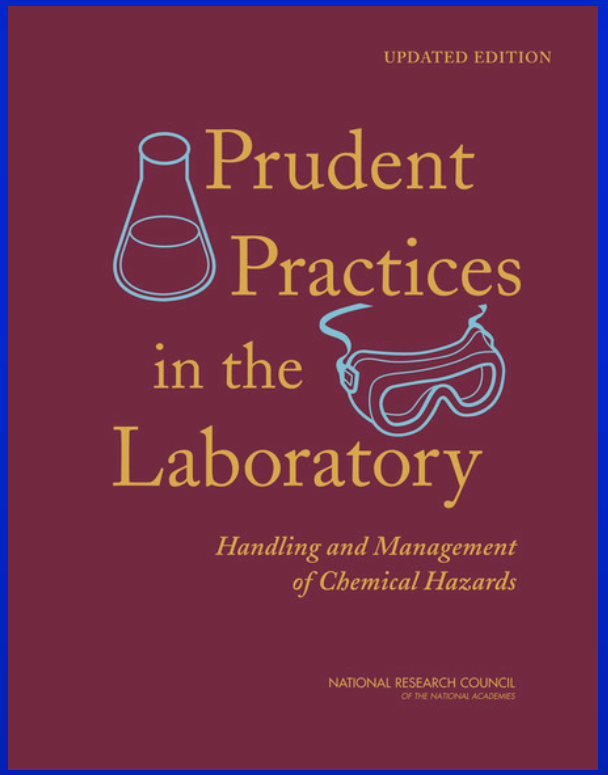
❑ PubChem LCSS

- A concise view of health and safety data for a given compound.
  - Flammability
  - Toxicity
  - Exposure limits
  - Exposure symptoms
  - First aid
  - Handling
  - Spill clean up
  - Many others …….



❑ PubChem LCSS

- Based on the format described by the National Research Council in "Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards" (2011)



Free PDF available from http://www.nap.edu/catalog/12654/prudent-practices-in-the-laboratory-handling-and-management-of-chemical.

❑ PubChem LCSS

- Supports chemical risk assessment in laboratories
- Provides information relevant to use of chemicals as described in the OSHA lab standard†.
  → Supplements the material safety data sheet (MSDS).

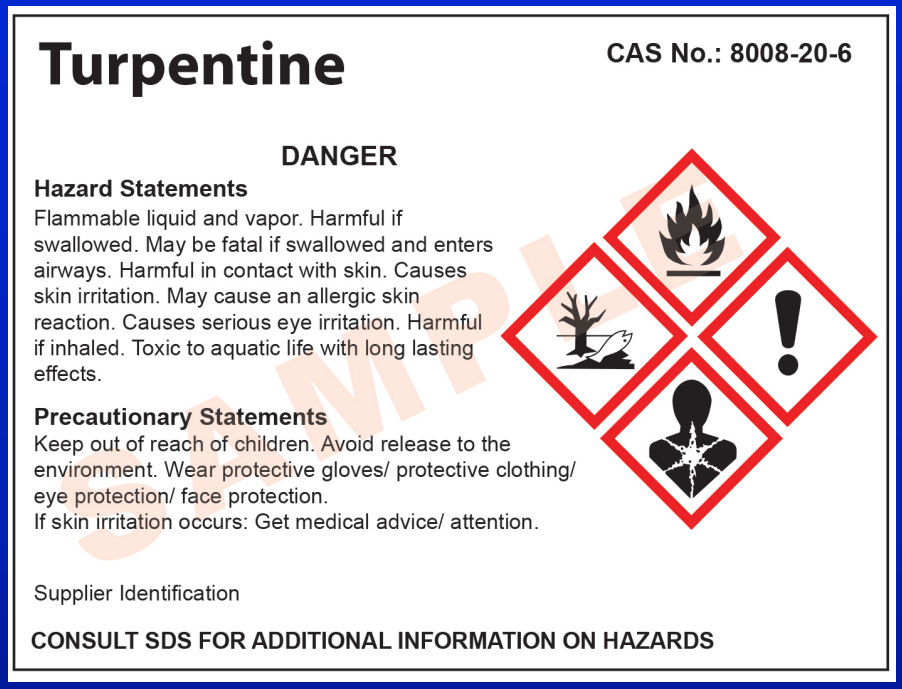
† *Toxic and Hazardous Substances: National Research Council Recommendations Concerning Chemical Hygiene in Laboratories (Non-Mandatory)*. 29 CFR §1910.1450 Appendix A. Occupational Safety and Health Administration (OSHA), Washington, DC, 2012. https://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=10107 (accessed Mar. 10, 2016).

❑ PubChem LCSS Coverage

- Globally Harmonized System of Classification and Labeling of Chemicals (GHS) (http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)
  - International standard for technical criteria for classifying chemicals according to their health, physical, and environmental hazards.

❑ PubChem LCSS Coverage

- Globally Harmonized System of Classification and Labeling of Chemicals (GHS) (http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)
  - Hazard communication requirements for product labels and safety data sheets.



Turpentine

CAS No.: 8008-20-6

DANGER

Hazard Statements

Flammable liquid and vapor. Harmful if swallowed. May be fatal if swallowed and enters airways. Harmful in contact with skin. Causes skin irritation. May cause an allergic skin reaction. Causes serious eye irritation. Harmful if inhaled. Toxic to aquatic life with long lasting effects.

Precautionary Statements

Keep out of reach of children. Avoid release to the environment. Wear protective gloves/ protective clothing/ eye protection/ face protection.
If skin irritation occurs: Get medical advice/ attention.

Supplier Identification

CONSULT SDS FOR ADDITIONAL INFORMATION ON HAZARDS

❑ PubChem LCSS Coverage

- Globally Harmonized System of Classification and Labeling of Chemicals (GHS) (http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html)

  - Global basis for harmonization of rules and regulations on hazardous chemicals

    → Improves regulatory efficiency
    Facilitates international trades

❑ PubChem LCSS Coverage

- PubChem LCSS is available for 5,130 compounds with GHS classification information

GHS classification source	# Compounds
EU REGULATION (EC) No 1272/2008 (a EU Regulation for classification, labelling and packaging of substances and mixtures)	3,263
International Chemical Safety Cards (ICSC) at International Labor Organization (ILO)	532
Chemical Management Center (CMC) at Japan National Institute of Technology and Evaluation (NITE)	2,723
Hazardous Substance Information System (HSIS) at Safe Work Australia	3,191
Total Unique Compounds	5,130

❑ PubChem LCSS Data Contents

- GHS Classification
- Synonyms
- Identifiers
- Physical Properties
- Toxicity Data
- Exposure Limits
- Health and Symptoms
- First Aid
- Flammability & Explosivity
- Stability and Reactivity
- Storage and Handling
- Cleanup and Disposal
- Additional Considerations

Data contents in PubChem Laboratory Chemical Safety Summary (LCSS)

- As of October 30, 2015
- Abbreviations in brackets indicate data sources.

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Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]
Odor [HSDB]
Boiling Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Melting Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]
Flash Point [HSDB, ICSC, NIOSH, OSHA]
Solubility [CAMEO, DRGBNK, HSDB, ICSC, NCI, NIOSH]
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Vapor Density [CAMEO, HSDB, ICSC, OSHA]
Vapor Pressure [CAMEO, HSDB, ICSC, NIOSH, OSHA]
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Decomposition [HSDB, ICSC]
Corrosivity [HSDB]
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Recommended Exposure Limit (REL) [NIOSH, OSHA]
Permissible Exposure Limit (PEL) [NIOSH, OSHA]
REL-Time-Weighted Average Concentration (REL-TWAC) [OSHA]
REL-Short-Term Exposure Limit (REL-STEL) [OSHA]
REL-Ceiling (REL-C) [OSHA]
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Effects of Long Term Exposure [ICSC]
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Radiation Limits and Potential [HSDB]
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Disposal Methods [HSDB]
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Toxic Combustion Products [HSDB]
Other Hazardous Reactions [HSDB]

http://confchem.ccce.divched.org/sites/confchem.ccce.divched.org/files/2015FallCCCENLP3fig5.pdf

❑ PubChem LCSS Data Sources

- CDC ATSDR Toxic Substance Portal
- NOAA CAMEO Chemicals
- Regulation (EC) No 12 1272/2008
- DrugBank
- EPA Air Toxics
- EPA Chemical Data Report
- HSDB
- ILO ICSC
- NCI Investigational Drugs
- NIOSH Pocket Guide
- OSHA Occupational Chemical DB
- PubChem

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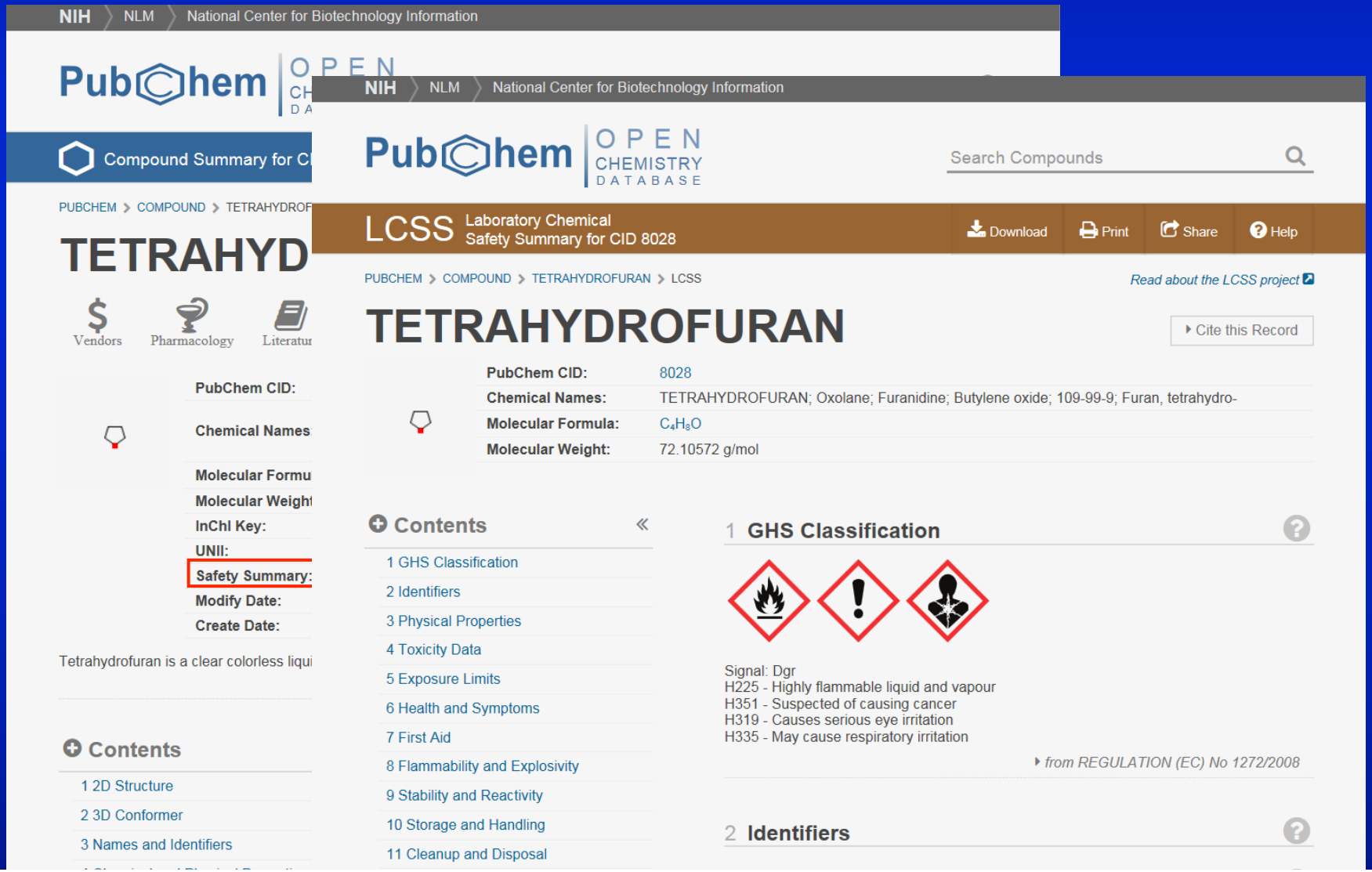
❑ Access to PubChem LCSS



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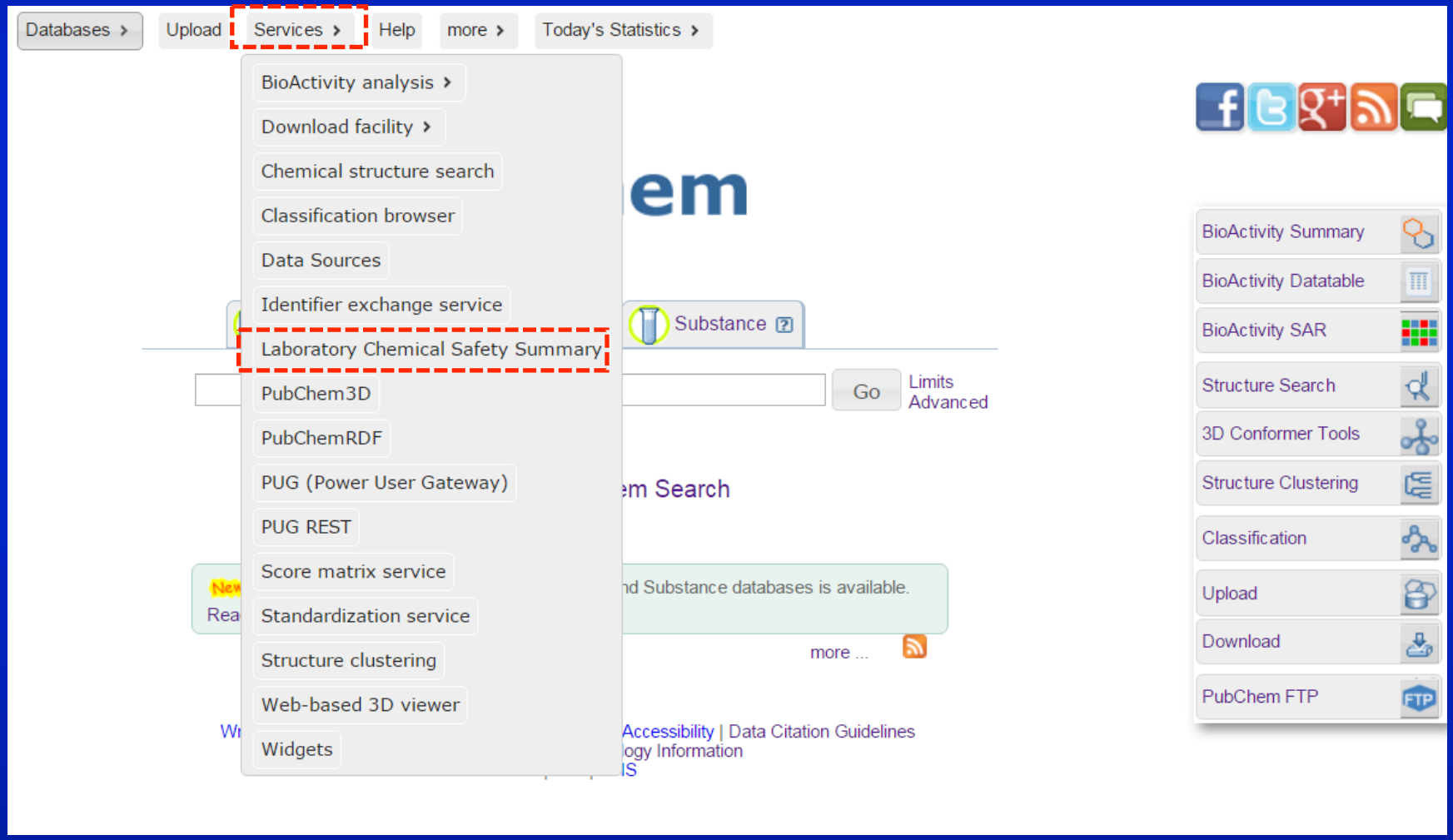

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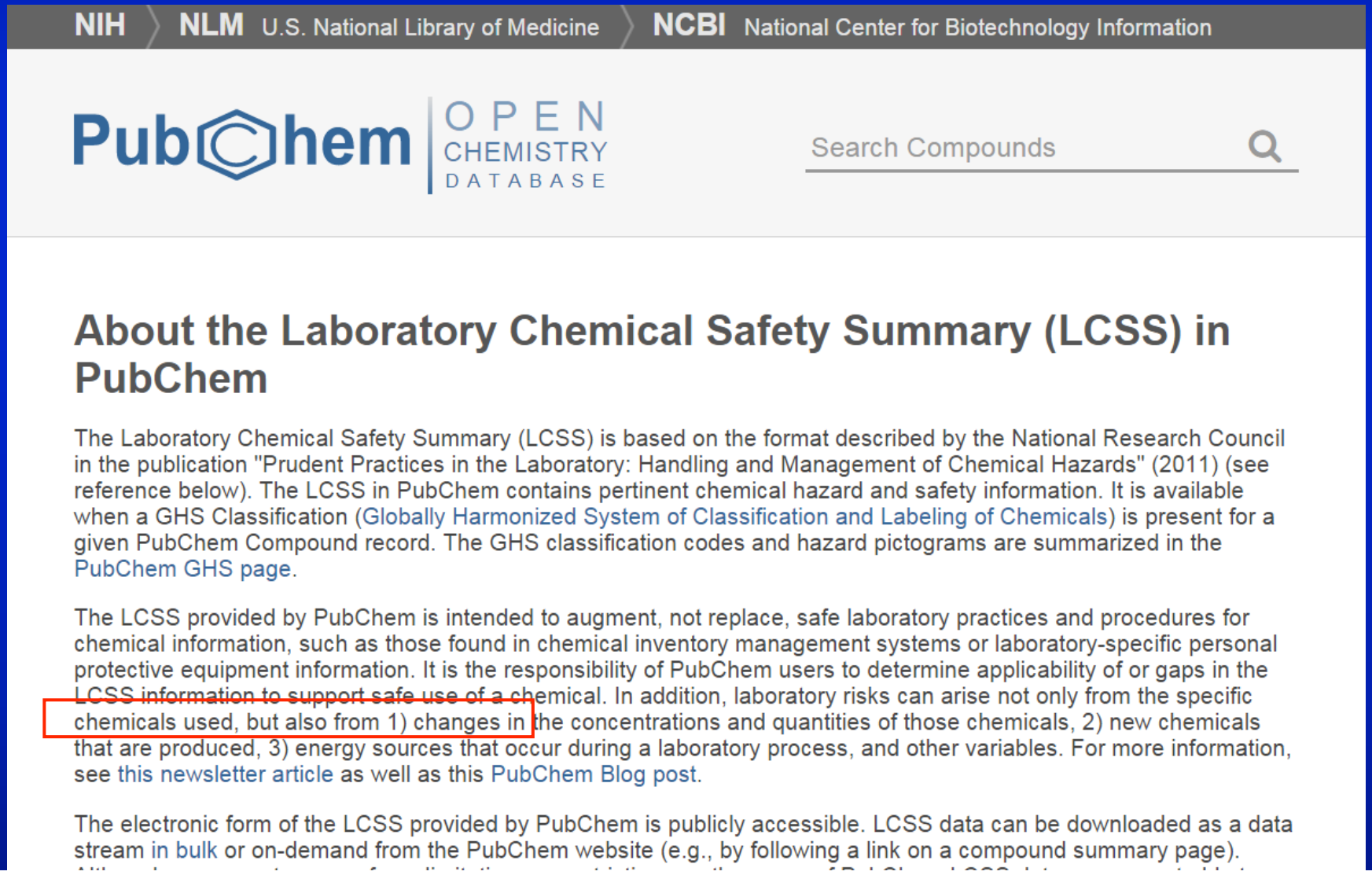

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1. 

Direct blue 301; 124605-82-9

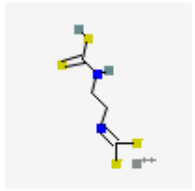
MW: 1278.433288 g/mol MF: $C_{33}H_{22}Li_4N_8Na_{16}O_{14}S_4$

IUPAC name: tetralithium;(3Z)-5-amino-3-[[4-[[4-[(2Z)-2-(8-amino-1-oxo-3...

Create Date: 2016-01-08

CID: 102601870

Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds

2. 

12427-38-2

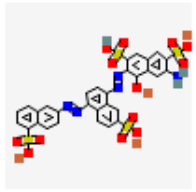
MW: 265.301885 g/mol MF: $C_4H_6MnN_2S_4$

IUPAC name: 2-(dithiocarboxyamino)ethyliminomethanedithiolate;manganese(...

Create Date: 2015-12-27

CID: 102460656

Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds PubMed (MeSH Keyword)

3. 

107246-80-0; 6-Amino-4-hydroxy-3-[7-sulfo-4-(5-sulfo-2-naphthylazo)-1-naphthylazo]-2,7-naphthalenedisulfonic acid tetralithium salt

MW: 811.505680 g/mol MF: $C_{30}H_{17}Li_4N_5O_{13}S_4$

IUPAC name: tetralithium;3-amino-5-oxido-7-sulfo-6-[[7-sulfonato-4-[(5-s...

Create Date: 2015-12-24

CID: 102117455

Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds

ISODRIN; 465-73-6

NIH > NLM > National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE

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Compound Summary for CID 102601870 | Download | Print | Share | Help

PUBCHEM > COMPOUND > DIRECT BLUE 301

Direct Blue 301

Cite this Record

$ Vendors

PubChem CID:	102601870
Chemical Names:	Direct blue 301; 124605-82-9; More...
Molecular Formula:	$C_{33}H_{22}Li_4N_8Na_{16}O_{14}S_4$
Molecular Weight:	1278.433288 g/mol
InChI Key:	DLNIVGKCMNJVJK-VVOGLQFISA-J
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)
Modify Date:	2016-03-15
Create Date:	2016-01-08

Contents

1 2D Structure

NIH › NLM › National Center for Biotechnology Information

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LCSS Laboratory Chemical Safety Summary for CID 102601870

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PUBCHEM › COMPOUND › DIRECT BLUE 301 › LCSS

Read about the LCSS project

Direct Blue 301

Cite this Record

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Contents

1 GHS Classification

Signal: Warning

GHS Hazard Statements
H317: May cause an allergic skin reaction [Warning Sensitization, Skin - Category 1]
H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard - Category 2]

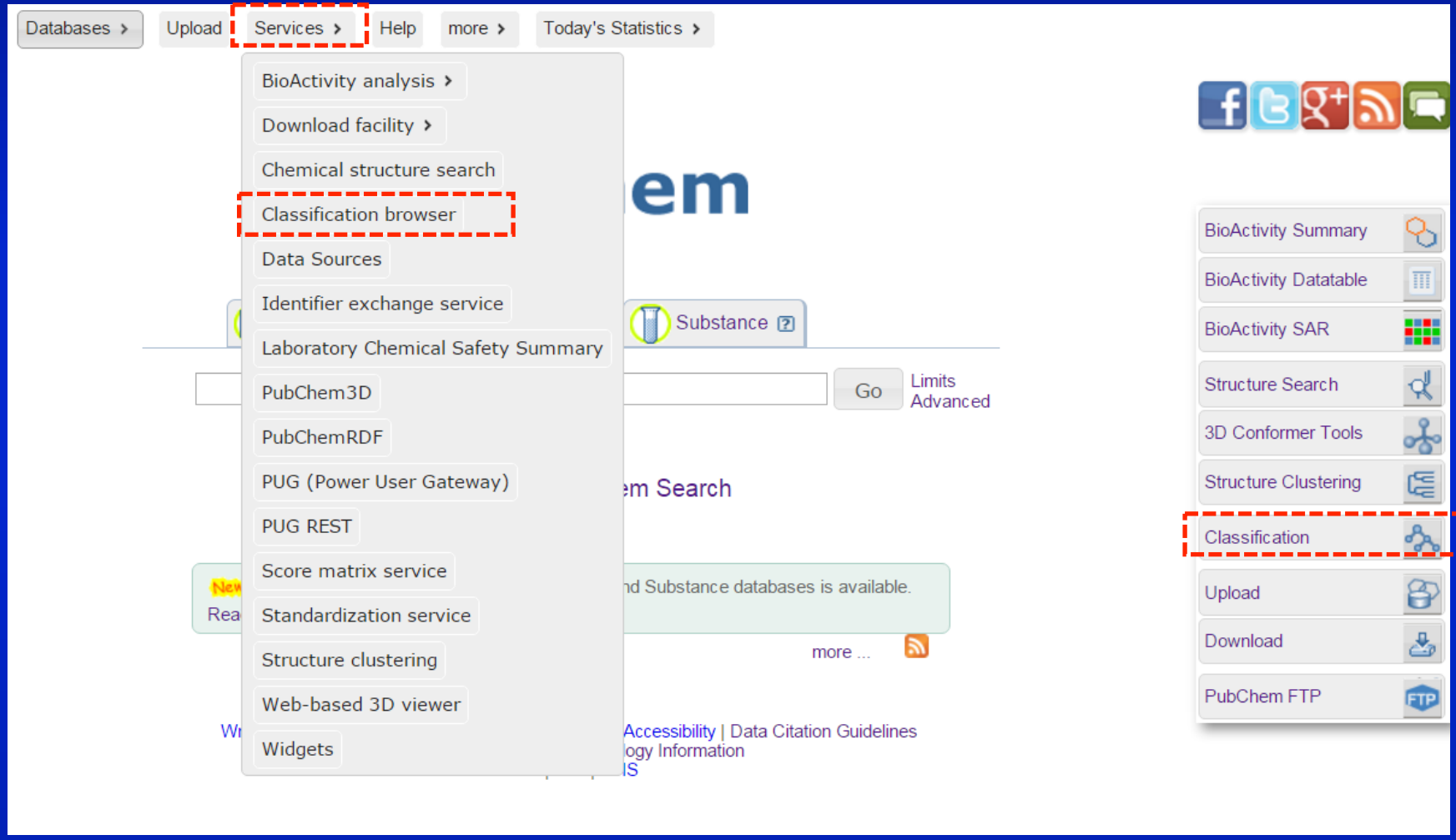
Precautionary Statements

❑ Access to PubChem LCSS

➢ Classification Browser (https://pubchem.ncbi.nlm.nih.gov/classification)

- Browse PubChem data using a classification of interest.
- Search for records annotated with the desired classification/term.
- Current available ontologies/classifications.

  - MeSH
  - ChEBI
  - FDA Pharm Classes
  - KEGG
  - LIPID MAPS classification system for lipids
  - PubChem Compound Table of Contents
  - PubChem BioAssay Classification
  - WHO ATC Code (Anatomical Therapeutic Chemical Classification System)
  - WIPO International Patent Classification 2014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Classification browser
Data Sources
Identifier exchange service
Laboratory Chemical Safety Summary
PubChem3D
PubChemRDF
PUG (Power User Gateway)
PUG REST
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Structure clustering
Web-based 3D viewer
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BioActivity Summary
BioActivity Datatable
BioActivity SAR
Structure Search
3D Conformer Tools
Structure Clustering
Classification
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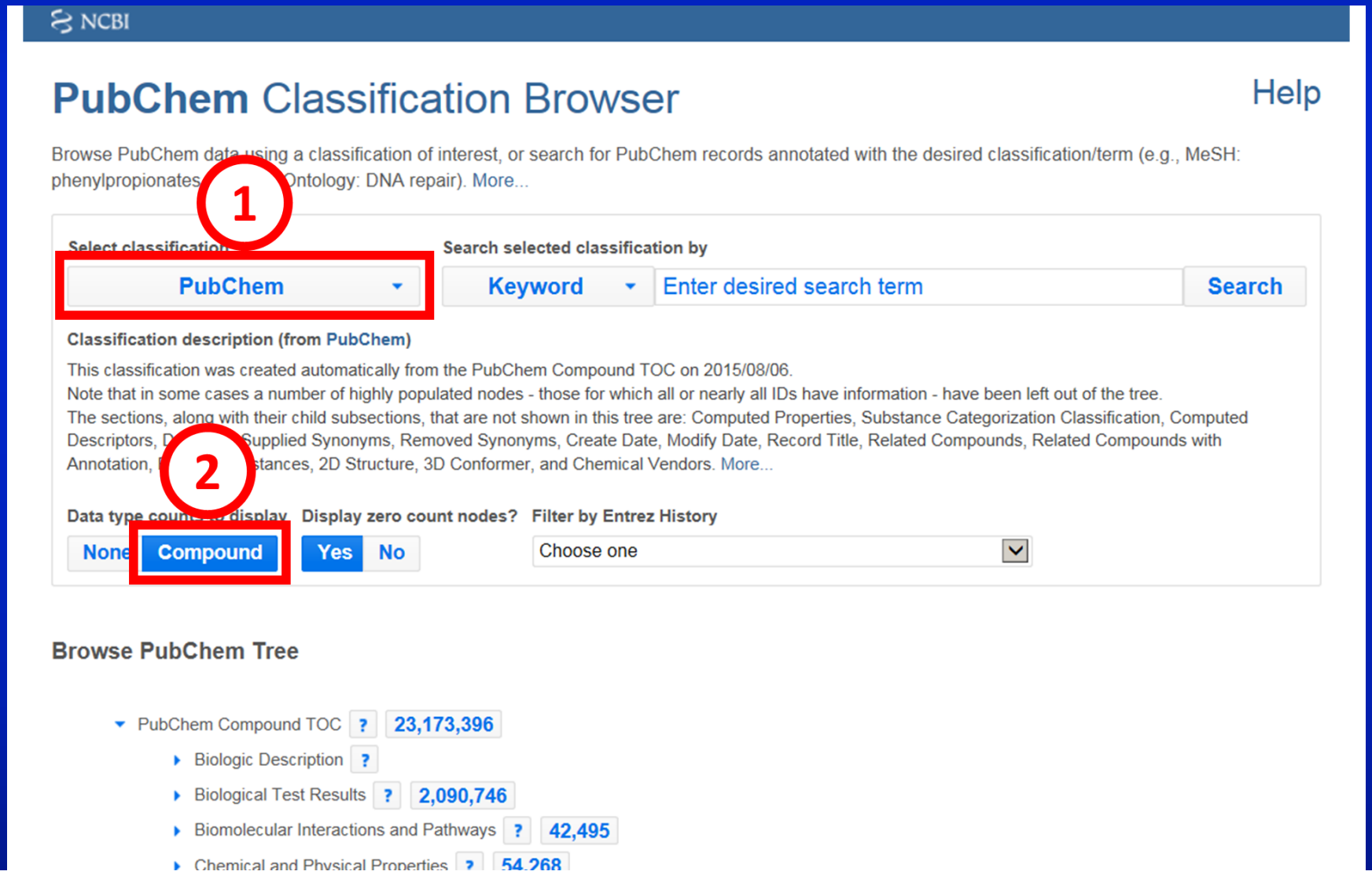
❑ Access to PubChem LCSS



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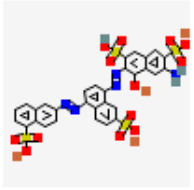
3. 

107246-80-0; 6-Amino-4-hydroxy-3-[7-sulfo-4-(5-sulfo-2-naphthylazo)-1-naphthylazo]-2,7-naphthalenedisulfonic acid tetralithium salt

MW: 811.505680 g/mol MF: $C_{30}H_{17}Li_4N_5O_{13}S_4$

IUPAC name: tetralithium;3-amino-5-oxido-7-sulfo-6-[[7-sulfonato-4-[(5-s...

Create Date: 2015-12-24

CID: 102117455

Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds

ISODRIN; 465-73-6

❑ Access to PubChem LCSS

- PubChem LCSS data are downloadable in XML, JSON, & ASN.1
- Bulk download via FTP
  (ftp://ftp.ncbi.nlm.nih.gov/pubchem/Compound/Extras/CID-LCSS.xml.gz)
- Additional PubChem data are available
  (through programmatic access route called PUG-REST)

Customization of LCSS
for specific procedures at individual institutions

❑ Limitations

- PubChem aggregates data from multiple sources without thorough accuracy check
  → Users need to review the accuracy and variability of data
- Ambiguity in name-structure associations
  formaldehyde vs. formalin (saturated water solution)
- Different units, precisions, and measurement conditions

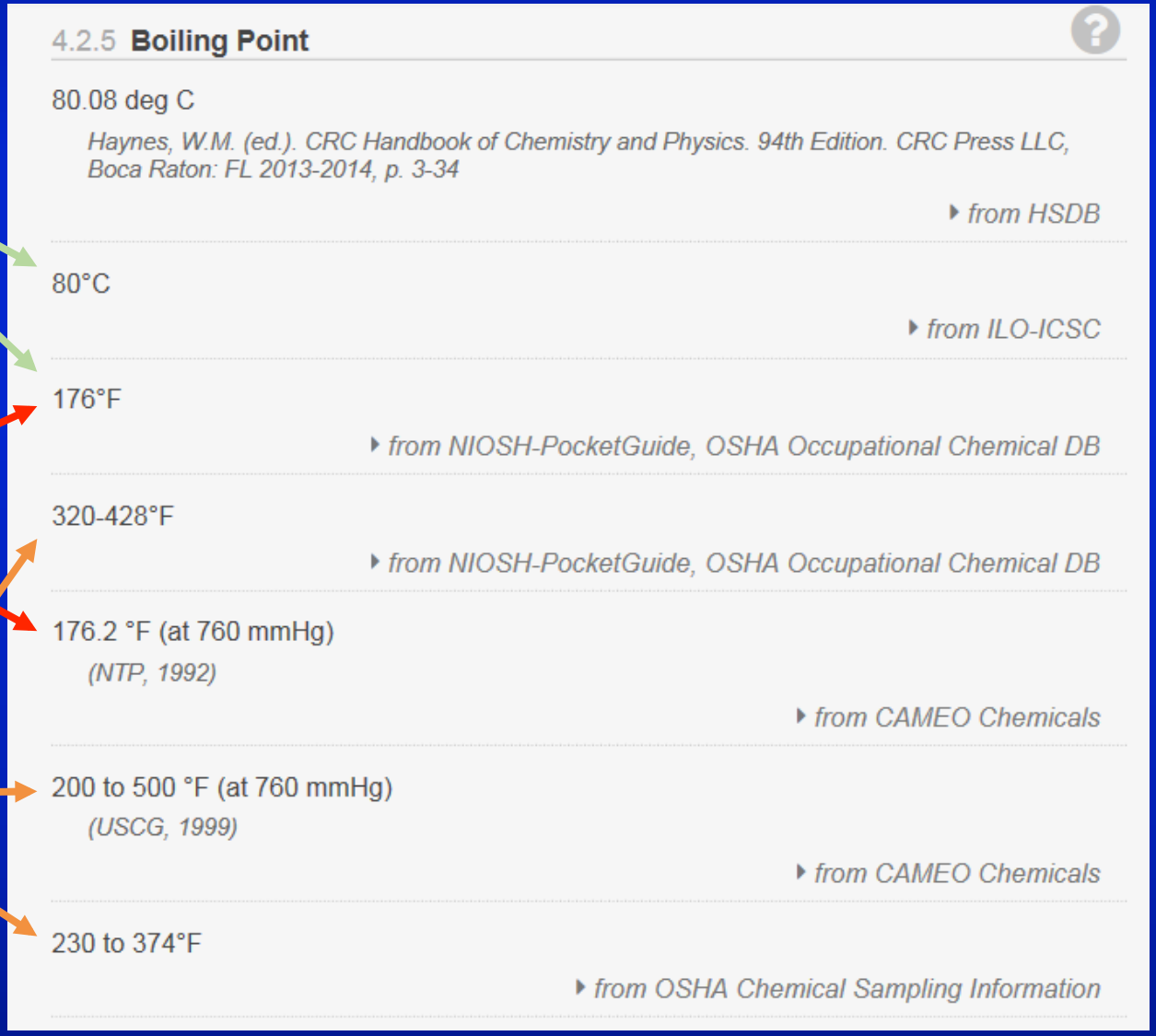
❑ Limitations

Different units

Different conditions & precisions

Naphtha (coal tar)

Mixture of Benzene, toluene & xylenes



4.2.5 **Boiling Point**

80.08 deg C

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 94th Edition. CRC Press LLC, Boca Raton: FL 2013-2014, p. 3-34

from HSDB

80°C

from ILO-ICSC

176°F

from NIOSH-PocketGuide, OSHA Occupational Chemical DB

320-428°F

from NIOSH-PocketGuide, OSHA Occupational Chemical DB

176.2 °F (at 760 mmHg)

(NTP, 1992)

from CAMEO Chemicals

200 to 500 °F (at 760 mmHg)

(USCG, 1999)

from CAMEO Chemicals

230 to 374°F

from OSHA Chemical Sampling Information

❑ Comparison between data sources

- GHS information is from four different sources.
  - EU Regulation
  - ILO
  - Japanese NITE
  - Safe Work Australia

Sometimes they provide very different GHS information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BioAssay
Compound
Substance
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Limits
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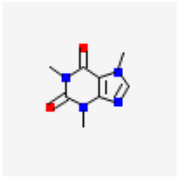
1. 

caffeine; Methyltheobromine; Guaranine ...

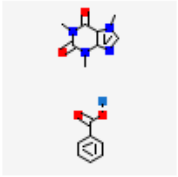
MW: 194.190600 g/mol MF: $C_8H_{10}N_4O_2$

IUPAC name: 1,3,7-trimethylpurine-2,6-dione

Create Date: 2004-09-16

CID: 2519

Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds PubMed (MeSH Keyword) Active in 124 of 2792 BioAssays

2. 

Caffeine sodium benzoate; Sodium **caffeine** benzoate; Annaca ...

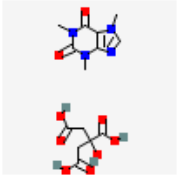
MW: 338.293769 g/mol MF: $C_{15}H_{15}N_4NaO_4$

IUPAC name: sodium;1,3,7-trimethylpurine-2,6-dione;benzoate

Create Date: 2008-02-05

CID: 23669229

Summary Similar Compounds Mixture/Component Compounds

3. 

Caffeine citrate; **Caffeine**, Citrated; 69-22-7 ...

MW: 386.314120 g/mol MF: $C_{14}H_{18}N_4O_9$

IUPAC name: 2-hydroxypropane-1,2,3-tricarboxylic acid;1,3,7-trimethylpur...

Create Date: 2005-03-26

CID: 6241

Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds PubMed (MeSH Keyword) Active in 1 of 148 BioAssays

Actions on your results

- **BioActivity Analysis** — Analyze the BioActivities of the compounds
- **Structure Clustering** — Cluster structures based on structural similarity
- **Structure Download** — Download the structures in various formats
- **Pathways** — Analyze pathways containing the compounds

Refine your results • What's this?

Chemical Properties

Rule of 5 (144)

BioActivity Experiments

BioAssays, Active (73)

BioAssays, Tested (109)

Protein 3D Structures (2)

Thermostabilised Adenosine A2a Receptor In Complex With Caffeine (1)

Crystal Structure Of A Chitinase Crchi1 From The Nematophagous Fungus

NIH › NLM › National Center for Biotechnology Information

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

Compound Summary for CID 2519 | Download | Print | Help

PUBCHEM › COMPOUND › CAFFEINE

Caffeine

Cite this Record

Vendors | Drug Information | Pharmacology | Literature | Patents | Bioactivities

PubChem CID:	2519
Chemical Names:	Caffeine; Methyltheobromine; Guaranine; 1,3,7-Trimethylxanthine; Cafeina; Koffein; More...
Molecular Formula:	$C_8H_{10}N_4O_2$
Molecular Weight:	194.1906 g/mol
InChI Key:	RYYVLZVUVIJVGH-UHFFFAOYSA-N
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)
Modify Date:	2016-03-15
Create Date:	2004-09-16

LCSS Laboratory Chemical Safety Summary for CID 2519

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PUBCHEM > COMPOUND > CAFFEINE > LCSS

Read about the LCSS project

Caffeine

Cite this Record

PubChem CID:	2519
Chemical Names:	Caffeine; Methyltheobromine; Guaranine; 1,3,7-Trimethylxanthine; Cafeina; Koffein
Molecular Formula:	$C_8H_{10}N_4O_2$
Molecular Weight:	194.1906 g/mol

Contents

1 GHS Classification

Signal: Warning

GHS Hazard Statements
H302: Harmful if swallowed [Warning Acute toxicity, oral - Category 4]

Precautionary Statements
P264: Wash ... thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P301+P312: IF SWALLOWED: call a POISON CENTER/doctor/... IF you feel unwell.
P330: Rinse mouth.
P501: Dispose of contents/container to ...

from EU REGULATION (EC) No 1272/2008

View GHS Classification from all (3) sources.

PUBCHEM > COMPOUND > CAFFEINE > SAFETY-AND-HAZARDS > HAZARDS-IDENTIFICATION > GHS-CLASSIFICATION

Caffeine

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from EU REGULATION (EC) No 1272/2008, Safe Work Australia - HSIS

EU & Australia provided the same information on caffeine

Signal: Danger

GHS Hazard Statements
H301: Toxic if swallowed [Danger Acute toxicity, oral - Category 3]
H332: Harmful if inhaled [Warning Acute toxicity, inhalation - Category 4]
H360: May damage fertility or the unborn child [Danger Reproductive toxicity - Category 1A, 1B]
H402: Harmful to aquatic life [Hazardous to the aquatic environment, acute hazard - Category 3]
H412: Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard - Category 3]

Precautionary Statements
P201: Obtain special instructions before use.
P202: Do not handle until all safety precautions have been read and understood.
P261: Avoid breathing dust/fume/gas/mist/vapors/spray.
P264: Wash ... thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P273: Avoid release to the environment.
P281: Use personal protective equipment as required.
P301+P310: IF SWALLOWED: Immediately call a POISON CENTER/doctor/...
P304+P312: IF INHALED: Call a POISON CENTER/doctor/... if you feel unwell.
P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P308+P313: IF exposed or concerned: Get medical advice/attention.
P312: Call a POISON CENTER or doctor/... if you feel unwell.
P321: Specific treatment (see ... on this label).
P330: Rinse mouth.
P405: Store locked up.
P501: Dispose of contents/container to ...

from NITE-CMC

Japan's GHS classifications are very different.

Signal: Danger

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H301: Toxic if swallowed [Danger Acute toxicity, oral - Category 3]
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▾ *from NITE-CMC*

Source Name: NITE-CMC
Record Name: caffeine
URL: http://www.safe.nite.go.jp/english/ghs/08-mhlw-0136e.html
Description: The chemical classification in this section was conducted by the Chemical Management Center (CMC) of Japan National Institute of Technology and Evaluation (NITE) in accordance with GHS Classification Guidance for the Japanese Government, and is intended to provide a reference for preparing GHS labelling and SDS for users.

GHS Classification Result

Chemical Name: caffeine
CAS: 58-08-2

Result:

ID: 20A2140
Classifier: Ministry of Health, Labour and Welfare (MHLW), Ministry of the Environment (MOE)
Year Classified: FY2008
Reference Manual: GHS Classification Guidance by the Japanese Government (Sep, 2008)

PHYSICAL HAZARDS

	Hazard class	Classification	Symbol	Signal word	Hazard statement	Precautionary statement	Rationale for the classification
1	Explosives	Not applicable	-	-	-	-	There are no chemical groups associated with explosive properties present in the molecules.
2	Flammable gases (including chemically unstable gases)	Not applicable	-	-	-	-	Solid (GHS definition)
3	Aerosols	Not applicable	-	-	-	-	Not aerosol products.
4	Oxidizing gases	Not applicable	-	-	-	-	Solid (GHS definition)
5	Gases under pressure	Not applicable	-	-	-	-	Solid (GHS definition)
6	Flammable liquids	Not applicable	-	-	-	-	Solid (GHS definition)
7	Flammable solid	Classification not possible	-	-	-	-	No data available.
8	Self-reactive substances and mixtures	Not applicable	-	-	-	-	There are no chemical groups present in the molecule associated with explosive or self-reactive properties.
9	Pyrophoric liquids	Not applicable	-	-	-	-	Solid (GHS definition)
10	Pyrophoric solids	Not classified	-	-	-	-	Its autoignition point is 540degC (IUCLID (2000)),

Symbol	Signal word	Hazard statement	Precautionary statement	Rationale for the classification
	Danger	H301: Toxic if swallowed	P301+P310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. P264: Wash ... thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P321: Specific treatment (see ... on this label). P330: Rinse mouth. P405: Store locked up. P501: Dispose of contents/container to ...	Since its twelve LD50 values for rats (261 – 383, 200 – 400, 192, 483, 233, 355, 247, 344, 421, 700, 50 – 500, and 261 – 383 mg/kg) have been reported in List 1 literature, and seven of them are within the guidance values of Category 3 and five Category 4 (SIDS (accessed in September 2008)), the substance was classified into Category 3.
		Vapours)						
							P304+P340: IF INHALED: Remove victim to fresh air	

❑ Summary

- PubChem LCSS is a concise view of health and safety information for a given compound
- Data are collected from many authoritative sources.
- Available to the public free of charge.
- Can be downloaded and annotated for customization.
- PubChem is actively collecting more GHS data to increase the LCSS coverage.

Thank you!