256th ACS National Meeting, Boston, August 2018

Chemical safety information in PubChem

Jian Zhang*, Paul Thiessen, Asta Gindulyte, Evan Bolton

U.S. National Library of Medicine
National Center for Biotechnology Information

Outlines …

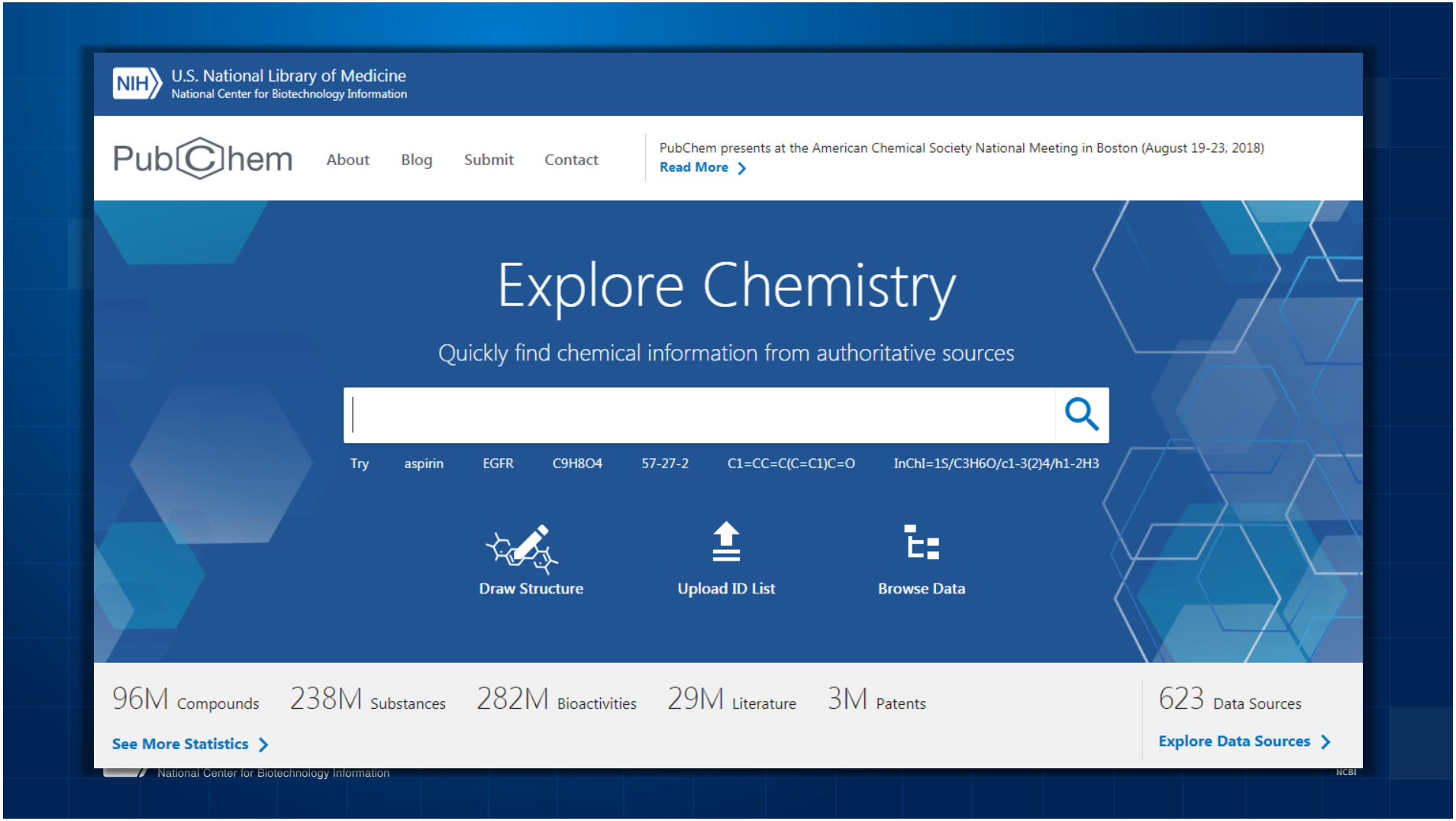
- What is PubChem .. an overview
- What data PubChem has ..
- Chemical safety data updates:
  - CAMEO Chemicals reactivity classification
  - Pistoia Alliance Chemical Safety Library reaction alerts
- How to access and retrieve safety data ..
- Summary

PubChem …

- A public chemical data repository .. A public data sharing platform to submit and share chemical data
- An open chemistry database .. Free chemical information
- A chemical information hub .. Data integrated from many sources with links to provenance
- A chemical information comparison center .. Data shopping comparison
- A chemical data index

Data Status .. https://pubchem.ncbi.nlm.nih.gov/

Compounds:	96,478,070
Substances:	247,243,896
BioAssays:	1,252,901
Tested Compounds:	2,978,541
Tested Substances:	4,994,132
BioActivities:	236,790,496
Protein Targets:	10,854
Gene Targets:	22,108
Data submitters:	623
Countries:	40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National Center for Biotechnology Information
PubChem
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PubChem presents at the American Chemical Society National Meeting in Boston (August 19-23, 2018)
Read More
Explore Chemistry
Quickly find chemical information from authoritative sources
Try
aspirin
EGFR
C9H8O4
57-27-2
C1=CC=C(C=C1)C=O
InChI=1S/C3H6O/c1-3(2)4/h1-2H3
Draw Structure
Upload ID List
Browse Data
96M Compounds
238M Substances
282M Bioactivities
29M Literature
3M Patents
623 Data Sources
See More Statistics
Explore Data Sources
National Center for Biotechnology Information
NCBI

Data …chemical centralized and beyond

- Structures – 2D, 3D, SMILES, InChI (key)
- Properties – MP, BP, MW, MF, solubility, flash point, vapor pressure, density, crystal, spectra, …
- Drug and medication
- Food additives
- Agrochemicals
- Safety and hazard
- Literature
- Patents
- Pathways
- Targets
- Toxicity
- Classifications
- Bioactivity
- Use and manufacture
- Nature products
- More ….

- Links to provenance

Where to find Chemical safety information in PubChem

- PubChem compound summary page – main web page that feed chemical information
- LCSS: Laboratory Chemical Safety Summary – Subset of chemical safety information page (Ref: *Prudent Practices in the Laboratory: Handling and Management of Chemical Hazards*)
- Classification browser – Classification tree style

Chemical safety inform summary …

3 major sections (headings)

- Chemical and Physical Properties
- Safety and Hazards
- Toxicity

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Contents

13 Safety and Hazards

13.1 Hazards Identification

13.1.1 GHS Classification

Signal: Danger

GHS Hazard Statements

Aggregated GHS information provide
Inventory. Each notification may be a

Reported as not meeting GHS hazard
please visit ECHA C&L website

Of the 52 notification(s) provided by

H302 (35.91%): Harmful if swallowed
H315 (80.13%): Causes skin irritation
H318 (77.52%): Causes serious eye da
H319 (18.59%): Causes serious eye ir
H372 (15.71%): Causes damage to or
target organ toxicity, repeated expos

Information may vary between notifi
percentage value in parenthesis indic
hazard codes. Only hazard codes wit

Precautionary Statement Codes

P260, P264, P270, P280, P301+P312,

Chemical safety information …

- Chemical and Physical Properties
- Safety and Hazard
- Toxicity

Safety and Hazards – 11 subheadings aligned with OSHA SDS

Hazards Identification
Safety and Hazard Properties
First Aid Measures
Fire Fighting Measures
Accidental Release Measures
Handling and Storage
Exposure Control and Personal Protection
Stability and Reactivity
Transport Information
Regulatory Information
Other Safety Information

Chemical safety information in compound summary …

Hazards Identification
- GHS Classification
- CLP Hazard Class and Category Codes
- EPA Safer Chemical
- Health Hazard
- Fire Hazard
- Explosion Hazard
- Hazards Summary
- Fire Potential
- Skin, Eye, and Respiratory Irritations

Safety and Hazard Properties
- LEL
- UEL
- Flammability
- Critical Temperature
- Critical Pressure
- Danger of Explosion
- NFPA Hazard Classification
- NFPA Fire Rating
- NFPA Reactivity Rating
- NFPA Health Rating
- NFPA Other

- TIHGas
- Isolation and Evacuation
- Spillage Disposal
- Cleanup Methods
- Disposal Methods
- Other Preventative Measures

Handling and Storage
- Nonfire Spill Response
- Safe Storage
- Storage Conditions

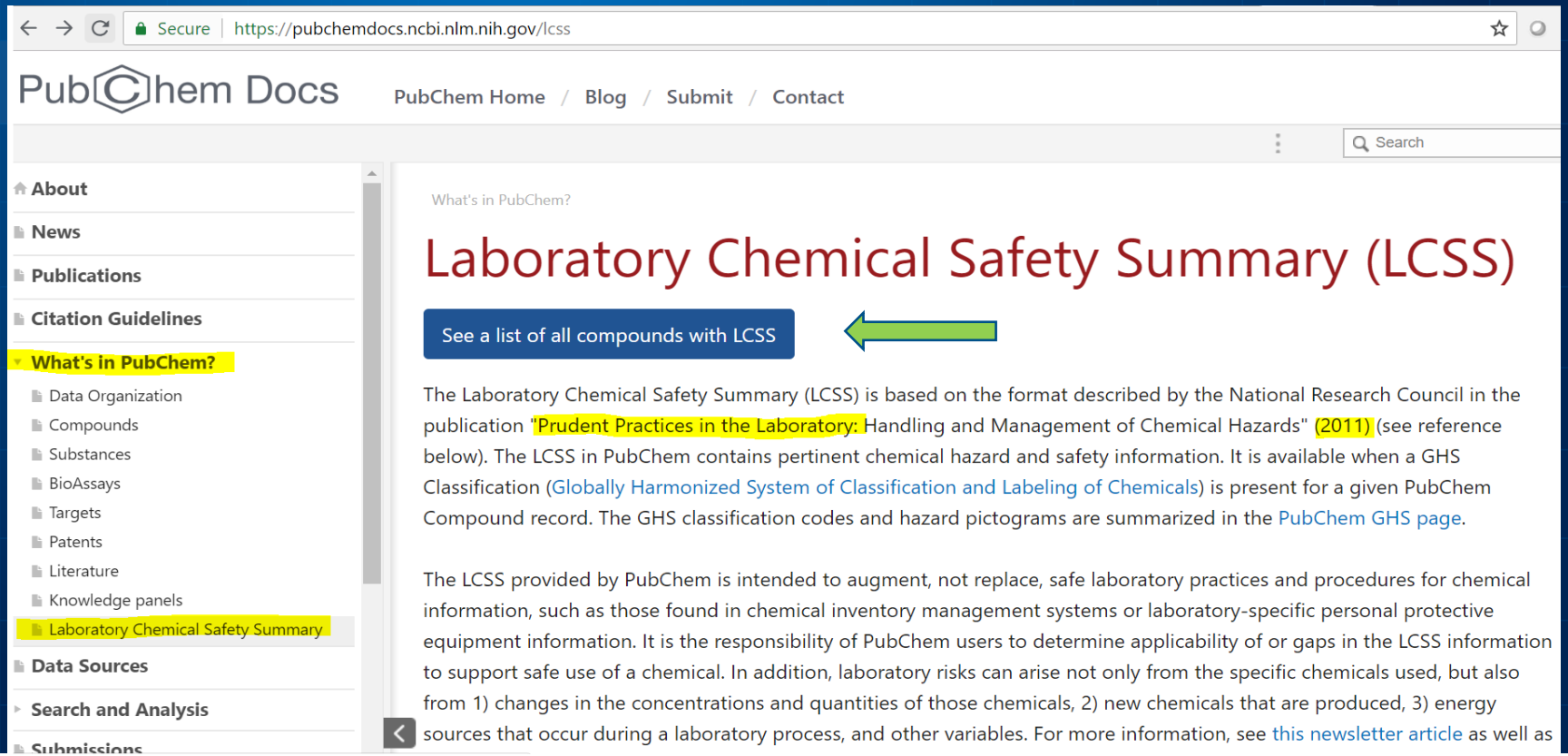
Exposure Control and Personal Protection
- REL
- PEL
- PEL-TWA
- PEL-STEL
- PEL-C
- REL-TWA
- REL-STEL
- REL-C
- IDLH
- Conversion
- Threshold Limit Values

Stability and Reactivity
- Air and Water Reactions
- Reactive Group
- Reactivity Alerts
- Reactivity Profile
- Reactivities and Incompatibilities

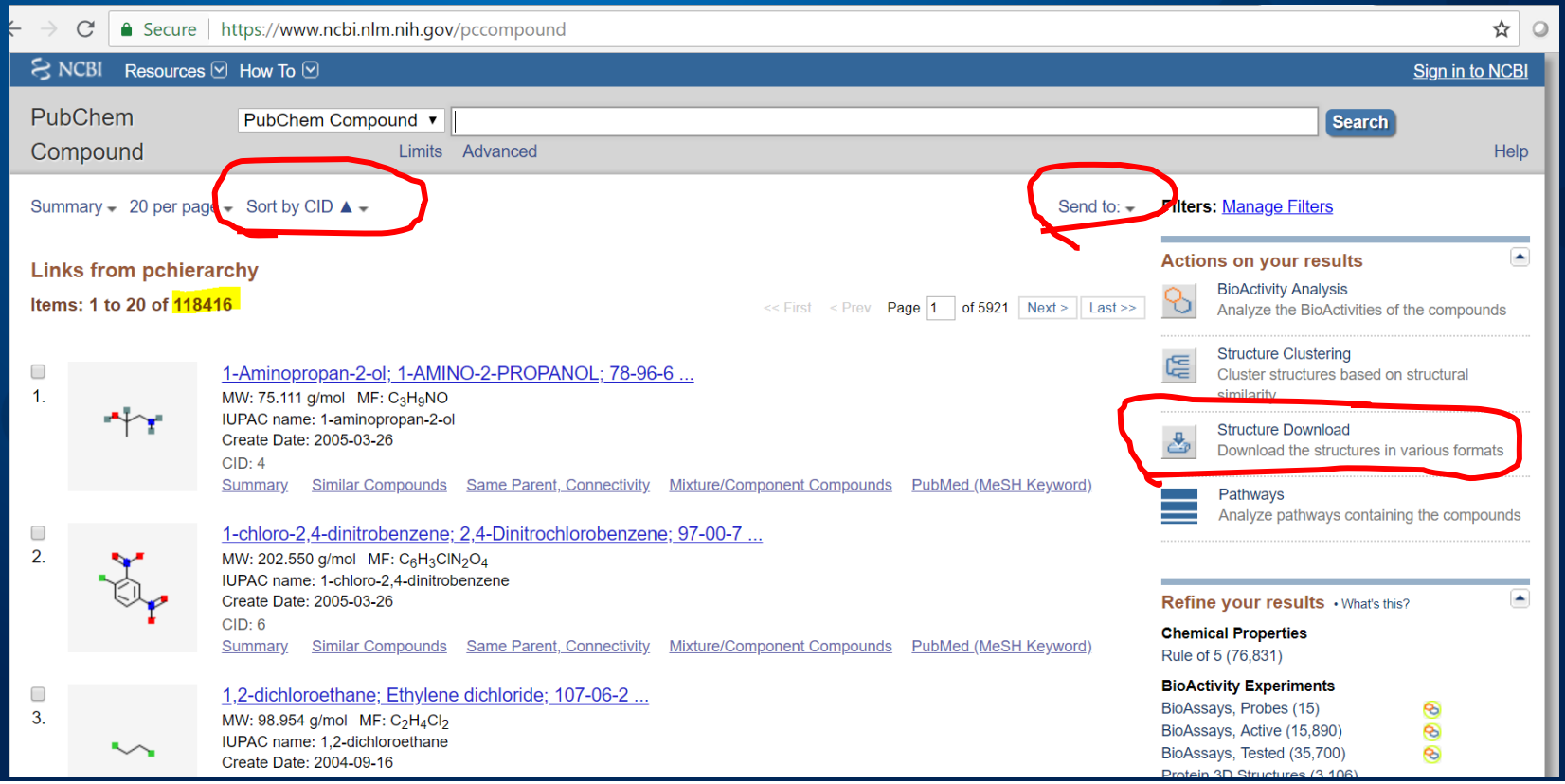
Transport Information
- DOT Emergency Guidelines
- Shipment Methods and Regulations
- DOT ID and Guide
- DOT Label
- Packaging and Labelling
- EC Classification
- UN Classification
- Emergency Response

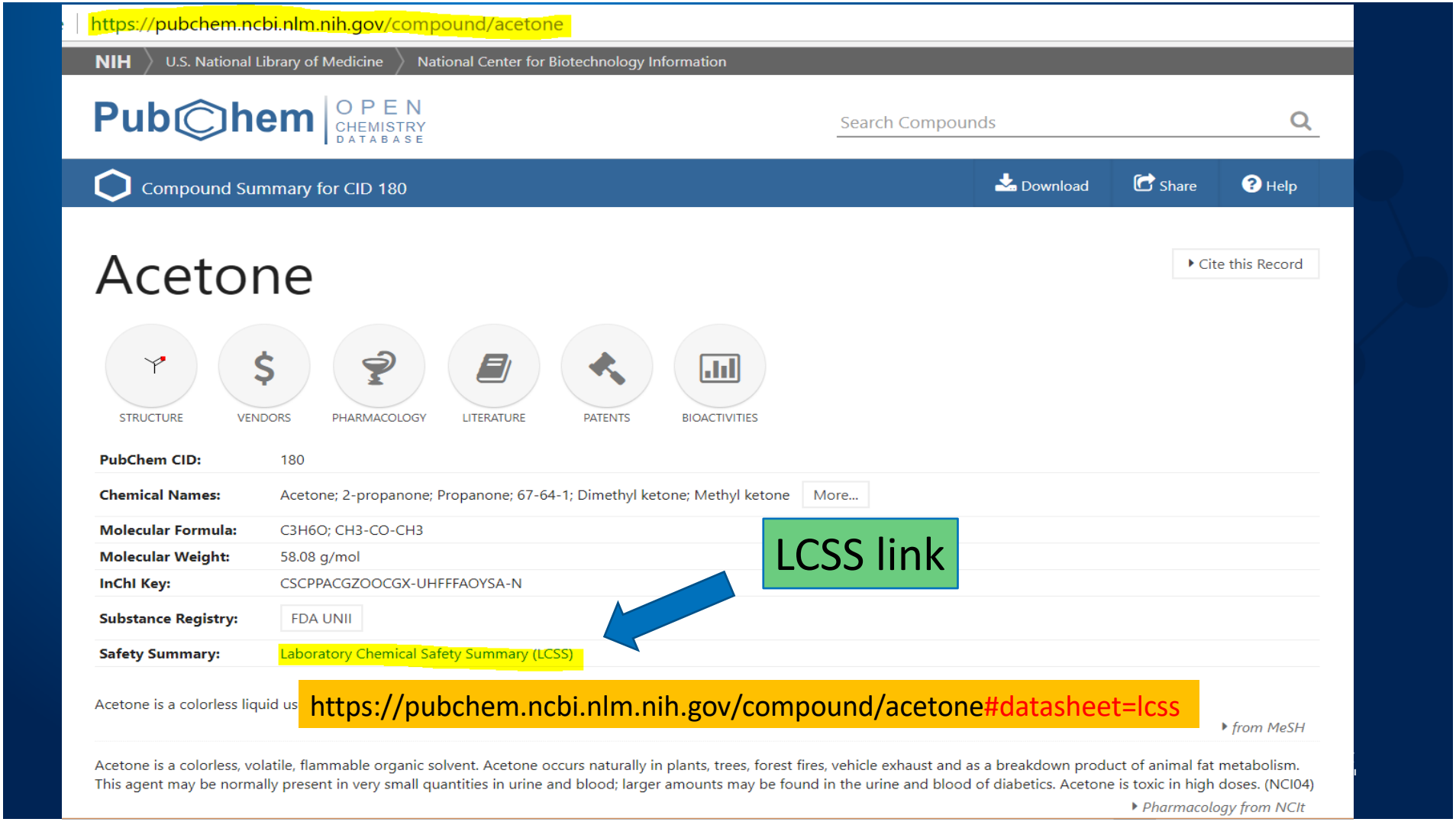
Regulatory Information
- DOT Emergency Response Guide
- Isolation Name
- Isolation Distance
- Atmospheric Standards
- Soil Standards
- Federal Drinking Water Standards
- Federal Drinking Water Guidelines

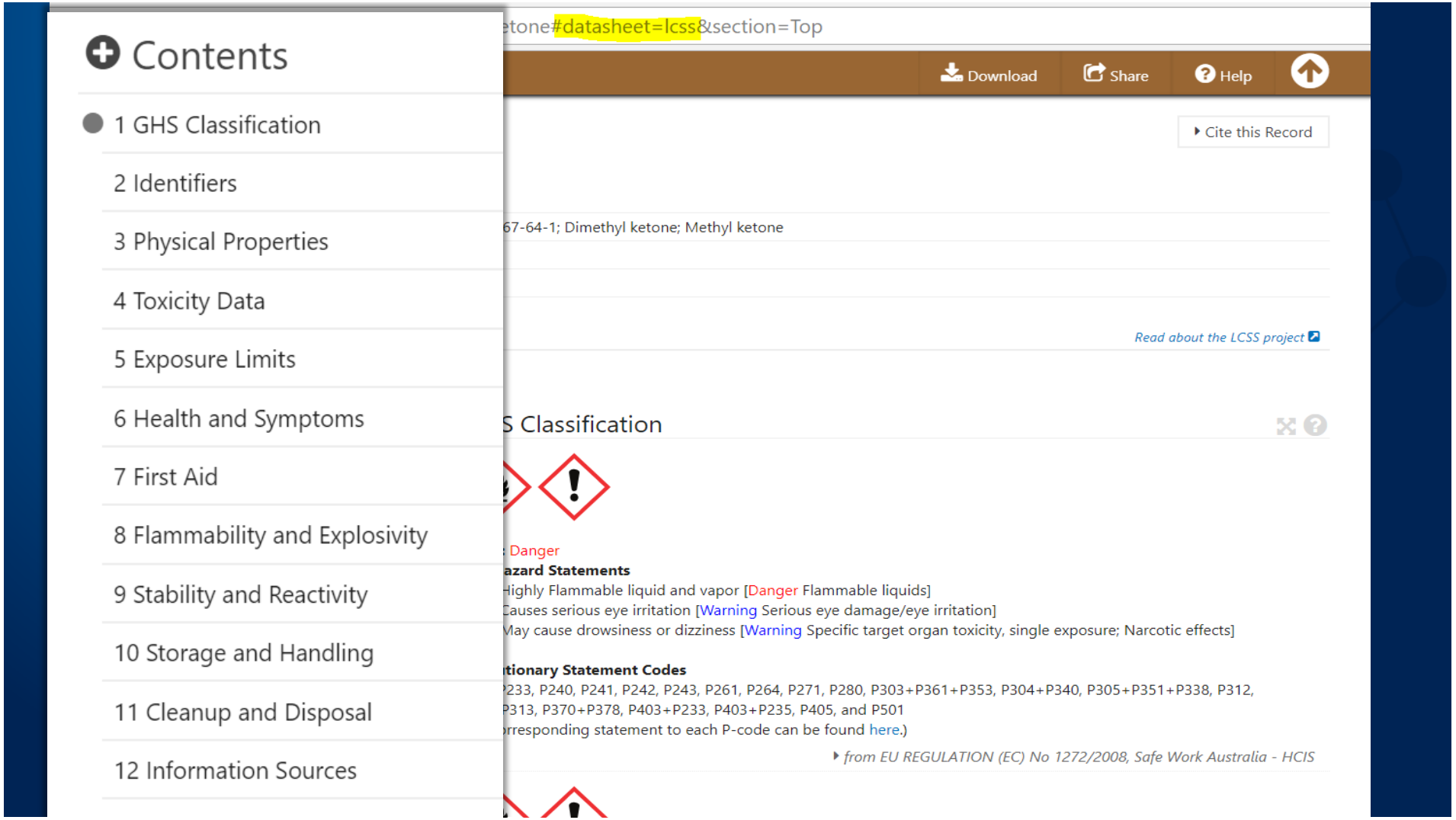
LCSS - Laboratory Chemical Safety Summary



LCSS - Laboratory Chemical Safety Summary




https://pubchem.ncbi.nlm.nih.gov/compound/acetone
NIH
U.S. National Library of Medicine
National Center for Biotechnology Information
PubChem
OPEN CHEMISTRY DATABASE
Search Compounds
Compound Summary for CID 180
Download
Share
Help
Acetone
Cite this Record
STRUCTURE
VENDORS
PHARMACOLOGY
LITERATURE
PATENTS
BIOACTIVITIES
PubChem CID: 180
Chemical Names: Acetone; 2-propanone; Propanone; 67-64-1; Dimethyl ketone; Methyl ketone
More...
Molecular Formula: C3H6O; CH3-CO-CH3
Molecular Weight: 58.08 g/mol
InChI Key: CSCPPACGZOOCGX-UHFFFAOYSA-N
Substance Registry: FDA UNII
Safety Summary: Laboratory Chemical Safety Summary (LCSS)
LCSS link
Acetone is a colorless liquid us
https://pubchem.ncbi.nlm.nih.gov/compound/acetone#datasheet=lcss
from MeSH
Acetone is a colorless, volatile, flammable organic solvent. Acetone occurs naturally in plants, trees, forest fires, vehicle exhaust and as a breakdown product of animal fat metabolism. This agent may be normally present in very small quantities in urine and blood; larger amounts may be found in the urine and blood of diabetics. Acetone is toxic in high doses. (NCI04)
Pharmacology from NCIt


Contents
1 GHS Classification
2 Identifiers
3 Physical Properties
4 Toxicity Data
5 Exposure Limits
6 Health and Symptoms
7 First Aid
8 Flammability and Explosivity
9 Stability and Reactivity
10 Storage and Handling
11 Cleanup and Disposal
12 Information Sources
etone#datasheet=lcss&section=Top
Download
Share
Help
Cite this Record
67-64-1; Dimethyl ketone; Methyl ketone
Read about the LCSS project
S Classification
Danger
azard Statements
Highly Flammable liquid and vapor [Danger Flammable liquids]
Causes serious eye irritation [Warning Serious eye damage/eye irritation]
May cause drowsiness or dizziness [Warning Specific target organ toxicity, single exposure; Narcotic effects]
tionary Statement Codes
233, P240, P241, P242, P243, P261, P264, P271, P280, P303+P361+P353, P304+P340, P305+P351+P338, P312,
313, P370+P378, P403+P233, P403+P235, P405, and P501
rresponding statement to each P-code can be found here.)
from EU REGULATION (EC) No 1272/2008, Safe Work Australia - HCIS

Classification browser …

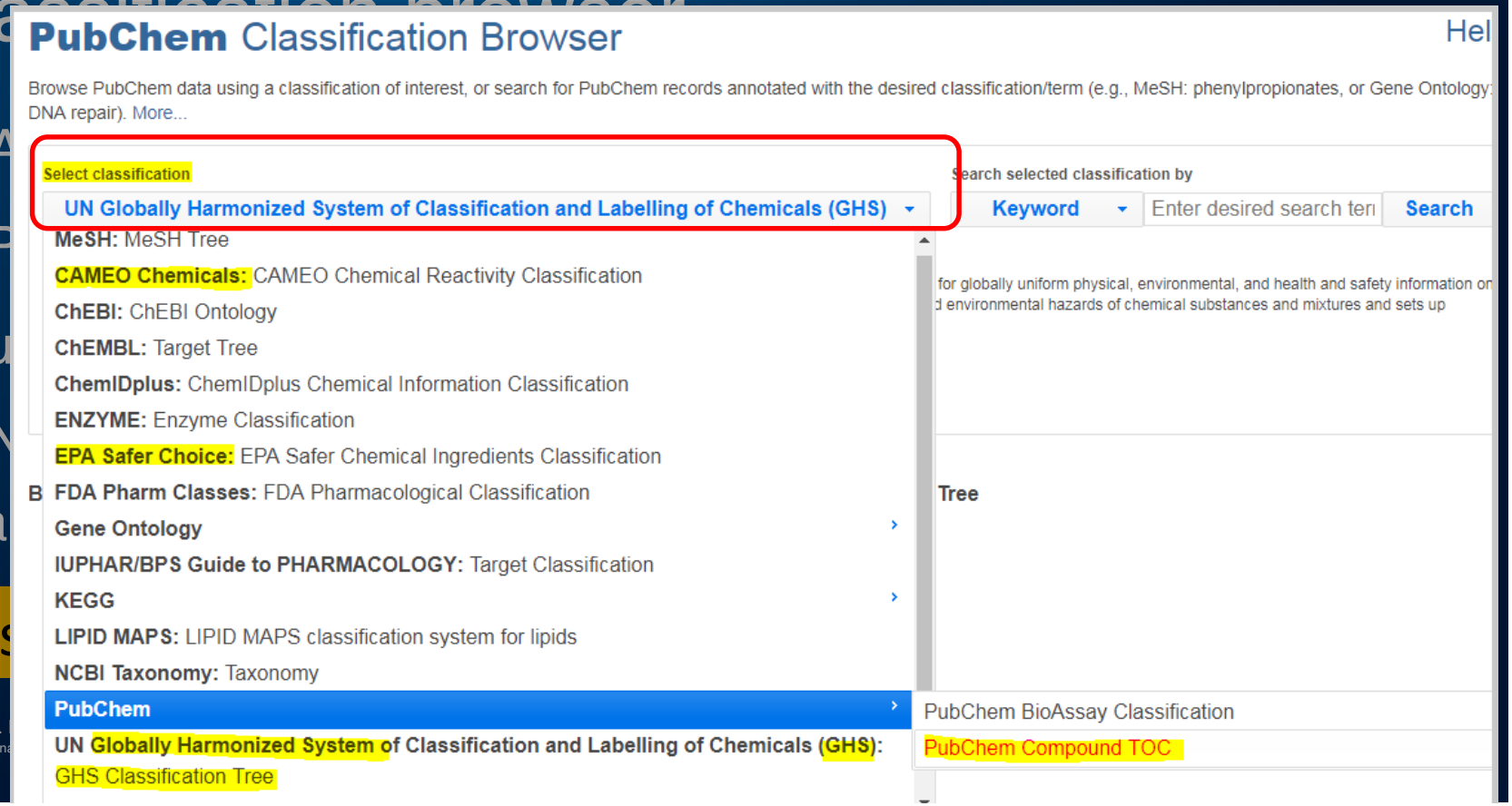
The classification browser allows users to browse the distribution of PubChem data among nodes in the hierarchy of interest, thereby providing an aggregate view of PubChem data. It also allows you to search for PubChem records annotated with the desired hierarchy/term, providing a powerful way to quickly find the subset of PubChem records.

Classification trees: major: 16. **Safety info related: 4**

Chemical Safety information from the Classification browser

- CA
- EP
- Pu
- UN
  La

https



Chemical safety information … Updates

- Cameo Chemicals reactivity classification
- Pistoia Alliance Chemical Safety Library

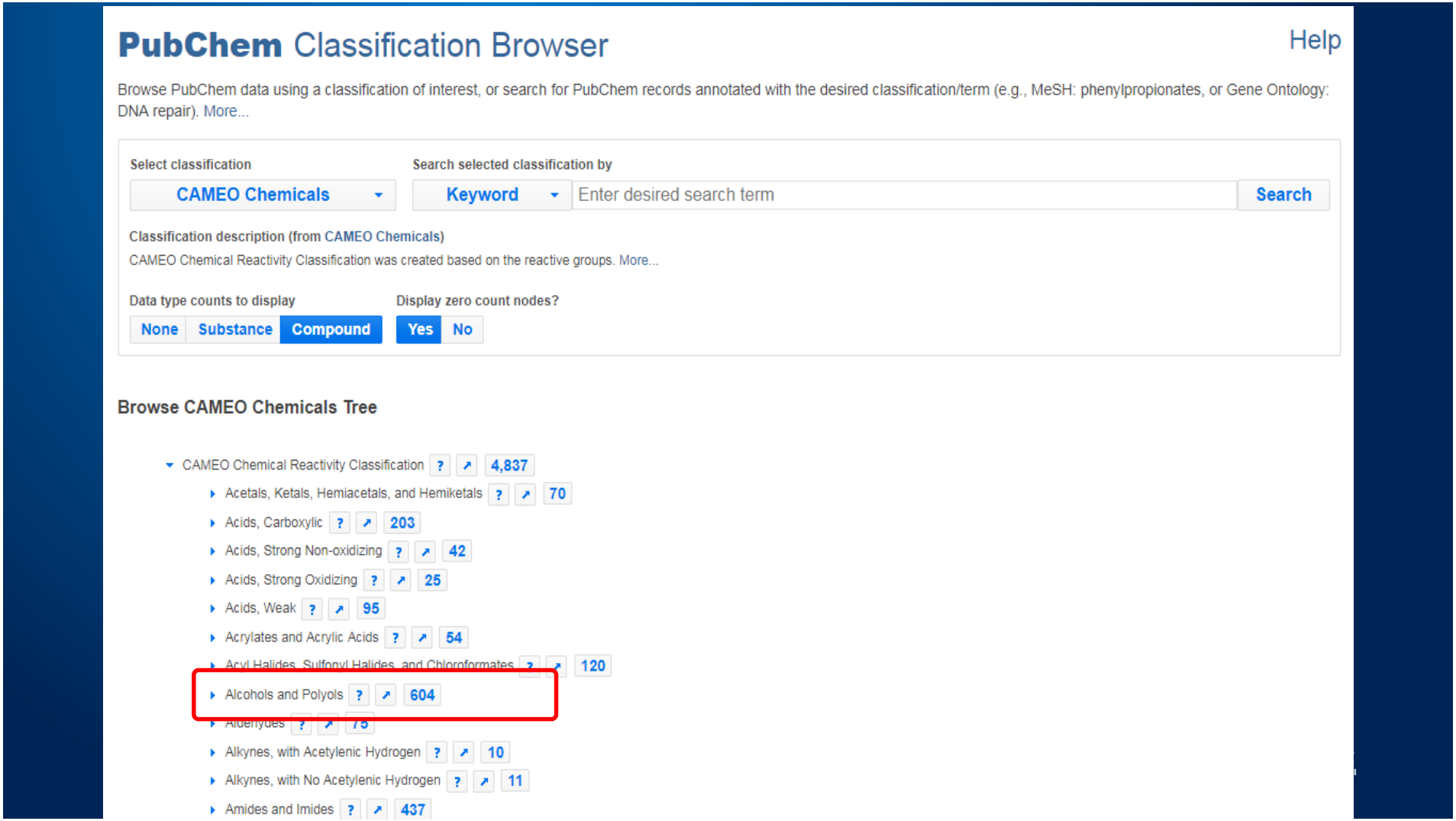
  CSL's Reaction alerts information

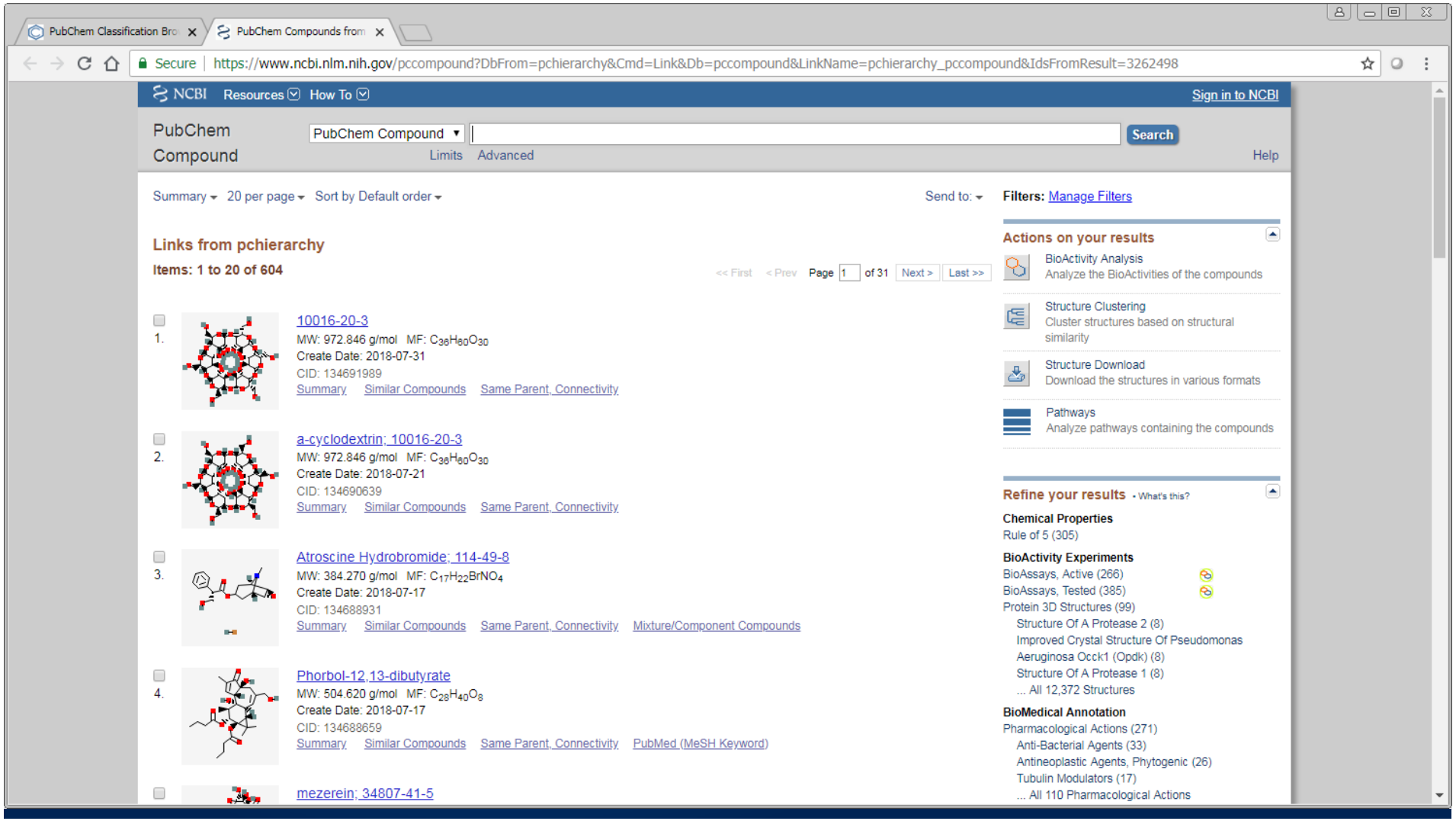
Update - CAMEO Chemicals Reactivity Classification

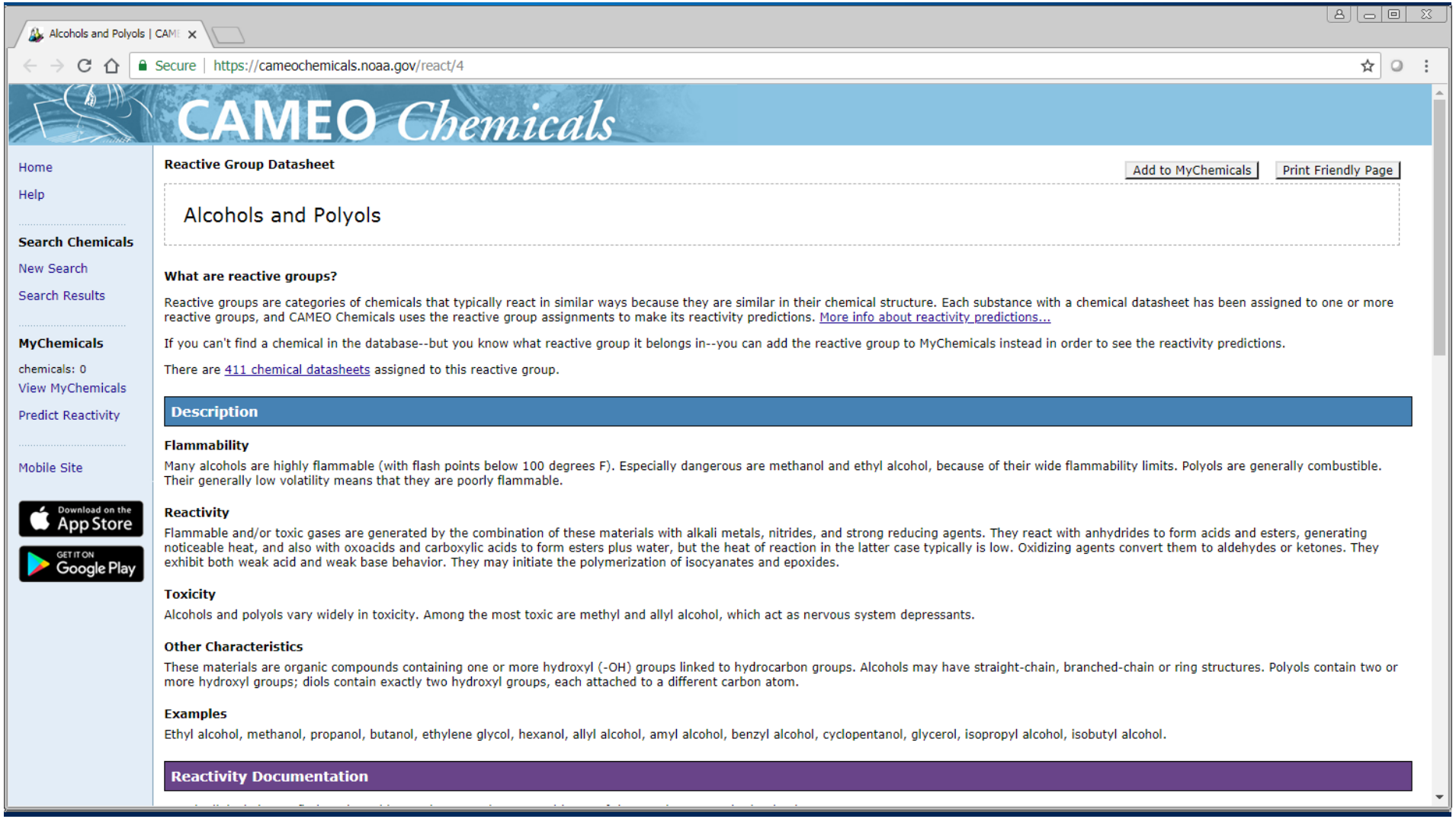
CAMEO Chemicals classify chemicals into 68 reactive categories according to structures and reactions. PubChem integrated the reactivity information and make it a special tree display for quick and convenient browsing

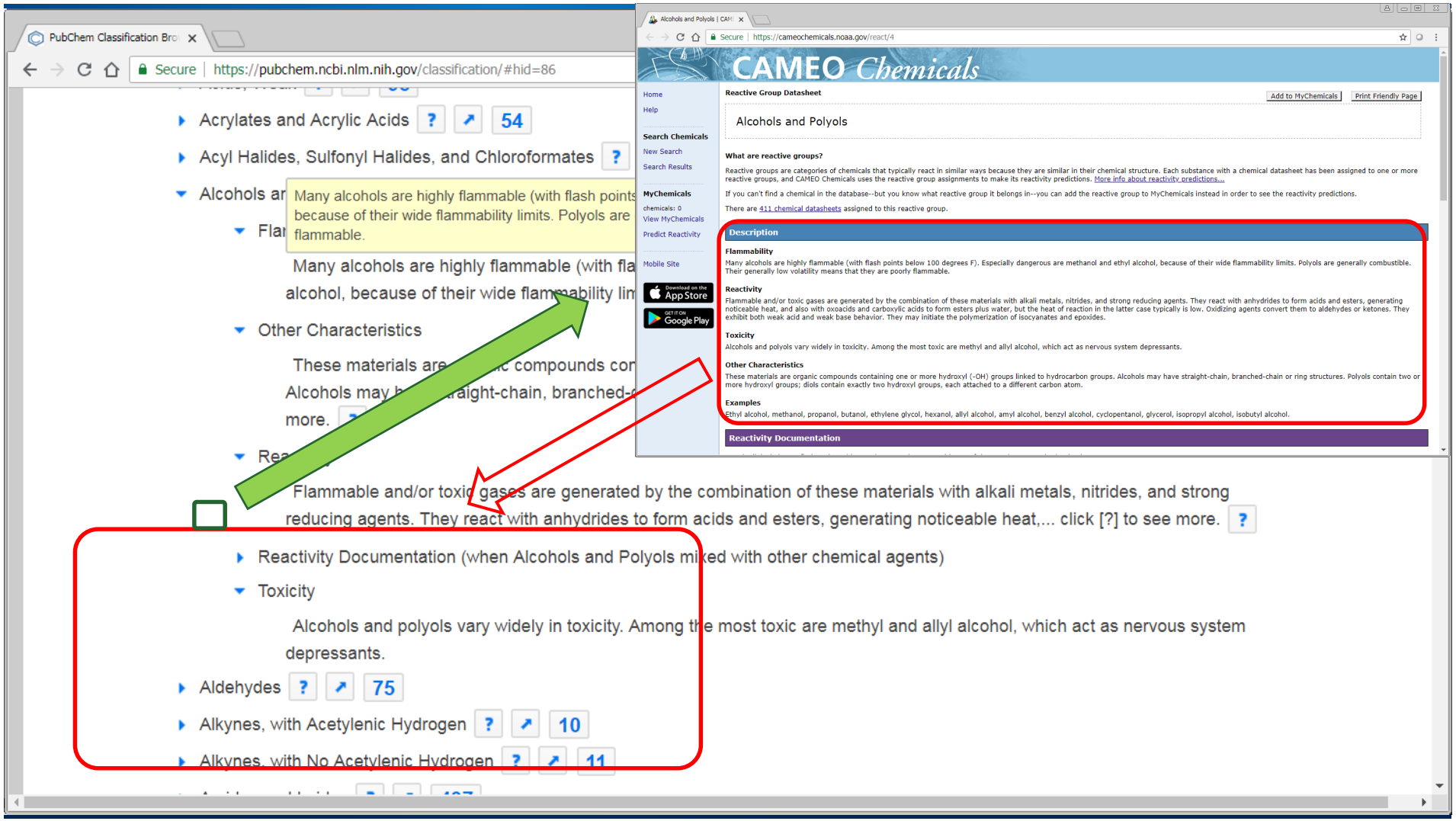
- Descriptions
  - Flammability
  - Reactivity
  - Toxicity
  - Others
- Reactivity Documentation

https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86


PubChem Classification Browser
Help
Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). More...
Select classification
CAMEO Chemicals
Search selected classification by
Keyword
Enter desired search term
Search
Classification description (from CAMEO Chemicals)
CAMEO Chemical Reactivity Classification was created based on the reactive groups. More...
Data type counts to display
None
Substance
Compound
Display zero count nodes?
Yes
No
Browse CAMEO Chemicals Tree
CAMEO Chemical Reactivity Classification 4,837
Acetals, Ketals, Hemiacetals, and Hemiketals 70
Acids, Carboxylic 203
Acids, Strong Non-oxidizing 42
Acids, Strong Oxidizing 25
Acids, Weak 95
Acrylates and Acrylic Acids 54
Acyl Halides, Sulfonyl Halides, and Chloroformates 120
Alcohols and Polyols 604
Aldehydes 75
Alkynes, with Acetylenic Hydrogen 10
Alkynes, with No Acetylenic Hydrogen 11
Amides and Imides 437


PubChem Classification Bro
PubChem Compounds from
Secure | https://www.ncbi.nlm.nih.gov/pccompound?DbFrom=pchierarchy&Cmd=Link&Db=pccompound&LinkName=pchierarchy_pccompound&IdsFromResult=3262498
NCBI Resources How To
Sign in to NCBI
PubChem Compound
PubChem Compound
Search
Limits Advanced
Help
Summary 20 per page Sort by Default order
Send to:
Filters: Manage Filters
Links from pchierarchy
Items: 1 to 20 of 604
<< First < Prev Page 1 of 31 Next > Last >>
1. 10016-20-3
MW: 972.846 g/mol MF: C36H60O30
Create Date: 2018-07-31
CID: 134691989
Summary Similar Compounds Same Parent, Connectivity
2. a-cyclodextrin; 10016-20-3
MW: 972.846 g/mol MF: C36H60O30
Create Date: 2018-07-21
CID: 134690639
Summary Similar Compounds Same Parent, Connectivity
3. Atroscine Hydrobromide; 114-49-8
MW: 384.270 g/mol MF: C17H22BrNO4
Create Date: 2018-07-17
CID: 134688931
Summary Similar Compounds Same Parent, Connectivity Mixture/Component Compounds
4. Phorbol-12,13-dibutyrate
MW: 504.620 g/mol MF: C28H40O8
Create Date: 2018-07-17
CID: 134688659
Summary Similar Compounds Same Parent, Connectivity PubMed (MeSH Keyword)
mezerein; 34807-41-5
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 (305)
BioActivity Experiments
BioAssays, Active (266)
BioAssays, Tested (385)
Protein 3D Structures (99)
Structure Of A Protease 2 (8)
Improved Crystal Structure Of Pseudomonas Aeruginosa Occk1 (Opdk) (8)
Structure Of A Protease 1 (8)
... All 12,372 Structures
BioMedical Annotation
Pharmacological Actions (271)
Anti-Bacterial Agents (33)
Antineoplastic Agents, Phytogenic (26)
Tubulin Modulators (17)
... All 110 Pharmacological Actions


Alcohols and Polyols | CAM
Secure | https://cameochemicals.noaa.gov/react/4
CAMEO Chemicals
Home
Help
Search Chemicals
New Search
Search Results
MyChemicals
chemicals: 0
View MyChemicals
Predict Reactivity
Mobile Site
Download on the App Store
GET IT ON Google Play
Reactive Group Datasheet
Add to MyChemicals
Print Friendly Page
Alcohols and Polyols
What are reactive groups?
Reactive groups are categories of chemicals that typically react in similar ways because they are similar in their chemical structure. Each substance with a chemical datasheet has been assigned to one or more reactive groups, and CAMEO Chemicals uses the reactive group assignments to make its reactivity predictions. More info about reactivity predictions...
If you can't find a chemical in the database--but you know what reactive group it belongs in--you can add the reactive group to MyChemicals instead in order to see the reactivity predictions.
There are 411 chemical datasheets assigned to this reactive group.
Description
Flammability
Many alcohols are highly flammable (with flash points below 100 degrees F). Especially dangerous are methanol and ethyl alcohol, because of their wide flammability limits. Polyols are generally combustible. Their generally low volatility means that they are poorly flammable.
Reactivity
Flammable and/or toxic gases are generated by the combination of these materials with alkali metals, nitrides, and strong reducing agents. They react with anhydrides to form acids and esters, generating noticeable heat, and also with oxoacids and carboxylic acids to form esters plus water, but the heat of reaction in the latter case typically is low. Oxidizing agents convert them to aldehydes or ketones. They exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides.
Toxicity
Alcohols and polyols vary widely in toxicity. Among the most toxic are methyl and allyl alcohol, which act as nervous system depressants.
Other Characteristics
These materials are organic compounds containing one or more hydroxyl (-OH) groups linked to hydrocarbon groups. Alcohols may have straight-chain, branched-chain or ring structures. Polyols contain two or more hydroxyl groups; diols contain exactly two hydroxyl groups, each attached to a different carbon atom.
Examples
Ethyl alcohol, methanol, propanol, butanol, ethylene glycol, hexanol, allyl alcohol, amyl alcohol, benzyl alcohol, cyclopentanol, glycerol, isopropyl alcohol, isobutyl alcohol.
Reactivity Documentation


PubChem Classification Bro
Secure | https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86
Acrylates and Acrylic Acids ? 54
Acyl Halides, Sulfonyl Halides, and Chloroformates ?
Alcohols ar
Many alcohols are highly flammable (with flash points because of their wide flammability limits. Polyols are flammable.
Fla
Many alcohols are highly flammable (with fla
alcohol, because of their wide flammability lin
Other Characteristics
These materials are compounds cor
Alcohols may h raight-chain, branched-
more.
Rea
Flammable and/or toxic gases are generated by the combination of these materials with alkali metals, nitrides, and strong reducing agents. They react with anhydrides to form acids and esters, generating noticeable heat,... click [?] to see more. ?
Reactivity Documentation (when Alcohols and Polyols mixed with other chemical agents)
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Aldehydes ? 75
Alkynes, with Acetylenic Hydrogen ? 10
Alkynes, with No Acetylenic Hydrogen ? 11
Alcohols and Polyols | CAM
Secure | https://cameochemicals.noaa.gov/react/4
CAMEO Chemicals
Home
Help
Search Chemicals
New Search
Search Results
MyChemicals
chemicals: 0
View MyChemicals
Predict Reactivity
Mobile Site
Download on the App Store
GET IT ON Google Play
Reactive Group Datasheet
Add to MyChemicals
Print Friendly Page
Alcohols and Polyols
What are reactive groups?
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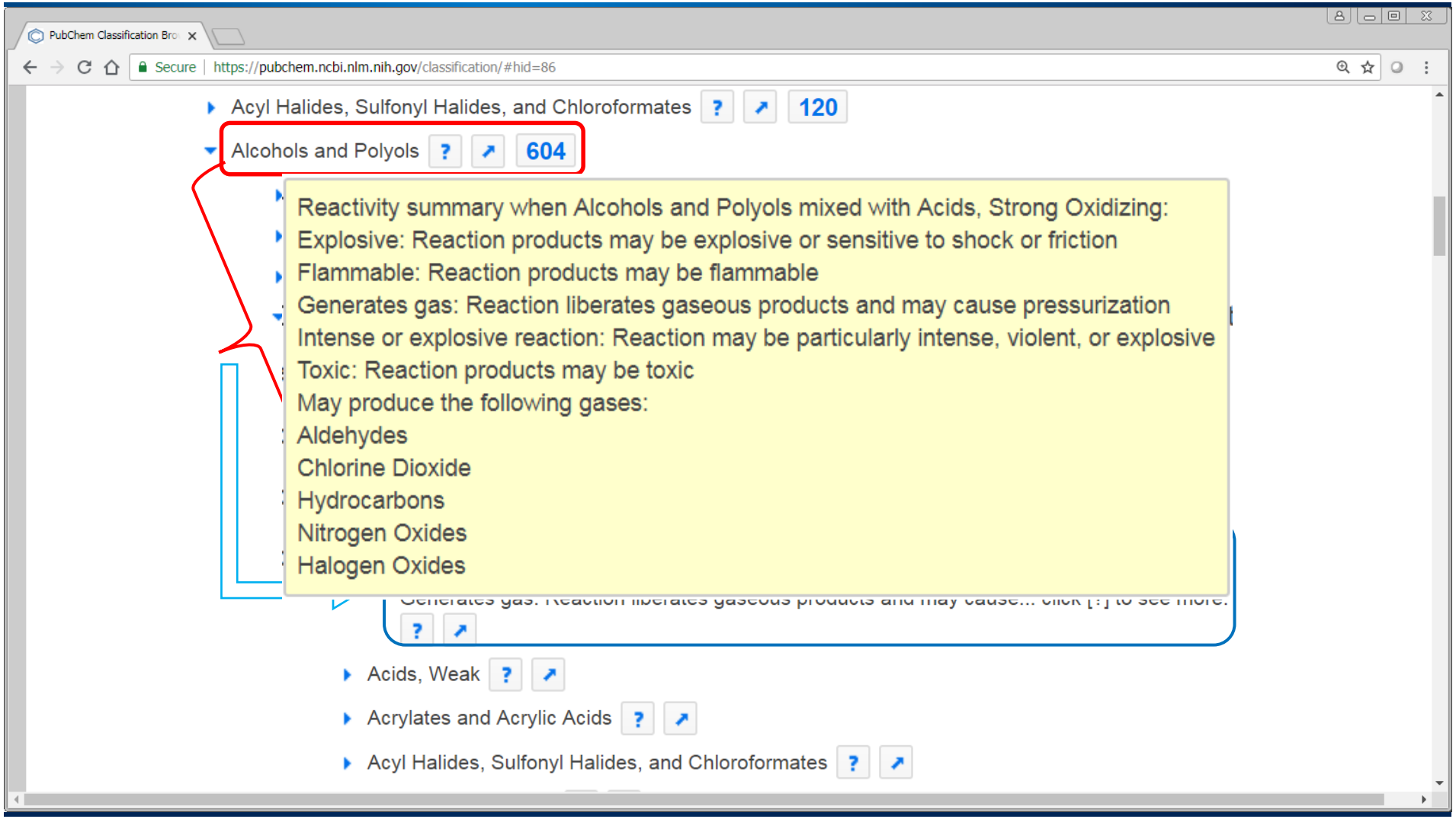
Reactivity Documentation

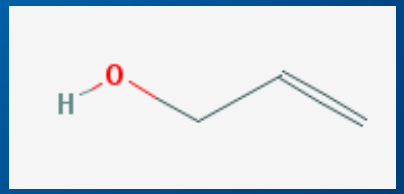
CAMEO Chemicals Reactivity Classification

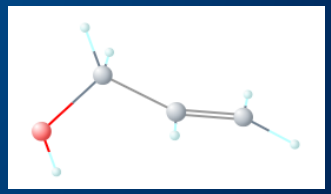
- Reactivity Documentation
  - Reactivity summary when one reactive group (chemical) mixed with another one.


PubChem Classification Bro
Secure | https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86
Acyl Halides, Sulfonyl Halides, and Chloroformates ? 120
Alcohols and Polyols ? 604
Reactivity summary when Alcohols and Polyols mixed with Acids, Strong Oxidizing:
Explosive: Reaction products may be explosive or sensitive to shock or friction
Flammable: Reaction products may be flammable
Generates gas: Reaction liberates gaseous products and may cause pressurization
Intense or explosive reaction: Reaction may be particularly intense, violent, or explosive
Toxic: Reaction products may be toxic
May produce the following gases:
Aldehydes
Chlorine Dioxide
Hydrocarbons
Nitrogen Oxides
Halogen Oxides
Acids, Weak ?
Acrylates and Acrylic Acids ?
Acyl Halides, Sulfonyl Halides, and Chloroformates ?

Case study: an individual compound vs classification tree

- Example: allyl alcohol
- CID 7858





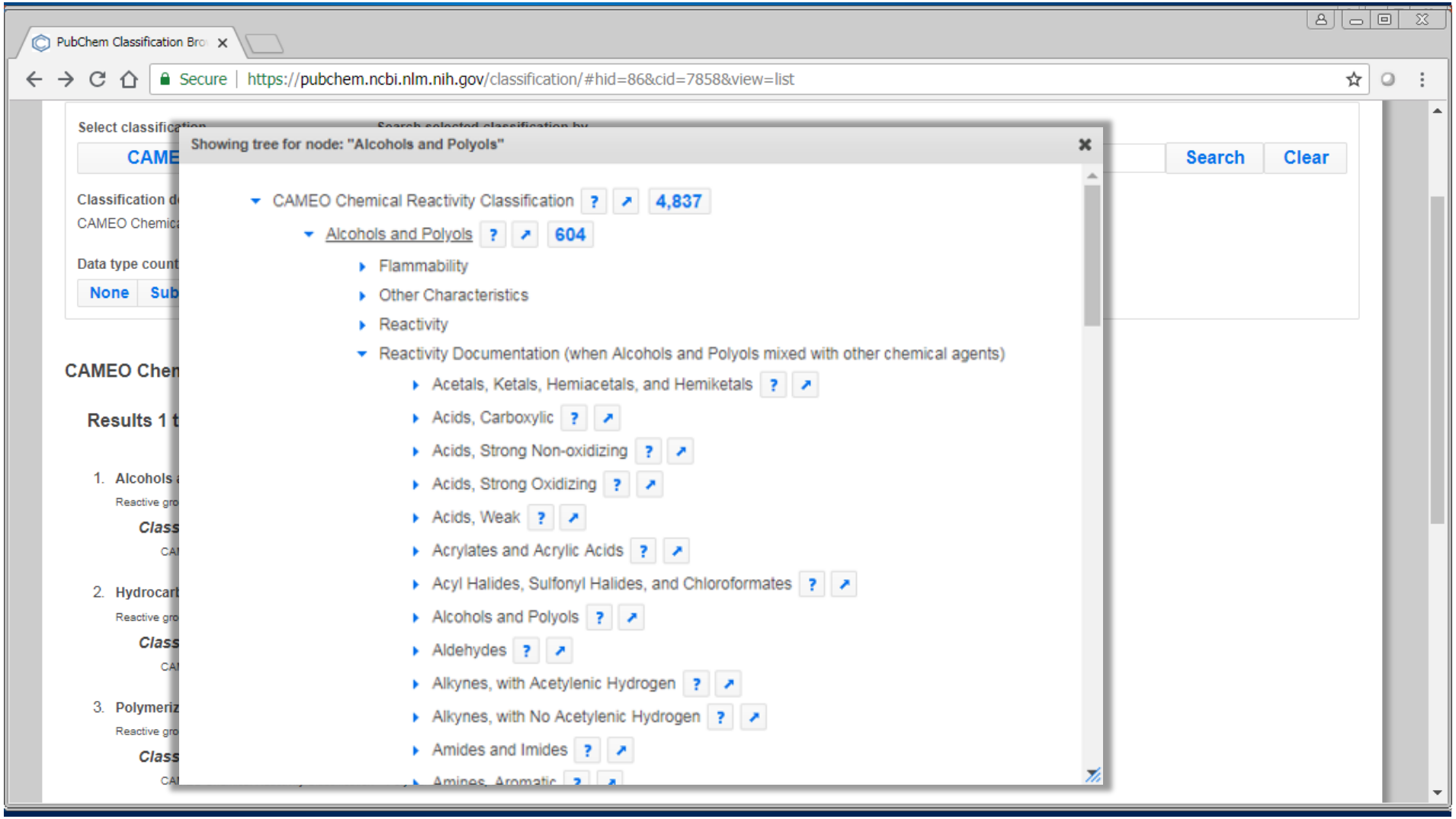
Space replacement: + or %20 or _

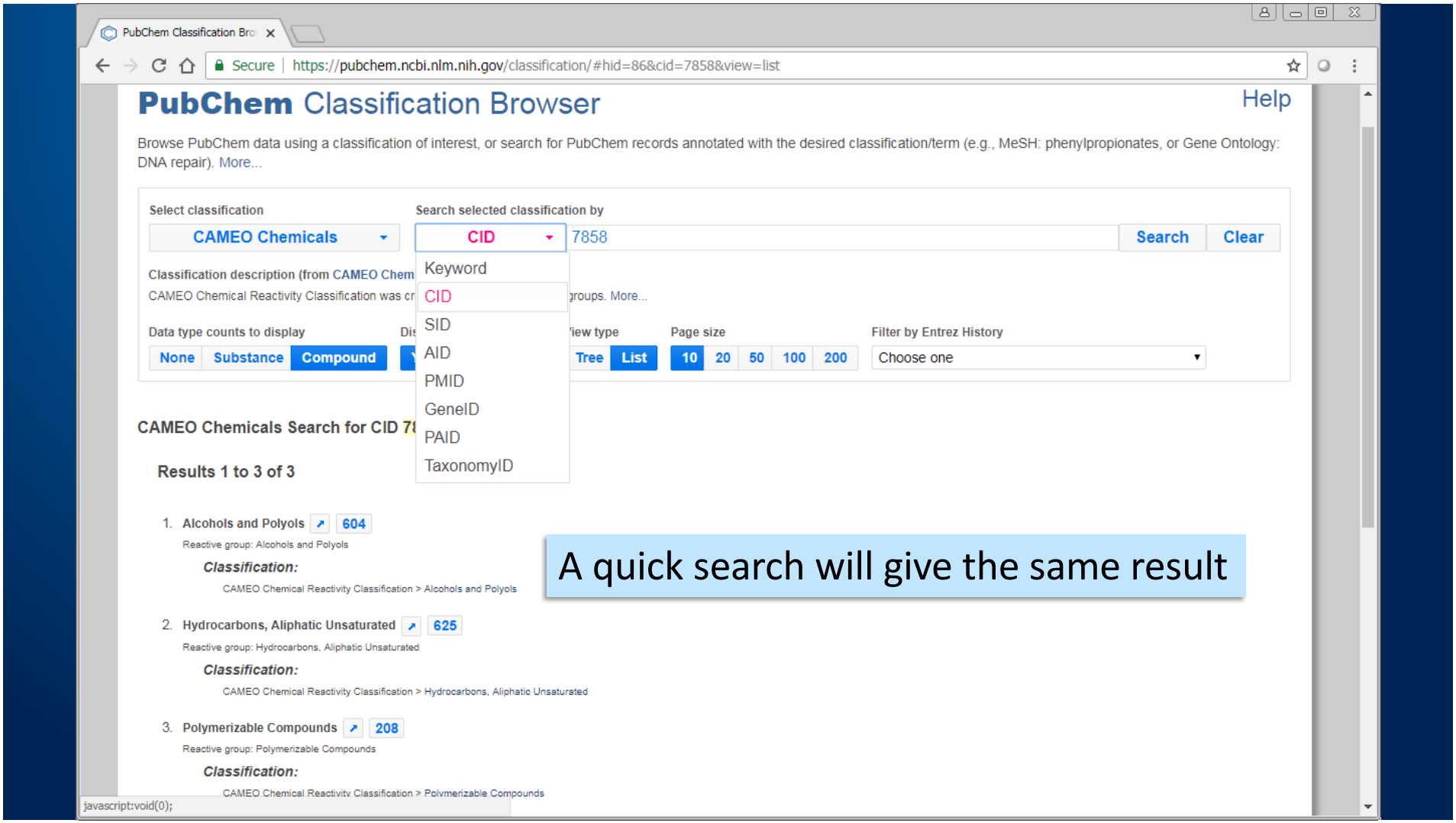
https://pubchem.ncbi.nlm.nih.gov/compound/allyl+alcohol

PubChem base URL

Database

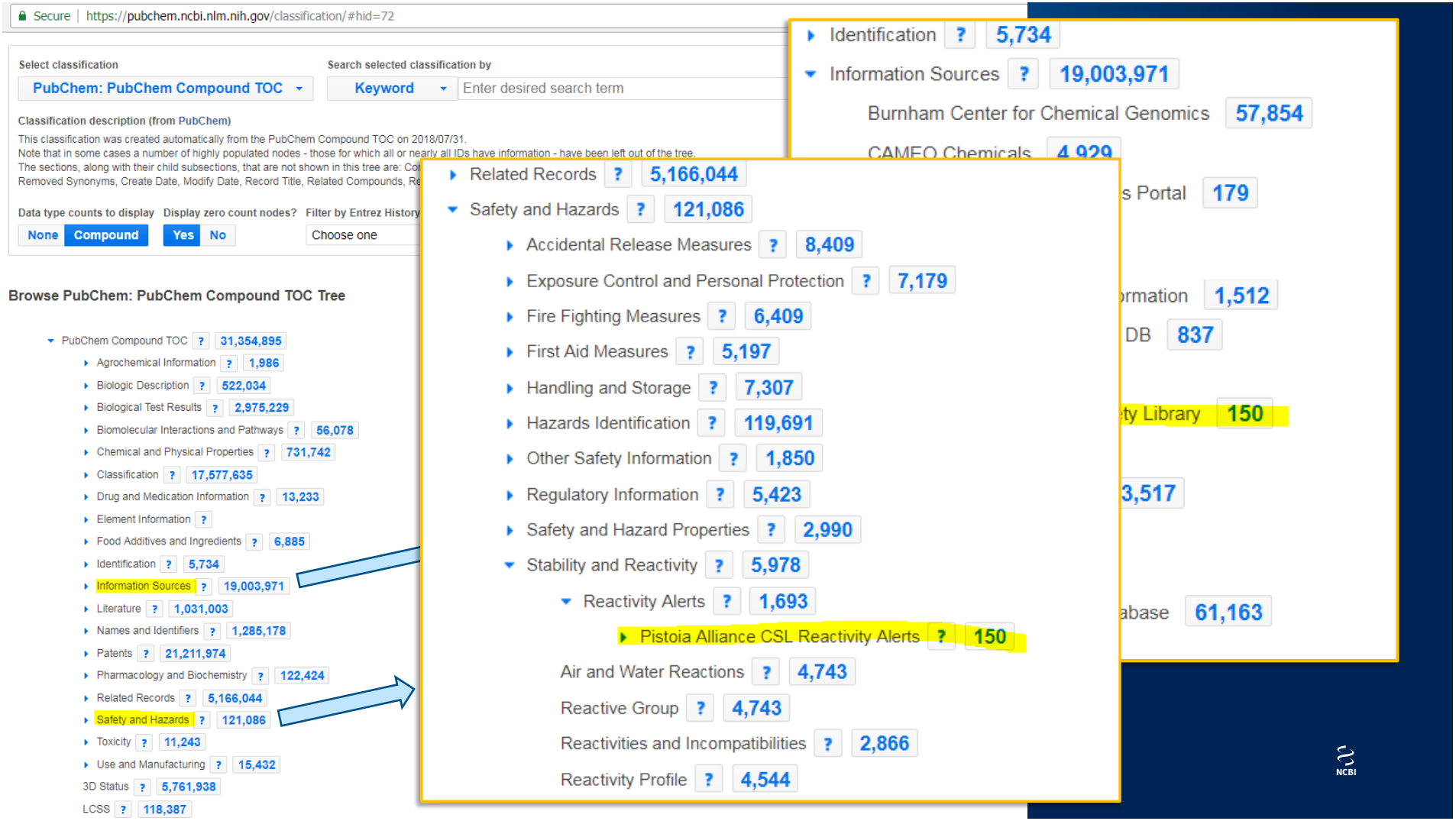
compound


PubChem Classification Bro
Secure | https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86&cid=7858&view=list
Search
Clear
Showing tree for node: "Alcohols and Polyols"
CAMEO Chemical Reactivity Classification 4,837
Alcohols and Polyols 604
Flammability
Other Characteristics
Reactivity
Reactivity Documentation (when Alcohols and Polyols mixed with other chemical agents)
Acetals, Ketals, Hemiacetals, and Hemiketals
Acids, Carboxylic
Acids, Strong Non-oxidizing
Acids, Strong Oxidizing
Acids, Weak
Acrylates and Acrylic Acids
Acyl Halides, Sulfonyl Halides, and Chloroformates
Alcohols and Polyols
Aldehydes
Alkynes, with Acetylenic Hydrogen
Alkynes, with No Acetylenic Hydrogen
Amides and Imides
CAMEO Chen
Results 1 t
1. Alcohols
2. Hydrocart
3. Polymeriz


PubChem Classification Bro
Secure | https://pubchem.ncbi.nlm.nih.gov/classification/#hid=86&cid=7858&view=list
PubChem Classification Browser
Help
Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). More...
Select classification
CAMEO Chemicals
Search selected classification by
CID
7858
Search
Clear
Keyword
CID
SID
AID
PMID
GeneID
PAID
TaxonomyID
Classification description (from CAMEO Chem
CAMEO Chemical Reactivity Classification was cr
groups. More...
Data type counts to display
None
Substance
Compound
Tree
List
Page size
10
20
50
100
200
Filter by Entrez History
Choose one
CAMEO Chemicals Search for CID 7
Results 1 to 3 of 3
1. Alcohols and Polyols 604
Reactive group: Alcohols and Polyols
Classification:
CAMEO Chemical Reactivity Classification > Alcohols and Polyols
2. Hydrocarbons, Aliphatic Unsaturated 625
Reactive group: Hydrocarbons, Aliphatic Unsaturated
Classification:
CAMEO Chemical Reactivity Classification > Hydrocarbons, Aliphatic Unsaturated
3. Polymerizable Compounds 208
Reactive group: Polymerizable Compounds
Classification:
CAMEO Chemical Reactivity Classification > Polymerizable Compounds
javascript:void(0);
A quick search will give the same result

Update: the reaction alerts from Pistoia Alliance CSL

Reactivity information when one chemical meet another one.


Secure | https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72
Select classification
PubChem: PubChem Compound TOC
Search selected classification by
Keyword
Enter desired search term
Classification description (from PubChem)
This classification was created automatically from the PubChem Compound TOC on 2018/07/31.
Note that in some cases a number of highly populated nodes - those for which all or nearly all IDs have information - have been left out of the tree.
The sections, along with their child subsections, that are not shown in this tree are: Co
Removed Synonyms, Create Date, Modify Date, Record Title, Related Compounds, Re
Data type counts to display
None
Compound
Display zero count nodes?
Yes
No
Filter by Entrez History
Choose one
Browse PubChem: PubChem Compound TOC Tree
PubChem Compound TOC ? 31,354,895
Agrochemical Information ? 1,986
Biologic Description ? 522,034
Biological Test Results ? 2,975,229
Biomolecular Interactions and Pathways ? 56,078
Chemical and Physical Properties ? 731,742
Classification ? 17,577,635
Drug and Medication Information ? 13,233
Element Information ?
Food Additives and Ingredients ? 6,885
Identification ? 5,734
Information Sources ? 19,003,971
Literature ? 1,031,003
Names and Identifiers ? 1,285,178
Patents ? 21,211,974
Pharmacology and Biochemistry ? 122,424
Related Records ? 5,166,044
Safety and Hazards ? 121,086
Toxicity ? 11,243
Use and Manufacturing ? 15,432
3D Status ? 5,761,938
LCSS ? 118,387
Related Records ? 5,166,044
Safety and Hazards ? 121,086
Accidental Release Measures ? 8,409
Exposure Control and Personal Protection ? 7,179
Fire Fighting Measures ? 6,409
First Aid Measures ? 5,197
Handling and Storage ? 7,307
Hazards Identification ? 119,691
Other Safety Information ? 1,850
Regulatory Information ? 5,423
Safety and Hazard Properties ? 2,990
Stability and Reactivity ? 5,978
Reactivity Alerts ? 1,693
Pistoia Alliance CSL Reactivity Alerts ? 150
Air and Water Reactions ? 4,743
Reactive Group ? 4,743
Reactivities and Incompatibilities ? 2,866
Reactivity Profile ? 4,544
Identification ? 5,734
Information Sources ? 19,003,971
Burnham Center for Chemical Genomics 57,854
CAMEO Chemicals 4,929
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DB 837
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3,517
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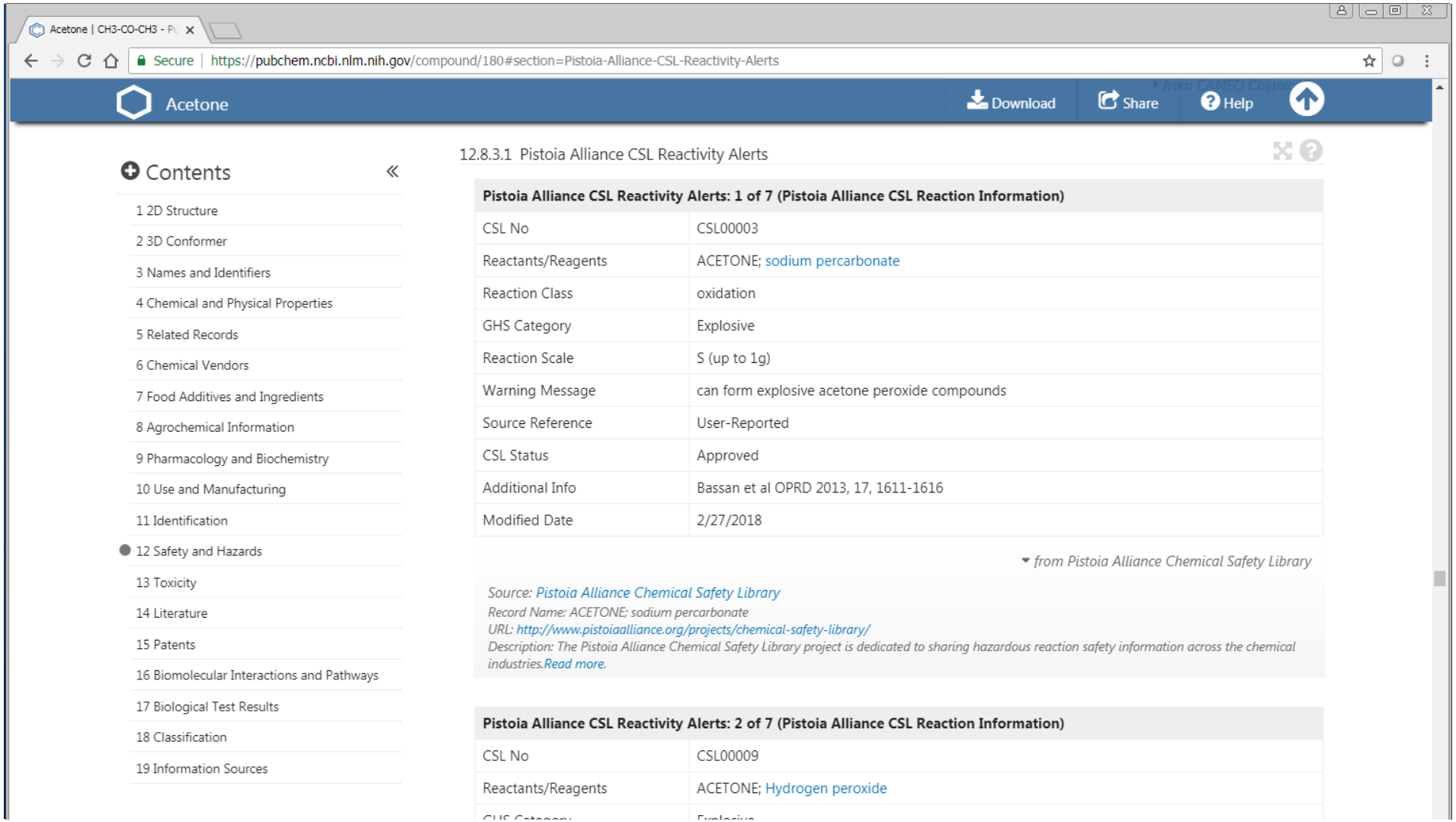
NCBI

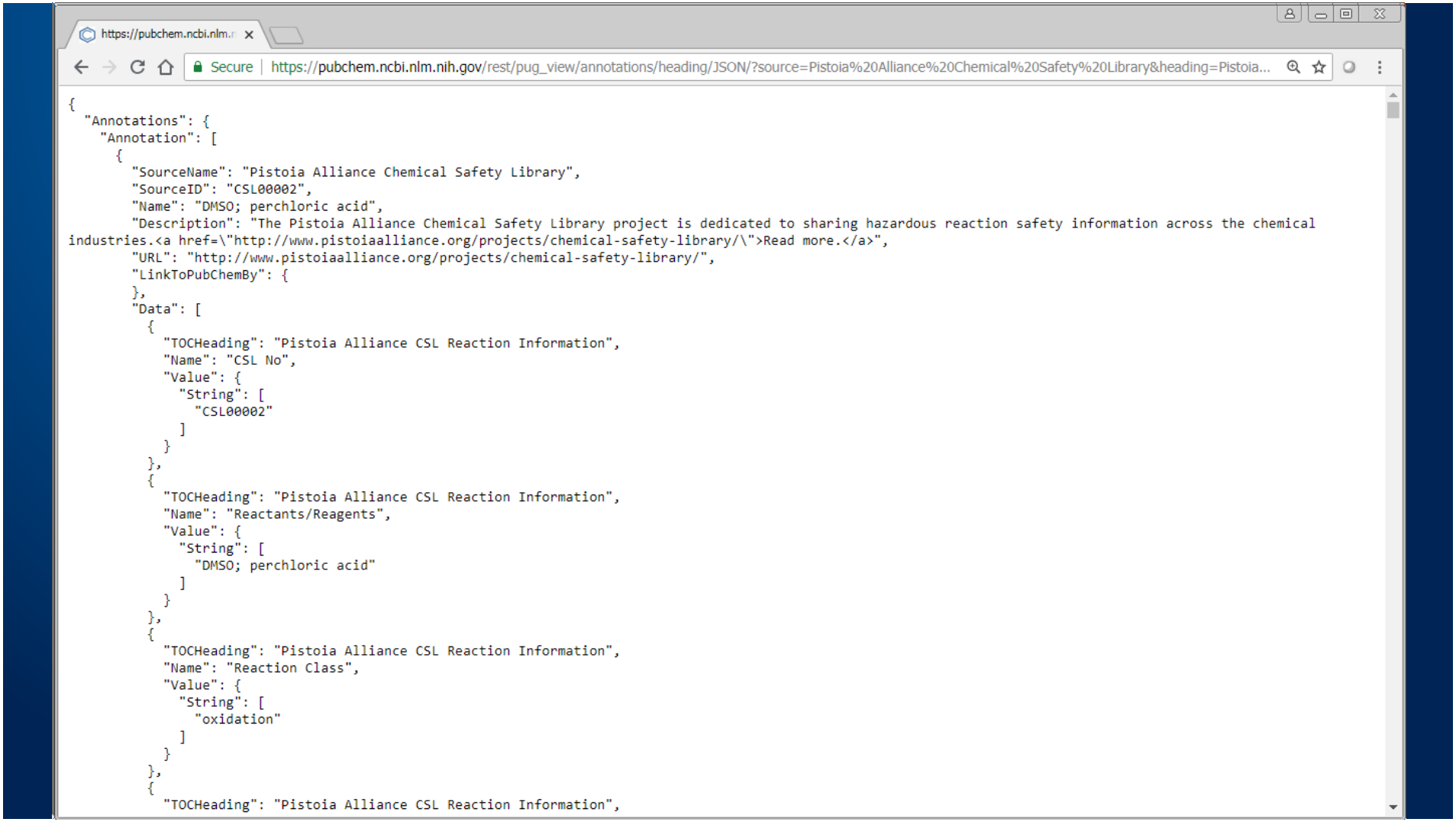

Acetone | CH3-CO-CH3 - Pu
Secure | https://pubchem.ncbi.nlm.nih.gov/compound/180#section=Pistoia-Alliance-CSL-Reactivity-Alerts
Acetone
Download
Share
Help
Contents
1 2D Structure
2 3D Conformer
3 Names and Identifiers
4 Chemical and Physical Properties
5 Related Records
6 Chemical Vendors
7 Food Additives and Ingredients
8 Agrochemical Information
9 Pharmacology and Biochemistry
10 Use and Manufacturing
11 Identification
12 Safety and Hazards
13 Toxicity
14 Literature
15 Patents
16 Biomolecular Interactions and Pathways
17 Biological Test Results
18 Classification
19 Information Sources
12.8.3.1 Pistoia Alliance CSL Reactivity Alerts
Pistoia Alliance CSL Reactivity Alerts: 1 of 7 (Pistoia Alliance CSL Reaction Information)
CSL No CSL00003
Reactants/Reagents ACETONE; sodium percarbonate
Reaction Class oxidation
GHS Category Explosive
Reaction Scale S (up to 1g)
Warning Message can form explosive acetone peroxide compounds
Source Reference User-Reported
CSL Status Approved
Additional Info Bassan et al OPRD 2013, 17, 1611-1616
Modified Date 2/27/2018
from Pistoia Alliance Chemical Safety Library
Source: Pistoia Alliance Chemical Safety Library
Record Name: ACETONE; sodium percarbonate
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.Read more.
Pistoia Alliance CSL Reactivity Alerts: 2 of 7 (Pistoia Alliance CSL Reaction Information)
CSL No CSL00009
Reactants/Reagents ACETONE; Hydrogen peroxide

Data Retrieving …

- Web page direct
- Using classification browser
- Using the sources page
- Using pug-view services – programmatic access

Data retrieving .. Sources page

https://pubchem.ncbi.nlm.nih.gov/sources/

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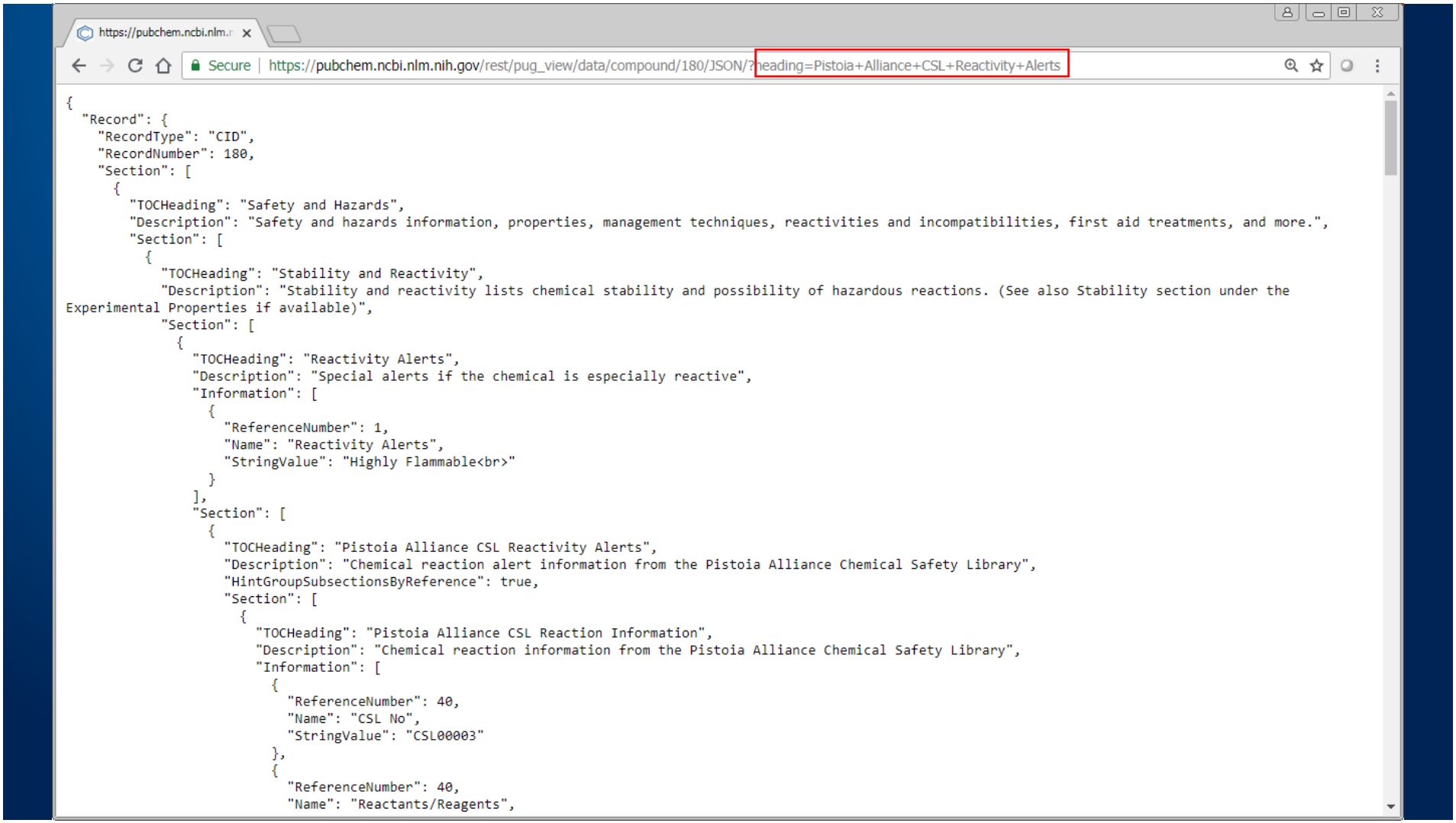
Data retrieving .. Pug_view APIs

PubChem Pug_view URL for Pistoia Alliance CSL data on acetone compound summary:

https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/compound/180/JSON/?heading=Pistoia+Alliance+CSL+Reactivity+Alerts


https://pubchem.ncbi.nlm.
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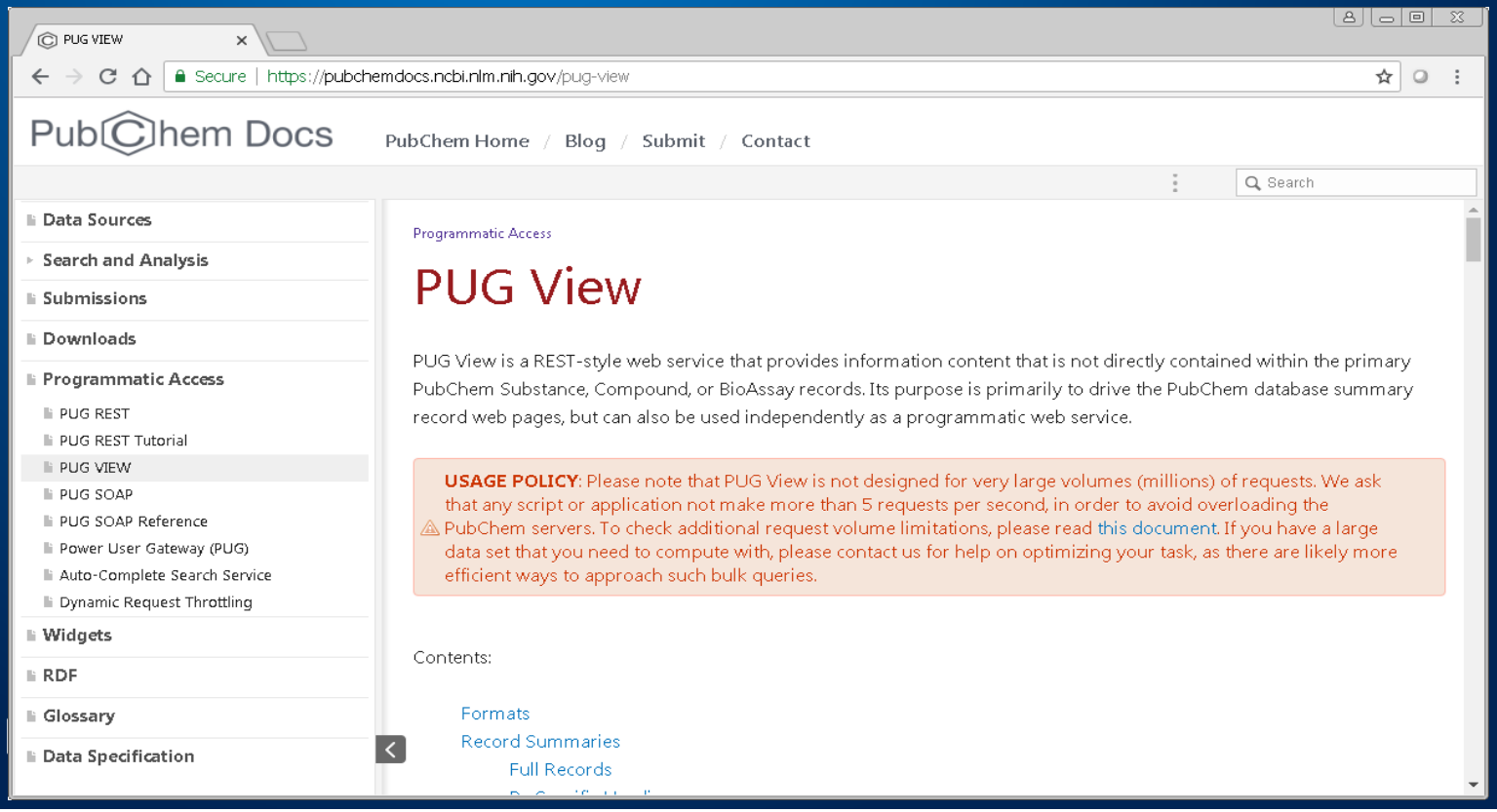
Data retrieving .. Pug_view APIs



Summary

- PubChem provides various chemical safety information as well as the link backs to original data sources.
- CAMEO Chemicals classification allows users find warning message and/or reaction activity potentials.
- Pistoia Alliance CSL's reactivity data is helpful for chemist especially the junior chemistry student when handle chemical reagents.
- The chemical data in PubChem can be retrieved in individual or batch compounds, with browsing or programmatical way.

Thanks you ...

This research was supported by the Intramural Research Program of the NIH, National Library of Medicine.

PubChem

Evan Bolton
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Tiejun Cheng
Jane He
Sunghwan Kim
Leon Li
Leonid Zaslavsky

CAMEO Chemicals

Pistoia Alliance

CHEMICAL SAFETY LIBRARY

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Gabrielle Whittick
Mark Manfredi
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Ralph Stuart