EPA Comptox Chemistry Dashboard: Web-based data integration hub for environmental chemistry and toxicology data

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Office of Research and Development

ISES 2017

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The CompTox Chemistry Dashboard

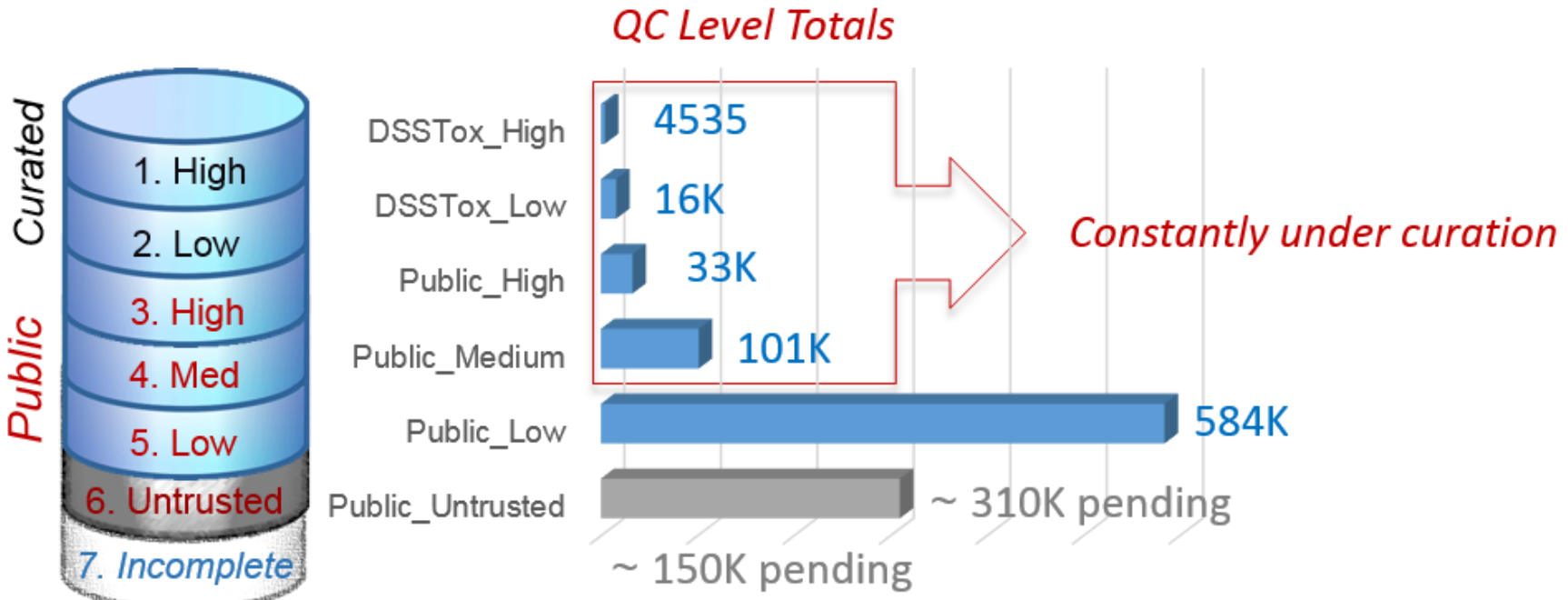
PRIMARY GOALS

- Deliver a web-based application serving up chemistry related data
- Provide public access to the results of over a decade of curation work
- Provide access to the results of our QSAR modeling work
- Transparency regarding our data and algorithms - Open Data mentality
- Deliver a central hub to link together websites of interest
- All data to be available as Open Data for download/reuse

SECONDARY GOAL

- **Develop a new cheminformatics architecture for all NCCT tools and data**

15 Years of Curating Chemistry Content



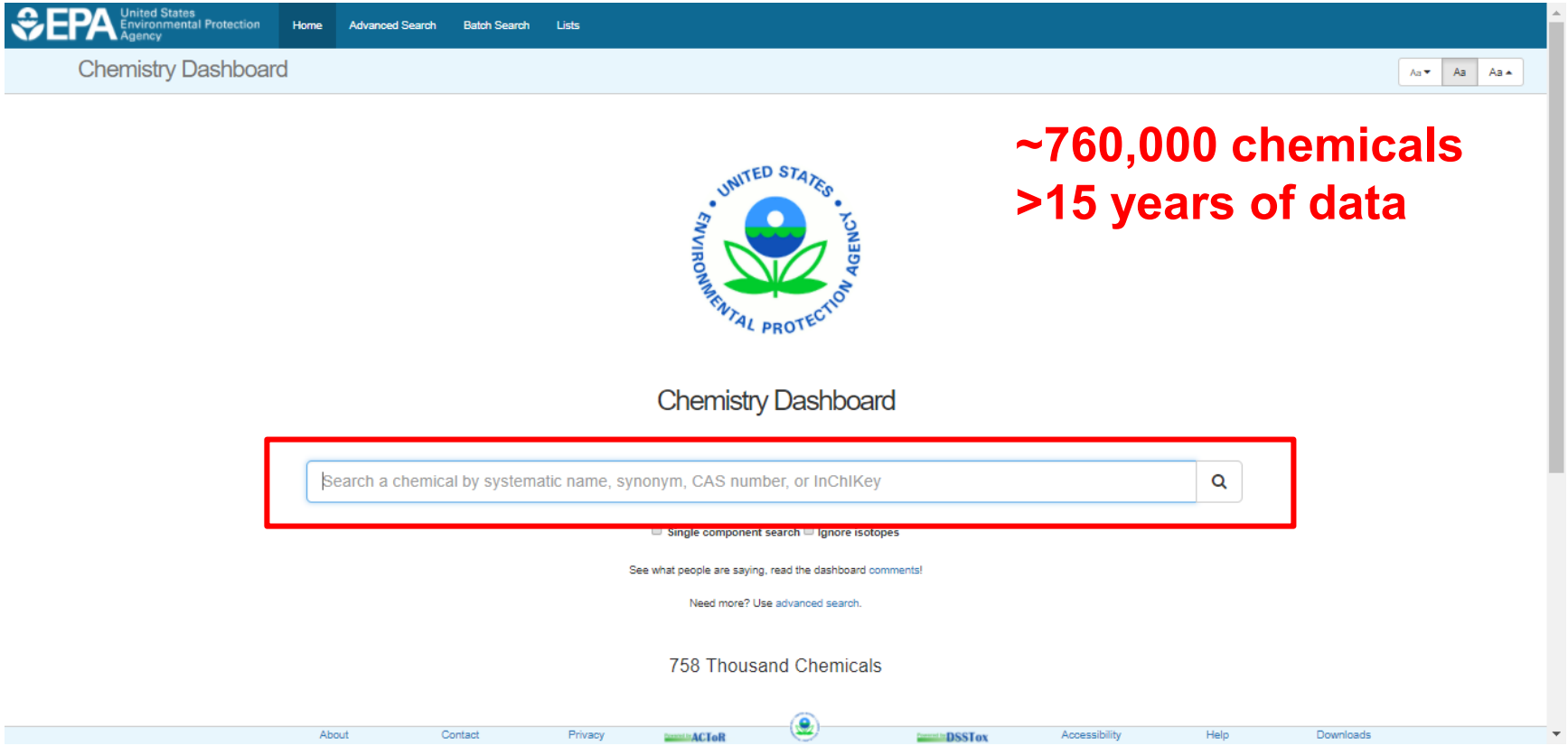
QC Levels

DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem
Public_Untrusted:	Postulated, but found to have conflicts in public sources

EPA United States Environmental Protection Agency

Comptox Chemistry Dashboard

https://comptox.epa.gov



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Comptox Chemistry Dashboard

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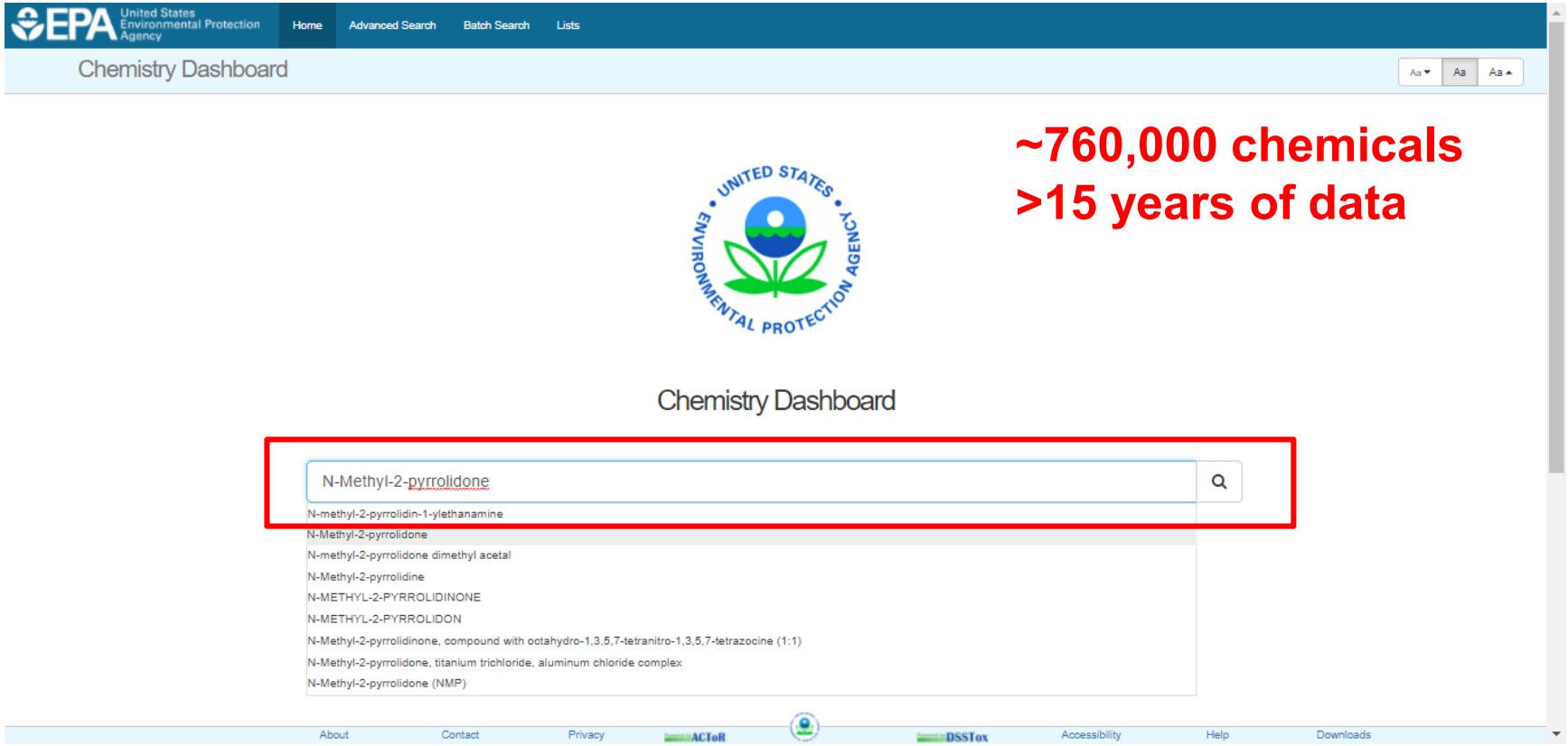

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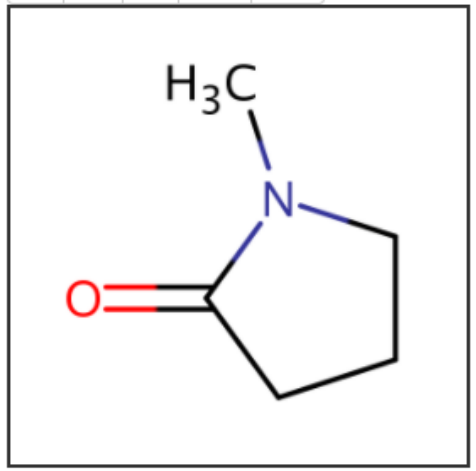
Chemical Page

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856

Searched by Synonym from Valid Source: Found 1 result for 'N-METHYLPYRROLIDONE'.



- Wikipedia
- Intrinsic Properties
  - **Molecular Formula:** C5H9NO — Find All Chemicals
  - **Average Mass:** 99.133 g/mol
  - **Monoisotopic Mass:** 99.068414 g/mol
- Structural Identifiers
- Related Compounds
- Presence in Lists
- Record Information

Chemical Properties | Env. Fate/Transport | Toxicity Values (Beta) | ADME (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Synonyms | Literature | External Links

Chemical Properties

- Summary
- LogP: Octanol-Water
- Water Solubility
- Density
- Flash Point
- Melting Point
- Boiling Point
- Surface Tension
- Thermal Conductivity
- Vapor Pressure
- Viscosity
- LogKoa: Octanol-Air

Download as: TSV | Excel | SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-0.380 (1)	-0.329 (5)	-0.380	-0.329	-0.380	-0.494 to -0.110	-
Water Solubility	10.1 (1)	6.68 (4)	10.1	6.68	10.1	1.48 to 12.8	mol/L
Density	-	1.02 (2)	-	1.02	-	1.01 to 1.03	g/cm^3
Flash Point	-	75.7 (2)	-	75.7	-	65.2 to 86.1	°C
Melting Point	-23.8 (8)	1.32e-01 (4)	-24.0	1.32e-01	-24.0 to -23.0	-10.2 to 25.9	°C
Boiling Point	203 (6)	199 (5)	204	199	202 to 204	191 to 202	°C
Surface Tension	-	33.8 (1)	-	33.8	-	-	dyn/cm
Thermal Conductivity	-	158 (1)	-	158	-	-	mW/(m*K)
Vapor Pressure	3.45e-01 (1)	5.21e-01 (4)	3.45e-01	5.21e-01	3.45e-01	1.71e-01 to 9.99e-01	mmHg
Viscosity	-	3.61 (1)	-	3.61	-	-	cP
LogKoa: Octanol-Air	-	3.84 (1)	-	3.84	-	-	-
Henry's Law	3.20e-09 (1)	9.15e-09 (1)	3.20e-09	9.15e-09	-	-	atm-m3/mole
Index of Refraction	-	1.47 (1)	-	1.47	-	-	-

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Multiple Prediction Algorithms

		Experimental
Source	**Result**	
PhysPropNCCT	-0.380	

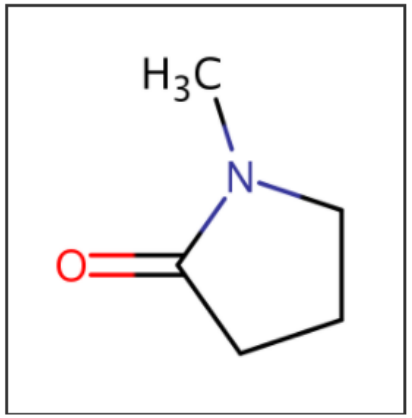
		Predicted
Source	**Result**	**Calculation Details**
EPISUITE	-0.110	Not Available
NICEATM	-0.494	Not Available
ACD/Labs Consensus	-0.345	Not Available
ACD/Labs	-0.398	Not Available
OPERA	-0.300	OPERA Model Report

OPERA Models: LogP: Octanol-Water

United States Environmental Protection Agency

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856



Model Results

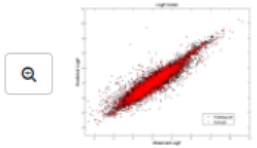
Predicted value: -0.300

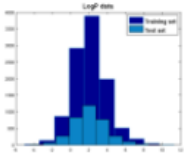
Global applicability domain: Inside

Local applicability domain index: 0.88

Confidence level: 0.81

Model Performance



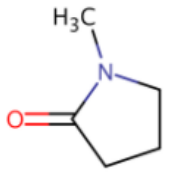


Weighted KNN model

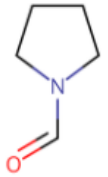
QMRF

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

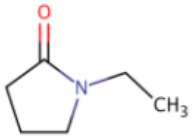
Nearest Neighbors from the Training Set



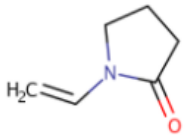
N-Methyl-2-pyrrolidone
Measured: -0.380
Predicted: -0.300



Prolinal
Measured: -0.320
Predicted: -0.226

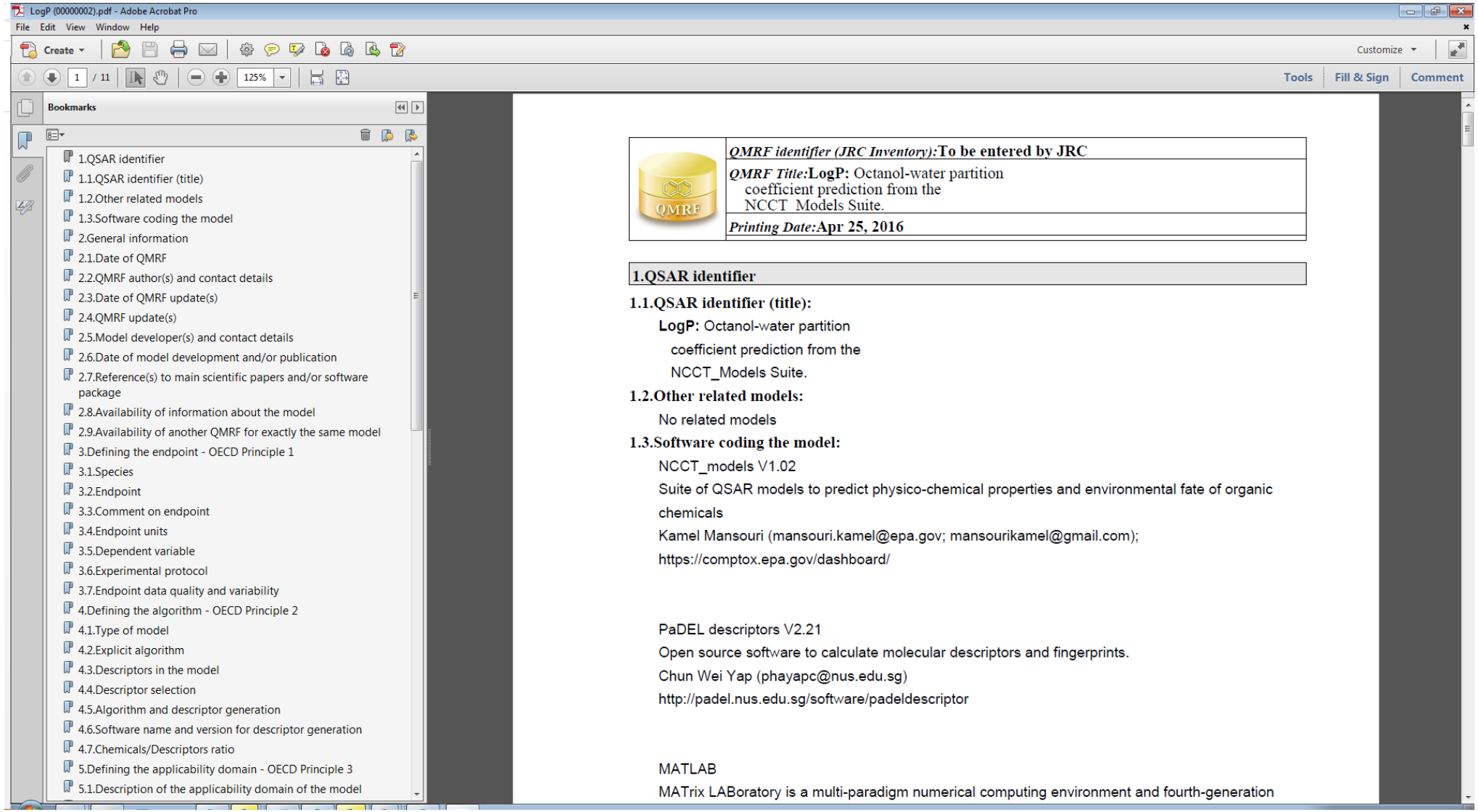


1-Ethyl-2-pyrrolidinone
Measured: -0.0400
Predicted: -0.211



N-Vinyl-2-pyrrolidone
Measured: 0.37
Predicted: 2.65e-01

Transparency: QSAR Modeling Reporting Format



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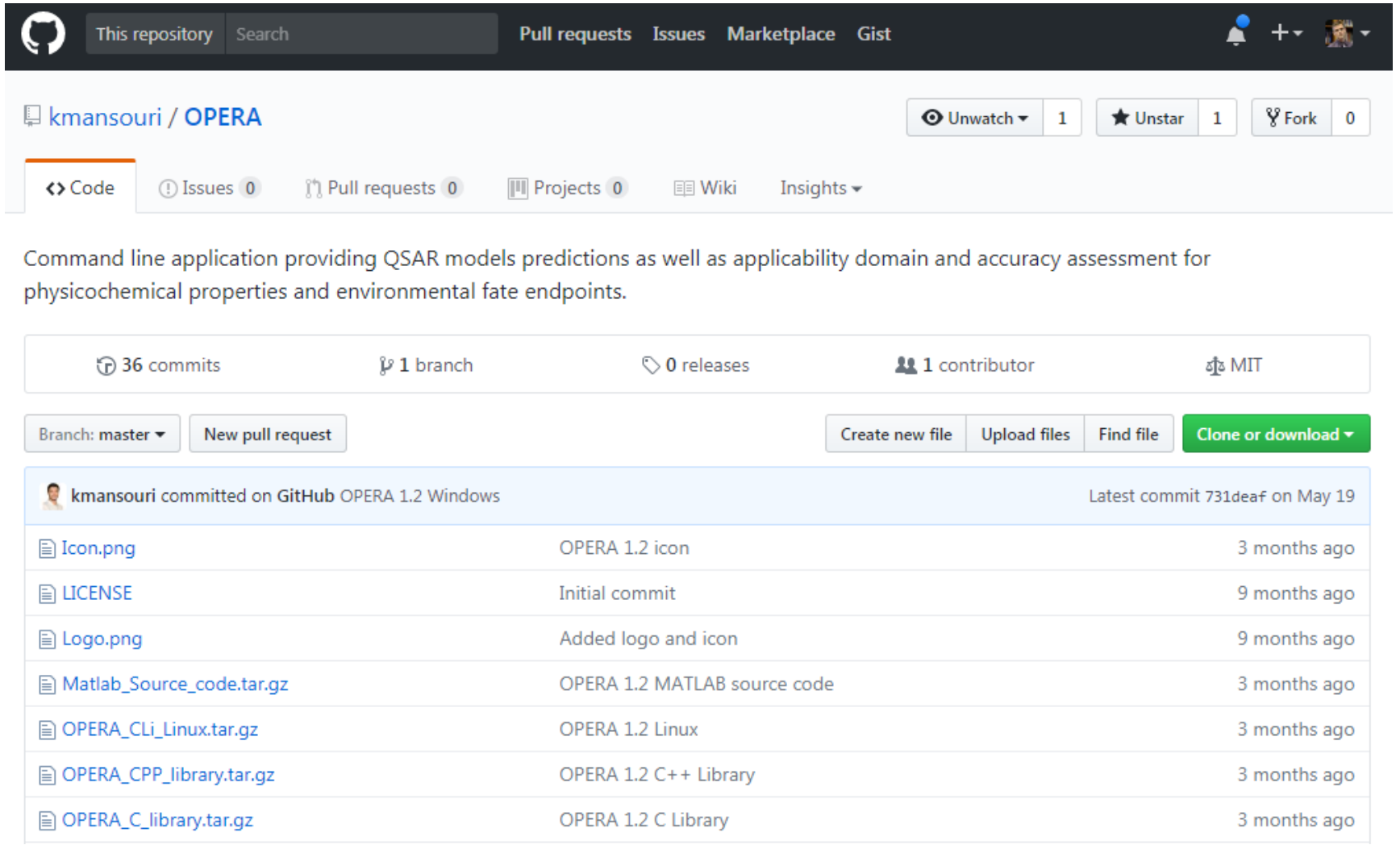
Transparency: OPERA on GitHub



https://github.com/kmansouri/OPERA.git

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Toxicity Values

- **Bioavailability Metric**
- Exposure Limit
- Point Of Departure
- Regulatory Toxicity Value
- Effect Level
- Misc Hazard Information
- Screening Level
- Uncertainty Factor

Download as: TSV | Excel

Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
TD50	-	20.7	mM/kg-day	-	-	-	-	-	DSSTox C...	ACToR
TD50	-	2050	mg/kg-day	-	-	-	-	-	DSSTox C...	ACToR
LEL	systemic	819	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	277	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
LEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
NEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
LEL	systemic	173	mg/kg-day	chronic	oral	chronic	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	115	mg/kg-day	chronic	oral	chronic	mouse	-	Study ID: ...	ToxRefDB
LEL	systemic	678	mg/kg-day	chronic	oral	chronic	rat	-	Study ID: ...	ToxRefDB
NEL	systemic	283	mg/kg-day	chronic	oral	chronic	rat	-	Study ID: ...	ToxRefDB
LEL	systemic	1230	mg/kg-day	subacute	oral	subacute	rat	-	Study ID: ...	ToxRefDB
NEL	systemic	493	mg/kg-day	subacute	oral	subacute	rat	-	Study ID: ...	ToxRefDB
LEL	systemic	2130	mg/kg-day	subacute	oral	subacute	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	920	mg/kg-day	subacute	oral	subacute	mouse	-	Study ID: ...	ToxRefDB

Chemical Properties | Env. Fate/Transport | Toxicity Values (Beta) | ADME (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Synonyms | Literature | External Links

Product Composition Details

Chemical Weight Fractions

Download as: TSV | Excel

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
citristrip canadian stripping...	home maintenance: stripper	0.65	0.7	MSDS	Retail Product Categories/...
citristrip stripping gel qcg7...	home maintenance: stripper	0.4	0.55	MSDS	Retail Product Categories/...
gumout 2 part professional...	auto products: auto fluids a...	0.3	0.4	MSDS	Retail Product Categories/...
minwax water based wipe ...	home maintenance: finish	0.06	0.06	MSDS	Retail Product Categories/...
10-02199- calico tip & glue...	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
artificial nail remover 728 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
calico tip & glue remover 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
kiss nail remover 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
waterborne clear wood fini...	home maintenance: finish	0.01	0.05	MSDS	Retail Product Categories/...

Chemical Properties | Env. Fate/Transport | Toxicity Values (Beta) | ADME (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Synonyms | Literature | External Links

In vitro Bioassay Data

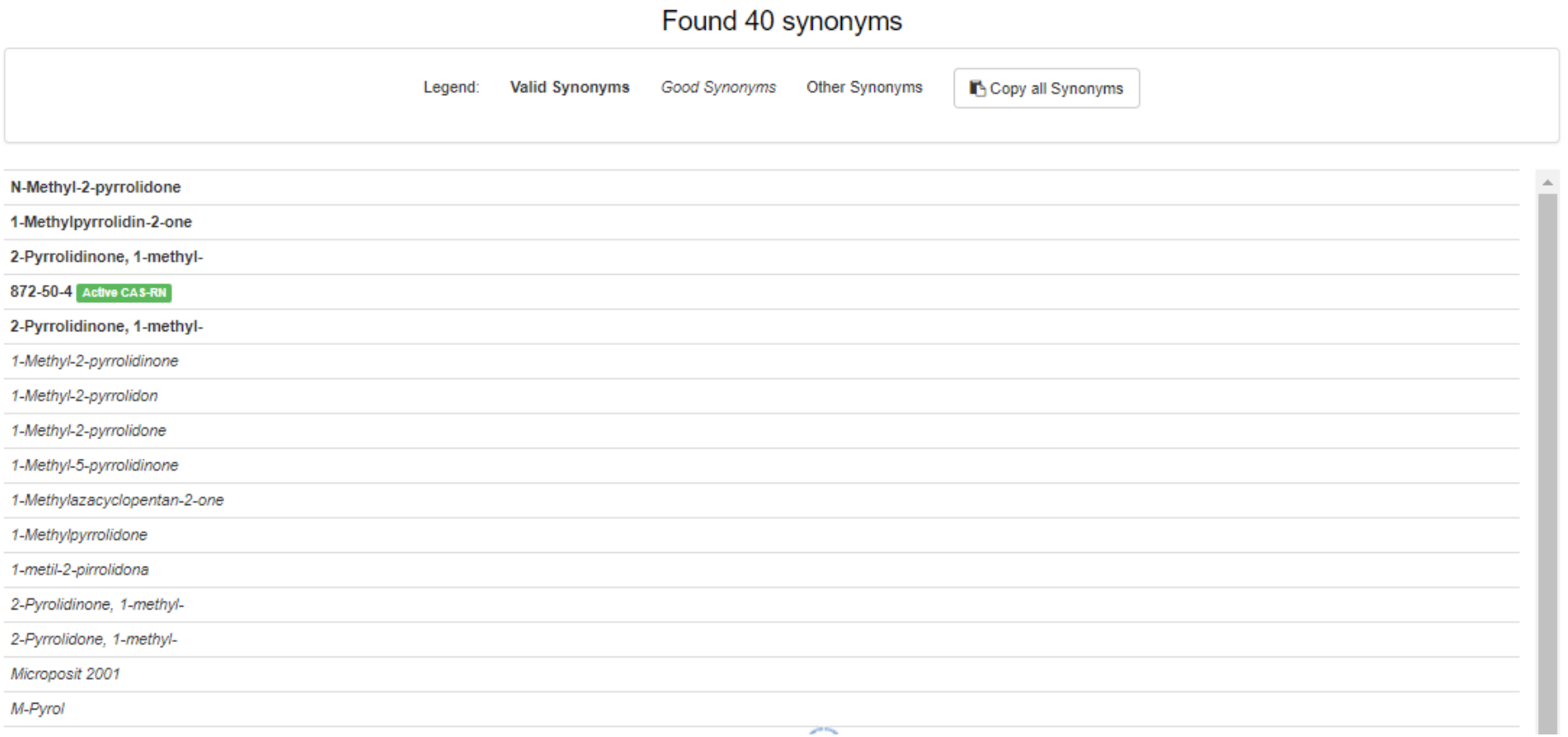
- *In vitro* **bioassays** are used to determine the biological activity of a substance – **ToxCast and Tox21 projects**
- A decade of measurements, and millions of dollars of data integrated into the dashboard

Download as: TSV | Excel Show: Inactive | Background

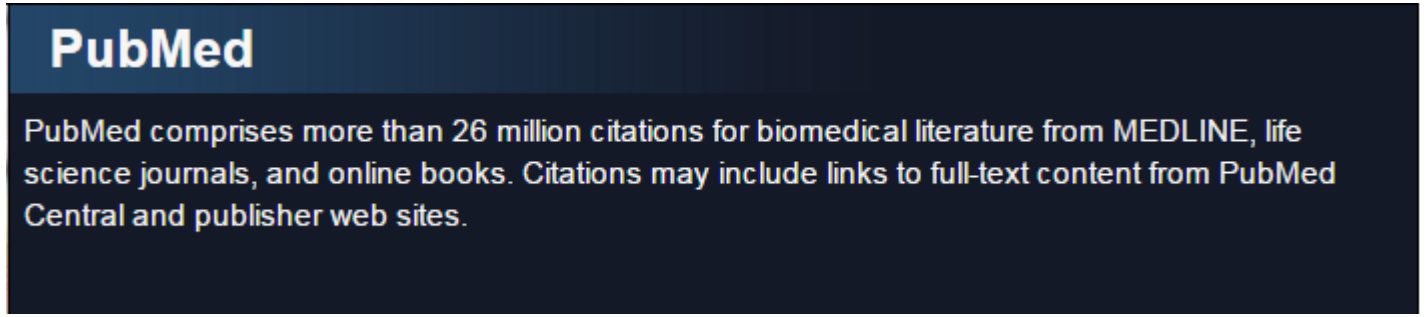
Assay Name	Hit Call	Top	Scaled Top	AC50	log AC50	Intended Target Family
TOX21_Aromatase_Inhibition	ACTIVE	60.7	1.94	28.1	1.45	cyp
TOX21_ERa_LUC_BG1_Agonist	ACTIVE	28.9	1.14	49.8	1.70	nuclear receptor
NVS_TR_hDAT	ACTIVE	55.8	2.79	31.8	1.50	transporter
BSK_CASM3C_SAA_up	ACTIVE	0.129	1.28	0.0116	-1.93	cell adhesion molecules
ATG_RXRb_TRANS_up	ACTIVE	3.58	3.47	23.5	1.37	nuclear receptor
APR_HepG2_MitoMembPot_72h_dn	ACTIVE	0.951	1.30	0.413	-0.384	cell morphology

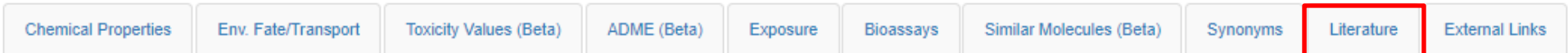
Chemical Properties | Env. Fate/Transport | Toxicity Values (Beta) | ADME (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Synonyms | Literature | External Links

Names and Identifiers



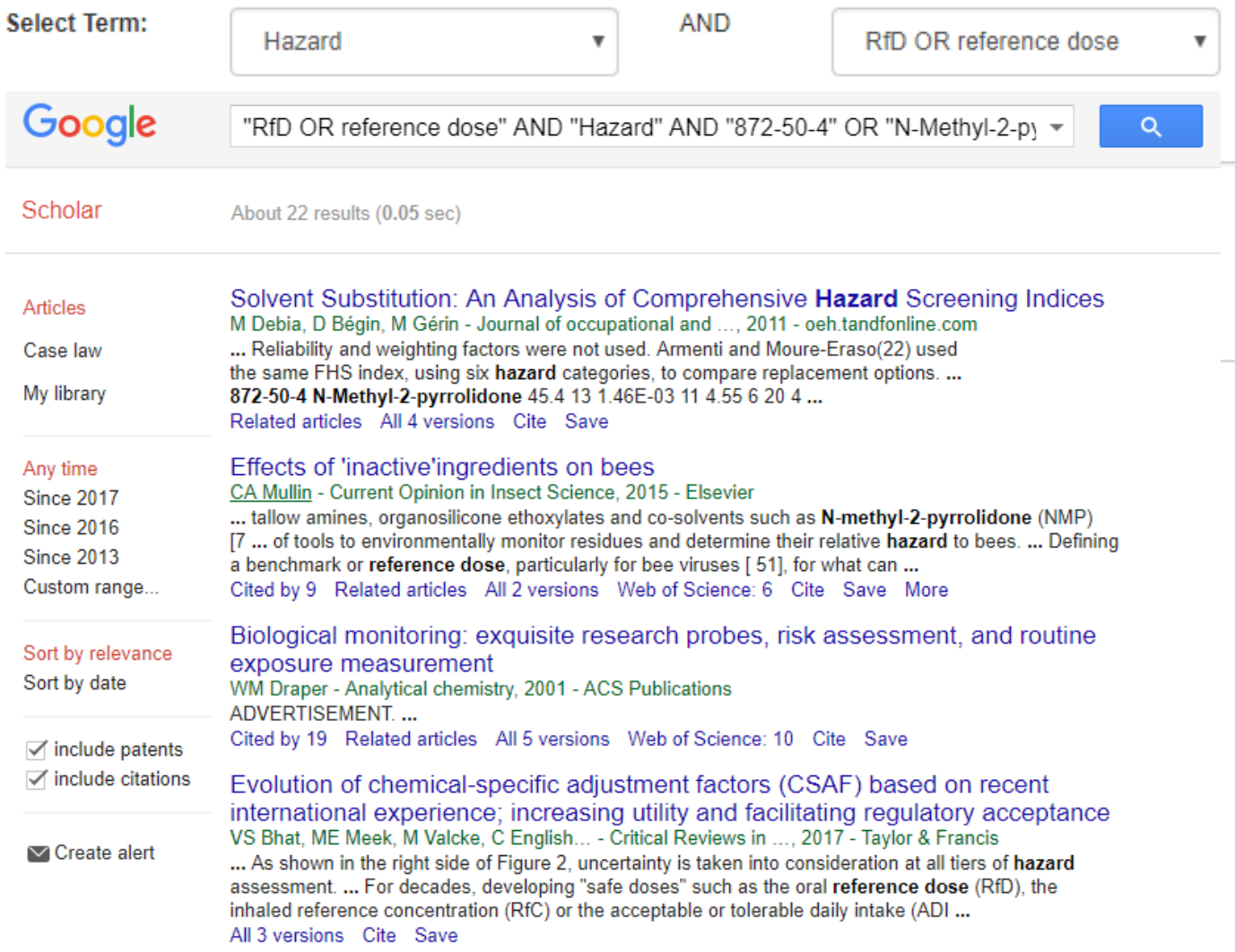
Integrated Literature Searching





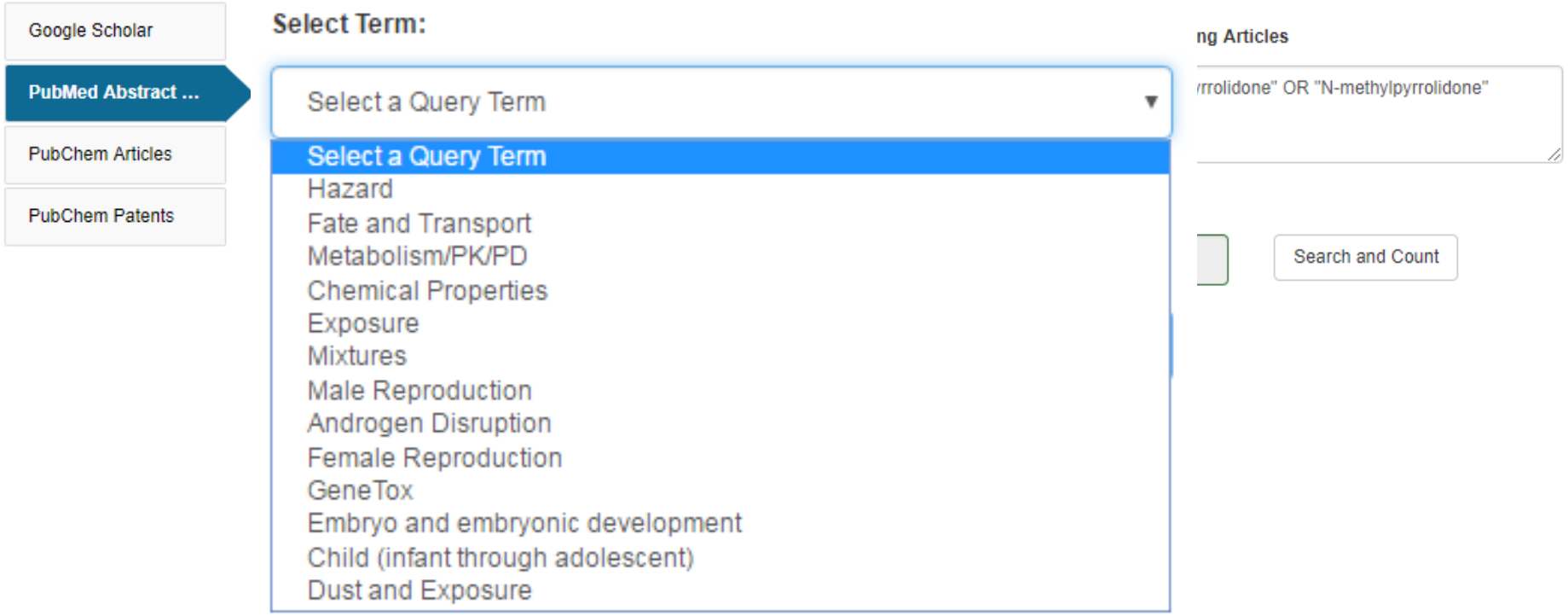
Integrated Literature Searching

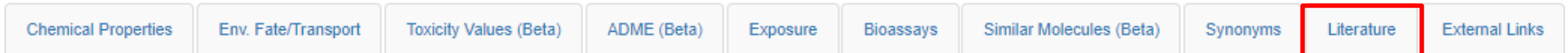
- Google Scholar
- PubMed Abstract S...
- PubChem Articles
- PubChem Patents



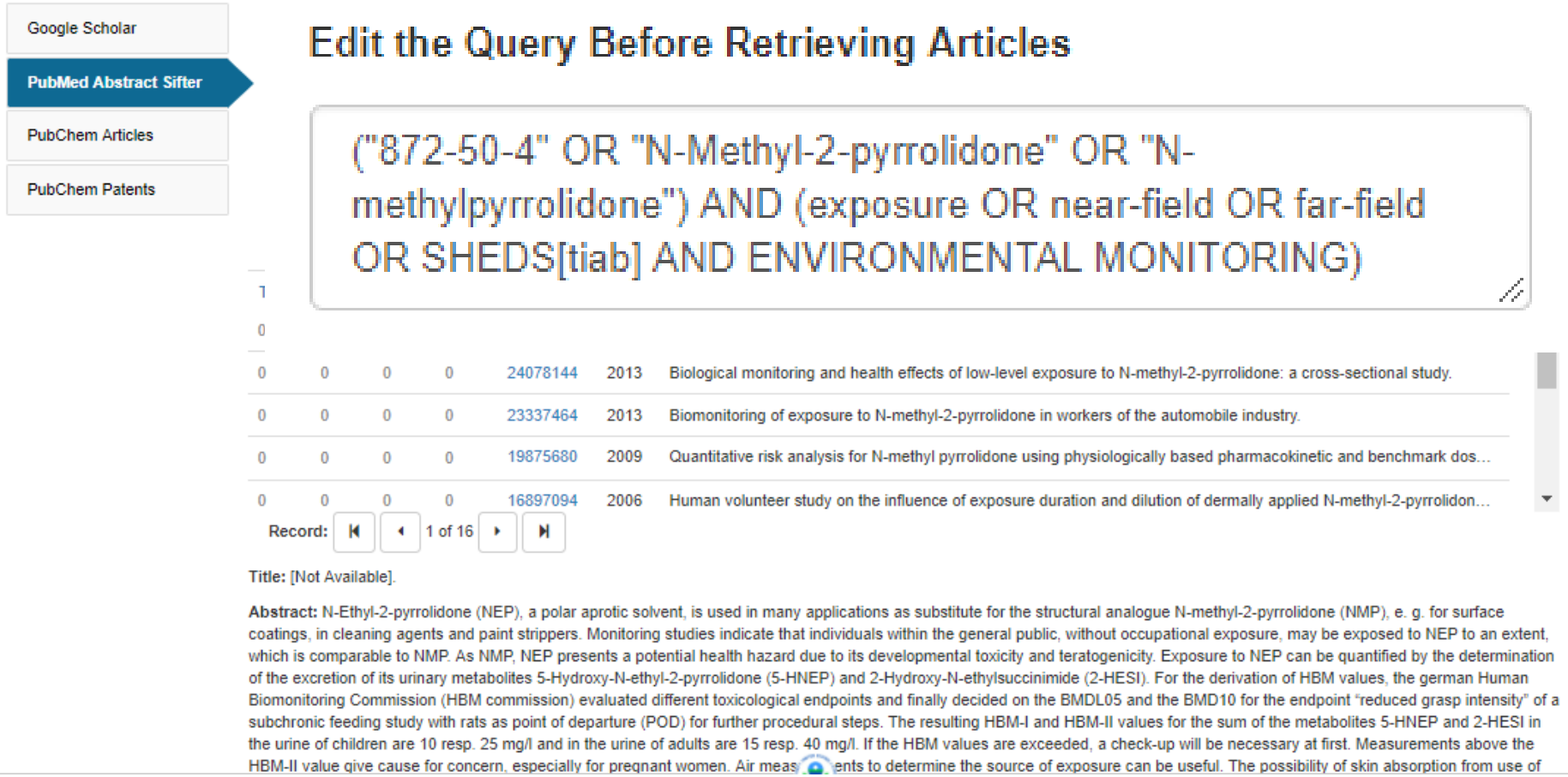
Chemical Properties | Env. Fate/Transport | Toxicity Values (Beta) | ADME (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Synonyms | **Literature** | External Links

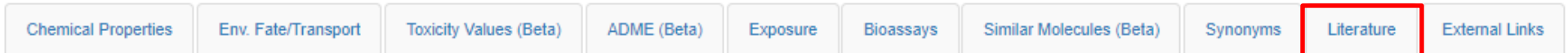
Integrated Literature Searching



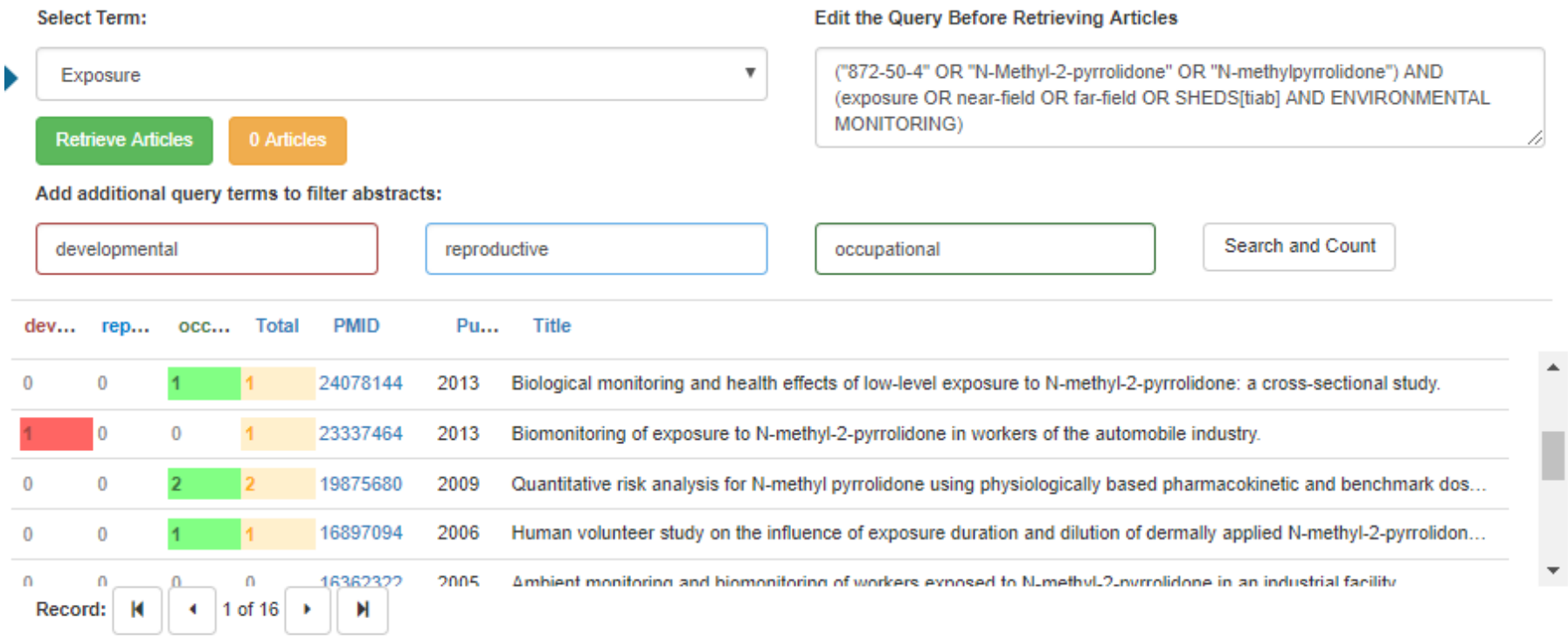


Integrated Literature Searching

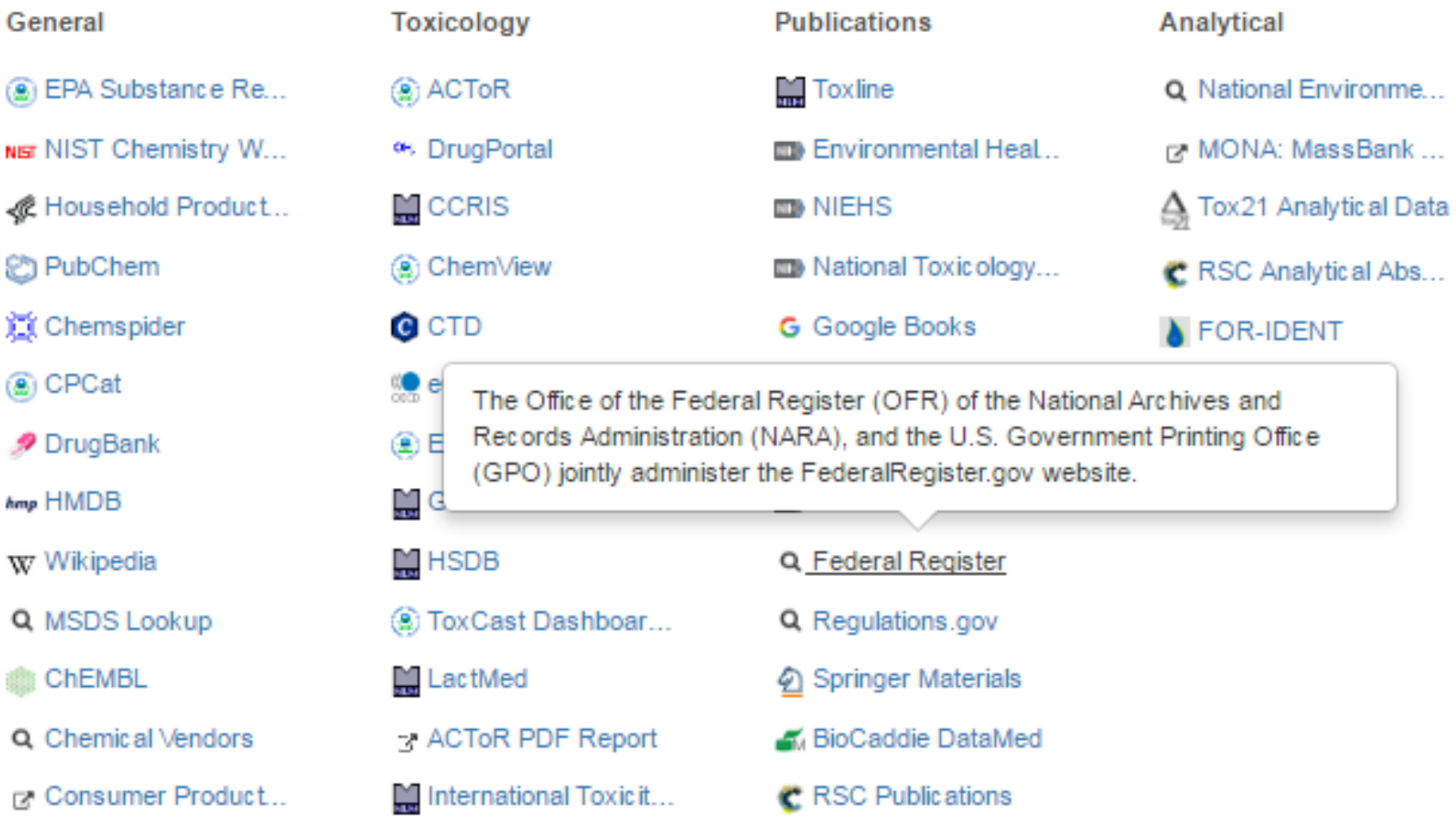




Pubmed Abstract Sifter



Links to Other Resources



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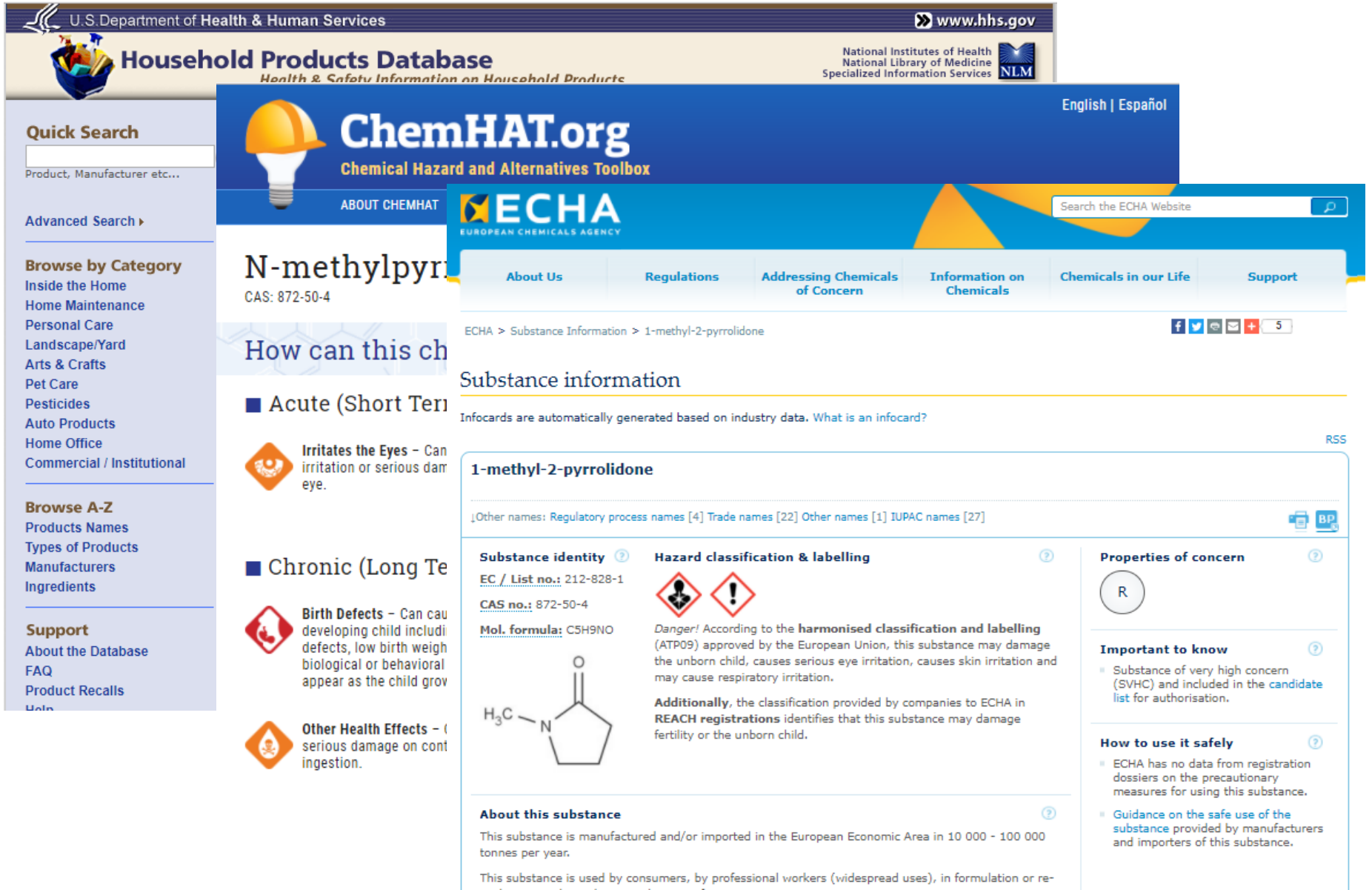
Example External Links…



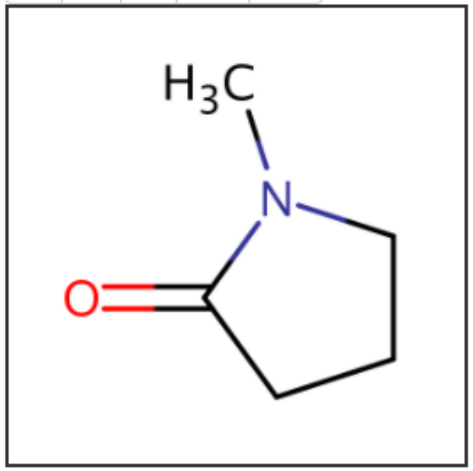
EPA United States Environmental Protection Agency

Managing structure relationships

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856

Searched by Synonym from Valid Source: Found 1 result for 'N-METHYLPYRROLIDONE'.



- Wikipedia
- Intrinsic Properties
- Structural Identifiers
- Related Compounds

Same Connectivity: 3 records (based on first layer of InChI)

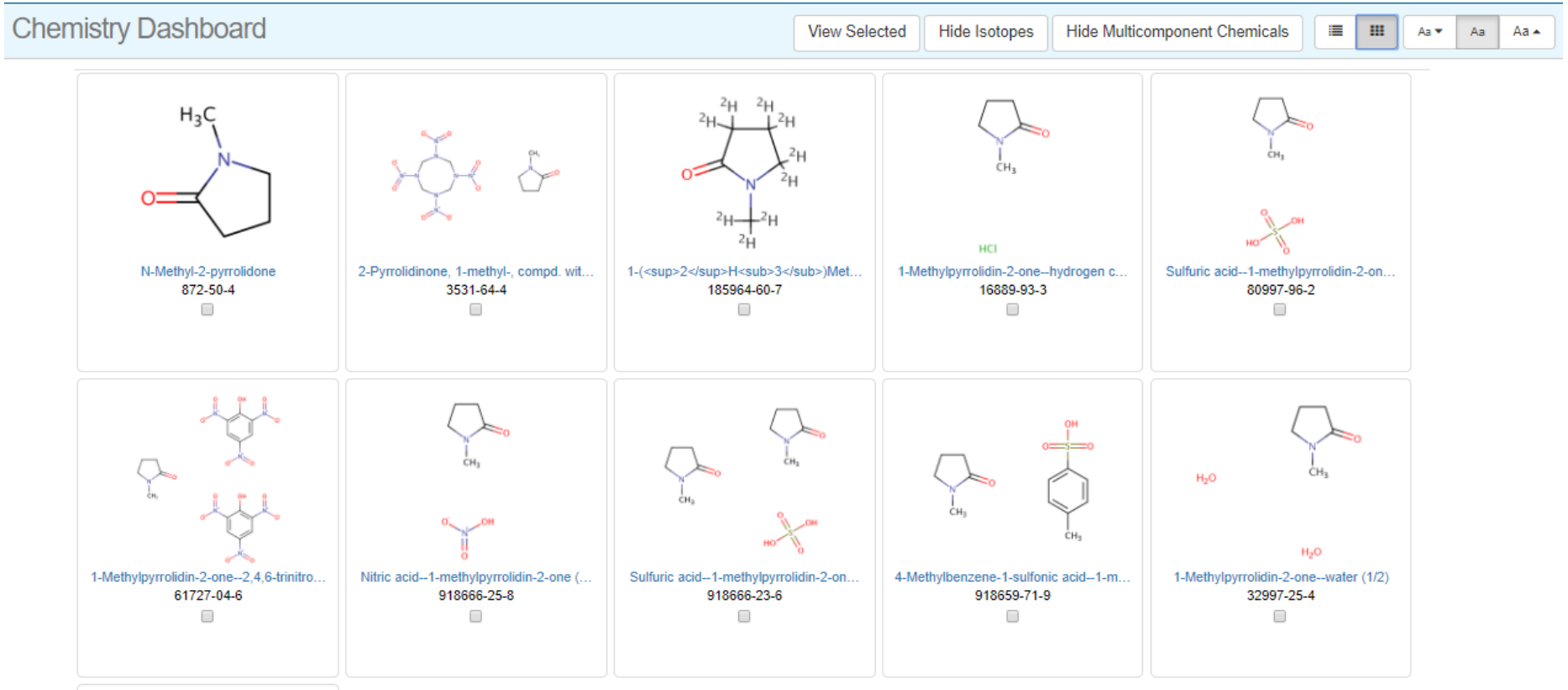
Mixtures, Components, and Neutralized Forms: 11 records (based on QSAR ready mappings and with the compound as a component of a mixture)

Similar Compounds: 970 records (based on Tanimoto coefficient > 0.8)

- Presence in Lists
- Record Information

United States Environmental Protection Agency

Managing structure relationships



Not just structures – “UVCBs”

United States Environmental Protection Agency

Poly (acrylamide-co-acrylic acid), partial sodium salt

62649-23-4 | DTXSID1049722

Searched by Approved Name: Found 1 result for 'Poly (acrylamide-co-acrylic acid), partial sodium salt'.

Record Information

Citation

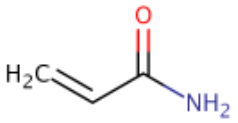
U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID1049722 (accessed February 12, 2017), Poly (acrylamide-co-acrylic acid), partial sodium salt

Data Quality 80%

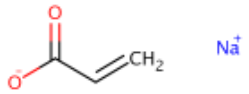
Manually curated and no conflicts in multiple public sources

Related Chemicals

Found 2 chemicals



Acrylamide
79-06-1



2-Propenoic acid, sodium salt
7446-81-3

EPA United States Environmental Protection Agency

UVCB Chemicals

- UVCB chemicals - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
- Many different types of UVCB chemicals
  - Surfactants with undefined composition
  - Petroleum Distillates
  - Gelatins, hydrozylates
  - Formaldehyde, reaction products with diethanolamine
  - Fatty acids, linseed-oil, compds. with triethylamine

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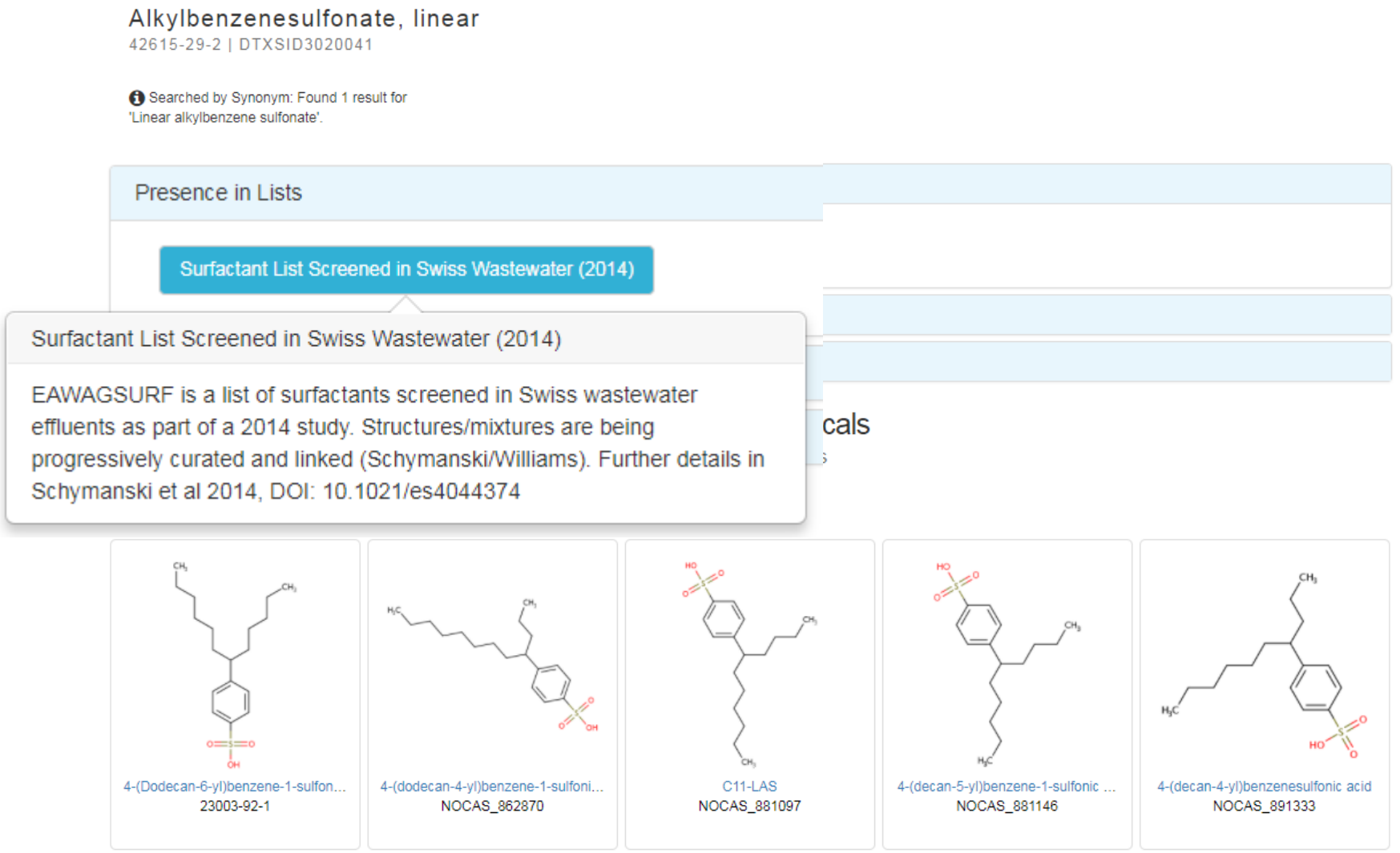
Managing UVCB Relationships



T.E.S.T services public ALPHA

- 96hr fathead minnow 50% lethal concentration (LC50)
- 48hr daphnia magna 50% lethal concentration (LC50)
- Tetrahymena pyriformis 50% growth inhibition conc. (IGC50)
- Oral rat 50% lethal dose (LD50)
- Bioconcentration Factor (BCF)
- Developmental Toxicity (DevTox)
- Ames Mutagenicity (Mutagenicity)
- Normal boiling point, Flash point, Melting point
- Surface tension, Viscosity, Water Solubility
- Thermal Conductivity, Vapor Pressure, Density

- EXAMPLE: https://comptox.epa.gov/dashboard/web-test/WS?smiles=ClC(Cl)(Cl)Cl

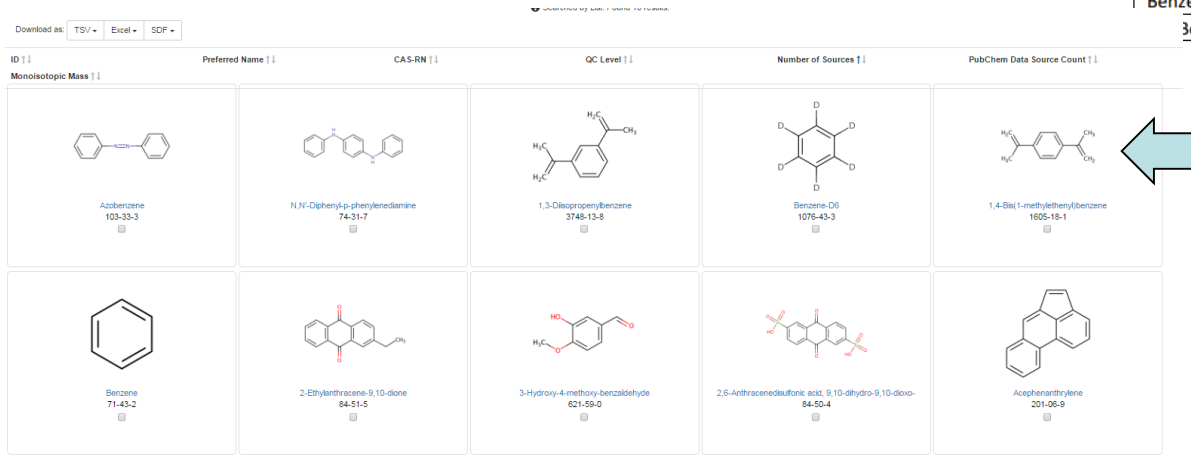
Use Cases

- I have a list of chemical names and CAS Registry Numbers

- What can the dashboard tell me about?
  - What are the chemical structures???
  - Are there predicted properties available?
  - Are there high throughput screening data?
  - What toxicity data are available?
  - Can I download the data for me to use?

Real World Applications – Names to Chemicals

Anthracene		120-12-7
Aromatic oil		
9,10-Anthracenedione, 2-ethyl	2-Ethylanthracene-9,10-dione	84-51-5
Azobenzene		103-33-3
Benz(e)acenaphthylene	Acephenanthrylene	201-06-9
Benzaldehyde, 3-hydroxyl-4-methoxy	3-Hydroxy-4-methoxy-benzaldehyde	621-59-0
Benz(a)anthracene		56-55-3
Benzene		71-43-2
Benzene, 1,3-bis(1-methylethenyl)-	1,3-bis(1-methylethenyl)benzene; 1,3-Diisopropenylbenzene	3748-13-8
Benzene, 1,4-bis(1-methylethenyl)-	1,4-Bis(1-methylethenyl)benzene	1605-18-1
Benzenediamine, N,N'-diphenyl-	N,N'-Diphenyl-p-phenylenediamine	74-31-7



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What about these chemicals????

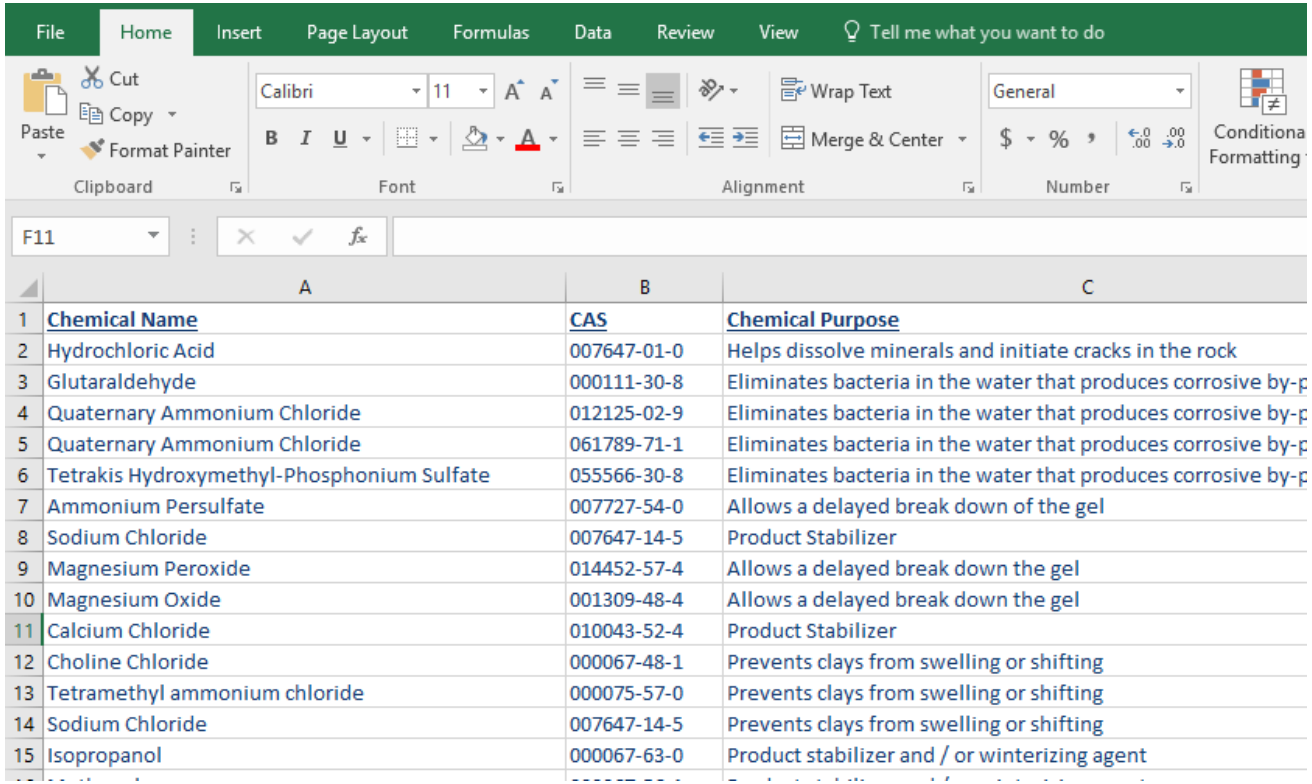
Frac Focus Chemical Disclosure Registry

HYDRAULIC FRACTURING HOW IT WORKS GROUNDWATER PROTECTION

What Chemicals Are Used

As previously noted, chemicals perform many functions in a hydraulic fracturing job. Although there are dozens to hundreds of chemicals which could be used as additives, there are a limited number which are routinely used in hydraulic fracturing. The following is a list of the chemicals used most often. This chart is sorted alphabetically by the Product Function to make it easier for you to compare to the fracturing records .

Chemical Name	CAS	Chemical Purpose	Product Function
Hydrochloric Acid	007647-01-0	Helps dissolve minerals and initiate cracks in the rock	Acid
Glutaraldehyde	000111-30-8	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	012125-02-9	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	061789-71-1	Eliminates bacteria in the water that produces corrosive by-products	Biocide



File Home Insert Page Layout Formulas Data Review View Tell me what you want to do

Cut Copy Format Painter Paste Clipboard

Calibri 11 Font

Wrap Text Merge & Center Alignment

General Number

Conditional Formatting

F11

	A	B	C
1	Chemical Name	CAS	Chemical Purpose
2	Hydrochloric Acid	007647-01-0	Helps dissolve minerals and initiate cracks in the rock
3	Glutaraldehyde	000111-30-8	Eliminates bacteria in the water that produces corrosive by-p
4	Quaternary Ammonium Chloride	012125-02-9	Eliminates bacteria in the water that produces corrosive by-p
5	Quaternary Ammonium Chloride	061789-71-1	Eliminates bacteria in the water that produces corrosive by-p
6	Tetrakis Hydroxymethyl-Phosphonium Sulfate	055566-30-8	Eliminates bacteria in the water that produces corrosive by-p
7	Ammonium Persulfate	007727-54-0	Allows a delayed break down of the gel
8	Sodium Chloride	007647-14-5	Product Stabilizer
9	Magnesium Peroxide	014452-57-4	Allows a delayed break down the gel
10	Magnesium Oxide	001309-48-4	Allows a delayed break down the gel
11	Calcium Chloride	010043-52-4	Product Stabilizer
12	Choline Chloride	000067-48-1	Prevents clays from swelling or shifting
13	Tetramethyl ammonium chloride	000075-57-0	Prevents clays from swelling or shifting
14	Sodium Chloride	007647-14-5	Prevents clays from swelling or shifting
15	Isopropanol	000067-63-0	Product stabilizer and / or winterizing agent

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What about these chemicals????

Batch Search

Please enter one identifier per line

Select Input Type(s)

- [ ] Chemical Name
- [x] CAS-RN
- [ ] InChIKey
- [ ] DSSTox Substance ID
- [ ] Exact Molecular Formula

Enter Identifiers to Search

```
007647-01-0
000111-30-8
012125-02-9
061789-71-1
055566-30-8
007727-54-0
007647-14-5
014452-57-4
001309-48-4
010043-52-4
```

Display All Chemicals | Download Chemical Data

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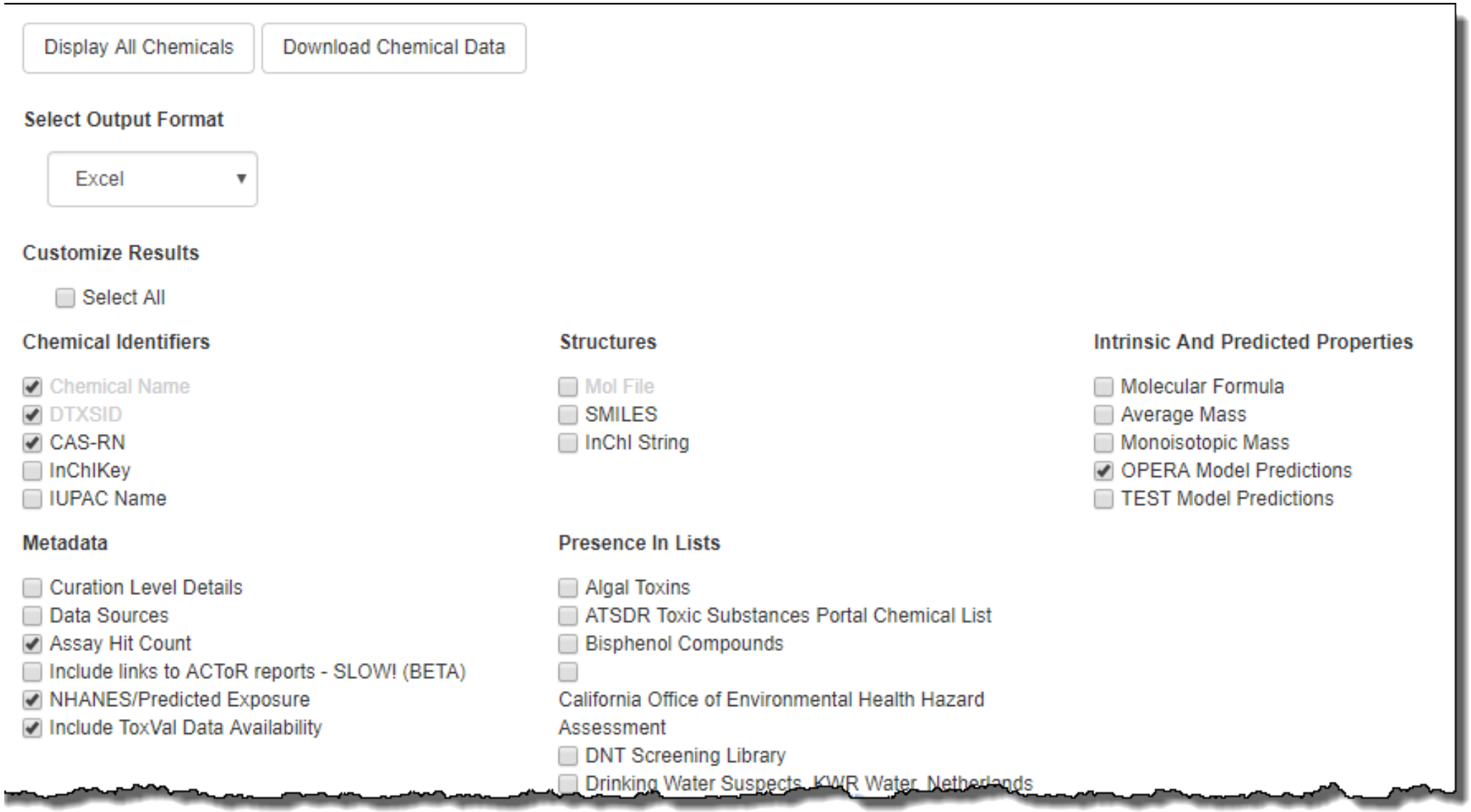
What about these chemicals????



What about these chemicals????

A	B	C	D	E	F	G	H	I	J
INPUT	DTXSID	PREFERRED NAME	CASRN	TOXCAST	TOXCAST	EXPOCAST	EXPOCAST	NHANES	TOXVAL DATA
007647-01-0	DTXSID2020711	Hydrochloric acid	7647-01-0	-	-	-	-	-	Y
000111-30-8	DTXSID6025355	Glutaraldehyde	111-30-8	12.86	71/552	Y	2.03e-05	-	Y
012125-02-9	DTXSID0020078	Ammonium chloride	12125-02-9	-	-	-	-	-	Y
061789-71-1	Checksum Failed	-							
055566-30-8	DTXSID0021331	Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	4.71	13/276	Y	3.47e-08	-	Y
007727-54-0	DTXSID9029691	Diammonium peroxydisulfate	7727-54-0	0.88	1/113	-	-	-	Y
007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
014452-57-4	DTXSID9049667	Magnesium peroxide	14452-57-4	-	-	-	-	-	Y
001309-48-4	DTXSID9049665	Magnesium oxide	1309-48-4	-	-	-	-	-	Y
010043-52-4	DTXSID5020235	Calcium chloride	10043-52-4	0.88	1/113	Y	9.45e-05	-	Y
000067-48-1	DTXSID4020325	Choline chloride	67-48-1	0.0	0/113	Y	4.94e-07	-	Y
000075-57-0	DTXSID6021749	Tetramethylammonium chloride	75-57-0	0.0	0/113	Y	5.33e-08	-	Y
007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
000067-63-0	DTXSID7020762	Isopropanol	67-63-0	9.73	11/113	Y	4.8e-05	-	Y
000067-56-1	DTXSID2021731	Methanol	67-56-1	0.0	0/113	Y	3.01e-05	-	Y
000064-18-6	DTXSID2024115	Formic acid	64-18-6	-	-	-	-	-	Y
000075-07-0	DTXSID5039224	Acetaldehyde	75-07-0	22.1	61/276	Y	2.57e-06	-	Y
064741-85-1	DTXSID0028169	Raffinates, petroleum, sorption process	64741-85-1	-	-	-	-	-	-
064742-47-8	DTXSID8028212	Distillates, petroleum, hydrotreated light	64742-47-8	-	-	-	-	-	Y

Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides

61789-71-7 | DTXSID6029381

Curating Chemistry Data is painful

	A	B	C
	INPUT	DTXSID	PREFERRED NAME
	007647-01-0	DTXSID2020711	Hydrochloric acid
	000111-30-8	DTXSID6025355	Glutaraldehyde
	012125-02-9	DTXSID0020078	Ammonium chloride
	061789-71-1	Checksum Failed	-
	055566-30-8	DTXSID0021331	Tetrakis(hydroxymethyl)ph
	007727-54-0	DTXSID9029691	Diammonium peroxydisulf
	007647-14-5	DTXSID3021271	Sodium chloride
	014452-57-4	DTXSID9049667	Magnesium peroxide

Chemical Name	CAS	Chemical Purpose	Product Fur
Hydrochloric Acid	007647-01-0	Helps dissolve minerals and initiate cracks in the rock	Acid
Glutaraldehyde	000111-30-8	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	012125-02-9	Eliminates bacteria in the water that produces corrosive by-products	Biocide
Quaternary Ammonium Chloride	061789-71-1	Eliminates bacteria in the water that produces corrosive by-products	Biocide

Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides

61789-71-7 | DTXSID6029381

Compare CAS Numbers:
61789-71-1 (**FAIL**) versus 61789-71-7 (**OCR failure**?)

What about these chemicals????

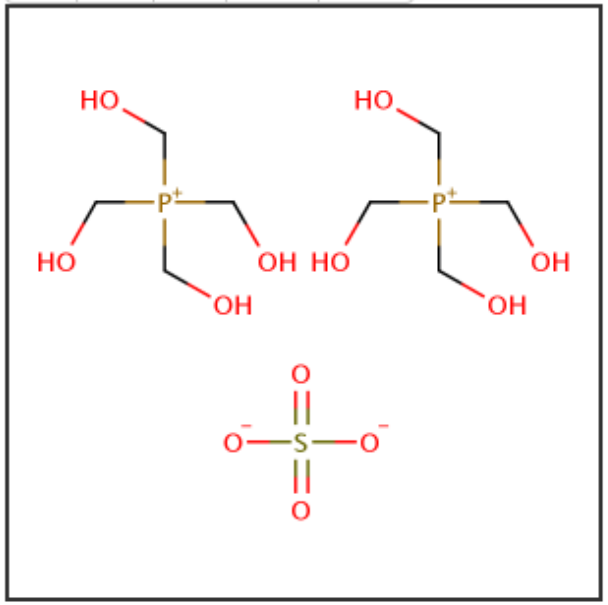
	A	B	C	D	E	F	G	H	I	J
	INPUT	DTXSID	PREFERRED NAME	CASRN	TOXCAST	TOXCAST	EXPOCAST	EXPOCAST	NHANES	TOXVAL DATA
	007647-01-0	DTXSID2020711	Hydrochloric acid	7647-01-0	-	-	-	-	-	Y
	000111-30-8	DTXSID6025355	Glutaraldehyde	111-30-8	12.86	71/552	Y	2.03e-05	-	Y
	012125-02-9	DTXSID0020078	Ammonium chloride	12125-02-9	-	-	-	-	-	Y
	061789-71-1	Checksum Failed	-							
	055566-30-8	DTXSID0021331	Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	4.71	13/276	Y	3.47e-08	-	Y
	007727-54-0	DTXSID9029691	Diammonium peroxydisulfate	7727-54-0	0.88	1/113	-	-	-	Y
	007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
	014452-57-4	DTXSID9049667	Magnesium peroxide	14452-57-4	-	-	-	-	-	Y
	001309-48-4	DTXSID9049665	Magnesium oxide	1309-48-4	-	-	-	-	-	Y
	010043-52-4	DTXSID5020235	Calcium chloride	10043-52-4	0.88	1/113	Y	9.45e-05	-	Y
	000067-48-1	DTXSID4020325	Choline chloride	67-48-1	0.0	0/113	Y	4.94e-07	-	Y
	000075-57-0	DTXSID6021749	Tetramethylammonium chloride	75-57-0	0.0	0/113	Y	5.33e-08	-	Y
	007647-14-5	DTXSID3021271	Sodium chloride	7647-14-5	-	-	-	-	-	Y
	000067-63-0	DTXSID7020762	Isopropanol	67-63-0	9.73	11/113	Y	4.8e-05	-	Y
	000067-56-1	DTXSID2021731	Methanol	67-56-1	0.0	0/113	Y	3.01e-05	-	Y
	000064-18-6	DTXSID2024115	Formic acid	64-18-6	-	-	-	-	-	Y
	000075-07-0	DTXSID5039224	Acetaldehyde	75-07-0	22.1	61/276	Y	2.57e-06	-	Y
	064741-85-1	DTXSID0028169	Raffinates, petroleum, sorption process	64741-85-1	-	-	-	-	-	-
	064742-47-8	DTXSID8028212	Distillates, petroleum, hydrotreated light	64742-47-8	-	-	-	-	-	Y

Single Click Navigation into the Chemical

Tetrakis(hydroxymethyl)phosphonium sulfate

55566-30-8 | DTXSID0021331

Searched by CAS-RN: Found 1 result for '55566-30-8'.



- Intrinsic Properties
- Structural Identifiers
- Related Compounds
- Presence in Lists
- Record Information

Citation

U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID0021331 (accessed October 16, 2017), Tetrakis(hydroxymethyl)phosphonium sulfate

Data Quality

Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers

United States Environmental Protection Agency

Data for Download

https://comptox.epa.gov/dashboard/downloads

Downloads

DSSTox Identifier to PubChem Identifier Mapping File — Posted: 11/14/2016

The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

SID	CID	DTXSID
316388891	20404	DTXSID30873143
316388890	10142816	DTXSID70873142
316388889	50742127	DTXSID40873139
316388888	19073841	DTXSID20873137
316388887	11505215	DTXSID00873135
316388886	25021861	DTXSID80873133
316388885	2784427	DTXSID60873131
316388884	6731	DTXSID00873130

DSSTox identifiers mapped to CAS Numbers and Names File — Posted: 11/14/2016

The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

	A	B	
1	**casrn**	**dsstox_substance_id**	**preferred_name**
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide

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Future Work

- Continue expansion and curation of data and types.
- Provide "**programmatic access**" to all data – connect to other Agency resources and allow other scientists to integrate their scientific applications.
- Continue to assemble and enhance chemical lists and data for specific projects. Make available to Agency researchers and for public use.
- Make new modules public – "Generalized Read Across", "EcoTox data"

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Conclusion

- Chemistry Dashboard for ~760,000 chemicals and associated data
  - Search for single chemical or batch-based searching
  - A focus on data curation and quality
- An **Integration Hub** – *in vitro* HTS, *in vivo* hazard toxicity, experimental and predicted physchem and fate and transport data
  - Transparency in predictions and access to Open Data
- Data downloads allows for reuse in other systems and integration of resources to support research

Acknowledgments

- The collective work of many
  - Chris Grulke
  - Andrew McEachran
  - Nancy Baker
  - Kathie Dionisio
  - Katharine Phillips
  - Kristin Isaacs
  - Jon Sobus
  - John Wambaugh
  - Richard Judson
  - Ann Richard
- Many colleagues across the agency

Antony Williams

Williams.Antony@epa.gov