http://www.orcid.org/0000-0002-2668-4821

The EPA CompTox Chemistry Dashboard and Underpinning Software Architecture – a platform for data integration for environmental chemistry data

Antony Williams[1], Chris Grulke[1], Daniel Chang[2], Kristan Markey[2] and Jeff Edwards[1]

1. *National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC*
2. *Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency, Washington, DC*
3. *Office of Science Coordination and Policy, U.S. Environmental Protection Agency, Washington, DC*

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

August 2017
ACS Fall Meeting, Washington, DC

The CompTox Chemistry Dashboard

PRIMARY GOALS

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

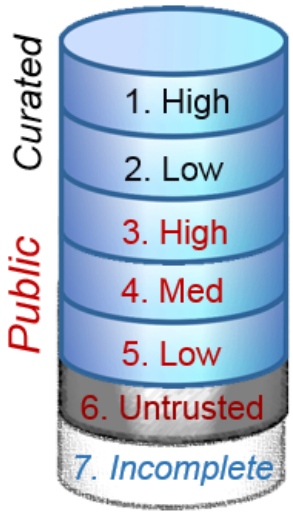
SECONDARY GOAL

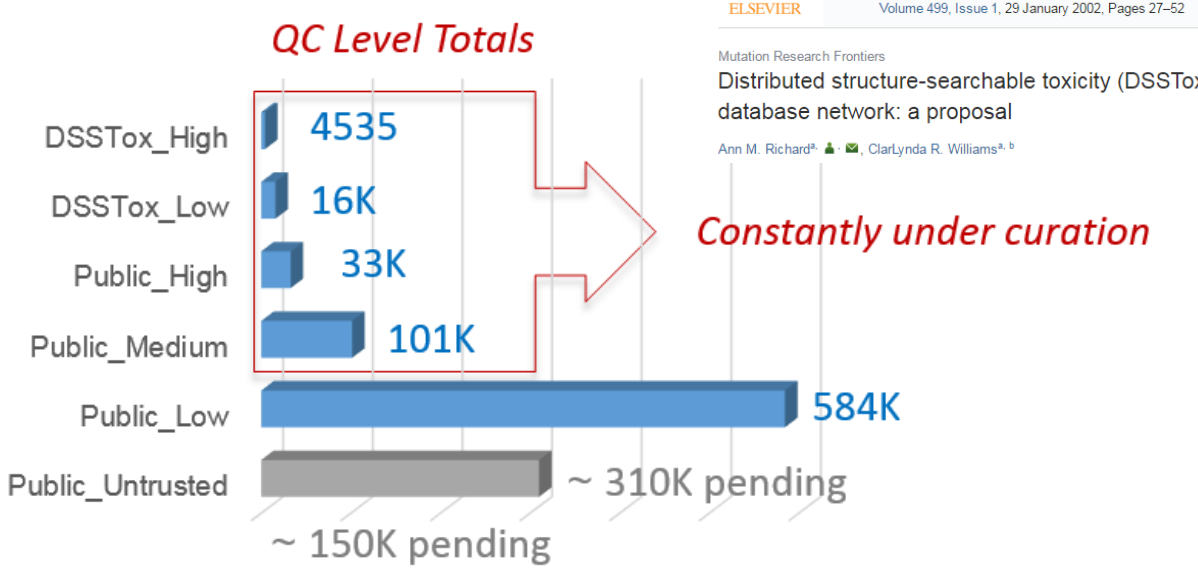
- Develop a cheminformatics architecture to serve as a high quality chemical foundation for all NCCT tools and data

The CompTox Chemistry Dashboard: An Overview

- A **publicly accessible website** delivering access:
  - ~760,000 chemicals and related property data
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - “Batch searching” for thousands of chemicals
- Day-to-day curation efforts for data quality

Our Chemistry Content





ELSEVIER
Mutation Research/Fundamental and Molecular Mechanisms of Mutagenesis
Volume 499, Issue 1, 29 January 2002, Pages 27–52

Mutation Research Frontiers

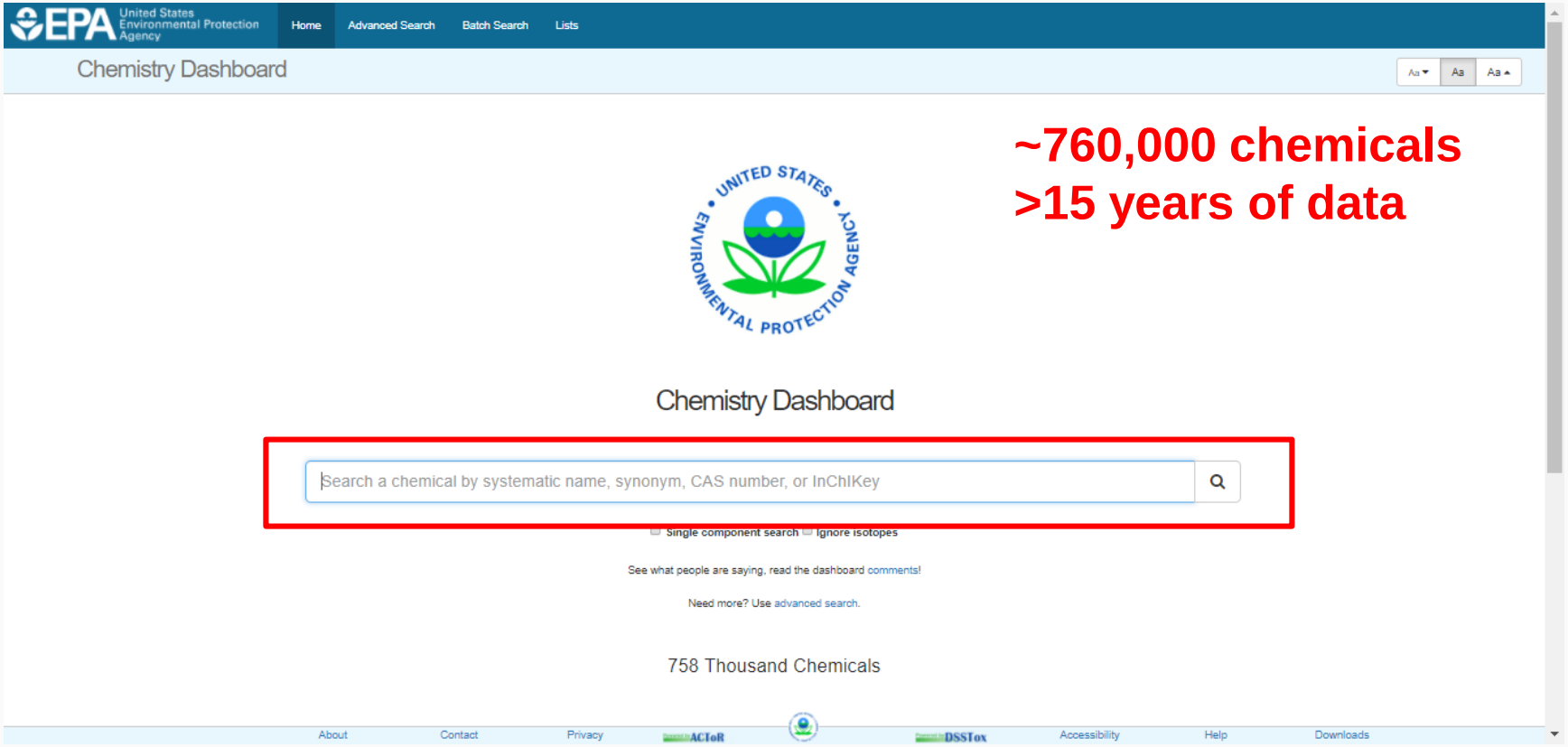
Distributed structure-searchable toxicity (DSSTox) public database network: a proposal

Ann M. Richard[a], ClarLynda R. Williams[a, b]

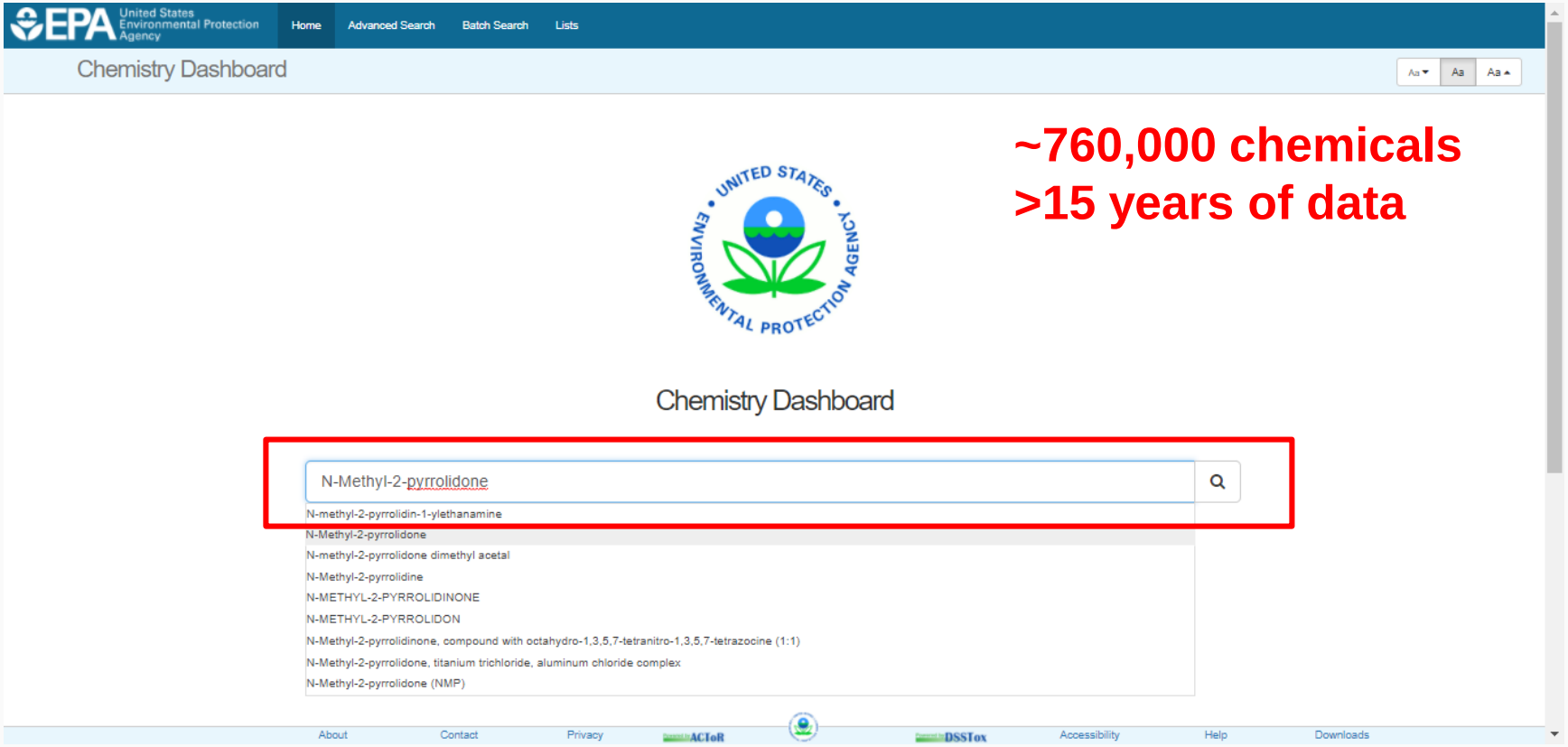
QC Levels

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

Comptox Chemistry Dashboard
https://comptox.epa.gov



Comptox Chemistry Dashboard
https://comptox.epa.gov

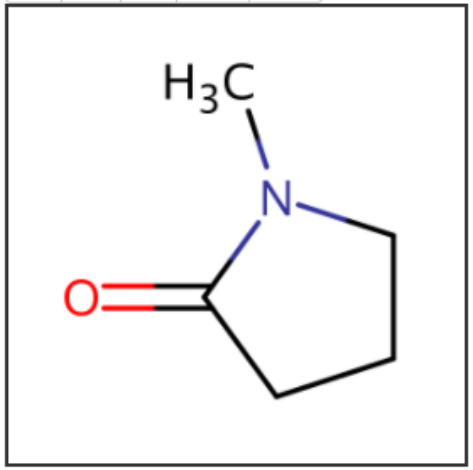


Chemical Page

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

EPA United States Environmental Protection Agency

- 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	-	-	-

Available Properties

- Solubility
- Melting Point
- Boiling Point
- LogP (Octanol-water partition coefficient)
- Atmospheric Hydroxylation Rate
- LogBCF (Bioconcentration Factor)
- Biodegradation Half-life
- Henry's Law Constant
- Fish Biotransformation Half-life
- LogKOA (Octanol/Air Partition Coefficient)
- LogKOC (Soil Adsorption Coefficient)
- Vapor Pressure

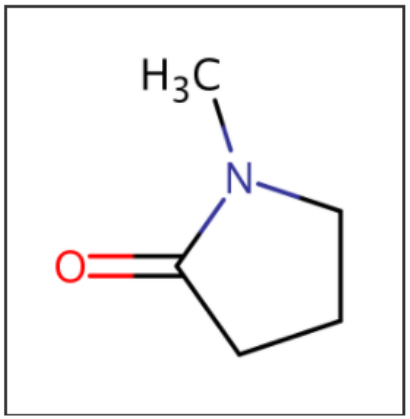
		Experimental
Source	**Result**	
PhysPropNCCT	-0.380	

		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

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856



Model Results

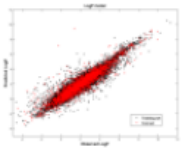
Predicted value: -0.300

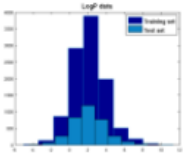
Global applicability domain: Inside

Local applicability domain index: 0.88

Confidence level: 0.81

Model Performance



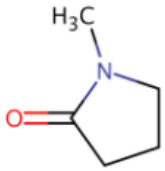


Weighted KNN model

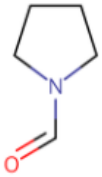
QMRF

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

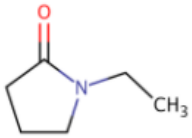
Nearest Neighbors from the Training Set



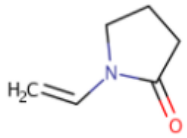
N-Methyl-2-pyrrolidone
Measured: -0.380
Predicted: -0.300



Prolinal
Measured: -0.320
Predicted: -0.226

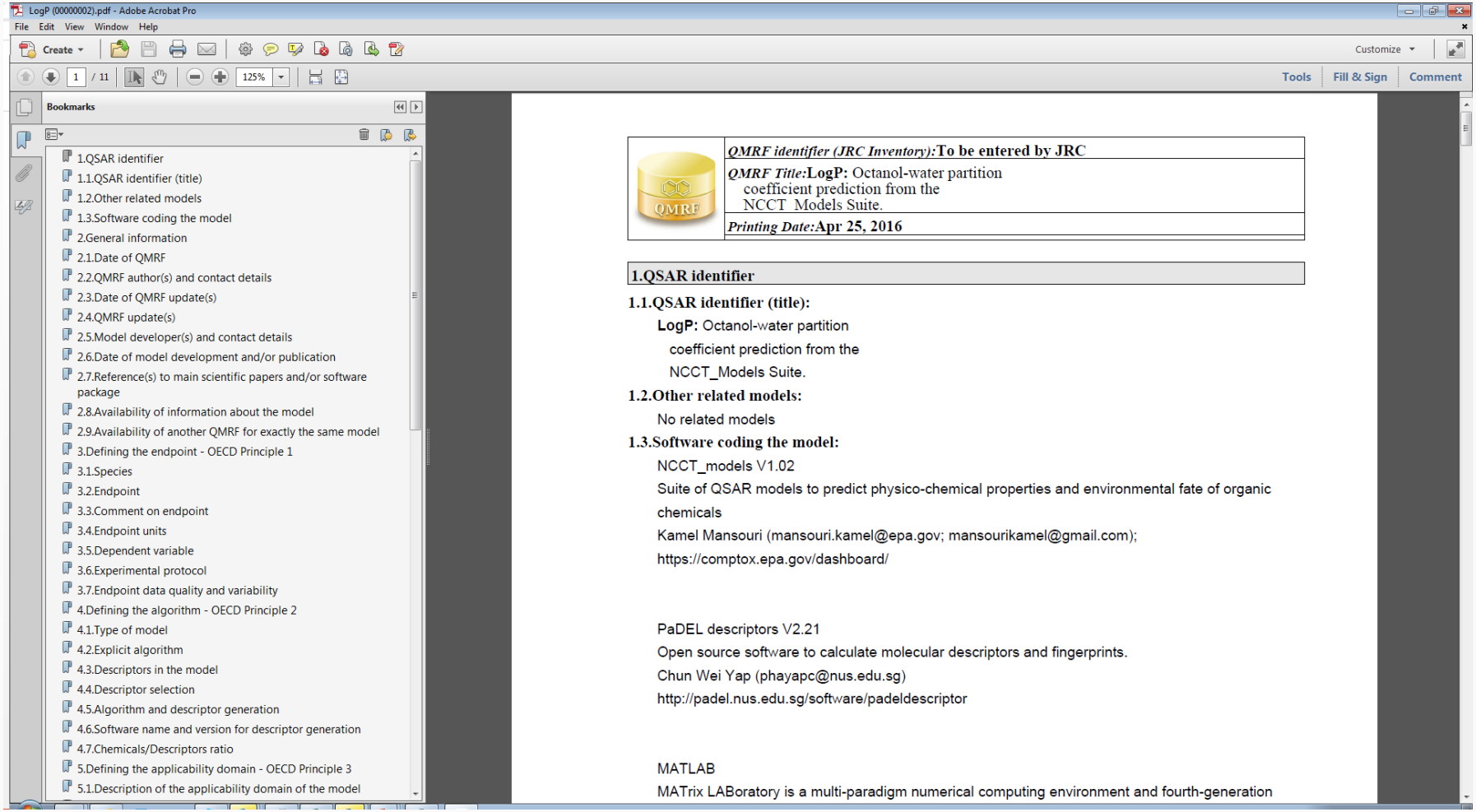


1-Ethyl-2-pyrrolidinone
Measured: -0.0400
Predicted: -0.211



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

QSAR Modeling Reporting Format



Toxicity Values

EPA United States Environmental Protection Agency

- **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	619	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

Product Composition Details

EPA United States Environmental Protection Agency

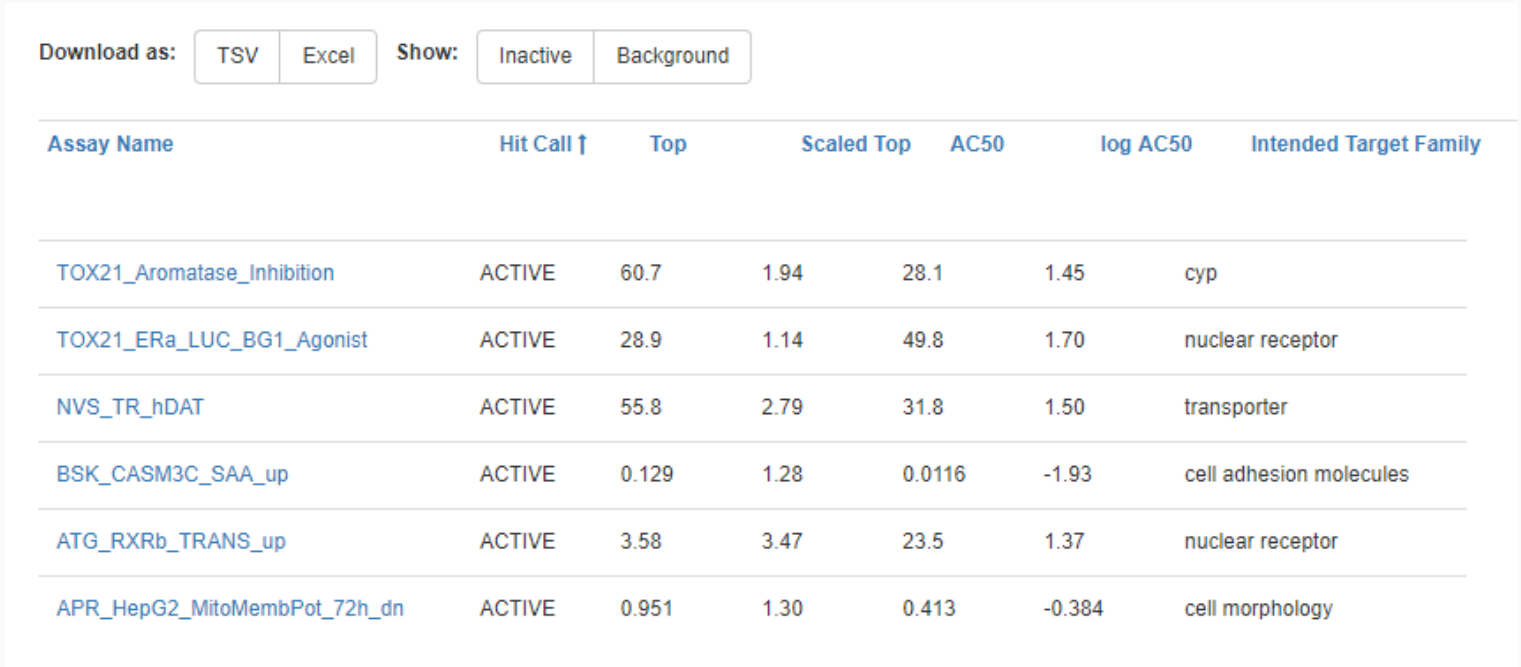
Chemical Weight Fractions

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/...

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

EPA United States Environmental Protection Agency

Found 40 synonyms

Legend: **Valid Synonyms** *Good Synonyms* Other Synonyms

Copy all Synonyms

N-Methyl-2-pyrrolidone

1-Methylpyrrolidin-2-one

2-Pyrrolidinone, 1-methyl-

872-50-4 Active CAS-RN

2-Pyrrolidinone, 1-methyl-

1-Methyl-2-pyrrolidinone

1-Methyl-2-pyrrolidon

1-Methyl-2-pyrrolidone

1-Methyl-5-pyrrolidinone

1-Methylazacyclopentan-2-one

1-Methylpyrrolidone

1-metil-2-pirrolidona

2-Pyrolidinone, 1-methyl-

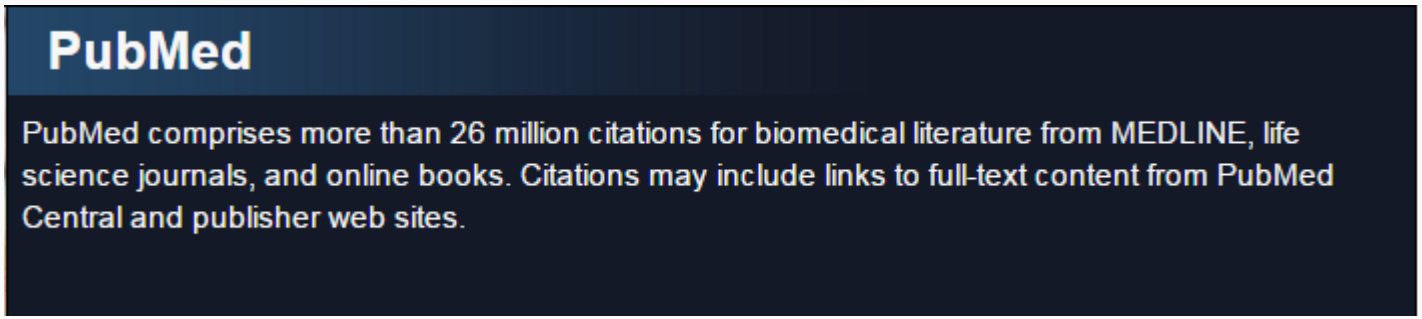
2-Pyrrolidone, 1-methyl-

Microposit 2001

M-Pyrol

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

EPA United States Environmental Protection Agency

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

Select Term: Hazard **AND** RfD OR reference dose

Google "RfD OR reference dose" AND "Hazard" AND "872-50-4" OR "N-Methyl-2-py

Scholar About 22 results (0.05 sec)

Articles
Case law
My library

Any time
Since 2017
Since 2016
Since 2013
Custom range...

Sort by relevance
Sort by date

include patents
include citations

Create alert

Solvent Substitution: An Analysis of Comprehensive Hazard Screening Indices
M Debia, D Bégin, M Gérin - Journal of occupational and ..., 2011 - oeh.tandfonline.com
... Reliability and weighting factors were not used. Armenti and Moure-Eraso(22) used the same FHS index, using six **hazard** categories, to compare replacement options. ... **872-50-4 N-Methyl-2-pyrrolidone** 45.4 13 1.46E-03 11 4.55 6 20 4 ...
Related articles All 4 versions Cite Save

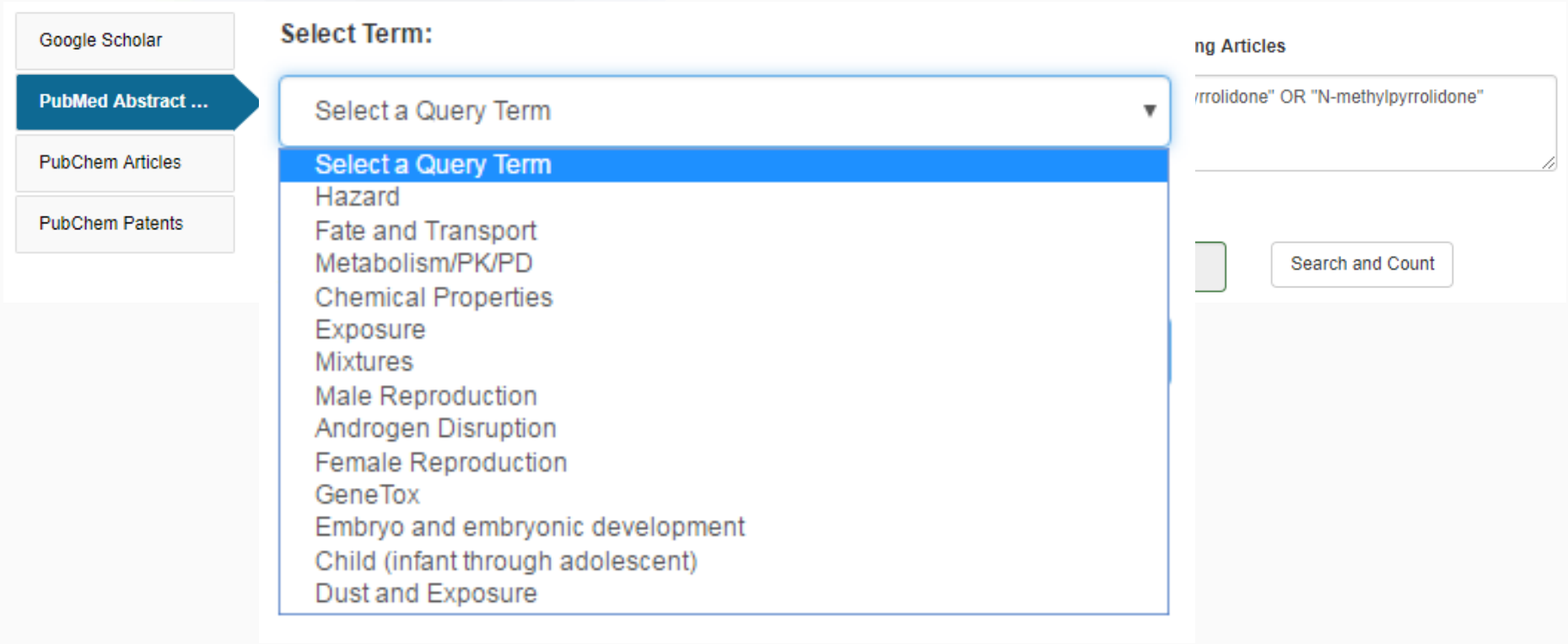
Effects of 'inactive'ingredients on bees
CA Mullin - Current Opinion in Insect Science, 2015 - Elsevier
... tallow amines, organosilicone ethoxylates and co-solvents such as **N-methyl-2-pyrrolidone** (NMP) [7 ... of tools to environmentally monitor residues and determine their relative **hazard** to bees. ... Defining a benchmark or **reference dose**, particularly for bee viruses [51], for what can ...
Cited by 9 Related articles All 2 versions Web of Science: 6 Cite Save More

Biological monitoring: exquisite research probes, risk assessment, and routine exposure measurement
WM Draper - Analytical chemistry, 2001 - ACS Publications
ADVERTISEMENT. ...
Cited by 19 Related articles All 5 versions Web of Science: 10 Cite Save

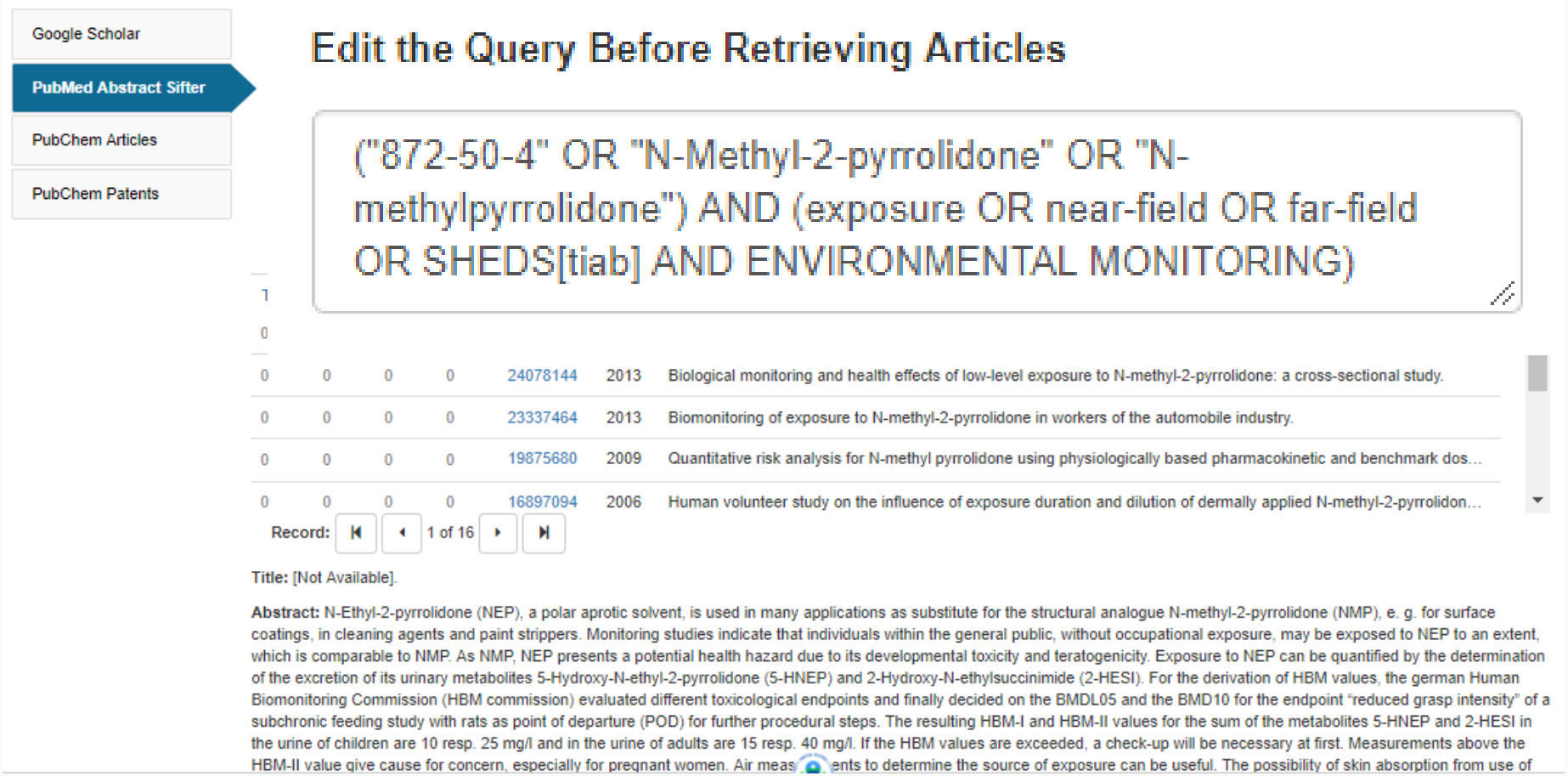
Evolution of chemical-specific adjustment factors (CSAF) based on recent international experience; increasing utility and facilitating regulatory acceptance
VS Bhat, ME Meek, M Valcke, C English... - Critical Reviews in ..., 2017 - Taylor & Francis
... As shown in the right side of Figure 2, uncertainty is taken into consideration at all tiers of **hazard** assessment. ... For decades, developing "safe doses" such as the oral **reference dose** (RfD), the inhaled reference concentration (RfC) or the acceptable or tolerable daily intake (ADI ...
All 3 versions Cite Save

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



Select Term:

Exposure

Retrieve Articles | 0 Articles

Edit the Query Before Retrieving Articles

("872-50-4" OR "N-Methyl-2-pyrrolidone" OR "N-methylpyrrolidone") AND (exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)

Add additional query terms to filter abstracts:

developmental | reproductive | occupational | Search and Count

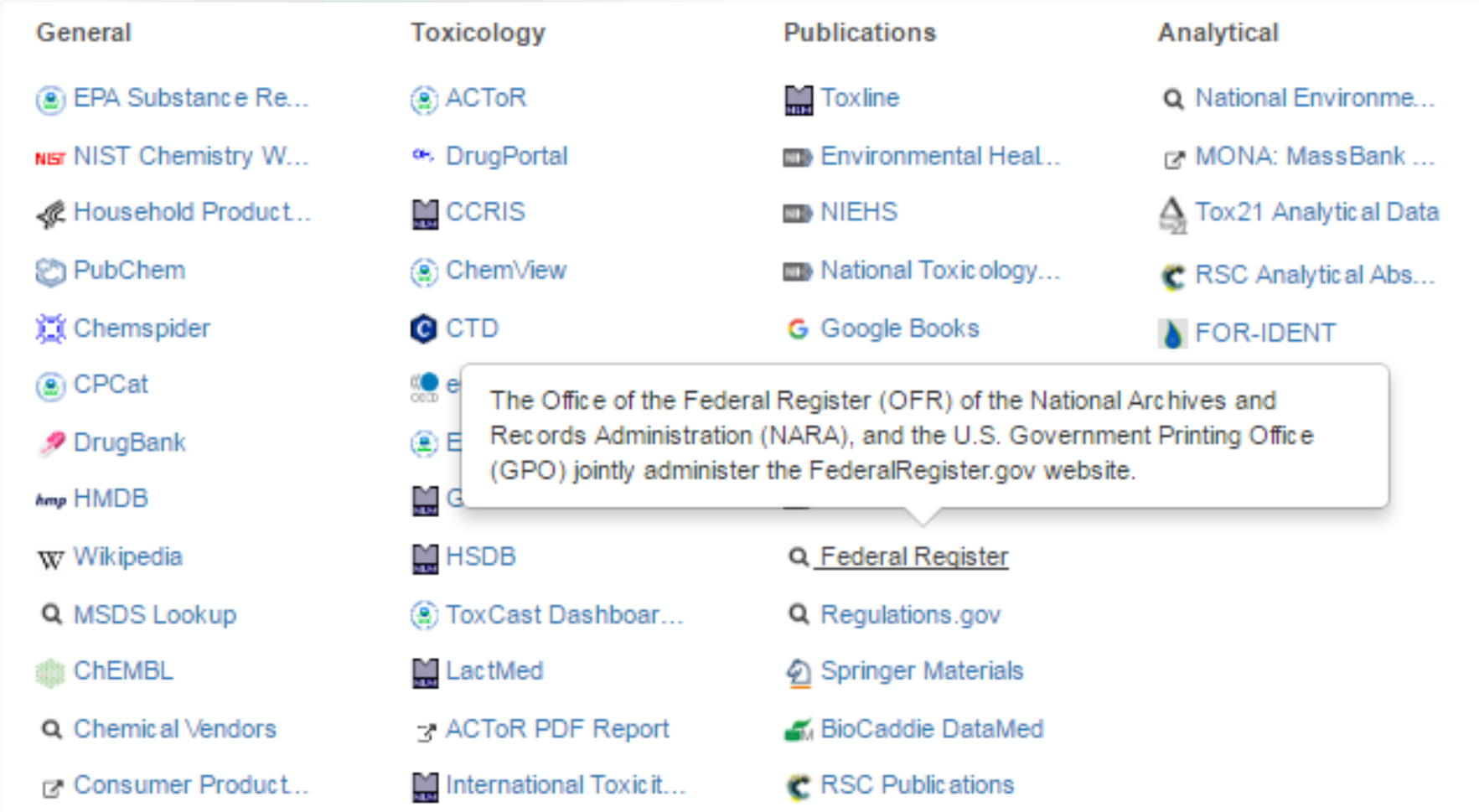
dev...	rep...	occ...	Total	PMID	Pu...	Title
0	0	1	1	24078144	2013	Biological monitoring and health effects of low-level exposure to N-methyl-2-pyrrolidone: a cross-sectional study.
1	0	0	1	23337464	2013	Biomonitoring of exposure to N-methyl-2-pyrrolidone in workers of the automobile industry.
0	0	2	2	19875680	2009	Quantitative risk analysis for N-methyl pyrrolidone using physiologically based pharmacokinetic and benchmark dos...
0	0	1	1	16897094	2006	Human volunteer study on the influence of exposure duration and dilution of dermally applied N-methyl-2-pyrrolidon...
0	0	0	0	16362322	2005	Ambient monitoring and biomonitoring of workers exposed to N-methyl-2-pyrrolidone in an industrial facility

Record: 1 of 16

Title: Stillbirth after occupational exposure to N-methyl-2-pyrrolidone. A case report and review of the literature.

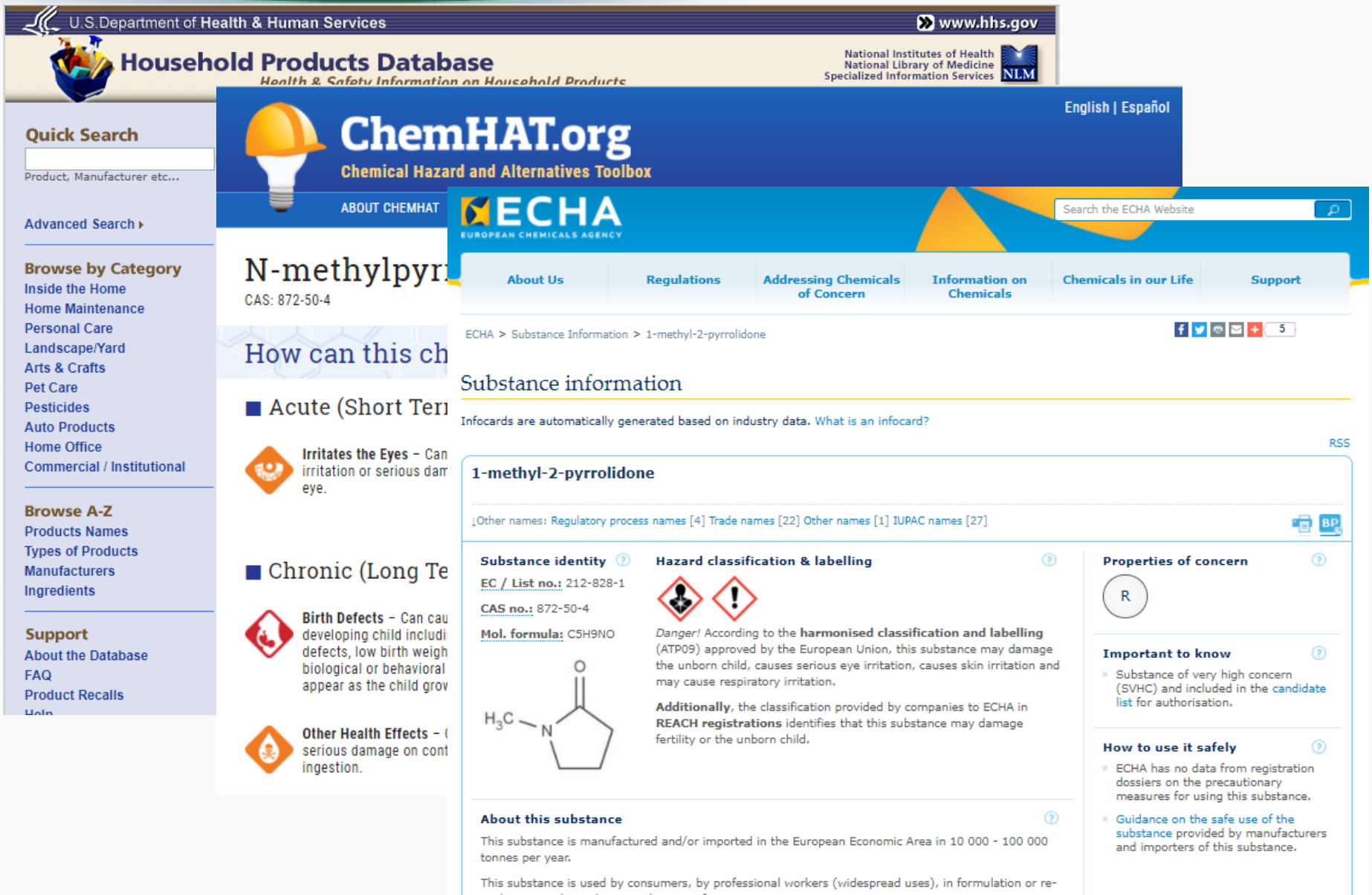
Abstract: N-methyl-2-pyrrolidone is a solvent that is increasingly used in a variety of industries, including petroleum refining, microelectronics, pesticide formulation, and veterinary medicine. Animal studies have demonstrated fetotoxic effects after maternal exposure to doses that have minimal to no adverse effect on the mothers. The fetotoxicity comprises resorption, stillbirth, and low birthweight and delayed ossification in surviving young. We report a human case of intrauterine growth retardation followed by fetal demise at 31 weeks gestation. The mother was a laboratory worker with no other apparent risk factors, who sustained occupational exposure to N-methyl-2-pyrrolidone throughout the first trimester of pregnancy. Laboratory work and solvent exposure have both previously been associated with adverse reproductive outcomes. Laboratories and other industries that use suspected reproductive toxins should have reproductive health policies in place that allow for decision-making based on toxicologic review, exposure assessment, and medical evaluation. These policies should allow for voluntary removal of prospective parents until environmental assessment and controls are instituted.

Links to Other Resources



Example External Links…

EPA United States Environmental Protection Agency



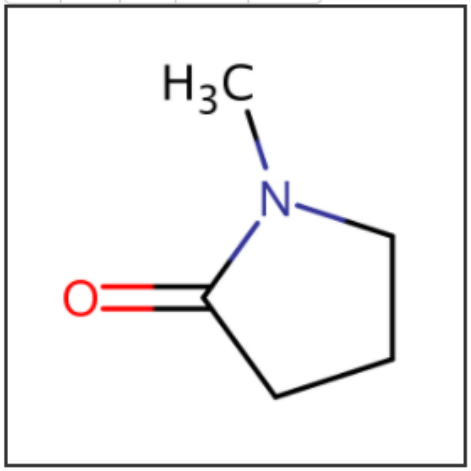
Managing structure relationships

EPA United States Environmental Protection Agency

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

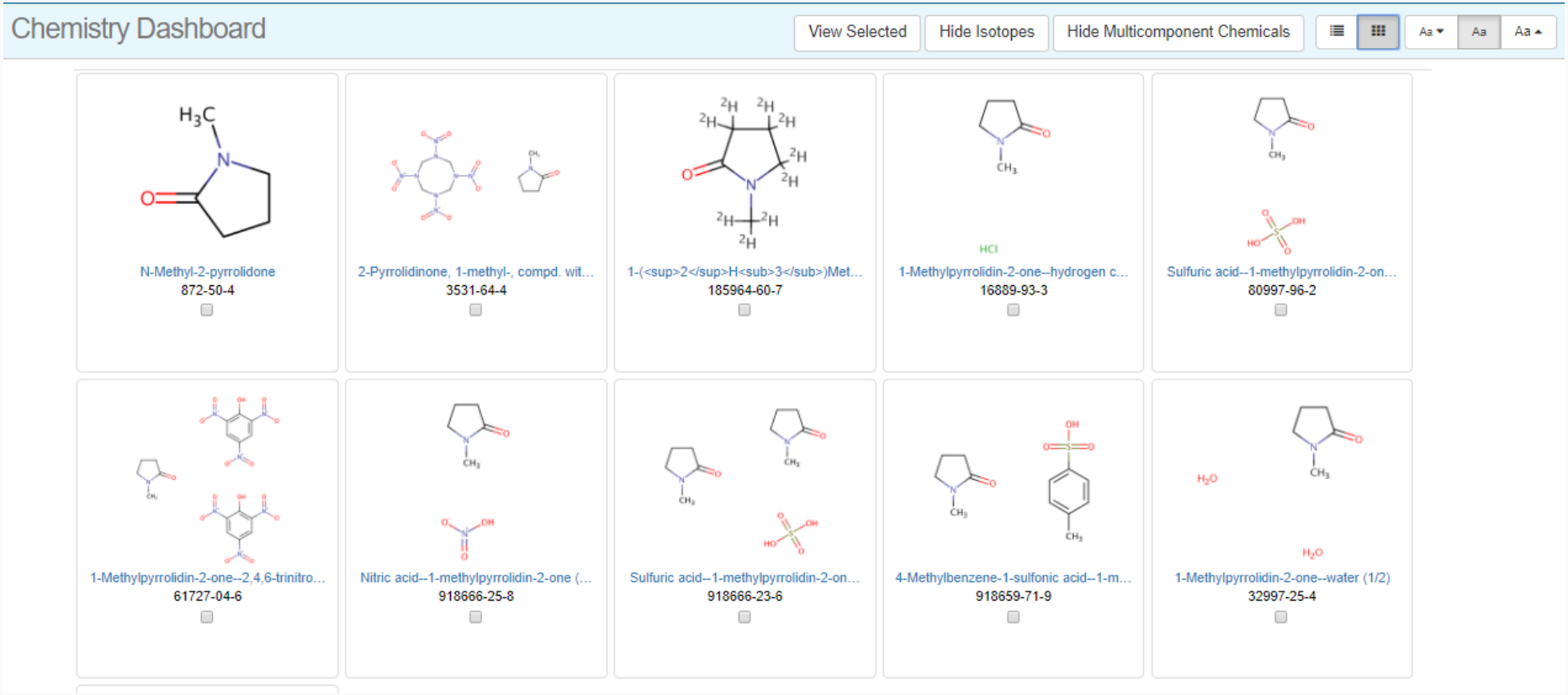
Same Connectivity: 3 records (based on first layer of InChI)

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

Managing structure relationships



Not just structures – “UVCBs”

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

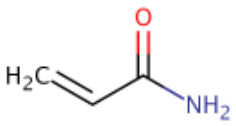
U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID1049722 (accessed February 12, 2017), Poly (acrylamide-co-acrylic acid), partial sodium salt

Data Quality 80%

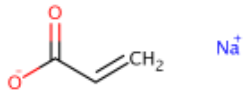
Manually curated and no conflicts in multiple public sources

Related Chemicals

Found 2 chemicals



Acrylamide
79-06-1



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

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

Managing UVCB Relationships

EPA United States Environmental Protection Agency

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

Searched by Synonym: Found 1 result for 'Linear alkylbenzene sulfonate'.

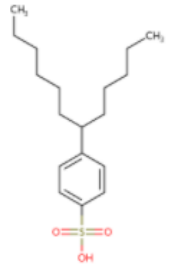
Presence in Lists

Surfactant List Screened in Swiss Wastewater (2014)

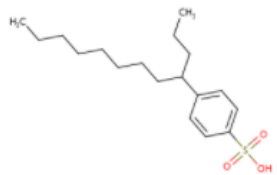
Surfactant List Screened in Swiss Wastewater (2014)

EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374

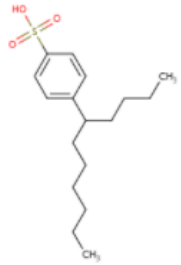
cals



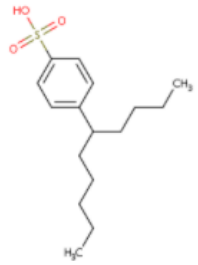
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



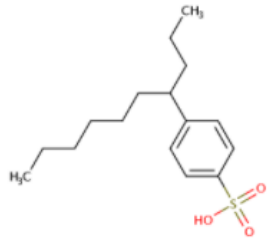
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



C11-LAS
NOCAS_881097



4-(decan-5-yl)benzene-1-sulfonic ...
NOCAS_881146



4-(decan-4-yl)benzenesulfonic acid
NOCAS_891333

Batch Searching for Data for Thousands of Chemicals

- What are these chemicals?

Chemicals Used in the Hydraulic Fracturing Process in Pennsylvania
Prepared by the Department of Environmental Protection
Bureau of Oil and Gas Management

Updated June 10, 2010

Chemical	Product Name
2,2-Dibromo-3-Nitrilopropionamide	Bio Clear 1000/Bio Clear 2000/ Bio-Clear 200/BioRid20L/ EC6116A
2-methyl-4-isothiazolin-3-one	X-Cide 207
5-chloro-2-methyl-4-isothiazolin-3-one	X-Cide 207
Acetic Acid	Fe-1A Acidizing Composition/ Packer Inhibitor
Acetic Anhydride	Fe-1A Acidizing Composition
Acetylene	GT&S Inc./ Airco
Alcohol Ethoxylated	C12-16 NE-200
Alkyl benzene sulfonic acid	Tetrolite AW0007/ FR-46
Ammonia (aqueous)	FAW-5
Ammonium Bifluoride	ABF 37%
Ammonium Persulfate	AP Break
Ammonium Bisulfite	Techni-Hib 604/ Fe OXCLEAR/ Packer Inhibitor
Ammonium chloride	Salt Inhibitor
Ammonium Salt (alkylpolyether	

Batch Searching for Data for Thousands of Chemicals

EPA United States Environmental Protection Agency

Select Input Type(s)

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

Enter Identifiers to Search

Sodium l-glutamate
4-Hydroxy-3-nitrophenylarsonic acid
4-Nitro-1,2-phenylenediamine
Methoxypromazine
1-Phenyl-3-methyl-5-pyrazolone
1-Phenyl-2-thiourea
Phenylbutazone
1,4-Benzenediamine
Prednisolone
Probenecid

Display All Chemicals | Download Chemical Data

Select Output Format

Excel

Customize Results

- [ ] Select All

Chemical Identifiers

- [x] Chemical Name
- [x] DTXSID
- [ ] CAS-RN
- [ ] InChIKey
- [ ] IUPAC Name

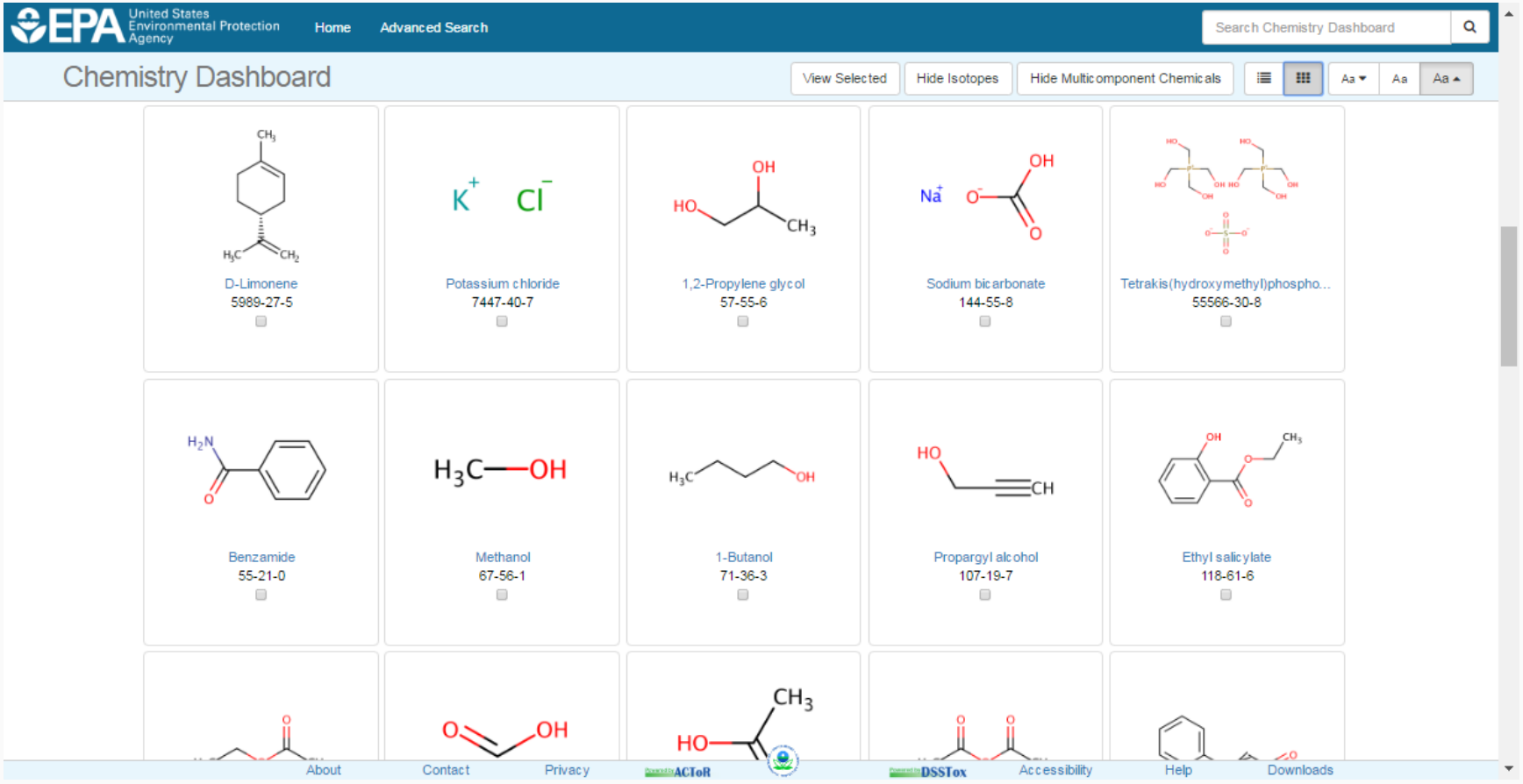
Structures

- [ ] Mol File
- [ ] SMILES
- [ ] InChI String

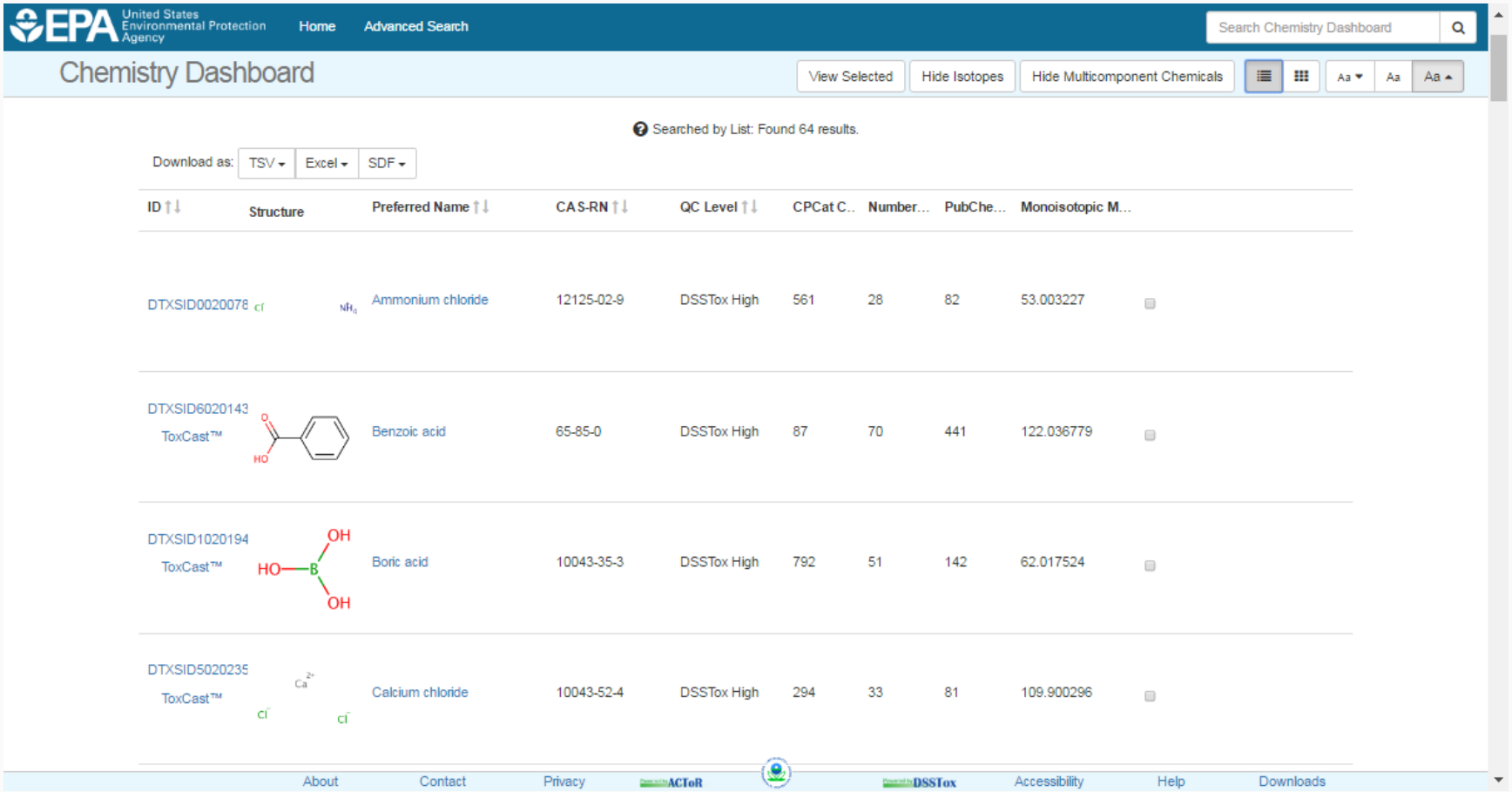
Intrinsic Properties

- [ ] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] OPERA and TEST Model Predictions

Access to associated data for review, modeling & download



Access to associated data for review, modeling & download



Real World Applications

- From chemical names to chemical data

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
1,4-Benzenediamine, N,N'-diphenyl-	N,N'-Diphenyl-p-phenylenediamine	74-31-7

Confidential Business Information

CBI is broadly defined as proprietary information, considered confidential to the submitter, the release of which would cause substantial business injury to the owner.

The Dashboard for CBI

- The dashboard code and data will be deployed in the Office of Pollution Prevention and Toxics (OPPT) supporting CBI data
  - Integrate OPPT CBI data in the database
  - Isolate all internet-based modules for the CBI environment – no external links, no literature searching, no PubChem data etc.
  - Rebuild OPERA models using CBI data (if the models improve can we release without training data?)

Collaborative QSAR Models

JOURNAL OF CHEMICAL INFORMATION AND MODELING

Article

pubs.acs.org/jcim

Developing Collaborative QSAR Models Without Sharing Structures

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SOFTWARE | OPEN ACCESS

eTOXlab, an open source modeling framework for implementing predictive models in production environments

Pau Carrió, Oriol López, Ferran Sanz and Manuel Pastor

Journal of Cheminformatics 2015 **7**:8 | https://doi.org/10.1186/s13321-015-0058-6

Received: 13 September 2014 | **Accepted:** 24 February 2015 | **Published:** 11 March 2015

Future Work

- Continue expansion and curation of data and types
- Provide "**programmatic access**" to all data – web services and application programming interface
- Continue to assemble and enhance chemical lists and data for specific projects
- Make new modules public – "Generalized Read Across", "EcoTox data"

Conclusion

- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- An **Integration Hub** to data – toxicity, environmental, property, bioassay, and expanding
- Data downloads allows for reuse in other systems and integration of resources to support research

Acknowledgments

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