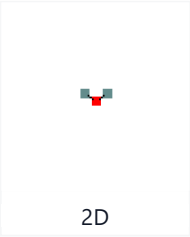
COMPOUND SUMMARY

Water

See also: Hydroxide (conjugate); Oxonium (conjugate); Hydrogen tritium oxide (related) ... View More ...

PubChem CID
962

Structure

2D

Chemical Safety
Laboratory Chemical Safety Summary (LCSS) Datasheet

Molecular Formula
H_2O

Synonyms
water
7732-18-5
Dihydrogen oxide
Distilled water
Sterile water
View More...

Molecular Weight
18.015 g/mol
Computed by PubChem 2.2 (PubChem release 2021.10.14)

Dates

Create: 2004-09-16
Modify: 2023-08-12

Description

Water appears as a clear, nontoxic liquid composed of **hydrogen** and **oxygen**, essential for life and the most widely used solvent. Include water in a mixture to learn how it could react with other chemicals in the mixture.

▸ CAMEO Chemicals

Water is an oxygen hydride consisting of an **oxygen** atom that is covalently bonded to two **hydrogen** atoms It has a role as an amphiprotic solvent, a member of greenhouse gas, a human metabolite, a Saccharomyces cerevisiae metabolite, an Escherichia coli metabolite and a mouse metabolite. It is an oxygen hydride, a mononuclear parent **hydride** and an inorganic **hydroxy** compound. It is a conjugate base of an **oxonium**. It is a conjugate acid of a **hydroxide**.

▸ ChEBI

Water (chemical formula: H2O) is a transparent fluid which forms the world's streams, lakes, oceans and rain, and is the major constituent of the fluids of organisms. As a chemical compound, a water molecule contains one **oxygen** and two **hydrogen** atoms that are connected by covalent bonds. Water is a liquid at standard ambient temperature and pressure, but it often co-exists on Earth with its solid state, ice; and gaseous state, steam (water vapor).

▸ DrugBank

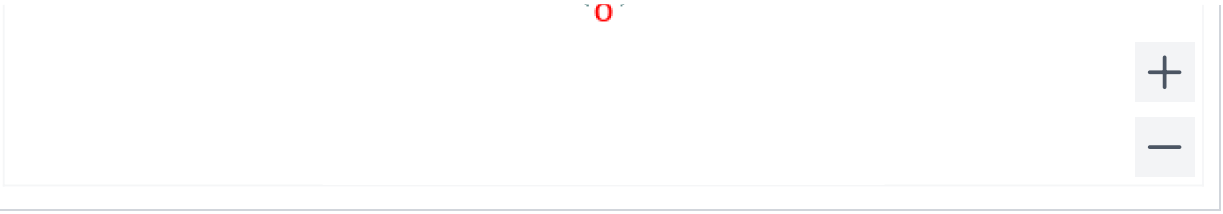
View More...

Contents

1 Structures

1.1 2D Structure

Chemical Structure Depiction



▸ PubChem

1.2 Crystal Structures

COD records with this CID as component

1000096	1001019	1004041	1007033	1007152	1007174	1007199	1007216	1008027	100
1000133	1001023	1004070	1007034	1007153	1007175	1007201	1007217	1008028	100
1000139	1001110	1004096	1007044	1007155	1007176	1007202	1007219	1008120	100
1000235	1001210	1004121	1007063	1007157	1007178	1007203	1007221	1008190	100
1000352	1001330	1004144	1007087	1007159	1007186	1007204	1007222	1008207	101
1000375	1001743	1006098	1007096	1007164	1007190	1007206	1007250	1008270	101
1000459	1001770	1007000	1007097	1007166	1007192	1007208	1007259	1008368	101
1000489	1001774	1007006	1007135	1007167	1007193	1007209	1007264	1008454	101
1001011	1001835	1007018	1007148	1007172	1007194	1007210	1008018	1008710	101
1001018	1004034	1007027	1007150	1007173	1007197	1007215	1008026	1008760	101

▸ Crystallography Open Database (COD)

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

oxidane

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

▸ PubChem

2.1.2 InChI

InChI=1S/H2O/h1H2

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ **PubChem**

2.1.3 InChIKey

XLYOFNOQVPJJNP-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ **PubChem**

2.1.4 Canonical SMILES

O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

▸ **PubChem**

2.2 Molecular Formula

H_2O

Computed by PubChem 2.2 (PubChem release 2021.10.14)

▸ **CAMEO Chemicals; Wikipedia; PubChem**

2.3 Other Identifiers

2.3.1 CAS

7732-18-5

▸ **CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals un...**

191612-63-2

▸ **CAS Common Chemistry**

146915-49-3

- CAS Common Chemistry

158061-35-9

- CAS Common Chemistry

191612-61-0

- CAS Common Chemistry

146915-50-6

- CAS Common Chemistry

17778-80-2

- EPA DSSTox

2.3.2 Related CAS

151517-95-2

Compound: Water, octadecamer

- CAS Common Chemistry

25766-61-4

Compound: Water, homopolymer

- CAS Common Chemistry

163734-19-8

Compound: Water, heneicosamer

- CAS Common Chemistry

151733-06-1

Compound: Water, tridecamer

- CAS Common Chemistry

155964-99-1

Compound: Water, undecamer

- CAS Common Chemistry

70232-06-3

Compound: Water, tetramer

- CAS Common Chemistry

181895-39-6

Compound: Water, octacosamer

- CAS Common Chemistry

139322-39-7

Compound: Water, octamer

- CAS Common Chemistry

144442-59-1

Compound: Water, nonamer

- CAS Common Chemistry

151517-94-1

Compound: Water, tetradecamer

- CAS Common Chemistry

151733-07-2

Compound: Water, heptadecamer

- CAS Common Chemistry

139322-38-6

Compound: Water, hexamer

- CAS Common Chemistry

163734-21-2

Compound: Water, pentacosamer

- CAS Common Chemistry

148076-13-5

Compound: Water, hexadecamer

▸ **CAS Common Chemistry**

148076-12-4

Compound: Water, dodecamer

▸ **CAS Common Chemistry**

163734-20-1

Compound: Water, docosamer

▸ **CAS Common Chemistry**

79800-59-2

Compound: Water, pentamer

▸ **CAS Common Chemistry**

142473-62-9

Compound: Water, decamer

▸ **CAS Common Chemistry**

31014-12-7

Compound: Water, trimer

▸ **CAS Common Chemistry**

142473-64-1

Compound: Water, eicosamer

▸ **CAS Common Chemistry**

151517-96-3

Compound: Water, tetracosamer

▸ **CAS Common Chemistry**

25655-83-8

Compound: Water, dimer

▸ **CAS Common Chemistry**

144442-58-0

Compound: Water, heptamer

CAS Common Chemistry

142473-63-0

Compound: Water, pentadecamer

CAS Common Chemistry

2.3.3 Deprecated CAS

558440-22-5, 558440-53-2, 1202864-49-0, 1371582-34-1, 652133-48-7

ChemIDplus

1202864-49-0, 558440-53-2

EPA DSSTox

2.3.4 European Community (EC) Number

231-791-2

European Chemicals Agency (ECHA)

686-299-4

European Chemicals Agency (ECHA)

2.3.5 NSC Number

147337

DTP/NCI

2.3.6 UNII

059QF0KO0R

- FDA Global Substance Registration System (GSRS)

2.3.7 DSSTox Substance ID

DTXSID6026296

- EPA DSSTox

DTXSID00170378

- EPA DSSTox

2.3.8 Nikkaji Number

J2.261.720F

- Japan Chemical Substance Dictionary (Nikkaji)

J408.680E

- Japan Chemical Substance Dictionary (Nikkaji)

J43.587B

- Japan Chemical Substance Dictionary (Nikkaji)

J2.656.835H

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.9 Wikipedia

Water

- Wikipedia

2.3.10 Wikidata

Q283

- Wikidata

Q427071

- Wikidata

Q81977184

- Wikidata

2.3.11 NCI Thesaurus Code

C65147

- NCI Thesaurus (NCIt)

2.3.12 RXCUI

11295

- NLM RxNorm Terminology

2.3.13 ChEMBL ID

CHEMBL1098659

- ChEMBL

2.4 Synonyms

2.4.1 MeSH Entry Terms

Hydrogen Oxide
Water

- Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

water
Water, mineral
Ultrex ii ultrapure
Water, sterile purified
7732-18-5

Dihydrogen oxide	Dihydrogen Monoxide	Water for injection	Water purified
Distilled water	aqua	Sterile water for irrigation	Pur-wash
Sterile water	DHMO	Sterile purified water	hydrogen hydroxide
Water vapor	agua	Water for hemodialysis	Sterile water for injection
Water, deionized	steam	acqua	EINECS 231-791-2
oxidane	Deionized water	dihydridooxygen	H2O
Purified water	Water, sterile	1,3-epoxy-	Sterile water for inhalation
Water, purified	Water, distilled	Wasser	UNII-059QF0KO0R

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name
Molecular Weight

Property Value
18.015 g/mol

Reference
Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name
XLogP3-AA

Property Value
-0.5

Reference
Computed by XLogP3 3.0 (PubChem release 2021.10.14)

Property Name
Hydrogen Bond Donor Count

Property Value
1

Reference
Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name
Hydrogen Bond Acceptor Count

Property Value

1

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Rotatable Bond Count

Property Value

0

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Exact Mass

Property Value

18.010564683 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Monoisotopic Mass

Property Value

18.010564683 g/mol

Reference

Computed by PubChem 2.2 (PubChem release 2021.10.14)

Property Name

Topological Polar Surface Area

Property Value

1Å²

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Heavy Atom Count

Property Value

1

Reference

Computed by PubChem

Property Name

Formal Charge

Property Value

0

Reference

Computed by PubChem

Property Name

Complexity

Property Value

0

Reference

Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)

Property Name

Isotope Atom Count

Property Value

0

Reference

Computed by PubChem

Property Name

Defined Atom Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name

Undefined Atom Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name

Defined Bond Stereocenter Count

Property Value

0

Reference

Computed by PubChem

Property Name
Undefined Bond Stereocenter Count

Property Value
0

Reference
Computed by PubChem

Property Name
Covalently-Bonded Unit Count

Property Value
1

Reference
Computed by PubChem

Property Name
Compound Is Canonicalized

Property Value
Yes

Reference
Computed by PubChem (release 2021.10.14)

▸ PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Water appears as a clear, nontoxic liquid composed of **hydrogen** and **oxygen**, essential for life and the most widely used solvent. Include water in a mixture to learn how it could react with other chemicals in the mixture.

▸ CAMEO Chemicals

Liquid

▸ EPA Chemicals under the TSCA; Human Metabolome Database (HMDB)

Clear colorless odorless liquid; [NTP]

▸ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.2.2 Color / Form

Colorless liquid

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 94th Edition. CRC Press LLC, Boca Raton: FL 2013-2014, p. 4-98

▸ Hazardous Substances Data Bank (HSDB)

Liquid

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1868

▸ Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Odorless

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. V3: 3692

▸ Hazardous Substances Data Bank (HSDB)

3.2.4 Taste

Tasteless

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. V3: 3692

▸ Hazardous Substances Data Bank (HSDB)

3.2.5 Boiling Point

212 °F at 760 mmHg

▸ CAMEO Chemicals

100

MSDS

▸ DrugBank

99.974 °C

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 94th Edition. CRC Press LLC, Boca Raton: FL 2013-2014, p. 4-98

▸ Hazardous Substances Data Bank (HSDB)

3.2.6 Melting Point

32 °F

▸ CAMEO Chemicals

0

MSDS

▸ DrugBank

0 °C

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1868

▸ Hazardous Substances Data Bank (HSDB); Human Metabolome Database (HMDB)

3.2.7 Solubility

Completely miscible

MSDS

▸ DrugBank

Water dissolves some amount of virtually every solid or gas with wich it comes in contact.

Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ Hazardous Substances Data Bank (HSDB)

Very soluble in ethanol, methanol, acetone

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 94th Edition. CRC Press LLC, Boca Raton: FL 2013-2014, p. 4-98

▸ Hazardous Substances Data Bank (HSDB)

55.5 mol/L

▸ Human Metabolome Database (HMDB)

3.2.8 Density

1

▸ CAMEO Chemicals

0.9950 g/cu cm at 25 °C

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1868

▸ Hazardous Substances Data Bank (HSDB)

Chemical and physical properties

Property	density
Comparison w/other substances	max at 4 °C, not at freezing pt; expands upon freezing
Importance to the environment	in lakes prevents freezing up and causes seasonal stratification
Property	MP and BP
Comparison w/other substances	abnormally high
Importance to the environment	permits water to exist as a liquid at earth's surface
Property	heat capacity
Comparison w/other substances	highest of any liquid except ammonia
Importance to the environment	moderates temperature by preventing extremes
Property	

heat of vaporization

Comparison w/other substances

one of the highest known

Importance to the environment

important to heat transfer in atmosphere and oceans; moderates temperature extremes

Property

surface tension

Comparison w/other substances

very high

Importance to the environment

regulates drop formation in clouds and rain

Property

absorption of radiation

Comparison w/other substances

large IR and UV regions; less in visible regions

Importance to the environment

important control on biological activity (photosynthesis) in water bodies and on atmospheric temperature

Property

solvent properties

Comparison w/other substances

excellent solvent for ionic salts and polar molecules because of dipolar nature

Importance to the environment

important in transfer of dissolved substances in hydrological cycle and in biological systems

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

Expands on freezing. Temp of max density 3.98 °C. density: 1.000000g/mL at 3.98 °C; 0.917 g/cc at 0 °C (ice); 0.999868 at 0 °C/4 °C (liquid)

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1868

▸ **Hazardous Substances Data Bank (HSDB)**

Weight of sea water: approximately 63.93 lb/cu ft at 15 °C; density of sea water: approximately 1.025 g/cu cm at 25 °C

van der Leeden et al; The Water Encyclopedia. 2nd ed., Geraghty & Miller Ground-Water Series., Chelsea MI: Lewis Pub pp. 808 (1990)

▸ **Hazardous Substances Data Bank (HSDB)**

Ice Properties

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

3.2.9 Vapor Pressure

23.75 [mmHg]

▸ **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

VP: 760 mm Hg at 100 °C

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. V3: 3692

▸ **Hazardous Substances Data Bank (HSDB)**

VP: 611.657 Pa at 273.16 K

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 94th Edition. CRC Press LLC, Boca Raton: FL 2013-2014, p. 6-13

▸ **Hazardous Substances Data Bank (HSDB)**

3.2.10 LogP

-1.38

HANSCH,C ET AL. (1995)

▸ **Human Metabolome Database (HMDB)**

3.2.11 Viscosity

Dynamic viscosity: 0.8949 cP at 25 °C; Kinematic viscosity: 0.8976 cP at 25 °C

van der Leeden et al; The Water Encyclopedia. 2nd ed., Geraghty & Miller Ground-Water Series., Chelsea MI: Lewis Pub pp. 808 (1990)

▸ Hazardous Substances Data Bank (HSDB)

3.2.12 Corrosivity

The solvent powers of water exerted in man-made conduit/pipe systems ... lead to ... corrosion and scaling

Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ Hazardous Substances Data Bank (HSDB)

3.2.13 Heat of Vaporization

9.717 kcal/mole

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1868

▸ Hazardous Substances Data Bank (HSDB)

3.2.14 Surface Tension

71.97 dyne/cm at 25 °C

van der Leeden et al; The Water Encyclopedia. 2nd ed., Geraghty & Miller Ground-Water Series., Chelsea MI: Lewis Pub pp. 808 (1990)

▸ Hazardous Substances Data Bank (HSDB)

3.2.15 Refractive Index

Index of refraction: 1.333

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. V3: 3692

▸ Hazardous Substances Data Bank (HSDB)

3.2.16 Kovats Retention Index

Standard non-polar

	319, 327
Semi-standard non-polar	317
Standard polar	1039, 1066

▸ NIST Mass Spectrometry Data Center

3.2.17 Other Experimental Properties

The polarity of water is an important factor in determining its solvent properties.

Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ Hazardous Substances Data Bank (HSDB)

... since **hydrogen** and **oxygen** each have 3 isotopes, there exist 18 possible molecular weights for water

Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ Hazardous Substances Data Bank (HSDB)

Apparent dipole moment: 6.24X10-30 C.m

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ Hazardous Substances Data Bank (HSDB)

Allotropic forms are ice (solid) and steam (vapor)

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. V3: 3692

▸ Hazardous Substances Data Bank (HSDB)

For more Other Experimental Properties (Complete) data for Water (12 total), please visit the **HSDB record page**.

▸ Hazardous Substances Data Bank (HSDB)

3.2.18 Chemical Classes

Other Classes -> Other Inorganic Compounds

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.3 SpringerMaterials Properties

Gibbs energy	Boiling point	Creep	Diffusion	E
Schoenflies notation	Chemical bond	Critical density	Diffusion of impurities	E
X-ray scattering	Chemical diffusion	Critical point	Diffusive flux	E
Absorbance	Chemical shift	Cross section	Dispersion	E
Acentric factor	Chemical structure	Crossover temperature	Elasticity	E
Activation energy	Composition	Crystal structure	Elastooptic coefficient	E
Activity	Compressibility	Crystallographic point group	Electric dipole moment	E
Adsorbate coverage	Compression	Density	Electrical resistivity	E
Azeotropes	Core level transition	Dielectric constant	Electron conductivity	F
Band structure	Corrosion	Dielectricity	Electronic structure	F

- SpringerMaterials

4 Spectral Information

4.1 1D NMR Spectra

1D NMR Spectra
NMRShiftDB Link

- NMRShiftDB

4.1.1 1H NMR Spectra

Spectra ID
3979

Instrument Type
JEOL

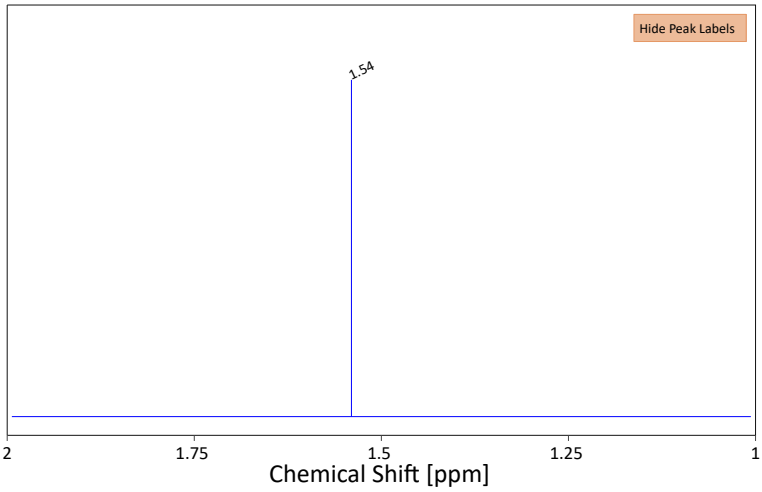
Frequency

400 MHz

Solvent
CD2Cl2

Shifts [ppm]:Intensity
1.54:1000.00

Thumbnail



▸ Human Metabolome Database (HMDB)

4.2 Mass Spectrometry

4.2.1 GC-MS

1 of 3 View All

NIST Number
7

Library
Main library

Total Peaks
5

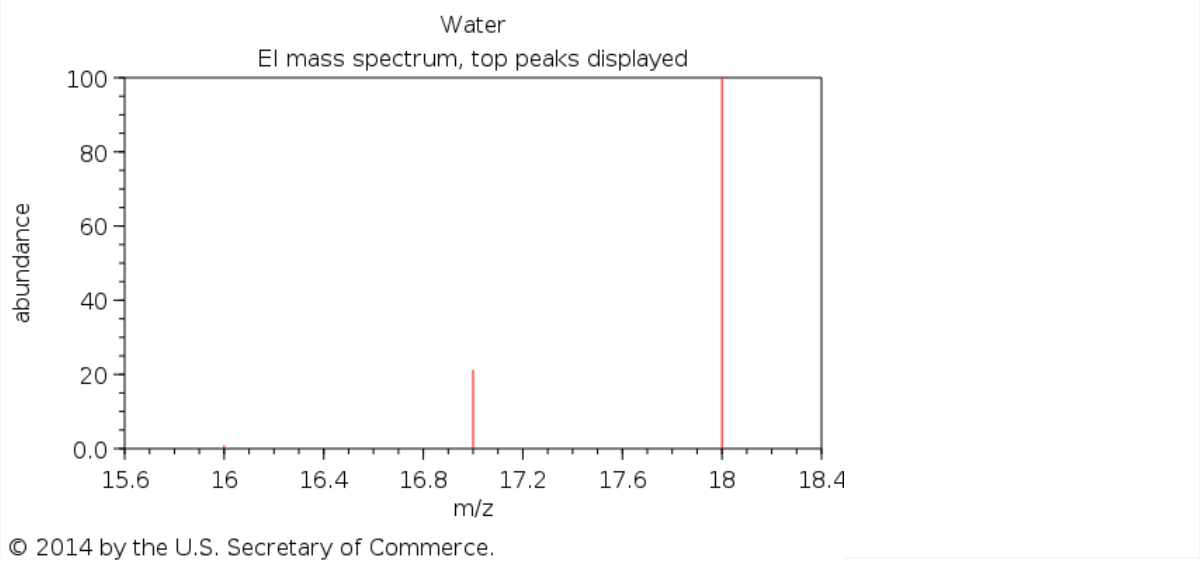
m/z Top Peak

18

m/z 2nd Highest
17

m/z 3rd Highest
16

Thumbnail



NIST Mass Spectrometry Data Center

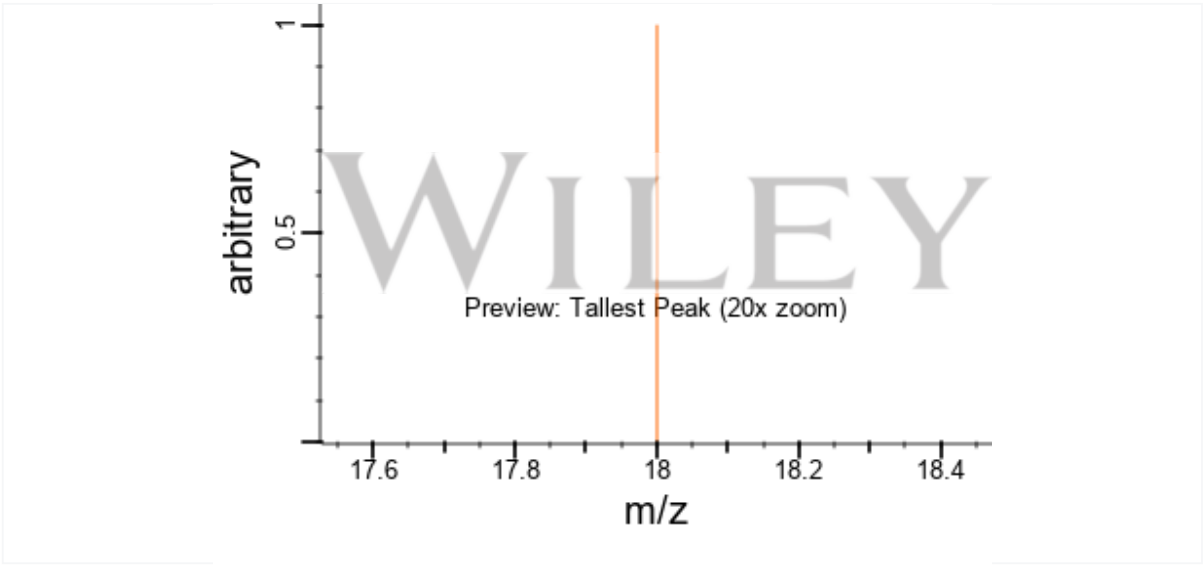
2 of 3 View All

Technique
GC/MS

Source of Spectrum
DigiLab GmbH (C) 2021

Copyright
Copyright © 2021 DigiLab GmbH and Wiley-VCH GmbH. All Rights Reserved.

Thumbnail



SpectraBase

4.2.2 MS-MS

1 of 2

Spectra ID
449782

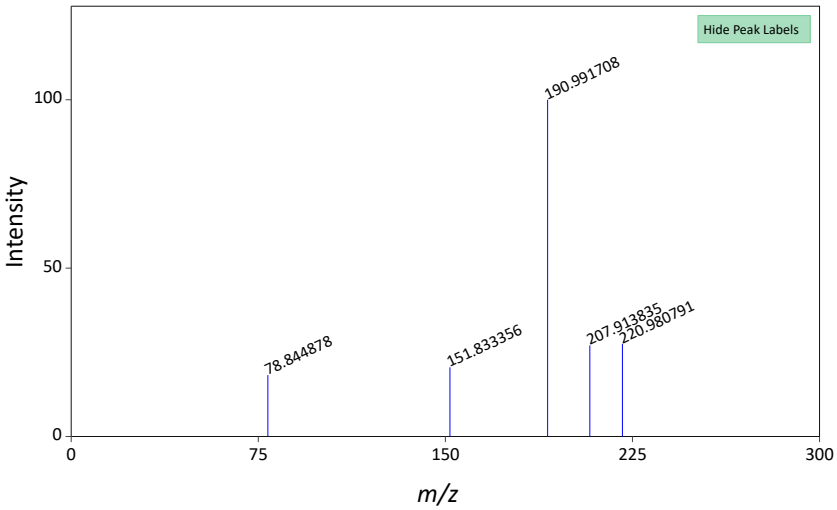
Instrument Type
Linear Ion Trap

Ionization Mode
positive

SPLASH
splash10-0006-0940000000-08a1813d85727d668cf4

Top 5 Peaks
190.991708 100
220.980791 27.51
207.913835 27.06
151.833356 20.54
78.844878 18.23

Thumbnail



Notes
instrument=Thermo Finnigan LTQ

▸ **Human Metabolome Database (HMDB)**

2 of 2

Spectra ID
449783

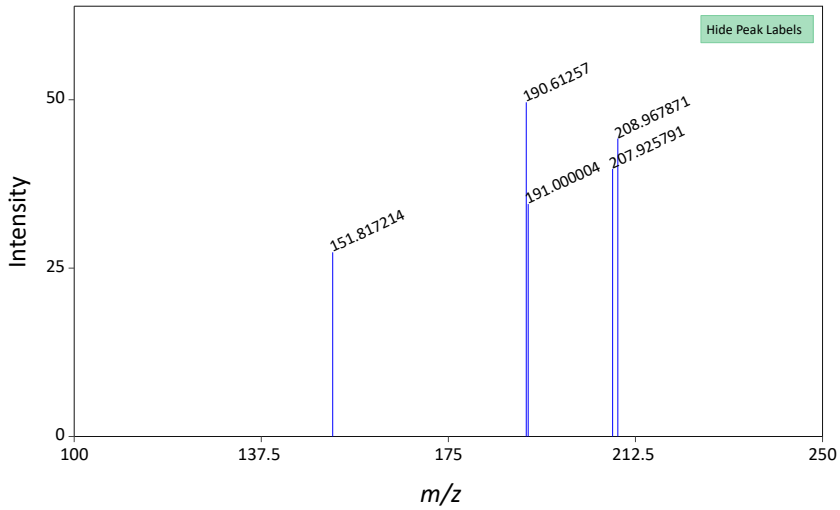
Instrument Type
Linear Ion Trap

Ionization Mode
positive

SPLASH
splash10-0a4l-0980000000-5b109ff45e0e5e5051ae

Top 5 Peaks
190.61257 49.62
208.967871 44.24
207.925791 39.74
191.000004 34.51
151.817214 27.35

Thumbnail



Notes
instrument=Thermo Finnigan LTQ

▸ **Human Metabolome Database (HMDB)**

4.3 IR Spectra

4.3.1 FTIR Spectra

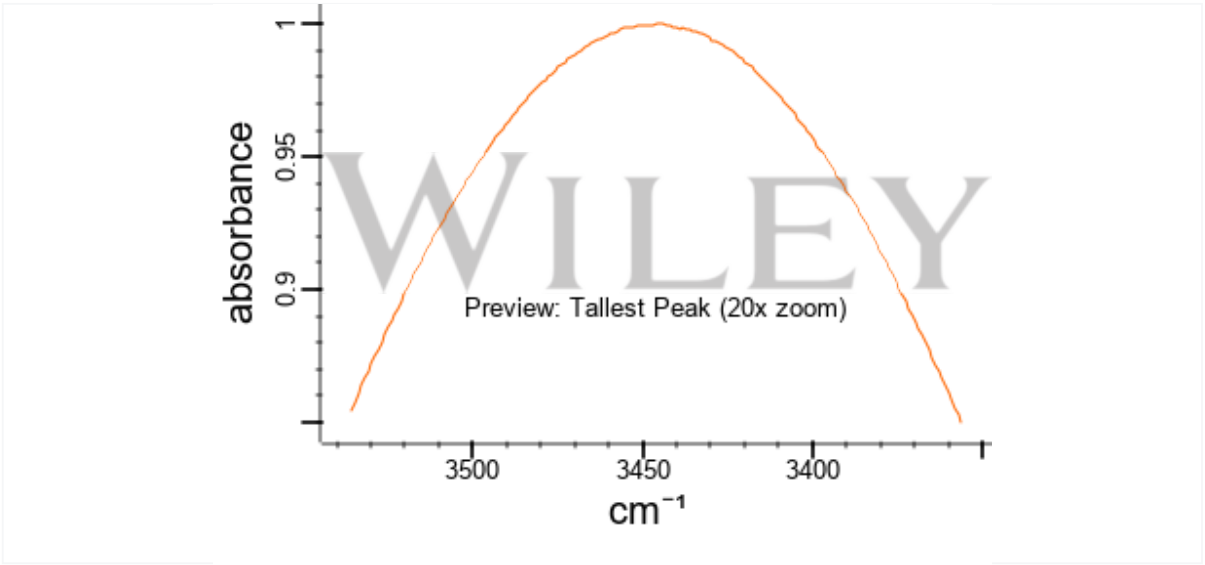
1 of 2

Technique
NEAT

Source of Sample
Fluka Chemie AG, Buchs, Switzerland

Copyright

Thumbnail



▸ SpectraBase

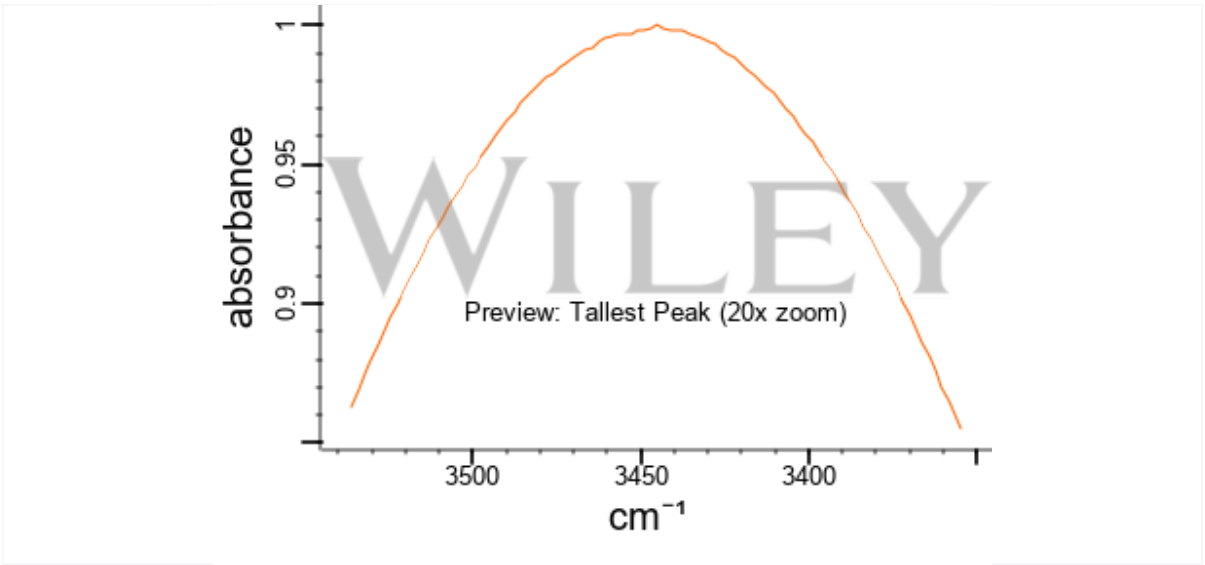
2 of 2

Instrument Name
Bruker IFS 88 C

Technique
Film

Copyright

Thumbnail



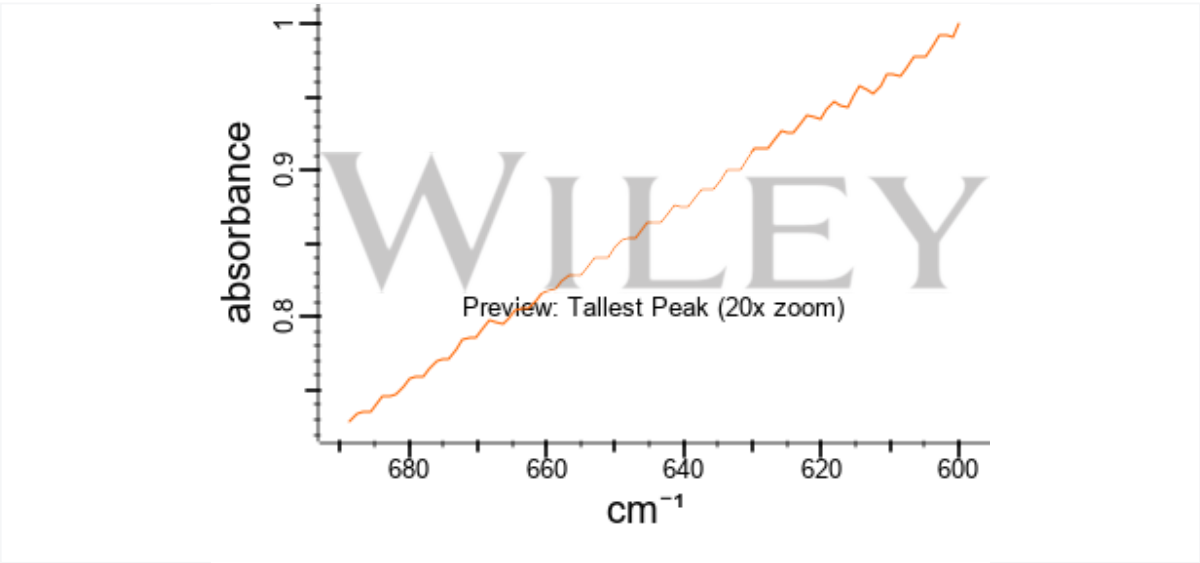
▸ SpectraBase

4.3.2 ATR-IR Spectra

Technique
ATR-Neat

Copyright

Thumbnail



▸ SpectraBase

4.3.3 Near IR Spectra

1 of 2

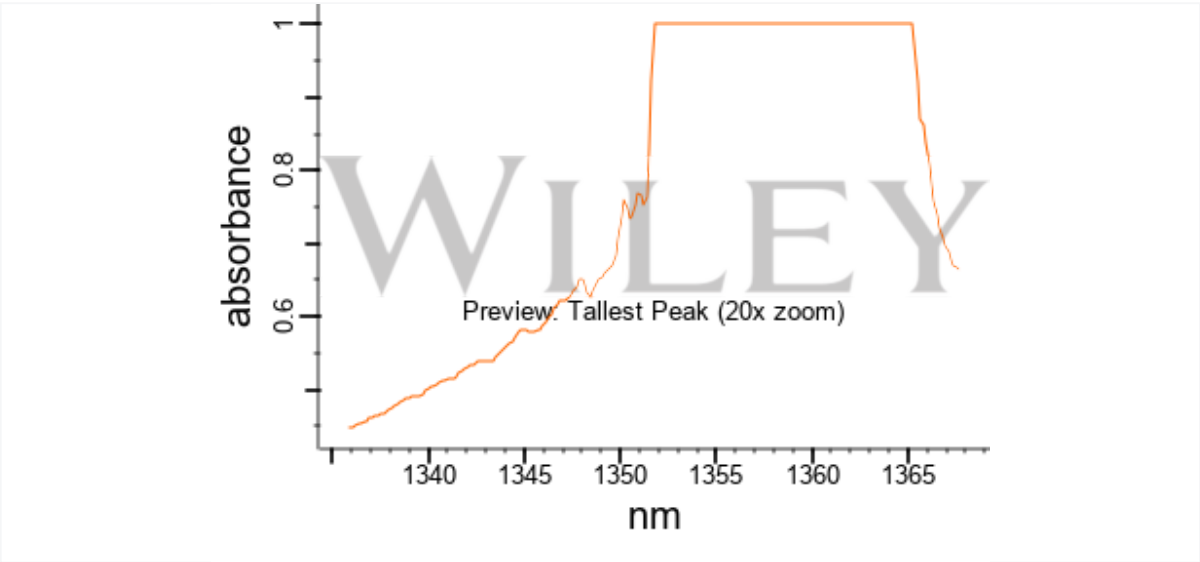
Instrument Name
BRUKER IFS 88

Technique
NIR

Source of Spectrum
Prof. Buback, University of Goettingen, Germany

Copyright

Thumbnail



▸ SpectraBase

2 of 2

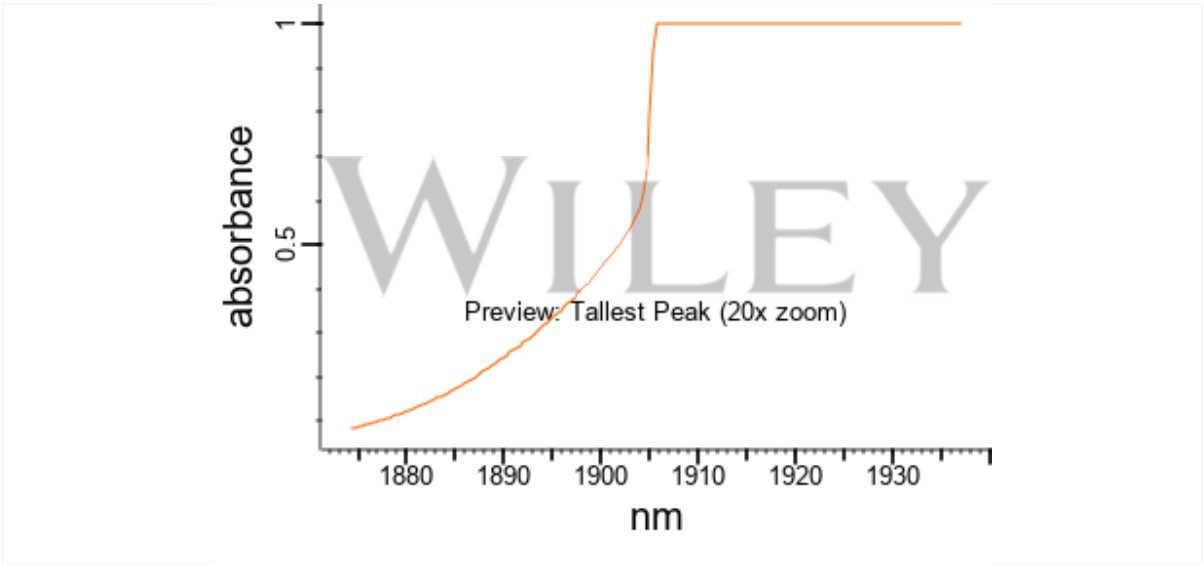
Instrument Name
BRUKER IFS 88

Technique
NIR

Source of Spectrum
Prof. Buback, University of Goettingen, Germany

Copyright

Thumbnail



SpectraBase

4.3.4 Vapor Phase IR Spectra

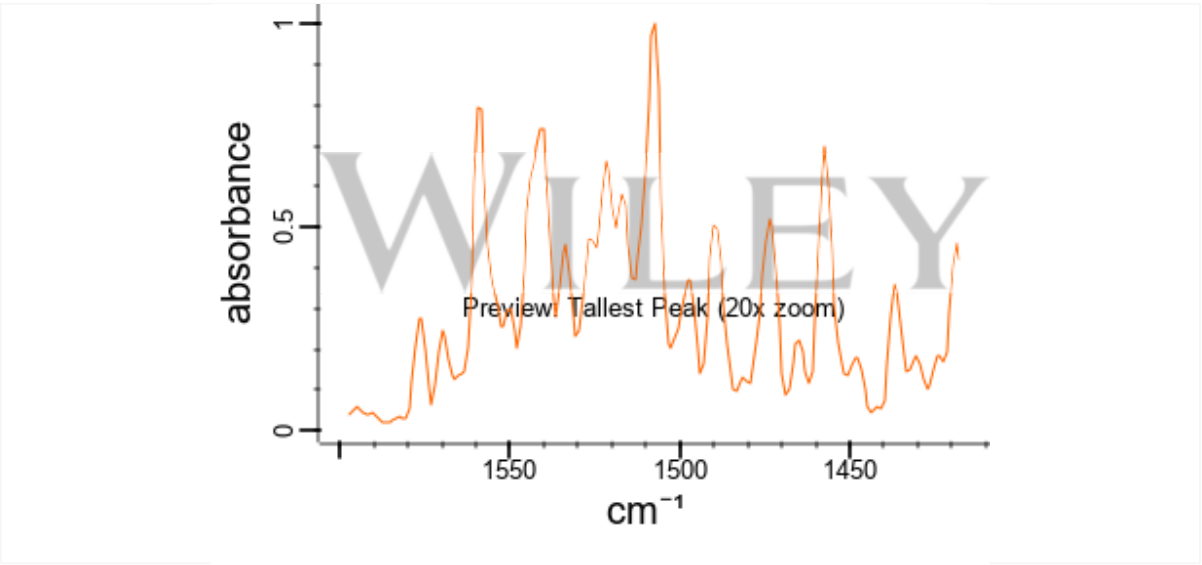
1 of 2

Instrument Name
DIGILAB FTS-14

Technique
Vapor Phase

Copyright

Thumbnail



▸ SpectraBase

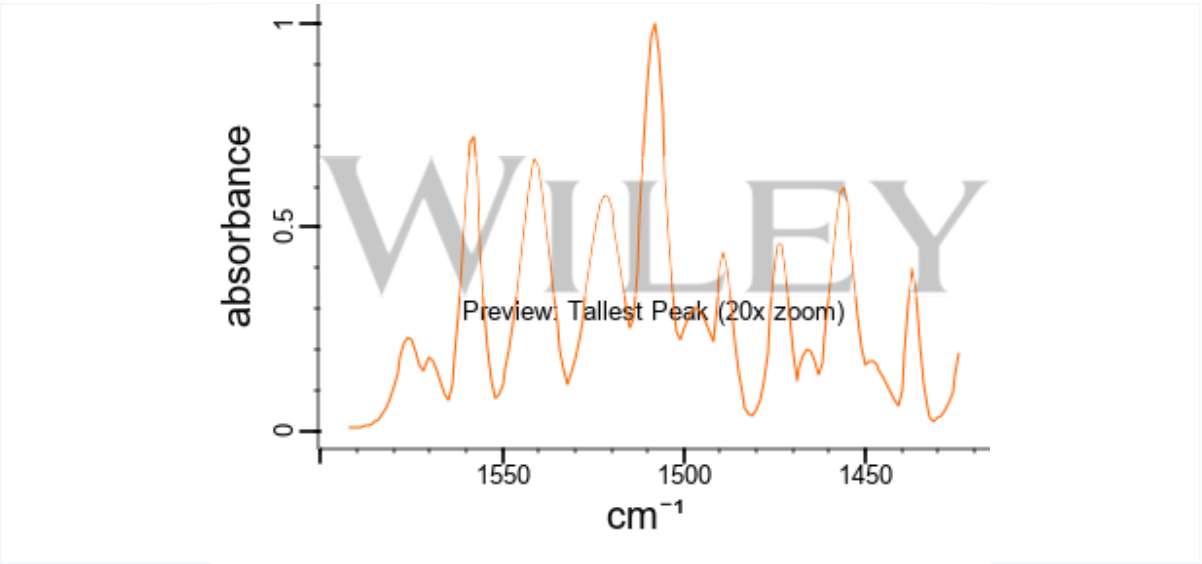
2 of 2

Instrument Name
Bruker IFS 85

Technique
Gas-GC

Copyright

Thumbnail



▸ SpectraBase

5 Related Records

5.1 Related Compounds with Annotation

56 items

Search

SORT BY Neighbor Type - A to Z

hydroxide, hydroxide ion, hydroxyl ion, oxidanide, 14280-30-9, ...

Compound CID: 961
Neighbor Type: 2D+3D
Annotation Types Count: 9

water, 7732-18-5, Dihydrogen oxide, Distilled water, Sterile water, ...

Compound CID: 962
Neighbor Type: 2D+3D
Annotation Types Count: 15

DEUTERIUM OXIDE, 7789-20-0, Heavy water, Deuterated water, Water-d2, ...

Compound CID: 24602

Page 1 of 12

▸ PubChem

5.2 Related Compounds

Same Connectivity Count
17

Mixtures, Components, and Neutralized Forms Count
187452

Similar Compounds Count
53

Similar Conformers Count
15

PubChem

5.3 Substances

5.3.1 Related Substances

All Count
399424

Same Count
1004

Mixture Count
398420

PubChem

5.3.2 Substances by Category

7 categories

Chemical Vendors (400) +

Curation Efforts (26) +

Governmental Organizations (456) +

Journal Publishers (4) +

Research and Development (29) +

Subscription Services (4) +

Legacy Depositors (112) +

PubChem

5.4 Other Relationships

Hydroxide (conjugate)


Oxonium (conjugate)

Hydrogen tritium oxide (related)

Diprotium Oxide (related)

PubChem

5.5 Entrez Crosslinks

PubMed Count
58

Protein Structures Count
434

Nucleotide Count
1

Taxonomy Count
14

Gene Count
72

PubChem

6 Chemical Vendors

33 vendors

Finetech Industry Limited

PubChem SID: 164839542
Purchasable Chemical: FT-0666297

PubChem SID: 273220380
Purchasable Chemical: FT-0696358

PubChem SID: 273220612
Purchasable Chemical: FT-0696590

VWR, Part of Avantor

PubChem SID: 384254820
Purchasable Chemical: 100514-824

PubChem SID: 384249344
Purchasable Chemical: 100514-852

PubChem SID: 384254821
Purchasable Chemical: 100514-856

Thermo Fisher Scientific

PubChem SID: 459195630
Purchasable Chemical: GID_900000000130581

PubChem SID: 459198715
Purchasable Chemical: GID_900000000185682

PubChem SID: 459198716
Purchasable Chemical: GID_900000000185694

abcr GmbH

PubChem SID: 329848147
Purchasable Chemical: AB171556

PubChem SID: 329848152
Purchasable Chemical: AB171653

PubChem SID: 316439279
Purchasable Chemical: AB204080

Alfa Chemistry

PubChem SID: 277333854
Purchasable Chemical: 7732-18-5

PubChem SID: 472849622
Purchasable Chemical: ACM17778802

PubChem SID: 433976156
Purchasable Chemical: ACM7732185

Sigma-Aldrich

PubChem SID: 329747105
Purchasable Chemical: 00612_SIAL

PubChem SID: 329748490
Purchasable Chemical: 07-6060_SAJ

PubChem SID: 329748491
Purchasable Chemical: 07-6061_SAJ

Starshine Chemical

PubChem SID: 464374287
Purchasable Chemical: starbld0295255

001Chemical

PubChem SID: 440049114
Purchasable Chemical: DY571327

CymitQuimica

PubChem SID: 470716835
Purchasable Chemical: CQ_7732-18-5

Cooke Chemical Co., Ltd

PubChem SID: 478258720
Purchasable Chemical: A3222712

PubChem SID: 478270133
Purchasable Chemical: A8395712

Acadechem

PubChem SID: 321936279
Purchasable Chemical: ACDS-067131

Ark Pharma Scientific Limited

PubChem SID: 340471458
Purchasable Chemical: N-0491

A2B Chem

PubChem SID: 444158717
Purchasable Chemical: AE03209

ChemFish Tokyo Co., Ltd.

PubChem SID: 442110305
Purchasable Chemical: 962

LGC Standards

PubChem SID: 483109488
Purchasable Chemical: VHG-CTR-0.1P-100

PubChem SID: 483109487
Purchasable Chemical: VHG-CTR-0.5P-100

PubChem SID: 483109486
Purchasable Chemical: VHG-CTR-1.0P-100

Santa Cruz Biotechnology, Inc.

PubChem SID: 472955016
Purchasable Chemical: sc-204391

PubChem SID: 472971205
Purchasable Chemical: sc-221533

PubChem SID: 473052580
Purchasable Chemical: sc-360260

AA BLOCKS

PubChem SID: 442914725
Purchasable Chemical: AA008N71

Oakwood Products

PubChem SID: 377011134
Purchasable Chemical: 101604

PubChem SID: 377011135
Purchasable Chemical: 101605

PubChem SID: 377011374
Purchasable Chemical: 102069

MolCore BioPharmatech

PubChem SID: 446275082
Purchasable Chemical: DY571327

PubChem SID: 405502458
Purchasable Chemical: MC571327

AKos Consulting & Solutions

PubChem SID: 152090145
Purchasable Chemical: AKOS015950726

VladaChem

PubChem SID: 329735696
Purchasable Chemical: VL145052

PubChem SID: 381003083
Purchasable Chemical: VL167276

PubChem SID: 381026070
Purchasable Chemical: VL281505-4L

Sinfoo Biotech

PubChem SID: 404830001
Purchasable Chemical: S051474

Strem Chemicals, Inc.

PubChem SID: 441102480
Purchasable Chemical: 98-8000

BLD Pharm

PubChem SID: 383826710
Purchasable Chemical: BD156594

MuseChem

PubChem SID: 355433590
Purchasable Chemical: I010717

MolPort

PubChem SID: 91689160
Purchasable Chemical: MolPort-003-926-090

Hunan Chemfish Pharmaceutical Co., Ltd.

PubChem SID: 475745806
Purchasable Chemical: CF104244

J&H Chemical Co.,ltd

PubChem SID: 468749448
Purchasable Chemical: JH179674

Yick-Vic Chemicals & Pharmaceuticals (HK) Ltd.

PubChem SID: 441066057
Purchasable Chemical: CC-1919A

3WAY PHARM INC

PubChem SID: 438594872
Purchasable Chemical: SWOT-61624

BOC Sciences

PubChem SID: 341118644
Purchasable Chemical: 7732-18-5

Tocris Bioscience

PubChem SID: 252157075
Purchasable Chemical: 3179

BenchChem

PubChem SID: 445527308
Purchasable Chemical: B1662957

▸ PubChem

7 Drug and Medication Information

7.1 Drug Indication

For diluting or dissolving drugs for intravenous, intramuscular or subcutaneous injection, according to instructions of the manufacturer of the drug to be administered.

▸ DrugBank

FDA Label

▸ DrugBank

7.2 FDA Approved Drugs

35 items

Search

SORT BY Marketing Status - Z to A

Drug
STERILE WATER IN PLASTIC CONTAINER

Ingredient(s)
STERILE WATER FOR IRRIGATION

Dosage Form/Route
LIQUID;IRRIGATION

Strength
100%

Marketing Status
Prescription

Company
B BRAUN

Application Number
016734

Production Number
001

Drug
STERILE WATER

Ingredient(s)
STERILE WATER FOR IRRIGATION

Dosage Form/Route

Page 1 of 7

▸ Drugs@FDA

7.3 FDA Orange Book

24 items

Search

SORT BY Trade Name - A to Z

Trade Name
STERILE WATER
Marketing Status
Prescription
Application Number
N017428
Applicant
BAXTER HEALTHCARE CORP

Trade Name
STERILE WATER IN PLASTIC CONTAINER
Marketing Status
Prescription
Application Number

Page 1 of 5

FDA Orange Book

7.4 FDA National Drug Code Directory

154 items

Search

SORT BY Start Marketing Date - Most Recent

Product NDC
42961-231
Start Marketing Date
2023-07-11
Dosage Form
SOLUTION

Strength
.984 mL/mL

Labeler
Cintas Corporation

Product NDC
83490-315

Start Marketing Date
2023-06-01

Dosage Form
INJECTION, SOLUTION

Strength
99.99 g/100mL

Page 1 of 31

National Drug Code (NDC) Directory

7.5 Drug Labels

Drug and label

374 items

Search

SORT BY Date - Most Recent

EYESALINE EMERGENCY EYEWASH (PURIFIED WATER) LIQUID

Drug: Purified water
Download: PDF label
Data File: XML
Ingredient (UNII): WATER (UNII:059QF0KO0R)
Indication: For flushing or irrigating the eye to reduce chances of severe injury caused by acid, alkali, or particulate contamination
Category: Human over the counter
Company: Honeywell Safety Products USA, Inc.
Date: 2023-06-20

FENDALL PURE FLOW (PURIFIED WATER) LIQUID

Drug: Purified water
Download: PDF label
Data File: XML

Ingredient (UNII): WATER (UNII:059QF0KO0R)
Indication: For flushing or irrigating the eye to reduce chances of severe injury caused by acid, alkali, or particulate contamination
Category: Human over the counter
Company: Honeywell Safety Products USA, Inc.
Date: 2023-06-20

SAIZEN (SOMATROPIN) KIT SAIZENPREP (SOMATROPIN) KIT

Drug: Sterile Water
Download: PDF label
Data File: XML
Description: SAIZEN is a human growth hormone produced by recombinant DNA technology. SAIZEN has 191 amino acid residues and a molecular weight of 22,125 daltons. Its amino acid sequence and structure are identical to the dominant form...
Indication: SAIZEN is a recombinant human growth hormone indicated for: Pediatric: Treatment of children with growth failure due to growth hormone deficiency (GHD) (1.1) Adult: Treatment of adults with either adult onset or childhood onset GHD. (1.2)
Category: Human prescription
Company: EMD Serono, Inc.
Date: 2023-06-19

SPY ELITE KIT (INDOCYANINE GREEN) KIT SPY-PHI KIT (INDOCYANINE GREEN) KIT SPY-MIS KIT (INDOCYANINE...

Drug: Water
Download: PDF label
Data File: XML

Page 1 of 75

DailyMed

Active ingredient and drug

381 items

Search

SORT BY Ingredient - A to Z

Ingredient
WATER (UNII:059QF0KO0R)

Drug
Sterile Water

Label
Drug PDF label

Data File

XML

Data SetID

236961cb-15c3-48aa-b7de-349bd062db71

Ingredient

WATER (UNII:059QF0KO0R)

Drug

Page 1 of 77

DailyMed

7.6 Clinical Trials

7.6.1 ClinicalTrials.gov

143 items

Search

SORT BY Date - Most Recent

Exogenous Ketone Ester in Women With Polycystic Ovary Syndrome.

CTID: NCT05762822
Phase: N/A
Status: Recruiting
Date: 2023-08-08

OH2 Administered by Intratumoral Injection

CTID: NCT05954091
Phase: Phase 1
Status: Not yet recruiting
Date: 2023-07-20

OH2 Oncolytic Viral Therapy in Non-Muscle-Invasive Bladder Cancer

CTID: NCT05232136
Phase: Phase 1/Phase 2
Status: Recruiting
Date: 2023-07-14

Duration of Cardiac Antimicrobial Prophylaxis Outcomes Study

CTID: NCT05447559
Phase: Phase 4
Status: Recruiting
Date: 2023-07-14

First-line Maintenance of QH2 Injection for Advanced Colorectal Cancer

Page 1 of 29

ClinicalTrials.gov

7.6.2 EU Clinical Trials Register

7 items

Search

SORT BY Date - Most Recent

A Phase 3, Multicenter, Open Label Study to Confirm the Diagnostic Potential of Intravenously Administered 15O- H2O to Identify Coronary Artery Disease During Pharmacological Stress and Resting Conditions Using PET Imaging

EudraCT: 2021-006295-17
Phase: Phase 3
Status: Trial now transitioned
Date: 2022-04-08

Efect of nebulized bicarbonate on bacterial infections in patients with cystic fibrosis. Randomized clinical trial

EudraCT: 2016-004033-25
Phase: Phase 2
Status: Ongoing
Date: 2017-06-19

Impact on Caesarean Section Rates Following Injections of Sterile Water

EudraCT: 2014-004343-12
Phase: Phase 3
Status: Completed
Date: 2015-10-07

A double-blind, randomised, placebo-controlled, Phase II study to evaluate ProCervix efficacy to clear HPV 16 and HPV 18 infection in women with normal cytology or ASCUS/LSIL

EudraCT: 2013-003358-25
Phase: Phase 2
Status: Completed, Ongoing

Date: 2013-11-25

Page 1 of 2

EU Clinical Trials Register

7.6.3 NIPH Clinical Trials Search of Japan

570 items

Search

SORT BY Date - Most Recent

AYD001 Phase III Clinical Trial
CTID: jRCT2031210570
Status: Recruiting
Date: 2022-01-21

Verification of effective oral care in preventing Ventilator-Associated pneumonia in ICU patients -A comparative study of oral care in the practical guide to oral care and conventional oral care-
CTID: jRCT1040210134
Status: Recruiting
Date: 2022-01-21

A study investigating the effect of Java ginger extract in patients with refractory leg neuropathic pain
CTID: jRCTs041210100
Status: Pending
Date: 2021-11-15

A phase 1 study of pimitespib and imatinib in patients with GIST
CTID: jRCT2011210044
Status: Recruiting
Date: 2021-11-01

A Research Study Looking at How NNC0385-0434 Tablets Work to Lower Blood Cholesterol in People With Heart Disease or a High Risk of Heart Disease
CTID: jRCT2031210399
Status: Recruiting
Date: 2021-10-29

Page 1 of 114

NIPH Clinical Trials Search of Japan

8 Food Additives and Ingredients

8.1 FDA Inventory of Effective Food Contact Substance Notifications - FCN

Food Contact Substance
A mixture containing peroxyacetic acid (CAS Reg. No. 79-21-0), hydrogen peroxide (CAS Reg. No. 7722-84-1), acetic acid (CAS Reg. No. 64-19-7), 1-hydroxyethylidene-1,1-diphosphonic acid (CAS Reg. No. 2809-21-4), and water (CAS Reg. No. 7732-18-5).

Manufacturer
Alex C. Fergusson, LLC (AFCO)

Effective Date
Jul 29, 2011

Intended Use
As an antimicrobial agent for meat and poultry carcasses.

Limitations/Specifications
The FCS will be added to: 1) process water used for washing, rinsing, cooling or otherwise for processing meat carcasses, parts, trim, and organs; and 2) process water applied to poultry parts, organs, and carcasses as a spray, wash, rinse, dip, chiller water, or scald water. In either application, the level of the components of the FCS in the process water will not exceed 220 ppm for peroxyacetic acid, 160 ppm for hydrogen peroxide, and 11 ppm for 1-hydroxyethylidene-1,1-diphosphonic acid.

National Environmental Policy Act
Environmental Assessment (in PDF, 89 kB)

FDA Decision
Finding of No Significant Impact (FONSI)

Notification
According to Section 409(h)(1)(C) of the Federal Food, Drug, and Cosmetic Act, food contact substance notifications (FCNs) are effective only for the listed manufacturer and its customers. Other manufacturers must submit their own FCN for the same food contact substance and intended use.

FDA Center for Food Safety and Applied Nutrition (CFSAN)

9 Pharmacology and Biochemistry

9.1 Absorption, Distribution and Excretion

Tritium radioactivity in mouse fetus taken from the pregnant female mouse which had been given **tritium** containing drinking water was measured to estimate the absorbed radiation dose from the incorporated **tritium**. BC3F1 female mice mated with ICR male were given drinking water containing various concentrations of **tritium** for whole pregnant period, from the morning when the vaginal plug was observed to the day just before term. At various times of the pregnant period, blood and fetuses were taken from the female mice to measure the **tritium** concentration using a Packard model of sample oxidizer. The absorbed radiation dose of the fetus from the incorporated **tritium** was estimated on the basis of the **tritium** concentration measured. The **tritium** concentration of the embryos increased gradually from the first pregnant day to reach the plateau level at the 7 to 9th day. The estimated radiation dose increased almost linearly depending on the **tritium** concentration in the drinking water. /**Tritium** containing drinking water/

Yamada T et al; J Radiat Res (Tokyo) 32 (1): 91 (1991)

- **Hazardous Substances Data Bank (HSDB)**

9.2 Human Metabolite Information

9.2.1 Tissue Locations

All Tissues

- **Human Metabolome Database (HMDB)**

9.2.2 Cellular Locations

Cytoplasm
Endoplasmic reticulum
Extracellular
Golgi apparatus
Lysosome
Mitochondria
Nucleus
Peroxisome

▸ Human Metabolome Database (HMDB)

9.2.3 Metabolite Pathways

11-beta-hydroxylase deficiency (CYP11B1)
17-alpha-hydroxylase deficiency (CYP17)
17-Beta Hydroxysteroid Dehydrogenase III Deficiency
2-aminoadipic 2-oxoadipic aciduria
2-Hydroxyglutric Aciduria (D And L Form)
2-ketoglutarate dehydrogenase complex deficiency
2-Methyl-3-Hydroxybutryl CoA Dehydrogenase Deficiency
21-hydroxylase deficiency (CYP21)
27-Hydroxylase Deficiency
3-Beta-Hydroxysteroid Dehydrogenase Deficiency
Total 46599 pathways, visit the HMDB page for details

▸ Human Metabolome Database (HMDB)

9.3 Biochemical Reactions

5,675 items

Search

SORT BY Rhea Accession - Increasing

Rhea Accession
RHEA:10000

Reaction
pentanamide + H_2O = pentanoate + NH_4^+

PubChem Enzyme
EC 3.5.1.50

Evidence PMID

Rhea Accession
RHEA:10008

Reaction
[protein]-dithiol + a hydroperoxide = [protein]-disulfide + an alcohol + H_2O

PubChem Enzyme

EC

Evidence PMID

Page 1 of 1,135

Rhea - Annotated Reactions Database

354,290 items

Search

SORT BY Taxonomy - A to Z

Reaction

H_2O + GTP ⟶ formate + H_2O + dihydroneopterin triphosphate

PubChem Pathway

tetrahydrofolate biosynthesis

Source

BioCyc

Taxonomy

Candida albicans SC5314

Reaction

ASA + H2O ⟶ H+ + ASA- + H2O

PubChem Pathway

Drug ADME

Source

Page 1 of 70,858

PubChem

9.4 Transformations

1 item

Predecessor

▸ NORMAN Suspect List Exchange

10 Use and Manufacturing

10.1 Uses

EPA CPDat Chemical and Product Categories

329 items

Search

SORT BY Category - A to Z

additive
Categorization Type: Reported Functional Use

adhesion/cohesion promoter
Categorization Type: OECD Functional Use

adhesive
Categorization Type: Reported Functional Use

admixture
Categorization Type: Reported Functional Use

anticaking agent
Categorization Type: OECD Functional Use

Page 1 of 66

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

▸ EPA Chemical and Products Database (CPDat)

Sources/Uses

The most universal solvent; [Merck Index] Used as a solvent, suspending agent, industrial coolant, diluent, moderator in nuclear reactors, nutrient, power source, hydration of lime, paper coatings, textile processing, debarking logs, filtration, washing and scouring, **sulfur** mining, hydrolysis, Portland cement, hydraulic systems, steam generation, and in foods and beverages; [NTP] Permitted for use as an inert ingredient in non-food pesticide products; [EPA]

Merck Index - O'Neil MJ, Heckelman PE, Dobbelaar PH, Roman KJ (eds). The Merck Index, An Encyclopedia of Chemicals, Drugs, and Biologicals, 15th Ed. Cambridge, UK: The Royal Society of Chemistry, 2013.

▸ **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

Industrial Processes with risk of exposure

Steel Producing [Category: Industry]

Electroplating [Category: Plate]

Petroleum Production and Refining [Category: Industry]

Pulp and Paper Processing [Category: Industry]

Textiles (Fiber & Fabric Manufacturing) [Category: Industry]

Painting (Solvents) [Category: Paint]

Mining [Category: Industry]

Sewer and Wastewater Treatment [Category: Industry]

Firefighting [Category: Other]

Leather Tanning and Processing [Category: Industry]

Photographic Processing [Category: Other]

Cement Producing [Category: Industry]

Textiles (Printing, Dyeing, or Finishing) [Category: Industry]

Dressing Hair [Category: Other]

Metal Extraction and Refining [Category: Industry]

▸ **Haz-Map, Information on Hazardous Chemicals and Occupational Diseases**

Physiologically water is classed as a nutrient substance.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1325

▸ **Hazardous Substances Data Bank (HSDB)**

Drinking, culinary purposes, bathing, washing, laundering, heating, air conditioning, agriculture, stock raising and gardens, for industrial processes and cooling, for water power and steam power, for fire protection, for disposal of wastes, for fishing, swimming, boating and other recreational purposes, for fish and wildlife propagation, and for navigation

Camp TR; Water and its Impurities. New York, NY: Reinhold Pub Co pp. 355 (1963)

▸ **Hazardous Substances Data Bank (HSDB)**

Estimated Water Use in the US.

Table: Use in Billion Gallons/Day

Category	Population X10+6
1950	150.7
1970	205.9
1985	242.2
2000	285.3

Category	Total Withdrawals
1950	180
1970	370
1985	399
2000	408

Category	rural self-supplied domestic
1950	2.1
1970	2.6
1985	3.32
2000	3.59

Category

livestock and aquaculture

1950

1.5

1970

1.9

1985

4.47

2000

no data

Category

irrigation

1950

89

1970

130

1985

137

2000

137

Category

thermoelectric power

1950

40

1970

170

1985

187

2000

195

Category

industrial

1950

37

1970

47

1985

39.5

2000

no data

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

- **Hazardous Substances Data Bank (HSDB)**

10.1.1 Use Classification

EPA Safer Chemical Functional Use Classes -> Solvents

- **EPA Safer Choice**

Safer Chemical Classes -> Green circle - The chemical has been verified to be of low concern

- **EPA Safer Choice**

Human Drugs -> FDA Approved Drug Products with Therapeutic Equivalence Evaluations (Orange Book) -> Active Ingredients

- **FDA Orange Book**

Cosmetics -> Solvent

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | ***DOI:10.5281/zenodo.2624118***

- **NORMAN Suspect List Exchange**

10.1.2 Industry Uses

Adhesives and sealant chemicals
Anti-adhesive agents
Lubricants and lubricant additives
Not Known or Reasonably Ascertainable
Sealant (barrier)

https://www.epa.gov/chemical-data-reporting

▸ EPA Chemicals under the TSCA

10.1.3 Consumer Uses

Adhesives and sealant chemicals
Emulsifier
Fragrance
Lubricants and lubricant additives
Sealant (barrier)

https://www.epa.gov/chemical-data-reporting

▸ EPA Chemicals under the TSCA

10.1.4 Household Products

Household & Commercial/Institutional Products

Information on 8712 consumer products that contain Water in the following categories is provided:

- Auto Products
- Commercial / Institutional
- Hobby/Craft
- Home Maintenance
- Home Office
- Inside the Home
- Landscaping/Yard
- Personal Care
- Pesticides
- Pet Care

▸ Consumer Product Information Database (CPID)

Household & Commercial/Institutional Products

Information on 0 consumer products that contain Aqua in the following categories is provided:

▸ Consumer Product Information Database (CPID)

10.2 Methods of Manufacturing

Derivation: (1) Oxidation of **hydrogen**; (2) end product of combustion; (3) end product of acid-base reaction; (4) end product of condensation reaction.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 1325

▸ **Hazardous Substances Data Bank (HSDB)**

10.3 Consumption Patterns

Agriculture consumes by far the most of any use category to which the accessible runoff worldwide is applied ... The number of acres irrigated with sprinkler and microirrigation systems has continued to increase and comprises more than half the total irrigated acreage.

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

Water Source Use in the US.

Table: Withdrawals in Billion gallons/day

Category	Population X10+6
1950	150.7
1970	205.9
1985	242.2
2000	285.3
Category	Groundwater
Category	fresh
1950	34

1970
68

1985
73.2

2000
83.3

Category
saline

1950
no data

1970
1.0

1985
0.65

2000
1.26

Category
Surface water

Category
fresh

1950
140

1970
250

1985
265

2000
262

Category
saline

1950
10

1970
53

1985

59.6

2000

61

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ Hazardous Substances Data Bank (HSDB)

10.4 U.S. Production

Aggregated Product Volume

2019: 100,000 - <500,000 lb

2018: <1,000,000 lb

2017: 100,000 - <500,000 lb

2016: 100,000 - <500,000 lb

https://www.epa.gov/chemical-data-reporting

▸ EPA Chemicals under the TSCA

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year
1986

Production Range (pounds)
>1 billion

Year
1990

Production Range (pounds)
>1 million - 10 million

Year
1994

Production Range (pounds)
>1 million - 10 million

Year
1998

Production Range (pounds)
>1 million - 10 million

Year
2002

Production Range (pounds)
>100 million - 500 million

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Water (7732-18-5). Available from, as of January 29, 2014: ***https://epa.gov/cdr/tools/data/2002-vol.html***

▸ **Hazardous Substances Data Bank (HSDB)**

Production volume for non-confidential chemicals reported under the 2006 Inventory Update Rule. Chemical: Water. Aggregated National Production Volume: 1 billion pounds and greater.

US EPA; Non-Confidential 2006 Inventory Update Reporting. National Chemical Information. Water (7732-18-5). Available from, as of January 29, 2014: ***https://cfpub.epa.gov/iursearch/index.cfm***

▸ **Hazardous Substances Data Bank (HSDB)**

Non-confidential 2012 Chemical Data Reporting (CDR) information on the production and use of chemicals manufactured or imported into the United States. Chemical: Water. National Production Volume: 10,000,000 - 50,000,000 lb/yr.

USEPA/Pollution Prevention and Toxics; 2012 Chemical Data Reporting Database. Water (7732-18-5). Available from, as of January 30, 2014: ***https://java.epa.gov/oppt_chemical_search/***

▸ **Hazardous Substances Data Bank (HSDB)**

10.5 General Manufacturing Information

Industry Processing Sectors

All Other Basic Inorganic Chemical Manufacturing
Construction
Petroleum Lubricating Oil and Grease Manufacturing
Wood Product Manufacturing

▸ **EPA Chemicals under the TSCA**

EPA TSCA Commercial Activity Status

Water: ACTIVE

https://www.epa.gov/tsca-inventory

▸ **EPA Chemicals under the TSCA**

Some bottled waters contain **fluoride**, and some do not. **Fluoride** can occur naturally in source waters used for bottling or be added. Most bottled waters contain **fluoride** at levels that are less than optimal for good oral health.

CDC; Drinking Water; Available from, as of February 4, 2014:
https://www.cdc.gov/healthywater/drinking/bottled/index.html

▸ **Hazardous Substances Data Bank (HSDB)**

People with compromised immune systems may want to take special precautions with the water they drink. In healthy individuals, the parasite Cryptosporidium can cause illness; however, for those with weakened immune systems, it can cause severe illness and possibly death. Look for bottled water treatments that protect against Cryptosporidium, which include: Reverse Osmosis Distillation Filtration with an absolute 1 micron filter.

CDC; Drinking Water; Available from, as of February 4, 2014:
https://www.cdc.gov/healthywater/drinking/bottled/index.html

▸ **Hazardous Substances Data Bank (HSDB)**

The proper amount of **fluoride** from infancy through old age helps prevent and control tooth decay. Community water fluoridation is a widely accepted practice for preventing and controlling tooth decay by adjusting the concentration of **fluoride** in the public water supply

CDC; Community Water Fluoridation; Available from, as of February 4, 2014:
https://www.cdc.gov/fluoridation/

▸ **Hazardous Substances Data Bank (HSDB)**

According to the EPA, approximately 286 million Americans receive their tap water from a community water system. These public water systems are monitored and regulated as set by the EPA. An estimated 15% of Americans, or about 45 million people, get their water from private ground water wells that are not subject to EPA regulations. Private ground water wells can provide safe, clean water. However, well water can also become contaminated, leading to illness. It is the responsibility of well owners to maintain and treat their well.

CDC; Drinking Water; Available from, as of February 4, 2014:
https://www.cdc.gov/healthywater/drinking/

▸ **Hazardous Substances Data Bank (HSDB)**

For more General Manufacturing Information (Complete) data for Water (10 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

11 Safety and Hazards

11.1 Hazards Identification

11.1.1 GHS Classification

GHS Hazard Statements

Not Classified

Reported as not meeting GHS hazard criteria by 1834 of 1842 companies (only ~ 0.4% companies provided GHS information). For more detailed information, please visit **ECHA C&L website.**

▸ **European Chemicals Agency (ECHA)**

11.1.2 EPA Safer Chemical

Chemical: Water

● Green circle - The chemical has been verified to be of low concern based on experimental and modeled data.

▸ **EPA Safer Choice**

11.1.3 Health Hazards

Water itself is nontoxic and is in fact essential for life. Solutes dissolved in water may be toxic, but those interactions are covered by the reactive groups that the solute belongs to.

▸ **CAMEO Chemicals**

11.2 Safety and Hazard Properties

11.2.1 Critical Temperature & Pressure

Critical temperature: 374.2 °C; critical pressure: 218 atm

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1868

▸ **Hazardous Substances Data Bank (HSDB)**

11.3 Stability and Reactivity

11.3.1 Air and Water Reactions

No rapid reaction with air. No rapid reaction with water.

- CAMEO Chemicals

11.3.2 Reactive Group

Water and Aqueous Solutions

- CAMEO Chemicals

11.3.3 Reactivity Alerts

11.3.1 CSL Reaction Information

1 of 4
CSL No CSL00038
Reactants/Reagents SODIUM BOROHYDRIDE; WATER
Function Group borohydride
GHS Category Gas Under Pressure
Warning Message Gas evolution. Ensure complete destruction of **borane** by using appropriate quench time and pH
Source Reference User-Reported
CSL Status Approved

Modified Date
5/31/2018

▸ Pistoia Alliance Chemical Safety Library

2 of 4

CSL No
CSL00075

Reactants/Reagents
WATER; DIETHYLAMINOSULFUR TRIFLUORIDE

GHS Category
Explosive

Warning Message
DAST alone at >90C explodes or in combination with water

Source Reference
User-Reported

CSL Status
Approved

Modified Date
8/7/2018

▸ Pistoia Alliance Chemical Safety Library

3 of 4

CSL No
CSL00111

Reactants/Reagents
WATER; Mercury(II) perchlorate hydrate; 2,6 lutidine; TETRAHYDROFURAN

Reaction Class
dithiane hydrolysis

Reaction Scale
M (up to 100g)

Warning Message
Explosion tetrahydrofuran, water, 2,6 lutidine, and mercury perchlorate hydrate

Source Reference
User-Reported

CSL Status
Approved

Additional Info
The reaction chemicals were scaled up, but the amount of solvent was not scaled up to an equivalent proportion. The amount of material used in the reaction was approximately 20 times more concentrated than the quantity specified in the literature. Electronic software was used to calculate the quantities of all reactants but not the quantity of solvent. Additionally, the lesser amount of solvent used in this reaction made it difficult for the magnetic stirrer bar to effectively mix
http://www.memphis.edu/ehs/pdfs/jan2012.pdf

Modified Date
5/24/2018

▸ Pistoia Alliance Chemical Safety Library

4 of 4

CSL No
CSL00132

Reactants/Reagents
WATER; Ammonium cerium(IV) nitrate; MALONIC ACID; POTASSIUM BROMATE

Reaction Class
oxidation

Function Group
bromate

GHS Category
Flammable,Oxidizer

Reaction Scale
Not Available

Warning Message

Chemical & Engineering News (15 Jun 1998) Vol. 76, No. 24, pp. 4. We wish to point out a safety hazard with a widely performed standard chemical demonstration that caused significant damage recently in a teaching laboratory in the chemistry department at the University of Tennessee, Knoxville. The Belousov-Zhabotinsky oscillator reaction described in Bassam Shakhashiri's" Chemical Demonstrations: A Handbook for Teachers of Chemistry," Vol. 2, involves the **cerium ammonium nitrate**-catalyzed redox reaction of **potassium bromate** with **malonic acid**. This reaction was carried out in an honors general chemistry laboratory without incident during the afternoon, but a fire was discovered in the lab two hours after everyone had left. It destroyed the wooden drawers beneath a stone benchtop before being extinguished by the fire department. Investigation revealed that the three chemicals used are stable when mixed dry, and react as expected when in dilute solution. However, when 0.5 g of each are mixed together, and between one drop and 3 mL of water added, a very exothermic reaction occurs with considerable fuming. All three chemicals are needed for this to initiate. When carried out on a piece of filter paper, ignition of the paper occurred. We suspect that in the teaching laboratory, dry chemicals were spilled during weighing, and, rather than being disposed of in the aqueous heavy-metal waste container, were placed in a trash can. This was stored under a sink with a leaky drainpipe, and the critical amount of moisture set off the reaction after everyone had left the room. There is a safety warning in the experimental procedure regarding bromates being strong oxidizing agents and indicating that mixtures with finely divided organic materials are easily ignited. The catalytic nature of the **cerium** salt on this is not indicated, however. We alert people to the hazardous nature of this particular mixture, under conditions that are not unusual.

Source Reference
ACS Safety Letters

CSL Status
Approved

Modified Date
2/28/2018

▸ **Pistoia Alliance Chemical Safety Library**

11.3.4 Reactivity Profile

Water reacts with many substances, including but not limited to alkali metals, hydrides, strong halogenating agents, and chlorosilanes. These reactions can be hazardous and may result in flammable or toxic gas production, or generation of excessive heat that may cause pressurization to occur. Another reactive hazard is heat of mixing. Mixing substances such as **sulfuric acid** or **sodium hydroxide** with water may generate significant heat. Additionally, water is a good solvent for polar molecules, so it can form aqueous solutions if it comes into contact with such molecules.

▸ **CAMEO Chemicals**

11.4 Other Safety Information

11.4.1 Special Reports

EPA; Water: Laboratory Certification.[EPA; Water: Laboratory Certification; Drinking Water Analytical Methods; Available from, as of February 4, 2014: http://water.epa.gov/scitech/drinkingwater/labcert/analyticalmethods.cfm#approved]

▸ Hazardous Substances Data Bank (HSDB)

12 Toxicity

12.1 Toxicological Information

12.1.1 Drug Induced Liver Injury

Compound
sterile water

DILI Annotation
No-DILI-Concern

Label Section
No match

References

M Chen, V Vijay, Q Shi, Z Liu, H Fang, W Tong. FDA-Approved Drug Labeling for the Study of Drug-Induced Liver Injury, Drug Discovery Today, 16(15-16):697-703, 2011. PMID:21624500 DOI:10.1016/j.drudis.2011.05.007

M Chen, A Suzuki, S Thakkar, K Yu, C Hu, W Tong. DILIrank: the largest reference drug list ranked by the risk for developing drug-induced liver injury in humans. Drug Discov Today 2016, 21(4): 648-653. PMID:26948801 DOI:10.1016/j.drudis.2016.02.015

▸ Drug Induced Liver Injury Rank (DILIrank) Dataset

12.1.2 Effects During Pregnancy and Lactation

◉ Summary of Use during Lactation

Information in this record refers to the use of water O 15 as a diagnostic agent. No information is available on the use of water O 15 during breastfeeding. United States and international authorities state that breastfeeding need not be interrupted after administration of radiopharmaceuticals containing oxygen-15.

◉ Effects in Breastfed Infants

Relevant published information was not found as of the revision date.

◉ Effects on Lactation and Breastmilk

Relevant published information was not found as of the revision date.

▸ Drugs and Lactation Database (LactMed)

12.1.3 Acute Effects

12 items

Search

Compound CID
962

Organism
infant

Test Type
TDLo

Route
oral

Dose
333 gm/kg

Effect
BEHAVIORAL: CONVULSIONS OR EFFECT ON SEIZURE THRESHOLD; GASTROINTESTINAL: HYPERMOTILITY, DIARRHEA

Reference
Archives of Disease in Childhood., 54(551), 1979 [PMID:485199]

Compound CID
962

Organism
man

Test Type

TDLo

Route

oral

Dose

Page 1 of 3

▸ ChemIDplus

12.1.4 Interactions

Because groundwater contamination is an important environmental concern, we examined the hepatic and renal effects of repeated exposure to a mixture of 25 chemicals frequently found in groundwater near hazardous-waste disposal sites and the effect of such exposure on **carbon tetrachloride** (CCl4) toxicity. Adult male F-344 rats received ad libitum deionized water and feed (Ad Lib Water) or ad libitum 10% MIX (referring to 10% of a technically achievable stock mixture) and feed for 14 d. Because exposure to the 25-chemical mixture via the drinking water resulted in decreased water and feed consumption, restricted deionized water and feed controls (Restricted Water) were included. On d 14, rats were gavaged with 0, 0.0375, 0.05, 0.075 or 0.15 mL CCl4/kg, and hepatic and renal toxicity assessed 24 hr later. Little or no hepatic and renal toxicity was observed in rats exposed to 10% MIX alone. No hepatic or renal lesions occurred that could be attributed to 10% MIX alone. Slight but statistically significant alterations, of uncertain biological significance, resulted from the water treatments: 10% MIX increased **alanine** aminotransferase, **urea nitrogen** (BUN), and BUN/**creatinine** ratio; Restricted Water increased 5'-nucleotidase and decreased alkaline phosphatase. Relative kidney weight was increased by both 10% MIX and Restricted Water. CCl4 resulted in significant dosage-dependent hepatotoxicity in all three water treatment groups but had little or no effect on renal indicators of toxicity. Relative to Ad Lib Water, significantly greater hepatotoxicity occurred in both 10% MIX and Restricted Water rats. The response to CCl4 in the Restricted Water rats was similar to that of 10% MIX rats, indicating that a substantial portion of the effect of 10% MIX on CCl4 hepatotoxicity is due to decreased water and feed intake.

PMID:7966440

Simmons JE et al; J Toxicol Environ Health 43 (3): 305-25 (1994)

▸ Hazardous Substances Data Bank (HSDB)

12.1.5 Antidote and Emergency Treatment

To evaluate the efficacy of **Ringer's lactate**, isotonic saline and hypertonic saline on the clinical and biochemical recovery of athletes with exercise-associated hyponatremic encephalopathy caused by fluid overload. We retrospectively reviewed serial blood **sodium** concentrations (Na+) and qualitative signs of recovery and time to recovery in two healthy menstruant females hospitalised with dilutional exercise-associated hyponatremic encephalopathy after withdrawal from the 2011 Comrades Marathon (89 km) and Argus Cycle Tour (109 km). Improvements in blood Na+ did not occur with intravenous administration of Ringer's lactate solution, but did occur with administration of isotonic and hypertonic saline. Qualitative improvements in mental status were not quantitatively related to the biochemical value of blood Na+ or subsequent return to normonatremia. Hyponatremia should be suspected in all female athletes presenting to the medical area of endurance races with vomiting, altered mental status and a history of high fluid intake. If a diagnosis of exercise-associated hyponatremia with cerebral encephalopathy is confirmed, the treatment of choice is administration of an intravenous bolus of hypertonic saline. Administration of **Ringer's lactate** should be discouraged, as this does not correct Na+ and appears to delay recovery.

PMID:23498039

Hew-Butler TD.et al; S Afr Med J. 102 (12): 927-30 (2012)

▸ **Hazardous Substances Data Bank (HSDB)**

/SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160

▸ **Hazardous Substances Data Bank (HSDB)**

/SRP:/ Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer **oxygen** by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool ... . Cover skin burns with dry sterile dressings after decontamination ... . /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160

▸ **Hazardous Substances Data Bank (HSDB)**

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema ... . Consider administering a beta agonist such as **albuterol** for severe bronchospasm ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV administration of D5W /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload ... . Treat seizures with **diazepam** or **lorazepam** ... . Use **proparacaine hydrochloride** to assist eye irrigation ... . /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 160-1

▸ **Hazardous Substances Data Bank (HSDB)**

For more Antidote and Emergency Treatment (Complete) data for Water (8 total), please visit the **HSDB record page**.

▸ **Hazardous Substances Data Bank (HSDB)**

12.1.6 Human Toxicity Excerpts

/SIGNS AND SYMPTOMS/ Human systemic effects by ingestion of very large amounts: body temperature increase, convulsions, diarrhea, fever, hypermotility, muscle contraction or spasticity, mydriasis, nausea or vomiting, tremors.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3692

▸ **Hazardous Substances Data Bank (HSDB)**

/CASE REPORTS/ Dilutional hyponatremia is a serious adverse effect of **desmopressin**, a vasopressin analog that is widely prescribed to manage monosymptomatic enuresis. The presentation of hyponatremia, largely related to cerebral dysfunction, can include severe signs like altered mental status and seizures. /The authors/ reviewed the literature dealing with altered mental status or seizures in enuretic subjects on **desmopressin**. The retained publications included patients who were described individually, revealing data on mode of administration, further identifiable factors predisposing to hyponatremia, presentation and

clinical course. /It was/ found 54 cases of hyponatremia secondary to **desmopressin** treatment presenting with altered mental status or seizures. In most cases the complication developed 14 days or less after starting **desmopressin**. An intranasal formulation had been used in 47 patients. Excess fluid intake was documented as a contributing factor in at least 22 cases. In 6 cases severe signs of hyponatremia developed in the context of intercurrent illnesses. Altered mental status or seizures are very rare but recognized complications of **desmopressin** in enuresis. This complication mostly develops in subjects managed with the intranasal formulation 14 days or less after starting the medication, following excess fluid intake and during intercurrent illnesses.

PMID:23619353

Lucchini B et al; Pediatr Urol 9 (6 Pt B): 1049-53 (2013)

▸ **Hazardous Substances Data Bank (HSDB)**

/CASE REPORTS/ A 62-year-old man with no major comorbidities became acutely hyponatremic on the second postoperative day following a routine carotid endarterectomy. He developed a headache, became hypertensive and confused, and then had a seizure and required intubation and admission to the intensive care unit. A CT angiogram of his head and carotid arteries was normal, as was a subsequent MRI head. His serum and urine osmolality were low. He was treated by fluid restriction and his hyponatraemia resolved over 3 days. On discontinuation of sedation the patient woke up appropriately. The cause of his hyponatremia was initially a mystery but when questioned by the medical team he admitted that he drank about 5 liters of water in the afternoon on the second postoperative day. At this point the diagnosis of dilutional hypervolemic hyponatremia secondary to water intoxication could be made.

PMID:23729677

Full text: ***https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3669829***

Parkinson F et al; BMJ Case Rep. 2013 May 30;2013. pii: bcr2012008299. doi: 10.1136/bcr-2012-008299.

▸ **Hazardous Substances Data Bank (HSDB)**

/CASE REPORTS/ A syndrome of hyponatremia associated with excessive beer drinking was first recognised in 1971. This syndrome has been referred to as beer potomania. Dilutional hyponatremia occurs due to excessive consumption of an exclusive beer diet which is poor in salt and protein. /The authors/ report a case of beer potomania who improved dramatically with introduction of solute load, with no subsequent neurological sequelae.

PMID:22736559

Full text: ***https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3047485***

Bhattarai N et al; BMJ Case Rep. 2010 Apr 29;2010. pii: bcr1020092414. doi: 10.1136/bcr.10.2009.2414.

▸ Hazardous Substances Data Bank (HSDB)

For more Human Toxicity Excerpts (Complete) data for Water (9 total), please visit the **HSDB record page**.

▸ Hazardous Substances Data Bank (HSDB)

12.1.7 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ The Sprague Dawley rat was used to assess the reproductive and teratologic effects of the highly treated reclaimed water derived from secondary wastewater by the Denver Water Department. A two-generation reproduction study with teratology phase was conducted using test groups receiving a 500x concentration of reclaimed wastewater or a 500x concentration of wastewater processed by an ultrafiltration process and control groups receiving commercially obtained distilled water or a 500x concentration of Denver's present high quality water. Fifty rats per sex in the first generation (F0) received the specified dosing regimen. From the offspring of this generation, 35 rats/sex/group (F1) received the appropriate drinking water through growth and maturation and during three breeding (F2a, b and c) and gestation periods... The evaluation of data from two generations of growth, breeding, gestation and lactation indicated no adverse reproductive effects from exposure to any of the dose-water regimens.

Lemen J et al; Toxicologist 11 (1): 113 (1991)

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Increasing usage of the energy generated by nuclear fission and fusion plants leads to release a large quantity of **tritiated water** (HTO) into the environment. From the point of radiation hazard, it is urgent needs to evaluate biological effect of HTO. In particular, it appears of interest to assess the effects on the development of fetuses exposed continuously by HTO throughout pregnancy. To determine the radiation effect of **tritiated water** on fetal development, BC3F1 female mice were provided various doses (50-500 uCi/mL) of HTO throughout pregnancy. The litter size decreased gradually as the doses became higher. The number of stillbirth per litter increased in turn. For lower doses of HTO, pre-implantation death would be a major factor for the reduction of the litter size. Fetal body weight, brain weight, head size and protein contents of the brain were examined in the fetuses irradiated. At relatively low dose (50 uCi/mL), no observable effect was found. But for higher doses, HTO had detrimental effect on the embryonal development. /**Tritiated water**/

Kurihara Y et al; J Radiat Res (Tokyo) 34 (1): 82 (1993)

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Objective: To determine the impact of new types of drinking water on health. Methods: Parents mice were fed with magnetized mineral water, activated water, purified water, mineral water, alkaline ionized water and natural water respectively for 3 months, and of offspring mice for 3 months. Results: To compare with natural water, activated water and magnetized mineral water could significantly increase the body weight of paternal mice (P < 0 .05), while mineral water and alkaline ionized water could significantly decrease the body weight of offspring male mice (P < 0.05), magnetized mineral water could significantly decrease the body weight of offspring mice (P < 0.05). Purified water could significantly decrease the neonatal mice weight (P < 0.05). Activated water and magnetized mineral water could significantly increase the neonatal mice number (P < 0.05). All the 5 new types of water had no effect on mice, pregnancy rate, gestation rate and birth livability. In offspring mice, SOD /superoxide dismutase/ activity could be increased significantly (P < 0.05) by treating with magnetized mineral water, activated water, purified water, mineral water, while alkaline ionized water could decrease the activity of SOD significantly (P < 0.05) . Conclusion: Five new types of drinking water could affect the body weight of mice, but had no effect on pregnancy rate, gestation rate and birth livability of mice. Magnetized mineral water, activated water, purified water and mineral water could increase SOD activity.

Zhou YH Chung-Kuo Kung Kung Wei Sheng (China Public Health) 19 (12):1429-30 (2003)

▸ Hazardous Substances Data Bank (HSDB)

/DEVELOPMENTAL NEUROTOXICITY/ Pregnant mice were injected intraperitoneally with different doses of **tritiated water** on day 13 of pregnancy. The litters received total cumulative absorbed beta-irradiation of 0 (control), 0.1, 0.2, 0.4 or 0.8 Gy due to exponentially decreasing exposure. The 0.4 Gy irradiation caused a significant reduction in brain weight but not in body weight examined at 8 weeks of age. The highest dose (0.8 Gy) inhibited both body and brain development. Histological examination showed that the cortical architecture and laminar organization were well preserved. Thickness of somatosensory cortex was decreased by the treatment, and there was significant difference between groups exposed to 0.4 Gy or more and the control. Quantitative analysis revealed that 8-week-old mice had a dose-related reduction in pyramidal cell densities. These effects were apparent in groups exposed to 0.2 Gy or more. The effect of prenatal exposure to chronic low dose-rate beta-irradiation from **tritiated water** may be a little greater than the same dose of acute X- or beta-irradiation. /**Tritiated water**/

Sun XZ; Teratology 57 (3): 5A (1998)

▸ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for Water (7 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

12.1.8 Non-Human Toxicity Values

LD50 Mice ip 25000 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3692

▸ Hazardous Substances Data Bank (HSDB)

LD50 Mice iv 25000 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3692

▸ Hazardous Substances Data Bank (HSDB)

LD50 Mice ip 190000 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 3692

▸ Hazardous Substances Data Bank (HSDB)

12.1.9 Ongoing Test Status

The following link will take the user to the National Toxicology Program (NTP) Test Agent Search Results page, which tabulates all of the "Standard Toxicology & Carcinogenesis Studies", "Developmental Studies", and "Genetic Toxicity Studies" performed with this chemical. Clicking on the "Testing Status" link will take the user to the status (i.e., in review, in progress, in preparation, on test, completed, etc.) and results of all the studies that the NTP has done on this chemical.[Available from, as of February 5, 2014: http://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm?fuseaction=ntpsearch.searchresults&searchterm=7732-18-5]

▸ Hazardous Substances Data Bank (HSDB)

12.1.10 Populations at Special Risk

Exercise Associated Hyponatremia (EAH) is an occurrence of endurance sports that can cause severe clinical manifestations such as cerebral edema or respiratory failure. EAH is a dilutional hyponatremia, variant of SIADH, characterized by a plasma concentration of **sodium** lower than 135 mEq/L. Female gender and the duration of the competitions are associated with higher risk of hyponatremia. The incidence of hyponatremia, in fact, increases with duration, especially 4-8 hours after the start of the race. Women seem to be at greater risk than men. The pathophysiological mechanisms include increased loss of **sodium** through sweating and excessive intake of hypotonic fluids during and after the sporting event. In the genesis of EAH seems to have a decisive role the inadequate secretion of AVP by non osmotic stimuli, including IL-6. Indications for the prevention of hyponatremia include education of athletes for adequate consumption of fluids and monitoring of changes in body weight. Following the identification of electrolyte imbalance, the treatment requires a water restriction and infusion of hypertonic solutions 3%, especially in cases of severe hyponatremia.

PMID:23099986

Urso C et al; Clin Ter 163 (5): e349-56 (2012)

▸ **Hazardous Substances Data Bank (HSDB)**

Dilutional hyponatremia, although not uncommon, is an underestimated problem in the pediatric population. In most cases, it results from excessive hydration or water retention, also described as the so-called water intoxication. One of the most known causes is the use of **desmopressin** in enuretic children. This drug enhances the free water reabsorption in the renal collecting ducts.

PMID:20622630

Boetzkes S et al; Pediatr Emerg Care 26 (7): 503-5 (2010)

▸ **Hazardous Substances Data Bank (HSDB)**

12.2 Ecological Information

12.2.1 Natural Pollution Sources

Water is absolutely essential to all life. The protoplasm of most living cells contains about 80% water. Most of the earth's surface is covered with water(1). The most striking feature of the earth is the extensive hydrosphere, lacking from neighboring planets. 97.22% of earth's water is captured in oceans, with approximately 2% of water locked up in polar icecaps and glaciers. Water found in land, including surface and groundwater, makes up <1% of the earth's water resources. Groundwater represents more than 97% of the usable freshwater resources and is a

major source of replenishment for surface water. Water resources are renewable but finite and scarce. Only freshwater flowing through the solar-powered hydrological cycle is renewable(2).

(1) Camp TR; Water and Its Impurities. New York, NY: Reinhold Publishing Corp pp. 355 (1963) (2) Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

The most abundant gas typically released into the atmosphere from volcanic systems is water vapor, followed by **cabon dioxide** and **sulfur dioxide**. Locally **sulfur dioxide** gas can lead to acid rain and air pollution downwind from a volcano(1).

*(1) USGS; Volcanic Gases and Their Effects. Available from, as of May 28, 2014: **https://volcanoes.usgs.gov/hazards/gas/***

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.2 Artificial Pollution Sources

Household leaks can waste more than 1 trillion gallons annually in the US. Ten percent of homes in the USA have leaks that waste 90 gallons or more of water per day(1).

*(1) US EPA; Water Sense. Fix A Leak Week. Available from, as of Mar 14, 2014: **https://www.epa.gov/watersense/our_water/fix_a_leak.html***

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.3 Environmental Fate

Water which evaporates from the surface of oceans, fresh watercourses, and vegetation is carried in the air to be precipitated as rainfall or snow. The molecules of water vapor in air are pure water; falling raindrops formed by their condensation are saturated with **nitrogen**, **oxygen** and other atmospheric gases. During precipitation, raindrops entrain dust, smoke particles and fumes. Rain which falls on land surfaces runs over the ground to the nearest watercourse, carrying with it eroded soil, decaying vegetation, microorganisms and colloidal and suspended matter. The remainder of the rain seeps into soil and flows underground. Except in areas where groundwater is over-pumped, this water eventually flows out into an open watercourse. In its transit through topsoil, this water dissolves **carbon dioxide** which makes it more acid. With passage through ground and rocks, it dissolves many minerals such as **calcium**, **magnesium**, **iron** and **manganese**; also sulfates, silicates and chlorides(1).

(1) Camp TR; Water and Its Impurities. New York, NY: Reinhold Publishing Corp pp. 355 (1963)

▸ Hazardous Substances Data Bank (HSDB)

Natural water systems contain numerous minerals and often a gas phase ... The distribution of chemical species in waters is strongly influenced by an interaction of mixing cycles and biological cycles. ... The maintenance of life in aquatic ecosystems results directly or indirectly from the steady impact of solar energy. Photosynthesis is carried out mostly by algae and water plants; it may be conceived as a disproportionation of water into an **oxygen** reservoir and **hydrogen** which forms high energy bonds with **carbon**, **nitrogen**, **sulfur**, and **phosphorus** compounds that are incorporated as organic matter in the biomass. ... The composition of natural waters is strongly influenced by the growth, distribution, and decay of algae and other organisms. Organisms regulate the oceanic and lacustrine composition and its variation with depth. Dissolved constituents are taken up by organisms. Their remains sink under the influence of gravity and are gradually destroyed by oxidation. The superposition of this particular cycle upon the ordinary mixing cycle in the ocean or in lakes accounts for the variation in depth and distribution of chemical properties.

Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ Hazardous Substances Data Bank (HSDB)

12.2.4 Environmental Abiotic Degradation

Hydrogeochemical cycles couple atmosphere, land, and water. Natural waters acquire their chemical characteristics by dissolution and by chemical reactions with solids, liquids, and gases with which they have come into contact during the various parts of the hydrological cycle(1).

(1) Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ Hazardous Substances Data Bank (HSDB)

ACID RAIN: From the oxidation of **carbon**, **sulfur**, and **nitrogen** during the combustion of fossil fuels, there is a buildup in the atmosphere (gas phase, aerosol particles, raindrops, snowflakes, and fog) of CO2 and the oxides of sulfur and **nitrogen**, which leads to acid-base interaction(1). Snow and rain that are generated from atmospheres that contain high concentrations of combustion-generated **sulphur dioxide** can be very acidic(2).

(1) Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006 (2) Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ Hazardous Substances Data Bank (HSDB)

12.2.5 Environmental Water Concentrations

Freshwater is now scarce in many regions of the world, resulting in severe ecological degradation, limits on agriculture and industrial production, threats to human health, and increased potential for international conflict(1).

(1) Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

Representative dissolved heavy metals in natural waters(1).

Source	East coast US rivers
Copper, nM	17
Zinc, nM	13
Cadmium, nM	0.095
Lead, nM	0.11
Source	Mississippi
Copper, nM	23
Zinc, nM	3
Cadmium, nM	23
Source	Amazon River
Copper, nM	24
Zinc, nM	0.3-0.8
Cadmium, nM	0.06

Source
Lake Constance

Copper, nM
5-20

Zinc, nM
15-60

Cadmium, nM
0.05-0.1

Lead, nM
0.2-0.5

Source
Lake Michigan

Copper, nM
10

Zinc, nM
9

Cadmium, nM
0.17

Lead, nM
0.25

Source
Lago Cristallina (Swiss Alps, 2200 m altitude)

Copper, nM
5

Zinc, nM
30

Cadmium, nM
0.5

Lead, nM
3

Source
Pacific Ocean

Copper, nM
0.5-5

Zinc, nM

0.1-10

Cadmium, nM

0.01-1

Lead, nM

0.005-0.08

Source
rainwater (near Zurich Switzerland)

Copper, nM

10-300

Zinc, nM

80-900

Cadmium, nM

0.4-7

Lead, nM

10-200

(1) Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

Typical analyses of surface and groundwaters in the US. Author-defined categories are: Type A - water supplies of New York City (Catskills source), San Francisco and Oakland (Sierra Nevada Mtns), many rivers and lakes in New England. Type B - typified by the Great Lakes, with the exception of Lake Superior, supplying Chicago, Cleveland, Buffalo, etc in the St Lawrence River Basin. Type C - 30-60 ft deep wells supplying Dayton, OH(1).

Constituent, mg/L
SiO2

A

9.5

B

1.2

C

10

Constituent, mg/L
Fe(III)

A

0.07

B

0.02

C

0.09

Constituent, mg/L

CA2+

A

4.0

B

36

C

92

Constituent, mg/L

Mg2+

A

1.1

B

8.1

C

34

Constituent, mg/L

Na+

A

2.6

B

6.5

C

8.2

Constituent, mg/L

K+

A

0.6

B

1.2

C

1.4

Constituent, mg/L
HCO3-

A
18.3

B
119

C
339

Constituent, mg/L
SO4(2-)

A
1.6

B
22

C
84

Constituent, mg/L
CL-

A
2.0

B
13

C
9.6

Constituent, mg/L
NO3-

A
0.41

B
165

C
434

Constituent, mg/L
Total dissolved solids

A	34
B	165
C	434

Constituent, mg/L	Total hardness as CaCo3
A	14.6
B	123
C	369

(1) Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ **Hazardous Substances Data Bank (HSDB)**

RAIN/SNOW: Composition of snow and rain(1).

Table: Concentrations in mg/L

Constituent	SiO2
Snow, Lake Tahoe, Nov, 1958	0.0
Rain, Menlo Park, CA, Jan 1958	1.2; 0.3

Constituent	Al (III)
Snow, Lake Tahoe, Nov, 1958	0.01

Constituent	Ca(+2)
Snow, Lake Tahoe, Nov, 1958	0.0
Rain, NC & VA, Aug 1962- Jul 1963	

0.65

Rain, Menlo Park, CA, Jan 1958

1.2; 0.8

Rain, Belgium

3.3

Constituent

Mg(+2)

Snow, Lake Tahoe, Nov, 1958

0.2

Rain, NC & VA, Aug 1962- Jul 1963

0.14

Rain, Menlo Park, CA, Jan 1958

0.7; 1.2

Rain, Belgium

0.36

Constituent

Na(+)

Snow, Lake Tahoe, Nov, 1958

0.6

Rain, NC & VA, Aug 1962- Jul 1963

0.56

Rain, Menlo Park, CA, Jan 1958

0.0; 9.4

Rain, Belgium

0.97

Constituent

K(+)

Snow, Lake Tahoe, Nov, 1958

0.6

Rain, NC & VA, Aug 1962- Jul 1963

0.11

Rain, Menlo Park, CA, Jan 1958

0.0; 0.0

Rain, Belgium

0.23

Constituent
NH4(+)

Snow, Lake Tahoe, Nov, 1958
0.0

Rain, Belgium
0.42

Constituent
HCO3(-)

Snow, Lake Tahoe, Nov, 1958
3

Rain, Menlo Park, CA, Jan 1958
7; 4

Rain, Belgium
0.0

Constituent
SO4(-2)

Snow, Lake Tahoe, Nov, 1958
1.6

Rain, NC & VA, Aug 1962- Jul 1963
2.18

Rain, Menlo Park, CA, Jan 1958
0.7; 7.6

Rain, Belgium
6.1

Constituent
Cl(-)

Snow, Lake Tahoe, Nov, 1958
0.2

Rain, NC & VA, Aug 1962- Jul 1963
0.57

Rain, Menlo Park, CA, Jan 1958
0.8; 17

Rain, Belgium
2.0

Constituent

NO2(-)

Snow, Lake Tahoe, Nov, 1958

0.02

Rain, Menlo Park, CA, Jan 1958

0.0; 0.02

Constituent

NO3(-)

Snow, Lake Tahoe, Nov, 1958

0.1

Rain, NC & VA, Aug 1962- Jul 1963

0.62

Rain, Menlo Park, CA, Jan 1958

0.2; 0.0

Rain, Belgium

2.2

Constituent

Total dissolved solids

Snow, Lake Tahoe, Nov, 1958

4.8

Rain, Menlo Park, CA, Jan 1958

8.2; 38

Constituent

pH

Snow, Lake Tahoe, Nov, 1958

5.6

Rain, Menlo Park, CA, Jan 1958

6.4; 5.5

Rain, Belgium

4.4

(1) Snoeyink VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 463 (1980)

▸ **Hazardous Substances Data Bank (HSDB)**

SEAWATER: Composition(1).

Constituent

Na+

Seawater at Salinity = 35%

10.77

Residence time, logT, years

7.7

Constituent

Mg+2

Seawater at Salinity = 35%

1.29

Residence time, logT, years

7.0

Constituent

Ca+2

Seawater at Salinity = 35%

0.4121

Residence time, logT, years

5.9

Constituent

K+

Seawater at Salinity = 35%

0.399

Residence time, logT, years

6.7

Constituent

Sr+2

Seawater at Salinity = 35%

0.0079

Residence time, logT, years

6.6

Constituent

Cl-

Seawater at Salinity = 35%

19.354

Residence time, logT, years

7.9

Constituent
SO4(-2)

Seawater at Salinity = 35%
2.712

Residence time, logT, years
6.9

Constituent
HCO3(-)

Seawater at Salinity = 35%
0.1424

Residence time, logT, years
4.9

Constituent
Br-

Seawater at Salinity = 35%
0.0673

Residence time, logT, years
8

Constituent
F-

Seawater at Salinity = 35%
0.0013

Residence time, logT, years
5.7

Constituent
B

Seawater at Salinity = 35%
0.0045

Residence time, logT, years
7.0

(1) Morgan JJ et al; Kirk-Othmer Encyclopedia of Chemical Technology. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 16 Jun 2006

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.6 Effluent Concentrations

Stormwater runoff carries urban pollution into rivers and lakes(1,2). Stormwater runoff is generated when rain and snowmelt do not soak into the ground but flow over land or impervious surfaces such as streets, parking lots, and building rooftops, accumulating debris, chemicals, sediment or other pollutants that could adversely affect water quality if the runoff is discharged untreated(1). Agriculture is the leading source of impairment to freshwater sources in the US. When excess fertilizer washes into rivers and lakes it causes algal blooms that lead to taste and health problems. **Nitrogen**-laden waters can also damage aquatic life leading to the formation of "dead zones"(2).

(1) US EPA; Waters By Type. Available from, as of Mar 13, 2014: ***https://water.epa.gov/type*** *(2) Nature Conservancy; Why is Our Water in Trouble? Threats to Freshwater Ecosystems. Available from, as of Mar 13, 2014:* ***https://www.nature.org/ourinitiatives/habitats/riverslakes/threatsimpacts/index.htm***

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.7 Sediment / Soil Concentrations

Wetlands are part of the foundation of water resources and are vital to the health of waterways and communities downstream. Wetlands feed downstream waters, trap floodwaters, recharge groundwater supplies, filter pollution, and provide fish and wildlife habitat. Wetlands include swamps, marshes and bogs. Wetlands also reduce flood risks(1). Forests, grasslands, wetlands, and flood plains stabilize water flow into rivers, lakes, and groundwater(2).

(1) US EPA; Waters By Type. Available from, as of Mar 13, 2014: ***https://water.epa.gov/type*** *(2) Nature Conservancy; Why is Our Water in Trouble? Threats to Freshwater Ecosystems. Available from, as of Mar 13, 2014:* ***https://www.nature.org/ourinitiatives/habitats/riverslakes/threatsimpacts/index.htm***

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.8 Plant Concentrations

The top 40 plants containing water(1).

Genus species
Aloe vera

Common name
Aloe

Part
Plant

Concn (ppm)
995,000

Genus species
Lycopersicon esculentum

Common name
Tomato

Part
Fruit

Concn (ppm)
982,000

Genus species
Amorphophallus knojac

Common name
Leopard Palm

Part
Leaf

Concn (ppm)
974,000

Genus species
Phaseolus lunatus

Common name
Lima Bean

Part
Leaf

Concn (ppm)
972,000

Genus species
Cucumis cativus

Common name
Cucumber

Part
Fruit

Concn (ppm)
971,000

Genus species

Lactuca sativa

Common name

Lettuce

Part

Leaf

Concn (ppm)

971,000

Genus species

Prunus persica

Common name

Peach

Part

Fruit

Concn (ppm)

964,000

Genus species

Prunus armeniaca

Common name

Apricot

Part

Fruit

Concn (ppm)

963,500

Genus species

Lagenaria siceraria

Common name

Calabash Gourd

Part

Fruit

Concn (ppm)

963,000

Genus species

Benincasa hispida

Common name

Waxgourd

Part
Fruit

Concn (ppm)
962,000

Genus species
Citrullus lanatus

Common name
Watermelon

Part
Fruit

Concn (ppm)
957,000

Genus species
Brassica chinensis

Common name
Bok-Choy

Part
Leaf

Concn (ppm)
956,400

Genus species
Brassica pekinensis

Common name
Chinese Cabbage

Part
Leaf

Concn (ppm)
954,000

Genus species
Aralia cordata

Common name
Udo

Part
Leaf

Concn (ppm)

953,000

Genus species
Opuntia ficus-indica

Common name
Indian Fig

Part
Bud

Concn (ppm)
962,600

Genus species
Cichorium intybus

Common name
Chicory

Part
Leaf

Concn (ppm)
951,000

Genus species
Nasturtium officinale

Common name
Watercress

Part
Herb

Concn (ppm)
951,000

Genus species
Asparagus officinalis

Common name
Asparagus

Part
Plant

Concn (ppm)
950,000

Genus species
Brassica oleracea var capitata var capitata

Common name
Red Cabbage

Part
Leaf

Concn (ppm)
950,000

Genus species
Luffa aegyptiaca

Common name
Luffa

Part
Fruit

Concn (ppm)
950,000

Genus species
Portulaca oleracea

Common name
Purslane

Part
Herb

Concn (ppm)
950,000

Genus species
Rheum rhabararum

Common name
Rhubarb

Part
Leaf; Stem

Concn (ppm)
950,000; 950,000

Genus species
Apium graveolens

Common name
Celery

Part

Petiole

Concn (ppm)

947,000

Genus species

Trichosanthes anguina

Common name

Snakegourd

Part

Fruit

Concn (ppm)

946,000

Genus species

Brassica oleacea var gemmifera var gemmifera

Common name

Brussel-Sprout

Part

Leaf

Concn (ppm)

945,500

Genus species

Brassica oleracea var viridis

Common name

Collards

Part

Leaf

Concn (ppm)

945,500

Genus species

Cylanthera pedata

Common name

Achocha

Part

Fruit

Concn (ppm)

945,000

Genus species
Petasites japonicus

Common name
Butterbur

Part
Petiole

Concn (ppm)
945,000

Genus species
Raphanus sativus

Common name
Radish

Part
Root

Concn (ppm)
945,000

Genus species
Pasiflora quadrangularis

Common name
Granadilla

Part
Fruit

Concn (ppm)
944,000

Genus species
Cichorium endivia

Common name
Endive

Part
Leaf

Concn (ppm)
943,800

Genus species
Phaseolus vulgaris subsp var vulgaris

Common name

Green Bean

Part

Fruit

Concn (ppm)

942,000

Genus species

Luffa aegyptiaca

Common name

Luffa

Part

Leaf

Concn (ppm)

940,000

Genus species

Tetragonia tetragonioides

Common name

New Zealand Spinach

Part

Leaf

Concn (ppm)

940,00

Genus species

Cucumis melo subsp ssp melo var cantalupensis

Common name

Cantaloupe

Part

Fruit

Concn (ppm)

938,000

Genus species

Capsicum annuum

Common name

Bell Pepper

Part

Fruit

Concn (ppm)
937,000

Genus species
Equisetum arvense

Common name
Horsetail

Part
Plant

Concn (ppm)
937,000

Genus species
Cucurbita spp

Common name
Summer Squash

Part
Fruit

Concn (ppm)
936,800

Genus species
Chrysanthemum coronarium

Common name
Garland Chrysanthemum

Part
Leaf

Concn (ppm)
935,000

Genus species
Momordica charantia

Common name
Bitter Melon

Part
Fruit

Concn (ppm)
934,000

Genus species

Brassica nigra

Common name

Black Mustard

Part

Leaf

Concn (ppm)

933,900

(1) USDA; Dr. Duke's Phytochemical and Ethnobotanical Databases. Plants with a chosen chemical. Water. Washington, DC: US Dept Agric, Agric Res Service. Available from, as of Feb 27, 2014: ***https://www.ars-grin.gov/duke/***

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.9 Other Environmental Concentrations

On an annual average, the earth's 149X10+6 sq km of dry land receives 745 mm of precipitation (111,000 cu km), of which 477 mm (71, 000 cu km) evaporates from the land and 40,000 cu km flows into the sea.

Weingartner H et al; Water, 1. Properties, Analysis and Hydrological cycle. Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (1999-2014). New York, NY: John Wiley & Sons. Online Posting Date: 15 Oct 2011

▸ **Hazardous Substances Data Bank (HSDB)**

12.2.10 Probable Routes of Human Exposure

Everything lives in a watershed - the area that drains to a common waterway, such as a stream, lake, estuary, wetland, aquifer, and ocean - and personal actions can directly affect a watershed.

(1) US EPA; Waters By Type. Available from, as of Mar 13, 2014: ***https://water.epa.gov/type***

▸ **Hazardous Substances Data Bank (HSDB)**

13 Associated Disorders and Diseases

7 items

Search

Disease
Death

Evidence Type
therapeutic

Evidence PMID
33901602

Disease
Brain Edema

Evidence Type
marker/mechanism

Page 1 of 2

▸ Comparative Toxicogenomics Database (CTD)

1 item

Indication
Solid tumour/cancer

ICD-11 Code
2A00-2F97

▸ Therapeutic Target Database (TTD)

14 Literature

14.1 Consolidated References

198,487 items

Search

SORT BY Publication Date - Most Recent

Screening, biochemical characterization and antibiotics resistance/susceptibility of bacteria isolated from native soil and water samples

Publication Name: Brazilian journal of biology = Revista brasleira de biologia
Publication Date: 2024
PMID: 35352774
DOI: 10.1590/1519-6984.254016

Pre-germination treatments of melon seeds for the production of seedlings irrigated with biosaline water

Publication Name: Brazilian journal of biology = Revista brasleira de biologia
Publication Date: 2024
PMID: 35043840
DOI: 10.1590/1519-6984.257314

Distribution and diversity of aquatic insects in different water bodies of Qatar

Publication Name: Brazilian journal of biology = Revista brasleira de biologia
Publication Date: 2024
PMID: 35293543
DOI: 10.1590/1519-6984.255950

Salt stress and organic fertilization on the growth and biochemical metabolism of Hylocereus costaricensis (red pitaya) seedlings

Publication Name: Brazilian journal of biology = Revista brasleira de biologia
Publication Date: 2024
PMID: 35613211
DOI: 10.1590/1519-6984.258476

Antibacterial effect of Asphodelus fistulosus aqueous and ethanolic crude extracts on gram positive

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PubChem

14.2 NLM Curated PubMed Citations

All NLM Curated PubMed Citations

administration and dosage
adverse effects
analysis
antagonists and inhibitors
biosynthesis
cerebrospinal fluid
chemistry
deficiency
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economics
immunology
isolation and purification
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pharmacology
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radiation effects
standards
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14.3 Thieme References

2,014 items

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Brønsted Acid Mediated Synthesis of 1,4-Dioxanes
DOI: 10.1055/s-0041-1738419
Publication Date: 2022
Publication Name: Synfacts

One-Pot Synthesis of 1,2,3-Triazole-Fused Polycyclic Systems via Sequential Annulation of 1,n-Enynes with Tosyl Azide
DOI: 10.1055/a-1892-0253
Publication Date: 2022
Publication Name: Synthesis

Copper(II)-Catalyzed[3+2]Annulation of Thioamides with AIBN: Facile Access to Highly Functionalized Thiazolidin-4-ones
DOI: 10.1055/a-1693-7535
Publication Date: 2022
Publication Name: Synthesis

Modern Synthesis and Chemistry of Stabilized Ketene N,O-Acetals
DOI: 10.1055/a-1713-8481
Publication Date: 2022
Publication Name: Synthesis

Photocatalytic Approach to α,α-Difluoroalkyl Alcohols
DOI: 10.1055/s-0041-1737546
Publication Date: 2022
Publication Name: Synthesis

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Thieme Chemistry

14.4 Wiley References

56 items

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Immobilization of a vanadium complex onto functionalized nanoporous MCM-41 and its application as a catalyst for the solvent-free chemoselective oxidation of sulfide to sulfoxide
DOI: 10.1002/aoc.3422
Publication Date: 2016
Publication Name: Appl. Organometal. Chem.

Polysiloxane microspheres functionalized with imidazole groups as a palladium catalyst support
DOI: 10.1002/aoc.3446
Publication Date: 2016
Publication Name: Appl. Organometal. Chem.

Nano-MoO3-modified MCM-22 for methane dehydroaromatization
DOI: 10.1002/aoc.3345
Publication Date: 2015
Publication Name: Appl. Organometal. Chem.

Solid-Phase Approach for the Synthesis of 2-Amido-1,3,4-oxadiazoles
DOI: 10.1002/jhet.1983
Publication Date: 2015
Publication Name: J. Heterocyclic Chem.

Synthesis and Chemical Reactivity of 4-Oxo-4H-1-benzopyran-3-carboxaldehyde
DOI: 10.1002/jhet.2001
Publication Date: 2014
Publication Name: Journal of Heterocyclic Chemistry

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Wiley

14.5 Depositor Provided PubMed Citations

30,216 items

Search

SORT BY Publication Date - Most Recent

Per- and polyfluoroalkyl substances (PFAS) inhibit cytochrome P450 CYP3A7 through direct coordination to the heme iron and water displacement

PMID: 36638633

Publication Date: 2023-03-01

Journal: Journal of inorganic biochemistry

Mitigating effect of L-carnitine against atrazine-induced hepatotoxicity: histopathological and biochemical analyses in albino rats

PMID: 36282381

Publication Date: 2023-02-01

Journal: Environmental science and pollution research international

Perfluorooctanoic acid (PFOA) promotes follicular growth and alters expression of genes that regulate the cell cycle and the Hippo pathway in cultured neonatal mouse ovaries

PMID: 36152675

Publication Date: 2022-11-01

Journal: Toxicology and applied pharmacology

Lycopene alleviates di(2-ethylhexyl) phthalate-induced splenic injury by activating P62-Keap1-NRF2 signaling

PMID: 35917956

Publication Date: 2022-10-01

Journal: Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association

The effects of oil sands process-affected water naphthenic acid fraction components on GDF15 secretion in extravillous trophoblast cells

PMID: 35259347

Publication Date: 2022-04-15

Journal: Toxicology and applied pharmacology

Page 1 of 6,044

PubChem

14.6 Chemical Co-Occurrences in Literature

Showing 3 of 25 View More

Chemical

Activated Charcoal

CID 5462310

Selected evidence

51,700 articles

View All

Alternatives to water oxidation in the photocatalytic water splitting reaction for solar hydrogen production

PMID 36938953; DOI 10.1039/d3nr00260h; Nanoscale 2023 Apr; 15(14):6521-6535 (Review Article)

Name matches: **carbon** *water*

A Review on Graphene (GN) and Graphene Oxide (GO) Based Biodegradable Polymer Composites and Their Usage as Selective Adsorbents for Heavy Metals in Water

PMID 36984407; DOI 10.3390/ma16062527; Materials (Basel, Switzerland) 2023 Mar; 16(6): (Review Article)

Name matches: **graphene** *water*

Bisphenols in water: Occurrence, effects, and mitigation strategies

PMID 37004822; DOI 10.1016/j.chemosphere.2023.138560; Chemosphere 2023 Mar; 328(?):138560 (Review Article)

Name matches: **carbon** *water*

Chemical

Oxygen

CID 977

Selected evidence

42,376 articles

View All

Recent Advances of Transition Metal Basic Salts for Electrocatalytic Oxygen Evolution Reaction and Overall Water Electrolysis

PMID 36862225; DOI 10.1007/s40820-023-01038-0; Nano-micro letters 2023 Mar; 15(1):57 (Review Article)

Name matches: **oxygen** *water*

Research on engineered electrocatalysts for efficient water splitting: a comprehensive review

PMID 36928479; DOI 10.1039/d2cp05522h; Physical chemistry chemical physics : PCCP 2023 Mar; 25(13):8992-9019 (Review Article)
Name matches: **oxygen** *water*

Trends in removal of pharmaceuticals in contaminated water using waste coffee and tea-based materials with their derivatives

PMID 36973862; DOI 10.1002/wer.10857; Water environment research : a research publication of the Water Environment Federation 2023 Mar; ?(?):e10857 (Review Article)
Name matches: **oxygen** *water*

Chemical

Sodium Chloride

CID 5234

Selected evidence

33,581 articles

View All

Salt and Water: A Review of Hypernatremia

PMID 36868726; DOI 10.1053/j.akdh.2022.12.010; Advances in kidney disease and health 2023 Mar; 30(2):102-109 (Review Article)
Name matches: **salt** *water*

Tailoring properties and performance of thin-film composite membranes by salt additives for water treatment: A critical review

PMID 36889093; DOI 10.1016/j.watres.2023.119821; Water research 2023 May; 234(?):119821 (Review Article)
Name matches: **salt** *water*

Pharmaceutical Methods for Enhancing the Dissolution of Poorly Water-Soluble Drugs

PMID 36917562; DOI 10.1089/adt.2022.119; Assay and drug development technologies 2023 Feb; 21(2):65-79 (Review Article)
Name matches: **salt** *water*

▸ **PubChem**

14.7 Chemical-Gene Co-Occurrences in Literature

Showing 3 of 100 View More

Gene/Protein/Enzyme

EC:1.15.1.1

Selected evidence

6,821 articles
View All

Plasma-Activated Water for Food Safety and Quality: A Review of Recent Developments
PMID 35682216; DOI 10.3390/ijerph19116630; International journal of environmental research and public health 2022 05; 19(11): (Review Article)
Name matches: **superoxide dismutase** *water*

Synergistic anticancer effects of crocin combined with deuterium-depleted water on HT-29 cells
PMID 36847076; DOI 10.1097/cad.0000000000001512; Anti-cancer drugs 2023 Feb; ?(?):
Name matches: **superoxide dismutase** *water*

[Gastroprotective and antidepressant-like effect of plum pectin (Prunus domestica L.) under water-immobilization stress in laboratory mice]
PMID 36883536; DOI 10.33029/0042-8833-2023-92-1-16-25; Voprosy pitaniia 2023; 92(1):16-25
Name matches: **superoxide dismutase** *water*

Gene/Protein/Enzyme

cat

Selected evidence

6,332 articles
View All

A subcritical water extract of soil grown Zingiber officinale Roscoe: Comparative analysis of antioxidant and anti-inflammatory effects and evaluation of bioactive metabolites
PMID 36843947; DOI 10.3389/fphar.2023.1006265; Frontiers in pharmacology 2023; 14(?):1006265
Name matches: **catalase** *water*

Synergistic anticancer effects of crocin combined with deuterium-depleted water on HT-29 cells
PMID 36847076; DOI 10.1097/cad.0000000000001512; Anti-cancer drugs 2023 Feb; ?(?):
Name matches: **catalase** *water*

Implications of atrazine concentrations in drinking water from Ijebu-North, Southwest Nigeria on the hypothalamic-pituitary-adrenal axis
PMID 36847489; DOI 10.1080/01480545.2023.2180025; Drug and chemical toxicology 2023 Feb; ?(?):1-9
Name matches: **catalase** *water*

Gene/Protein/Enzyme

avp

Selected evidence

4,642 articles
View All

Glucocorticoids and Water Balance: Implications for Hyponatremia Management and Pituitary Surgery
PMID 37062279; DOI 10.1159/000530701; Neuroendocrinology 2023 Apr; ?(?): (Review Article)
Name matches: **arginine vasopressin** *water*

Hyponatraemia and hypernatraemia: Disorders of Water Balance in Neurosurgery
PMID 33389341; DOI 10.1007/s10143-020-01450-9; Neurosurgical review 2021 Oct; 44(5):2433-2458 (Review Article)
Name matches: **antidiuretic hormone; arginine vasopressin** *water*

Activation of AQP2 water channels by protein kinase A: therapeutic strategies for congenital nephrogenic diabetes insipidus
PMID 34224008; DOI 10.1007/s10157-021-02108-6; Clinical and experimental nephrology 2021 Oct; 25(10):1051-1056 (Review Article)
Name matches: **antidiuretic hormone** *water*

PubChem

14.8 Chemical-Disease Co-Occurrences in Literature

Showing 3 of 25 View More

Disease

Drug-Related Side Effects and Adverse Reactions

Selected evidence

39,891 articles
View All

A Current Review of Water Pollutants in American Continent: Trends and Perspectives in Detection, Health Risks, and Treatment Technologies
PMID 36901509; DOI 10.3390/ijerph20054499; International journal of environmental research and public health 2023 Mar; 20(5): (Review Article)
Name matches: **toxicity** *water*

Toxicological aspect of water treated by chlorine-based advanced oxidation processes: A review
PMID 36958544; DOI 10.1016/j.scitotenv.2023.163047; The Science of the total environment 2023 Mar; 878(?):163047 (Review Article)
Name matches: **toxicity** *water*

Bisphenols in water: Occurrence, effects, and mitigation strategies
PMID 37004822; DOI 10.1016/j.chemosphere.2023.138560; Chemosphere 2023 Mar; 328(?):138560 (Review Article)
Name matches: **toxicity** *water*

Disease

Infections

Selected evidence

28,859 articles

View All

Enteric pathogen reduction targets for onsite non-potable water systems: A critical evaluation

PMID 36848851; DOI 10.1016/j.watres.2023.119742; Water research 2023 Feb; 233(?):119742 (Review Article)

Name matches: **infections** *water*

A meta-analysis on the distribution of pathogenic Vibrio species in water sources and wastewater in Africa

PMID 37028683; DOI 10.1016/j.scitotenv.2023.163332; The Science of the total environment 2023 Apr; ?(?):163332 (Review Article)

Name matches: **infections** *water*

Biosecurity and water, sanitation, and hygiene (WASH) interventions in animal agricultural settings for reducing infection burden, antibiotic use, and antibiotic resistance: a One Health systematic review

PMID 37164518; DOI 10.1016/s2542-5196(23)00049-9; The Lancet. Planetary health 2023 05; 7(5):e418-e434 (Review Article)

Name matches: **infection; infections** *water*

Disease

Edema

Selected evidence

16,157 articles

View All

Water-Resistant Conductive gels toward Underwater Wearable Sensing

PMID 36857417; DOI 10.1002/adma.202211758; Advanced materials (Deerfield Beach, Fla.) 2023 Mar; ?(?):e2211758 (Review Article)

Name matches: **swelling** *water*

Ethnomedicinal uses, phytochemistry, and pharmacological relevance of Justicia procumbens (Oriental Water Willow) - A promising traditional plant

PMID 37385576; DOI 10.1016/j.jep.2023.116819; Journal of ethnopharmacology 2023 Jun; 317(?):116819 (Review Article)

Name matches: **edema** *water*

Review of net water uptake in the management of acute ischemic stroke

PMID 35278122; DOI 10.1007/s00330-022-08658-x; European radiology 2022 Aug; 32(8):5517-5524 (Review Article)

Name matches: **edema** *water*

▸ PubChem

15 Patents

US9034300
US9259494
US9849199
US7316997
US7144577
US5861379
US8314066
US8435945
US7881777
US6915154
US8647605
US9421280
US8406860
US8892190
US8185176
US10631746

▸ DrugBank

15.1 Depositor-Supplied Patent Identifiers

20 items

Search

SORT BY Priority Date - Most Recent

Quantification of absolute blood flow in tissue using fluorescence-mediated photoplethysmography
Publication Number: US-10631746-B2
Priority Date: 2014-10-09
Grant Date: 2020-04-28

Method for treating local infection
Publication Number: US-2015045720-A1
Priority Date: 2013-08-08

Composition and method for medical imaging of body cavities
Publication Number: US-9034300-B2
Priority Date: 2009-10-16
Grant Date: 2015-05-19

Composition and method for medical imaging of body cavities

Publication Number: US-9259494-B2

Priority Date: 2009-10-16

Grant Date: 2016-02-16

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PubChem

Link to all deposited patent identifiers

PubChem

15.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=XLYOFNOQVPJJNP-UHFFFAOYSA-N

PATENTSCOPE (WIPO)

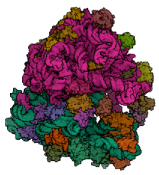
16 Interactions and Pathways

16.1 Protein Bound 3D Structures

159 items

Search

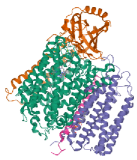
SORT BY Resolution - Increasing



70S ribosome from Staphylococcus aureus

PDB Code: 5LI0

Resolution: 0 Å



Cytochrome c oxidase structure in F-state

PDB Code: 7AU3

Resolution: 0 Å

Structure image

The 1.52 angstrom CryoEM structure of the [NiFe]-hydrogenase Huc from Mycobacterium smegmatis - catalytic dimer (Huc2S2L)

Page 1 of 32

▸ RCSB Protein Data Bank (RCSB PDB)

View 434 proteins in NCBI Structure

▸ PubChem

16.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code
HOH

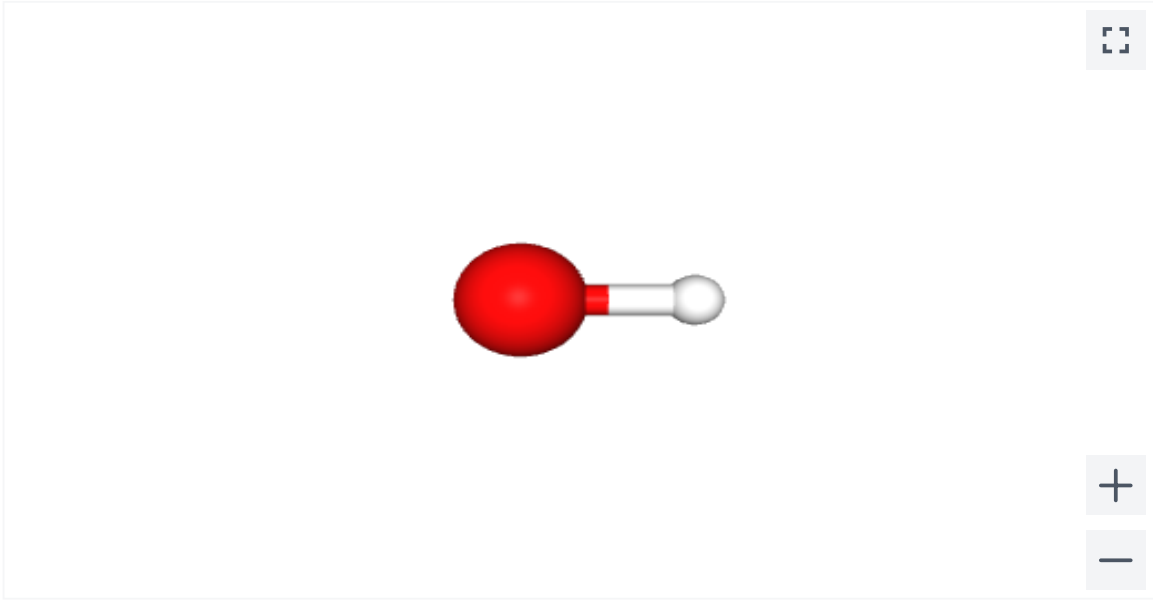
PDBe Structure Code
1NHE

PDBe Conformer

Interactive Chemical Structure Model

Ball and Stick | Sticks | Wire-Frame | Space-Filling

Show Hydrogens | Animate



▸ Protein Data Bank in Europe (PDBe)

16.2 Chemical-Target Interactions

101 items

Search

SORT BY Data Source - A to Z

Structure

Gene

AHR

Taxonomy

Homo sapiens (human)

Action

Mineral waters results in increased activity of AHR protein

Evidence IDs

PMID:22490669

Data Source

Comparative Toxicogenomics Database (CTD)

Structure

Gene

CYP1A1

Taxonomy

Homo sapiens (human)

Action

Mineral waters results in increased expression of CYP1A1 mRNA

Evidence IDs

PMID:22490669

Page 1 of 21

▸ Comparative Toxicogenomics Database (CTD)

16.3 Pathways

71,291 items

Search

SORT BY Taxonomy - A to Z

pseudouridine degradation
Source: PlantCyc
External ID: PWY-6019
Taxonomy: Aquilegia coerulea

phospholipid remodeling (phosphatidylcholine, yeast)
Source: PlantCyc
External ID: PWY-7416
Taxonomy: Aquilegia coerulea

ACP metab

Source: PlantCyc
External ID: PWY-6012
Taxonomy: Aquilegia coerulea

L-ascorbate degradation V
Source: PlantCyc
External ID: PWY-6959
Taxonomy: Aquilegia coerulea

Page 1 of 14,259

PubChem

17 Biological Test Results

17.1 BioAssay Results

1,575 items

Search

SORT BY Activity Value - Increasing

NCI In Vivo Anticancer Drug Screen. Data for tumor model Lewis Lung Carcinoma (subcutaneous) in B6D2F1 (BDF1) mice

Activity: Inactive

BioAssay AID: 270
Substance SID: 429743
Compound CID: 962

NCI In Vivo Anticancer Drug Screen. Data for tumor model Lewis Lung Carcinoma (subcutaneous) in B6D2F1 (BDF1) mice

Activity: Inactive

BioAssay AID: 270
Substance SID: 429743
Compound CID: 962

NCI In Vivo Anticancer Drug Screen. Data for tumor model Lewis Lung Carcinoma (subcutaneous) in B6D2F1 (BDF1) mice

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▸ PubChem

18 Taxonomy

2 items

Structure

Taxonomy
Homo sapiens (human)

Data Source
Human Metabolome Database (HMDB)

Structure

▸ E. coli Metabolome Database (ECMDB)

19 Classification

19.1 MeSH Tree

1 item View in Classification Browser

MeSH Tree > Chemicals and Drugs Category > Inorganic Chemicals > Electrolytes > Ions > Anions

Water

A clear, odorless, tasteless liquid that is essential for most animal and plant life and is an excellent solvent for many substances. The chemical formula is hydrogen oxide (H2O). (McGraw-Hill Dictionary of Scientific and Technical Terms,

▸ Medical Subject Headings (MeSH)

19.2 NCI Thesaurus Tree

1 item View in Classification Browser

NCI Thesaurus Tree > Drug, Food, Chemical or Biomedical Material > Food or Food Product > Food Component

Water

H2O, a clear, colorless, odorless, tasteless liquid that freezes into ice below 0 degrees centigrade and boils above 100 degrees centigrade

▸ NCI Thesaurus (NCIt)

19.3 ChEBI Ontology

2 items View in Classification Browser

ChEBI Ontology > chemical entity > molecular entity > inorganic molecular entity > inorganic hydride > chalcogen hydride

water

An oxygen hydride consisting of an oxygen atom that is covalently bonded to two hydrogen atoms

ChEBI Ontology > chemical entity > atom > main group element atom > p-block element atom

oxygen atom

▸ ChEBI

19.4 KEGG: Drug

1 item View in Classification Browser

Therapeutic category of drugs in Japan > 7 Agents not mainly for therapeutic purpose > 71 Dispensing medicines > 713 Solvents

Water (JP18/USP); Purified water (JP18); Purified water in containers (JP18); Water, purified (USP); Sterile purified water in containers (JP18); Water for injection (JP18); Water for injection in

▸ KEGG

19.5 KEGG: JP15

1 item View in Classification Browser

Drugs listed in the Japanese Pharmacopoeia

Water

KEGG

19.6 KEGG: Risk Category of Japanese OTC Drugs

1 item View in Classification Browser

Risk category of Japanese OTC drugs > Third-class OTC drugs > Inorganic and organic chemicals

Water (JP18/USP)

KEGG

19.7 EPA Safer Choice

2 items View in Classification Browser

Solvents

EPA Safer Chemical Ingredients Classification

Solvents

EPA Safer Choice

19.8 ChemIDplus

47 items View in Classification Browser

ChemIDplus Chemical Information Classification

CCRIS

Chemical Carcinogenesis Research Information System - Carcinogenicity, mutagenicity, tumor promotion and tumor inhibition data from the National Cancer Institute (NCI). CCRIS provides historical information from the years 1985 - 2011. It is no longer updated.

ChemIDplus Chemical Information Classification

CGB

Coast Guard Bulk Hazardous Materials - Coast Guard Bulk Hazardous Materials.Hazardous Materials Standards Division, Coast Guard, U.S. Department of Homeland Security

ChemIDplus Chemical Information Classification

CTD

Comparative Toxicogenomics Database - CTD selects and organizes gene, sequence, chemical, reference, and taxonomic data about gene-chemical interactions. It is hosted at North Carolina State University (NCSU).

ChemIDplus Chemical Information Classification

ChEBI

Chemical Entities of Biological Interest - Dictionary of molecular entities focused on "small" chemical compounds. ChEBI is part of the EMBL-European Bioinformatics Institute.

ChemIDplus Chemical Information Classification

ClinicalTrials.gov

ClinicalTrials.gov - ClinicalTrials.gov offers up-to-date information for locating federally and privately supported clinical trials for a wide range of diseases and conditions

Page 1 of 10

▸ ChemIDplus

19.9 CAMEO Chemicals

1 item View in Classification Browser

Water and Aqueous Solutions

Reactive group: Water and Aqueous Solutions

▸ CAMEO Chemicals

19.10 UN GHS Classification

1 item View in Classification Browser

Not Classified

No hazards have been classified (by majority companies[ECHA] or information source

▸ UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

19.11 EPA CPDat Classification

329 items View in Classification Browser

EPA CPDat Classification > Functional Use
adhesion/cohesion promoter

EPA CPDat Classification > Functional Use
anticaking agent

EPA CPDat Classification > Functional Use
binder

EPA CPDat Classification > Functional Use
chelating agent

EPA CPDat Classification > Functional Use
cleaning agent

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▸ EPA Chemical and Products Database (CPDat)

19.12 NORMAN Suspect List Exchange Classification

36 items View in Classification Browser

NORMAN Suspect List Exchange Classification
Solvent

S32 | REACH2017 | 2017 List of REACH Chemicals

A 2017 list of REACH chemicals including InChIKeys and spectral information, provided by N. Alygizakis and J. Slobodnik, EI. Dataset DOI:10.5281/zenodo.2653020

S74 | REFTPS | Transformation Products and Reactions from Literature

This dataset is designed to provide an entry point for users to contribute transformation products and reactions documented in the literature for addition to the NORMAN SLE and PubChem Transformations section. Dataset DOI:10.5281/zenodo.4318838

S77 | FCCDB | Food Contact Chemicals Database v5.0

The Food Contact Chemicals database (FCCdb, DOI:10.5281/zenodo.3240108) is a compilation of information on over 12,000 intentionally added food contact chemicals extracted from publicly available sources such as legislation or industry inventories for different types of food contact materials and selected sources of hazard information, as described by Groh et al. 2021 (see DOI:10.1016/j.envint.2020.106225). Structural information for ~6000 entries where clear mappings could be found was added by P. Chirsir into FCCdb Version 5, prior to hosting it on the NORMAN Suspect List Exchange (see Dataset DOI:10.5281/zenodo.4625495). Further detailed descriptions for each sub-category in the classification tree can be found in the ReadMe tab of the FCCdb spreadsheet file, or in the respective sub-category tooltips ('?' boxes).

S37 | LITMINEDNEURO | Neurotoxicants from literature mining PubMed

A list of chemicals associated with neurotoxicity compiled through systematic literature mining of PubMed using MeSH

Page 1 of 8

▸ NORMAN Suspect List Exchange

19.13 EPA DSSTox Classification

51 items View in Classification Browser

CompTox Chemicals Dashboard Chemical Lists

[ACSREAG] LIST: ACS Reagent Chemicals

Short_Description: The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials.

Long_Description: The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials. These specifications have become the de facto standards for chemicals used in many high-purity applications. In addition to detailing these specifications, ACS Reagent Chemicals provides general physical properties and analytical uses for all reagent chemicals as well as guidelines for standard analytical methods. The online book is available at https://pubs.acs.org/isbn/9780841230460

CompTox Chemicals Dashboard Chemical Lists

[BLOODEXPOSOME] LIST: BLOODEXPOSOME Chemicals identified as part of the blood exposome

Short_Description: Chemicals identified as part of the blood exposome

Long_Description: Barupal et al report on Generating the Blood Exposome Database Using a Comprehensive Text Mining and Database Fusion Approach. The database can be used for prioritizing chemicals for systematic reviews, developing target assays in exposome research, identifying compounds in untargeted mass spectrometry, and biological interpretation in metabolomics data. (Last remapped February 17th 2023)

CompTox Chemicals Dashboard Chemical Lists

[CALWATERBDS] WATER: California Water Boards Additive Information

Short_Description: California Central Valley water board oil field additive constituents list

Long_Description: California Central Valley water board oil field additive constituents list (Additive Information Updated June 2018)

CompTox Chemicals Dashboard Chemical Lists

[CANADADSL] Canadian Domestic Substances List 2019

Short_Description: The domestic substances list (DSL) is the sole standard against which a substance is judged to be"new"to Canada.

Long_Description: On May 4, 1994, Environment and Climate Change Canada published the domestic substances list (DSL) in Part II of the Canada Gazette. The DSL is an inventory of approximately 23 000 substances manufactured in, imported into or used in Canada on a commercial scale. It is based on substances present in Canada, under certain conditions, between January 1, 1984 and December 31, 1986. The DSL is the sole standard against which a substance is judged to be"new"to Canada. With few exemptions, all substances not on this list are considered new and must be reported prior to importation or manufacture in order that they can be assessed to determine if they are toxic or could become toxic to the environment or human health.

CompTox Chemicals Dashboard Chemical Lists

[CIGARETTES] TOBACCO|SMOKING|WIKILIST: Additives in cigarettes

Short_Description: This is a partial list of the 599 additives in cigarettes submitted to the United States Department of Health and Human Services in April 1994.

Long_Description: This is a partial list of the 599 additives in cigarettes submitted to the United States Department of Health and Human Services in April 1994. It applies, as documented, only to American manufactured cigarettes

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▸ EPA DSSTox

19.14 Consumer Product Information Database Classification

10 items View in Classification Browser

- Auto Products
- Commercial / Institutional
- Hobby/Craft
- Home Maintenance
- Home Office

Page 1 of 2

▸ Consumer Product Information Database (CPID)

19.15 LOTUS Tree

2 items View in Classification Browser

LOTUS Tree > Chemical Tree > Shikimates and Phenylpropanoids
Aminoacids

LOTUS Tree > Chemical Tree > Amino acids and Peptides
Aminoacids

▸ LOTUS - the natural products occurrence database

19.16 FDA Drug Type and Pharmacologic Classification

5 items View in Classification Browser

FDA Drug Type and Pharmacologic Classification
HUMAN OTC DRUG

FDA Drug Type and Pharmacologic Classification > Pharmacologic Class
Blood Coagulation Factor [EPC]

FDA Drug Type and Pharmacologic Classification > Pharmacologic Class
Calcium [CS]

FDA Drug Type and Pharmacologic Classification > Pharmacologic Class
Cations, Divalent [CS]

FDA Drug Type and Pharmacologic Classification > Pharmacologic Class
Increased Coagulation Factor Activity [PE]

▸ National Drug Code (NDC) Directory

19.17 EPA Substance Registry Services Tree

28 items View in Classification Browser

EPA SRS List Classification
Safer Chemical Ingredients List

SCIL :: The Safer Chemical Ingredients List (SCIL) is a list of chemical ingredients, arranged by functional-use class, that the Safer Choice Program has evaluated and determined to be safer than traditional chemical ingredients. This list is designed to help manufacturers find safer chemical alternatives that meet the criteria of the Safer Choice Program.

EPA SRS List Classification
Wisconsin Department of Natural Resources

WDNR :: Substances compiled by WDNR

EPA SRS List Classification
2012 Chemical Data Reporting

2012 CDR :: This list contains chemicals that were reported to EPA's 2012 Chemical Data Reporting (CDR). Companies that manufacture (including import) certain chemicals at certain volumes in the U.S. must report to EPA every four years through its CDR. The vast majority of chemicals on this 2012 CDR list needed to be reported, but some of these chemicals were not required to be reported. EPA uses the CDR data to support many health, safety, and environmental protection activities.

EPA SRS List Classification
Green Chemistry Expert System

GCES :: The Green Chemistry Expert System (GCES) is a tool currently under development by the U.S. EPA, which will allow users to build a green chemical process, design a green chemical, or survey the field of green chemistry. Its primary purpose is to guide users in the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. This new approach to pollution prevention is the central focus of EPA`s Green Chemistry Program. The GCES will be a primary source of linear structural formulas in the CRS.

EPA SRS List Classification

High Production Volume Challenge Program / Voluntary Childrens Chemical Evaluation Program Information System

HPVIS :: The HPVIS/VCCEP Information System will allow EPA to receive and manage documents and data generated for the High Production Volume (HPV) Initiative, the Voluntary Children's Chemical Evaluation Program (VCCEP), and other EPA initiatives. It will also track the status of submitters` commitments, test plans, and other milestones. HPVIS is a critical component of the Office of Pollution Prevention and Toxics` ability to fulfill its mandate under the Toxic Substances Control Act (TSCA). OPPT has succeeded in meeting the information needs of TSCA for many years, primarily by managing the data flow through incremental, evolutionary improvements in information management.

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▸ EPA Substance Registry Services

20 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. CAMEO Chemicals

LICENSE
CAMEO Chemicals and all other CAMEO products are available at no charge to those organizations and individuals (recipients) responsible for the safe handling of chemicals. However, some of the chemical data itself is subject to the copyright restrictions of the companies or organizations that provided the data.
https://cameochemicals.noaa.gov/help/reference/terms_and_conditions.htm?d_f=false

WATER

https://cameochemicals.noaa.gov/chemical/30024

CAMEO Chemical Reactivity Classification

https://cameochemicals.noaa.gov/browse/react

2. CAS Common Chemistry

LICENSE
The data from CAS Common Chemistry is provided under a CC-BY-NC 4.0 license, unless otherwise stated.
https://creativecommons.org/licenses/by-nc/4.0/

Water, tetramer, radical ion(1-)

https://commonchemistry.cas.org/detail?cas_rn=191612-63-2

Water, dimer, radical ion(1-)

https://commonchemistry.cas.org/detail?cas_rn=146915-49-3

Water, dimer, radical ion(1+)

https://commonchemistry.cas.org/detail?cas_rn=158061-35-9

Water

https://commonchemistry.cas.org/detail?cas_rn=7732-18-5

Water, trimer, radical ion(1-)

https://commonchemistry.cas.org/detail?cas_rn=191612-61-0

Water, hexamer, radical ion(1-)

https://commonchemistry.cas.org/detail?cas_rn=146915-50-6

Water, octadecamer

https://commonchemistry.cas.org/detail?cas_rn=151517-95-2

Water, homopolymer

https://commonchemistry.cas.org/detail?cas_rn=25766-61-4

Water, heneicosamer

https://commonchemistry.cas.org/detail?cas_rn=163734-19-8

Water, tridecamer

https://commonchemistry.cas.org/detail?cas_rn=151733-06-1

Water, undecamer

https://commonchemistry.cas.org/detail?cas_rn=155964-99-1

Water, tetramer

https://commonchemistry.cas.org/detail?cas_rn=70232-06-3

Water, octacosamer

https://commonchemistry.cas.org/detail?cas_rn=181895-39-6

Water, octamer

https://commonchemistry.cas.org/detail?cas_rn=139322-39-7

Water, nonamer

https://commonchemistry.cas.org/detail?cas_rn=144442-59-1

Water, tetradecamer

https://commonchemistry.cas.org/detail?cas_rn=151517-94-1

Water, heptadecamer

https://commonchemistry.cas.org/detail?cas_rn=151733-07-2

Water, hexamer

https://commonchemistry.cas.org/detail?cas_rn=139322-38-6

Water, pentacosamer

https://commonchemistry.cas.org/detail?cas_rn=163734-21-2

Water, hexadecamer

https://commonchemistry.cas.org/detail?cas_rn=148076-13-5

Water, dodecamer

https://commonchemistry.cas.org/detail?cas_rn=148076-12-4

Water, docosamer

https://commonchemistry.cas.org/detail?cas_rn=163734-20-1

Water, pentamer

https://commonchemistry.cas.org/detail?cas_rn=79800-59-2

Water, decamer

https://commonchemistry.cas.org/detail?cas_rn=142473-62-9

Water, trimer

https://commonchemistry.cas.org/detail?cas_rn=31014-12-7

Water, eicosamer

https://commonchemistry.cas.org/detail?cas_rn=142473-64-1

Water, tetracosamer

https://commonchemistry.cas.org/detail?cas_rn=151517-96-3

Water, dimer

https://commonchemistry.cas.org/detail?cas_rn=25655-83-8

Water, heptamer

https://commonchemistry.cas.org/detail?cas_rn=144442-58-0

Water, pentadecamer

https://commonchemistry.cas.org/detail?cas_rn=142473-63-0

3. ChemIDplus

Water

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0007732185

ChemIDplus Chemical Information Classification

https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

4. DrugBank

Water

https://www.drugbank.ca/drugs/DB09145

5. DTP/NCI

water

https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=147337

6. EPA Chemicals under the TSCA

Water

https://www.epa.gov/chemicals-under-tsca

7. EPA DSSTox

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

Water

https://comptox.epa.gov/dashboard/DTXSID6026296

Atomic oxygen

https://comptox.epa.gov/dashboard/DTXSID00170378

CompTox Chemicals Dashboard Chemical Lists

https://comptox.epa.gov/dashboard/chemical-lists/

8. European Chemicals Agency (ECHA)

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https://echa.europa.eu/web/guest/legal-notice

Water

https://echa.europa.eu/substance-information/-/substanceinfo/100.028.902

water

https://echa.europa.eu/information-on-chemicals

Water

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/69840

9. FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

WATER

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/059QF0KO0R

10. Hazardous Substances Data Bank (HSDB)

LICENSE
https://www.nlm.nih.gov/web_policies.html

Water

https://pubchem.ncbi.nlm.nih.gov/source/hsdb/8183

11. Human Metabolome Database (HMDB)

Water

http://www.hmdb.ca/metabolites/HMDB0002111

HMDB0002111_msms_449782

https://hmdb.ca/metabolites/HMDB0002111#spectra

12. Wikipedia

water

https://en.wikipedia.org/wiki/Water

13. Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Water

https://haz-map.com/Agents/18668

14. ChEBI

Water

http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:15377

ChEBI Ontology

http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

15. E. coli Metabolome Database (ECMDB)

https://ecmdb.ca/compounds/M2MDB000142

16. NCI Thesaurus (NCIt)

https://www.cancer.gov/policies/copyright-reuse

https://ncithesaurus.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=ncit&code=C65147

NCI Thesaurus Tree

https://ncit.nci.nih.gov

17. ChEMBL

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http://www.ebi.ac.uk/Information/termsofuse.html

https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1098659/

18. ClinicalTrials.gov

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https://clinicaltrials.gov/ct2/about-site/terms-conditions#Use

https://clinicaltrials.gov/

19. Comparative Toxicogenomics Database (CTD)

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http://ctdbase.org/about/legal.jsp

Mineral Waters

https://ctdbase.org/detail.go?type=chem&acc=D008900

Water

https://ctdbase.org/detail.go?type=chem&acc=D014867

20. Therapeutic Target Database (TTD)

Sterile Water

https://idrblab.net/ttd/data/drug/details/D0SQ1W

21. Consumer Product Information Database (CPID)

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https://www.whatsinproducts.com/contents/view/1/6

Water

https://www.whatsinproducts.com/chemicals/view/1/738/007732-18-5

Aqua

https://www.whatsinproducts.com/chemicals/view/1/5877/07732-18-5

Consumer Products Category Classification

https://www.whatsinproducts.com/

22. Crystallography Open Database (COD)

23. DailyMed

LICENSE
https://www.nlm.nih.gov/copyright.html

Drug: 059QF0KO0R | PURIFIED WATER | STERILE PURIFIED WATER | STERILE WATER | STERILE WATER FOR INHALATION .. total 8

https://dailymed.nlm.nih.gov/dailymed/

24. Drug Induced Liver Injury Rank (DILIrank) Dataset

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https://www.fda.gov/about-fda/about-website/website-policies#linking

sterile water

https://www.fda.gov/science-research/liver-toxicity-knowledge-base-ltkb/drug-induced-liver-injury-rank-dilirank-dataset

25. Drugs and Lactation Database (LactMed)

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https://www.nlm.nih.gov/copyright.html

Water O 15

https://www.ncbi.nlm.nih.gov/books/n/lactmed/LM1145/

26. Drugs@FDA

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https://www.fda.gov/about-fda/about-website/website-policies#linking

BACTERIOSTATIC WATER FOR INJECTION IN PLASTIC CONTAINER | PUR-WASH | PURIFIED WATER .. total 8

https://www.accessdata.fda.gov/scripts/cder/daf/

27. EPA Chemical and Products Database (CPDat)

LICENSE

https://comptox.epa.gov/dashboard/DTXSID6026296#exposure

EPA CPDat Classification

https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

28. EPA Safer Choice

Water

https://www.epa.gov/saferchoice/safer-ingredients

EPA Safer Chemical Ingredients Classification

https://www.epa.gov/saferchoice

29. FDA Orange Book

https://www.fda.gov/drugs/drug-approvals-and-databases/approved-drug-products-therapeutic-equivalence-evaluations-orange-book

30. NORMAN Suspect List Exchange

Water

NORMAN Suspect List Exchange Classification

https://www.norman-network.com/nds/SLE/

31. EU Clinical Trials Register

https://www.clinicaltrialsregister.eu/

32. FDA Center for Food Safety and Applied Nutrition (CFSAN)

FCN Number 1089

https://www.cfsanappsexternal.fda.gov/scripts/fdcc/index.cfm?set=FCN&id=1089

33. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J2.261.720F

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J408.680E

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J43.587B

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J2.656.835H

34. National Drug Code (NDC) Directory

STERILE WATER FOR INJECTION

https://www.fda.gov/drugs/drug-approvals-and-databases/national-drug-code-directory

35. NIPH Clinical Trials Search of Japan

https://rctportal.niph.go.jp/en/

36. NIST Mass Spectrometry Data Center

Water

http://www.nist.gov/srd/nist1a.cfm

37. SpectraBase

Water

https://spectrabase.com/spectrum/7hySgwgTbsW

Water

https://spectrabase.com/spectrum/9qMhGSf79sG

WATER

https://spectrabase.com/spectrum/5dxrV5ZbsPc

Water

https://spectrabase.com/spectrum/H7KdKI7UNSz

WATER DISTILLED

https://spectrabase.com/spectrum/BnpcCEB1yUv

Water

https://spectrabase.com/spectrum/l0LqRdA3ay

Water

https://spectrabase.com/spectrum/7K3onlwNjkd

Water

https://spectrabase.com/spectrum/4riq7S9O8mF

Water

https://spectrabase.com/spectrum/HBvwEyjf7Tn

38. NLM RxNorm Terminology

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https://www.nlm.nih.gov/research/umls/rxnorm/docs/termsofservice.html

water

https://rxnav.nlm.nih.gov/id/rxnorm/11295

39. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/87690734

40. Pistoia Alliance Chemical Safety Library

LICENSE
https://www.cas.org/sites/default/files/documents/chemical-safety-library-terms.pdf

SODIUM BOROHYDRIDE; WATER

http://www.pistoiaalliance.org/projects/chemical-safety-library/

41. Protein Data Bank in Europe (PDBe)

http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/HOH

42. RCSB Protein Data Bank (RCSB PDB)

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Data files contained in the PDB archive (ftp://ftp.wwpdb.org) are free of all copyright restrictions and made fully and freely available for both non-commercial and commercial use. Users of the data should attribute the original authors of that structural data.
https://www.rcsb.org/pages/policies

https://www.rcsb.org/

43. Rhea - Annotated Reactions Database

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https://www.rhea-db.org/rhea?query=CHEBI:15377

44. SpringerMaterials

water

https://materials.springer.com/substanceprofile/docs/smsid_uatzaqfmzswvnmaj

45. Thieme Chemistry

https://pubchem.ncbi.nlm.nih.gov/substance/?source=22163&sourceid=1024111-500000000

46. Wikidata

Q283

https://www.wikidata.org/wiki/Q283

Hydroxyl_radical

https://www.wikidata.org/wiki/Q427071

Atomic oxygen

https://www.wikidata.org/wiki/Q81977184

47. Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=128024

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=137732

48. Medical Subject Headings (MeSH)

Water

https://www.ncbi.nlm.nih.gov/mesh/68014867

MeSH Tree

http://www.nlm.nih.gov/mesh/meshhome.html

49. PubChem

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

50. KEGG

Therapeutic category of drugs in Japan

http://www.genome.jp/kegg-bin/get_htext?br08301.keg

Drugs listed in the Japanese Pharmacopoeia

http://www.genome.jp/kegg-bin/get_htext?br08311.keg

Risk category of Japanese OTC drugs

http://www.genome.jp/kegg-bin/get_htext?br08312.keg

51. UN Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

52. LOTUS - the natural products occurrence database

LICENSE
The code for LOTUS is released under the GNU General Public License v3.0.
https://lotus.nprod.net/

LOTUS Tree

https://lotus.naturalproducts.net/

53. EPA Substance Registry Services

LICENSE
https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

54. PATENTSCOPE (WIPO)

SID 403031219

https://pubchem.ncbi.nlm.nih.gov/substance/403031219