LIBRARY RESOURCES FOR CHEMISTRY

Cardinal Meyer Library
Marian University

LIBRARY RESOURCES

Connect to databases or websites through the Library's webpage so that you can access online books or articles:

http://www.marianuniversity.edu/welcome-to-cardinal-meyer-library/

CHEMISTRY REFERENCE BOOKS

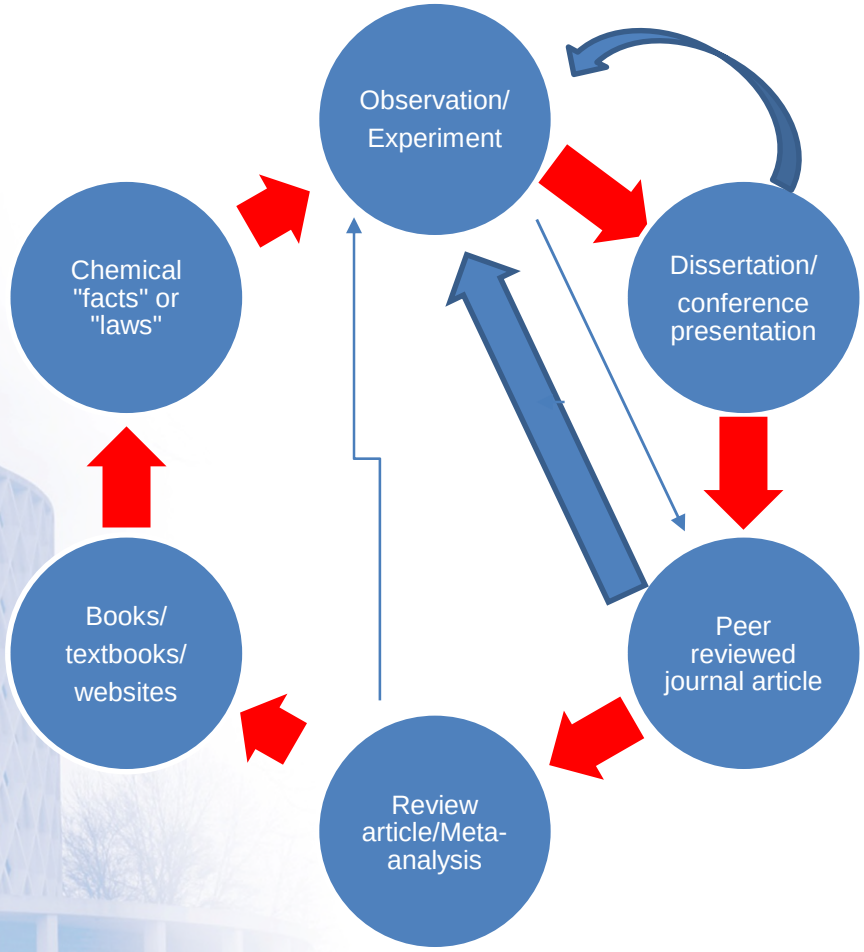
- Dictionary of Organic Compounds, R547.003 D554
- Physicians' Desk Reference: R615.1 P578 [drug package inserts]
- Merck Index: R615.103 M555m

*R at the front means reference area

540=Chemisty; 625=Pharmaceuticals

Entries usually give the original citation on a chemical's discovery.

SCHOLARLY PROCESS



EBOOKS

- Kaye & Laby Tables of Physical & Chemical Constants (16th Ed.)

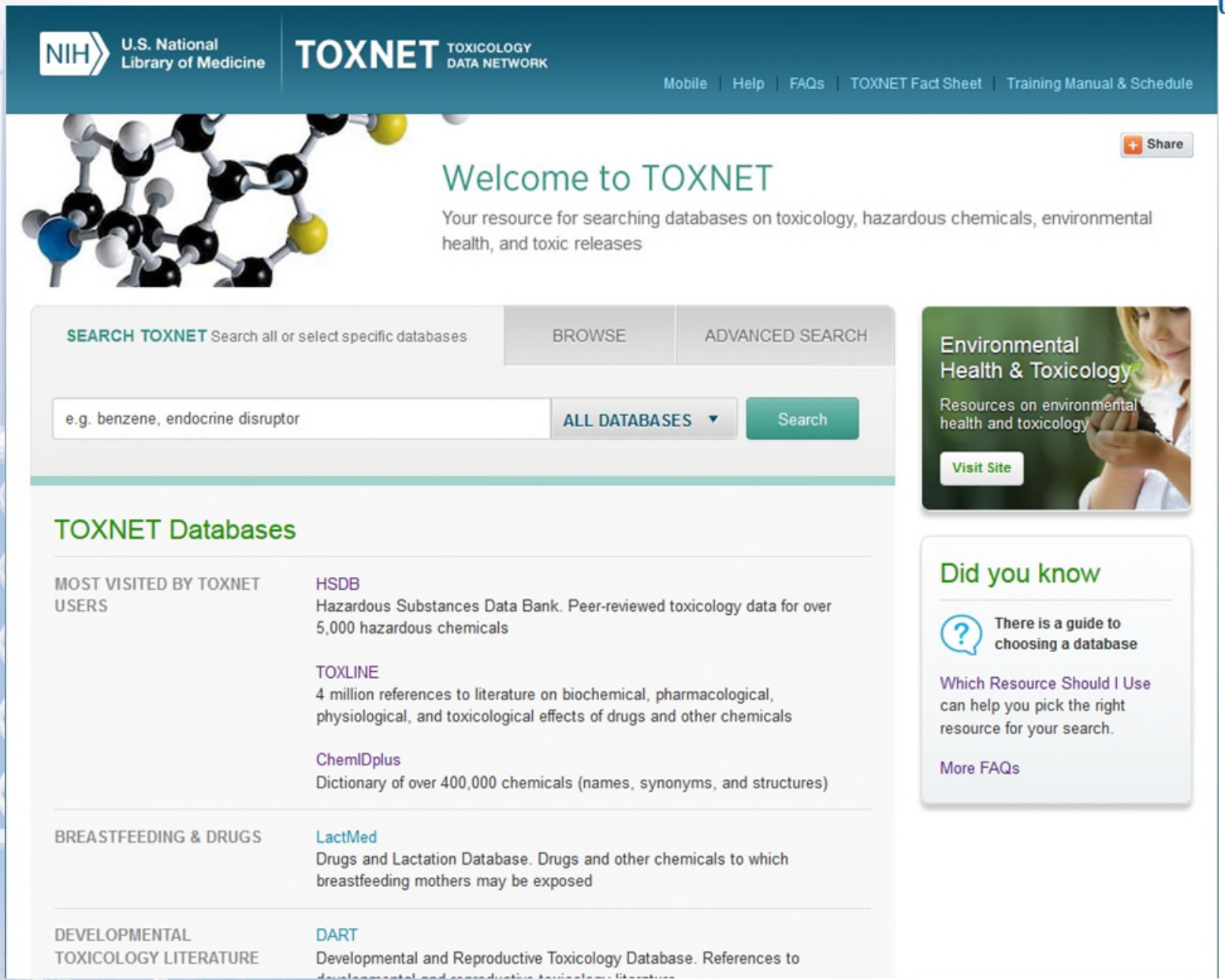
The entire, unedited contents of the 16th edition (1995), containing tables of data, formulae, graphs and charts. Topics from fundamental constants to fiber optics, superconductivity to Raman spectroscopy, etc.

Chemistry Resources

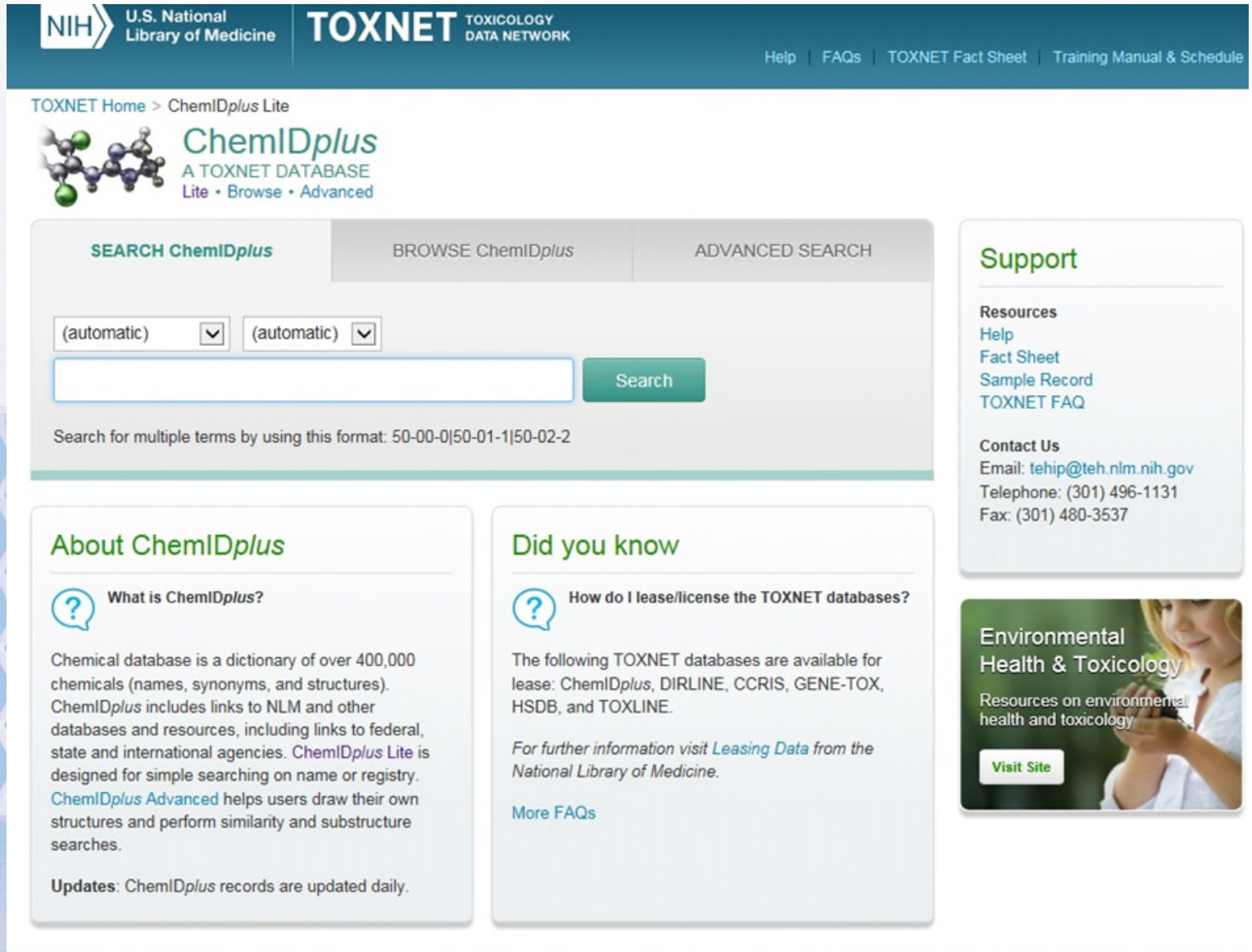
- ChemSpider (UK--free!): http://www.chemspider.com/
- PubChem (USA--free!): (http://pubchem.ncbi.nlm.nih.gov/
- PubChem Searcher (free)
- ToxNet: (free) http://toxnet.nlm.nih.gov/

TOXNET

MARIAN UNIVERSITY



ChemIDPlus


NIH U.S. National Library of Medicine
TOXNET TOXICOLOGY DATA NETWORK
Help | FAQs | TOXNET Fact Sheet | Training Manual & Schedule
TOXNET Home > ChemIDplus Lite
ChemIDplus
A TOXNET DATABASE
Lite • Browse • Advanced
SEARCH ChemIDplus
BROWSE ChemIDplus
ADVANCED SEARCH
(automatic)
(automatic)
Search
Search for multiple terms by using this format: 50-00-0|50-01-1|50-02-2
About ChemIDplus
What is ChemIDplus?
Chemical database is a dictionary of over 400,000 chemicals (names, synonyms, and structures). ChemIDplus includes links to NLM and other databases and resources, including links to federal, state and international agencies. ChemIDplus Lite is designed for simple searching on name or registry. ChemIDplus Advanced helps users draw their own structures and perform similarity and substructure searches.
Updates: ChemIDplus records are updated daily.
Did you know
How do I lease/license the TOXNET databases?
The following TOXNET databases are available for lease: ChemIDplus, DIRLINE, CCRIS, GENE-TOX, HSDB, and TOXLINE.
For further information visit Leasing Data from the National Library of Medicine.
More FAQs
Support
Resources
Help
Fact Sheet
Sample Record
TOXNET FAQ
Contact Us
Email: tehip@teh.nlm.nih.gov
Telephone: (301) 496-1131
Fax: (301) 480-3537
Environmental Health & Toxicology
Resources on environmental health and toxicology
Visit Site

BENZENE RESULTS

TOXNET > ChemIDplus > Substance

ChemIDplus
A TOXNET DATABASE
Lite • Browse • Advanced

Name/Synonym | equals | BENZENE | Search

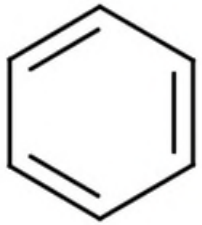
Start New Query | Modify Query | Search History | Switch to Summary View

Substance Name: Benzene
RN: 71-43-2
UNII: J64922108F
InChIKey: UHOVQNZJYSORNB-UHFFFAOYSA-N

Note
Toxic, volatile, flammable liquid hydrocarbon byproduct of coal distillation. It is used as an industrial solvent in paints, varnishes, lacquer thinners, gasoline, etc. Benzene causes central nervous system damage acutely and bone marrow damage chronically and is carcinogenic. It was formerly used as parasiticide.

Molecular Formula
C6-H6

Molecular Weight
78.1134



All | Classifications | Links to Resources | Names & Synonyms | Registry Numbers | Structure Descriptors | Toxicity | Physical Properties

Classification Codes

Classification Codes

- Agricultural Chemical
- Drug / Therapeutic Agent
- Human Data
- Mutation Data
- Out-Dated Pesticide
- Reproductive Effect
- Skin / Eye Irritant
- Tumor Data

Superlist Classification Codes

- 2007 CERCLA Priority List, Rank: 6
- 2011 CERCLA Priority List, Rank: 6
- Known to be a Carcinogen
- Overall Carcinogenic Evaluation: Group 1
- Reportable Quantity (RQ) = 10 lb
- TWA 0.5 ppm; STEL 2.5 ppm; skin; Confirmed human carcinogen; BEI
- TWA see 1910.1028; Also see Table Z-2 for the limits applicable in the operations or sectors excluded in 1910.1028

Links to Resources

NLM Resources (File Locators)

- CCRIS
- ClinicalTrials.gov
- DailyMed
- DART
- DrugPortal
- MedlinePlusAll
- MeSH
- MeSH Heading
- PubChem
- PubMed
- TOXMAP
- TRI2000
- TRI2001
- TRI2002
- TRI2003
- TRI2011
- TRI2012
- TRI2013
- TRI2014
- TRI2015

CAS Registry Number

TOXNET > ChemIDplus > Substance

ChemIDplus
A TOXNET DATABASE
Lite • Browse • Advanced

Name/Synonym | equals | BENZENE | Search

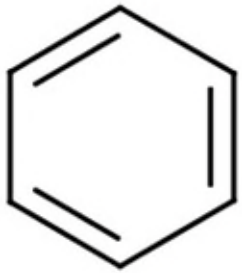
Start New Query | Modify Query | Search History | Switch to Summary View

Substance Name: Benzene
RN: 71-43-2
UNII: J64922108F
InChIKey: UHOVQNZJYSORNB-UHFFFAOYSA-N

Note
Toxic, volatile, flammable liquid hydrocarbon byproduct of coal distillation. It is used as an industrial solvent in paints, varnishes, lacquer thinners, gasoline, etc. Benzene causes central nervous system damage acutely and bone marrow damage chronically and is carcinogenic. It was formerly used as parasiticide.

Molecular Formula
C6-H6

Molecular Weight
78.1134



All | Classifications | Links to Resources | Names & Synonyms | Registry Numbers | Structure Descriptors | Toxicity | Physical Properties

Registry Numbers

CAS Registry Number
71-43-2

FDA UNII
J64922108F

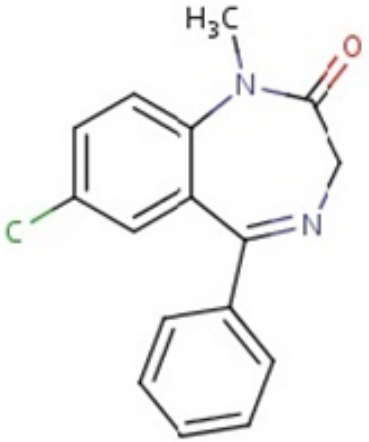
Other Registry Numbers
1053658-43-7
174973-66-1
54682-86-9

System Generated Number
0000071432

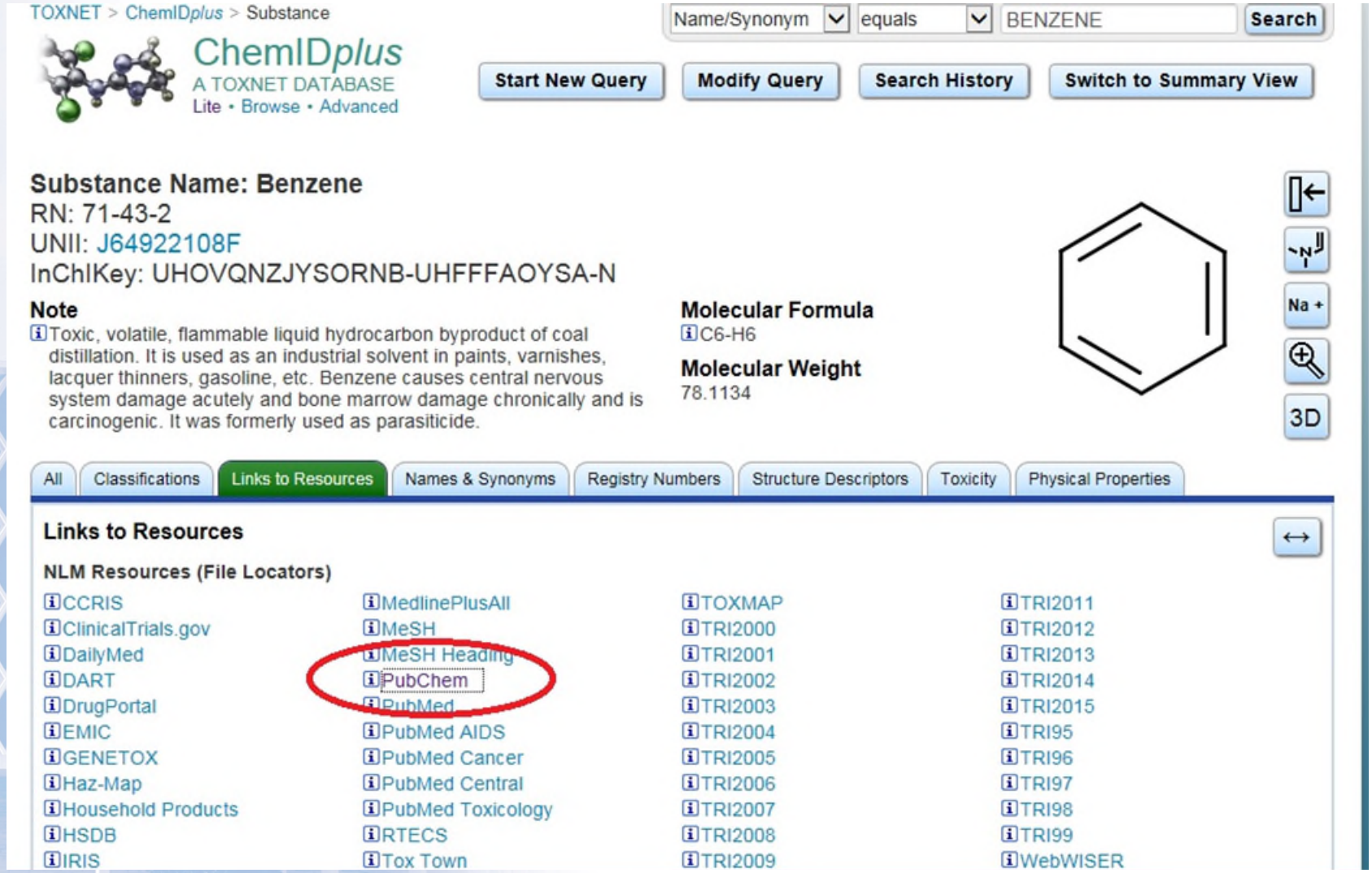
Chemical Abstracts Registry Number

- Used to find a substance over many databases like an Social Security number for a person

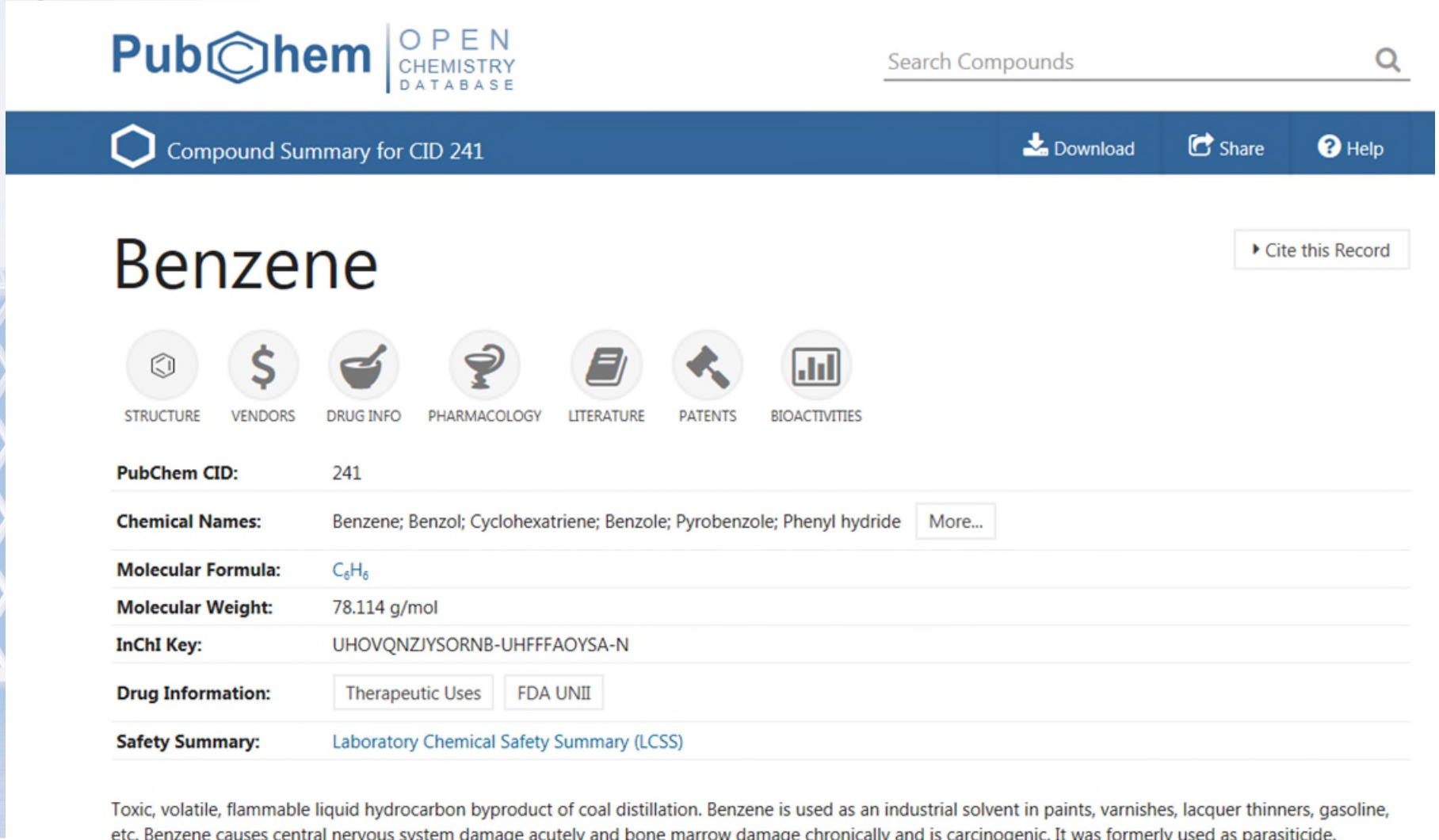
DIAZEPAM
CASRN: 439-14-5



LINKS TO RESOURCES



PubChem


PubChem OPEN CHEMISTRY DATABASE
Search Compounds
Compound Summary for CID 241
Download
Share
Help
Benzene
Cite this Record
STRUCTURE
VENDORS
DRUG INFO
PHARMACOLOGY
LITERATURE
PATENTS
BIOACTIVITIES
PubChem CID: 241
Chemical Names: Benzene; Benzol; Cyclohexatriene; Benzole; Pyrobenzole; Phenyl hydride More...
Molecular Formula: C6H6
Molecular Weight: 78.114 g/mol
InChI Key: UHOVQNZJYSORNB-UHFFFAOYSA-N
Drug Information: Therapeutic Uses FDA UNII
Safety Summary: Laboratory Chemical Safety Summary (LCSS)
Toxic, volatile, flammable liquid hydrocarbon byproduct of coal distillation. Benzene is used as an industrial solvent in paints, varnishes, lacquer thinners, gasoline, etc. Benzene causes central nervous system damage acutely and bone marrow damage chronically and is carcinogenic. It was formerly used as parasiticide.

HAZARDOUS SUBSTANCES DATA BASE

MARIAN UNIVERSITY

HSDB: DIAZEPAM CASRN: 439-14-5 This record appears in multiple databases.

View record in another database: HSDB | Download this Record | Print | Select Record | My List | Permalink

TABLE OF CONTENTS

Show Selected Items | Clear | Expand all | Collapse all

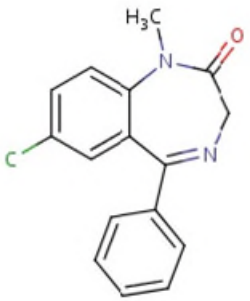
- Full Record
- Human Health Effects
- Emergency Medical Treatment
- Animal Toxicity Studies
- Metabolism/ Pharmacokinetics
- Pharmacology
- Environmental Fate & Exposure
- Environmental Standards & Regulations
- Chemical/Physical Properties
- Chemical Safety & Handling
- Manufacturing/Use Information
- Laboratory Methods
- Special References
- Synonyms and Identifiers
- Administrative Information

Show Selected Items | Clear

CLICK TO HIDE

DIAZEPAM

CASRN: 439-14-5



FULL RECORD DISPLAY

Displays all fields in the record.

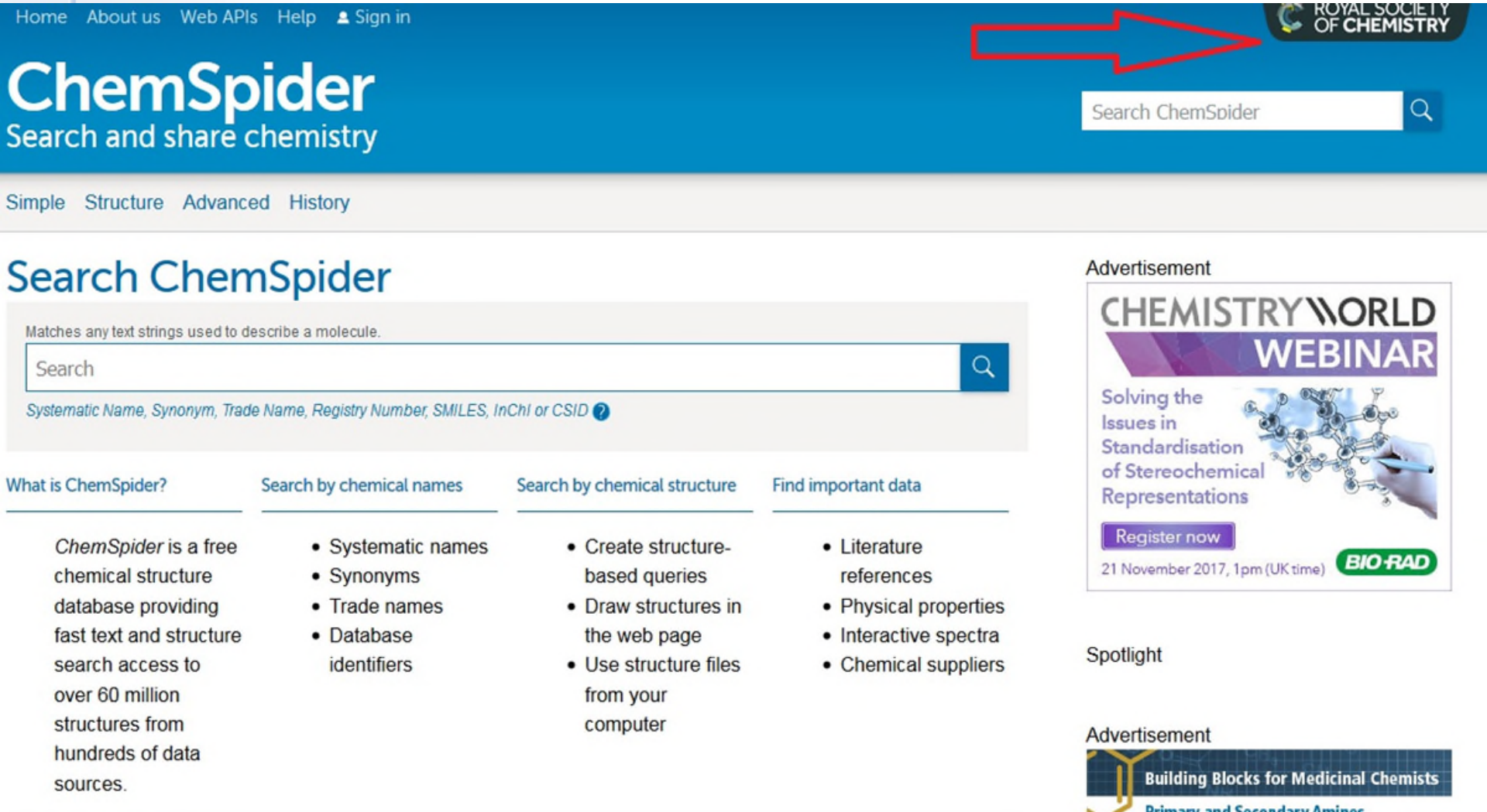
For other data, click on the Table of Contents

Human Health Effects:

Toxicity Summary:

IDENTIFICATION: Diazepam is classified as a psycholeptic, anxiolytic benzodiazepine derivative. Diazepam is a crystalline solid. Diazepam is very slightly soluble in water, soluble in alcohol and freely soluble in chloroform. Indications: Treatment of anxiety disorders, seizures and status epilepticus. Symptoms of drug withdrawal associated with the chronic abuse of ethanol, benzodiazepines, barbiturates, and other CNS depressants. Skeletal muscle spasticity and acute muscular spasms, including tetanus and cerebral palsy. Treatment of insomnia: Anxiety and/or desire for producing amnesia prior to surgery, dental, and endoscopic procedures. Conscious sedation for short anesthesia, alone or in combination with an opioid. Continuous infusion for sedation or seizures in the intensive care setting. HUMAN EXPOSURE: Main risks and target organs: Central nervous system, causing depression of respiration and consciousness. Summary of clinical effects: Central nervous system (CNS)

ChemSpider


Home About us Web APIs Help Sign in
ROYAL SOCIETY OF CHEMISTRY
ChemSpider
Search and share chemistry
Search ChemSpider
Simple Structure Advanced History
Search ChemSpider
Matches any text strings used to describe a molecule.
Search
Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID
What is ChemSpider?
ChemSpider is a free chemical structure database providing fast text and structure search access to over 60 million structures from hundreds of data sources.
Search by chemical names
Systematic names
Synonyms
Trade names
Database identifiers
Search by chemical structure
Create structure-based queries
Draw structures in the web page
Use structure files from your computer
Find important data
Literature references
Physical properties
Interactive spectra
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Solving the Issues in Standardisation of Stereochemical Representations
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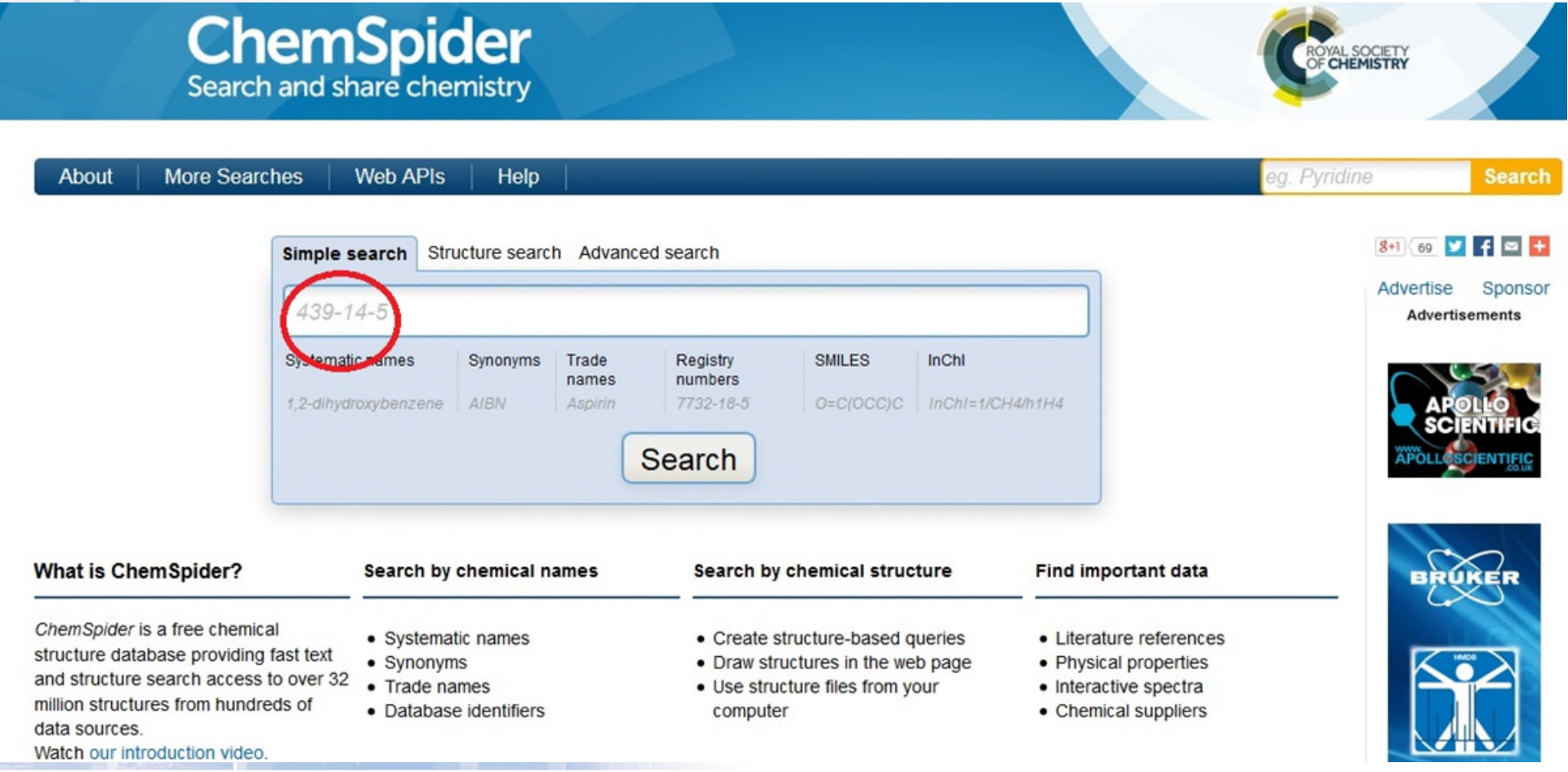
Spotlight
Advertisement
Building Blocks for Medicinal Chemists

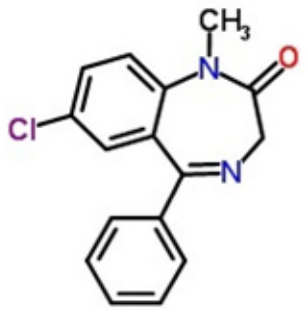
ChemSpider

- Example: diazepam registry number seach



ChemSpider Results

Search term: **439-14-5** (Found by approved synonym)



Cell 2D 3D Save Zoom

Diazepam

ChemSpider ID: **2908**

Molecular Formula: $C_{16}H_{13}ClN_2O$

Average mass: 284.740 Da

Monoisotopic mass: 284.071655 Da

▼ Systematic name

7-Chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one

▶ SMILES and InChIs

▶ Cite this record

anxiolytic drug | **muscle relaxant** | **sedative**

▶ Names and Identifiers

▶ ChemSpider Searches

▼ Properties

Experimental data | **Predicted** - ACD/Labs | **Predicted** - EPISuite | **Predicted** - ChemAxon

Data supplied by datasources and users.

- **Experimental Physico-chemical Properties**

  Experimental Melting Point:

  125 °C **Oxford University Chemical Safety Data (No longer updated)** More details

Structural Searching

- PubChem Searcher

Platform-independent chemical structure drawing tool. Provides translation into InChI/SMILES/etc., as well as exporting to image and chemical information files (i.e. MDL, ChemDraw, ISIS, etc.).

- Cn3D Searcher

Cn3D ("see in 3D") is a helper application for web browsers that allows viewing of 3-dimensional structures from NCBI's Entrez Structure database. Cn3D is provided for Windows and Macintosh, and can be compiled on Unix. Cn3D simultaneously displays structure, sequence, and alignment, and now has powerful annotation and alignment editing features

- Xminstry

A web-based, Java-free, HTML5-free structure drawing tool. Can import from programs on Windows with a small add-on. Can export to a variety of image and structure formats.

- Accelrys Draw

Accelrys Draw is a simple program for drawing chemical structures. Requires registration. Other tools also available.

- Jmol

Jmol is an open-source, Java-based viewer for viewing 3D chemical structures, and contains features for viewing chemicals, crystals, materials and biomolecules.

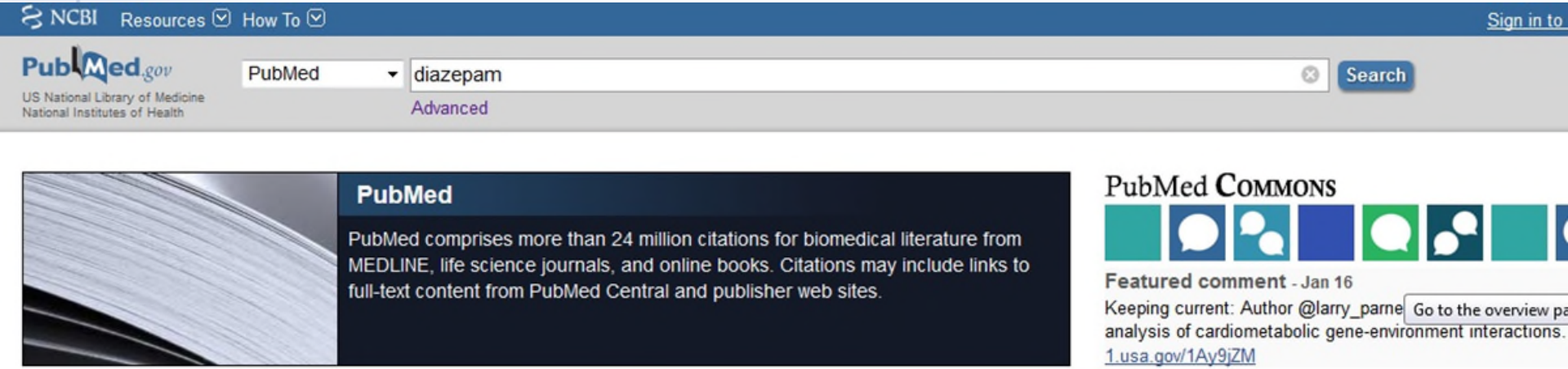
CHEMICAL PROPERTIES

CalTech Library chemistry website

Special thanks to CalTech Chemistry librarian, Donna T. Wrublewski, Ph.D., MRSC

The properties of many organic chemicals have been established for long enough that the information is available in open source and free resources.

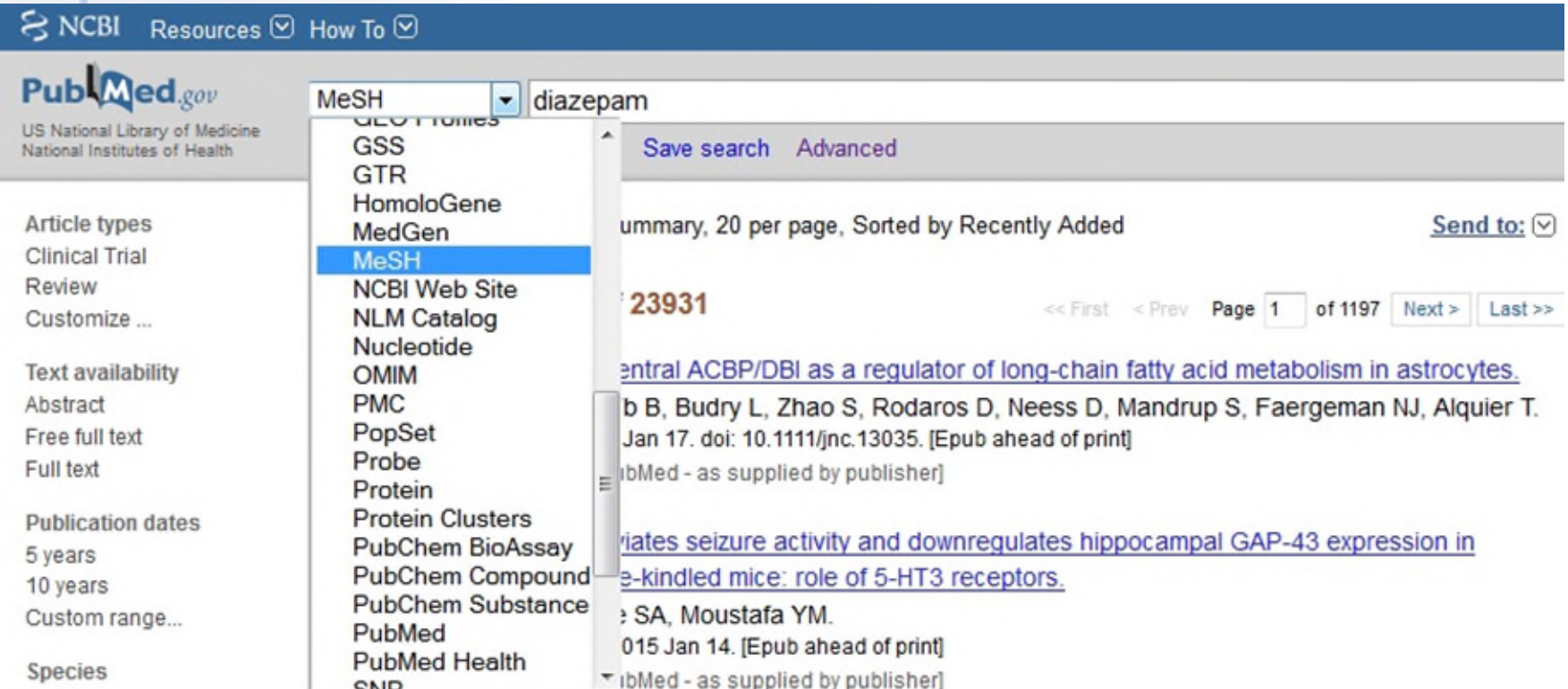
PubMed



PubMed will automatically suggest search terms as you type in your topic. You can select from these terms or search by the topic you typed.

PubMed Subjects

Narrow results by using the drop down and choosing MeSH (Medical Subject Heading)



MeSH

- Click on the best subject

isplay Settings: Summary, 20 per page Send to:

esults: 13

Diazepam

A benzodiazepine with anticonvulsant, anxiolytic, sedative, muscle relaxant, and amnesic properties and a long duration of action. Its actions are mediated by enhancement of GAMMA-AMINOBUTYRIC ACID activity.
Year introduced: 1965(1963)

Diazepam Binding Inhibitor

An 86-amino acid polypeptide, found in central and peripheral tissues, that displaces **diazepam** from the benzodiazepine recognition site on the gamma-aminobutyric acid receptor (RECEPTORS, GABA). It also binds medium- and long-chain acyl-CoA esters and serves as an acyl-CoA transporter. This peptide regulates lipid metabolism.
Year introduced: 2002

Receptors, GABA-A

Cell surface proteins which bind GAMMA-AMINOBUTYRIC ACID and contain an integral membrane chloride channel. Each receptor is assembled as a pentamer from a pool of at least 19 different possible subunits. The receptors belong to a superfamily that share a common CYSTEINE loop.
Year introduced: 1994

MeSH Subheadings

- Click desired boxes

Diazepam

A benzodiazepine with anticonvulsant, anxiolytic, sedative, muscle relaxant, and amnesic properties and a long duration of action. Its actions are mediated by enhancement of GAMMA-AMINOBUTYRIC ACID activity.
Year introduced: 1965(1963)

PubMed search builder options
Subheadings:

☐ administration and dosage	☐ classification	☑ pharmacology
☐ adverse effects	☐ contraindications	☐ physiology
☐ agonists	☐ diagnostic use	☐ poisoning
☐ analogs and derivatives	☐ economics	☐ radiation effects
☐ analysis	☐ etiology	☐ secretion
☐ antagonists and inhibitors	☐ history	☐ standards
☐ biosynthesis	☐ immunology	☐ statistics and numerical data
☐ blood	☐ isolation and purification	☐ supply and distribution
☐ cerebrospinal fluid	☐ metabolism	☐ therapeutic use
☐ chemical synthesis	☐ organization and administration	☐ toxicity
☐ chemistry	☑ pharmacokinetics	☐ urine

☑ Restrict to MeSH Major Topic.
☐ Do not include MeSH terms found below this term in the MeSH hierarchy.

Tree Number(s): D03.438.079.080.070.216
MeSH Unique ID: D003975
Registry Number: Q3JTX2Q7TU
Entry Terms:

- 7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
- Diazemuls

PubMed

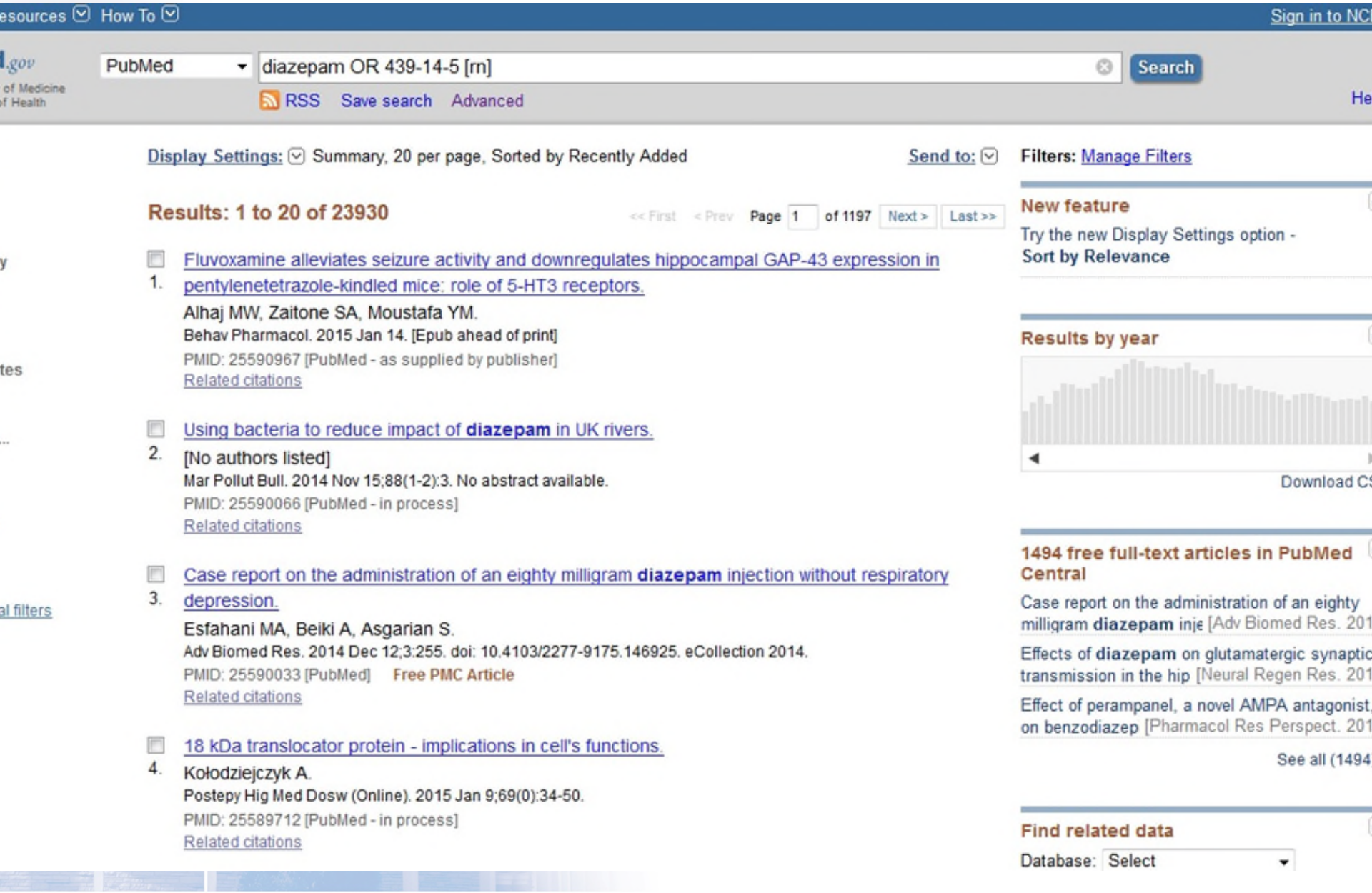
The results will appear as follows:

To view the abstract (summary) of an article, click on the title.

To narrow down the list of results, use the Filter Your Results option or use the Also Try options to begin a new search.

PUBMED RESULTS

MARIAN UNIVERSITY



esources How To Sign in to NC

.gov of Medicine f Health

PubMed diazepam OR 439-14-5 [rn] Search

RSS Save search Advanced He

Display Settings: Summary, 20 per page, Sorted by Recently Added Send to: Filters: Manage Filters

Results: 1 to 20 of 23930

<< First < Prev Page 1 of 1197 Next > Last >>

1. Fluvoxamine alleviates seizure activity and downregulates hippocampal GAP-43 expression in pentylenetetrazole-kindled mice: role of 5-HT3 receptors.
   Alhaj MW, Zaitone SA, Moustafa YM.
   Behav Pharmacol. 2015 Jan 14. [Epub ahead of print]
   PMID: 25590967 [PubMed - as supplied by publisher]
   Related citations

2. Using bacteria to reduce impact of **diazepam** in UK rivers.
   [No authors listed]
   Mar Pollut Bull. 2014 Nov 15;88(1-2):3. No abstract available.
   PMID: 25590066 [PubMed - in process]
   Related citations

3. Case report on the administration of an eighty milligram **diazepam** injection without respiratory depression.
   Esfahani MA, Beiki A, Asgarian S.
   Adv Biomed Res. 2014 Dec 12;3:255. doi: 10.4103/2277-9175.146925. eCollection 2014.
   PMID: 25590033 [PubMed] Free PMC Article
   Related citations

4. 18 kDa translocator protein - implications in cell's functions.
   Kołodziejczyk A.
   Postepy Hig Med Dosw (Online). 2015 Jan 9;69(0):34-50.
   PMID: 25589712 [PubMed - in process]
   Related citations

New feature

Try the new Display Settings option - **Sort by Relevance**

Results by year

Download CS

1494 free full-text articles in PubMed Central

Case report on the administration of an eighty milligram **diazepam** inje [Adv Biomed Res. 201

Effects of **diazepam** on glutamatergic synaptic transmission in the hip [Neural Regen Res. 201

Effect of perampanel, a novel AMPA antagonist, on benzodiazep [Pharmacol Res Perspect. 201

See all (1494

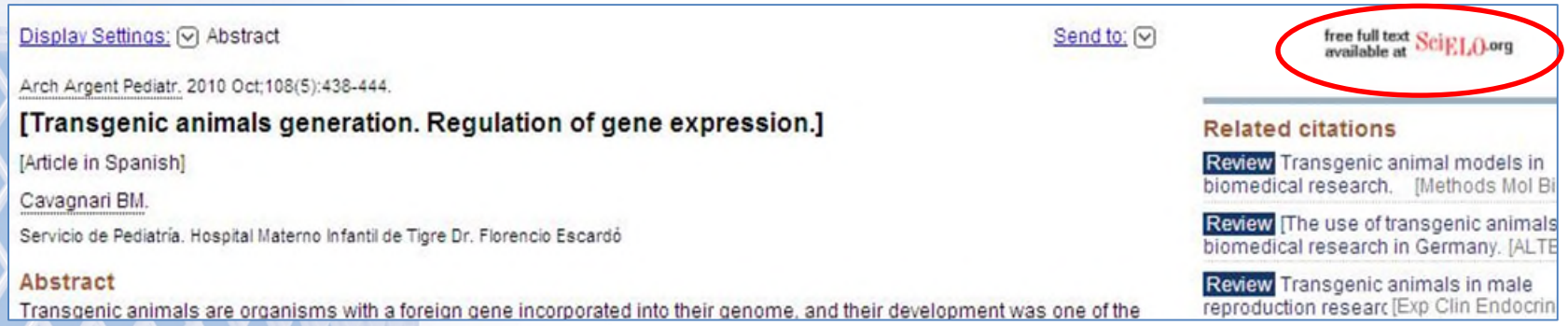
Find related data

Database: Select

PubMed

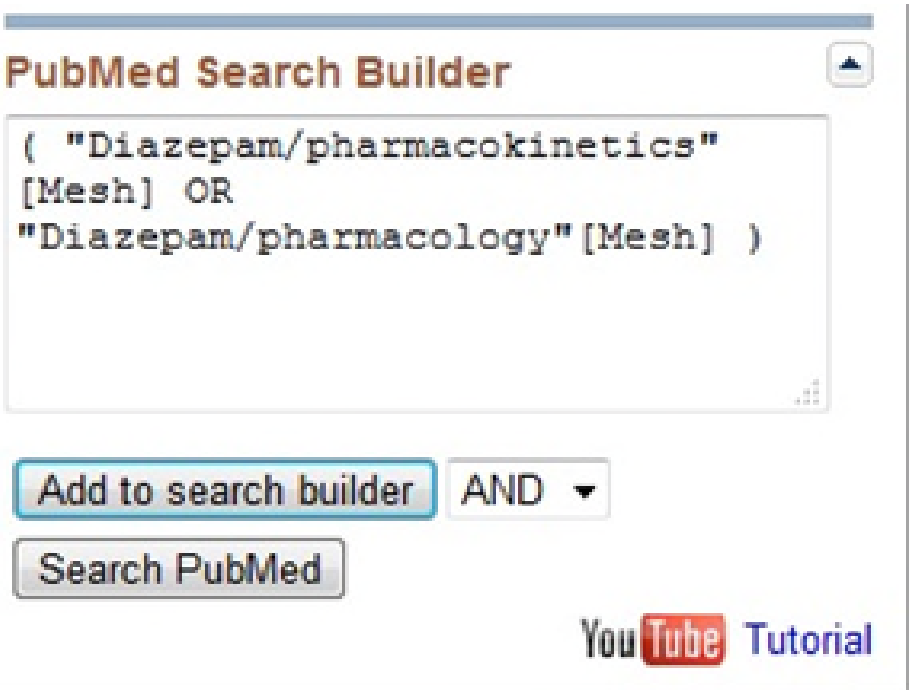
Some articles available in PubMed have the full text of the article available.

- To access the full text, click the link on the abstract page to access the full text.



MeSH: ADD TO SEARCH

- Click on the far right: Add to Search Builder
- Click on Search PubMed



PubMed Search History

- Compare the results from using Diazepam as free text, subject headings, Major topic, subheadings:

History

Download history Clear history

Search	Add to builder	Query	Items found	Time
#13	Add	Search **("Diazepam"[Majr]) AND ("Diazepam/pharmacokinetics"[Majr] OR "Diazepam/pharmacology"[Majr])**	5516	12:46:06
#12	Add	Search **("Diazepam/pharmacokinetics"[Mesh] OR "Diazepam/pharmacology"[Mesh])**	11159	12:45:23
#11	Add	Search **"Diazepam"[Mesh]**	16947	12:37:32
#1	Add	Search **diazepam**	23931	12:24:58
#10	Add	Search **diazepam[MeSH Major Topic]**	8671	12:23:03

LARGE UNIVERSITIES AND CORPORATIONS OWN MORE CHEMICAL SOURCES:

- Chemical Abstracts/SciFinder: chemical structures, properties, reactions and articles
- Reaxys: chemical structures, properties and reactions)
- Web of Science (Science Citation Index): Trace the research by who used a source or cited an author

Chemistry citations

American Chemical Society (ACS) Style Guide (3rd Edition, 2006) is available online

Bunnett, J. F.; Kearley, F. J., Jr.; *J. Org. Chem.*, **1971**, *36*, 184-186.

The authors are listed last name, first initial(s).

The journal is italicized and listed in abbreviated form (more about that below).

The year is listed in bold font.

The journal volume is listed in italicized font.

The starting and ending pages are listed separated by a hyphen.

Sometimes you will see the title given between the author names and the journal abbreviation, but usually not. This is because titles can be very long and include non-standard symbols or fonts.

Journal Abbreviations

- CASSI - Chemical Abstracts Services Source Index is a listing of both journal abbreviations and full titles. You can use this to translate an abbreviation, or, knowing the full journal title, find its accepted abbreviation to use in your citation. However, it is limited to publications indexed by CAS.
- NLM's Abridged Index Medicus (AIM) - biological and clinical journals indexed in the AIM may have a different abbreviation, more info can be found on the linked page.

Recommended Databases

Academic Search Premiere (EBSCO) includes 430 chemistry journals some in fulltext. Many articles will need to be requested through interlibrary loan.

Science Direct includes 2052 books and journal titles in chemistry published by Elsevier including a few open source or fulltext owned by Marian. Most will need to be retrieved through interlibrary loan.

SAGE --fulltext journals from Sage Publishing including some in chemistry such as *Analytical Chemistry Insights*

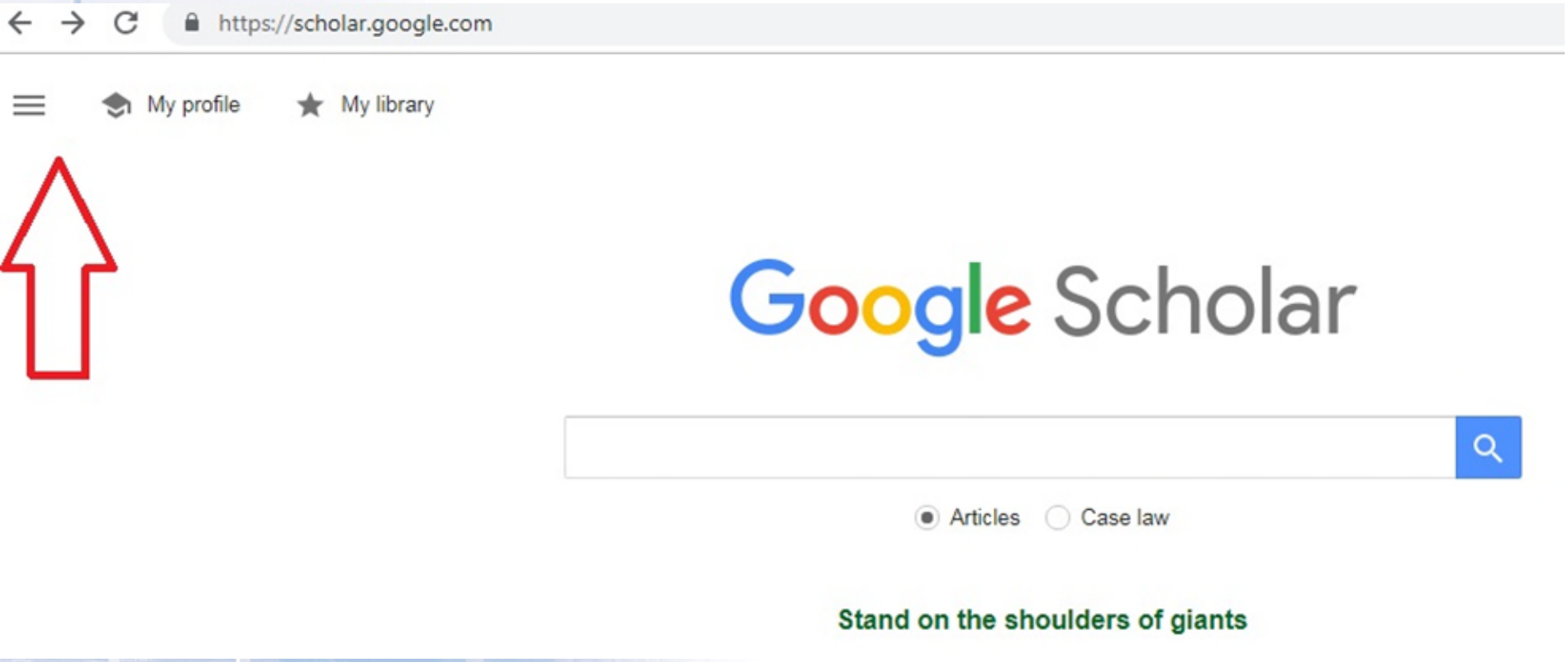
MEDLINE/PubMed provides authoritative medical information including articles related to chemistry. Some articles will be in fulltext but most will require interlibrary loan.

Google Scholar

- On campus, more fulltext articles should be available since Marian subscriptions should be recognized.
- May be best for very old materials since they are not covered by copyright and are in public domain.
- Citation searching
- Not vetted or peer reviewed!

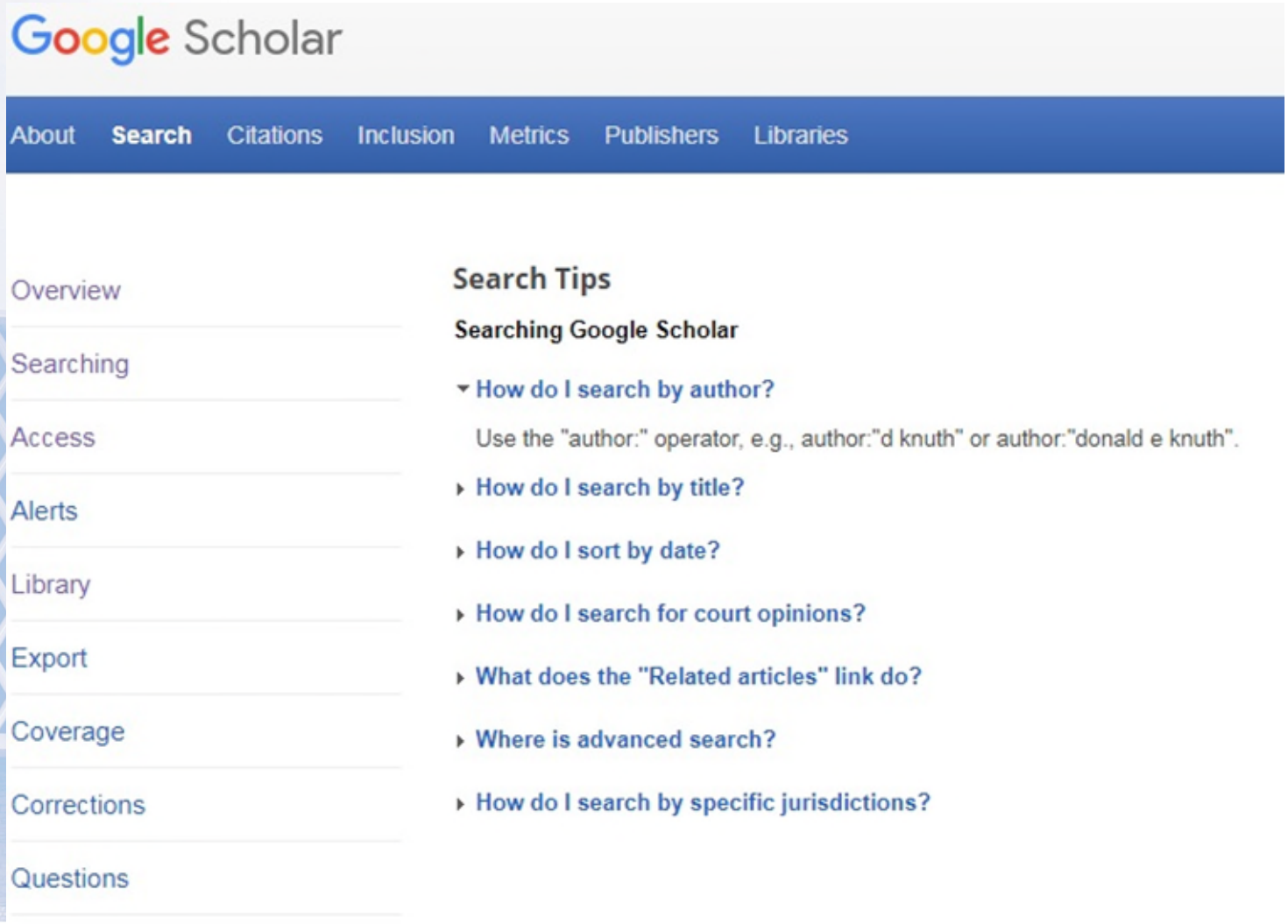
Google Scholar

- Click here to use Advanced Search
- Click on the very bottom Help to perform citation searches

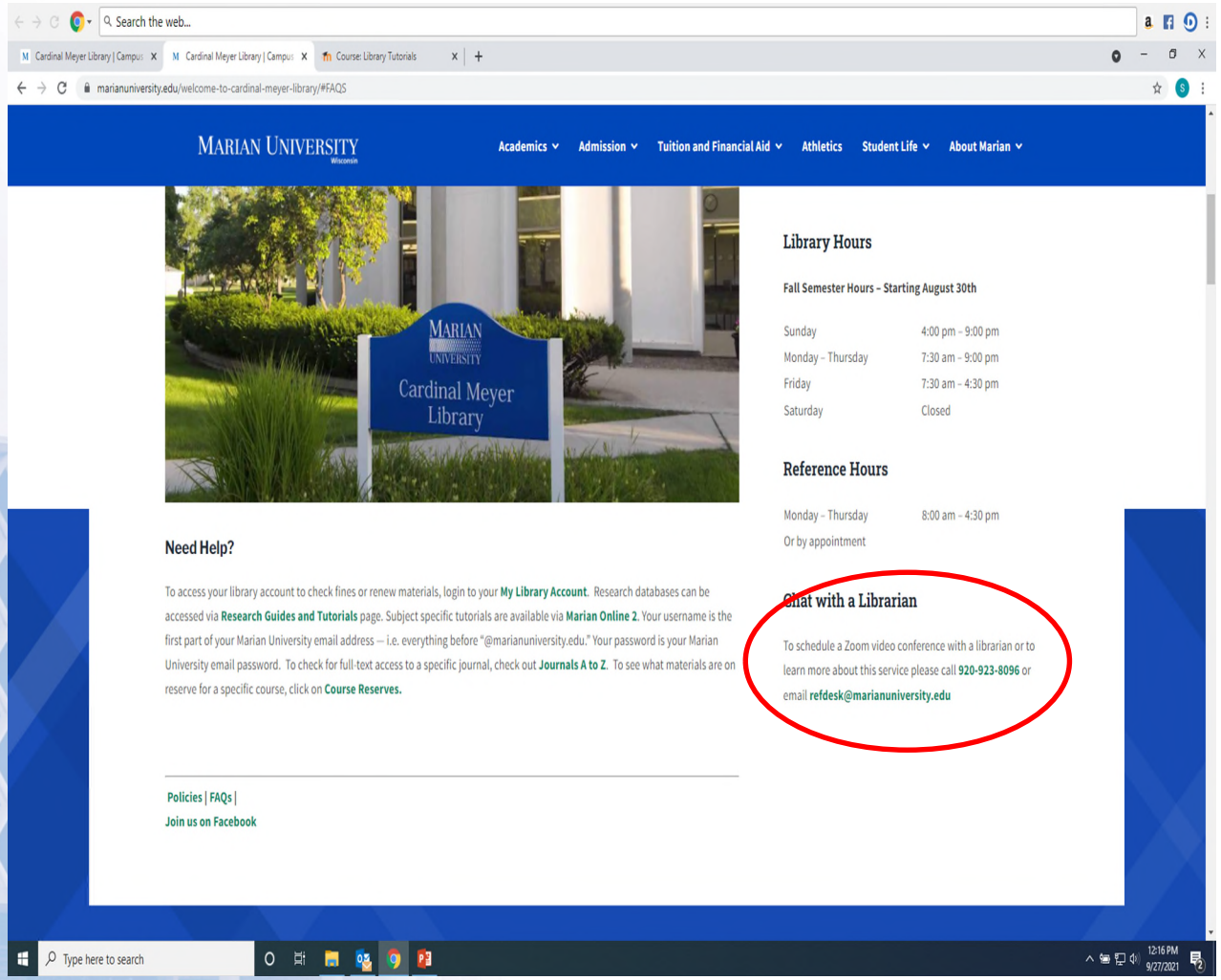


Google Scholar

- Use the advanced methods to find citations, articles, sort by date, etc.



Questions?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