

Sesión computacional

Uso de SciFinderⁿ en Farmacoquímica



Introducción

SciFinder-n es una plataforma desarrollada por el Chemical Abstracts Service (CAS) que permite el acceso a información científica confiable y actualizada sobre sustancias químicas, reacciones, literatura científica y patentes. Es una herramienta ampliamente utilizada en investigación académica e industrial, especialmente en áreas como la química medicinal, farmacología y desarrollo de fármacos. En el campo de la Farmacoquímica, SciFinder-n facilita la búsqueda y análisis de estructuras químicas, propiedades fisicoquímicas, rutas de síntesis y relaciones estructura-actividad, lo que lo convierte en un recurso fundamental para el estudio y diseño de medicamentos. Esta práctica tiene como finalidad familiarizar al estudiante con el uso de SciFinder-n y su aplicación en el análisis integral de un fármaco.

Objetivo de la práctica

1. Buscar sustancias químicas en SciFinder-n.
2. Interpretar información fisicoquímica y estructural relevante.
3. Identificar síntesis y reacciones asociadas a un fármaco.
4. Localizar y analizar artículos científicos y patentes.
5. Relacionar la información química con su uso farmacológico.

CONTEXTO DE LA PRÁCTICA

El estudiante trabajará con un fármaco de interés farmacológico asignado por el docente.

PARTE 1. BÚSQUEDA DE LA SUSTANCIA

Ingresar a SciFinder-n y buscar el fármaco en la sección “Substances”.

Identificar: número CAS, fórmula molecular, peso molecular y estructura química.

The screenshot shows the SciFinder search interface. At the top, the CAS SciFinder logo is visible. Below the logo, the user's name "Brayan Alberto Marti..." is displayed. A search bar contains the text "Diazepam". Below the search bar, a list of search results is shown, with "Diazepam" selected. The list includes: Diazepam-Lipuro, Diazepam receptors, Diazepam reineckate, Diazepam demethylase, Diazepam demethylases, Diazepam-niacin mixt., Diazepam 3-hydroxylase, diazepam N-demethylase, and Diazepam hydrochloride.

The screenshot shows the SciFinder search results page for Diazepam. The search bar contains "Diazepam". The results are sorted by Relevance and viewed in Full view. The first result is selected, showing the chemical structure of Diazepam (4-chloro-7-methyl-5H-1,2-diazepin-6-one) and its properties.

2 Results

Sort: Relevance View: Full

1

439-14-5
C₁₆H₁₃ClN₂O
Diazepam

Properties	Value	Condition
Molecular Weight	284.74	-
Melting Point (Experimental)	132 °C	-
Boiling Point (Predicted)	497.380±45.00 °C	Press: 760.00 Torr
Density (Predicted)	1.261±0.14 g/cm ³	Temp: 25 °C; Press: 760 Torr
pKa (Experimental)	3.40 (basic)	-

Experimental Properties | Spectra

35K 445 56

2

PARTE 2. PROPIEDADES FISICOQUÍMICAS

Revisar propiedades como pKa, logP/logD y solubilidad.

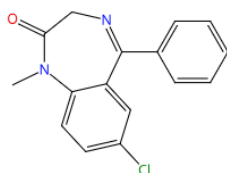
Relacionar estas propiedades con la absorción y uso farmacológico.

[Return to Results](#)

[Prev](#) (1 of 2) [Next](#)

CAS Registry Number: 439-14-5

35K 445 56



C₁₆H₁₃ClN₂O

2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl- (8CI, 9CI, ACI)



Patents Containing Substance in Claims

Preparation of kavalactone analogs as beta-adrenergic receptor antagonists from kava (Piper methysticum)

Patent Number: WO2026019925

Publication Date: 2026-01-22

Preparation of perfect, pure and uniform cochleates for drug delivery

Patent Number: WO2026010571

Publication Date: 2026-01-08

Device for extracting analytes from biological samples

Patent Number: IN202511097900

Publication Date: 2025-12-12

[View All Patents](#)

Properties	Value	Condition
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CAS SciFinder

Diazepam



[Expand All](#) | [Collapse All](#)

Other Names and Identifiers

Experimental Properties

Biological	Chemical	Lipinski	Structure Related	Thermal
Property		Value	Condition	Source
Median Lethal Dose		3700 mg/kg	Organism: rat; Route: oral	(1) CAS
Median Lethal Dose		2100 mg/kg	Organism: mouse; Route: oral	(2) CAS
Median Lethal Dose		2000 mg/kg	Organism: mouse; Route: subcutaneous	(3) CAS
Median Lethal Dose		2000 mg/kg	Organism: rat; Route: subcutaneous	(3) CAS
Median Lethal Dose		1850 mg/kg	Organism: mouse; Route: oral	(1) CAS
Median Lethal Dose		720 mg/kg	Organism: mouse; Route: oral	(4) CAS
Median Lethal Dose		710 mg/kg	Organism: rat; Route: oral	(5) APC
Median Lethal Dose		355 mg/kg	Organism: mouse; Route: intraperitoneal	(6) CAS
Median Lethal Dose		275 mg/kg	Organism: mouse; Route: intravenous	(7) CAS
Median Lethal Dose		102 mg/kg	Organism: rat; Route: injection	(8) CAS
Median Lethal Dose		51 mg/kg	Organism: mouse; Route: intravenous	(7) CAS
Median Lethal Dose		49 mg/kg	Organism: mouse; Route: intravenous	(7) CAS
Median Lethal Dose		12 mg/kg	Organism: mouse; Route: intramuscular	(9) CAS

PARTE 3. SÍNTESIS Y REACCIONES

Buscar reacciones asociadas al fármaco.

Seleccionar una ruta sintética y describir reactivos, tipo de reacción y condiciones.

The screenshot shows the CAS SciFinder interface for the search term "Diazepam". The search bar at the top contains "Diazepam" and a search icon. Below the search bar, there is a "Return to Results" link. The main content area displays the CAS Registry Number "439-14-5" with a "Get Reactions" button. Below this, there are three icons representing different metrics: a document icon for "35K", a flask icon for "445", and a shopping cart icon for "56". The chemical structure of Diazepam is shown in the center. To the right, there is a "Patents Containing" section with the title "Preparation of kavala antagonists from kav:" and the patent number "WO20260" and publication date "2026-01-".

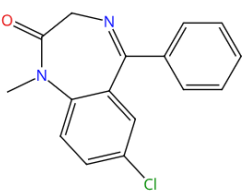
The screenshot shows the CAS SciFinder interface for the search term "439-14-5". The search bar at the top contains "439-14-5" and a search icon. Below the search bar, there is a "View Related Results" dropdown menu. The main content area displays the search results for "439-14-5". The left sidebar shows the "Filter Results" section with "Behavior" and "Substance Role" filters. The "Substance Role" filter is set to "Product (239)". The main content area shows a reaction scheme for "Scheme 1 (1 Reaction)". The reaction scheme shows the synthesis of Diazepam from a starting material and a reagent. The starting material is a complex heterocyclic structure, and the reagent is a sulfonamide derivative. The product is Diazepam. The reaction is labeled "Scheme 1 (1 Reaction)" and "Steps: 1 Yield: 97%". There is a "Suppliers (56)" button below the reaction scheme.

PARTE 4. BÚSQUEDA BIBLIOGRÁFICA

Seleccionar dos artículos científicos recientes relacionados con la actividad farmacológica. Analizar la relación estructura-actividad.

CAS Registry Number: 439-14-5

35K 445 56



$C_{16}H_{13}ClN_2O$

7-chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one (8CI, 9CI, ACI)

Patents Containing Substance in Claims

- Preparation of kavalactone analogs as beta-adrenergic receptor antagonists from kava (Piper methysticum)
Patent Number: WO2026019925
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- Preparation of perfect, pure and uniform cochleates for drug delivery
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Publication Date: 2026-01-08
- Device for extracting analytes from biological samples
Patent Number: IN202511097900
Publication Date: 2025-12-12

View All Patents

CAS Scifinder

Enter a query... Draw

References for 439-14-5

View Related Results

35,063 Results Sort: Relevance View: Partial Abstract

1

Assessment of sedative activity of Chrysin: Behavioral approach with pharmacokinetics, toxicological profile and molecular docking

By: Al Hasan, Md Sakib; Bhuiya, Md Shimul; Sheikh, Salehin; Bithi, Sumaya Akter; Saim, Md Abu; Kamil, Hossam; Ansari, Siddique Akber; Ahammed, Nowreen Tabassum; Islam, Muhammad Torequl

Sleep medicine (2025), 126, 88-96 | Language: English, Database: MEDLINE

The purpose of this study was to investigate the sedative effects of Chrysin (CHR) along with modulatory effects on diazepam (DZP) and flumazenil (FLU) in an animal sleep model produced by thiopental sodium (TS). Additionally, we explored the pharmacokinetics and potential GABA_A receptor interactions of CHR through computational studies. Swiss albino mice were treated with intraperitoneal administration of CHR (5 and 10 mg/kg), DZP (2 mg/kg), and FLU (0.1 mg/kg) either alone or in combination. Sleeping onset and duration were measured following TS administration. Molecular docking was performed.

View More


Full Text 3 0 14

2

Tangeretin enhances sedative activity of diazepam in Swiss mouse through GABA_A receptor interaction: In vivo and in silico approaches

Analyze Results

Top Document Types



Patent Offices

PARTE 5. PATENTES (OPCIONAL)

Identificar una patente relacionada con el fármaco y describir su objetivo.

The screenshot shows the CAS SciFinder interface. At the top, there is a search bar with the text "Enter a query..." and a "Draw" button. Below the search bar, there is a "Return to Home" link and the text "References for 439-14-5". The main content area is divided into three panels:

- Filter Results:** On the left, there is a "Filter Results" panel with a "Filter by" button and an "Exclude" button. Below it, there is a "Search Within Results" section with a search box and a "Search" button. At the bottom, there is a "Document Type" section with checkboxes for "Journal (31K)", "Patent (2624)", and "Review (1234)".
- Search Results:** The main panel shows "Filtering: Document Type: Patent" and "2,624 Results". Below this, there is a "Sort: Relevance" and "View: Partial Abstract" dropdown. The first result is "1" and is titled "Pharmaceutical composition containing Perilla frutescens and Mentha piperita extract for preventing and treating sleep disorder". The abstract text reads: "The invention relates to a pharmaceutical composition for preventing or treating sleep disorders that improves sleep quality by reducing sleep latency and prolonging sleep duration in animal models, and thus can be effectively used as a composition for effectively improving sleep in which the composition is a natural substance with few side effects. The pharmaceutical composition for preventing or treating sleep disorders, comprising a mixture of a Perilla frutescens extract and a peppermint (Mentha piperita) extract as an active ingredient." Below the abstract, there are buttons for "PatentPak", "Full Text", and a "1" icon.
- Analyze Results:** On the right, there is an "Analyze Results" panel with a "Top Document Types" section. It contains a bar chart with a large purple bar labeled "Journal" and a smaller green bar labeled "Patent". Below the chart, there are buttons for "Patent", "Journal", "Report", "Review", and "Full Text".

Producto final a entregar

- Reporte corto que incluya:
 - Datos de la sustancia
 - Propiedades fisicoquímicas
 - Ruta sintética seleccionada
 - Análisis de literatura
 - Conclusiones farmacológicas