

CAS INNOVATIONS IN MAKING SCIENCE DISCOVERABLE

CAS SciFinder 2026

劉全哲 博士 Customer Success Manager

CAS

A division of the
American Chemical Society



What is a database?

- A collection of information organized in such a way that a computer program can quickly select desired pieces of data.

You can think of a database as an electronic filing system.

What do we need database?

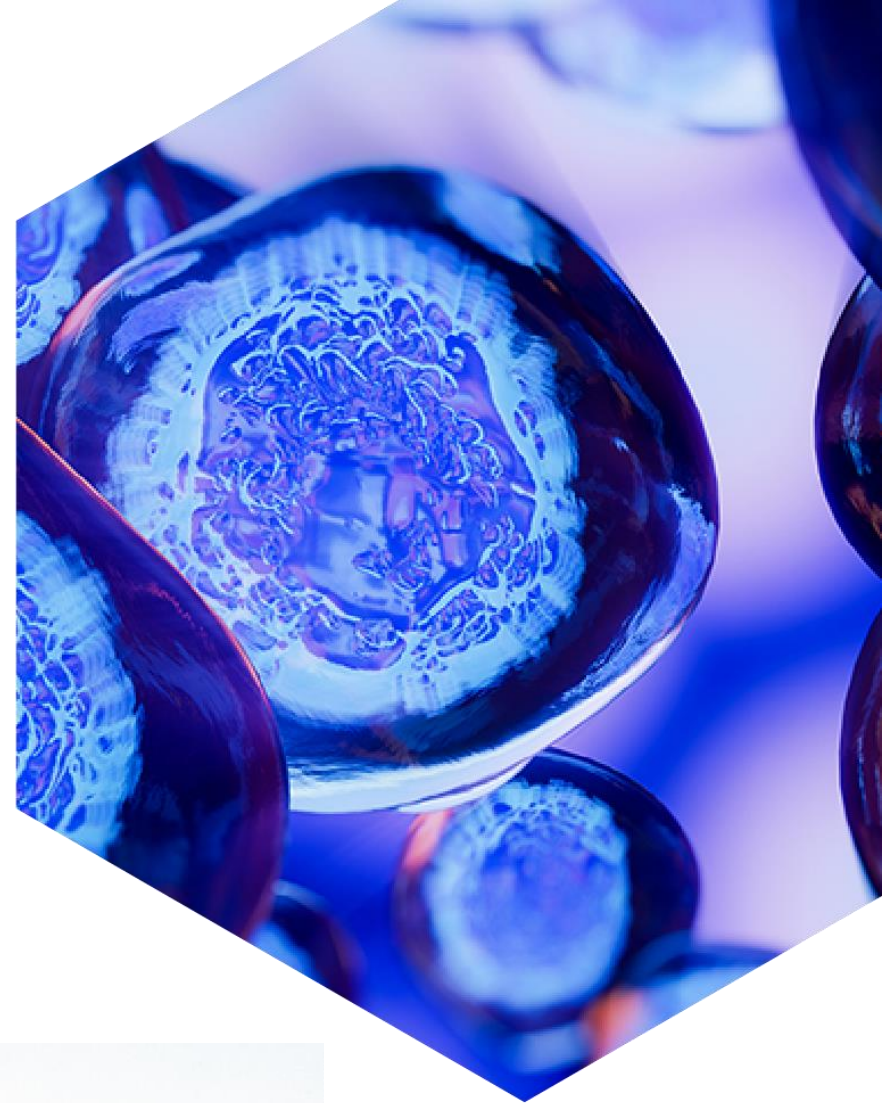
- Data is easier to manager
 - Too much data in one reference
 - Too many references
 - Too many language for reference
- Databases can better enforce data quality
- Leads to better data integration
- Databases are used to store, organize and retrieve data, quickly!!

About CAS

Founded in 1907, chemists around the world understood the value to research in aggregating scientific information.

Today we are a global organization of expert scientists, technologists, and business leaders with a long and successful history of harnessing scientific information to support valuable research insights.

Approximately 1,600 staff members – including CAS scientists, speaking 50 languages among them (600+ Ph.D. Scientists)



CAS connects you to the world's published science for better insights



Over
50K
scientific journals
and documents

Over
250
million substances

Over
50
languages
translated

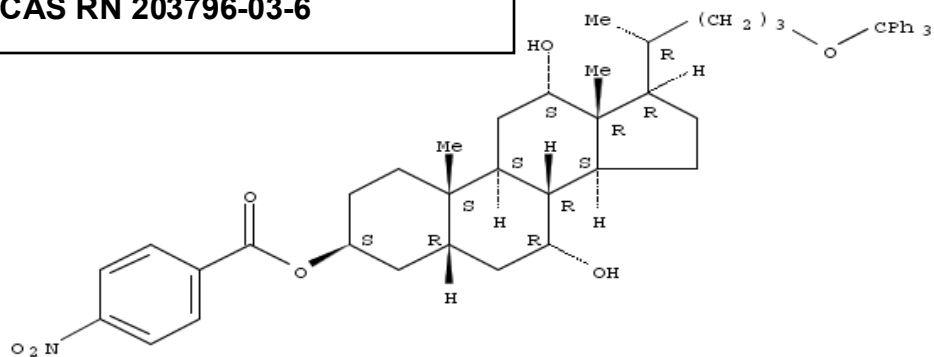
109
patent offices
worldwide

CAS scientists find the chemistry, and save you time!

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

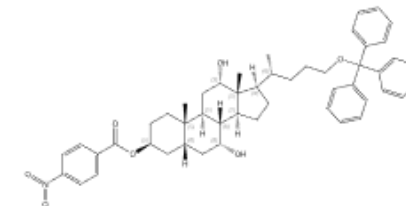
5 Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO₃ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na₂SO₄. The desired product (2.72 g, 85% yield) was obtained as white powder after
10 SiO₂ chromatography (Et₂O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529, 1489, 1448, 1345 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H) 5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98
15 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ¹³C NMR (CDCl₃, 75 MHz) δ 164.21, 150.56, 144.70, 136.79, 130.77, 128.88, 127.86, 126.98, 123.70, 86.47, 73.24, 73.00, 68.70, 64.22, 47.79, 46.79, 42.15, 39.76, 37.47, 35.52, 35.34, 34.23, 33.79, 32.46, 31.12, 28.74, 27.12 (thioglyce

CAS RN 203796-03-6



Absolute stereochemistry.

203796-03-6



Absolute stereochemistry shown

C₅₀H₅₉NO₇
Cholane-3,7,12-triol, 24-(triphenylmethoxy)-, 3-(4-nitrobenzoate), (3β, 5β, 7α, 12α)-

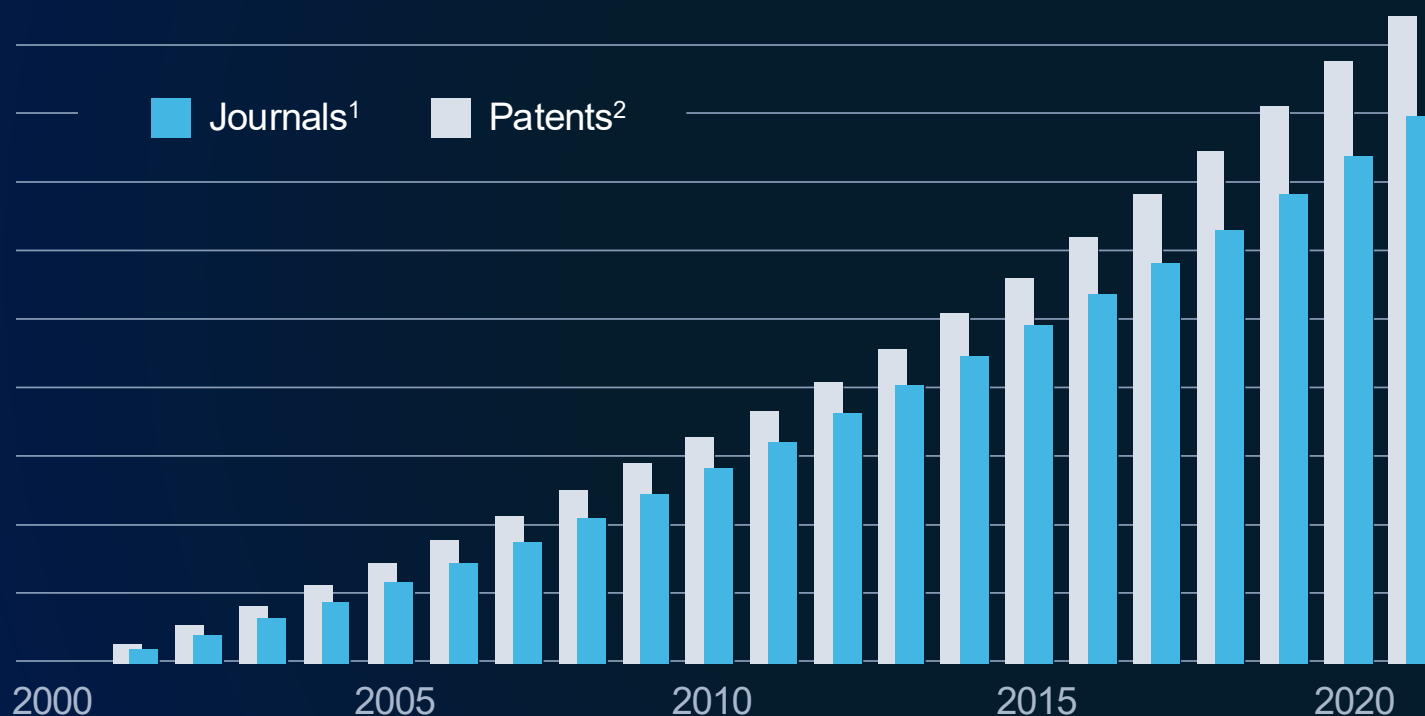
Role: Reactant, Synthetic Preparation, Reactant or Reagent, Preparation



American Chemical Society

The volume and complexity of scientific information is escalating exponentially

Growth of published science last 20 years



HIGH VOLUME

Limits holistic perspective

LACK OF CONSISTENCY

Hinders effective analysis

POOR COMPATIBILITY

Reduces digitalization ROI

1. Hanson, Mark & Gomez Barreiro, Pablo & Crosetto, Paolo; Brockington, Dan. (2023). The strain on scientific publishing. [10.48550/arXiv.2309.15884](https://arxiv.org/abs/10.48550/arXiv.2309.15884)

2. WIPO statistics database. Last updated: November 2023

Expanding our scientific domain coverage

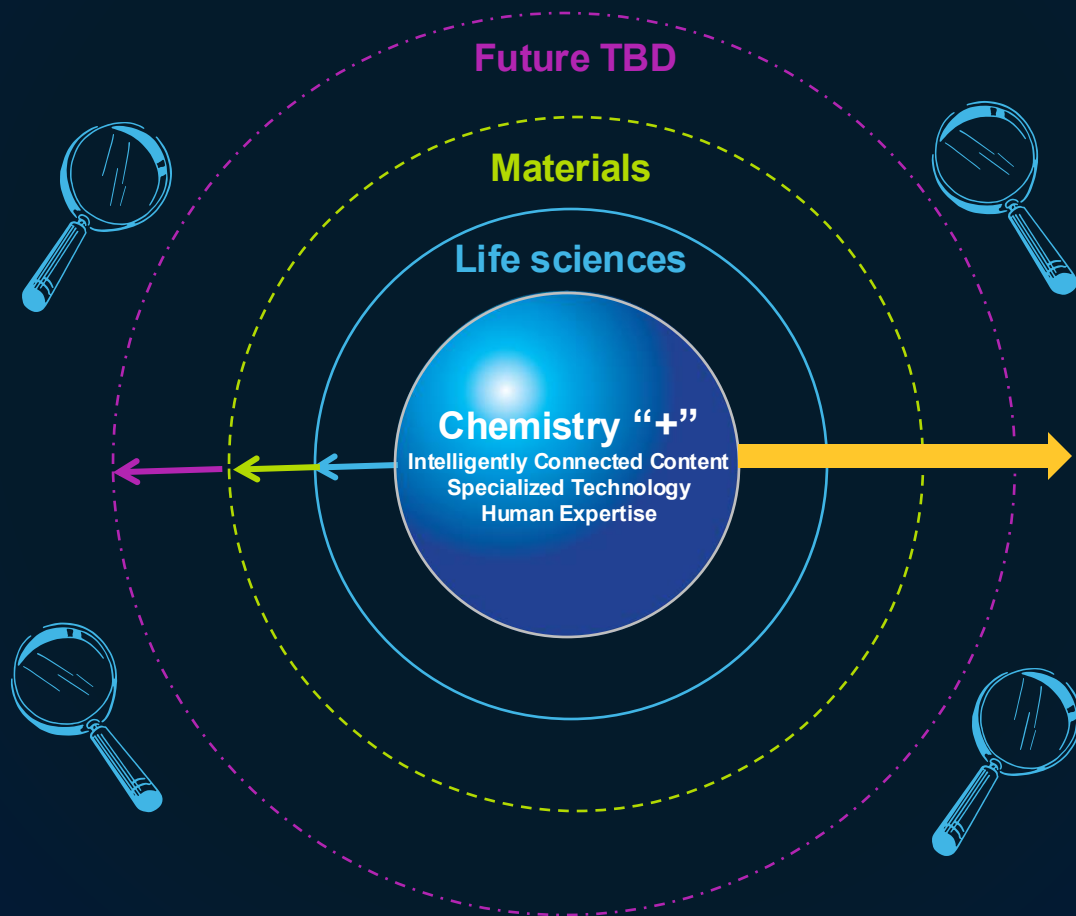
We are evolving to cover a gap in your research and decision-support needs

CAS SciFinder Discovery Platform™

- Synthesis planning
- Data confirmation
- Published research analysis

STN IP Protection Suite

- Synthesis planning
- Prior art search
- Data confirmation
- Published research analysis
- IP landscape



CAS BioFinder™

- Lead analysis and prioritization
- Toxicology projection
- Disease targeting

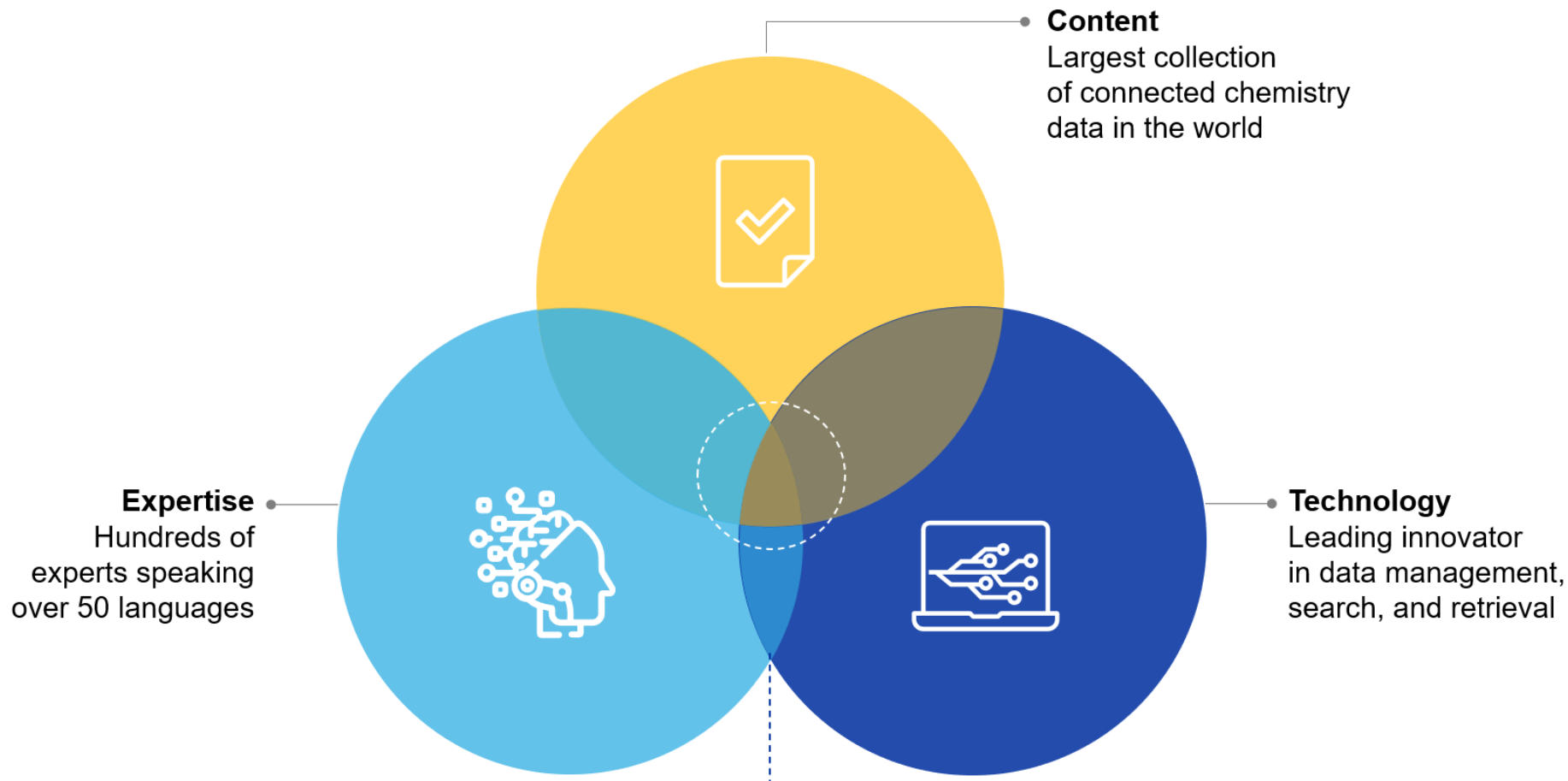
CAS Custom ServicesSM

- Premium/All-Access
- Internal/external data integration
- AI/ML predictive models
- Specialized solution development

Materials science solution (future)

- Applications
- Commercial analysis

CAS Custom Services: Maximizing the Strategic Impact of Scientific Information



We transform scientific data into actionable, evidence-based insights.

CAS Data Solutions for a Client-Focused Engagement

Content Management: Internal Data Discovery

*Do you know what you know?
Don't waste knowledge and
past investments*

Digitization

Data Extraction

Data Normalization

Taxonomies

System Search

Knowledge Management: Data Design

*Your research is generating
more data than ever, what to
do about it*

Substance Registry

Domain Modeling &
Governance

Structure Normalization

Data Migration

Content System Audit

External Data Connection

Prediction: AI

*AI should excite you, not
concern you. Make content
advances work for you*

Training Data Sets
(Algorithm Development)

Custom AI Data Curation

AI Data Support

Retrieval Augmented
Generation (RAG) Solutions

AI-Based Research Area
Assessments

Data-Enabled Risk Management

*Sci-information doesn't just
help innovate, it can also
protect your business*

Responsible Synthesis
Design

Substance Supply Chain
Analysis

Substance Regulatory
Status & Safety

Toxicology Literature
Review

Commercial Sourcing

Alternatives Analysis

Search

*Sometimes we all need an
extra set of experienced eyes
or additional help*

IP Custom Search

- Landscape
- State of the Art
- Freedom to Operate
- Novelty
- Pre-Patent Examination
- Written Opinions

And much more! Do you have an informatics project but don't see a corresponding CAS offering? We can explore your need, bring in an expert services team specialist, and we'll see if we can't help you ensure a successful project outcome!

For training purposes only. Do not distribute or present to customers at this time.

CAS SciFinder Discovery platform

*SciFinder

Top 5 key searching function

- Reference searching
- Reaction searching
- Substance searching
- Supplier searching
- Retrosynthesis

*CAS Formulation

*CAS Analytical Methods

The screenshot shows the CAS SciFinder Discovery platform interface. At the top, there is a navigation bar with the CAS SciFinder logo and a user profile for Titer C Liu. Below the navigation bar, a greeting says "Good Morning, Titer C". The main search area features a search bar with the text "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and a "Draw" button. Below the search bar, there is a dropdown menu for "Author/Inventor Name" with a placeholder text "Enter last name, first name middle name." and an example "Example: Schubert, J A". There is also a button to "Add Advanced Search Field". Below the search area, there is a "Featured Search" section with four cards: "Prior Art Discovery" (Discover prior art in patents and non-patent literature using AI-enhanced search technologies), "Patent Markush" (Search Patent Markush by structure and view associated references), "Retrosynthetic Analysis" (Make reaction plans with conditions, yields, catalysts, and experimental procedures), and "Search CAS Lexicon" (Build powerful searches using CAS concepts, chemical classes, and taxonomy). A "View All" link is visible on the right side of the featured search section.

Reference searching

CAS SciFinder halves the time needed to perform literature reviews*

The screenshot displays the CAS SciFinder web interface. At the top left is the CAS SciFinder logo. On the top right, there are notification and user profile icons, with the user name "Titer C Liu". Below the header, a navigation bar includes "All", "Substances", "Reactions", "References" (highlighted), and "Suppliers". A "For You" button with a "NEW" badge is also present. The main search area features a large search bar with the text "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." and a "Draw" button. Below the search bar, a dropdown menu is open for "Author/Inventor Name", showing options like "Authors/Inventors", "Publication Name", "Organization", "Title", "Abstract/Keywords", "Concept", "Substances", "Life Science Data", "Publication Year", "Document Identifier", and "Patent Identifier". The "Life Science Data" option is highlighted with a purple box. To the right of the dropdown, there is a text input field with the placeholder "Enter last name, first name middle name." and an "Example: Schubert, J A". Below the search area, there are three featured cards: "Patent Markush" (with a ribbon icon), "Retrosynthetic Analysis" (with a hexagonal icon), and "Search CAS Lexicon" (with a grid icon). A "View All" link is located to the right of these cards. The background of the interface is a dark blue abstract pattern.

CAS SciFinder halves the time needed to perform literature reviews*

Perform literature reviews

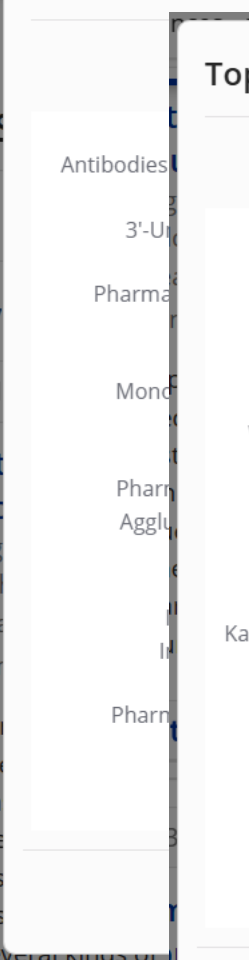
Keep up to date with the world's published scientific patent and journal literature across multiple disciplines using the most advanced relevance engine for scientific research.

- An easy-to-read display lets user quickly browse reference
- Filters are available to further narrow results...by year, source type, and organization

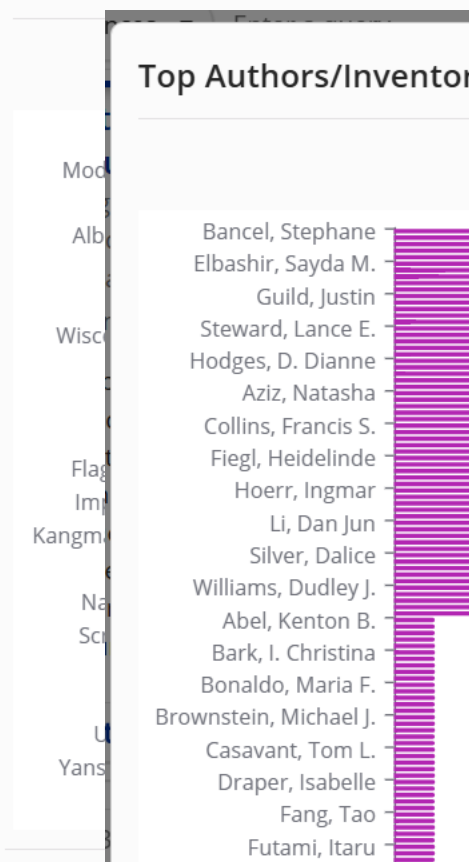
The screenshot displays the CAS SciFinder search results interface. On the left, a 'Filter Results' sidebar includes options for 'Analyze Results', 'Behavior' (Filter by/Exclude), and various filters like 'Search Within Results', 'Document Type', 'Substance Role', 'Organization', 'Publication Year', 'Language', 'Database', 'Publication Name', and 'Concept'. The main search results area shows 2,101 results, with the first result selected. The selected result is a patent titled 'Risperidone oral formulation from aqueous solution not containing sorbitol' by Janssen Pharmaceutica N.V. The abstract describes a stable aqueous solution of risperidone for oral administration. On the right, an 'Analyze Results' panel shows a bar chart of 'Top Document Types' (Journal, Review, Report, Patent, Clinical Trial) and 'Top Substance Roles'.

Result Analyze

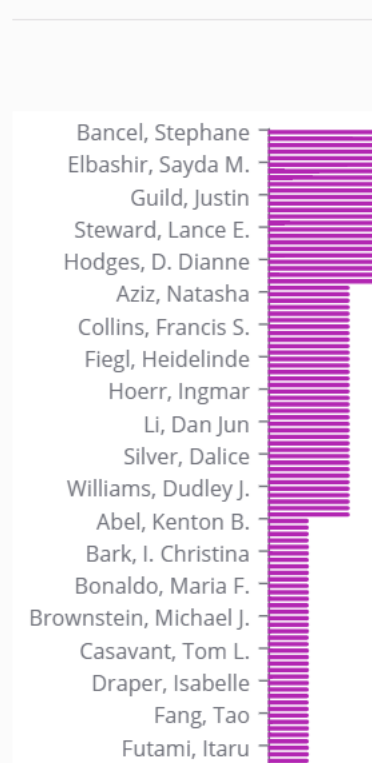
Top Concepts



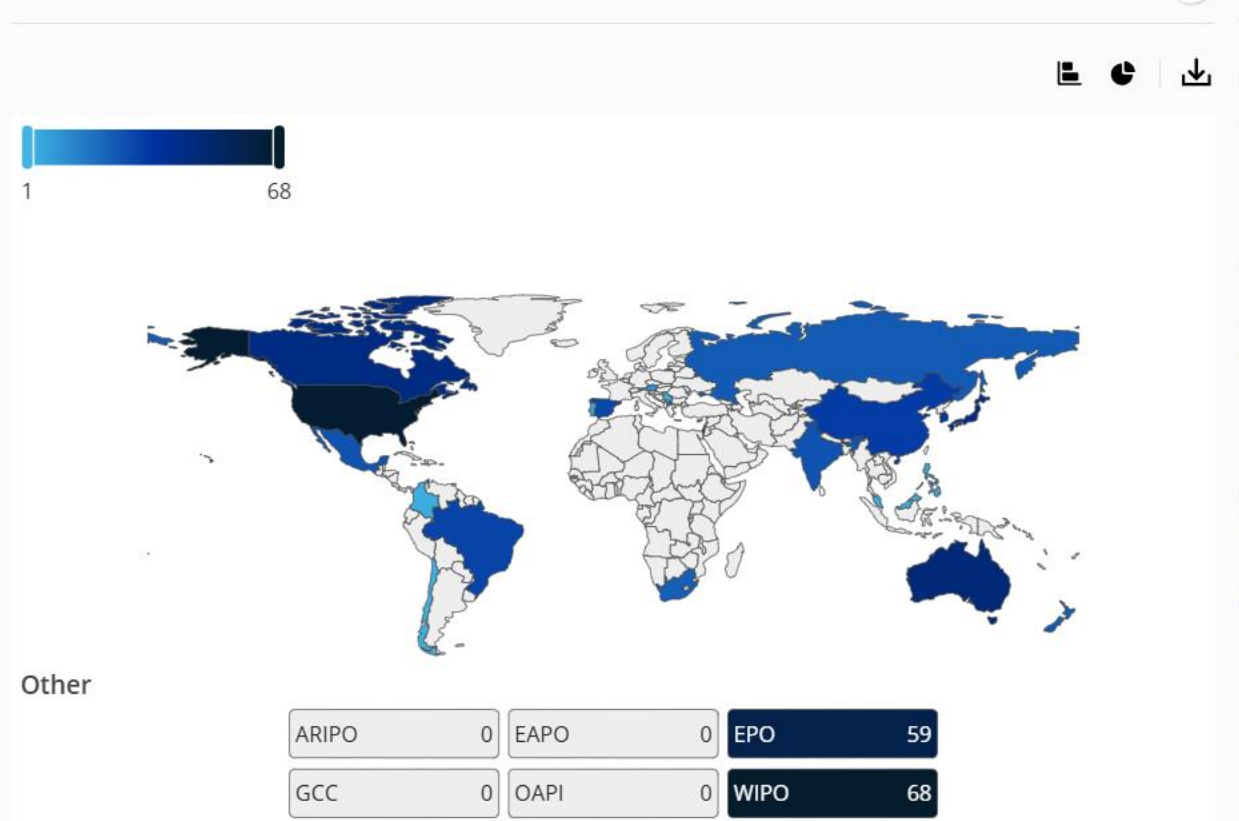
Top Assignees/Organizations



Top Authors/Inventors



Patent Offices



Process for preparation of risperidone

3 1 1 Citation Map



In this Patent

Inventors: Zhang, Guiling; Zhu, Yidong; Fan, Chuanwen; Zhang, Minghui; Wang, Jingyi

Patent Family

Patent

WO200

CN1013

CN1013

GB2464

GB2464

US2010

Priority

Priority

CN2007

WO200

Claims

Claims text

1 What

A ris

Chara

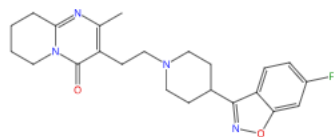
Classifications

Patent	Classification	Codes
WO2009012721 A1	IPCI	C07D 471/04
CN101353347 A	IPCI	C07D 471/04
	CPCI	C07D 471/04
CN101353347 B	IPCI	C07D 471/04
	CPCI	C07D 471/04
GB2464854 A	IPCI	C07D 471/04
	CPCI	C07D 471/04; C07D 471/04
GB2464854 B	IPCI	C07D 471/04
	CPCI	C07D 471/04; C07D 471/04
US20100130740 A1	IPCI	C07D 471/04

Substances

3

106266-06-2

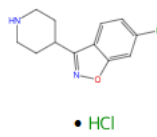


C₂₃H₂₇FN₄O₂

Risperidone

Role: Industrial Manufacture, Synthetic Preparation, Preparation

84163-13-3

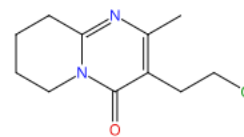


C₁₂H₁₃FN₂O.C1H

1,2-Benzisoxazole, 6-fluoro-3-(4-piperidinyl)-, hydrochloride (1:1)

Role: Reactant, Reactant or Reagent

63234-80-0



C₁₁H₁₅ClN₂O

4H-Pyrido[1,2-a]pyrimidin-4-one, 3-(2-chloroethyl)-6,7,8,9-tetrahydro-2-methyl-

Role: Reactant, Reactant or Reagent



PatentPak:

Why waste time slogging through dense patent material with direct access to and understanding of the chemistry within the document

Patent chemistry is fully annotated with structures, nomenclature and more!

The screenshot displays the PatentPak interface. At the top, there is a navigation bar with the PatentPak logo, page number (28/37), zoom controls, and download options (PDF, PDF+). The main content area is divided into two sections: 'Key Substances in Patent' on the left and 'CLAIMS' on the right. The 'Key Substances' section lists three substances with their CAS RNs and chemical structures. The first substance is CAS RN 2752-65-0. The second is CAS RN 81624-55-7. The third is CAS RN 81624-55-7, with the CAS Name: 1,2-Ethanediamine, N,N,N',N'-tetrakis[(6-methyl-1H-benzimidazol-2-yl)methyl]-. The 'CLAIMS' section contains six numbered claims. Claim 1 describes a pharmaceutical composition comprising at least one NPM inhibitor, at least one anti-cancer agent, and a pharmaceutically acceptable carrier. Claim 2 specifies the NPM inhibitor is an siRNA. Claim 3 specifies the NPM inhibitor is gambogic acid. Claim 4 specifies the NPM inhibitor is NSC 348884. Claim 5 specifies the anti-cancer agent is a target cancer therapy. Claim 6 specifies the target cancer therapy is sorefenib. Two purple boxes highlight specific locations: one around the chemical structure of the second substance, and another around the text 'NSC 348884' in claim 4, which has a location pin icon next to it.

Important chemistry locations are identified by CAS expert scientists

Substance searching

CAS SciFinder[®] Alerts 2 Saved Titer C Liu

Searching for...

- All
- Substances**
- Reactions
- References
- Suppliers
- Sequences
- Retrosynthesis

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Enter a query... Draw Q

Examples: C₆H₆ | (C₈H₈)_x | C₂₂H₂₆CuN₂O₅.C₂H₃N

Learn more about SciFinder[®] Advanced Search.

View All Search History

Feedback

Rerun Search

Recent Search History

May 5, 2023

- Substances** 11:46 AM

Molecular Formula ×

- Molecular Formula
- CAS Registry Number >
- Chemical Identifier >
- Document Identifier
- Patent Identifier
- Experimental Spectra** >
 - Proton NMR
 - Carbon-13 NMR
 - Nitrogen-15 NMR
 - Fluorine-19 NMR
 - Phosphorus-31 NMR
- Bioactivity Data **NEW** >
- Biological >
- Chemical Properties >
- Density >
- Electrical >
- Lipinski >
- Magnetic >
- Mechanical > 32)
- Optical and Scattering > e (160K), 192)

CAS SciFinder provides access to the world's most trusted substance resource, CAS REGISTRY®

Inform your research with the one true source for authoritatively identifying a chemical substance and its related chemical structures, chemical names, regulatory information, and properties, including the CAS Registry Number®, as well as reaction schemes, product yields and more.

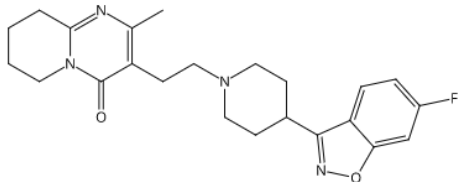
The screenshot displays the 'Substances' section of the CAS SciFinder interface, showing a grid of chemical entries. The interface includes a search bar, navigation tabs for 'References', 'Reactions', and 'Suppliers', and a 'Sort: Relevance' dropdown. The grid contains the following entries:

- 1821732-51-7**: 2-Azetidinone, 4-ethyl-4-methyl-, (4S)-. Absolute stereochemistry shown. 0 References, 0 Reactions, 1 Supplier.
- 39155-99-2**: 2-Azetidinone, 4-ethenyl-4-methyl-, (S)-. Absolute stereochemistry shown. 1 Reference, 0 Reactions, 1 Supplier.
- 39155-98-1**: 2-Azetidinone, 4-ethenyl-4-methyl-, (R)-. Absolute stereochemistry shown. 1 Reference, 0 Reactions, 3 Suppliers.
- 28982-78-7**: (C₇H₁₃NO)_x 2-Azetidinone, 4-methyl-4-propyl-, (+)-, polymers. Rotation (+). 1 Reference, 0 Reactions, 0 Suppliers.
- 45652-80-0**: 2-Azetidinone, 4-methyl-4-propyl-, (+)-. Rotation (+). 0 References, 0 Reactions, 0 Suppliers.
- 27063-09-8**: 2-Azetidinone, 4-methyl-4-propyl-, (-)-. Rotation (-). 0 References, 0 Reactions, 0 Suppliers.

Substances information

CAS Registry Number: 106266-06-2

References (13K) Reactions (218) Suppliers (122) [Download](#) [Email](#) [Save](#)



C₂₃H₂₇FN₄O₂
 4H-Pyrido[1,2-a]pyrimidin-4-one, 3-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-2-methyl-, (9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	410.49	-
Melting Point (Experimental)	170 °C	-
Boiling Point (Predicted)	572.4±60.0 °C	Press: 760 Torr
Density (Predicted)	1.38±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	8.07±0.10	Most Basic Temp: 25 °C

[Experimental Properties](#) | [Spectra](#)

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

Other Names and Identifiers

Experimental Properties

Property	Value	Condition	Source
Median Lethal Dose	29.7 mg/kg	Organism: rat; Route: intravenous	(1) APC
Median Lethal Dose	18.3 mg/kg	Organism: dog; Route: oral	(1) APC
Median Lethal Dose	14.1 mg/kg	Organism: dog; Route: intravenous	(1) APC
ADME (Absorption, Distribution, Metabolism, Excretion) - 16 Sources	See Full Text		(2-17) CAS
Half-Life (Biological) - 7 Sources	See Full Text		(18-24) CAS
LC50 - 1 Source	See Full Text		(25) CAS

Sources
 (1) (2000) 1280 pages, CAS

Structure Activity Relationships [CAS LIFE SCIENCES](#)

Absorption, Distribution, Metabolism, and Excretion Data [CAS LIFE SCIENCES](#)

Toxicity [CAS LIFE SCIENCES](#)

Target Function Parameter Disease Organism [Download](#)

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
5-HT2A receptors	-	5-HT2C receptor activity	19.7 nM	Schizophrenia	-	View Detail	(1) CAS
Adrenoceptor A1	-	α1 receptor activity	2.8 nM	Schizophrenia	-	View Detail	(1) CAS
Dopamine D3 receptors	-	D3 receptor activity	10.9 nM	Schizophrenia	-	View Detail	(1) CAS
HEK293 cells and Chang liver cells	Antagonist	IC50	>600 ug/ml	Depression	Mouse	View Detail	(2) CAS
HEK293 cells and Chang liver cells	Antagonist	IC50	238.8 ug/ml	Depression	Mouse	View Detail	(2) CAS
Histamine H1 receptors	-	H1 receptor activity	26.1 nM	Schizophrenia	-	View Detail	(1) CAS
-	-	Adiposity index	Ligand didn't show any significant difference in adiposity index	-	-	View Detail	(3) CAS
-	-	APO level	17.92 mg/kg	Schizophrenia	-	View Detail	(1) CAS
-	-	AUC	Ligand significantly increased AUC values	-	-	View Detail	(3) CAS
-	-	Behavior	1628.3 cm	-	-	View Detail	(3) CAS
-	-	Behavior	1573.7 cm	-	-	View Detail	(3) CAS
-	-	Behavior	0.21	-	-	View Detail	(3) CAS
-	-	Behavior	0.34	-	-	View Detail	(3) CAS
-	-	Behavior	0.38	-	-	View Detail	(3) CAS
-	-	Behavior	0.28	-	-	View Detail	(3) CAS
-	-	Behavior	0.40	-	-	View Detail	(3) CAS
-	-	Behavior	0.43	-	-	View Detail	(3) CAS
-	-	Behavior	47.3	-	-	View Detail	(3) CAS
-	-	Behavior	58.8	-	-	View Detail	(3) CAS
-	-	Behavior	2119.17 cm	-	-	View Detail	(3) CAS
-	-	Behavior	56.1	-	-	View Detail	(3) CAS
-	-	Behavior	62	-	-	View Detail	(3) CAS
-	-	Behavior	73.2	-	-	View Detail	(3) CAS
-	-	Behavior	65.8	-	-	View Detail	(3) CAS
-	-	Behavior	1778 cm	-	-	View Detail	(3) CAS
-	-	Behavior	1768.33 cm	-	-	View Detail	(3) CAS
-	-	Behavior	1937.2 cm	-	-	View Detail	(3) CAS

CAS SciFinder reduces the time needed to analyze the IP landscape*

Access industry-leading capabilities like patent Markush searching, and content such as patents that have been chemically annotated by our scientists, so you can stay on top of the technology landscape.

The screenshot displays the CAS SciFinder interface with a search results page. On the left, a 'Filter Results' sidebar is visible, showing options for 'Patent Markush Match' (As Drawn (54), Substructure (58)), 'Behavior' (Filter by, Exclude), and 'Patent Office' (World Intellectual Property Organization (22), Korea, Republic of (8), European Patent Organization (7), United States (7), China (5), View All). A 'CA Section' filter is also present. The main content area shows three results, each with a chemical structure and associated patent details:

- WO2020015665 Markush Details**
Semiconductor device and solar cell
Assignee: Toray Advanced Materials Research Laboratories (China) Co., Ltd.
World Intellectual Property Organization, WO2020015665 A1 2020-01-23 | Language: Chinese, Database: CAplus
Patent Status: ● Dead
Patent claim 4
Buttons: PatentPak, Full Text
Note: There are no notes to display for this structure.
- KR2066207 Markush Details**
Polyamic acid composition for polyimide and adhesive for flexible copper clad laminated film
Assignees: INNOX Advanced Materials Co., Ltd.; Korea Research Institute of Chemical Technology
Korea, Republic of, KR2066207 B1 2020-01-14 | Language: Korean, Database: CAplus
Patent Status: ● Alive
Patent claim 1
Buttons: PatentPak, Full Text
31: alkyl <containing 1-5 C>
96: alkyl <containing 1-5 C>
- KR2090193 Markush Details**
Polyamic acid composition for polyimide as adhesive for flexible copper foil laminated film
Assignees: INNOX Advanced Materials Co., Ltd.; Korea Research Institute of Chemical Technology
Korea, Republic of, KR2090193 B1 2020-03-17 | Language: Korean, Database: CAplus
Patent Status: ● Alive
Patent claim 1
Buttons: PatentPak, Full Text
91: alkyl <containing 1-5 C>

Reaction: Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus

The screenshot displays a web interface for a chemical reaction database. On the left is a sidebar with various filters. The main area shows a reaction scheme for the synthesis of a complex molecule. Below the scheme are two identical 'Reaction Summary' panels, each with a table of reagents, catalysts, solvents, and conditions. To the right of these panels is a text block providing a reference for the reaction.

Structure Match

- As Drawn (5)
- Substructure (18)

Filter by

- Substance Role
 - Product (13)
 - Reactant (5)
- Yield
 - 90-100% (4)
 - 80-89% (2)
 - 70-79% (4)
 - 50-69% (1)
 - 30-49% (2)
- Number of Steps
 - 1 (13)
- Experimental Protocols
 - MethodsNow Available (2)
 - Procedure Available (6)
- Reaction Type
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes

Source Reference

- Publication Year
- Document Type
- Language

Reactions (13)

References

View - Select -

📄 📧 ★ Save

Scheme 1 (2 Reactions) View

CCOC(=O)C(COC(=O)C)C(=O)OCC + C1=CC=CC=C1O >> CCOC(=O)C(COC(=O)C)C(=O)OCC1=CC=CC=C1O

Steps: 1
Yield: 92%

🛒 Suppliers (3) 🛒 Suppliers (6)

Reaction Summary

Reagents	Sodium acetate Acetic acid, manganese(3+) salt (3:1)	Steps: 1 Yield: 92%
Catalysts	-	
Solvents	Acetic acid	
Conditions	-	

[View Reaction Detail](#) | [Experimental Protocols](#)

Carbon-carbon bond-forming reactions promoted by trivalent manganese
[View Reference Detail](#)
By: Melikyan, Gagik G.
Organic Reactions (Hoboken, NJ, United States) (1997).
No pp. given
[Full Text](#)

Reaction Summary

Reagents	Sodium acetate Acetic acid, manganese(3+) salt (3:1)	Steps: 1 Yield: 92%
Catalysts	-	
Solvents	Acetic acid	
Conditions	-	

[View Reaction Detail](#) | [Experimental Protocols](#)

[View 2 Reactions](#)

[Collapse Scheme](#)

Intuitive information layouts fosters quick comprehension

Design efficient bench strategies and work plans

Find practical methods and pathways for production synthesis, extracted directly from the literature.

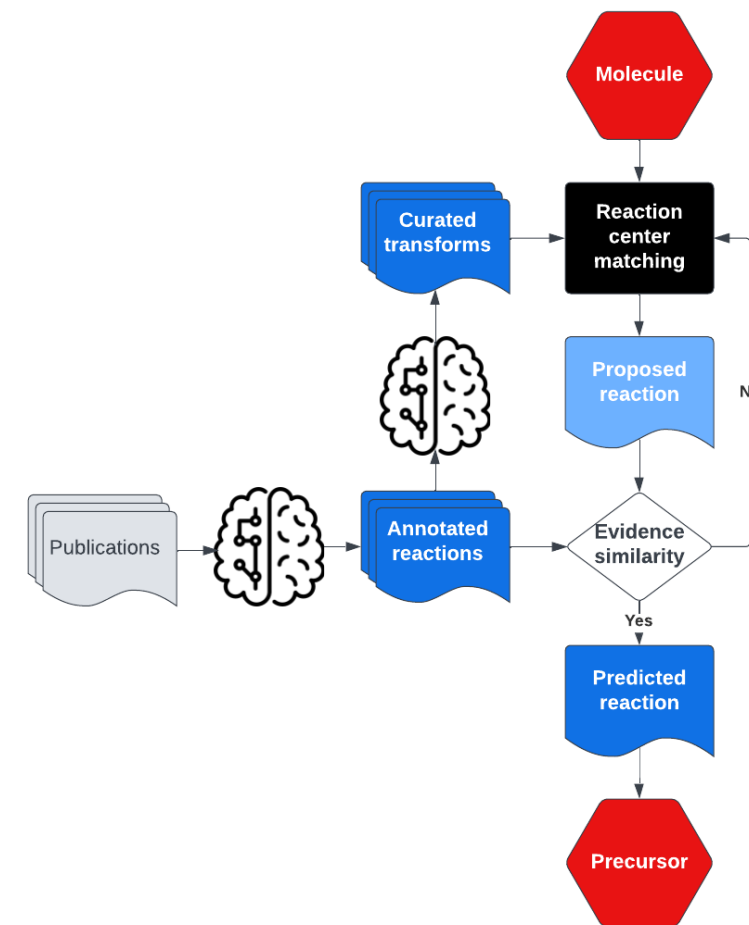
Identify opportunities for new breakthroughs in synthetic methods.

Experimental Protocols	
Synthetic Methods	
Products	Ruthenium, carbonylchloro[2-[1-(hydroxy-κO)-2-naphthalenyl]-1-diazene-carbothioamidato-κN ² ,κS] (triphenylphosphine)-, Yield: 80%
Reactants	Carbonylchlorohydrotris(triphenylphosphine)ruthenium 2-(1-Oxo-2(1H)-naphthalenylidene)hydrazinecarbothioamide
Solvents	Benzene
Procedure	<ol style="list-style-type: none">1. Add the appropriate ligand (0.023-0.029 g, 0.1 mmol) in 1:1 M ratio to a solution of Ruthenium(II) complex (0.1 g, 0.1 mmol) in benzene (20 cm³).2. Heat the mixture under reflux for 5 h on water bath.3. Concentrate the resulting solution to 3 cm³.4. Precipitate the product by the addition of petroleum ether (60-80 °C).5. Recrystallize the mixture using CH₂Cl₂.6. Dry the residue under vacuum to obtain the product.
Transformation	Aromatization of Six-Membered Rings Coordination of a Metal to Carbon and Heteroatom Ligand Substitution
Characterization Data	
▼ Ruthenium, carbonylchloro[2-[1-(hydroxy-κO)-2-naphthalenyl]-1-diazene-carbothioamidato-κN ² ,κS] (triphenylphosphine)-	
CAS Method Number 3-478-CAS-9063944	

Retrosynthesis – How it works

Evidence based validation of predictive chemistry

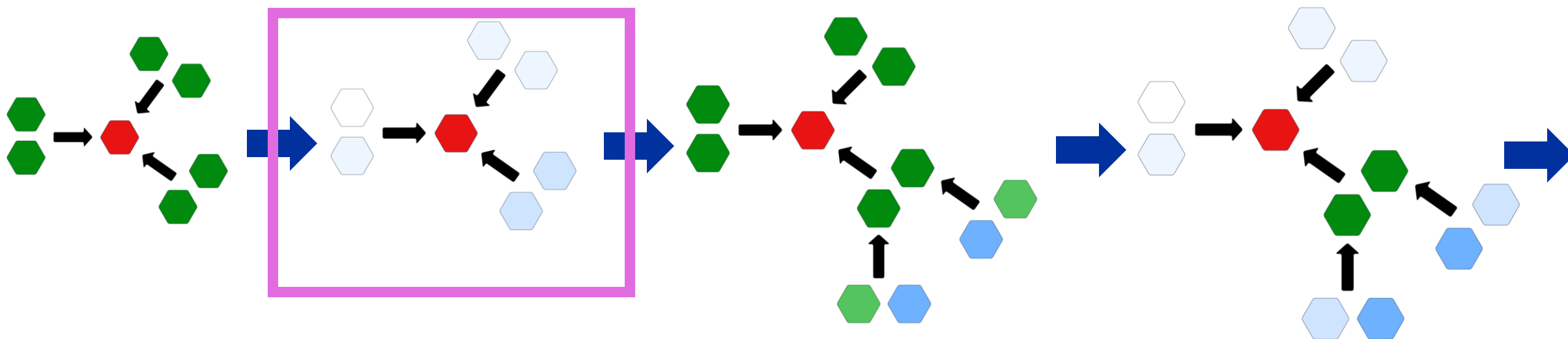
- CAS Reactions are used to generate all potential predicted reactions, then used again to provide specific evidence to evaluate each proposed reaction.
- Similarity to published chemistry is the criteria for accepting predicted reactions.
- Displayed evidence is ordered by relevance to that specific predicted reaction.



Retrosynthesis – How it works

Route guidance by substance-trained AI model

At each step, the top alternatives are selected by synthetic accessibility inference scores.



Explore the best directions for finding starting materials

Innovate with retrosynthesis plans in real time

Retrosynthesis plans are generated in real-time for both experimental and predictive targets.

Review and evaluate plan steps and alternatives collaboratively, accelerating innovation.

View evidence directly within your plan, enabling precise comparison of alternative predictive synthetic pathways.



Retrosynthesis – Interactive Search

Real time results

Retrosynthesis Plan Options for drawn structure

Set Rules Supporting Predicted Reactions [Learn more](#)

Common

Uncommon (includes common rules)

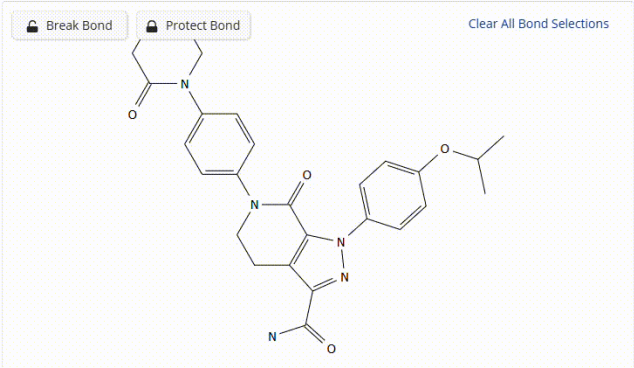
Rare (includes common and uncommon rules)

Set Starting Materials Cost Limit [Learn more](#)

USD/mol

[Continue to Retrosynthesis Plan](#)

Break and Protect Bonds (Optional)
Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. [Learn more](#)



First in the world real-time retrosynthesis planning!

Our solutions are continuously evolving

CAS SciFinder powered by AI

Good Evening, Aurora

What are you looking for? Draw Q

- Exploratory Search**
Search similar patents and non-patent literature powered by AI-enhanced technology.
- Patent Markush**
Lorem ipsum dolor sit amet consectetur. Nulla cras mi dui aliquet tincidunt.
- Advanced Search**
Search methods using criteria like keywords, analytes, matrices, and more.

History For You

Prior Art Discovery ensures researchers can find relevant prior art leveraging proprietary AI trained by CAS experts

Our solutions are continuously evolving

CAS SciFinder powered by AI

The screenshot displays the CAS SciFinder web interface. At the top left is the CAS SciFinder logo. A search bar contains the text 'Draw' and a magnifying glass icon. Below the search bar, there are tabs for 'History' and 'For You', with 'For You' being the active tab. The main content area is titled 'Your Content Recommendations' and features a grid of eight article cards. Each card contains a title, a brief description, and citation information (journal name, volume, issue, year, language, and database). The cards are arranged in two rows of four. The first row includes articles on TADDOL-derived catalysts, bitter taste mechanisms, organometallic peptide libraries, and anti-tuberculosis activity. The second row includes articles on air quality implications, graphene thermal conductivity, exercise capacity decline, and indoor PV device testing. Each card has a three-dot menu icon in the bottom right corner.

CAS SciFinder

Draw

History **For You**

Your Content Recommendations

- Application scope and limitations of TADDOL-derived chiral ammonium salt phase-transfer catalysts.**
Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Possible novel mechanism for bitter taste mediated through cGMP**
Journal of neurophysiology (1999), 18(4), 3432-34 | Language: English, Database: MEDLINE
- The development of organometallic OBOC peptide libraries and sequencing of N-terminal rhenium(...)**
Canadian Journal of Chemistry (2015), 18(4), 3432-34 | Language: English, Database: CAplus
- Design, synthesis and anti-tuberculosis activity of 1-adamantyl-3-heteroaryl ureas with...**
Bioorganics & Medicinal Chemistry(2013), 18(4), 3432-34 | Language: English, Database: CAplus and MEDLINE
- Air quality implications of the Deepwater Horizon oil spill**
Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Thermal Conductivity of Graphene in Corbino Membrane Geometry**
Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Only slow decline in exercise capacity in the natural history of patients with congenital heart dise...**
Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE
- Indoor PV devices testing**
Molecules (Basel, Switzerland)(2013), 18(4), 3432-34 | Language: English, Database: MEDLINE

- Natural language search
- Personalized recommendations
- Scientifically accurate summaries

AI-powered Result Summaries!

CAS SciFinder NSAID use in geriatric dogs

AI Summary

Based on the search results, here's a summary of key findings related to nsaid and geriatric and dogs:

The search results encompass a wide array of studies focusing on the use of non-steroidal anti-inflammatory drugs (NSAIDs) in geriatric dogs, ranging from their effectiveness in managing pain and arthritis to their impact on anesthesia and recovery. Key findings include the successful use of NSAIDs like firocoxib for pain management in geriatric dogs over extended periods, the importance of careful monitoring and dosage adjustments when administering NSAIDs to elderly dogs, and the potential for NSAIDs to cause adverse effects such as gastrointestinal disturbances. Additionally, the studies highlight the need for comprehensive pain management strategies that may include NSAIDs alongside other treatments, and the necessity of considering the unique physiological characteristics of geriatric dogs when prescribing medications.

Key Findings:

- 1. NSAID Use for Pain Management:**
 - Firocoxib (Previcox) is effective in managing pain associated with osteoarthritis in geriatric dogs for up to 90 days (2)
- 2. NSAID Effects on Kidney Function:**
 - Acute kidney injury (AKI) has been observed in young dogs after general anesthesia for non-emergency surgeries, but no clear connection to NSAIDs was identified (3)
- 3. NSAID Impact on Cartilage Metabolism:**
 - Some NSAIDs may have a negative impact on cartilage metabolism, while others might not affect it or could even have a slight positive effect
- 4. NSAID Safety During Anesthesia:**
 - Statement 1: A study found that the use of an antiemetic protocol including maropitant, famotidine, and fentanyl in geriatric dogs resulted in vomiting, nausea, and aspiration pneumonia
- 5. NSAID Alternatives and Complementary Therapies:**
 - A study evaluated the effectiveness of Ashwagandha combined with TENS (Transcutaneous Electrical Nerve Stimulation) for managing osteoarthritis in geriatric dogs, suggesting potential alternatives to NSAIDs
- 6. NSAID Formulation Development:**
 - Carprofen microspheres have been developed as a controlled-release formulation for the administration of carprofen, a non-steroidal anti-inflammatory drug (NSAID) commonly used in geriatric dogs to alleviate arthritis symptoms. This formulation aims to improve the therapeutic efficacy and reduce side effects associated with traditional NSAID treatments
- 7. NSAID Pharmacology and Efficacy**
 - Many NSAIDs have been shown to be effective in inhibiting gastric acid secretion in dogs

Twelve previously healthy non-geriatric dogs present for acute kidney injury after general anaesthesia for non-emergency surgical procedures in the UK. The Journal of small animal practice (2020), 61(6), 363-367 | Database: MEDLINE

Are these the results you're expecting to see? Was this helpful?

CAS SciFinder AI is always improving. [suggest improvements](#) or [learn more.](#)

References

- **References by Author**

- *Query Examples:*

- smith, john

- john smith on MEIS1 gene

- **References by Journal**

- *Query Example:* documents published in jacs

- **References by Document Type**

- *Query Example:* patents about waterborne coating

Substances and Their Properties

Search for a substance by property or a substance's physical, experimental, and predicted properties using simple keywords, with or without Boolean operators, and natural language

– *Example queries:*

- amines with boiling point <100
- what is the glass transition point of PMMA
- boiling point of 79-09-4
- benoxaprofen median lethal dose
- ketones with H acceptors >2
- acids with pKa <0.5
- substances that self-ignite over 70 F
- compounds with melting point between 114.6-115.5 degrees C

- ibuprofen carbon nmr
- spectra of benzene
- 51234-28-7 spectra
- Visible Absorption Spectrum of CH₂Cl₂
- GHS data for toluene
- where can I find the regulation information on sulfur dioxide
- how hazardous is the chemical nitrogen dioxide
- safety regulations for chlorine
- benzene cost
- cost of 51234-28-7
- who sells acetone
- where to buy triostin a
- source for 1,2,4-trimethylbenzene

Reaction

- *Water as a solvent for synthesis of toluene*
- What can I synthesize with Fmoc-Gly-OH and iron catalyst?
- Chromium dichloride catalyzed Nozaki-Hiyama-Kishi reactions
- how to synthesize benzenamine, 3-methoxy- with copper catalyst
- protocols to make toluene catalyzed by copper
- how to make ibuprofen
- suzuki coupling procedures
- synthesis of ibuprofen with 80-86% yield with PdCl_2 catalyst
- Water as a solvent for synthesis of toluene with high yield
- Michael addition yield = 80

Sequence Search

Why is it important to an Academic Account

Sequences are important for investigators to probe...

- Underlying genomic and proteomic mechanisms.
- Answer questions associated with physiological phenomena, pathological conditions, environmental sciences, agricultural inventions, etiological factors...

CAS provides the world's largest biosequence collection and integrated BLAST/CDR/Motif searching.

- >70M biosequences curated by CAS scientists.
- >700 million additional proteins and nucleotides.

CAS SciFinder Discovery Platform for Molecular Biologists

Enhancing biological research with biosequence searching in SciFinderⁿ

UNMATCHED CONTENT

Newly enhanced collection of 700M+ proteins and nucleotides from 60+ patent authorities dating back to 1957

SPECIALIZED TECHNOLOGY

Multiple search options to support your sequence search needs, including BLAST, CDR search for antibody and T-cell receptors, and Motif search

HUMAN EXPERTISE

Human and machine-curated biosequence collection including sequences not found in electronic sequence listings and other databases

The screenshot displays the 'Biosequences' search interface. On the left, a 'Searching for...' sidebar lists categories: All, Substances, Reactions, References, Suppliers, and Biosequences (highlighted). The main area is titled 'Biosequences' and includes a search input field with a sample sequence: ATCGATCCAGATCGACTAGCTACGATCGATCGACTAGCTAGCATCAGTACGATCGATTACGGGGCTAGCATAGCTACGACTAGATCGATCGACUATCGATCCGUACT. Below the input are tabs for 'BLAST', 'CDR', and 'Motif', along with 'Upload Sequence' and 'Clear Search' buttons. On the right, search parameters are set: 'Sequence Type' is 'Nucleotide', 'Search Within' is 'Nucleotides', and 'Search Databases' includes 'CAS Biosequences' and 'NCBI Public Database'. The 'Limit Total Sequence Results to:' is set to 100. An 'Advanced Biosequence Search' section contains various parameters: 'Sequence Identity %' (100), 'Query Coverage %' (100), 'BLAST Algorithm' (MegaBlast), 'Match with Gaps?' (Yes), 'Word Size' (28), 'E-Value' (10), 'Gap Costs' (Linear), 'Reward for Match, Penalty for Mismatch' (-2), and 'Exclude Low Complexity Regions' (No). A 'Start Biosequence Search' button is at the bottom right.

CAS SciFinder Discovery Platform for Analytical Chemists

CAS Analytical Methods is a single source for in-depth scientific methods

- Save time with easy access to method details from millions of disclosed procedures
- Compare analytical methods side-by-side to understand key similarities and differences
- Organize experimental details in an easy-to-read format
- Get materials, instrumentation, and conditions

The screenshot displays the CAS SciFinder Discovery Platform interface. On the left, there is a sidebar with search filters: 'Analyte' (Palmitic acid (24), Stearic acid (22), Oleic acid (21), Arachidonic acid (19), Linoleic acid (18)), 'Matrix' (Blood plasma (24), Blood serum (2)), 'Method Category', 'Technique', and 'Year'. A 'Return to Advanced Search' link is at the top of the sidebar. The main area shows 'Results (24)' with a 'Sort Relevance' dropdown. A single result is displayed: 'Analysis of Palmitic acid in Blood plasma by High-performance liquid chromatography-mass spectrometry' with CAS MN: 2-107-CAS-39800. The result includes buttons for 'View Details & Instructions' and 'Add to Compare'. Below the title, a table lists key details: Analyte (Palmitic acid; Heptadecanoic acid; Fatty acids), Matrix (Blood plasma), Other Materials (Material: Ascentis C18 (2.7 μm, 2.1 x 150 mm) column), Method Category (Bioassay), Technique (High-performance liquid chromatography-mass spectrometry; Extraction), and Equipment Used (Liquid chromatography (LC) system; mass spectrometer (MS); Speed Vac).

Test and validate innovations

Search and filter hundreds of thousands of analytical methods extracted from published references to find the best option for your work.

CAS Method Number 1-101-CAS-433277	Method Category Active Pharmaceutical Ingredient and Metabolite Analysis	Technique Photodiode array detectors; Reversed-phase HPLC		
Analyte Nintedanib	Matrix -	Material YMC Pack C18 column (size: 250 x 4.6 mm; 5 µm particle size)	Reagent -	Biological Reagent -
Equipment Used LC system, Shimadzu Solvent delivery pump, Shimadzu Degasser, Shimadzu Autosampler, Shimadzu Column thermostat, Shimadzu Pump, LC-20AD XR, Shimadzu Autoinjector, SIL-20AC XR, Shimadzu PDA detector, SPD-M20A, Shimadzu		Instructions Preparation of stock and standard solutions <ol style="list-style-type: none">1. Transfer an accurately weighed 25 mg of nintedanib into 25 mL volumetric flask.2. Add sufficient amount of diluent (acetonitrile:water (90:10)) to dissolve it and dilute up to 25 mL to obtain 1000 µg/mL concentrations.3. Transfer an aliquot of 5 mL from the stock solution into 50 mL volumetric flask and dilute volume up to 50 mL with diluent to obtain 100 µg/mL concentrations.4. Transfer an aliquots of stock solution (1.75, 2.5, 3.75, 5.0, 6.25 and 7.5 mL) separately into 50 mL volumetric flasks and dilute to volume 50 mL with diluent to obtain 25, 50, 75, 100, 125 and 150 µg/mL concentrations. Reverse phase high performance liquid chromatography (RP-HPLC)-photo diode array (PDA) detection <ol style="list-style-type: none">1. Perform high performance liquid chromatography using LC system (Make & Model: Shimadzu; pump: LC-20AD XR, auto injector: SIL-20AC XR, PDA detector: SPD-M20A) equipped with binary solvent delivery pump, degasser, autosampler and column thermostat using Empower Software (Version 3, Future release 1).2. Carry out chromatographic separation using YMC Pack C18 column (size: 250 x 4.6 mm; 5 µm particle size).3. Set the column oven temperature at 25 °C.4. Use water pH 3.0 with orthophosphoric acid as mobile phase A and acetonitrile as mobile phase B.5. Set the gradient program as follows: time: 00:00; mobile phase A: 50; mobile Phase-B: 50; time: 04:00; mobile phase A: 50; mobile phase-B: 50; time: 05:00; mobile phase A: 0; mobile Phase-B: 100; time: 09:00; mobile phase A: 0; mobile phase-B: 100; time: 09:10; mobile phase A: 50; mobile Phase-B: 50; time: 12:00; mobile phase A: 50; mobile Phase-B: 50.6. Set the flow rate at 1.0 mL/min.7. Inject 10 µL of sample.8. Detect the sample at 210 nm.		
Conditions Instrument column: YMC Pack C18 column (size: 250 x 4.6 mm; 5 µm particle size); column oven temperature: 25 °C; mobile phase A: water pH 3.0 with orthophosphoric acid; mobile phase B: acetonitrile; flow rate: 1.0 mL/min; injection volume: 10 µL detection wavelength: 210 nm		Validation Linearity Range 25 - 150 µg/mL		
Source				

CAS Analytical Methods

Why is it important to an Academic Account?

Collection of diverse methods indexed to help solve chemical problems or teach research techniques.

Procedures from +5000 journals & peer reviewed publications.

- Including top journals like: Food Chemistry, Analytical Chemistry, and Analyst.

Coverage spans from wastewater analysis to active pharmaceutical ingredient analysis.

- Step-by-step methods curated by CAS and formatted to take into the lab.
- Easily locate relevant methods.
 - Advanced search, faceting, and compare options.

CAS SciFinder Discovery Platform for Formulation Scientists

Develop safe and effective products with CAS Formulus®

FASTER ITERATION

Understand a formulation's effectiveness with quick access to the best information for active ingredients and excipients

MORE EFFICIENCY

Get insights beyond literature and interact with formulations data curated from patents, journals, and product inserts more effectively

COMPREHENSIVENESS

Evaluate ingredients, find alternative suppliers, and explore regulatory requirements in one easy interface

The screenshot displays the CAS Formulus web interface. At the top, the logo 'CAS Formulus' is on the left, and navigation links for 'Help & Support', 'History', and 'Account' are on the right. Below the header, there are two main sections: 'Search for' and 'Create a Formulation'. Under 'Search for', there are two buttons: 'Formulations' (highlighted in blue) and 'Ingredients'. Under 'Create a Formulation', there is a blue button labeled 'Launch Formulation Designer'. To the right of these buttons is a search input field with a magnifying glass icon and a search button. Below the search field, there is a text prompt: 'Search for Formulations by Ingredient, Purpose, Form, Function, etc.' and a link to 'Try Advanced Search for a more precise search experience'. At the bottom right, a light blue box contains text: 'Formulation Designer uses our highly curated content collection to provide you with a template based on your selections for industry, purpose, physical form, and active/featured ingredients.'

Develop differentiating formulations and manufacture-to-scale

Evaluate a formulation's effectiveness with quick access to the best information for active ingredients and excipients.

Formulations

Formulations (1,530,182) | Suggested References | Sort: Relevance

Filter by

- Industry
 - Agrochemical
 - Cosmetics & Personal Care
 - Pharmaceutical
- Purpose
 - Hair dyes (115K)
 - Pharmaceutical formulations (79K)
 - Drug delivery systems (68K)
 - Cosmetics and Personal care products (52K)
 - Antitumor agents (42K)
- Physical Form
 - Tablets (187K)
 - Solutions (121K)
 - Liquids (68K)
 - Capsules (43K)
 - Gels (39K)
- Information Included
 - Component Amount (1.4M)
 - Process (771K)

View All

Montelukast Sodium Chewable Tablets: Antiasthmatics

Location: Article Table 1
Purpose: Antiasthmatics
Target: Asthma, Homo sapiens
Delivery Route: Oral drug delivery systems
Physical Form: Tablets

Component	Function	Amount Reported
Cyclopropaneacetic acid, 1-[[[(1 <i>R</i>)-1-[3-[(1 <i>E</i>)-2-(7-chloro-2-quinolinyl)ethenyl]phenyl]-3-[2-(1-hydroxy-1-methylethyl)phenyl]propyl]thio]methyl]-, sodium salt (1:1)	-	5 mg
Sodium carboxymethyl starch	disintegrant	10 mg
Mannitol	excipient	307.5 mg
modified karaya gum	diluent	150 mg

Additional components reported

View Formulation Detail

12 Similar Formulations - View All (opens in a new window)

Journal: Preparation and evaluation of montelukast sodium chewable tablets using modified karaya gum
Pharmacia Sinica
Language: English
View Reference Detail

Thank you !

謝謝 !

For more information

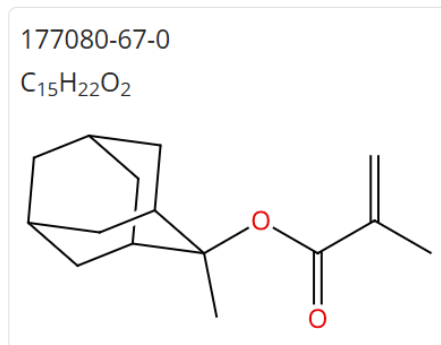
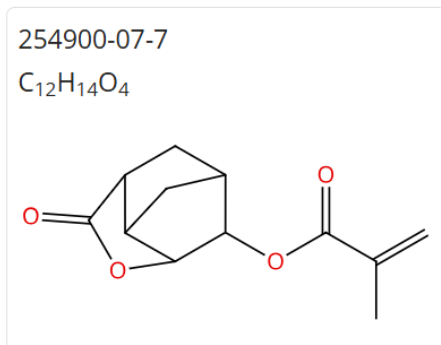
CAS Representative Office

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+886-975-765358



- 請查詢貴單位發表,並限制在2025年以後的文獻.
- 含有Mo金屬的所有物質,特別是有機金屬化合物.
- 高分子搜尋



- 抗凝血藥物 Apixaban的分析方法與逆合成分析
- What is the advantage of Perovskite Solar Cells?