

劉全哲
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CAS SciFinderN

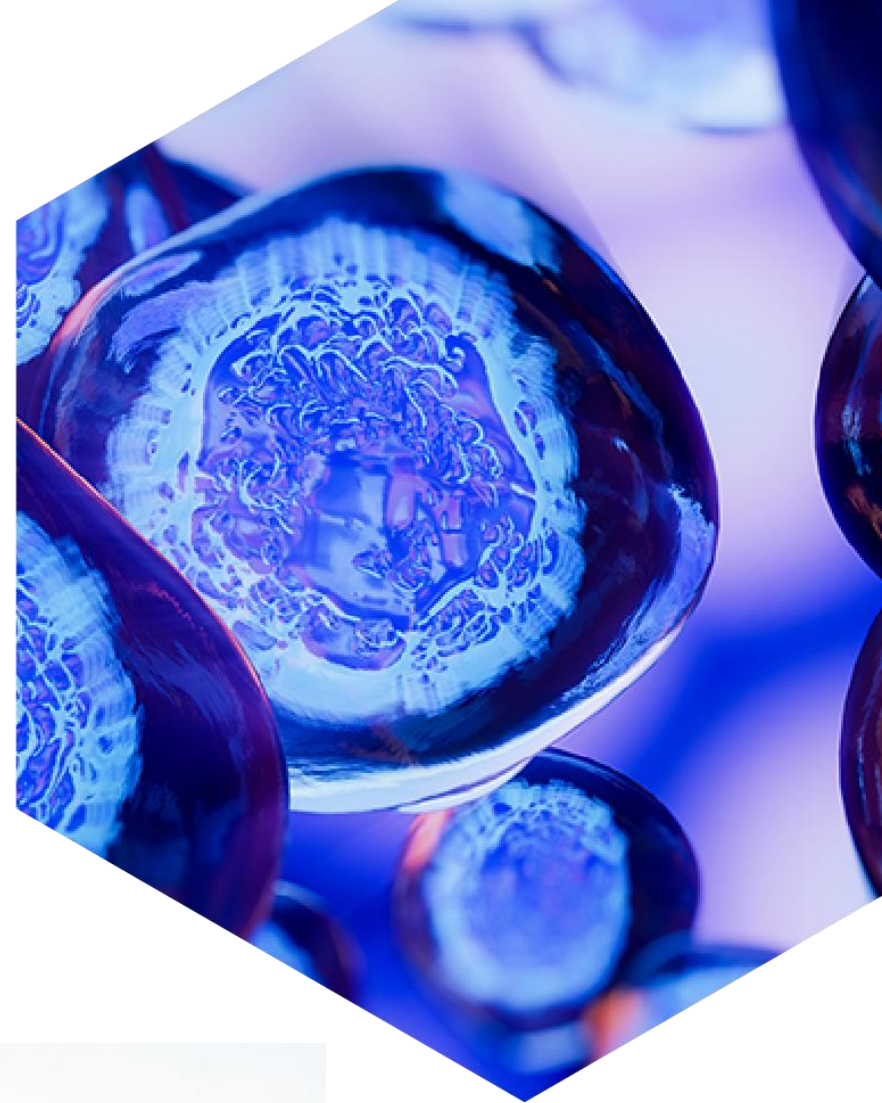


About CAS

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.

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PHARMA



48

of the top 50

ACADEMIC



100

of the top 100

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20

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10

of the top 10 global
patent offices

1. Pharm Exec's Top 50 Companies 2020. 2. ShanghaiRanking's Global Ranking of Academic Subjects 2020.
3. Genetic Engineering & Biotechnology News Top 25 Biotech Companies of 2019. 4. C&EN's Global Top 50
for 2020. 5. WIPO IP Facts and Figures 2019.

CAS has the most comprehensive collection of connected science



Over
50K
scientific journals
and documents

Over
250
million
substances

Over
50
languages
translated

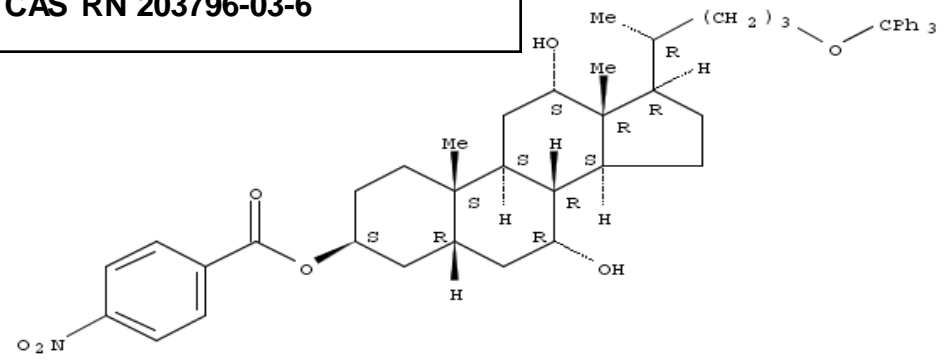
64
patent offices
worldwide

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.

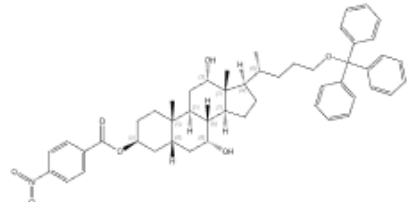
Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO₃ solution followed by extraction 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 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 (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



Scifinderⁿ Discovery platform

*SciFinderN

Top 6 key searching function

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

*CAS Formulation

*CAS Analytical Methods

The screenshot displays the SciFinderN web interface. At the top, the CAS SciFinder logo is on the left, and user account information (Alerts with 44 notifications, Saved items, and user name Titer C Liu) is on the right. The main content area is divided into two columns. The left column, titled 'Searching for...', contains a vertical list of search categories: All, Substances, Reactions, References (highlighted in blue), Suppliers, Sequences, and Retrosynthesis. The right column, titled 'References', features a search bar with the placeholder 'Enter a query...', a 'Draw' button, and a search icon. Below the search bar is an 'Author Name' field with a dropdown arrow and a placeholder 'Enter last name, first name middle name.', followed by an example 'Schubert, J A' and a close button. A '+ Add Advanced Search Field' button is also present. A blue banner for 'Launch CAS Lexicon' is visible, explaining its function. At the bottom, the 'Recent Search History' section shows a search from May 2, 2023, at 2:58 PM for 'References' related to 'plectranthus amboinicus', resulting in 377 hits. A 'Rerun Search' button is located to the right of the history entry. A 'View All Search History' link and a 'Feedback' button are also visible in the bottom right corner.

Perform Reference searching

CAS SciFinder[®] halves the time needed to perform literature reviews*

The screenshot displays the CAS SciFinder web interface. At the top, the CAS SciFinder logo is on the left, and navigation links for Alerts (with a notification badge), Saved, and the user profile (Titer C Liu) are on the right. The main content area is divided into three sections. On the left, a sidebar titled 'Searching for...' contains buttons for 'All', 'Substances', 'Reactions', 'References' (which is highlighted in blue), 'Suppliers', 'Sequences', and 'Retrosynthesis'. The central 'References' section features a search bar with the text 'cancer and lung'. Below the search bar, there are two rows of search criteria, each starting with 'AND' and a dropdown menu. The first row has 'Author Name' selected with a placeholder 'Enter last name, first name middle name.' and an example 'Schubert, J A'. The second row has 'Target' selected with a placeholder 'Multiple entries must be delimited by a space.' A dropdown menu is open for the 'Target' field, listing various search criteria: Authors, Publication Name, Organization (highlighted in blue), Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked with a 'NEW' badge), Publication Year, Document Identifier, Patent Number, and Publisher. To the right of the search criteria, there is a 'Draw' button and a search button with a magnifying glass icon. Below the search bar, there is a link 'Learn more about SciFinder[®] Advanced Search.' and a blue box containing text about the CAS General Thesaurus. At the bottom left, the 'Recent Search History' section shows a search from 'May 5, 2023' for 'Substances' at '11:46 AM'. At the bottom right, there is a 'Rerun Search' button and a 'Feedback' button with a speech bubble icon. The CAS logo and 'A division of the American Chemical Society' text are in the bottom right corner.

CAS SciFinder[®]

Alerts 2 Saved Titer C Liu

Searching for...

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

References

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

cancer and lung

AND Author Name Enter last name, first name middle name. Example: Schubert, J A

AND Target Multiple entries must be delimited by a space.

+ Add Another Search Criterion

Launch the CAS General Thesaurus enables you to browse the CAS General Thesaurus to find indexed concepts and build a Reference query with up to 1,000 indexed search terms.

[Learn more about SciFinder[®] Advanced Search.](#)

Recent Search History

May 5, 2023

Substances 11:46 AM

Substructure (160K)

Rerun Search

Feedback

CAS A division of the American Chemical Society

Perform literature reviews

CAS SciFinder[®] halves the time needed to 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 web interface. At the top, the search bar contains 'plectranthus amboinicus'. Below the search bar, there are tabs for 'Substances', 'Reactions', 'Citing', and 'Knowledge Graph'. The left sidebar contains a 'Filter Behavior' section with 'Filter by' and 'Exclude' buttons. Under 'Document Type', there are checkboxes for Journal (332), Patent (45), Review (17), Clinical Trial (1), and Commentary (1). Under 'Language', there is a dropdown menu. Under 'Publication Year', there is a bar chart showing the distribution of publications from 1992 to 2023, with a 'View Larger' link. Below the chart, there are input fields for 'No Min' and 'No Max' with an 'Apply' button. The main content area shows 379 results. The first result is titled 'Chemical profile, antiproliferative and antibacterial activities and docking studies of essential oil and hexane fraction of hydrosol from fresh leaf of Plectranthus amboinicus (Lour.) Spreng.' by Ibrahim, Enas I. E.; Yagi, Sakina; Tzanova, Tzvetomira; Schohn, Herve; Uba, Abdullahi Ibrahim; Zengin, Gokhan. The second result is titled 'Development of electrospun Plectranthus amboinicus loaded PCL polymeric nanofibrous scaffold for skin wound healing application: in-vitro and in-silico analysis' by Rathinavel, Saranya; Sugumar, Moogambigai; Swaminathan, Elamathi; Kubendren, Sudharshan; Samvasivan, Kalaimagal; Sangeetha, Dharmalingam. The interface also includes buttons for 'Full Text', 'Substances', 'Reactions', 'Citing', and 'Citation Map' for each result.

Reference Detail

Substances (6) React

Patent

Patent Information

Patent Number

WQ2007076701

Publication Date

2007-07-12

Application Number

WQ2006-CN3694

Application Date

2006-12-29

Kind Code

A1

Assignee

Zensun (Shanghai) Science & Technology Limited, China

Source

World Intellectual Property Organization

Database Information

AN: 2007:762994

CAN: 147:134439

CAplus

Language

English

Concepts

Alzheimer disease

Animal gene

Modifier: NRG1, NR

Role: Biological Stud

Activity; Therapeuti

Anti-Alzheimer age

Antidiabetic agents

Antitumor agents

Cardiac hypertroph

Cardiomyocyte

Modifier: growth an

Cardioprotective a

Cardiovascular dis

Cell differentiation

Modifier: cardiomy

Cell proliferation

Modifier: cardiomy

Controlled-release

Diabetes mellitus

Substances

135729-61-2

C1=CC=C(C=C1)C2=CC=CC=C2

Absolute stereoche

C19H24N2O

Palonosetron

Role: Pharmacolog

Use, Biological Stud

50-18-0

ClC1=CC=CC=C1

C7H15Cl2N2O2P

Cyclophospham

Role: Adverse Effect

Pharmacological Ac

Biological Study, Us

Formulations

Collagen Formulation: Anticancer Agents

[View Formulus® Detail](#)

Location: Article Page 3, 6

Purpose: Antitumor agents

Target: cancer

Component	Function	Amount Reported
Group: cyclic dinucleotides stock solution	-	-
cyclic dinucleotides	-	6.67 µg
endotoxin-free water	solvent	-
Phosphate-buffered saline solutions	buffer	-
collagen stock solution	carrier	3.5-5 mg/mL

Stingel Formulation: Anticancer Agents

[View Formulus® Detail](#)

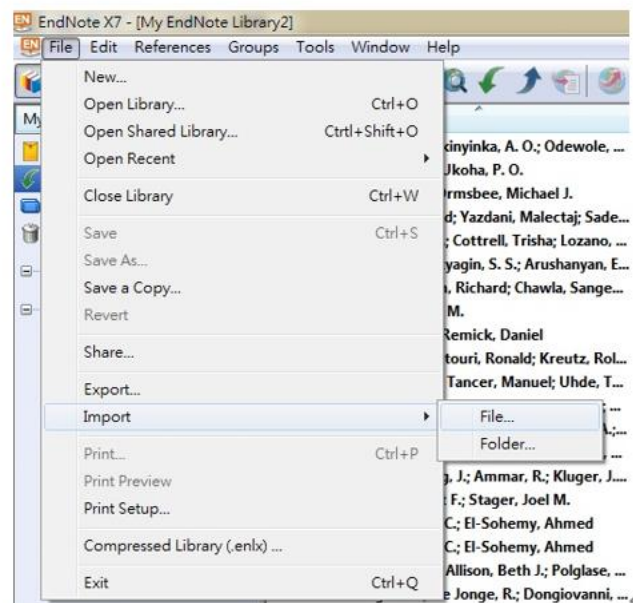
Location: Article Page 3, 6



EndNote output

The screenshot shows the CAS SciFinder web interface. A search for "cancer" has been performed, and a list of results is displayed. A dialog box titled "Download Reference Results" is open, allowing the user to select the file type (PDF), display options (Result Summary or Result Details), and file name (Reference_20230505_2132). The dialog also includes options to select the quantity of results (All Results, Selected Results, or Range) and to include specific information (Task History, Abstract, Concepts, Substances, Formulations, Analytical Methods, Citations). A "Download" button is visible at the bottom of the dialog.

若點選 .ris 檔無法直接開啟至 EndNote，也可另開啟 EndNote，在工具列點選 File→Import→File，將儲存的 .ris 檔案匯入。←



在 Import File 選擇檔案來源，Import Option 選擇 Reference Manager (RIS)，也可將 SciFinderN 的文獻檢索結果匯至 Endnote。←

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!

PATENTPAK
A CAS SOLUTION

PAGE 28 / 37 ZOOM PDF PDF+

Key Substances in Patent

CAS RN 2752-65-0

Analyst Markup Locations (1)
Page 28

CAS RN 81624-55-7

CAS Name
1,2-Ethanediamine,
N,N,N',N'-tetrakis[(6-methyl-1H-benzimidazol-2-yl)methyl]-

Substance Detail
Reactions (0)
Suppliers (15)
References (7)
Edit Structure

CLAIMS

What is claimed is:

1. A pharmaceutical composition, comprising:
at least one NPM inhibitor;
at least one anti-cancer agent; and
a pharmaceutically acceptable carrier.
2. The pharmaceutical composition of claim 1, wherein the NPM inhibitor is an siRNA that inhibits NPM expression.
3. The pharmaceutical composition of claim 1, wherein the NPM inhibitor is gambogic acid.
4. The pharmaceutical composition of claim 1, wherein the NPM inhibitor is NSC 348884.
5. The pharmaceutical composition of claim 1, wherein the anti-cancer agent is a target cancer therapy.
6. The pharmaceutical composition of claim 5, wherein the target cancer therapy is
sorefenib.

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

-

Molecular Formula

AND

+ Add A

Molecular Formula

CAS Registry Number

Chemical Identifier

Document Identifier

Patent Identifier

Experimental Spectra

Bioactivity Data NEW

Biological

Chemical Properties

Density

Electrical

Lipinski

Magnetic

Mechanical

Optical and Scattering

Proton NMR

Carbon-13 NMR

Nitrogen-15 NMR

Fluorine-19 NMR

Phosphorus-31 NMR

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

Learn more about SciFinder[®] Advanced Search.

Recent Search History

May 5, 2023

Substances

11:46 AM

View All Search History

Feedback

Rerun Search

Mine substances and reactions

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 CAS SciFinder interface for searching substances. The top bar shows 'Substances (3,884)' with a sort dropdown set to 'Relevance' and a 'View: Partial' option. Below the bar are tabs for 'References', 'Reactions', and 'Suppliers'. The main content area is a grid of substance cards. Each card includes a checkbox, a CAS number, a 'View Detail' link, a chemical structure, a description of stereochemistry, a molecular formula, a chemical name, and counts for references, reactions, and suppliers.

CAS Number	Chemical Name	Formula	References	Reactions	Suppliers
1821732-51-7	2-Azetidinone, 4-ethyl-4-methyl-, (4S)-	C ₆ H ₁₁ NO	0	0	1
39155-99-2	2-Azetidinone, 4-ethenyl-4-methyl-, (S)-	C ₆ H ₉ NO	1	0	1
39155-98-1	2-Azetidinone, 4-ethenyl-4-methyl-, (R)-	C ₆ H ₉ NO	1	0	3
28982-78-7	2-Azetidinone, 4-methyl-4-propyl-, (+)-, polymers	(C ₇ H ₁₃ NO) _x	1	0	0
45652-80-0	2-Azetidinone, 4-methyl-4-propyl-, (+)-	C ₇ H ₁₃ NO	0	0	0
27063-09-8	2-Azetidinone, 4-methyl-4-propyl-, (-)-	C ₇ H ₁₃ NO	0	0	0
127083-86-7					
127129-14-0					
1401295-99-5					

Substances information

CAS Registry Number: 106266-06-2

References (13K)

Reactions (218)

Suppliers (122)

Download

Email

Save

CN1CCCC1CCc2nc3ccccc3n2

C₂₃H₂₇N₄O₂

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

Biological	Chemical	Lipinski	Structure Related	Thermal
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) 1380 pages, CASplus

Structure Activity Relationships

Absorption, Distribution, Metabolism, and Excretion Data

Toxicity

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

Inform IP strategy

CAS SciFinderⁿ 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.

Patent Markush Match

As Drawn (6)

Substructure (151)

Filter by

Patent Office

- ☐ World Intellectual Property Organization (5)
- ☐ Korea, Republic of (1)

Patent Markush (6)

References

☐ KR2010125109
View Reference Detail

Patent claim 1

PATENTPAK Full Text

54: alkyl <containing 1-10 C> (opt. substd. by G2)
119: alkyl <containing 1-10 C> (opt. substd. by G2)

☐ WO2014052836
View Reference Detail

Patent claim 1

PATENTPAK Full Text

184,185,187,188,190: opt. substd. by 1 or more G11

☐ WO2003072657
View Reference Detail

Patent claim 7

PATENTPAK Full Text

17: alkyl <containing 1-10 C> (opt. substd. by 1 or more G21)
22: alkyl <containing 1-10 C> (opt. substd. by 1 or more G21)

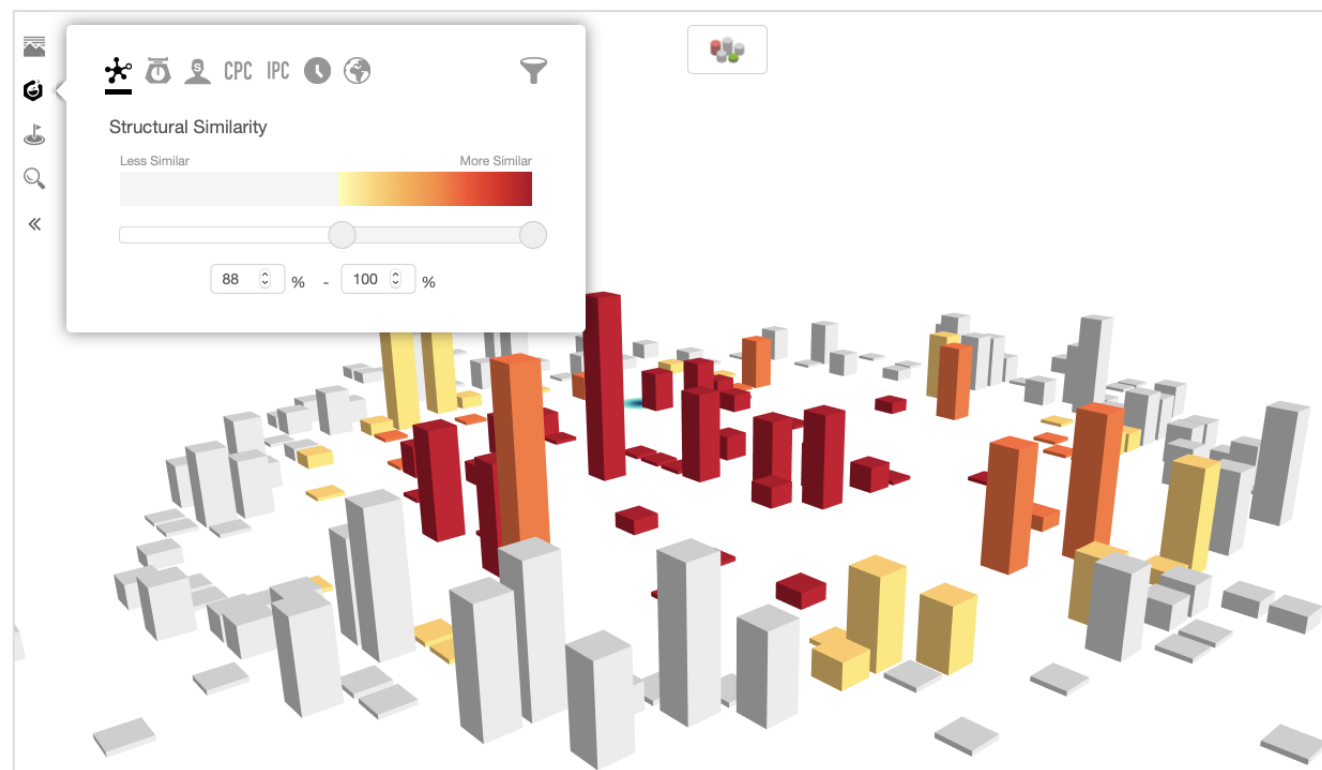
*CAS SciFinderⁿ Productivity Survey 2020

Visualize search results

CAS SciFinder[®] offers visual context for substance and biosequence result sets

Graphically explore the structural similarity of chemicals compared to one another and the patents associated with them.

Review visualized biosequence search results and evaluate sequence space from an IP perspective.



Reaction: Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus

The screenshot displays the CAS Reactions interface. On the left, a sidebar contains various filtering options under '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), and 'Source Reference' (Publication Year, Document Type, Language). The main area shows 'Reactions (13)' with a 'Scheme 1 (2 Reactions) View'. The reaction scheme depicts the conversion of a complex ester and furan to a bicyclic product. Below the scheme, two identical 'Reaction Summary' boxes are shown, detailing reagents (Sodium acetate, Acetic acid, manganese(3+) salt (3:1)), catalysts, solvents (Acetic acid), and conditions. A 'Full Text' button is available for each summary. The interface also includes 'Suppliers' links for reactants and products, and a 'Collapse Scheme' button at the bottom.

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-diazenecarbothioamidato-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-diazenecarbothioamidato-κN²,κS] (triphenylphosphine)-

CAS Method Number 3-478-CAS-9063944

Retro-Synthetic Planning

CAS SciFinder[®]

Reactions ▼ Enter a query...

Draw

Q

2

Retrosynthesis Plan Options for 106266-06-2

Powered by ChemPlanner[®]

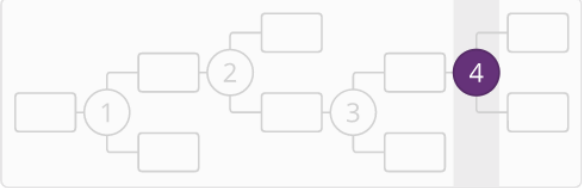
Select Synthetic Depth

1

2

3

☒ 4



[Learn more.](#)

Set Rules Supporting Predicted Reactions

☒ Common

☐ Uncommon (includes Common Rules)

☐ Rare (includes Common and Uncommon Rules)

[Learn more.](#)

Set Starting Materials Cost Limit

1000

USD/mol ▼

[Learn more.](#)

☒ Email me when my plan is complete

Create Retrosynthesis Plan

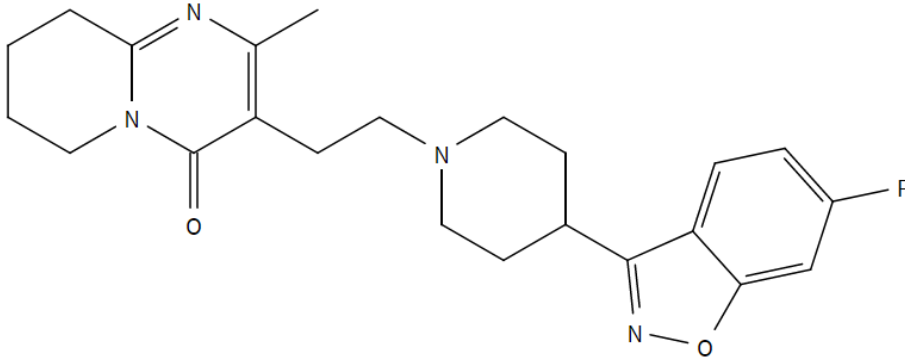
Break and Protect Bonds

[Learn more.](#)

Break Bond

Protect Bond

Clear All Bond Selections



Feedback

A division of the American Chemical Society

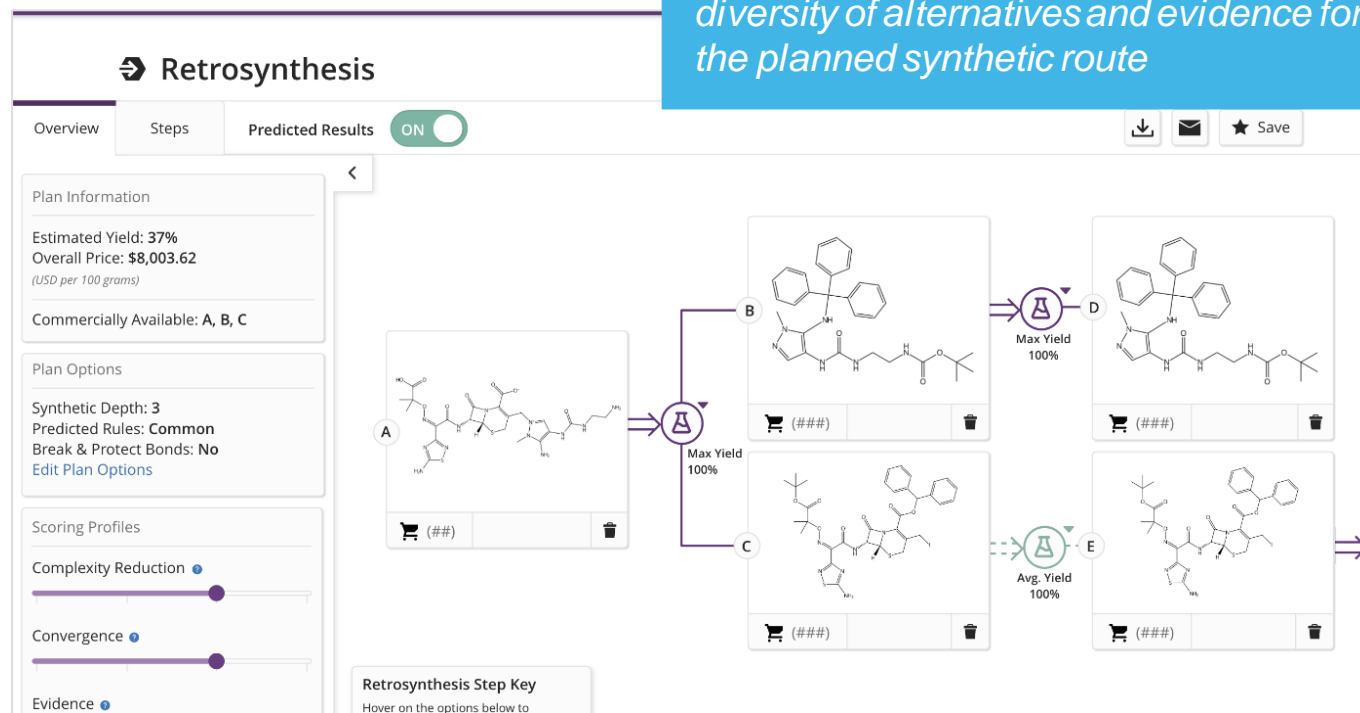
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CAS SciFinder Discovery Platform for Synthetic Planning

CAS SciFinder[®] is a catalyst for unlocking research productivity

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- Scale up levels of production synthesis
- Identify opportunities for new breakthroughs in methods development

Researchers can clearly understand the diversity of alternatives and evidence for the planned synthetic route



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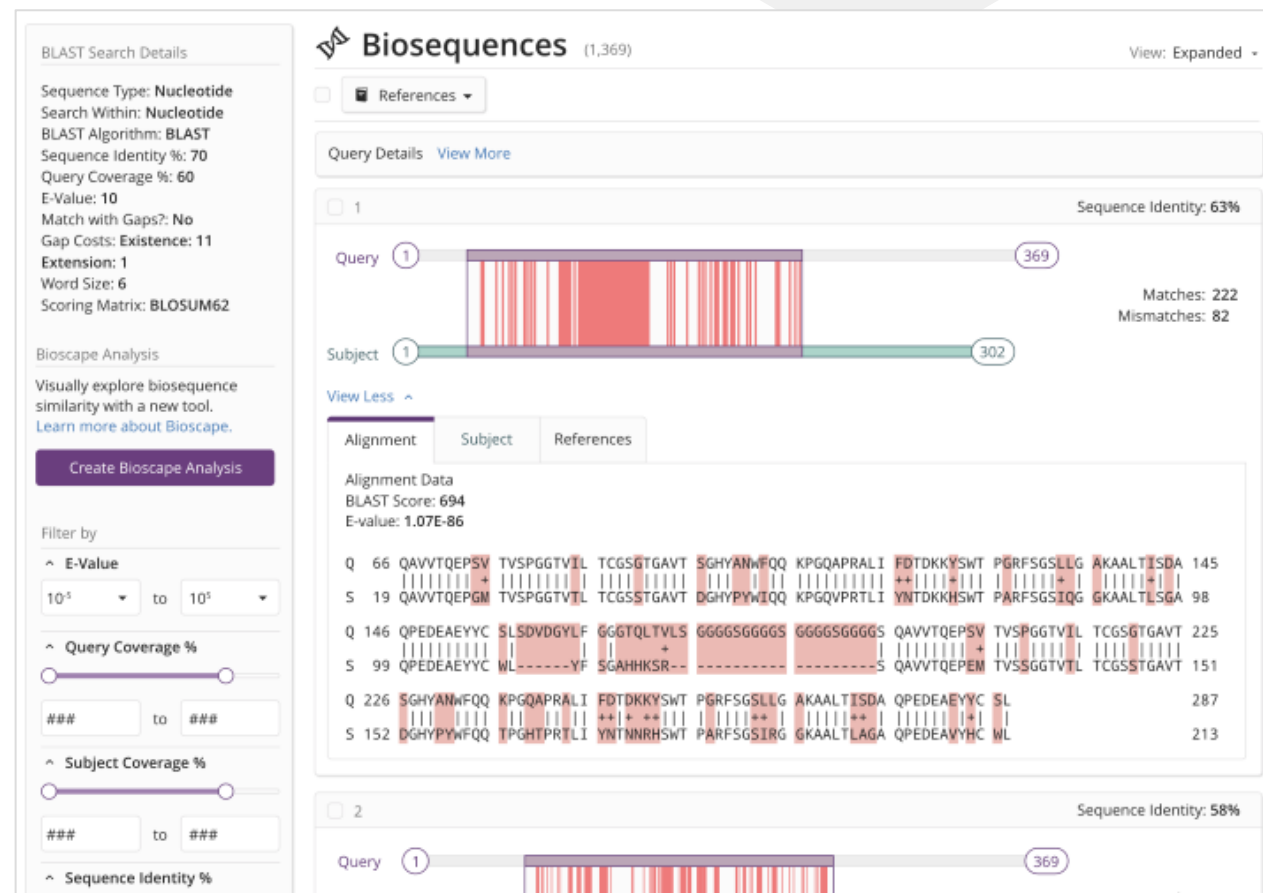
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Filter by Exclude

^ Preferred Suppliers

☐ No Preference (85)

^ Supplier

☐ KANTO CHEMICAL (5)

☐ ALDRICH (3)

☐ ASW MedChem Product List (3)

☐ AK Scientific Product Catalog (2)

☐ Alchem Pharmtech Product List (2)

View All

^ Purity

☐ ≥99% (2)

☐ 95-98% (63)

☐ 90-94% (3)

^ Quantity






☐ Milligrams (6)

☐ Grams (51)

☐ Kilograms (23)

Shopping Cart Suppliers (85) Sort: Ships Within ▾

☐

Supplier	Substance	Details	Availability
<input type="checkbox"/> 1			
 1PlusChem Product List United States Updated Mar 31, 2021 	1125-88-8 Benzaldehyde Dimethyl Acetal Order Number: 1P0034Y6	Purity 95-98% Quantity 100g ▾	USD 40 Maintained in stock Ships within 1 week View Detail Order from Supplier
<input type="checkbox"/> 2			
 A2B Chem Product List United States Updated Mar 22, 2021 	1125-88-8 Benzaldehyde dimethyl acetal Order Number: AB45582	Purity 95-98% Quantity 100g ▾	USD 14 Maintained in stock Ships within 1 week View Detail Order from Supplier
<input type="checkbox"/> 3			
 AA BLOCKS LLC Product List	1125-88-8 Benzaldehyde dimethyl acetal Order Number: AA0034EQ	Purity 95-98% Quantity	USD 16 Maintained in stock Ships within 1 week

GHS Hazard Statements

CAS Registry Number: 79-41-4

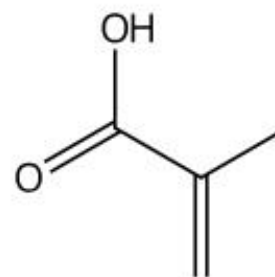
References (105K)

Reactions (51K)

Suppliers (69)



Save



^ GHS Hazard Statements

Code	Hazard Statement	Source
H402	Harmful to aquatic life	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria, Expert Curated, Japan GHS Classifications (Japanese), Merck Life Science OY (Sigma-Aldrich), Redox Pty Ltd, Sigma-Aldrich (as MilliporeSigma, Merck), Tokyo Chemical Industry Co (TCI America), Tokyo Chemical Industry Co (TCI Europe)
H400	Very toxic to aquatic life	Pfaltz&Bauer
H373	May cause damage to organs through prolonged or repeated exposure	Expert Curated, New Zealand Hazardous Substances and New Organisms (HSNO) Act - Classification of Chemicals, Tokyo Chemical Industry Co (TCI America), Tokyo Chemical Industry Co (TCI Europe)
H372	Causes damage to organs through prolonged or repeated exposure	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria, Expert Curated, Japan GHS Classifications (Japanese), Tokyo Chemical Industry Co (TCI America), Tokyo Chemical Industry Co (TCI Europe)
H370	Causes damage to organs	Expert Curated, Japan GHS Classifications (Japanese)
H350i	May cause cancer by inhalation	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H350	May cause cancer	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria
H341	Suspected of causing genetic defects	European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling - most serious notifications, European Chemical Agency (ECHA) Classification&Labelling Inventory - Notified classification and labelling according to CLP criteria

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 'Results' section of the CAS SciFinder platform. On the left, a sidebar contains filters for 'Analyte' (listing Palmitic acid (24), Stearic acid (22), Oleic acid (21), Arachidonic acid (19), and Linoleic acid (18)), 'Matrix' (listing Blood plasma (24) and Blood serum (2)), 'Method Category', 'Technique', and 'Year'. The main content area shows a search result for 'Analysis of Palmitic acid in Blood plasma by High-performance liquid chromatography-mass spectrometry' with CAS MN: 2-107-CAS-39800. Below the title, there are buttons for 'View Details & Instructions' and 'Add to Compare'. A table of details follows, listing 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).

[Return to Advanced Search](#)

Results (24) Sort Relevance ▾

☐ 📌 ★ 🔍 Compare (0/3)

☐ **Analysis of Palmitic acid in Blood plasma by High-performance liquid chromatography-mass spectrometry**
CAS MN: 2-107-CAS-39800

[View Details & Instructions](#) [Add to Compare](#)

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
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.

Equipment Used

HPLC System, Merck Hitachi

Ultraturrax, T25 basic, IKA Werke

UV-VISIBLE Spectrophotometer, V-630, Jasco, Japan

Homogeniser, A10, IKA

Rotavapor, Heidolph

Vacuum system, Buchner

Conditions

Chromatographic

Mobile phase, acetonitrile/methanol/dichloromethane (75:21:4 v/v/v) and 0.1% BHT + 0.05% triethylamine (MeOH + 0.05 M ammonium acetate); flow rate, 1.5 mL/min; injection volume, 20 μ L, temperature, 20 $^{\circ}$ C

Instructions

Sample extraction by traditional method

1. Collect fresh tomato samples (fresh matter, juices, purees, pulp, concentrates and sauces) homogenize coarse pieces in an IKA Werke Ultraturrax (T25 basic) model A10 laboratory homogenizer.
2. Weigh amount of homogenized sample and add 90 ml of a mixture of THF - methanol 1:1 (v/v) and of magnesium carbonate.
3. Filter the solution with a Buchner vacuum system and wash with a THF - methanol mixture.
4. Separate the phases in an amber separating funnel after the addition to the mixture of 50 ml of 40 - 60 $^{\circ}$ C petroleum ether and 50 ml of NaCl 10% aqueous solution.
5. Wash THF - methanol - water phase twice with 50 ml of petroleum ether.
6. Carry out filtration on anhydrous sodium sulphate of the ether aliquots containing the **analyte** and collection of the same in a rotavapor vial.
7. Evaporate the ether phase up to almost total dryness using a Rotavapor.
8. Retrieve and collect the extract with a solution of THF + 0.1% of BHT in a 20 ml amber vial.

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

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COMPREHENSIVENESS

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

The screenshot displays the CAS Formulus web application. At the top, the header includes the CAS logo, the word 'Formulus', and navigation links for 'Help & Support', 'History', and 'Account'. The main content area is divided into two columns. The left column features a 'Search for' section with two buttons: 'Formulations' (highlighted in blue) and 'Ingredients'. Below this is a 'Create a Formulation' section with a 'Launch Formulation Designer' button. The right column contains a search bar with the placeholder text 'Search for Formulations by Ingredient, Purpose, Form, Function, etc.' and a magnifying glass icon. Below the search bar, there is a link to 'Try Advanced Search for a more precise search experience'. At the bottom of the right column, a light blue box contains text describing the Formulation Designer: '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)

View All

Physical Form

☐ Tablets (187K)

☐ Solutions (121K)

☐ Liquids (68K)

☐ Capsules (43K)

☐ Gels (39K)

View All

Information Included

☐ Component Amount (1.4M)

☐ Process (771K)

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](#)

Case:

1. Revlimid → multiple myeloma

2. Humira

藥品	2022 銷售額 (美元)	2021 銷售額 (美元)	成長率	公司	適應症
Comirnaty (tozinameran)	408億	403億	1.2%	Pfizer/BioNTech	COVID-19 mRNA疫苗
Spikevax (elasomeran)	218億	177億	23.2%	Moderna	COVID-19 mRNA疫苗
Humira (adalimumab)	216億	212億	1.9%	AbbVie	類風濕性關節炎
Keytruda (pembrolizumab)	210億	172億	22.1%	Merck & Co.	癌症免疫療法
Paxlovid(Nirmatrelvir/Ritonavir)	190億	1億	18900.0%	Pfizer	COVID-19口服抗病毒藥物
Eliquis (apixaban)	118億	108億	9.3%	BMS / Pfizer	抗凝血劑
Biktarvy (bictegravir, emtricitabine, tenofovir alafenamide)	104億	86億	20.9%	Gilead	HIV-1抗反轉錄病毒複方製劑
Eylea (aflibercept)	103億	99億	4.0%	Bayer/Regeneron	黃斑部退化病變
Stelara (ustekinumab)	101億	96億	5.2%	Janssen Biotech	中至重度斑塊性乾癬
Revlimid (lenalidomide)	100億	129億	-22.5%	BMS	多發性骨髓瘤 (MM)

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Senior Account Consultant
Tliu2@acs-i.org

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of researchers agree
CAS SciFinderⁿ allows them
to be more innovative than
other research solutions.*

SPEED



77%

of researchers agree
CAS SciFinderⁿ allows them
to work more quickly than
other research solutions.*

CONFIDENCE

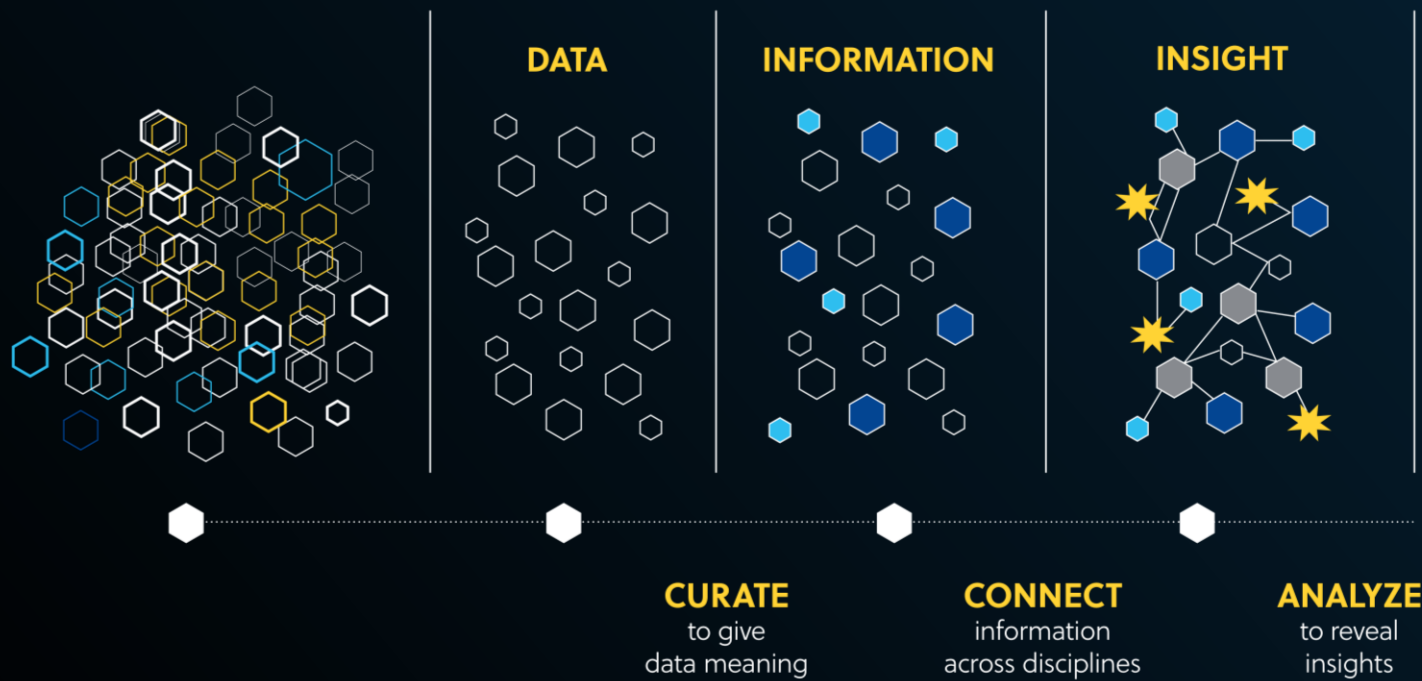


84%

of researchers agree
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to work more confidently
compared to other research solutions.*

*CAS SciFinderⁿ Productivity Survey 2020.

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