



**SciFINDER**<sup>®</sup>  
A CAS SOLUTION

ACS International Ltd  
vhyttinen@cas.org

**SciFinder**<sup>®</sup>

Premier CAS solutions to explore all chemistry  
**MethodsNow, PatentPak, ChemZent, SciFinder<sup>n</sup>**

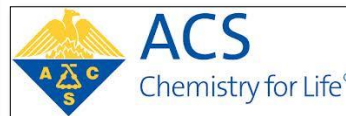
Veli-Pekka Hyttinen

May 23, 2018

# CAS supports the mission of the ACS

## ACS Mission

To improve people's lives through the transforming power of chemistry.



## CAS Mission

To provide the world's best digital research environment to search, retrieve, analyze and link chemical information.

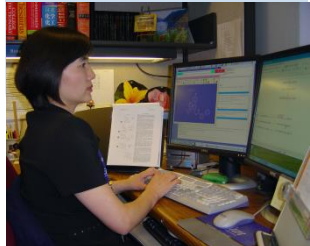


# CAS scientists analyze, summarize and make scientific information accessible to colleagues worldwide

Source  
Selection



Document  
Indexing



Reaction  
Indexing



Markush  
Indexing



Authority  
Processing



Proprietary, standardized indexing in CAS databases ensures consistent, comprehensive search results.

# CAS scientists find the chemistry, and save you time!

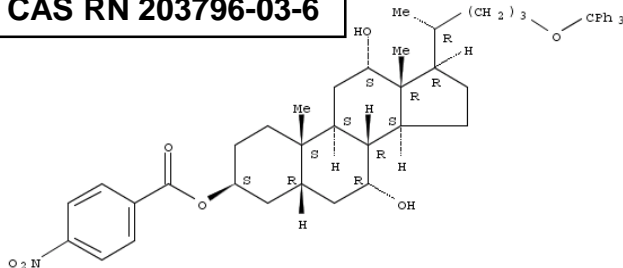
Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

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 NaHCO<sub>3</sub> solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>.

The desired product (2.72 g, 85% yield) was obtained as white powder after SiO<sub>2</sub> chromatography (Et<sub>2</sub>O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529, 1489, 1448, 1345 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 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); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz) δ 164.21, 150.56, 144.70, 136.79, 130.77, 64.22, 47.79, 46.79, 42.18, 28.74, 27.71, 26.85, 26.33.

(thioglycerol+Na<sup>+</sup> matrix)

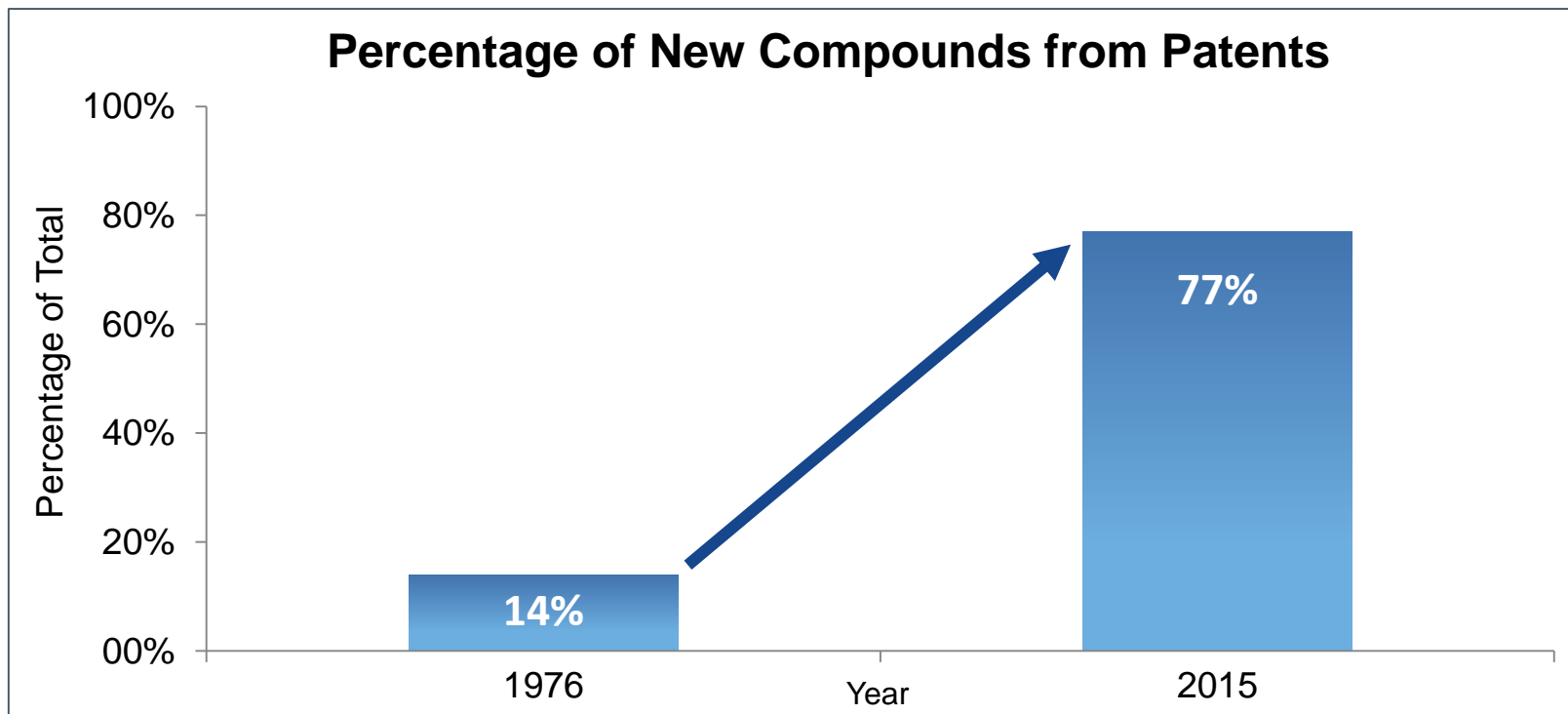
CAS RN 203796-03-6



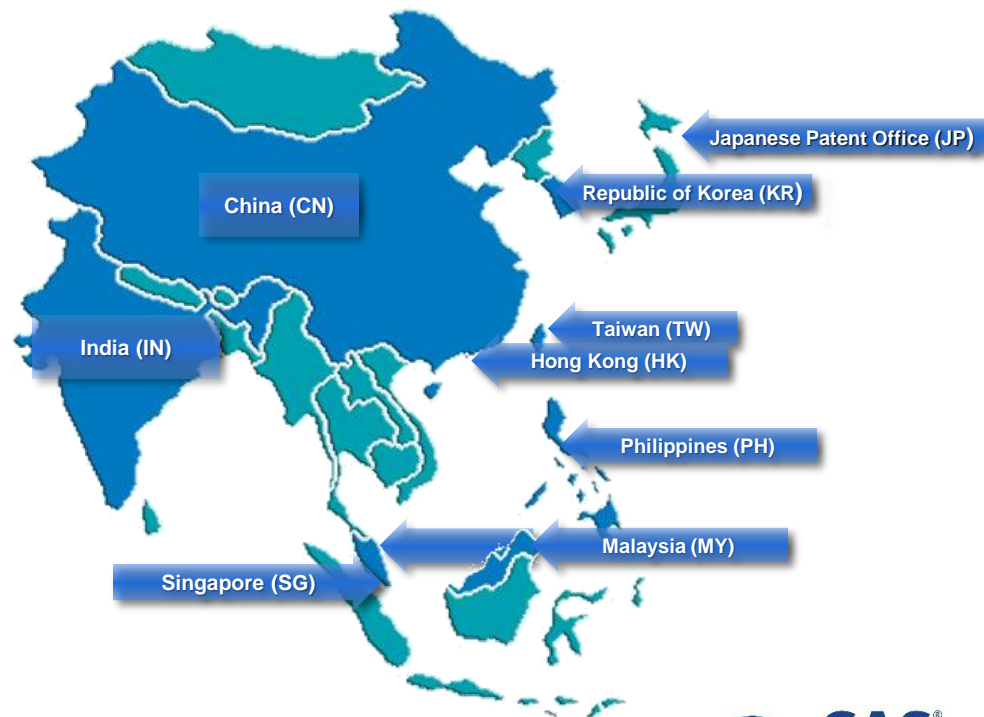
Absolute stereochemistry.



## Increasingly, new compounds in the literature are first disclosed in patents



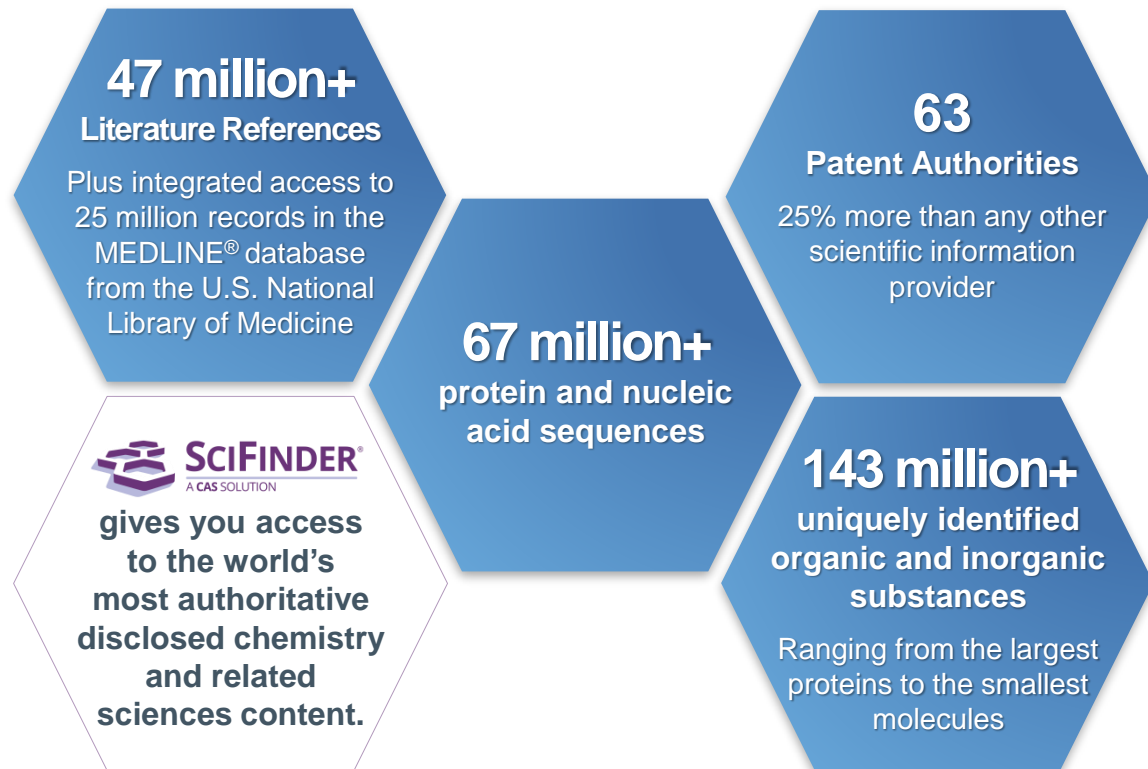
## CAlus coverage of patents from Asia is unmatched



**CAS**<sup>®</sup>

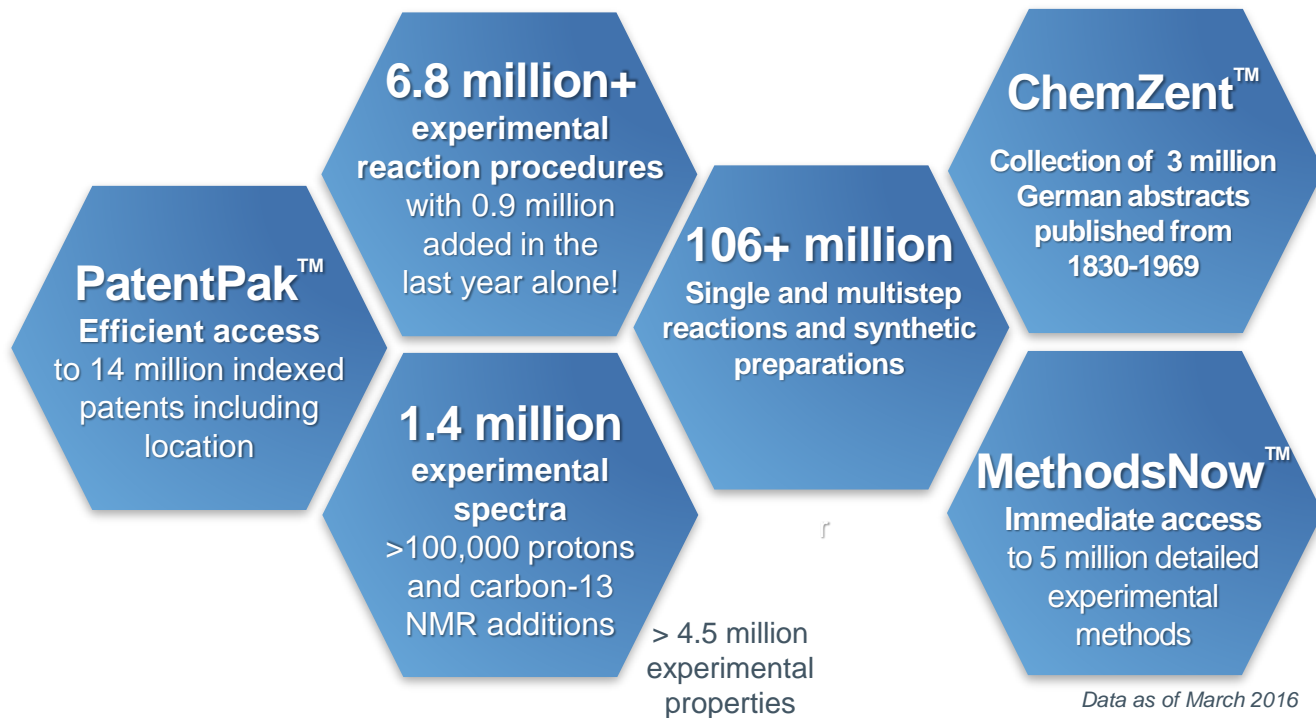
A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

**CAS analyzes the world's disclosed research to keep SciFinder the most valuable tool supporting your organization's research enterprise**



*Data as of March 2016*

# SciFinder saves you time by delivering valuable information to advance your research





# SciFinder – EXPLORE REFERENCES

curated and indexed 47+mill C.A. plus references from 10,000+ journals and 63 patent offices; and 25+mill MEDLINE references from 5,000 journals

The screenshot shows the SciFinder interface. At the top, there's a navigation bar with 'CAS Solutions', 'SciFINDER A CAS SOLUTION', 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this is a secondary bar with 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar contains 'REFERENCES' (with sub-items: Research Topic, Author Name, Comparison Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). The main area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field containing 'NANOTECHNOLOGY IN CANCER THERAPY' and a 'Search' button. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. To the right, there are sections for 'SAVED ANSWER SETS' and 'KEEP ME POSTED' with various search results and dates.

**REFERENCES**

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags



## Get References – Quick View

✕

### Quick View

**Development of a Rapid LC-MS/MS Method for the Quantification of Cannabidiol, Cannabidivarin,  $\Delta^9$ -Tetrahydrocannabivarin, and Cannabigerol in Mouse Peripheral ...**

[Other Sources](#)

By Piscitelli, Fabiana; Pagano, Ester; Lauritano, Anna; Izzo, Angelo A.; Di Marzo, Vincenzo  
 From Analytical Chemistry (Washington, DC, United States) (2017), 89(8), 4749-4755. | Language: English, Database: CAPLUS

Cannabis has been known as a medicine for several thousand years across many cultures and its beneficial effects are mostly due to the presence of cannabinoids, unique natural products, whose pharmacol. is going to gain increasing interest in the scientific community. The discovery of the main psychoactive constituent of Cannabis sativa L.,  $\Delta^9$ -tetrahydrocannabinol ( $\Delta^9$ -THC), led to the identification of at least 100 addnl. phytocannabinoids, including cannabidiol (CBD), cannabidivarin (CBDV),  $\Delta^9$ -tetrahydrocannabivarin ( $\Delta^9$ -THCV), and cannabigerol (CBG). These mols. are gaining growing interest for their medical properties; however, further research is needed to assess the differences in their pharmacokinetic and pharmacodynamic profiles. The aim of this study was to set up a rapid and accurate method, by using the LC-MS-IT-TOF technol., to detect and quantify CBD, CBDV,  $\Delta^9$ -THCV, and CBG in biol. matrixes. Data show that the method developed here is linear in the calibration range; recoveries from mouse tissues were in the 50-60% range and sensitivity was 2 ng/mL for CBDV, 4 ng/mL for CBG and THCV, and 7 ng/mL for CBD. The method is rapid, precise and accurate, and it will represent a fundamental tool to evaluate the pharmacokinetic and pharmacodynamic properties of selected phytocannabinoids in tissues from different animal models, and develop new cannabinoid-based medicine.

Reference Images
Substance Images

# SciFinder – EXPLORE SUBSTANCES

143+ million organic and inorganic small molecules, 67+ million bio sequences and 1,1+ million MARKUSH structures from patents – structures; names, molecular formulae

The screenshot displays the SciFinder interface for searching substances. The main content area is titled "SUBSTANCES: CHEMICAL STRUCTURE". It features a "Structure Editor" with "Java" and "Non-Java" tabs, showing a chemical structure of a substituted furanone. Below the editor is a "Search Type" section with radio buttons for "Exact Structure", "Substructure" (selected), and "Similarity", and a checkbox for "Show precision analysis". A "ChemDraw" logo is present with the text "Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More". A blue "Search" button and a link to "Advanced Search" are at the bottom of the search area. The left sidebar contains "REFERENCES" and "SUBSTANCES" sections, with "SUBSTANCES" highlighted and its sub-items: "Chemical Structure", "Markush", "Molecular Formula", "Property", and "Substance Identifier". The right sidebar shows "SAVED ANSWER SETS" with a list of search results and "KEEP ME POSTED" with a list of recent activity.

**SUBSTANCES**

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier



# SciFinder – EXPLORE REACTIONS

106+ million reactions/synthetic preparations by substructures, CAS Nr, InChi, Smiles

CAS Solutions

SciFinder  
A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome Veli-Pekka Hyttinen

Explore | Saved Searches | SciPlanner

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

REACTIONS: REACTION STRUCTURE

Structure Editor:

Java Non-Java

Search Type:

- Allow variability only as specified
- Substructure

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More

Import CXF

Search

Advanced Search

SAVED ANSWER SETS

- WO2012040623 (PP)
- WO 2015011082
- surface mod not semicond
- curtius reactions (17)
- azabicyclo sss conv
- Reaction ketones to alcohols
- reaction - ketone to alcohol
- aldehyde reactions new
- ring closing metathesis 1
- suzuki catalyst patents
- Autosaved Reference Set

View All | Import

KEEP ME POSTED

- Thiolates in water
- Mar 04, 2017(24)
- Jan 28, 2017(10)
- China Nerin Eng SMELTING
- Oct 08, 2016(3)
- Warfarin PROPH
- Jan 30, 2016(1)

View All

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

# Categorize and analyze options make it easy to find relevant information

**Categorize**

1. Select a heading and category.      2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in biology (221)	<b>Select All</b> <b>Deselect All</b>	
General chemistry	Animal pathology (69)	<input type="checkbox"/> Interferons 7	
Biotechnology	Animal pathology (69)	<input type="checkbox"/> Antibodies and Immunoglobulins 5	
Synthetic chemistry	<b>Immunology (72)</b>	<input type="checkbox"/> Interferons, $\alpha$ 5	
Genetics & protein chemistry	Processes & systems (44)	<input type="checkbox"/> Vaccines 5	
Physical chemistry	Endocrinology (48)	<input type="checkbox"/> Interleukin 2 3	
Polymer chemistry	Anatomy (27)	<input type="checkbox"/> Interleukin 4 3	
<b>Biology</b>	Substances in adverse effects (16)	<input type="checkbox"/> Leukotriene B4 3	
Technology		<input type="checkbox"/> RANTES (chemokine) 3	
Analytical chemistry		<input type="checkbox"/> Spleen 3	
Environmental chemistry		<input type="checkbox"/> Tumor necrosis factor $\alpha$ 3	
		<input type="checkbox"/> Anti-HIV agents, vaccines 2	
		<input type="checkbox"/> CD4 antigens 2	
		<input type="checkbox"/> CXC chemokines 2	
		<input type="checkbox"/> Etanercept 2	
		<input type="checkbox"/> High throughput screening 2	

Biology > Immunology

**SUBSTANCES**

Get References   Get Reactions   Get Commercial Sources

Analyze   Refine

Sort by: CAS Registry Number

0 of 1 Substance Selected

Analyze by:

- Target Indicators
- Bioactivity Indicators**
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role

Transport proteins (all) 1

Show More

1. **28911-01-5**

~2061   ~34

**C<sub>17</sub> H<sub>12</sub> Cl<sub>2</sub> N<sub>4</sub>**  
4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-

Regulatory Information  
Spectra  
Experimental Properties

Key Substances in Patent

CAS RN 7440-38-2D

As

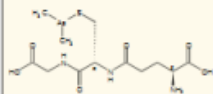
comps.

[Search in SciFinder](#) | [View Detail](#)

Analyst Markup Location

- page 2
- page 3

CAS RN 69819-86-9

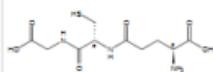


[Search in SciFinder](#) | [View Detail](#)

Analyst Markup Location

- page 3
- page 3
- page 19
- page 21

CAS RN 70-18-8

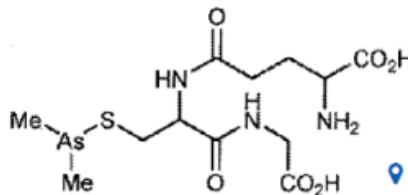


[Search in SciFinder](#) | [View Detail](#)

Analyst Markup Location

- page 19

[0005] The present invention provides novel crystalline forms of organic arsenical compounds having anti-cancer properties. In certain embodiments, the present invention provides a crystalline form of a compound having a structure of formula (I) (darinaparsin)



(I)

[0006] wherein the crystalline form has a melting point greater than or equal to 185 °C. In some embodiments, the crystalline form has a melting point in the range of about 185-200 °C. In some embodiments, the crystalline form has a melting point in the range of about 187-200 °C, e.g., 187-197 °C. In some embodiments, the crystalline form has a melting point in the range of about 190-200 °C. In other embodiments, the invention provides a crystalline form of a compound having a structure of formula (I) (darinaparsin) wherein the crystal form has an X-ray-powder diffraction pattern comprising characteristic peaks at one or more of the following angles: about 16.6°, about 17.4°, about 18.4°, about 19.3°, about 20.0°, about 21.0°, about 22.0°, about 23.3° and about 25.0°.

[0007] In some embodiments, the X-ray powder diffraction pattern of a crystalline form of a compound having a structure of formula (I) (darinaparsin) expressed in terms of 2θ, at one or more of the following angles: about 14.4°, about 19.3°, about 22.0°, about 23.3° and about 25.0°. In some embodiments, the X-ray powder diffraction pattern of the crystalline form of a compound having a structure of formula (I) (darinaparsin) has



**PATENTPAK™**  
A CAS SOLUTION



# METHODSNOW™ – Step-by-step experimental protocols

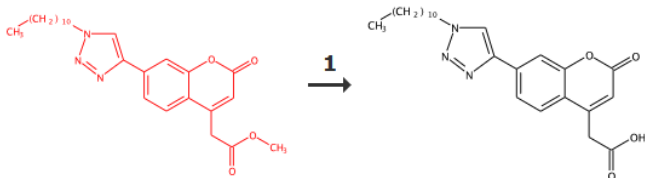
A CAS SOLUTION

## MethodsNow

### 7-Triazolylcoumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule mi

By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha  
From Tetrahedron, 68(30), 6038-6053; 2012  
Published by Elsevier Ltd.

Reaction Steps **1** 2 3 4



<b>Products</b>	2H-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-, 75%, CAS RN 1384966-77-1
<b>Reactants</b>	2H-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-, methyl ester, 1384966-75-9
<b>Reagents</b>	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
<b>Solvents</b>	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

Print

## MethodsNow

<b>Procedure</b>	<ol style="list-style-type: none"><li>1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H-1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0.780 mmol) in THF/water(25 mL/25 mL) at room temperature.</li><li>2. Stir the reaction mixture for 3 hours at room temperature.</li><li>3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid.</li><li>4. Partition the reaction mixture between ethyl acetate and water.</li><li>5. Extract the aqueous layer with ethyl acetate.</li><li>6. Dry the combined organic layer over magnesium sulfate.</li></ol>
<b>Scale</b>	milligram
<b><sup>1</sup>H NMR</b>	<sup>1</sup> H NMR (300 MHz, acetone- d <sub>6</sub> ): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, J = 8.1 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, J = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, J = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, J = 6.8 Hz, 3H).
<b><sup>13</sup>C NMR</b>	<sup>13</sup> C NMR (125 MHz, DMF-d <sub>2</sub> , 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).
<b>IR</b>	IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm <sup>-1</sup> .
<b>HRMS</b>	HRMS (EI): m/z calculated for C <sub>24</sub> H <sub>31</sub> N <sub>3</sub> O <sub>4</sub> : 425.2315 [M <sup>+</sup> ]; found: 425.2315.
<b>Mass Spec</b>	MS (ESI): m/z: 426 [M+H <sup>+</sup> ].
<b>MP</b>	235.5±0.8 °C.
<b>CAS Method Number</b>	3-352-CAS-78415

Print/Export

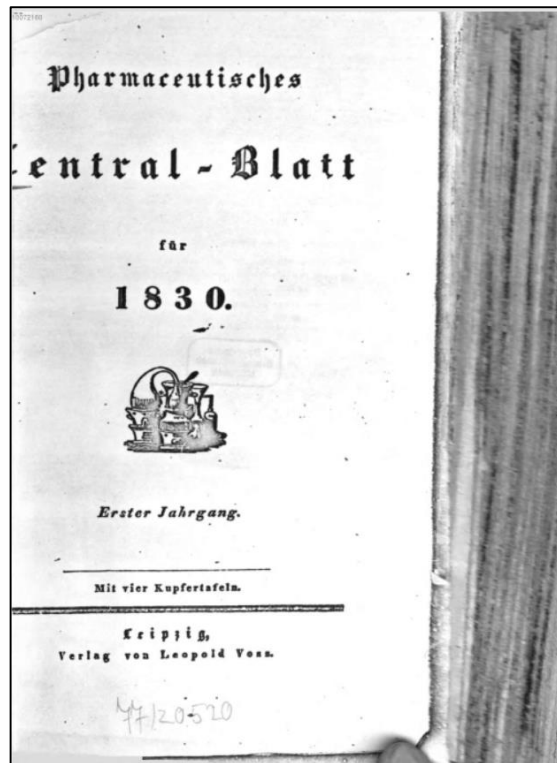
Close



SCIFINDER®  
A CAS SOLUTION

# Chemisches Zentralblatt predates the introduction of Chemical Abstracts by almost 80 years

- Published German language abstracts from 1830-1969
- Chronicles the birth of chemistry as a science
  - Before 1800, chemistry was more alchemy (i.e. how to turn lead into gold) than actual science
- Searchable substance structures in 3 million machine translated abstracts



First Issue:  
Note, the name changed several times before 1856



# SciFinder-n Get to actionable results more quickly with a streamlined new interface

Streamlined search navigation saves you clicks

Immediately run past searches

The screenshot displays the SciFinder-n search interface. At the top, there are navigation links for 'Saved', 'History', and 'Account'. The main search area features a search bar with the text 'treatment of cancer' and a search button. Below the search bar, there are tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. A 'Recent Searches' section is visible, showing a search for 'high temperature low density plasma' (424K) and an 'Advanced Search' for 'Memorial Sloan-Kettering Cancer Ctr.'. A chemical structure drawing is shown in a pop-up window, with 'Edit Drawing' and 'Remove' buttons. The interface is clean and modern, with a focus on search navigation and results.

More conveniently search structures and text

# SciFinder-n Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus

The screenshot displays the SciFinder-n interface for a reaction search. On the left, a 'Structure Match' sidebar offers filtering options: 'As Drawn (5)', 'Substructure (18)', and 'Filter by' categories including Substance Role (Product, Reactant), Yield (90-100%, 80-89%, 70-79%, 50-69%, 30-49%), Number of Steps (1), Experimental Protocols (MethodsNow Available, Procedure Available), Reaction Type, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, Source Reference, Publication Year, Document Type, and Language. The main area, titled 'Reactions (13)', shows 'Scheme 1 (2 Reactions) View' with a chemical reaction scheme. Below the scheme are 'Suppliers (3)' and 'Suppliers (6)' buttons. A 'Reaction Summary' table lists reagents (Sodium acetate, Acetic acid, manganese(3+) salt (3:1)), catalysts (-), solvents (Acetic acid), and conditions (-). It also indicates 'Steps: 1' and 'Yield: 92%'. A 'Full Text' button is available. The summary is titled 'Carbon-carbon bond-forming reactions promoted by trivalent manganese' and includes a reference: 'By: Melikyan, Gagik G. Organic Reactions (Hoboken, NJ, United States) (1997). No pp. given'. A second, identical summary is shown below. At the bottom, there are 'View 2 Reactions' and 'Collapse Scheme' options.

Intuitive information layouts fosters quick comprehension

# One idea can lead you to another - SciFinder<sup>n</sup> has you covered!

The screenshot displays the SciFinder web application interface. At the top, a browser window shows five tabs, all labeled 'SciFinder', which are circled in purple. Below the browser, the SciFinder logo and navigation menu are visible. The main content area is titled 'References (3,103)' and features a search bar with a magnifying glass icon. The search results are filtered by 'Substances', 'Reactions', and 'Cited By'. Two search results are shown: 'Multikinase inhibitors: a new option for the treatment of thyroid cancer' and 'sorafenib for the treatment of renal cancer'. Each result includes the author, journal information, and an abstract. The interface also includes a sidebar with filters for 'Structure Match', 'Document Type', 'Language', and 'Publication Year', along with a bar chart showing the distribution of results by year.

Simultaneous searches can be performed in new browser/windows

# SciFinder-n Citation Mapping helps you understand where to go next in your literature review

**SciFinder**  
References ▾ Enter a query... Draw 🔍 ★ ⌚ 👤

## 🔗 Citation Map

Identification and characterization of a *Pantoea citrea* gene encoding glucose dehydrogenase that is essential for causing pink disease of pineapple

**Abstract:** *Pantoea citrea*, a member of the family Enterobacteriaceae, causes pink disease of pineapple, whose symptom is characterized by the formation of pink to brown discolorations of the infected portions of the pineapple fruit cylinder upon canning. Mol. genetic approaches were applied to elucidate the mechanism responsible for this fruit discoloration. A *P. citrea* mutant strain, CMC6, defective in its ability to cause pink disease and fruit discoloration, was generated by nitrosoguanidine mutagenesis. A DNA fragment that restored these activities was isolated by screening a genomic cosmid library.

By: Cha, Jae-Soon; Pujol, Catherine; Kado, Clarence I.  
Applied and Environmental Microbiology (1997), 63(1), 71-76 | Language: English, Database: CAPUS

View Reference Detail View More ▾

### References This Document Cites

Basic local alignment search tool 34K Citations 🔍	Basic local alignment search tool. 34K Citations 🔍
DNA sequencing with chain-terminating inhibitors 16K Citations 🔍	DNA sequencing with chain-terminating inhibitors. 16K Citations 🔍
A simple method for displaying the hydrophobic character of a protein.	A simple method for displaying the hydrophobic character of a protein.

### References Citing This Document

The commercial production of chemicals using pathway engineering 155 Citations 🔍	The biochemistry, physiology and genetics of PQQ and PQQ-containing enzymes 131 Citations 🔍
Gluconobacter oxydans: its biotechnological applications 42 Citations 🔍	Immune evasion of the human pathogenic yeast <i>Candida albicans</i> : Pra1 is a Factor H, FHL-1 and plasminogen binding surface protein 40 Citations 🔍
The periplasmic serine protease inhibitor ecotin protects bacteria against neutrophil elastase 120 Citations 🔍	The epidemiology and management of seedborne bacterial disease... 18 Citations 🔍
Multigene editing in the <i>Escherichia coli</i> genome via the CRISPR-Cas9 system 39 Citations 🔍	Quinoprotein ethanol dehydrogenase of <i>Pseudomonas aeruginosa</i> is a homodimer. Sequence of the gene and deduced structural properties of the enzyme 26 Citations 🔍
Genetic and biochemical characterization of the pathway in <i>Pantoea citrea</i> leading to pink disease of pineapple	Mathematical modeling of in vitro enzymatic

Interactive map allows speedy identification of important research (maybe even that one paper you wouldn't otherwise find!)