



SciFINDER[®]
A CAS SOLUTION

ACS International Ltd
vhyttinen@cas.org

SciFinder[®]

Решения для химиков от CAS:
MethodsNow, PatentPak, ChemZent

Veli-Pekka Hyttinen
April, 2018



SciFINDER[®]
A CAS SOLUTION

Ученые CAS анализируют, общаются и делают доступной научную информацию коллегам по всему миру

Отбор
источников



Индексирование



Реакции



Структуры
Маркуша



Процессинг



Применение в базах данных CAS специально разработанной технологии **стандартизированного индексирования** обеспечивает высокое качество информации в результатах поиска.



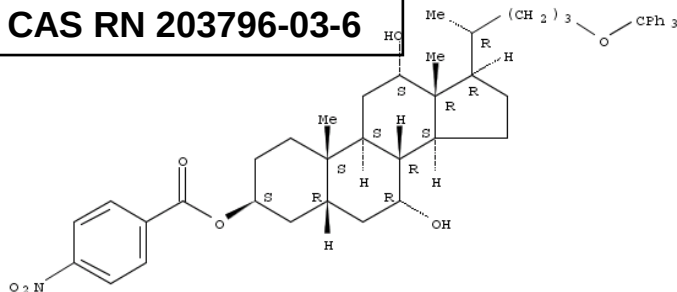
CAS[®]

A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

Сотрудники CAS находят химическую информацию и экономят Ваше время!

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, 1.56 Hz, 2 H); 0.70 (2.18 Hz, 13C NMR (CDCl₃, 75 MHz) δ 161.01, 159.55

CAS RN 203796-03-6



Absolute stereochemistry.



CAS[®]

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AMERICAN CHEMICAL SOCIETY

CAPLUS® – библиография 10,000+ журналов (185 стран) патенты из 63 ведомств	47+ млн. ссылок (5,000 ежедневно), Рефераты и индексирование с 1802 г., цитаты с 1997–
REGISTRY® – соединения Органические и неорганич. структуры, последовательности	141+ млн. малых молекул (20,000+ ежедневно), 67+ млн. Последо-ватель-ностей, 7,0+ млрд. свойств
CASREACT® – реакции Структурные диаграммы, детали	+ млн. реакций и синтезов с 1840г.
CHEMLIST® – регулируемая химия REACH, EINECS, US. Gov/Fed. Register	388,000 регулируемых соединений с 1979 г.
CHEMCATS® – поставщики реактивов Химические каталоги	млн. соединений от поставщиков (28+ млн. уникальных CAS-номеров) с ценами
MARPAT® – структуры Маркуша 440k патентов, INPI с1961 г.	1,4+ млн.структур Маркуша (75 новых патентов ежедневно)
MEDLINE – библиография 5,200 биомедицинских журналов	25+ млн.библиографических NLM-ссылок с 1947 г.

Основные возможности SciFinder – мощного инструмента для поддержки научной деятельности в Вашей организации

**141 млн.+
уникальных
соединений**

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ссылок**

+ интегрированный доступ к 24 миллионам ссылок из базы данных MEDLINE®

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реакций**

Почти в 2 раза больше чем у ближайшего конкурента

63

**патентных
ведомств**

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SCIFINDER®
A CAS SOLUTION

Предоставляет доступ к
максимальному
объему публичной
информации по химии.

SciFinder – поиск ссылок на патенты и журнальные статьи по темам, именам авторов и организаций

The screenshot displays the SciFinder web interface. At the top, there is 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'. The main content area is titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field with the text 'NANOTECHNOLOGY IN CANCER THERAPY' and a 'Search' button. To the left of the search field, there is a sidebar with a 'REFERENCES' section containing a list of search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Below this is a 'SUBSTANCES' section with options like Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. At the bottom left is a 'REACTIONS' section with 'Reaction Structure'. To the right of the search field, there is a 'SAVED ANSWER SETS' section with a list of search results, including 'WO2012040623 (PP)', 'WO 2015011083', 'surface and not semiconducting reactions (17)', 'azabicyclo sss conv', 'Reaction ketones to alcohols', 'reaction - ketone to alcohol', 'aldehyde reactions new', 'ring closing metathesis 1', 'suzuki catalyst patents', and 'Autosaved Reference Set'. Below this is a 'KEEP ME POSTED' section with a list of updates, including 'Thiolates in water', 'China Nerin Eng SMELTING', and 'Warfarin PROPH'. On the far right, there is a 'REFERENCES' section with a list of search criteria: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, and Tags. Two arrows point from the 'REFERENCES' section on the right to the search input field and the 'Search' button.

REFERENCES: RESEARCH TOPIC

Search

Advanced Search

SAVED ANSWER SETS

WO2012040623 (PP)

WO 2015011083

surface and not semiconducting 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

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags



SciFinder – поиск химических веществ по названиям, структурам, структурам Маркуша и молекулярным формулам

SciFinder®

Preferences | SciFinder Help | Sign Out

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

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

Search Type:

- ☐ Exact Structure
- ☒ Substructure
- ☐ Similarity

☐ Show precision analysis

ChemDraw

Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

SAVED ANSWER SETS ?

selective reduction of nitro group

Lipitor_fragment_patents_from _sss

143950-76-9

water_desalination_reviewarticle

MarkShannon1

macrocycles_protein

Autosaved Substance Set

View All | Import

KEEP ME POSTED ?

carbon nanotubes

Sep 06, 2014(258)

Aug 30, 2014(256)

Aug 23, 2014(268)

View All

SUBSTANCES

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



SciFinder – поиск реакций и синтетических препаратов по структурам

The screenshot displays the SciFinder web interface. At the top, there is 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'. The left sidebar contains a list of categories: REFERENCES, SUBSTANCES, and REACTIONS. The 'REACTIONS' category is highlighted, and 'Reaction Structure' is selected. The main content area is titled 'REACTIONS: REACTION STRUCTURE'. It features a 'Structure Editor' with 'Java' and 'Non-Java' tabs. A chemical structure of a substituted benzene ring with a hydroxyl group and a fused ring system is shown. Below the structure, there is a text prompt: 'Click image to change structure or view detail.' To the right of the structure editor, there is a 'Search Type' section with two radio buttons: 'Allow variability only as specified' and 'Substructure'. Below this is a 'ChemDraw' logo and a link to 'Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. Learn More'. At the bottom of the main content area, there is a 'Search' button and a link to 'Advanced Search'. On the right side of the interface, there are two sections: 'SAVED ANSWER SETS' and 'KEEP ME POSTED'. The 'SAVED ANSWER SETS' section lists various search results, including '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', and 'Autosaved Reference Set'. The 'KEEP ME POSTED' section lists 'Thiolates in water' (Mar 04, 2017(24), Jan 28, 2017(10)) and 'China Nerin Eng SMELTING' (Oct 08, 2016(3)).

The inset image shows a close-up of the 'Structure Editor' interface. It has two tabs: 'Java' and 'Non-Java'. A chemical structure of a substituted benzene ring with a hydroxyl group and a fused ring system is shown. Below the structure, there is a text prompt: 'Click image to change structure or view detail.'



SciFinder allows you to explore and analyze the breadth of CAS content so you can be more effective in your work

Stay current
in your field
and keep
track of
competition

Quickly find
and analyze
information
(research topic,
structure,
reaction)

Share ideas
with colleagues
and
collaborators

The screenshot displays the SciFinder web interface. At the top, there's a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' tabs. A search bar contains the text 'Keep Me Posted "Hydrogenation of Alkenes"[Apr 16, 2016] (3)'. Below this, there are buttons for 'Get Substances', 'Get Reactions', 'Get Related Citations', and 'Tools'. A 'Send to SciPlanner' button is highlighted in the top right. The main content area shows a list of references. The first reference is titled '1. Ph(i-PrO)SiH2: An Exceptional Reductant for Metal-Catalyzed Hydrogen Atom Transfers'. It includes a chemical structure diagram of a metal complex with a silane ligand and a list of bullet points: 'Catalyst loading to 0.05 mol%', 'Diverse organic solvents', and 'Reaction rates increased'. The second reference is identical to the first. The interface also includes a 'References' section with 'Analyze', 'Refine', and 'Categorize' tabs. The 'Analyze by' dropdown is set to 'Author Name', showing a list of authors: Martinez Ruben M, Obradors Carla, Shenvi Ryan A, Hanninen Mikko M, and Hayes Paul G.

SciFinder Smart Search



Natural phrase search covers

- synonyms : cancer → e.g. tumor
- word forms : freeze → frozen
- plural forms : mouse → mice
- abbreviations : oxidn
- truncations : solv → solvable, solved ...

You can add each synonym term in brackets separated with comma

- > determination of dioxin in food (chicken, poultry, egg)
- > heart disease (cardiovascular disease, coronary disease, heart attack)

Please note that SciFinder smart search does not automatically retrieve all kind of food (bread, milk etc.)

Применение фильтров Categorize и Analyze облегчает поиск релевантной информации

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in biology (221)
General chemistry	Animal pathology (69)
Biotechnology	Immunology (72)
Synthetic chemistry	Processes & systems (44)
Genetics & protein chemistry	Endocrinology (48)
Physical chemistry	Anatomy (27)
Polymer chemistry	Substances in adverse effects (16)
Biology	
Technology	
Analytical chemistry	
Environmental chemistry	

Biology > Immunology

2. Select index terms of interest.

Index Terms	Count
Select All Deselect All	
☐ Interferons	7
☐ Antibodies and Immunoglobulins	5
☐ Interferons, α	5
☐ Vaccines	5
☐ Interleukin 2	3
☐ Interleukin 4	3
☐ Leukotriene B4	3
☐ RANTES (chemokine)	3
☐ Spleen	3
☐ Tumor necrosis factor α	3
☐ Anti-HIV agents, vaccines	2
☐ CD4 antigens	2
☐ CXC chemokines	2
☐ Etanercept	2
☐ High throughput screening	2

SUBSTANCES ?

Analyze Refine

Analyze by: ?

- Target Indicators
- Bioactivity Indicators**
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role
- Transport proteins (all) 1

Show More

Get References Get Reactions Get Commercial Sources

Sort by: CAS Registry Number

0 of 1 Substance Selected

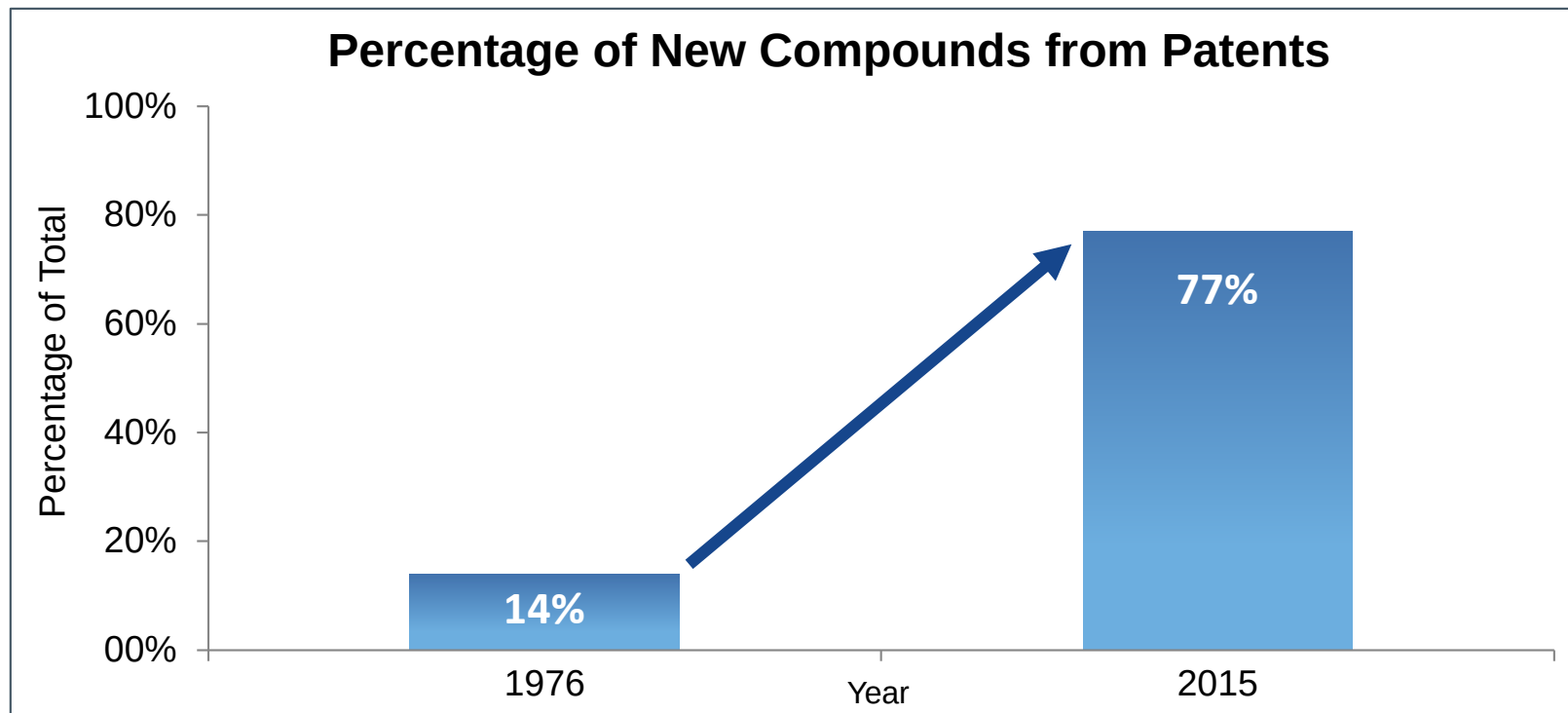
1. **28911-01-5**

~2061 ~34

C₁₇ H₁₂ Cl₂ N₄
4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-

Regulatory Information
Spectra
Experimental Properties

Новые химические соединения все чаще впервые описываются в патентах





PATENTPAK[®]

A CAS SOLUTION

- Быстрый поиск релевантных химических соединений в патентах
- **Патентное приложение для быстрого поиска релевантной химической информации в патентах, не выходя из SciFinder!**
- **Ежедневное обновление 14+ млн патентов из 31 стран**





PATENTPAK®
A CAS SOLUTION

- Постоянный доступ к **полным текстам патентов** из **основных патентных ведомств по всему миру**
- Семейства патентов на **разных языках**
- Поиск соединений
- **Интерактивный визуализатор** **связанный с SciFinder**

PatentPak™

PAGE 3 / 27 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 7440-38-20

As

compds.

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

SUMMARY OF THE INVENTION

[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)

CN(C(=O)N(C(=O)N(C(=O)O)CSC(As)(C)C)C(=O)O)C(=O)O

(I)

herein the crystalline form has a melting point greater than or equal to 185 °C. In certain embodiments, the crystalline form has a melting point in the range of about 185-200 °C. In other embodiments, the crystalline form has a melting point in the range of about 187-200 °C, or about 190-200 °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 diffraction pattern comprising characteristic peaks, expressed in terms of 2θ, at one or more of the following angles: about 16.6°, about 17.4°, about 21.4° and about 25.2°.



METHODSNow™

A CAS SOLUTION

- Презентация нового решения для поиска и анализа информации в самой большой в мире коллекции научных методов
- Индексирование качества CAS и новая, добавленная стоимость шаблонов ключевых методов из важных полнотекстовых источников
- Обнаруживает более 4,5 миллиона синтетических поэтапных протоколов и 0,5 миллиона аналитических методов, ориентированных на фармацевтику, сельское хозяйство и химические вещества
- Подробная информация для аналитических исследователей, таких как матрица, аналит, инструменты и возможности сравнения



SciFINDER®

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METHODSNow™
A CAS SOLUTION

Один продукт - два интерфейса

MethodsNow-Synthesis

SciFinder

Reaction Structure substructure > reactions (9)

REACTANTS

ANALYZE

Group by: No Grouping | Sort by: Relevance

1. View Reaction Detail [Link](#) [Send to SciFinder](#)

Single Step: Hover over any structure for more options.

Overview

MethodsNow™

Procedure

Stir the mixture of 7-ethyl-4-methoxy-2-oxo-1,4-dihydroquinoline-3-carboxylic acid (400 mg, 1.68 mmol), 1-azobiscyclohexane (380 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.

2. Add water to the mixture.

3. Work up.

Analysis: Environmental Data

¹H NMR, ¹³C NMR, IR

View with MethodsNow

MethodsNow-Analysis

CAS Solutions

METHODSNow™

★ Saved | Account

Search

Enter keyword, matrix, analyte, etc.

Advanced Search

Browse Method Categories

Agricultural Applications / Analysis	Fuels / Geology / Biofuels	Pharmacology / Toxicology
Bioassays	Historical Analysis / Dating	Polymer Analysis
Biomolecule Isolation	Miscellaneous	Water Analysis
Environmental Analysis	Organic Compound Analysis	
Food Analysis	Organometallics / Inorganics	

Recent Searches

Browse: Pesticide Residue Analysis



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MethodsNow Synthesis – Пошаговые экспериментальные протоколы

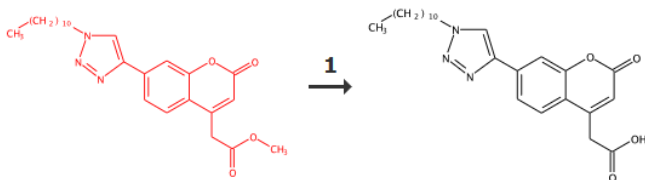
MethodsNow

7-Triazoly coumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule microarrays

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



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

Print

MethodsNow

Procedure

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.
2. Stir the reaction mixture for 3 hours at room temperature.
3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid.
4. Partition the reaction mixture between ethyl acetate and water.
5. Extract the aqueous layer with ethyl acetate.
6. Dry the combined organic layer over magnesium sulfate.

Scale

milligram

¹H NMR

¹H NMR (300 MHz, acetone-*d*₆): 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).

¹³C NMR

¹³C NMR (125 MHz, DMF-*d*₂, 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).

IR

IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm⁻¹.

HRMS

HRMS (EI): *m/z* calculated for C₂₈H₃₁N₃O₄: 425.2315 [*M*⁺]; found: 425.2315.

Mass Spec

MS (ESI): *m/z*: 426 [*M*+H⁺].

MP

235.5±0.8 °C.

CAS Method Number

3-352-CAS-78415

Print/Export

Close



MethodsNow Analysis – сравнить аналитические методы

CAS Solutions

METHODSNow™
A CAS SOLUTION

★ Saved Account

Search

Enter keyword, matrix, analyte, etc.

wastew

- wastewater
- wastewater treatment
- wastewater treatment anaerobic sludge
- wastewater treatment plants
- wastewater treatment sludge

Agricultural Applications / Analysis

Bioassays

Biomolecule Isolation

Environmental Analysis

Food Analysis

Fuels / Geology / Biofuels

Historical Analysis / Dating

Miscellaneous

Organic Compound Analysis

Organometallics / Inorganics

Pharmacology / Toxicology

Polymer Analysis

Water Analysis

Recent Searches

hplc lycopene analysis

METHODSNow wastewater sludge

Return to Results

Compare Protocols

Expand All Collapse All

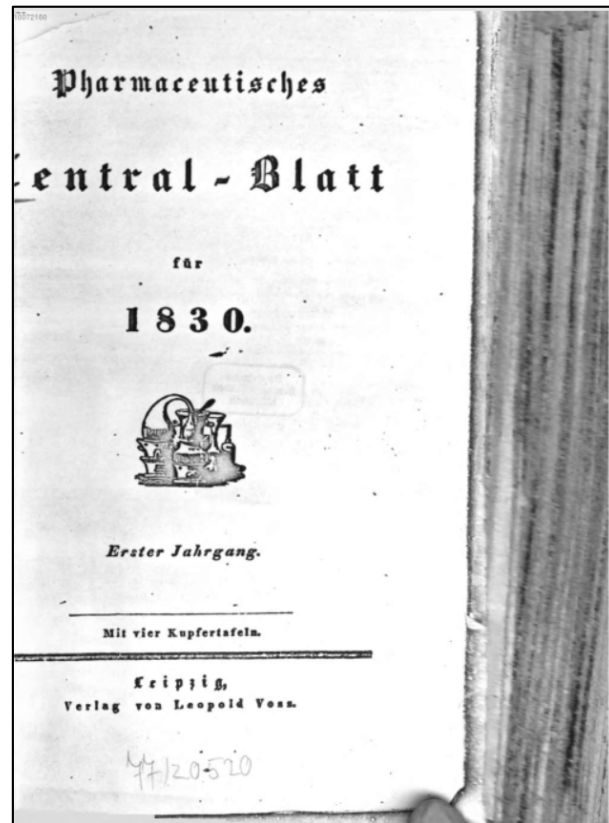
	1	2
Title	Analysis of Carbamazepine in Wastewater by Atmospheric pressure chemical ionization mass spectrometry	Analysis of Carbamazepine in Wastewater by Atmospheric pressure chemical ionization mass spectrometry
CAS Method Number	1-101-CAS-29149	1-101-CAS-27867
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis: Water / Wastewater / Sludge Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis: Water / Wastewater / Sludge Analysis
Technique	Atmospheric pressure chemical ionization mass spectrometry	Atmospheric pressure chemical ionization mass spectrometry
Analyte	Carbamazepine	Carbamazepine
Matrix	Wastewater; Wastewater treatment sludge	Wastewater; Wastewater treatment sludge
Other Materials	Environmental cartridges; Glass-fiber (0.45mm); LachWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W, continuous).	Environmental cartridges; Glass-fiber (0.45mm); Stainless steel vessel (34 mL); LachWell 96-well polypropylene plate cavities; Infrared (IR) laser diode (980 nm, 20 W, continuous).
Equipment Used	Milli-Q/Milli-RO system, Millipore, Milford, MA, USA; Microwave Accelerated Reaction System, CEM Corporation, North Carolina, USA; Vacuum pump, Welch Retschle Thomas, USA; View All >	Milli-Q/Milli-RO system, Millipore, Milford, MA, USA; ASE extractor, 350, Dionex, Sunnyvale, CA, USA; Vacuum pump, Welch Retschle Thomas, USA; LDTD-APC ionization source, View All >
Source	Carbamazepine in municipal wastewater and wastewater sludge; Ultrafast quantification by laser diode thermal desorption-atmospheric pressure chemical ionization View All >	Carbamazepine in municipal wastewater and wastewater sludge; Ultrafast quantification by laser diode thermal desorption-atmospheric pressure chemical ionization View All >



CHEMZENT™
A CAS SOLUTION

Chemisches Zentralblatt

- Основана в 1830 году для абстрактной литературы по химии на немецком языке
- Опубликован 3 миллиона немецких рефератов журнала 1830-1969
- CAS индексировал вещества и создал машинный перевод из тезисов



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



SCIFINDER®
A CAS SOLUTION