

汤健钊

高级客户顾问

jtang@acs-i.org

如何使用SciFinder获取医药信息

南方医科大学

2018.11.08



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市



CAS——构建最高质量的化学数据库



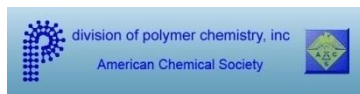
arXiv.org

Aldrichimica ACTA

ACS
chemical
biology



BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY



J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical
Neuroscience



THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters

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A CAS SOLUTION

CAS——构建最高质量的化学数据库



CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水

染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学



CAS数据库最具价值的内容——人工索引

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751 PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014
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Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

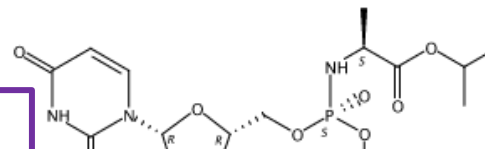
Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

Substances

[1190307-88-0P Sofosbuvir](#)
Absolute stereochemistry.

Page 2 in [PATENTPAK](#)



Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

CAS最新动向—解决方案

PatentPak™

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A Solution Powered by CAS

 **METHODSNOW™**
A CAS SOLUTION

 **CHEMZENT™**
A CAS SOLUTION

 **SCIFINDER®**
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CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

6. Preparation of substituted nucleosides, nucleotides and analogs thereof as antiviral agents

Quick View PATENTPAK

By Beigelman, Le...
From PCT Int. App...

Patent No.	Kind	Language
WO 2016100441	A1	English

Disclosed he...
phosphate, R...
methods of t...
medicament

Patent Family

US 20160176911	A1	English
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atkina, Natalia
Language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R' is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prepd. and tested as antiviral agent and of a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

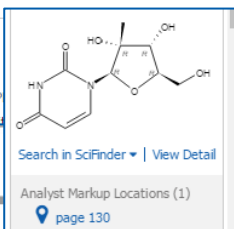
By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoguo; Lin, Yanfeng
From Faming Zhuanli Shenqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAPLUS

The prep. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methyluridine with

ZOOM

DOWNLOAD PDF

8. Q...
By F...



CAS RN 1206126-39-7

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 130

CAS RN 1206126-41-1

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 130

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
23 June 2016 (23.06.2016)

WIPO | PCT

(51) International Patent Classification:
C07H 19/10 (2006.01) C07H 19/13 (2006.01)
C07H 19/20 (2006.01) A61K 31/7072 (2006.01)
C07H 19/11 (2006.01) A61K 31/7076 (2006.01)
C07H 19/213 (2006.01) A61K 31/708 (2006.01)
C07H 19/067 (2006.01) A61P 31/14 (2006.01)
C07H 19/073 (2006.01)

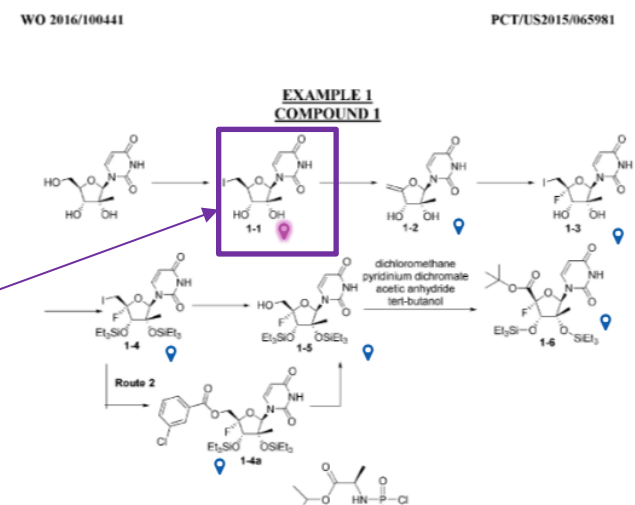
(81) Designated States (kind of national protection):
AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KZ, LA, LC, LK, LR, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SS, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TD, TJ, TM, UZ, UA, UG, UZ, VC, VN, ZA, ZM, ZW), European (AL, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KZ, LA, LC, LK, LR, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW), African and Asian (AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KZ, LA, LC, LK, LR, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW), African and Asian (AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KZ, LA, LC, LK, LR, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TD, TJ, TM, UZ, UA, UG, UZ, VC, VN, ZA, ZM, ZW), European (AL, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KZ, LA, LC, LK, LR, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW), African and Asian (AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, KZ, LA, LC, LK, LR, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RO, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).

(21) International Application Number: PCT/US2015/065981

(22) International Filing Date: 16 December 2015 (16.12.2015)

(25) Filing Language: English



CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求

SciFinder
SciPlanner
Reaction Structure substructure > reactions (9)
Analyze Reagent
Reagent
E/N
K₂CO₃
Et₃N
Show More
Set References Tools
Critical Inv. for Shipping Sort by Relevance
Send to SciPlanner Display Options
1. View Reaction Detail Link Vendor Reactions
Single Step hover over any structure for more options.
Overview
Microcosm™
Procedure
1. Stir the mixture of 7-methyl-4-methoxy-2-methyl-2H-chromen-2-one (480 mg, 1.05 mmol), 1-iodooctane (388 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.
View more...
Available Experimental Data
1H NMR, 13C NMR, IR, HRMS, Mass Spec, MP
View with MethodsNow

嵌在SciFinder中的合成模块

CAS Solutions
METHODS NOW
atorvastatin
Return to Home
Sort Relevance
Analyze
Atorvastatin (227)
Atorvastatin calcium (211)
Ezetimibe (80)
Amlodipine besylate (56)
Fenofibrate (46)
View All
Matrix
Pharmaceutical tablets (293)
Blood plasma (60)
Tablets (49)
Pharmaceutical capsules (34)
Garcinia atroviridis (20)
View All
Method Category
Technique
Reversed-phase HPLC (152)
Spectrophotometry (101)
UV-visible spectroscopy (71)
HPLC (57)
Liquid chromatographic UV detectors (43)
View All
Results (528)
Sort Relevance
Compare (0/3)
Add to Compare
View Details & Instructions
Analyte Atorvastatin
Matrix Blood plasma
Other Materials Material: 60 F254 silica gel HP TLC plates
Method Category Active Pharmaceutical Ingredient and Metabolite Analysis
Technique High-performance thin layer chromatography
Equipment Used Automatic TLC Sampler 3
Source HPTLC determination of atorvastatin in plasma
Jamshidi, A.; Nateghi, A. R.
Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlage GmbH
Document Sources
Abstract

单独的分析界面

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciFinder覆盖的数据库



SciFinder覆盖医学专家每日阅读的医学领域出版物

- Zhonghua Tangniaobing Zazhi
- Biomedical Chromatography
- Romanian Biotechnological Letters
- Pharmaceutical Patent Analyst
- Asian Pacific Journal of Tropical Biomedicine
- International Journal of Molecular Medicine
- Archives of Pharmacal Research
- BioMedical Research
- Journal of the Egyptian Medical Association
- European Journal of Medicinal Chemistry
- Klinische Wochenschrift

- *ACS Synthetic Biology*
- *Annual Review of Biochemistry*
- *Biochemistry and Cell Biology*
- *Cellular Physiology and Biochemistry*
- *Journal of Biological Chemistry*
- *Journal of Cellular Biochemistry*
- *Molecular and Cellular Biochemistry*
- *Preparative Biochemistry and Biotechnology*

- *Advanced Drug Delivery Reviews*
- *Annual Review of Pathology: Mechanisms of Disease*
- *Anti-Inflammatory Anti-Allergy Agents in Medicinal Chemistry*
- *Circulation Research*
- *Immunity*
- *Journal of the American Medical Association*
- *Journal of Experimental Medicine*
- *Nature Reviews Drug Discovery*
- *Trends in Immunology*

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New Commercial Source Logos



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SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder main interface with several key components and annotations:

- Top Navigation:** CAS Solutions, SCIFINDER A CAS SOLUTION, Preferences | SciFinder Help, and Sign Out.
- User Greeting:** Welcome Helen Zhu.
- Tool Bar:** Explore, Saved Searches, and SciPlanner.
- Left Sidebar (Annotations):**
 - REFERENCES:** Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags.
 - SUBSTANCES:** Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier.
 - REACTIONS:** Reaction Structure.
- Search Area (Annotation: 检索入口):** A search box with a "Search" button and an "Advanced Search" link. Examples provided include "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds".
- Right Panel (Annotation: 已保存的结果集):** A list of saved answer sets including CSF1R, jmc, EP 19870107847, Daclatasvir-1, SUB result, EX result, MF result, polymer1, structure search, and Autosaved Substance Set. Below this is a "KEEP ME POSTED" section with a link to "Learn how to: Create Keep Me Posted".

已保存的结果集

检索入口

定题追踪

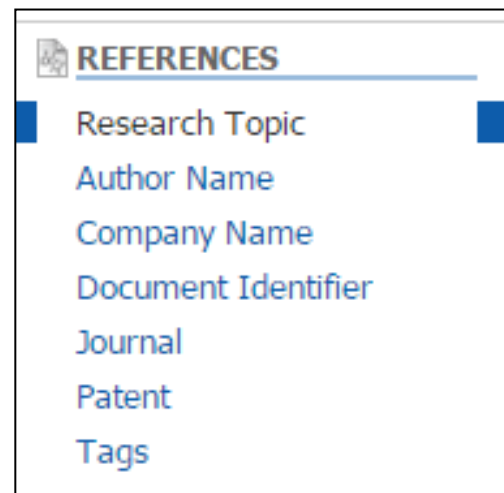
SciFinder检索——文献检索

■ 文献检索方法

- 主题检索
- 作者名检索
- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献

■ 检索策略推荐

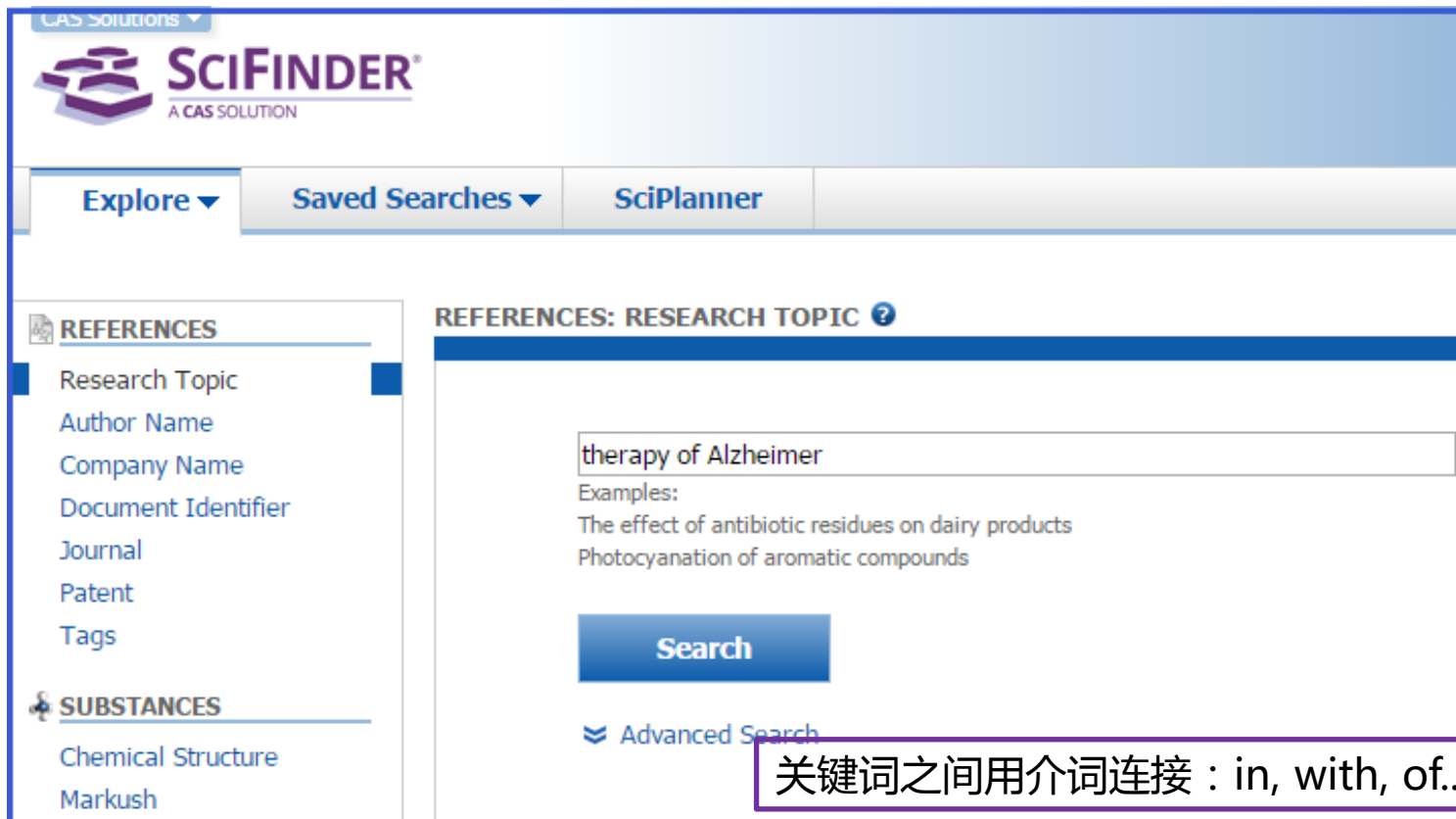
- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献
- 关注某科研人员的文献：作者名检索
- 关注某机构科研进展：机构名检索



文献检索——主题

主题检索：阿尔茨海默症的治疗

检索式：therapy of Alzheimer



The screenshot displays the SciFinder search interface. At the top, the SciFinder logo is visible, along with navigation tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. On the left, a sidebar menu lists search criteria under 'REFERENCES' (Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags) and 'SUBSTANCES' (Chemical Structure, Markush). The main search area is titled 'REFERENCES: RESEARCH TOPIC' and contains a search input field with the text 'therapy of Alzheimer'. Below the input field, there are 'Examples:' such as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples. At the bottom of the search area, there is a link for 'Advanced Search'. A purple box highlights the text '关键词之间用介词连接：in, with, of...' at the bottom right of the search area.

主题检索的候选项

Explore ▾ Saved Searches ▾ SciPlanner

Research Topic "therapy of Alzheimer"

REFERENCES ⓘ

Select All Deselect All

1 of 5 Research Topic Candidates Selected

	References
<input type="checkbox"/> 1507 references were found containing "therapy of Alzheimer" as entered.	1507
<input checked="" type="checkbox"/> 18649 references were found containing the two concepts "therapy" and "Alzheimer" closely associated with one another.	18649
<input type="checkbox"/> 61620 references were found where the two concepts "therapy" and "Alzheimer" were present anywhere in the reference.	61620
<input type="checkbox"/> 6313362 references were found containing the concept "therapy".	6313362
<input type="checkbox"/> 230575 references were found containing the concept "Alzheimer".	230575

Get References

“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中；

“were present anywhere in the reference”表示同时出现在一篇文献中；

按被引次数排序— Citing References

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "therapy of Alzheimer" > references (18649) > refine "china" (1085) > refine by categories > Effects of ginger root extract...

REFERENCES ⓘ Get Substances Get Reactions Get Related Citations Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize Sort by: Citing References ▾ ↓

Accession Number
Author Name
Citing References
Publication Year
Title

Display Options Page: 1 of 933

Analyze by: ⓘ	
Author Name ▾	
Perry George	123
Smith Mark A	121
Zhu Xiongwei	80
Bush Ashley I	67
Masters Colin L	65
Selkoe Dennis J	58
Brinton Roberta Diaz	57
Giacobini Ezio	55
De Strooper Bart	54
Iqbal Khalid	52

1. **The amyloid hypothesis of Alzheimer's disease: progress and problems on the road to therapeutics**
By Hardy, John; Selkoe, Dennis J.
From Science (Washington, DC, United States) (2002), 297(5580), 353-356. | Language: English, Database: CAPLUS
A review. It has been more than 10 yr since it was first proposed that the neurodegeneration in **Alzheimer's** disease (AD) may be caused by deposition of amyloid β -peptide ($A\beta$) in plaques in brain tissue. According to the amyloid hypothesis, accumulation of $A\beta$ in the brain is the primary influence driving AD pathogenesis. The rest of the disease process, including formation of neurofibrillary tangles contg. tau protein, is proposed to result from an imbalance between $A\beta$ prodn. and $A\beta$ clearance.

2. **Alzheimer's disease: genes, proteins, and therapy**
By Selkoe, Dennis J.
From Physiological Reviews (2001), 81(2), 741-766. | Language: English, Database: CAPLUS
A review with 216 refs. Rapid progress in deciphering the biol. mechanism of **Alzheimer's** disease (AD) has arisen from the application of mol. and cell biol. to this complex disorder of the limbic and assocn. cortices. In turn, new insights into fundamental aspects of protein biol. have resulted from research on the disease. This beneficial interplay between basic and applied cell biol. is well illustrated by advances in understanding the genotype-to-phenotype relationships of familial **Alzheimer's** disease. All four genes definitively linked to inherited forms of the disease to date have bee...

3. **The amyloid hypothesis of Alzheimer's disease: progress and problems on the road to therapeutics**
By Hardy John; Selkoe Dennis J
From Science (New York, N.Y.) (2002), 297(5580), 353-6. | Language: English, Database: MEDLINE
It has been more than 10 years since it was first proposed that the neurodegeneration in **Alzheimer's** disease (AD) may be caused by deposition of amyloid beta-peptide

Citing Reference: 帮助找到最重要的文献

文献检索结果

The screenshot displays the SciFinder search results page for the topic "therapy of Alzheimer". The interface includes a top navigation bar with "Explore", "Saved Searches", "SciPlanner", "Save", "Print", and "Export" options. A yellow warning banner at the top states "Duplicates not removed. Answer set exceeds 10,000 reference limit." Below this, the search topic is identified as "Research Topic 'therapy of Alzheimer' > references (18649)".

Key annotations in Chinese are present:

- "文献分析工具" (Literature Analysis Tool) points to the "Analyze" tab in the left sidebar.
- "获取原文" (Get Full Text) points to the "Other Sources" link for the first reference.

The left sidebar shows an "Analyze by:" section with a dropdown menu set to "Author Name". A list of authors and their corresponding reference counts is displayed:

Author Name	Count
Perry George	123
Smith Mark A	121
Zhu Xiongwei	80
Bush Ashley I	67
Masters Colin L	65
Selkoe Dennis J	58
Brinton Roberta Diaz	57
Giacobini Ezio	55
De Strooper Bart	54

The main content area shows two references:

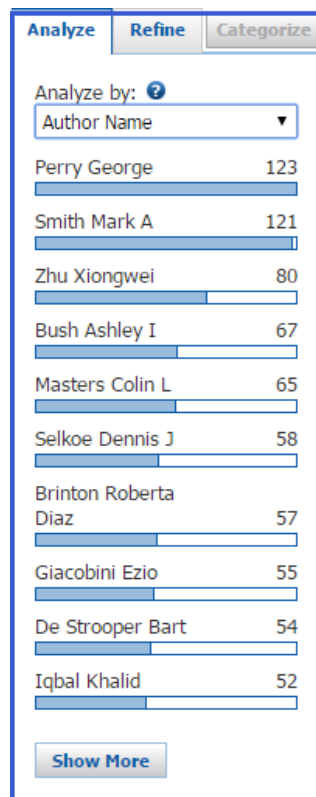
- 1. Combining BACE1 inhibition with metal chelation as possible therapy for Alzheimer's disease**
By Henary, Maged M.; Dost, Tyler L.; Owens, Eric A.; Punganuru, Surendra Reddy
Edited by Atta-ur-Rahman; Choudhary, Muhammad Iqbal
From Drug Design and Discovery in Alzheimer's Disease (2014), 547-565. | Language: English, Database: CAPLUS
A complex disease such as **Alzheimer's** requires an arsenal of **therapies** to help combat and stabilize its advancement. Despite considerable scientific progress, current **therapeutic** approaches for **Alzheimer's** treatment offer only limited and transient benefits to patients. Therefore, in response to the mol. complexity of this disease, a new strategy has recently emerged aimed at simultaneously targeting multiple pathol. processes involved in the pathogenesis cascade. β -secretase plays a crit. role in β -amyloid formation, a major constituent of amyloid plaques in **Alzheimer's** disease (AD) brain ...
- 2. BACE1 inhibitors: attractive therapeutics for Alzheimer's disease**
By Decourt, Boris; Macias, MiMi; Sabbagh, Marwan; Adem, Abdu
Edited by Atta-ur-Rahman; Choudhary, Muhammad Iqbal
From Drug Design and Discovery in Alzheimer's Disease (2014), 518-546. | Language: English, Database: CAPLUS
One of the neuropathol. hallmarks of **Alzheimer's** disease (AD) is the presence of brain senile plaques made up principally of aggregated amyloid beta ($A\beta$) peptides. $A\beta$ is produced during the consecutive proteolysis of the transmembrane amyloid precursor protein (APP) by β - and γ -secretases. Genetic and pharmacol. manipulations have demonstrated the major β -secretase in AD that makes the initial cleavage required for synthesis of $A\beta$ is the beta-site APP-cleaving enzyme 1 (BACE1). It is therefore very tempting to consider inhibiting BACE1 as a potential AD **therapeutic** intervention. Here, we r...

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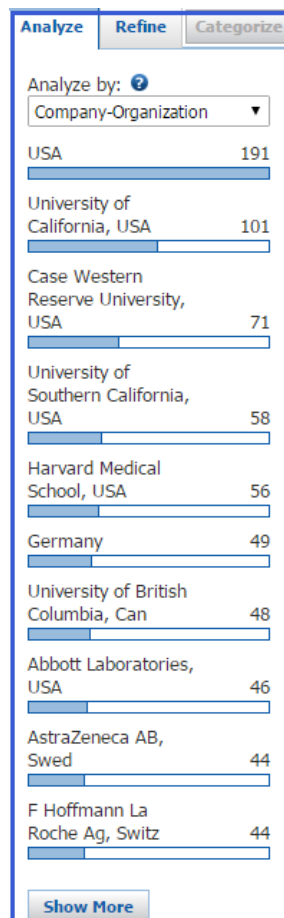


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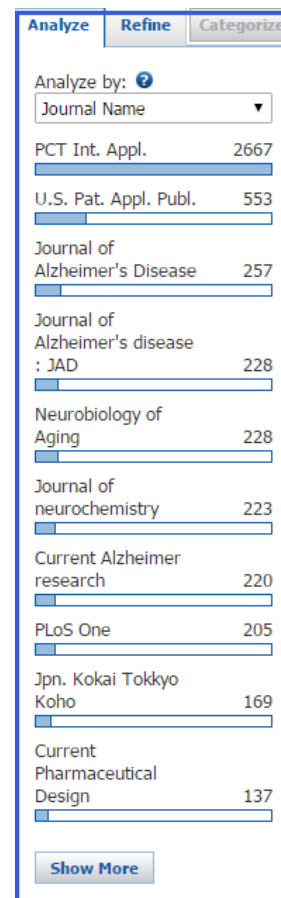
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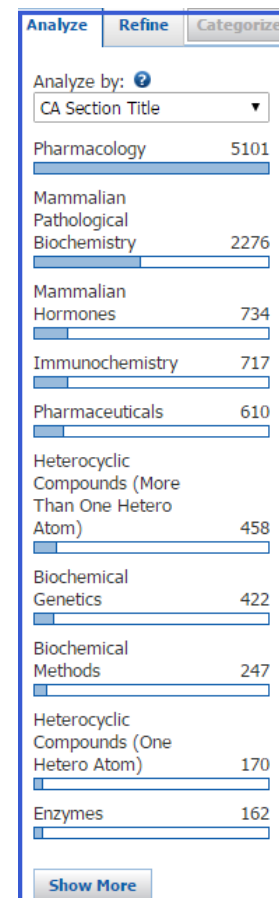
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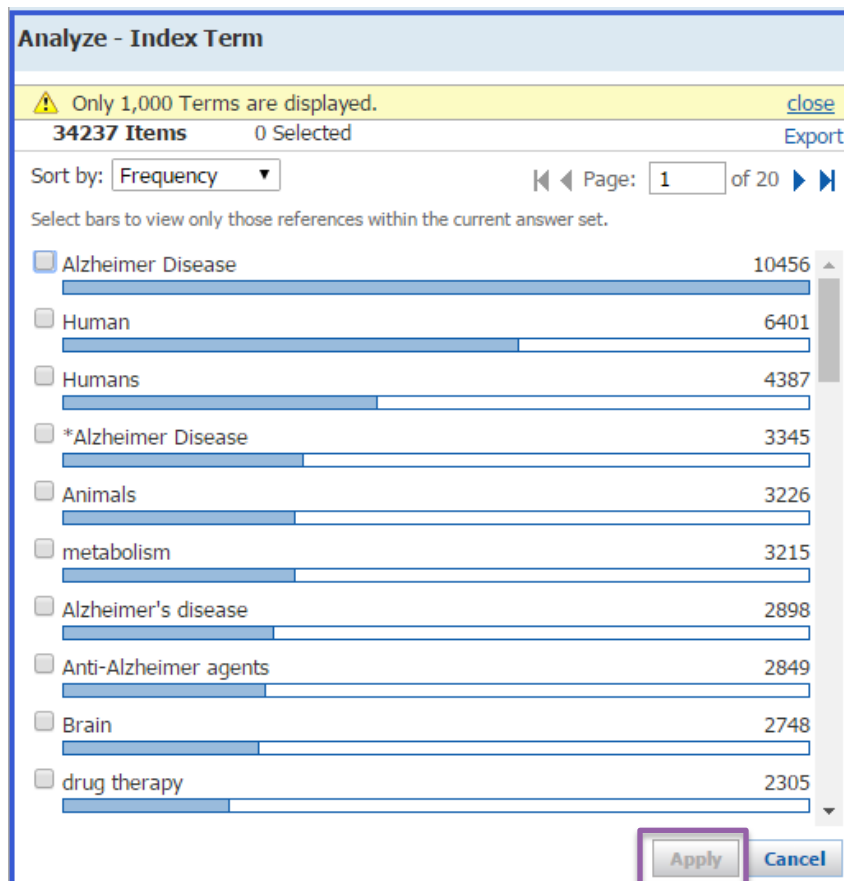
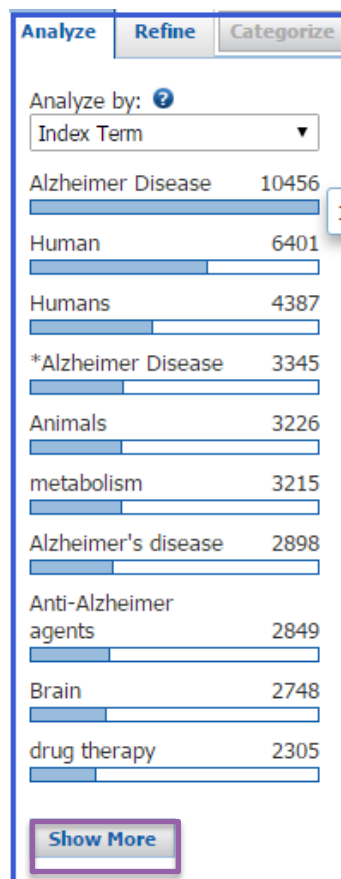
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Tang Xi Can	8

1. Streptozotocin Induces Mild Cognitive Impairment at Appropriate Doses in Mice as Determined by Long-Term Potentiation and the Morris Water Maze

By Li, Dong; Huang, Yan; Cheng, Bin; Su, Jie; Zhou, Wen-Xia; Zhang, Yong-Xiang; Abbate, Carlo
From Journal of Alzheimer's Disease (2016), 54(1), 89-98. | Language: English, Database: CAPLUS

Alzheimer's disease (AD) is a progressive neurodegenerative disease, and effective therapeutic drugs in the clinic are still lacking. Ideally, AD progression could be stopped at an early stage, such as at the mild cognitive impairment (MCI) stage. MCI refers to the clin. condition between normal aging and dementia. Patients with MCI experience memory loss but do not meet the criteria for the diagnosis of clin. probable AD. However, few MCI animal models have been established. Here, we used in vivo long-term potentiation (LTP) recording and the Morris water maze (MWM) to evaluate the effec...

2. Design of electrochemical biosensors with peptide probes as the receptors of targets and the inducers of gold nanoparticles assembly on electrode surface

By Xia, Ning; Wang, Xin; Yu, Jie; Wu, Yangyang; Cheng, Shuchao; Xing, Yun; Liu, Lin
From Sensors and Actuators, B: Chemical (2017), 239, 834-840. | Language: English, Database: CAPLUS

We reported a general way to design electrochem. biosensors with peptide probes as the receptors of targets and the inducers of gold nanoparticles (AuNPs) assembly on electrode surface. To demonstrate the feasibility of our strategy, human chorionic gonadotropin (hCG) was first detd. as a model analyte. Specifically, the hCG-binding peptide triggered the aggregation of AuNPs in soln.; by modifying the electrode with the hCG-binding peptide, the peptide-induced AuNPs assembly was achieved on the electrode surface, resulting in the formation of a network of AuNPs and a significant fall of char...

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1. **Effects of ginger root extract on animal inflammatory factors in rats with Alzheimer's disease**
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By Zeng, Gao-feng; Zhang, Zhi-yong; Lu, Li; Xiao, De-qiang; Zong, Shao-hui; He, Jian-ming
From Guangdong Yixue (2013), 34(7), 1014-1016. | Language: Chinese, Database: CAPLUS
Objective: To study the effect of ginger root ext. on expression and relationship of nuclear factor- κ B (NF- κ B) and interleukin-1 β (IL-1 β) in the hippocampus of rats with β -amyloid protein (A β) caused Alzheimer's disease (AD), and explore the possible therapeutic effects and mechanism of ginger ext. on AD. Methods: 60 SD healthy rats, half male and half female, were randomly divided into sham operation (SOP) group and operation (OP) group, resp. 10 and 50, SOP group was intracerebroventricularly injected with normal saline, OP group was intracerebroventricularly injected with A β 25-35. After...

2. **Ameliorative effects of huperzine A on Alzheimer's disease associated mitochondrial dysfunction and its potential molecular mechanisms**
Quick View Other Sources
By Ye, Chun-yan; Zhang, Hai-yan
From Zhongguo Xinyao Yu Linchuang Zazhi (2012), 31(12), 701-706. | Language: Chinese, Database: CAPLUS
A review. Alzheimer's disease (AD) was a common neurodegenerative disease, of which the most widely used therapeutic drug was acetylcholinesterase inhibitor (AChEI). Huperzine A, an alkaloid developed by Chinese scientists, was a potent AChEI. Recent work revealed that besides the acetylcholinesterase inhibitory effect, huperzine A could also significantly benefit mitochondria in various models like middle cerebral artery occlusion (MCAO) rat, APP/PS1 transgenic mice and β -amyloid (A β) injured isolated mitochondria. This review summarized the pivotal roles of mitochondria in AD processing ...

3. **UPLC-TOF MS-Based Metabonomic Study on Coadministration of Huperzine A and Ligustrazine Phosphate for Treatment of Alzheimer's Disease**
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By Shi, Jun; Wang, Yiming; Luo, Guoan
From Chromatographia (2011), 74(11-12), 827-832. | Language: English, Database: CAPLUS
This work was designed to assess the holistic efficacy of concurrent treatment with huperzine A (HA) and ligustrazine phosphate (LP) in the a metabonomics characteristics of the poly-therapy in treating Alzheimer's disease (AD). Metabolic profiling of the brain was performed using coupled to time-of-flight mass spectroscopy (UPLC-TOF MS). Principal component anal. and partial least squares discriminant anal. were

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1. Effects of ginger root extract on animal inflammatory factors in rats with Alzheimer's disease

By: Zeng, Gao-feng; Zhang, Zhi-yong; Lu, Li; Xiao, De-qiang; Zong, Shao-hui; He, Jian-ming

Objective: To study the effect of ginger root ext. on expression and relationship of nuclear factor kappa B (NF- κ B) and interleukin-1 β (IL-1 β) in the hippocampus of rats with β -amyloid protein (A β) caused Alzheimer's disease (AD), and explore the possible therapeutic effects and mechanism of ginger ext. on AD. Methods: 60 SD healthy rats, half male and half female, were randomly divided into sham operation (SOP) group and operation (OP) group, resp. 10 and 50, SOP group was intracerebroventricular injected with normal saline, OP group was intracerebroventricular injected with A β 25-35. After the modeling, the OP group were randomly divided into ginger ext. low dose group (OP+LGRE group), ginger ext. middle dose group (OP+MGRE), ginger ext. high dose group (OP+HGRE group), huperzine A group (OP+HPA group) and control group (group OP+BC). All rats received intragastric administration (group OP+BC was treated with normal saline) after 4 wk, the NF- κ B, IL-1 β immunohistochem. staining was used to compare the changes of rat brain inflammation system index and pathol. Results: In OP+HGRE group, OP+HPA group, IL-1 β NF- κ B pos. expression was significantly higher; the intervention had no significant effect of group OP+LGRE, OP+MGRE. Conclusion: ginger ext. can improve the pos. expression activity of NF- κ B and IL-1 β on AD rats.

Indexing

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Section cross	
Concepts 重要概念	
Alzheimer disease Pharmaceutical natural products	Anti-Alzheimer agents Zingiber officinale
effects of ginger root ext. on animal inflammatory factors in rats with Alzheimer's disease	
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...ors in rats with Alzheimer's disease	

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Pages1014-1016
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2013
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COMPANY/ORGANIZATION

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Guangxi Medical University
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CAN162:419412
CAPLUS

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Guangdong Yixue Bianjibu

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Chinese

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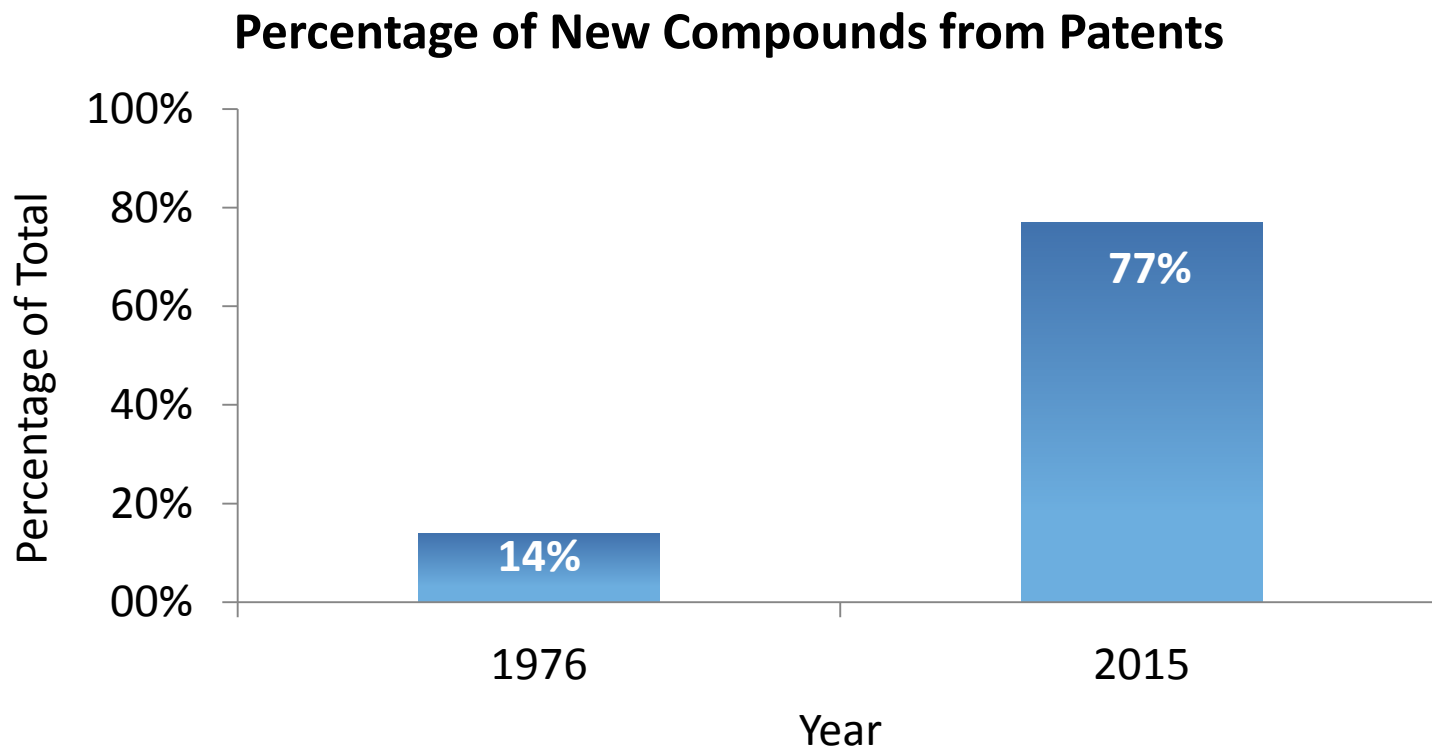
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8. Preparation of 6-fluoro-9-methyl- β -carboline for the treatment of ear disease

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By Rommelspacher
From Eur. Pat. Appl.

Patent No.	Kind	Language
EP 2853533	Interactive	German

Patent Family

WO 2015044434	A2	German
WO 2015044434	A3	German

... methyl- β -carboline (I) and pharmaceutical compns. thereof useful in the treatment of acute and chronic inner ear diseases. ... 6-1-methyl-1H-Indole-3-ethanamine hydrochloride with 2,2-dihydroxyacetic acid followed by decarboxylation and redn. and

9. Preparation of fluoro-substituted 9-methyl- β -carbolines for the treatment of ear diseases

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By Rommelspacher, Hans; Enzensperger, Christoph
From PCT Int. Appl. (2015), WO 2015044434 A2 20150402. | Language: German, Database: CAPLUS

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CAS RN 24335-20-4

HCl

Beispiele

Beispiel 1a: Synthese von 6-Fluor-9-methyl-β-carbolin

5 Analog zur Vorschrift von Ho und Walker (Beng T. Ho und K. E. Walker; *Org. Synth.* 1971, 51, 136 oder *Org. Synth.* 1988, Coll. Vol. 3, 3, 5 mmol (800 mg) 5-Fluor-1-methyltryptamin (AKos GmbH, Steinen) gelöst und mit einer

10 Glyoxalsäurehydrat (Figur 1a, Formel III) in 810 wird dann eine Lösung aus 3,4 mmol (190,4 wobei der pH auf etwa 4 eingestellt wird. Raumtemperatur gerührt und zur Vervollständigung der Kristallisation noch eine weitere Stunde ins Eisbad gestellt. Der orange-beige Niederschlag des Betains (Figur 1a, Formel IVa) wird abfiltriert und mit wenig Eiswasser gewaschen.

15 Zur Decarboxylierung wird der noch feuchte Filterkuchen des Betains (Figur 1a, Formel IVa) in einen Kolben überführt und in verdünnter Salzsäure (6,48 mL Wasser und 918 µL konzentrierte Salzsäure) gelöst. Die Reaktionsmischung wird unter

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C₁₈ H₁₆ N₂ O
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Molecular Weight
276.33

Melting Point (Experimental)
Value: 166 °C

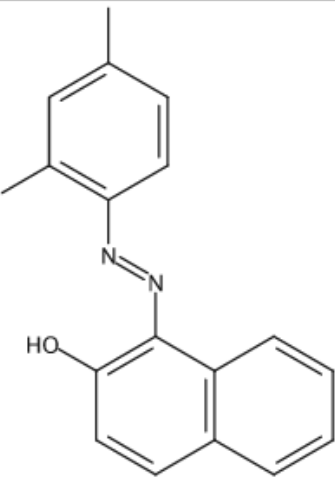
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Value: 476.7±40.0 °C | Condition: Press: 760 Torr

Density (Predicted)
Value: 1.14±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
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H Donors	1		(21)
H Donor/Acceptor Sum	4		(21)
logP	5.471±1.252	Temp: 25 °C	(21)
Molecular Weight	276.33		(21)

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- H Acceptors
- H Donors
- Koc
- logD
- logP
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- Mass Solubility (g/L)
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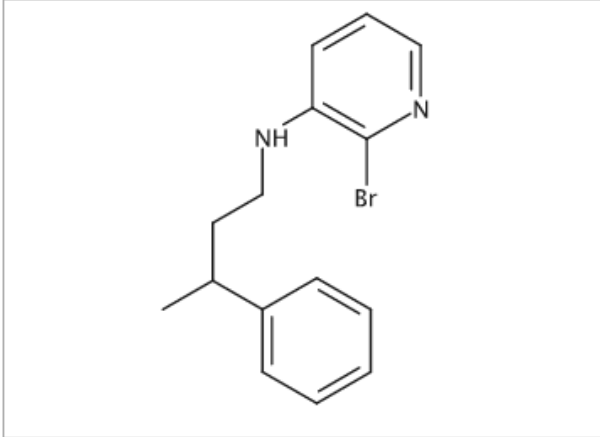
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Only retrieve substances

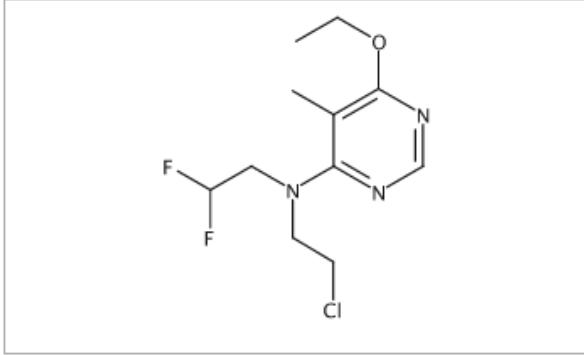
1. 1986293-22-4



$C_{15}H_{17}BrN_2$
3-Pyridinamine, 2-bromo-*N*-(3-phenylbutyl)-

Key Physical Properties

2. 1986293-21-3



$C_{11}H_{16}ClF_2N_3O$
4-Pyrimidinamine, *N*-(2-chloroethyl)-*N*-(2,2-difluoroethyl)-6-ethoxy-5-methyl-

Key Physical Properties

4. 1986293-16-6

5. 1986293-14-4

4500多万个结构，
如何筛选黄酮类物质？

物质结果集的筛选——Refine

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Atom Short

Get substances that match your query using:

- Exact search
- Substructure search

OK

Cancel

$C_{15}H_{10}O_2$ 222.24

锁环工具：避免在被锁定的环结构上出现新的环结构

SUBSTANCES ?

Analyze Refine

Refine by: ?

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.

Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

Refine

物质检索结果集

Explore ▾ Saved Searches ▾ SciPlanner

Property "Predicted - Molecular Weight, ..." > substances (45142315) > refine "substructure" (16901)

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: Relevance ▾

0 of 16901 Substances Selected

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Structure Editor:

Java Non-Java

Click image to change structure or view detail.
Search type: **Substructure**

1. 1373355-19-1

~3

$C_{17}H_{14}O_2$
4,7-Dimethylflavone

▶ Key Physical Properties

2. 912915-64-1

~6 ~3

$C_{15}H_{10}O_4$
4,7-Dihydroxyflavone

▶ Key Physical Properties

4. 6665-68-5

~38 ~7

5. 22395-22-8

~269 ~67

从4500多万个结构中
筛选出16901个黄酮类物质

物质检索——分子式

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: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

无机金属盐：金属离子和阴离子间用点 (.) 分开

1. 151-21-3

(Component: 151-41-7)

~84904 ~276

C₁₂H₂₆O₄S.Na
Sulfuric acid monododecyl ester sodium salt (1:1)

▶ **Key Physical Properties**

- Regulatory Information
- Spectra
- Experimental Properties

分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前;如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

物质检索——结构

The screenshot displays the SciFinder web interface for searching chemical structures. On the left is a navigation menu with three main sections: REFERENCES, SUBSTANCES, and REACTIONS. Under SUBSTANCES, 'Chemical Structure' is highlighted with a purple box. The main content area is titled 'SUBSTANCES: CHEMICAL STRUCTURE' and features a 'Structure Editor' window with 'Java' and 'Non-Java' tabs and a 'Click to Edit' prompt. To the right, the 'Search Type' section includes radio buttons for 'Exact Structure', 'Substructure' (which is selected), and 'Similarity', along with a 'Show precision analysis' checkbox. A 'ChemDraw' logo is visible in a box at the bottom right of the main area. At the bottom of the interface, there is an 'Import CXF' link, a large blue 'Search' button, and a footer containing 'Advanced Search' and an 'Always Show' checkbox.

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 to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw

Launch a SciFinder substance or reaction

Import CXF

Search

[Advanced Search](#) Always Show

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing chemical structures, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has radio buttons for 'Structure', 'Reaction', and 'Markush', and search options for 'Exact search', 'Substructure search', and 'Similarity search'. The interface also features a command line at the bottom with the text 'C H O S N P Cl Br F I Si' and a 'Scale 100' indicator. Numerous callout boxes in Chinese point to specific tools and features, such as '橡皮' (Eraser), '铅笔' (Pencil), '元素周期表' (Periodic Table), '常用基团' (Common Groups), 'R基团定义工具' (R-group definition tool), '可变位置连接工具' (Variable position connection tool), '模版工具' (Template tool), '索套选择工具' (Lasso selection tool), '原子锁定工具' (Atom locking tool), '镜面旋转工具' (Mirror rotation tool), '单双键, RS构型, 不确定键定义工具' (Single/double bond, RS configuration, uncertain bond definition tool), '常见环, 多元环工具' (Common rings, multi-ring tools), '负电子' (Negative charge), '正电子' (Positive charge), 'C原子和单键恢复工具' (C atom and single bond recovery tool), '结构检索选择' (Structure search selection), and '结构和反应切换功能' (Structure and reaction switching function).

橡皮

结构和反应切换功能

铅笔

元素周期表

可变基团

重复基团工具

碳链工具

选择工具

环锁定工具

旋转工具

正电子

C原子和单键恢复工具

常用基团

R基团定义工具

可变位置连接工具

模版工具

索套选择工具

原子锁定工具

镜面旋转工具

结构检索选择

单双键, RS构型, 不确定键定义工具

常见环, 多元环工具

负电子

Structure Editor

Draw or change

Shortcut Keys

Drawing Editor:

Structure

Reaction

Markush

Get substances that match your query using:

Exact search

Substructure search

Similarity search

确定

取消

C H O S N P Cl Br F I Si

Scale 100

(query)

物质检索——精确结构检索

The screenshot displays the 'Structure Editor' window. At the top left, a callout box points to the 'I' icon in the toolbar, containing the text: '通过CAS RN转换结构：CAS RN: 50-36-2'. The central workspace shows a chemical structure of a bicyclic amine derivative with a benzoyl group and a methoxy group. On the right side, the 'Drawing Editor' panel is visible, with 'Structure' selected. Below it, the search options are: 'Exact search' (selected), 'Substructure search', and 'Similarity search'. A callout box highlights the 'Exact search' option with the text: '精确结构检索'. At the bottom of the window, the molecular formula $C_{17}H_{21}NO_4$ and the molecular weight 303.36 are displayed.

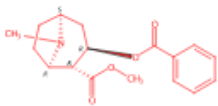
精确结构检索结果

Get References | Get Reactions | Get Commercial Sources | Tools | Create Posted

Sort by: Relevance

0 of 6 Substances Selected

1. **668-19-9**



Absolute stereochemistry.

C₁₇H₂₁N O₄
8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, (1*R*, 2*R*, 3*R*, 5*S*)-

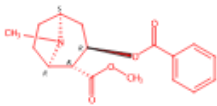
▶ Key Physical Properties
Spectra

可卡因

2. **114599-38-1**

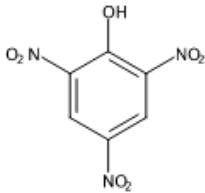
可卡因组合物

668-19-9
C₁₇H₂₁N O₄



Absolute stereochemistry.

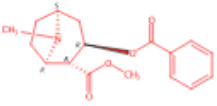
88-89-1
C₆H₃N₃O₇



C₁₇H₂₁N O₄ · C₆H₃N₃O₇
Alcocaine, picrate (6CI)

3. **109496-04-0**

(Component: 668-19-9)



* HCl

Absolute stereochemistry.

C₁₇H₂₁N O₄ · Cl H
Alcocaine, hydrochloride (6CI)

盐酸可卡因

物质检索——精确结构检索

精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

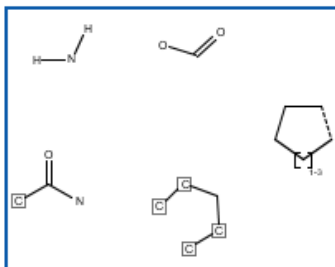
物质检索——亚结构检索

作用机理

 编辑本段

帕拉米韦是Babu等在分析唾液酸、扎那米韦、奥司他韦与NA的互相作用机制及构效关系的基础上设计并合成的环戊烷衍生物，与环连接的基团有亲水的羧基和胍基，以及疏水的异戊基和乙酰氨基，4个极性不同的基团分别作用于流感病毒NA结构中不同的活性位点区域。羧基部分与NA活性位点的3个精氨酸残基Arg118, Arg292,

SUBSTANCES: CHEMICAL STRUCTURE ?



Click image to change structure or view detail.

Import CXF

Search

 Advanced Search Always Show

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Formula Weight Return only substances in this formula weight range:

Min: Max:

Characteristics Single component
 Commercially available
 Included in references

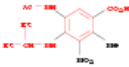
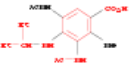
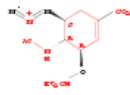
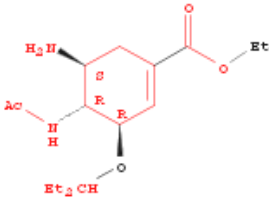
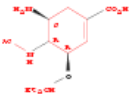
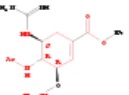
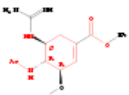
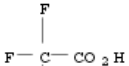
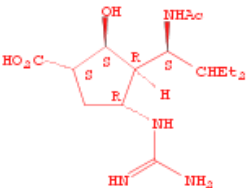
单组分物质

Classes Alloys
 Coordination compounds
 Incompletely defined
 Mixtures
 Polymers
 Organics, and others not listed

有机物质

物质检索——亚结构检索

0 of 704 Substances Selected

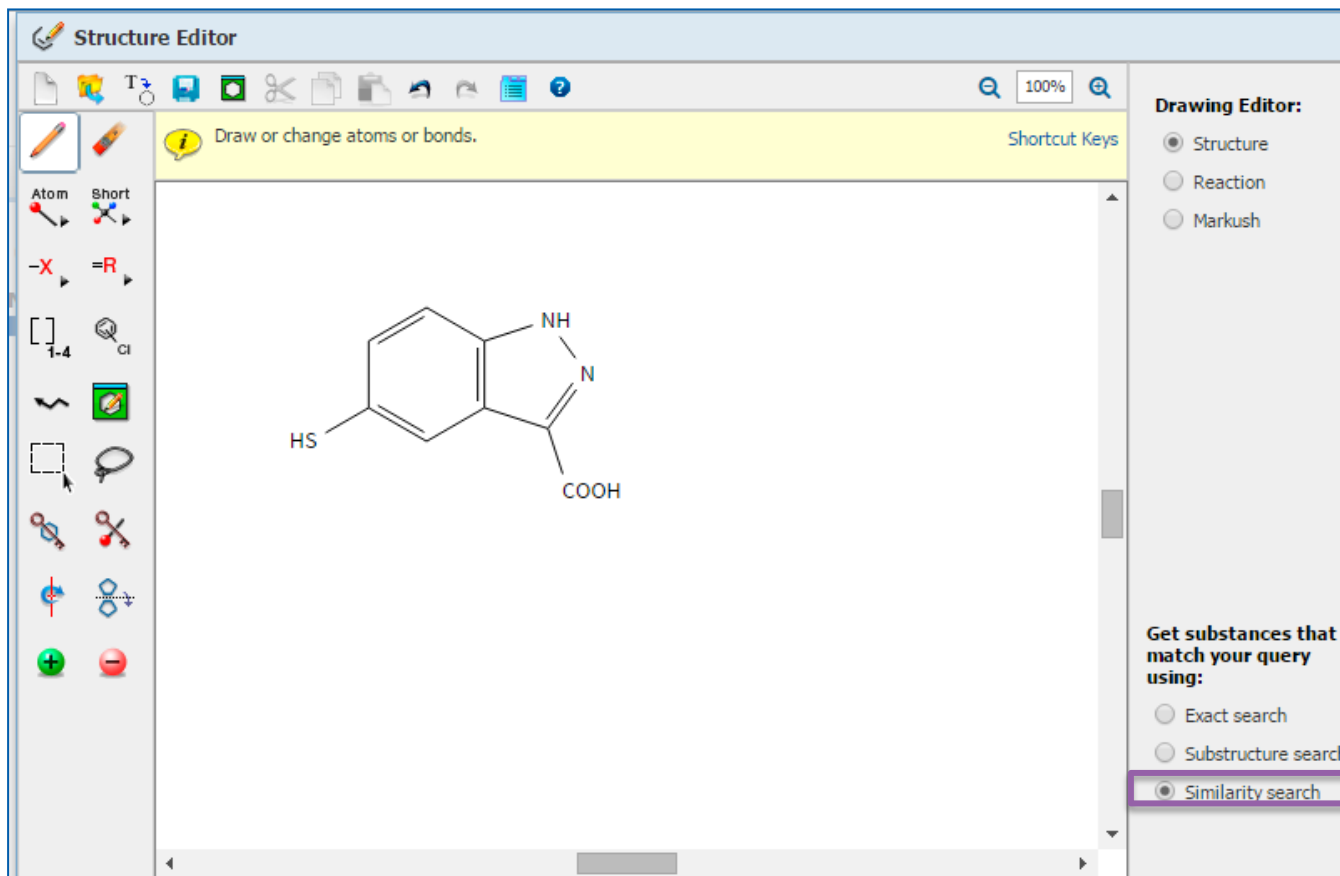
<p>1. Substance Detail 127971-59-9</p>  <p>C₁₅ H₂₁ N₃ O₅ Benzoic acid, 5-(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-3-nitro-</p> <p>Experimental Properties</p>	<p>2. Substance Detail 127971-80-6</p>  <p>C₁₇ H₂₅ N₃ O₄ Benzoic acid, 3,5-bis(acetylamino)-4-[(1-ethylpropyl)amino]-2-methyl-</p>	<p>3. Substance Detail 182367-45-9</p>  <p>Relative stereochemistry.</p> <p>C₁₄ H₂₂ N₄ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-azido-3-(1-ethylpropoxy)-, (3a,4β,5a)-(9CI)</p>	<p>4. Substance Detail 182367-47-1</p> <h2>达菲核心成分</h2>  <p>C₁₆ H₂₈ N₂ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, ethyl ester, (3a,4β,5a)-(9CI)</p>
<p>5. Substance Detail 182367-71-1</p>  <p>Relative stereochemistry.</p> <p>C₁₄ H₂₄ N₂ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-amino-3-(1-ethylpropoxy)-, (3R,4R,5S)-rel</p>	<p>6. Substance Detail 182367-73-3</p>  <p>Relative stereochemistry.</p> <p>C₁₇ H₃₀ N₄ O₄ 1-Cyclohexene-1-carboxylic acid, 4-(acetylamino)-5-[(aminoiminomethyl)amino]-3-(1-ethylpropoxy)-, ethyl ester, (3R,4R,5S)-rel</p>	<p>7. Substance Detail 182367-74-4</p> <div style="border: 1px solid black; padding: 5px;"> <p>182367-73-3 C₁₇ H₃₀ N₄ O₄</p>  <p>Relative stereochemistry.</p> </div> <div style="border: 1px solid black; padding: 5px;"> <p>76-05-1 C₂ H F₃ O₂</p>  </div>	<p>182368-47-4</p> <p>1. Substance Detail 330600-85-6</p> <h2>帕拉米韦</h2>  <p>C₁₅ H₂₈ N₄ O₄ Cyclopentanecarboxylic acid, 3-[[[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[(aminoiminomethyl)amino]-2-hydroxy-, (1S,2S,3R,4R)-</p>

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

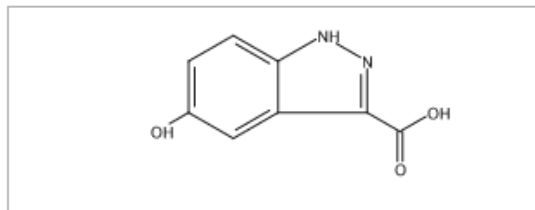
相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

1H-Indazole-3-carboxylic acid, 5-hydroxy-

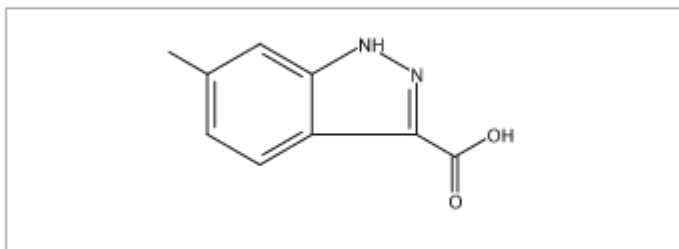
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

1H-Indazole-3-carboxylic acid, 6-methyl-

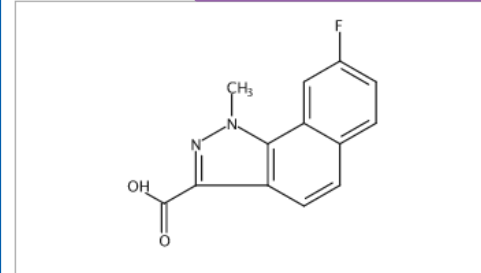
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[σ]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties



SCIFINDER®
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

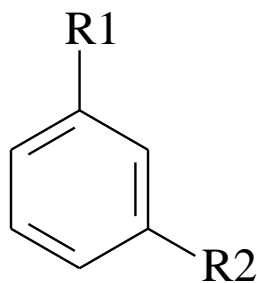
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

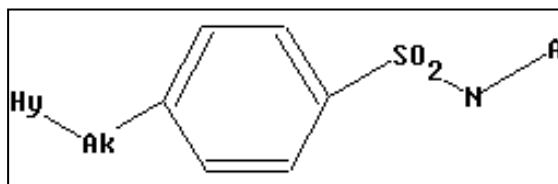
Markush检索

- 具体物质[Specific Substance]：
 - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 预测性物质[Prophetic Substance]：
 - 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
 - 专利中所陈述的预测物质，不会被分配CAS RN
 - Markush检索，能检索到通过结构检索检不到的专利



R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH—halogen,
|
CH₃



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围。

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

100%

Drawing Editor:

- Structure
- Reaction
- Markush

Get Markush patents where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK
Cancel

A C H O S N P Cl Br F I Si

Markush检索

SCIFINDER[®]
A CAS SOLUTION

Welcome Helen Zhu

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Markush substructure > references (1969) > Compounds and methods for anti...

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Tools ▾ Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize

Sort by: Accession Number ▾ ↓

0 of 1969 References Selected

Display Options

Analyze by: Document Type ▾

Patent	1969
Journal	1

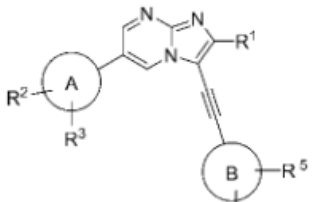
Show More

全部是专利

1. **Compounds and methods for anticoagulation therapy**
PATENTPAK
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**
PATENTPAK
By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R¹ = H or halogen; ring A Ph or pyridyl; R², R³ (same or different) = hydrogen, halogen, C₁₋₄ alkyl or C₁₋₄ alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R² and R³ are at the adjacent substitution position, R² and R³ together with ring A form C₅₋₈ carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R⁴, R⁵ (same or different) = H, halogen, hydroxy, amino, -C(O)OR^a, -C(O)NR^b, SO₃H, SO₂NR^aR^b, SO₂R^b, or NR^aSO₂R^b; R^a, R^b (same...

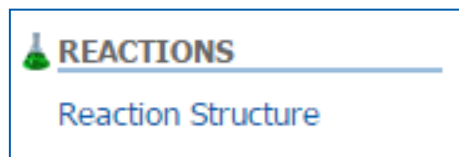
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

结构式



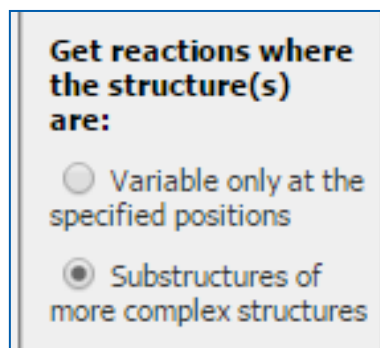
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

The screenshot shows the Structure Editor window with various toolbars and a central canvas. The interface includes a top toolbar with icons for file operations, a left toolbar with drawing tools, a right sidebar with 'Drawing Editor' settings, and a bottom toolbar with element selection and bond types. The central canvas is currently empty. The status bar at the bottom shows 'CH₄' and '16.04'.

Reaction Arrow (反应箭头): Points to the reaction arrow icon in the left toolbar.

Reaction Role Tools (反应角色工具): Points to the reaction role icons (green circle with '+', red circle with '-') in the left toolbar.

Reaction Atom Marking Tools (反应原子标记工具): Points to the atom marking icons (black arrow, red arrow with 'A', blue arrow with 'B') in the left toolbar.

Functional Group List (官能团列表): Points to the 'alcohol', 'ketone', and 'aldehyde' icons in the left toolbar.

Reaction Position Marking Tools (反应位置标记工具): Points to the reaction position marking icons (blue arrow with '1', black arrow with '2') in the left toolbar.

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The interface includes a drawing toolbar on the left with various tools for creating and editing chemical structures. The 'Drawing Editor' panel on the right contains search options for 'Get reactions where the structure(s) are:'. A callout box points to the search options with the text '精确反应检索'.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Atom Short

$-X$ $=R$

reactant: c1ccc(cc1)[N+](=O)[O-]

product: Nc1ccccc1

Drawing Editor:

- Structure
- Reaction
- Markush

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK

Cancel

$C_7H_7NO_2 \cdot C_7H_9N$ 137.14 . 107.16

精确反应检索

反应检索结果

浏览记录，发现很多反应来自同一篇文章，
通过Group by Document合并。

获取相似反应

Get References Tools

Group by: **Document** (Selected) Sort by: Relevance

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step *Hover over any structure for more options.*

Cc1ccc(cc1)[N+](=O)[O-] → Cc1ccc(cc1)N

~102 100% ~122

Overview
Steps/Stages
1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes
solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References
Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

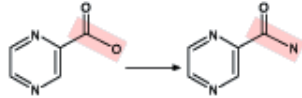
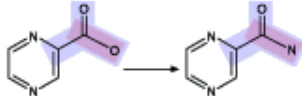
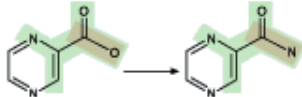
Narrow：反应中心及扩展的原子和键

Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (2934)

- Medium - Reaction centers plus adjacent atoms and bonds (109)

- Narrow - Reaction centers plus extended atoms and bonds (95)


按照反应类型排序

Group by: Transformation ▾ Sort by: Frequency ▾ ↓

▾ 0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azo Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N-Ar} \text{O}^-$$

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

REACTIONS ? Get References Tools Send to SciPlann

Analyze Refine

Analyze by: ?
Reagent

H ₂	148
NaBH ₄	51
N ₂ H ₄ -H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ •HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

Show More

Group by: No Grouping Sort by: Relevance ↓

0 of 512 Reactions Selected Page: 1 of 11

1. View Reaction Detail Link Similar Reactions

Single Step *Hover over any structure for more options.*

~102 **100%** **~122**

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

[Quick View](#) [Other Sources](#)

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

Experimental Procedure



General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

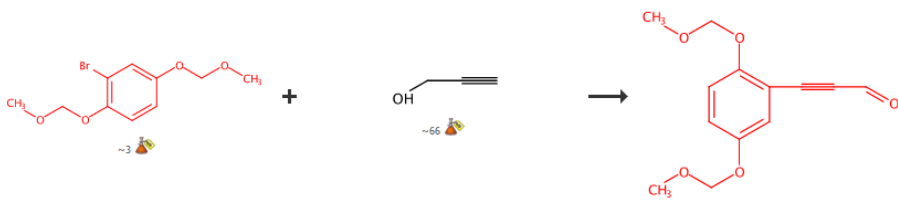
SciFinder囊括最大的反应实验过程合集

Experimental Procedure:

我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么?
- 查免费的Supporting Information? 可能只有图谱。

2 Steps Hover over any structure for more options.



Overview

Steps/Stages

- 1.1 C: Pd(PPh₃)₄; S: BuNH₂; 21 h, 100°C
- 2.1 R: DMSO, R: Cl(O=)CC(=O)Cl, S: CH₂Cl₂, 15 min, -78°C
- 2.2 S: CH₂Cl₂, -78°C; 2 h, -78°C
- 2.3 R: Et₃N, 30 min, -78°C; -78°C → rt
- 2.4 R: H₂O, R: NH₄Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, scale method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, Stages: 4
Most stages in any one step: 4

Experimental Procedure

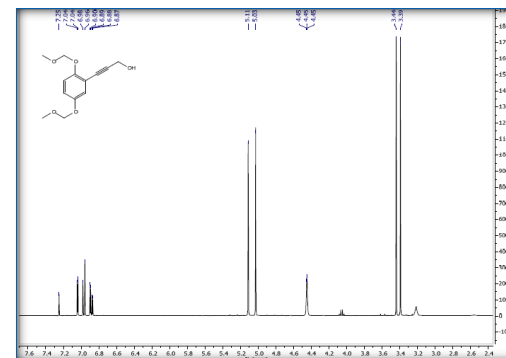


Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ and **16**⁸ were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and Pd(PPh₃)₄ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10-50%). **3-[2,5-bis(methoxymethoxy)phenyl]prop-2-yn-1-ol**⁸ (**8**). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); ¹³C NMR (CDCl₃, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]⁺ (calcd for C₁₃H₁₆O₅ 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (332 μ L, 4.68 mmol) in dry CH₂Cl₂ (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol **8** (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH₂Cl₂ (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et₃N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. **3-[2,5-bis(methoxymethoxy)phenyl]prop-2-ynal** (**9**). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



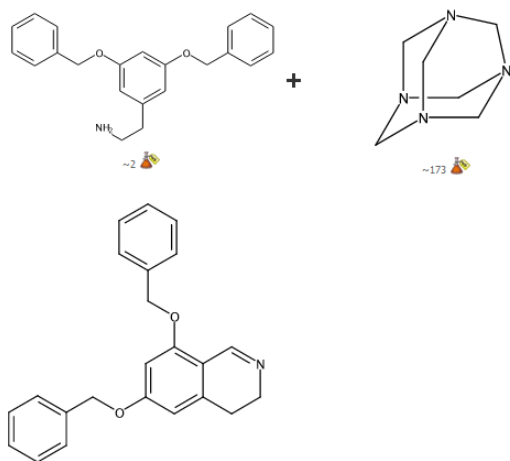
MethodsNow Synthesis

MethodsNow

Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wiha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger
From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012
Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



多步反应中，原文没有描述
的实验过程以灰色标示

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	<ol style="list-style-type: none"> 1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethanamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon. 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H₂O. 4. Basify with potassium carbonate and extract with CH₂Cl₂. 5. Wash the combined organic layers with brine. 6. Dry over MgSO₄ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
¹H NMR	(CDCl ₃ , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, <i>J</i> = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
¹³C NMR	(CDCl ₃ , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν _{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm ⁻¹
HRMS	(FAB+) calcd for C ₂₃ H ₂₂ N ₂ (M+H ⁺) 344.1651; found 344.1658
Mass Spec	(FAB+) <i>m/z</i> 344 (M+H ⁺)
State	yellow solid
CAS Method Number	3-614-CAS-200055

物质信息

实验过程

图谱信息

保存/导出方法

Print/Export

Close

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化

The screenshot displays the Structure Editor software interface. The main workspace shows a chemical structure of benzothiazole with an R1 group attached to the 2-position. The R-group Definitions panel is open, showing a list of R-groups (R1 to R10) and a table of atoms. The 'Atoms' table is expanded, and the element 'S' (Sulfur) is highlighted in a purple box. The 'R1 = O, S' field is also visible.

Atoms																	
H																	He
Li	Be									B	C	N	O	F		Ne	
Na	Mg									Al	Si	P	S	Cl	Ar		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	**															
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

亚结构反应检索

The screenshot displays the Structure Editor interface. The main workspace shows a chemical reaction: a reactant (a benzimidazole ring with an R1 substituent and a hydrogen atom on the imidazole ring) reacting to form a product (the same benzimidazole ring with an R1 substituent and an Ak substituent). A purple arrow points from the Ak variable in the product to the Ak variable in the search filter menu.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Variables

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
AK	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

OK
Cancel

Formula is not available

亚结构反应检索

The screenshot displays the Structure Editor window. At the top, a yellow message bar reads "Click an atom to block substitution." The main workspace shows a chemical reaction: a benzimidazole derivative with a hydrogen atom at the 2-position (labeled "reactant") reacts to form the same derivative with an "Ak" group at the 2-position (labeled "product").

On the right side, the "Drawing Editor" panel has three radio buttons: "Structure", "Reaction" (which is selected), and "Markush". Below this, the section "Get reactions where the structure(s) are:" contains two radio buttons: "Variable only at the specified positions" and "Substructures of more complex structures" (which is selected and highlighted with a purple box).

At the bottom of the interface, there is a search bar containing "Ak", a list of chemical elements (C, H, O, S, N, P, Cl, Br, F, I, Si), and a "Formula is not available" status message.

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

REACTIONS Get References Tools

Analyze Refine

Group by: No Grouping Sort by: Number of Steps

0 of 249 Reactions Selected

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step *Hover over any structure for more options.*

CCCCCICI + C1=CC=C2C(=C1)N=C(S2)C3CCCCC3 → C1=CC=C2C(=C1)N=C(S2)C3CCCCC3 **83%**

Overview

Steps/Stages

- 1.1 R:LiO-Bu-*t*, C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

Notes

catalyst prepared and used, screw c
Reagents: 2, Catalysts: 1, Solvents:

References

Synthesis of quinoline-based NNN-p
for C-H bond alkylation of azoles wi
Quick View [Other Sources](#)
By Patel, Ulhas N. et al
From *Organometallics* 35(11), 1785-1793-

ACS / Proprietary and Confidential / Do Not Distribute

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

3 Steps *Hover over any structure for more options.* **点击Send to SciPlanner** [Display Options](#)

Overview

Steps/Stages

- 1.1 R: NH₃, R: t-BuOK, R: t-BuOOH, S: THF
- 2.1 R: NaH, S: THF
- 3.1 R: POCl₃, reflux

Notes

Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1

References

Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

进入SciPlanner 新建文件

SciPlanner SciPlanner_11_19_2015_112612 **将刚推送过来的反应拖至编辑面板**

Workspace Edit View GoTo

- New
- Open
- Save
- Duplicate
- Import
- Export
- Print
- Close

Your Workspace is empty.

Drag items from the reference, substance, and reaction libraries (on the right) to this area.

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile

打开中间产物的标准菜单
选择Synthesize this

1 2 3

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

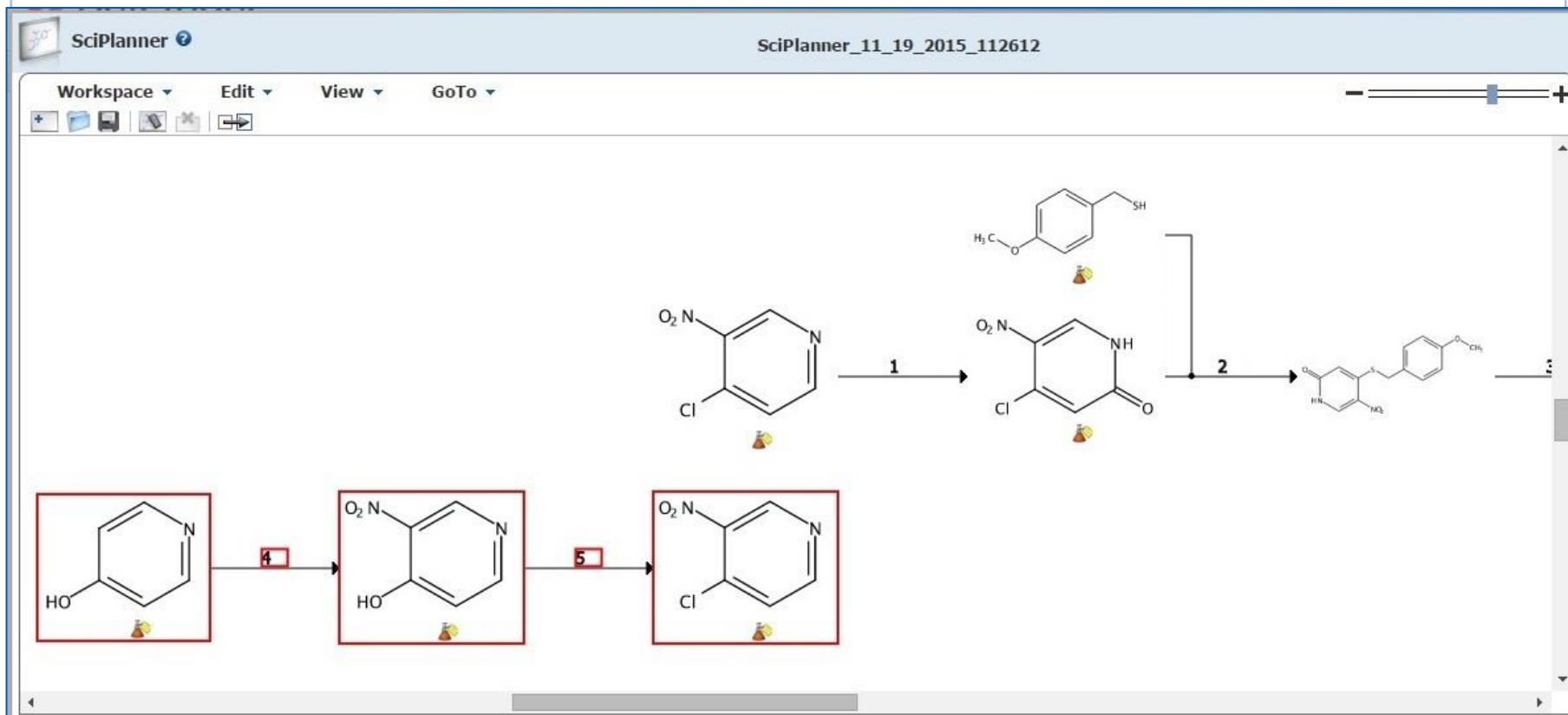
2 Steps Hover over any structure for more options.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

~161 ~192

SciPlanner使用简介

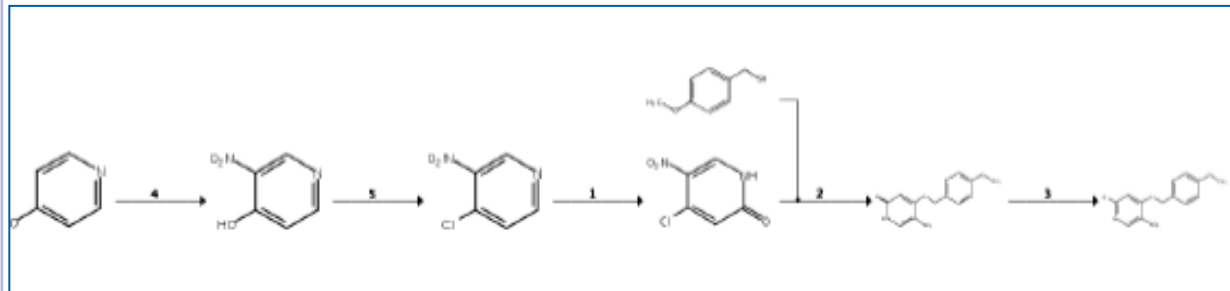


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

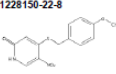
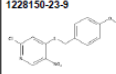
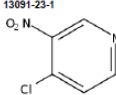
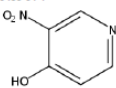
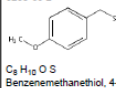
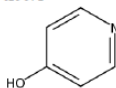
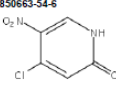
SciPlanner使用简介

The screenshot displays the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_11_19_2015_112612". Below the title bar is a menu bar with "Workspace", "Edit", "View", and "GoTo". A "Workspace" dropdown menu is open on the left, listing options: "New", "Open", "Save", "Duplicate", "Import", "Export", "Print", and "Close". The "Export" option is highlighted in blue. In the center, a chemical reaction scheme is shown with three steps: 4, 5, and 1. Step 4 shows a starting material reacting to form a 5-nitro-2-hydroxypyridine intermediate. Step 5 shows the intermediate reacting to form a 5-nitro-2-chloropyridine intermediate. Step 1 shows the final product, a 5-nitro-2-chloropyridine derivative. A pink callout box with a pointer to the "Export" menu item contains the text: "点击 Workspace, 选择 Export 导出结果". Another pink callout box with a pointer to the reaction scheme contains the text: "用鼠标将两个同样的结构拖至重叠, 两条反应合并". A third pink callout box with a pointer to the "Export" dialog box contains the text: "选择适当的输出格式, 输出结果". The "Export" dialog box is open on the right, showing options for "Offline Review" (Portable Document Format (*.pdf), Citations (*.ris), Image (*.png)) and "Saving Locally" (SciPlanner eXchange (*.pkx)). The "Details" section includes a "File Name" field with the text "SciPlanner_11_19_2015_112612" and a "Title" field. The "Include" section has checkboxes for "SciPlanner Image", "Reaction Details", "Substance Details", and "Reference Details", all of which are checked. "Export" and "Cancel" buttons are at the bottom right of the dialog box.

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K₂CO₃, S:H₂O, cooled, pH 10</p>	<p>Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2</p> <p>Transformation:</p> <p>1. Formation of Alkyl Halides from Alcohols</p>	90%
<p>References</p> <p>High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes</p> <p>By Poloek, Anurach et al</p> <p>From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
<p>1228150-22-8</p>  <p>C₁₃H₁₂N₂O₄S 2-(1H)-Pyridinone, 4-[[[4-(methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p>  <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[[4-(methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p>  <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p>  <p>C₅H₄N₂O₂ 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p>  <p>C₈H₁₀O₂S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p>  <p>C₅H₄N₂O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p>  <p>C₆H₃ClN₂O₃ 2-(1H)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - **MethodsNow**
- SciFinder常见问题及解决

MethodsNow™是一个完整的 CAS 解决方案



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- 分析与合成两个模块
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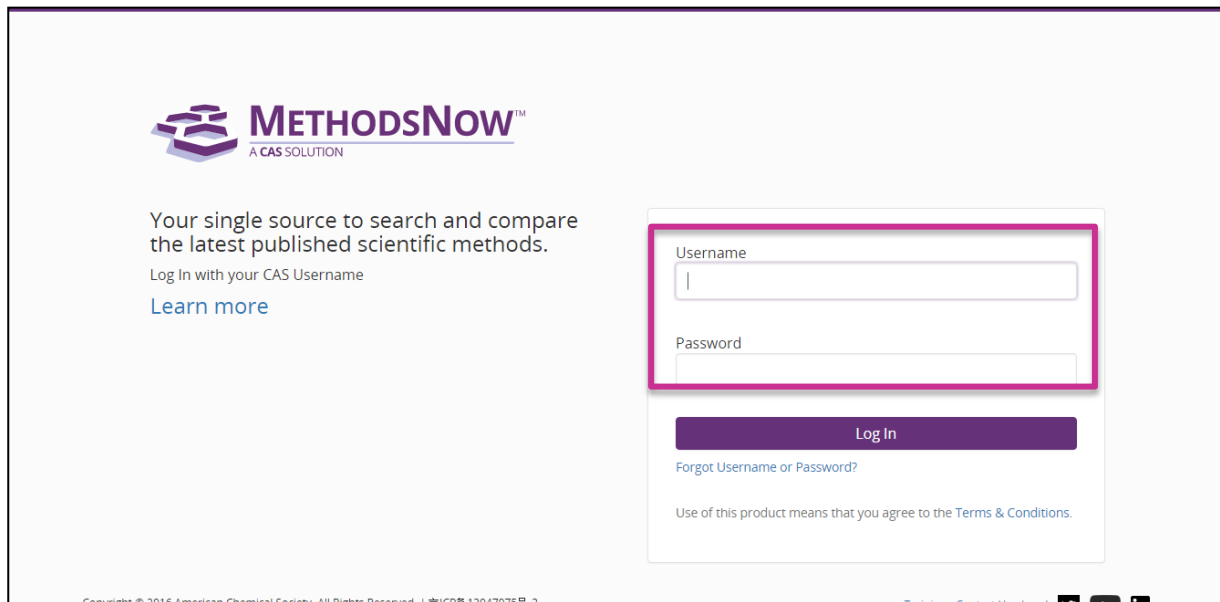



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- Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析...
- Historical Analysis / Dating: 考古分析，同位素分析
- Environmental Analysis: 土壤/空气/水分析，农药残留分析...
- Agricultural Applications / Analysis: 除草剂分析...
- Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析...
- Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工...
- Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析...

目前有13个大类，45个小类。某些子项目属于多种方法分类

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MethodsNow – Analysis(www.methodsnow.com)

检索/高级检索



方法分类



历史检索



The screenshot shows the MethodsNow website interface. At the top, there is a navigation bar with the logo 'METHODSNOW A CAS SOLUTION' and links for 'Saved' and 'Account'. Below the navigation bar is a search section with the heading 'Search' and a search input field. A callout bubble points to the search button with the text '保存结果集'. Below the search section is a 'Browse Method Categories' section with a grid of category links. A callout bubble points to one of the category links with the text '点击一个类别 浏览相关方法'. Below the categories is a 'Recent Searches' section with a list of search terms. A callout bubble points to the 'X' icon next to a search term with the text '点击“X” 删除检索历史'. Another callout bubble points to the search term 'hplc lycopene analysis' with the text '点击历史检索 重新运行检索'.

高级检索

The image shows two overlapping screenshots of the CAS MethodsNow Advanced Search interface. The top screenshot shows the main search area with a 'Keyword' field and a dropdown menu for logical operators. A callout box points to the operator dropdown with the text '逻辑运算符 : and, or, not'. Another callout box points to a close button on the right with the text '删除检索条件'. The bottom screenshot shows a dropdown menu for search criteria, with a callout box listing the options: '检索选项 : 关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名'. The dropdown menu includes 'Publication Name', 'Keyword', 'Analyte', 'Matrix', 'Method Category', 'Technique', 'CAS Method Number', and 'Publication Name' (highlighted).

CAS Solutions **METHODSNow** A CAS SOLUTION ★ Saved Account

← Return to Home

Advanced Search

逻辑运算符 : and, or, not

Keyword

AND Matrix

AND Analyte

Add Search Criteria

增加检索条件

删除检索条件

CAS Solutions **METHODSNow** A CAS SOLUTION ★ Saved Account

← Return to Home

Advanced Search

检索选项 : 关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名

Publication Name

Keyword

Analyte

Matrix

Method Category

Technique

CAS Method Number

Publication Name

案例：氟比洛芬中的杂质分析

CAS Solutions



Saved



Account

Search

此处只需输入一个关键词即可，MethodsNow会自动进行同义词查找

Enter keyword, matrix, analyte, etc.

impuri



A impurities

Browse Method Categories

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

impurities



结果显示

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impurities

导出方法 保存方法 (3)

Res

典型分析方法标题格式：通过某技术手段在某基质中分析某物质

Analysis of Impurities in 2-Thiophenepropanoic acid, α -[[2-butyl-1-[(4-carboxyphenyl)methyl]-1H-imidazol-5-yl]methylene]-, (αE)-, methanesulfonate (1:1) by HPLC
CAS MN: 1-101-CAS-58103

View Details & Instructions 查看方法详情

Add to Compare 方法对比

Analyte Impurities

Matrix 2-Thiophenepropanoic acid, α -[[2-butyl-1-[(4-carboxyphenyl)methyl]-1H-imidazol-5-yl]methylene]-, (αE)-, methanesulfonate (1:1)

Other Materials Material: Column (250 mm x 4.6 mm x 5.0 μ m)

Method Category Active Pharmaceutical Ingredient and Metabolite Analysis

Technique HPLC

Equipment Used HPLC system

Return to Home

Analyte

- Copper (296)
- Iron (218)
- Lead (204)
- Nickel (202)
- Impurities (201)

View All

Matrix

- Pharmaceutical tablets (456)
- Drugs (170)
- Tablets (142)
- River waters (134)
- Drinking waters (127)

View All

Method Category

Technique

限定分析物、基质、方法等条件

结果筛选

CAS Solutions **METHODSNOW**™ A CAS SOLUTION

impurities

Sort Relevance

Compare (0/3)

fonate (1:1) by

Add to Compare

imidazol-5-

Matrix

Alphabetically By Count

- Drainage waters (1)
- Drinking waters (127)
- Drug delivery systems (78)
- Drugs (170)
- Duck meat (6)
- Dust (2)
- Dysprosium oxide (Dy₂O₃) (2)
- Echinodorus macrophyllus (1)
- Edible oils (3)
- Fe (1)

- [[α,α'-[1,2-Ethanediyldi(imino-κM)]bis[2-(hydroxy-κO)benzeneacetato-κO]](2-)]manganese (3)
- Ethanol (2)
- Ethanolamine (1)
- Ethene, homopolymer (3)
- (Ethylenediaminetetraacetato)manganate(2-) (2)
- Ethylene oxide-propylene oxide block copolymer (1)

- Flammulina velutipes (1)
- Flaxseed (7)
- Flours and Meals (1)
- Flower (4)
- Fluorine-18 fluorodeoxyglucose (1)
- Fluorite (CaF₂) (2)
- Fluorosilicic acid (1)
- Flupirtine maleate (1)
- Flurbiprofen (11)
- Foeniculum vulgare (1)

← Prev 1 ... 3 4 5 6 7 ... 13 Next → Go to page: 5 Go

Apply Cancel

Technique HPLC

Equipment Used HPLC system

Return to Home

Analyte

- Copper (296)
- Iron (218)
- Lead (204)
- Nickel (202)
- Impurities (201)

View All

Matrix

- Pharmaceutical ta (456)
- Drugs (170)
- Tablets (142)
- River waters (134)
- Drinking waters (1)

View All

Method Category

Technique

结果显示

Analysis of (+)-Flurbiprofen in Tablets by Reversed-phase HPLC

CAS MN: 1-101-CAS-47394

Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis

Technique: Reversed-phase HPLC; UV-visible spectroscopy

Materials	Role	Image	CAS RN
(-)-Flurbiprofen	analyte	View Structure	51543-40-9
(-)-Ketoprofen	analyte	View Structure	56105-81-8
(+)-Ibuprofen	analyte	View Structure	51146-56-6
(+)-Pranoprofen	analyte	View Structure	103813-85-0
Naproxen	analyte	View Structure	22204-53-1
(-)-Pranoprofen	analyte	View Structure	132880-23-0
(+)-Ketoprofen	analyte	View Structure	22161-81-5
(+)-Flurbiprofen	analyte	View Structure	51543-39-4
(-)-Ibuprofen	analyte	View Structure	51146-57-7

实验材料

Source

High-performance enantiomer separation of nonsteroidal anti-inflammatory drugs (NSAIDs) by 3 μm reversed-phase chiral columns and application to the optical purity testing of naproxen drug substances and its formulations

Tanaka, Moe; Nagamatsu, Kumi; Nishi, Hiroyuki

Analytical Sciences (2014), 30 (3), 397 - 406. Japan Society for Analytical Chemistry

CODEN: ANSCEN | ISSN: 09106340 | DOI: 10.2116/analsci.30.397

[Document Sources](#)

Abstract

The enantiomer separation of 5 nonsteroidal anti-inflammatory drugs (NSAIDs), such as ibuprofen, ketoprofen (KP) and naproxen (NX), which are included in The Japanese Pharmacopoeia 16th edition (JP16), was investigated by employing 4 kinds of 3 μm reversed-phase chiral columns (AD-3R, AS-3R, OD-3R, and OJ-3R). Except for KP, the enantiomers of 4 NSAIDs were successfully separated by 1 of the 4 columns. Among 5 NSAIDs, only NX was used as a single enantiomer (S-form, active form) in the clin. field (JP16); therefore, optical purity testing method of NX is required for its quality evaluation. Among 4 CSPs, the method was developed by an AS-3R column, which showed good enantioselectivity for NX enantiomers. By optimizing the conditions, the resolution (R_s) of 2.55 was obtained for NX enantiomers within approx. 6 min. The minor enantiomer R-form eluted before the main active enantiomer S-form. Finally, the developed method was applied to the optical purity testing of NX active pharmaceutical ingredients (APIs) and its formulations (tablet and

文献信息

Equipment Used

HPLC apparatus, Kyoto, Japan

HPLC system, Shimadzu

UV/VIS spectrophotometer, UV-2550, Shimadzu, Japan

Injector, Rheodyne 7725i

设备条件

Instructions

Enantiomer separation by HPLC (water and ACN (3:2))

1. Prepare sample solutions of racemic NSAIDs (nonsteroidal anti-inflammatory drugs) with MeOH at a concentration of approximately 1 mg/mL.
2. Prepare a sample solution for NX, through mixing the active S(+)-form and the minor enantiomer R(-)-form at a ratio of approximately 1:1.
3. Prepare a solution of a paraben mixture by combining each 10 mL of a 100 mg/100 mL MeOH solution of uracil, Me (methyl *p*-hydroxybenzoate) paraben, Et (ethyl *p*-hydroxybenzoate) paraben, iPr (isopropyl *p*-hydroxybenzoate) paraben, nPr (*n*-propyl *p*-hydroxybenzoate) paraben, and Bu (*n*-butyl *p*-hydroxybenzoate) paraben to a 100-mL volumetric flask.
4. Add water to the volume (10 mg each/100 mL).
5. Use uracil as a t_0 marker substance, because it was not retained under the applied HPLC conditions.
6. Investigate HPLC separations of enantiomers of five NSAIDs a mixture of paraben by employing four kinds of the 3 μm reversed-phase chiral columns (AD-3R) under the following conditions: column temperature, 25°C (room temperature); flow rate, 1.0 mL/min; detection, UV 254 nm (210 nm for IB).
7. Employ a mixture of water and ACN (3:2) as mobile phase.
8. Inject a constant volume (2-5 μL) of the sample solution manually through a Rheodyne 7725i injector (20 μL loop).

Validation

Retention Time	4.36 (enantiomer-1 pranoprofen), 4.76 (enantiomer-2 pranoprofen) (t_{R1}/min , t_{R2}/min respectively)
	7.77 (enantiomer-1 naproxen), 8.70 (enantiomer-2 naproxen) (t_{R1}/min , t_{R2}/min respectively)
	11.2 (enantiomer-1 ibuprofen), 12.3 (enantiomer-2 ibuprofen) (t_{R1}/min , t_{R2}/min respectively)

实验步骤及数据有效性

对比不同分析方法

Compare Methods



导出对比
PDF文件

Expand All | Collapse All

	1	2	3
Title	Analysis of (+)-Flurbiprofen in Tablets by Reversed-phase HPLC	Analysis of (+)-Flurbiprofen in Tablets by Reversed-phase HPLC	Analysis of (+)-Flurbiprofen in Tablets by Capillary electrophoresis
CAS Method Number	1-101-CAS-47394		
Method Category	Active Pharmaceutical Ingre Metabolite Analysis		
Technique	Reversed-phase HPLC; UV-v spectroscopy		
Analyte	(-)-Flurbiprofen; (-)-Ketoprof Ibuprofen; (+)-Pranoprofen; (-)-Pranoprofen; (+)-Ketoprof View All		
Matrix		Ketoprofen; (±)-Pranoprofen; Flurbiprofen; Ibuprofen; Tablets; Capsule (microbial)	(±)-Pranoprofen; Flurbiprofen; Ibuprofen; Ketoprofen; Tablets; Capsule (microbial)
Other Materials		C18 column (5 µm, 4.6 mm i.d. x 15 cm); Membrane filter (0.45 µm pore size); Capillary tube (i.d. 50 µm, 60 cm) View All	CHIRALPAK AD-H (5 µm, 4.6 mm i.d. x 25 cm)
Equipment Used		HPLC apparatus, Kyoto, Japan; HPLC system, Shimadzu; UV/VIS spectrophotometer, UV-2550, View All	UV/VIS spectrophotometer, UV-2550, Shimadzu, Japan; HPLC system, Shimadzu; HPLC apparatus, Kyoto, View All
Source		High-performance enantiomer separation of nonsteroidal anti- inflammatory drugs (NSAIDs) by 3 View All	High-performance enantiomer separation of nonsteroidal anti- inflammatory drugs (NSAIDs) by 3 View All
Method		Enantiomer separation by HPLC (water and ACN (3:2)) 1. Prepare sample solutions of View All	Enantiomer separation by HPLC (<i>n</i> - hexane/acetone/acetic acid (80:20:1)) 1. For a comparison, with View All
			Ketoprofen; Flurbiprofen; (±)- Pranoprofen; Ibuprofen; Tablets; Capsule (microbial)
			Membrane filter (0.45 µm pore size); Capillary tube (i.d. 50 µm, 60 cm length; effective length, 50 cm)
			P/ACE MDQ system, Beckman; Ultrasonic bath, AU-16C, Tokyo-rika, Tokyo, Japan; Injector, Rheodyne View All
			High-performance enantiomer separation of nonsteroidal anti- inflammatory drugs (NSAIDs) by 3 View All
			Enantiomer separation by CE (capillary electrophoresis) 1. Perform CE separation with an View All

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到8以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取SciFinder账号-未授权IP地址



Unauthorized IP Address

User registration is available only from IP addresses specified by the key contact at your organization. Please try to register again from an authorized location.

如果注册时遇到未授权IP地址的提示：

新用户注册时如出现IP地址未授权的提示，请发邮件至 china@acs-i.org，写明校名、院系、年级、院系联系人(导师或者辅导员)及联系电话、本人真实姓名和邮箱,请附上学生证或者教职工卡的正反面照片，同时表明需要注册SciFinder账号,并请在24小时查收邮件完成注册。



如何获取SciFinder账号

The screenshot displays the SciFinder registration interface, divided into three main sections:

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features dropdown menus for Area of Research and Job Title.
- USERNAME AND PASSWORD--**: Includes input fields for Username (with a *Tips* link), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for Answer (with a *Why?* link).

At the bottom of the form are two buttons: **Register>>** and **Clear All**.

请注意：

1. 必须输入真实姓名和**自己**邮箱。
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、*)

例：abc@123

4. 从下拉列表中选择一个密码提示问题并给出答案。
单击 Register (注册)。

如何获取SciFinder账号



账号注册成功，登录scifinder.cas.org开始使用SciFinder

SciFinder使用注意事项

- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

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