

CAS SciFinder Discovery Platform (Academic)

全面高效获取医药信息



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大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush)
 - 反应检索
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 序列检索*
 - 分析实验方法 (CAS Analytical Methods)
 - 配方/制剂信息检索 (CAS Formulus*)
- 常见问题及解答

CAS 致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻



HINDSIGHT

Connecting past discoveries to build a better future

连接前人的发现，建设更美好的未来

INSIGHT

Revealing unseen relationships that spark ideas and speed discovery

揭示能激发想法和加速发现的，未预见的联系

FORESIGHT

Identifying trends and emerging opportunities to accelerate growth

确定加速增长的趋势和新机遇

CAS 具有最全面的学科连接内容合集



Over
55K
scientific journals
and documents

Over
274
million substances

Over
50
languages
translated

Over
64
patent offices
worldwide

CAS独特的内容合集

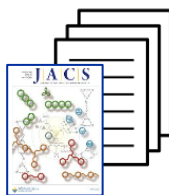
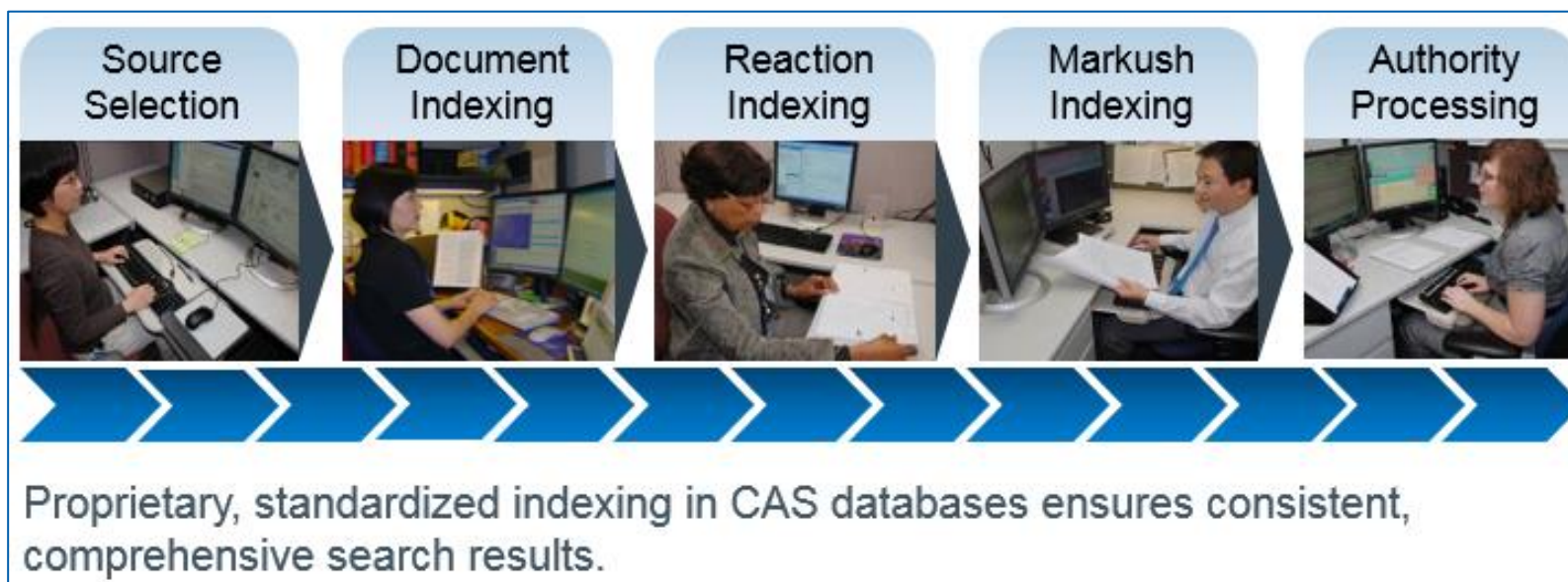


来源：

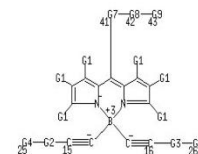
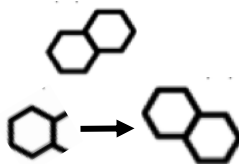
<https://www.cas.org/cas-data>

<https://www.cas.org/about/cas-content>

CAS科学家的智力标引



1990
Smith, M.
anthracene



Androst-4-en-3-one,
17-hydroxy-17-
methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

CAS解决方案与服务



Discovery

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need



Intellectual Property

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets



Custom Solutions

CAS Custom ServicesSM

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

CAS SciFinder Discovery Platform (Academic)平台解决方案

CAS SciFinderⁿ ——加速科学发现的业界领先的科学工具

业界最领先的相关性搜索引擎，提供和化学相关的各学科文献、物质、反应和生物序列等检索内容，检索智能、高效、简单。可用于基金申请的文献准备、为新课题制定实验计划、寻求学术合作者、进行逆合成分析以及更多其他的教学和科研活动。

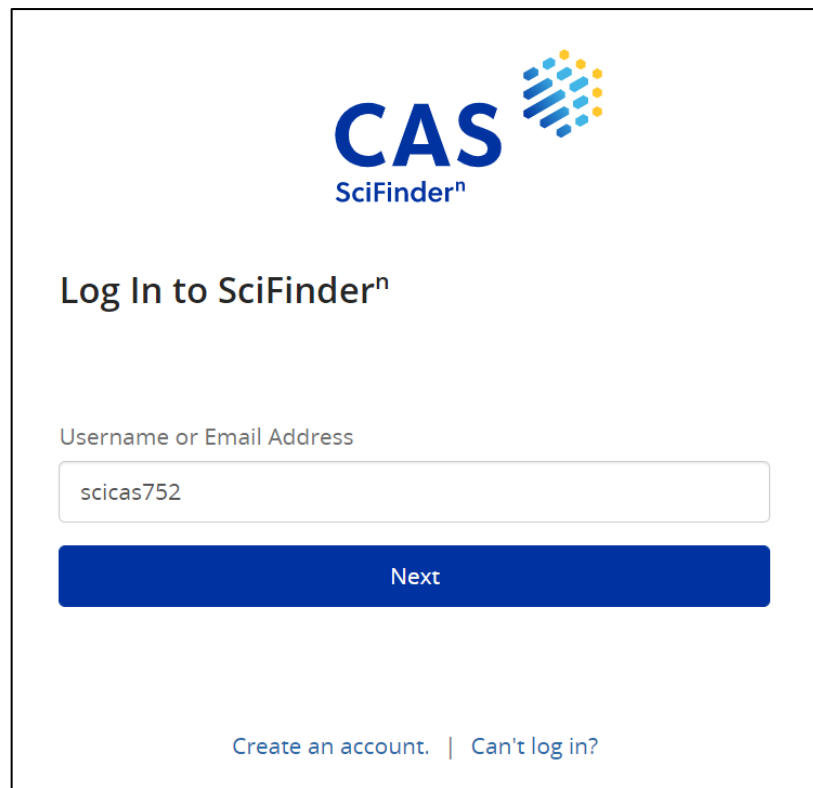
CAS Analytical Methods ——借助CAS科学家深度加工的科学方法，提升研究效率

分析方法解决方案涵盖来自期刊中的化学分析方法，提供检索和对比功能，可快速获得能直接在实验室操作的分析方法。可为法医学、食品科学、农学、制药、环境等学科的教学和实验提供帮助。

CAS Formulus ——助力开发安全、有效的产品

集成配方（制剂）数据与工作流程的解决方案，提供来自期刊、专利和产品说明中的配方详情。可检索制药、化妆品、食品、农化、油墨、涂料等众多领域中的配方，及其工艺、成分、目标成分的常见配伍成分、设计配方、和探索合规要求等。

CAS SciFinderⁿ 登录网址: <https://SciFinder-n.cas.org>



CAS SciFinderⁿ

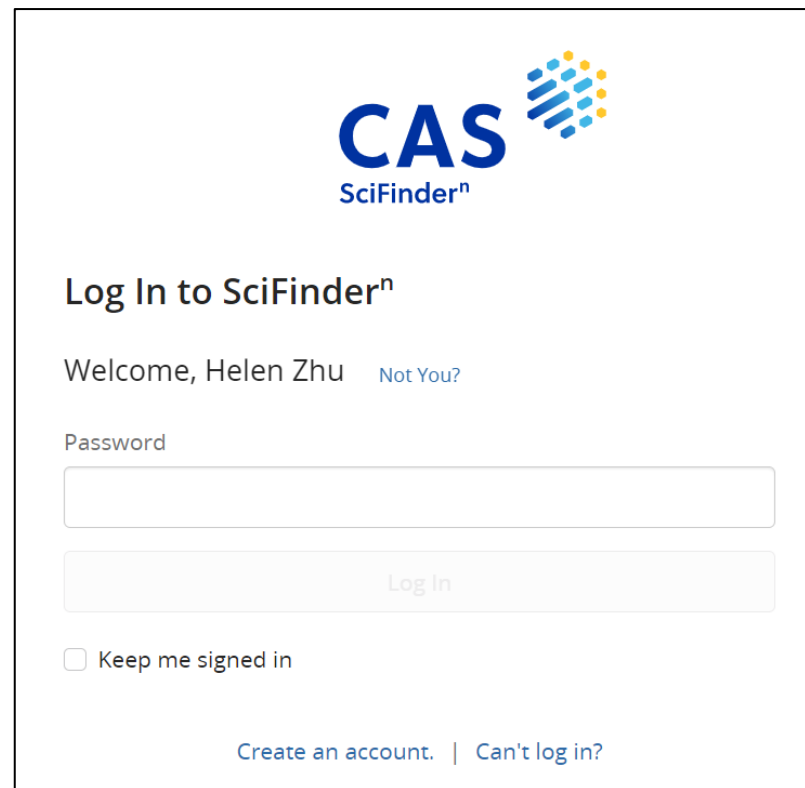
Log In to SciFinderⁿ

Username or Email Address

scicas752

Next

[Create an account.](#) | [Can't log in?](#)



CAS SciFinderⁿ

Log In to SciFinderⁿ

Welcome, Helen Zhu [Not You?](#)

Password

Log In

Keep me signed in

[Create an account.](#) | [Can't log in?](#)

使用CAS SciFinder账号登录

CAS SciFinder[®]主界面

The screenshot shows the CAS SciFinder main interface with several callouts in Chinese:

- 检索历史** (Search History) - points to the top right navigation area.
- 账户信息** (Account Information) - points to the user profile 'Helen Zhu'.
- 已保存结果集及信息更新结果集** (Saved result sets and information updated result sets) - points to the 'Saved' and 'Alerts' icons.
- 灵活的检索选项** (Flexible search options) - points to the search input field and the 'Draw' button.
- 便捷地合并文本与结构检索** (Conveniently merge text and structure search) - points to the 'Draw' button.
- 重新运行检索式** (Rerun search) - points to the 'Rerun Search' button.
- 修改检索式** (Modify search) - points to the 'Edit Search' button.
- 近期检索历史** (Recent search history) - points to the 'Recent Search History' section.

The interface includes a left sidebar with navigation options like 'CAS SciFinder[®]', 'CAS Analytical Methods', and 'CAS Formulus'. The main search area features a search bar with a 'Draw' button and a 'Molecular Formula' dropdown. Below the search bar, there are examples of search queries and a link to 'Learn more about SciFinder[®] Advanced Search'. The bottom section displays 'Recent Search History' with a table of search results.

Date	Search Type	Results
March 22, 2023	References	9035-69-2 (3,790 Results)
		4:08 PM

大纲

- CAS及CAS SciFinderⁿ简介
- 常见检索方式
 - 文献检索
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 - 逆合成反应路线设计 (CAS Retrosynthesis*)
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 - 分析实验方法 (CAS Analytical Methods)
 - 配方/制剂信息检索 (CAS Formulus*)
- 常见问题及解答



大纲

- CAS SciFinderⁿ中的文献检索
 - 主题词检索及布尔逻辑算符的运用
 - 文献检索结果集的筛选
 - 引文地图的应用
 - 文献结果集的导出和检索历史管理
 - 定位专利原文中的重要信息
 - 利用ChemZent丰富化学历史知识

视频链接:

https://american-chemical-society.zoom.us/rec/share/9PrTtd4gKFB245SuJax26so0a4WAHC9MsgB74Bt3mPRK9TgcwZI753ROg4eHHseL.I_K0dQtNjGzGJK5y

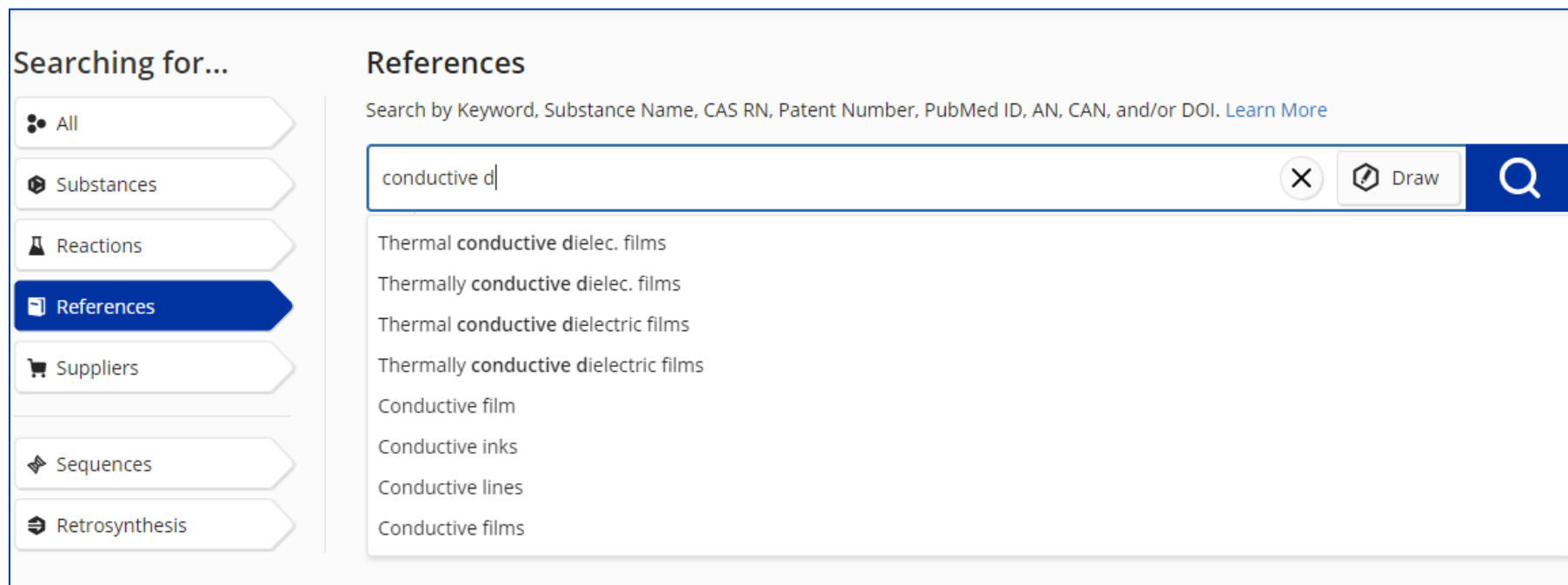


文献检索

- 文献检索方法
 - 主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
 - 各种字段：作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商
 - 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，再获得文献或文本+结构联合检索
 - 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—主题词检索及布尔逻辑算符的使用

主检索框：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI



The screenshot shows a search interface with a left sidebar and a main search area. The sidebar, titled "Searching for...", contains several categories: All, Substances, Reactions, References (highlighted in blue), Suppliers, Sequences, and Retrosynthesis. The main search area is titled "References" and includes a search box with the text "conductive d". Below the search box, a list of suggestions is displayed: Thermal conductive dielec. films, Thermally conductive dielec. films, Thermal conductive dielectric films, Thermally conductive dielectric films, Conductive film, Conductive inks, Conductive lines, and Conductive films. The search box also features a clear button (X), a "Draw" button, and a search button (Q).

基于科学家创建的叙词表，充分利用自动提示检索词，启发检索思路

文献检索—主题词检索及布尔逻辑算符的使用

The screenshot displays the SciFinder search interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances, Reactions, References (highlighted in blue), Suppliers, Sequences, and Retrosynthesis. The main search area is titled "References" and includes a search bar with the query "chronic heart failure" and "traditional chinese medicine". Below the search bar, there is a dropdown menu set to "AND" and another dropdown menu set to "Author Name" with a text input field containing "Enter last name, first name middle name." and an example "Schubert, J A". A "Draw" button and a search button are also visible. A link to "Learn more about SciFinder[®] Advanced Search." is present. At the bottom, there is a "Launch CAS Lexicon" button and a description: "CAS Lexicon enables you to browse the CAS General Thesaurus to find indexed concepts and substances to build a Reference query with up to 1,000 indexed search terms."

- 布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not
- “ ” 不允许词形变化，但可出现单数或复数；
- () 优先运算，括号中表达式还可以和其他术语交互
- 支持通配符*或?，如 medic*可代表medical, medicine, medication, medicinal等
(*代表0或多个字符；? 代表0或1个字符)

文献检索—主题词检索及布尔逻辑算符的使用

"cardiac disease" not "acute heart failure"
检索：心脏疾病，排除急性心衰

References search for ""cardiac disease" not "acute heart failure""

Substances Reactions Citing Knowledge Graph Save and Alert

Filter Behavior 25,170 Results Sort: Publication Date: Newest View: Partial Abstract

Filter by Exclude

Document Type

- Journal (24K)
- Patent (683)
- Review (6,155)
- Biography (27)
- Book (12)

View All

Language

- English (22K)
- German (609)
- Japanese (488)
- French (485)
- Chinese (397)

View All

Publication Year

1

Whole exome sequencing with a focus on **cardiac disease**-associated genes in families of sudden unexplained deaths in Yunnan, southwest of China

By: Wei, Si-Jie; Du, Jin-Liang; Wang, Yue-Bing; Qu, Peng-Fei; Ma, Lin; Sun, Zhong-Chun; Tang, Xue; Liu, Kai; Xi, Yan-Mei; Nie, Sheng-Jie; et al

BMC Genomics (2023), 24(1), 57 | Language: English, Database: CAlus and MEDLINE

Abstract: Objectives: To explore the causes of sudden unexpected death (SUD) and to search for high-risk people, whole exome sequencing (WES) was performed in families with SUDs. Methods: Whole exome sequencing of 25 people from 14 SUD families were screened based on **cardiac disease**-associated gene variants, and their echocardiograms and electrocardiograms (ECG) were also examined. The protein function of mutated genes was predicted by SIFT, PolyPhen2 and Mutation Assessor. Results: In the group of 25 people from 14 SUD families, 49 single nucleotide variants (SNVs) of **cardiac disease**-associate...

View More

Full Text Substances (0) Reactions (0) Citing (0) Citation Map

2

Effects of Aficamten on cardiac contractility in a feline translational model of hypertrophic cardiomyopathy

By: Sharpe, Ashley N.; Oldach, Maureen S.; Rivas, Victor N.; Kaplan, Joanna L.; Walker, Ashley L.; Kovacs, Samantha I.; Hwee, Darren T.; Cremin, Peadar; Morgan, Bradley P.; Malik, Fady I.; et al

Scientific Reports (2023), 13(1), 32 | Language: English, Database: CAlus and MEDLINE

Hypertrophic cardiomyopathy (HCM) is the most prevalent inherited **cardiac disease** in humans and cats and lacks efficacious pharmacol. interventions in the preclin. phase of disease. LV outflow tract obstruction (LVOTO) is commonly observed in HCM-affected patients and is a primary driver of heart failure symptoms and reduced quality of life. Novel

Feedback

("cardiac disease" not "acute heart failure") and "traditional chinese medicine"
检索：排除心衰的心脏疾病，且与中医药相关

References search for "("cardiac disease" not "acute heart failure") and "traditional chinese medicine""

Substances Reactions Citing Knowledge Graph Save and Alert

Filter Behavior 183 Results Sort: Publication Date: Newest View: Partial Abstract

Filter by Exclude

Document Type

- Journal (158)
- Patent (25)
- Review (38)
- Clinical Trial (3)
- Historical (4)

View All

Language

- English (151)
- Chinese (23)
- Korean (5)
- Japanese (2)
- German (1)
- Ukrainian (1)

View All

Publication Year

1

Phytochemical screening and in vitro anti-inflammatory activity of aqueous extract of cinnamomum verum (bark)

By: Chandrawanshi, Anand; Katare, Vivekanand; Mangrole, Sadhna; Jain, Prabhat Kumar

Indo American Journal of Pharmaceutical Sciences (2023), 10(1), 156-159 | Language: English, Database: CAlus

Traditional **herbal medicines** are naturally occurring, plant-derived substances with minimal or no requirement of industrial processing that has been used to treat illness within local or regional healing practices. The utilization and application of plants for healing purposes predate human history and lead to the origin of much modern medicine. Traditional **herbal medicines** are naturally occurring, plant-derived substances with minimal or no requirement of industrial processing that has been used to treat illness within local or regional healing practices. The utilization and application of pl...

View More

Full Text Substances (0) Reactions (0) Citing (0) Citation Map

2

Virtual screening analysis of natural flavonoids as trimethylamine (TMA)-lyase inhibitors for coronary heart disease

By: Zhou, Peng; Zhao, Xiao-Ni; Ma, Yao-Yao; Tang, Tong-Juan; Wang, Shu-Shu; Wang, Liang; Huang, Jin-Ling

Journal of Food Biochemistry (2022), 46(12), e14376 | Language: English, Database: CAlus and MEDLINE

A review. Coronary **heart disease** (CHD) is defined by atherosclerosis, which can result in stenosis or blockage of the arterial leading to ischemic **cardiac diseases** such as angina and myocardial infarction. Accumulating evidence indicates that the gut microbiota plays a vital role in the beginning and progression of CHD. The gut microbial metabolite, trimethylamine-N-oxide (TMAO), is intimately linked to the pathophysiol. of CHD. TMAO is formed when trimethylamine (TMA) is converted by flavin-containing monooxygenases in the hepatocytes. Therefore, inhibition of TMA production is essent...

View More

Feedback

使用布尔逻辑运算符，精准构建检索主题

高级检索—高效实现多项自定义组合检索

Searching for...

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

References

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

"chronic heart failure" and "traditional chinese medicine" [X] Draw [Q]

AND [X] Author Name Zhang, Boli [X]

- AND
- OR
- NOT
- Author Name
- Authors
- Publication Name
- Organization
- Title
- Abstract/Keywords
- Concept
- Substances
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

* 检索方法可单独使用，也可联用

主检索框：关键词、物质名称、CAS RN、DOI等

高级检索字段：作者名、期刊名、机构名、题目、摘要、概念词、物质标识符、出版商

结构检索

CAS Lexicon—利用词库选词获得准确结果

可在CAS 词库层级中浏览CAS标引的概念词（Concepts）和物质，建立用于检索文献的检索式（建立的检索式中最多可使用1000个词）

References

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

Enter a query...

Draw

Author Name Enter last name, first name middle name

+ Add Advanced Search Field

Learn more about SciFinder

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

检索并浏览CAS Lexicon词库中的层级，勾选适合的主题词：

Preferred Term、Broader Terms、Narrower Terms、Related Terms

Search CAS Lexicon

Heart failure Search Concept

Your Query You may include up to 1,000 terms in a search. Clear All

Heart failure X

Post-myocardial infarction heart failure X

Heart failure - Related Terms (2 Concepts) X

^ Preferred Term

Heart failure

This will search synonyms: Cardiac **failure**; Cardiac insufficiency; Cardiovascular **failure**; Congestive cardiac insufficiency; Congestive **failure heart**; Congestive **heart failure**; Congestive **heart** insufficiency; Coronary **heart failure**; Coronary insufficiency; **Heart** decompensation; **Heart** hypodynamia; **Heart** insufficiency; Myocardial **failure**; Myocardial insufficiency; Progressive **heart failure**

[View fewer synonyms](#)

^ Broader Terms (2) Select All

Heart disease

Organ failure

^ Narrower Terms (3) Select All

Acute heart failure

Select a boolean operator OR

Add Term(s)

^ Related Terms (10)

Acetazolamide

Amrinone lactate

Cardiopulmonary resuscitation

Cardiotonics

Congestive hepatopathy

Diuretics

High cardiac output

Inotropics

Low cardiac output

Sacubitril-valsartan mixt.

文献结果集—排序与筛选

References search for ""chronic heart failure" and "traditional chinese medicine""

Substances Reactions Citing Knowledge Graph

748 Results

Sort: Publication Date: Newest View: Partial Abstract

Filter Behavior

- Filter by Exclude
- Document Type
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CA Section
- CAS Solutions
- Bioactivity Data
- Formulation Purpose
- Database
- Search Within Results
- Filter Content Report

1

XinLi formula, a traditional Chinese decoction, all... the interaction of AGTR1 and AQP1

By: Wei, Xiao-Hong; Liu, Wen-Jing; Jiang, Wei; Lan, Tao-Hua; Pan, H...
Phytomedicine (2023), 113, 154722 | Language: English, Database...

XinLi formula (XLF) is a **traditional Chinese medicine** used in clin... remarkable curative effect. However, the mechanism remains unknown... the goal of the current investigation was to determine how XLF affected CHF in a rat model of the condition brought on by ligation of the left anterior descending coronary artery, and to investigate the underlying mechanism. Cardiac function was detected by echocardiog. The contents of myocardial enzymes, Ang II, ALD, TGF-β1, and inflammatory factors were measured by ELISA. Myocardial injury and myo...

View More

Full Text

Substances (0) Reactions (0) Citing (0) Citation Map

2

Qiangxin recipe improves doxorubicin-induced chronic heart failure by enhancing KLF5-mediated glucose metabolism

By: Yuan, Chenyue; Wu, Zong; Jin, Cuiliu; Cao, Weiwei; Dong, Yaorong; Chen, Jiahui; Liu, Chenping
Phytomedicine (2023), 112, 154697 | Language: English, Database: CAlus and MEDLINE

Qiangxin recipe (QXF) is a well-known **Chinese herbal medicine** commonly used in Asia for thousands of years to treat cardiovascular diseases, but its underlying mechanism remains unclear. This study aimed to illustrate whether Qiangxin Recipe (QXF) induce glucose metabolism and inhibit cardiomyocyte apoptosis by promoting the activation of the transcription factor Kruppel like factor 5 (KLF5). In vitro experiments, we constructed an H9C2 cardiomyocyte injury model using doxorubicin and use RNA-seq data anal. to detect the mechanism of QXF. In in vivo experiments, C57 BL/6 mice injected with do...

View More

Full Text

Substances (2) Reactions (0) Citing (0) Citation Map

知识图谱

排序：更快查找相关信息

Relevance

- Times Cited
- Accession Number: Ascending
- Accession Number: Descending
- Publication Date: Newest
- Publication Date: Oldest

聚类筛选项节省时间，一目了然。无需逐步二次检索和限定，直接勾选即可定位所需信息

文献类型

文献语言

研究发展趋势

CAS标引的
技术术语

CAS学科
研究方向

二次检索

下载报告

3 American

文献结果集—聚类筛选Concept

Concept ✕

Top Count Alphanumeric Search

<input type="checkbox"/> Chronic heart failure (369)	<input type="checkbox"/> Myocardium (33)	<input type="checkbox"/> Polygonatum odoratum (18)
<input type="checkbox"/> Pharmaceutical natural products (331)	<input type="checkbox"/> Schisandra chinensis (33)	<input type="checkbox"/> Protein phosphorylation (18)
<input type="checkbox"/> Homo sapiens (223)	<input type="checkbox"/> Alisma orientale (32)	<input checked="" type="checkbox"/> Traditional medicine diagnostic patterns (18)
<input type="checkbox"/> Human (223)	<input type="checkbox"/> Leonurus japonicus (31)	<input type="checkbox"/> Tumor necrosis factors (18)
<input type="checkbox"/> Heart failure (176)	<input type="checkbox"/> Pharmaceutical granules (31)	<input type="checkbox"/> Ventricular Function, Left (18)
<input type="checkbox"/> Cardioprotective agents (111)	<input type="checkbox"/> Rats, Sprague-Dawley (31)	<input type="checkbox"/> Circulation (17)
<input checked="" type="checkbox"/> Panax ginseng (111)	<input type="checkbox"/> Apoptosis (30)	<input type="checkbox"/> Diastolic blood pressure (17)
<input type="checkbox"/> Salvia miltiorrhiza (108)	<input type="checkbox"/> Cardiovascular agents (30)	<input type="checkbox"/> Heart disease (17)
<input type="checkbox"/> Astragalus membranaceus (102)	<input type="checkbox"/> Female (30)	<input type="checkbox"/> Pharmaceutical natural products, licorice (17)
<input type="checkbox"/> Drugs, Chinese Herbal (98)	<input checked="" type="checkbox"/> Heart rate (30)	<input type="checkbox"/> Systolic blood pressure (17)
<input type="checkbox"/> Aconitum carmichaelii (82)	<input type="checkbox"/> Cardiomyocyte (28)	<input type="checkbox"/> Cardiac fibrosis (16)
<input checked="" type="checkbox"/> Chinese medicine (78)	<input type="checkbox"/> Signal transduction (28)	<input type="checkbox"/> Mitochondria (16)
<input type="checkbox"/> Animals (77)	<input type="checkbox"/> Ventricular remodeling (28)	<input type="checkbox"/> Pharmaceutical natural products, GinSeng (16)
<input type="checkbox"/> Humans (76)	<input type="checkbox"/> Citrus reticulata (27)	<input type="checkbox"/> Phytotherapy (16)
<input type="checkbox"/> Cinnamomum cassia (71)	<input type="checkbox"/> Mandarin (27)	
	<input checked="" type="checkbox"/> Biomarkers (25)	

Apply Cancel

Concept ✕

Top Count Alphanumeric Search

Concept Name

metabol* Search

11 Selected

<input checked="" type="checkbox"/> Amino acid metabolism disorders (1)	<input checked="" type="checkbox"/> Lipid metabolism (1)	<input type="checkbox"/> Metabolites (3)
<input checked="" type="checkbox"/> Drug metabolism (2)	<input type="checkbox"/> Metabolic acidosis (2)	<input type="checkbox"/> Metabolome (2)
<input type="checkbox"/> Drug metabolites (1)	<input type="checkbox"/> Metabolic disorders (1)	<input type="checkbox"/> Metabolomics (10)
<input type="checkbox"/> Drug-metabolizing enzymes (1)	<input checked="" type="checkbox"/> Metabolic pathways (1)	<input checked="" type="checkbox"/> Secondary metabolites (1)
<input checked="" type="checkbox"/> Energy metabolism (13)	<input type="checkbox"/> Metabolism (3)	
<input type="checkbox"/> Energy metabolism, animal (3)	<input type="checkbox"/> Metabolism, animal (1)	

Apply Cancel

通过Concept纵览并精准定位感兴趣的核心研究点

文献结果集—聚类筛选CA Section

^ CA Section

- Pharmacology (400)
- Unavailable (241)
- Pharmaceuticals (70)
- Mammalian Pathological Biochemistry (31)
- Pharmaceutical Analysis (4)
- Biochemical Methods (1)
- Mammalian Hormones (1)

[View Fewer](#)

通过CA Section快速
锁定学科研究方向

文献结果集—保存及下载

结果集的合并、交集和去重

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The screenshot shows a search interface for "chronic heart failure" with various filters on the left. Three callout boxes provide instructions: 1. A box at the top points to the 'Merge, Intersection, and Deduplication' icon. 2. A box on the right points to the 'Save Results and Create Alert' dialog, which includes options for saving (Query Only, Selected Answers, All Answers) and alert frequency (No Alerts, As Available, Weekly, Monthly). 3. A box at the bottom points to the 'Download Reference Results' dialog, which allows selecting file types (PDF, RIS, etc.), quantity (All Results, Selected Results, Range), and display options (Result Summary, Result Details). The CAS logo is visible in the bottom right corner.

文献详情

Evaluation of the effect of Shengxian Decoction on doxorubicin-induced chronic heart failure model rats and a multicomponent pharmacokinetic study after oral administration in normal and model rats

它引文献 引文地图

Substances (19) Reactions (0) Citing (6) Citation Map Save

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Language
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By: Huang, Cuiyun; Qiu, Shi; Fan, Xiangcheng; Jiao, Guangyang; Zhou, Xun; Sun, Mei; Weng, Nan; Gao, Shouhong; Tao, Xia; Zhang, Feng; et al
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Shengxian Decoction (SXT), a well-known **Traditional Chinese Medicine** (TCM) formula composed of Astragali Radix, Bupleuri Radix, Cimicifugae Rhizoma, Anemarrhenae Rhizoma and Platycodonis Radix, is clin. considered as an effective formula against cardiovascular diseases. However, the exact effective substance of SXT in treating **chronic heart failure** (CHF) still remains unclear. In the current study, we investigated the benefit of SXT in doxorubicin (DOX)-induced CHF rats and established a UHPLC-MS/MS method to simultaneously determine 18 key compounds in a subsequent comparative pharmacokinetic study in normal and CHF rats. Histopathol. studies, transmission electron microscopy, and echocardiog. were applied to assess the therapeutic effect of SXT on DOX-induced CHF rats, which indicated that SXT significantly ameliorated DOX-induced CHF, similar to enalapril. In addition, we successfully established a UHPLC-MS/MS method to determine the pharmacokinetics of the components in rat plasma, which was validated with good linearity, inter-day and intra-day precisions and accuracies, matrix effects, extraction recovery, and stability values. Our results showed that only astragaloside IV showed increased plasma exposure in the CHF rats, while saikosaponin A, quercetin, timosaponin B-II, ferulic acid, isoferulic acid and formononetin decreased compared to their pharmacokinetic characteristics in the normal and CHF rats. This study demonstrates that SXT enjoys obvious therapeutic effect on DOX-induced CHF rats, and the altered metabolism of some compounds in SXT is affected by the pathol. state of CHF rats. Our findings provide a better understanding of the in vivo exposure to complex compounds of SXT, supporting effective substance screening and further investigation of the therapeutic mechanism.

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- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
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Substances:
对原文中重点研究的物质信息一目了然；由Role了解文献对物质研究的学科方向

物质角色

^ Concepts

Blood plasma	Mortality rate
Blood serum	Pathology
Body weight	
Chronic heart failure	
Heart	
Metabolism	
Mitochondria	

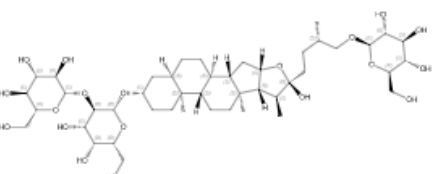
^ MEDLINE® Medical Subject Headings

Animals	Heart Failure
Astragalus propinquus	Qualifier: chemically induced; drug therapy
Cardiovascular Agents	Male
Qualifier: pharmacokinetics; therapeutic use	Mass S
Chromatography, High Pressure Liquid	Medici
Chronic Disease	Rats

^ Substances

Substances (19)

136656-07-0

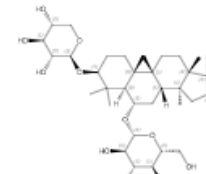


Absolute stereochemistry shown, Rotation (-)

C₄₅H₇₆O₁₉
Timosaponin B II

Role: Pharmacological Activity, Pharmacokinetics, Therapeutic Use, Biological Study, Uses

84687-43-4



Absolute stereochemis

C₄₁H₆₈O₁₄
Astragaloside IV

Role: Pharmacological Activity, Pharmacokinetics, Therapeutic Use, Biological Study, Uses



文献详情—引文地图

Citation Map for Evaluation of the effect of Shengxian Decoction on doxorubicin-induced chronic heart failure model rats and a multicomponent comparative pharmacokinetic study after oral administration in normal and model rats

By: Huang, Cuiyun; Qiu, Shi; Fan, Xiangcheng; Jiao, Guangyang; Zhou, Xun; Sun, Mei; Weng, Nan; Gao, Shouhong; Tao, Xia; Zhang, Feng; et al
Biomedicine & Pharmacotherapy (2021), 144, 112354 | Language: English, Database: CAPlus and MEDLINE

Full Text ▾

Filter By Cited By Citing

Filter Behavior
Filter by Exclude

Document Type

- Journal (49)
- Review (9)
- Clinical Trial (2)
- Report (1)

Author

- Dong, Xin (2)
- Gao, Shouhong (2)
- Jiang, Bo (2)
- Lipshultz, Steven E. (2)
- Sallan, Stephen E. (2)

[View All](#)

Concept

- Animals (29)
- Male (23)
- Humans (19)
- Rats (16)
- Rats, Sprague-Dawley (15)

[View All](#)

Citations

Citation Map Key

- Cited by Root Document
- References Citing Root Document

Sulforaphane protection against the development of doxorubicin-induced chronic heart failure is associated with Nrf2 Upregulation
By: Bai, Yang; Chen, Qiang; Sun, Yun-Peng; Wang, Xuan; Lv, Li; Zhang, Li-Ping; Liu, Jin-Sha; Zhao, Song; Wang, Xiao-Lu
Cardiovascular Therapeutics (2017)

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专利文献

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The screenshot shows the CAS PatentPak interface. On the left, there is a sidebar with 'Key Substances in Patent' and a list of CAS RNs with their respective chemical structures. The main area displays a patent document in Japanese, including a chemical structure (式(5)) and a reaction scheme. The interface includes navigation controls like 'PAGE', 'ZOOM', and 'DOWNLOAD'.

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The screenshot shows the patent details page for 'Elastomer and wearable device with good sweat and water resistance'. The page includes a title, patent number (JP2021138895), publication date (2021-09-16), application number (JP2020-40000), and application date (2020-03-09). It also lists the assignee (Sumitomo Bakelite Co., Ltd., Japan) and the source (Japan, CODEN: JKOXAF). The page features a 'Patent Family' table and 'IPC Data' section. A callout box highlights the text '获取现有技术文献' (Obtain existing technical literature) and another callout box highlights '专利族信息' (Patent family information).

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
JP2021138895	Japanese	A	PDF PDF+ Viewer	2021-09-16	JP2020-40000	2020-03-09

Patent	Class	Patent Family Classification Codes
JP2021138895	IPC1	C08L 0083/04; C08L 0083/07; C08K 0003/36; A41D 0013/00; A41D 0031/00; A41D 0031/04

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References search for "enzyme and reduction" + drawn structure

Substances Reactions Citing Knowledge Graph Save and Alert

Structure Match: As Drawn (0) Substructure (8,881)

Filter Behavior: Filter by Exclude

Document Type Language Publication Year Available at My Institution Author Publication Name Concept

Database: Cplus (8,605) MEDLINE (6,814) CHEMZENT (31)

Search Within Results Filter Content Report Download filter data from this result set

Filtering: Database: CHEMZENT 31 Results Sort: Relevance View: Partial Abstract

Fabric change of CARB azole in rats and rabbit
By: Johns, S. R.; Wright, S. E.
Chemisches Zentralblatt (1966), 137(5), 01578-01578 | Language: German, Database: CHEMZENT

Machine Translated: After administration of carbazoles is 3-hydroxy carbazole, conjugate with glucuronic acid in the urine separated Hauptstoffwechselprod. in rats and rabbits. The hydroxylation in 3-position is in accordance with the etching oxidizing enzymes at the position of greatest electron density. For the investigation of werden carbazole-14 C is used. Experiments: 14C-carbazole (I), Melting Point 242-244 ° (from benzene) by diazotization and reduction of 14C-aniline to 14C-phenylhydrazine (240-245 ° F) with cyclohexanone in 14C-tetrahydrocarbazol is converted. Dehydrogenation to Pd-C gives I. Respect m...

Cobamide and ribo nucleotide reduction. 3. Part The content of the Cobamid-abhängigen Ribonucleosid-triphosphatreduktase in Lactobacillus leichmanii influencing factors
By: Ghambeer, R. K.; Blakley, R. L.
Chemisches Zentralblatt (1968), 139(28), 160-160 | Language: German, Database: CHEMZENT

Machine Translated: Hysic. Res. common. 20 (1965) 20. — the content of ribo nucleoside triphosphate reductase (I) in extracts of L. leichmanii depends on the age of the culture. During the linear growth if I-Geh. with increasing age up to the end of the linear phase on and falls then. Extracts from stationary cells exhibit no significant I-Aktivität. The rapid I-Synth. during the linear growth by chloramphenicol and ActinomycinD inhibited. The decrease of I-Geh. after completion of the linear growth is based not on the presence one increased amount proteolyt. Enzymes nor on incomplete release of said enzyme. The ...

Nr. 5-1559 E-6. Pharmakologie, Therapie, Toxikologie, Hygiene 1966

68-74, 1963; Washington, D.C. George Washington Univ., School of Med., Dep. of Pharmacol.; engl.) — Die i.p. Injektion von 1 mg des adeninnanalogen Purin-antimetaboliten 4-Aminopyrazolopyrimidin (I) verursachte bei Mäusen einen Anstieg der Gessantleberlipide innerhalb 24 Std. auf das 3-4fache. Hieran waren an erster Stelle die Neutrallipide, in geringerem Ausmaß auch das Cholesterin (II) beteiligt, während der Phospholipid (III)-Geh. unverändert blieb. I-Gabe hemmte den in vitro-Einbau von ¹⁴C₁₁-Acetat (IV) in die Lipide von Leberschnitten, hatte aber wenig Einfl. auf die Ox. von IV u. ¹⁴C₁₁-Palmitat (V) in vitro. Die Plasmalipidkonz. sank nach I-Applikation u. war durch einen Abfall der Triglyceride u. des II hervorgerufen. III u. freie Fettsäuren waren nicht beteiligt. V wurde von den Lebern der mit I behandelten Tiere schlechter aufgenommen als von den Lebern der Kontrolltiere. Obgleich der Einbau von ¹⁴C₁₁-Oxetsäure in RNS durch I gehemmt wurde, konnte kein verminderter Einbau von ¹⁴C₁₁-Glycin in Leber- u. Plasmaproteine festgestellt werden. Die normalerweise massive Hyperlipidämie nach Gabe von Triton WR-1339 wurde durch I verhindert. VI. schließt aus den Unters., daß I wahrscheinlich die Sekretion von Triglyceriden aus der Leber hemmt. H. Zöllner 4607

1559 Stoffwechsel des Carbazols in Ratten und Kaninchen. S. R. Johns und S. E. Wright. (J. med. Chem. 7, 158-161, 1964; Sydney, Univ. of Sydney, Dep. of Pharmacy; engl.) — Nach Gabe von Carbazol ist 3-Hydroxycarbazol, konjugiert mit Glucuronsäure, das im Harn ausgeschiedene Hauptstoffwechselprod. bei Ratten u. Kaninchen. Die Hydroxylierung in 3-Stellung ist in Übereinstimmung mit dem Angriff oxydierender Enzyme an der Stellung mit der größten Elektronendichte. Für die Unters. wurde Carbazol-¹⁴C verwendet. Versuche: ¹⁴C-Carbazol (I), F. 242-244° (aus Bzl.) durch Diazotierung u. Red. von ¹⁴C-Anilin zu ¹⁴C-Phenylhydrazinhydrochlorid (F. 240-245°), das mit Cyclohexanon in ¹⁴C-Tetrahydrocarbazol übergeführt wird. Dehydrierung an Pd-C ergibt I. Hergestellt Bezugsubstanzen: 1-Hydroxycarbazol, F. 160-162° durch Cyclisierung von Cyclohexan-1,2-diaminophenylhydrazon (F. 183-195°) in ethanol. Essigsäure über 1.2.3.4-Tetrahydro-1-oxocarbazol (F. 169°), das an Pd-C dehydriert wird. 3-Hydroxycarbazol (II), F. 260-261° über folgende Stufen: p-Methoxyphenylhydrazinhydrochlorid (III), F. 198-200° (aus A.) durch Diazotierung u. Red. von p-Anisidin. — 6-Methoxy-1.3.4-tetrahydrocarbazol (IV), C₁₃H₁₁NO, F. 94-95° (aus A.), durch Rk. von III mit Cyclohexanon in wss. Essigsäure (50%ig) bei Ggw. von Natriumacetat. 3-Methoxycarbazol (V) C₁₃H₁₁NO, N-Butyl-, Äthyl-, Bromid, DL₂₀ 384, Curarisierungswirkg., 30,7, chololyt. Aktivität, 0,04; N-Cyclohexyl-, Äthyl-, Bromid, 33,5/28/0,02; N-Phenyl-, Äthyl-, Bromid, 17,5/20/0,09; N-Phenyl-, Benzyl-, Bromid, 11/13/0,14; N-β-Phenyl-, Äthyl-, Bromid, 21/22/0,1; N-Octyl-, Äthyl-, Bromid, 6,8/6,7/1,5; Lauryl-, Äthyl-, Bromid, 21,5/12,6/16; N-Butyl-, Hydrochlorid, 115/-/0,02; N-Cyclohexyl-, HCl, 75/-/0,02; N-Phenyl-, HCl, 47,5/-/cholinerq.; N-β-Phenyl-, HCl, 60/-/0,03; N-Octyl-, HCl, 47/-/0,5; N-Lauryl-, HCl, 37,5/-/1,5; N,N-dialkylcarbaminsäure-β-di-äthylaminoäthylester; Äthyl-, Bromid: diäthyl-, DL₂₀ 28, Curarisierungswirkg., 28, spasmody. Aktivität, 50 (Papaverin = 100), 0,05 (I = 100), Antihistaminaktivität, — (Promethazin = 100); diäthyl-, 8/11/2100/6/4,3; dicyclohexyl-, 2,2/4,8/2300/2,4/0,05; Diphenyl-, 9,5/11,6/310/0,13/0,03; Di-[β-phenäthyl]-, 6,5/6,5/570/0,38/0,07; Dibutyl-, Benzyl-, Bromid, 7,5/5,5/200/0,11/-; Carbazol (II), Äthyl-, Bromid, 3,3/4,0/730/0,26/0,20; Acridin (III), Äthyl-, Bromid, 5,8/4,5/770/0,4/0,20; Phenozazin (IV), Äthyl-, Bromid, 4,0/5,3/1400/1,3/0,5; Phenothiazin (V), Äthyl-, Bromid, 3,0/4,0/800/0,8/0,5; Hydrochlorid: Dibutyl-, 38/-/1000/3,0/3,0; Dicyclohexyl-, 22/-/1130/2,4/0,1; Diphenyl-, 42,5/-/770/4,5/0,1; Di-[β-phenäthyl]-, 10,3/-/400/0,14/0,2; II, 20/-/280/0,1/0,3; III, 35/-/1800/1/1; IV, 24,5/-/770/0,8/1; V, 25/-/12000/16/30. K. Maier 4607

1561 Wirkung von Chlorcyclizin und anderen Stoffen auf die Toxizität verschiedener Organophosphat-Anticholinesterasen. Richard M. Welch und J. M. Coon. (J. Pharmacol. exp. Therap., 143, 192-98, 1964; Philadelphia, Pa., Jefferson Med. Coll., Dep. of Pharmacol.; engl.) — W. untersuchten versch. Substanzen mit bekannter Wirkg. auf die Lebermikrosomen-Enzymsyst. auf deren Wirkg. auf die Toxizität einiger Organophosphat-insektizide an Mäusen. Eine Vorbehandlung der Tiere täglich über 4 Tage mit Chlorcyclizin (I), Phenobarbital (II), SKF-525 A (α,α-Diphenyl-α-propyl-essigsäure-β-äthylaminodihylester · HCl; III) oder Cyclohexan zeigte einen deutlichen Schutz gegen die Toxizität von Malathion, Parathion (IV) u. EPN (p-Nitrophenyl-thionbenzolphosphorsäureäthylester). Eine I-Vorbehandlung erhöhte außerdem wesentlich die orale DL₅₀ von Paraoxon (V). TEPP (Tetraäthylpyrophosphat) u. Physostigmin. Eine s.c.-Dosis von I, II oder III schützte gegen IV. Die Umwandlung von IV in V durch Mäuseleber erfolgte etwa 2mal so schnell, wenn das Tier 4 Tage vorher mit I vorbehandelt wurde. Eine I-Dosis senkte deutlich die Serum-Paraoxonase (VI; A-Esterase), erhöhte aber dagegen gering die Leber-VI. I erhöhte innerhalb von 24 Std. das Verhältnis Lebergew. zu Körpergew. um ...

- ChemZent是最古老的德国化学文摘的英文版，唯一提供可用英文获取德国化学文摘的解决方案
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文献检索—主题词+结构联合检索

The screenshot shows the CAS SciFinder interface. At the top, the search query is "herb and medic*" and the search type is "References". A chemical structure of a pentacyclic triterpenoid is drawn and overlaid on the search results. The left sidebar shows filter options, with "Substance Role" expanded to show a list of roles: Biological Study (334), Uses (214), Analytical Study (83), Preparation (49), Occurrence (33), Language, Publication Year, Available at My Institution, and Author. The main results area shows two entries. The first entry is "Pentacyclic triterpenoids from the medicinal herb, Centella asiatica (L.) Urban" with 368 results. The second entry is "Effects of Gymnema sylvestre extract on the pharmacokinetics and pharmacodynamics of glimepiride in streptozotocin induced diabetic rats" with 2 results. A blue arrow points from the "Substance Role" filter in the sidebar to the "Substance Role" panel on the right.

The "Substance Role" panel is shown with the "By Count" tab selected. It displays 8 selected roles from a list of 17. The selected roles are: Therapeutic Use (204), Pharmacological Activity (132), Analyte (83), Purification or Recovery (43), Natural Product Occurrence (33), Cosmetic Use (15), and Adverse Effect (6). The unselected roles are: Biological Study (334), Uses (214), Biological Study, Unclassified (127), Analytical Study (83), Preparation (49), Occurrence (33), Properties (23), Food or Feed Use (16), Reactant (6), and Reactant or Reagent (6). The panel includes "Apply" and "Cancel" buttons at the bottom.

物质在文献中的研究角色

文献检索小结

1. 使用布尔逻辑算符and、or、not连接主题词
2. 利用CAS Lexicon选词精准检索文献
3. 通过聚类筛选工具快速获得目标文献
4. 从引文地图拓展检索，获得更多灵感
5. 用PatentPak提高专利阅读效率
6. 主题词+结构联合检索快速获得文献

物质检索

- 物质检索方法
 - 物质标识符：化学名称，CAS RN
 - 文献标识符：专利号、文献号、PubMed ID、DOI
 - 分子式
 - 物性参数
 - 谱图数据
 - 结构式
- 检索策略推荐
 - 有机化合物，金属配合物，天然产物：结构检索
 - 无机物，合金：分子式检索
 - 高分子化合物：分子式检索和结构检索

物质检索

通过物质名称、CAS RN，文献标识符检索物质

Searching for...

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

Substances

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

Enter a query...

Draw

Molecular Formula

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

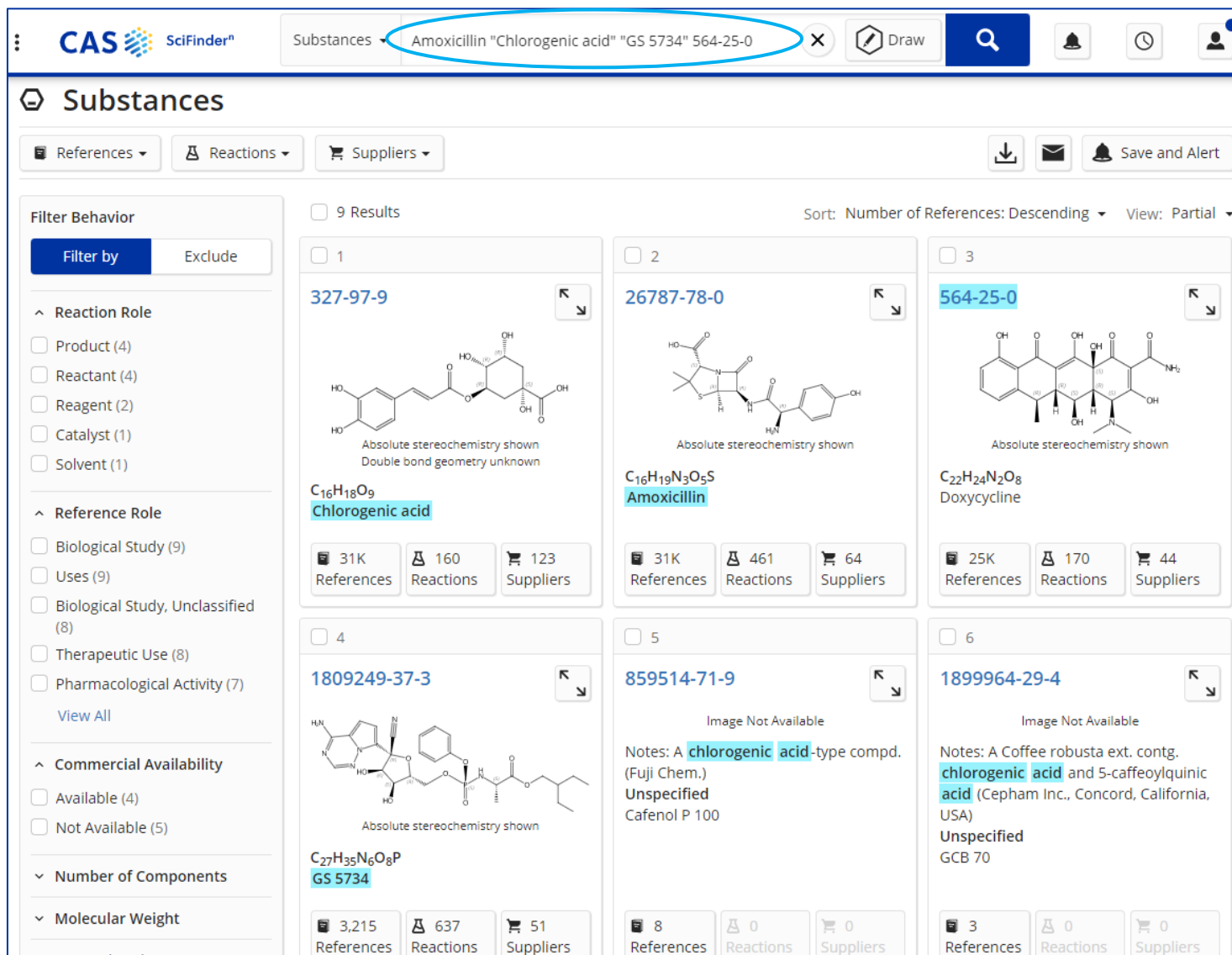
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打开结构绘制面板进行结构检索

物质检索—物质名称、CAS RN、代码



The screenshot shows the CAS SciFinder search results for the query "Amoxicillin "Chlorogenic acid" "GS 5734" 564-25-0". The search bar contains the query, and the results are displayed in a grid of six cards. Each card shows a chemical structure, a CAS RN, and the number of references, reactions, and suppliers. The results are sorted by the number of references in descending order.

CAS RN	Chemical Name	References	Reactions	Suppliers
327-97-9	Chlorogenic acid	31K	160	123
26787-78-0	Amoxicillin	31K	461	64
564-25-0	Doxycycline	25K	170	44
1809249-37-3	GS 5734	3,215	637	51
859514-71-9	Unspecified Cafenol P 100	8	0	0
1899964-29-4	Unspecified GCB 70	3	0	0

- 物质检索框中可同时检索多个物质识别符（物质名称或CAS RN）；
- 双引号“ ”可精准识别物质识别符；
- 不同的物质使用空格隔开，支持高达2000个字符

物质检索—物质名称中间或词尾使用通配符*或？

The image displays two screenshots of the CAS SciFinder search interface. The left screenshot shows a search for 'flavone*' resulting in 4,467 substances. The right screenshot shows a search for 'flavone?' resulting in 20 substances. A text box at the bottom center states: '物质名称中使用通配符可以检索多个物质' (Using wildcards in substance names can retrieve multiple substances).

Left Screenshot (Search: flavone*)

- Substances: 4,467
- Sort: Relevance
- View: Partial
- Filter Behavior: Filter by (selected), Exclude
- Commercial Availability: Available (1,873), Not Available (2,594)
- Reaction Role: Product (1,934), Reactant (729), Reagent (15), Catalyst (12), Solvent (1)
- Reference Role: Preparation (3,950), Synthetic Preparation (2,005), Biological Study (1,445), Properties (1,219), Biological Study, Unclassified (1,127)
- Stereochemistry: View All
- Number of Components: View All
- Substance Class: View All
- Isotopes: View All
- Metals: View All
- Molecular Weight: View All

Right Screenshot (Search: flavone?)

- Substances: 20
- Sort: Relevance
- View: Partial
- Filter Behavior: Filter by (selected), Exclude
- Commercial Availability: Available (1), Not Available (19)
- Reference Role: Biological Study (18), Uses (17), Therapeutic Use (12), Biological Study, Unclassified (8), Pharmacological Activity (8)
- Number of Components: View All
- Substance Class: View All
- Isotopes: View All
- Metals: View All
- Experimental Property: View All
- Bioactivity Indicator: View All

物质检索—文献标识符及结果集排序

CAS SciFinder[®] Substances US20060106041

Substances search for "US20060106041"

References Reactions Suppliers Save and Alert

Filter Behavior

Filter by Exclude

Reaction Role

- Product (45)
- Reactant (29)
- Reagent (10)
- Catalyst (11)
- Solvent (7)

Reference Role

- Preparation (45)
- Synthetic Preparation (45)
- Reactant (32)
- Reactant or Reagent (32)
- Biological Study (23)

View All

Commercial Availability

- Available (41)
- Not Available (4)

45 Results Sort: Relevance View: Partial

1 68-12-2 CN(C)C=O C₃H₇NO Dimethylformamide 158K References 3.9M Reactions 245 Suppliers

2 100-39-0 c1ccccc1CCBr C₇H₇Br Benzyl bromide 63K References 190K Reactions 65 Suppliers

4 77-78-1 COS(=O)(=O)OC C₂H₆O₄S Dimethyl sulfate

5 98-09-9 c1ccccc1S(=O)(=O)Cl C₆H₅ClO₂S Benzenesulfonyl chloride

6 100-07-2 COc1ccc(cc1)C(=O)Cl C₈H₇ClO₂ 4-Methoxybenzoyl chloride

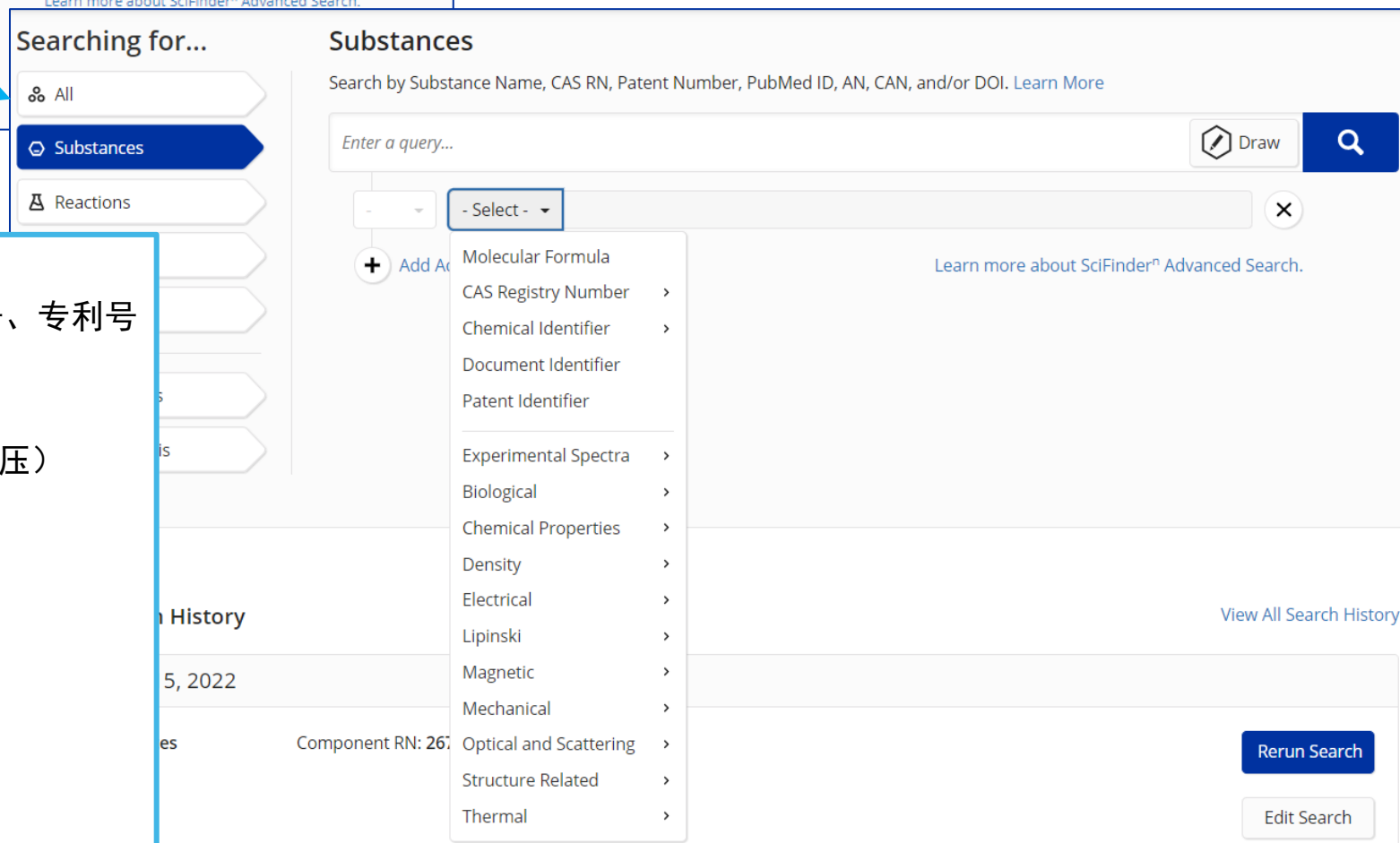
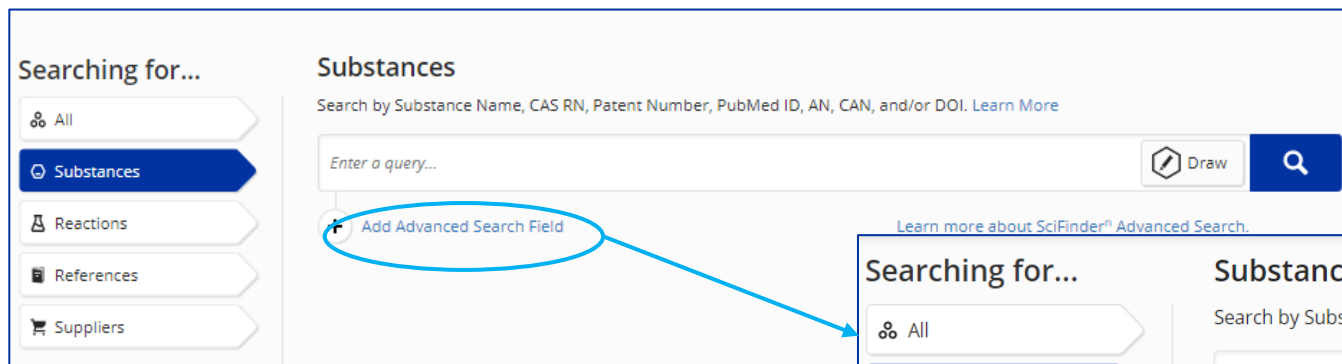
Relevance

- CAS RN: Ascending
- CAS RN: Descending
- Molecular Formula: Ascending
- Molecular Formula: Descending
- Molecular Weight: Ascending
- Molecular Weight: Descending
- Number of References: Ascending
- Number of References: Descending
- Number of Suppliers

利用物质排序快速
查找目标物质：
相关度
CAS RN
分子式
分子量
文献量
供应商数量

帮助用户迅速获得关
注文献中的物质信息

物质检索—Advanced Search



高级检索字段：

CAS RN（物质、组份）、物质标识符、分子式、文献号、专利号

实验谱图（¹H, ¹³C, ¹⁵N, ¹⁹F, ³¹P NMR）

生物（生物富集因子、LD50）

化学（Koc, LogD, LogP、溶解度、分子量、pKa、蒸汽压）

密度属性（密度、摩尔体积）

电学（电导/电导率、电阻/电阻率）

Lipinski（自由旋转键、H受体/供体）

磁（磁力矩）

机械属性（拉伸强度）

光散射（旋光性、折射率）

结构（极性表面积）

热学（熔点、沸点、闪电、玻璃转化温度、蒸发焓）

物质检索—分子式

Na₂SO₄: H₂O₄S.2Na

Searching for...

Substances

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

Enter a query...

Molecular Formula H₂SO₄.2Na

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

Learn more about SciFinder[®] Advanced Search.

Filter Behavior

Filter by Exclude

Reaction Role

Product (2)

Reagent (2)

Catalyst (1)

Reference Role

Process (6)

Uses (6)

Biological Study (5)

Properties (5)

Analytical Study (4)

Commercial Availability

Available (4)

Not Available (5)

Number of Components

Substances search for "H₂O₄S.2Na" Molecular Formula

References Reactions Suppliers

9 Results

Sort: Relevance View: Partial

1 7757-82-6

2 13759-07-4

3 14262-80-7

4 225640-22-2

5 20581-68-4

6 911392-46-6

Chemical structures and associated data (References, Reactions, Suppliers) are displayed for each result.

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：铁钴镍合金 Co. Fe. Ni
- 无机含氧盐：阳离子和阴离子用点（.）分开；阴离子以氢补齐至电中性

物质检索—联合检索

H谱特征峰化学位移数据: 7 to 8, 2.2, 3 to 4

C谱特征峰化学位移数据: 44.5 to 45

分子量: 500--545之间

Searching for...

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

Substances

Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI

Enter a query...

Molecular Weight: 500 to 545
Predicted values only.

AND Proton NMR: 7 to 8, 2.2, 3 to 4
Allowance of ± 0.2 ppm.

AND Carbon-13 NMR: 44.5 to 45
Allowance of ± 2 ppm.

[Add Advanced Search Field](#)

Substances search for 3 Advanced Fields

References Reactions Suppliers

7,330 Results Sort: CAS RN: Ascending View: Partial

Filter Behavior

Filter by Exclude

Reaction Role

- Product (7,254)
- Reactant (2,125)
- Reagent (8)
- Catalyst (128)

Reference Role

- Preparation (7,309)
- Synthetic Preparation (7,196)
- Biological Study (2,381)
- Reactant (2,308)
- Reactant or Reagent (2,308)

[View All](#)

Bioactivity Data

Commercial Availability

- Available (1,477)
- Not Available (5,853)

Number of Components

Molecular Weight

Stereochemistry

1 752-13-6
Absolute stereochemistry shown
C25H28N4O10
Riboflavin, 2',3',4',5'-tetraacetate
300 References 730 Reactions 9 Suppliers

2 1262-14-2
Absolute stereochemistry shown
C33H44O6
Dihydrocelestrol diacetate
34 References 15 Reactions 1 Supplier

3 2222-07-3
Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown
C30H42O7
Cucurbitacin I
462 References 13 Reactions 44 Suppliers

4 3022-92-2
Absolute stereochemistry shown
C23H39N5O5S2
Malformin A₁
Protein/Peptide Sequence
Sequence Length: 5
107 References 11 Reactions 15 Suppliers

5 5945-86-8
Absolute stereochemistry shown
C30H36O9
Nimbin
363 References 129 Reactions 27 Suppliers

6 6997-41-7
Absolute stereochemistry shown
C34H48O3
3 β -(Benzoyloxy)cholest-5-en-7-one
47 References 47 Reactions 15 Suppliers

物质详情

CAS Registry Number: 2222-07-3

References (462) Reactions (13) Suppliers (44)

Download Email Save

Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

$C_{30}H_{42}O_7$
19-Norlanosta-1,5,23-triene-3,11,22-trione, 2,16,20,25-tetrahydroxy-9-methyl-, (9β,10α,16α,23E)- (9Cl, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	514.65	-
Boiling Point (Predicted)	698.3±55.0 °C	Press: 760 Torr
Density (Predicted)	1.26±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	8.51±0.70	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

- Other Names and Identifiers
- Experimental Properties
- Experimental Spectra
- Structure Activity Relationships
- Toxicity
- Predicted Properties
- Predicted Spectra
- Bioactivity Indicators
- Target Indicators
- Regulatory Information
- Additional Details

折叠菜单显示物质各类信息

物质详情

Experimental Spectra

¹H NMR ¹³C NMR

View Proton NMR Spectrum

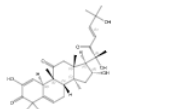
Proton NMR Spectrum - 2 Sources

Sources

- (1) Seger, Christoph; Magnetic Resonance in Chemistry, (2005), 43(6), 489-491, CAplus
- (2) Wu, Pei-Lin; Chemical & Pharmaceutical Bulletin, (2004), 52(3), 345-349, CAplus
- (3) Molavi, Ommoleila; Molecular Pharmaceutics, (2010), 7(2), 364-374, CAplus

Proton NMR Spectrum for 2222-07-3

2222-07-3



Absolute stereochemistry shown, Rotation (-)
Double bond geometry shown

C30H42O7

CAS Name
Cucurbitacin I

Conditions

Working Frequency
300 MHz

Solvent
[Chloroform-d \(865-49-6\)](#)

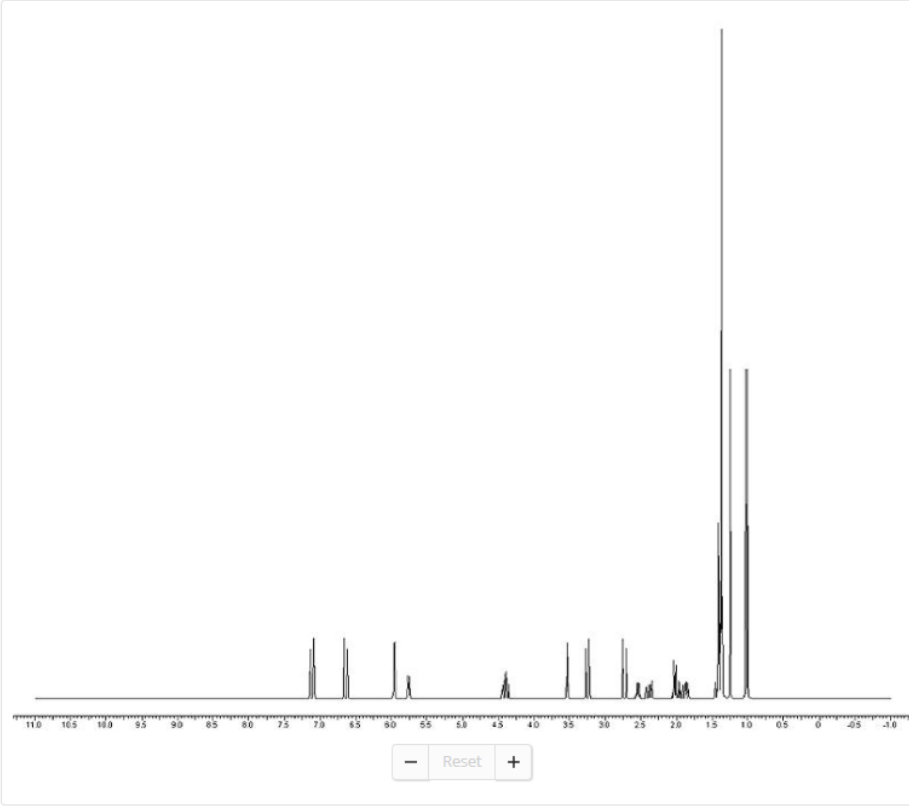
Temperature
27 °C

Spectrum Summary

Spectrum ID
06mrc5a1_34.H

Peak Data
7.11, 6.64, 5.96, 5.76, 4.4, 3.53,
3.25, 2.73, 2.54, 2.38, 2.03, 1.99,
1.87, 1.42, 1.41 (3H), 1.38 (3H), 1.37
(6H), 1.36 (3H), 1.25 (3H), 1.03 (3H),
1.0 (3H) ppm

Source
Spectral data were obtained from
Advanced Chemistry Development,
Inc.



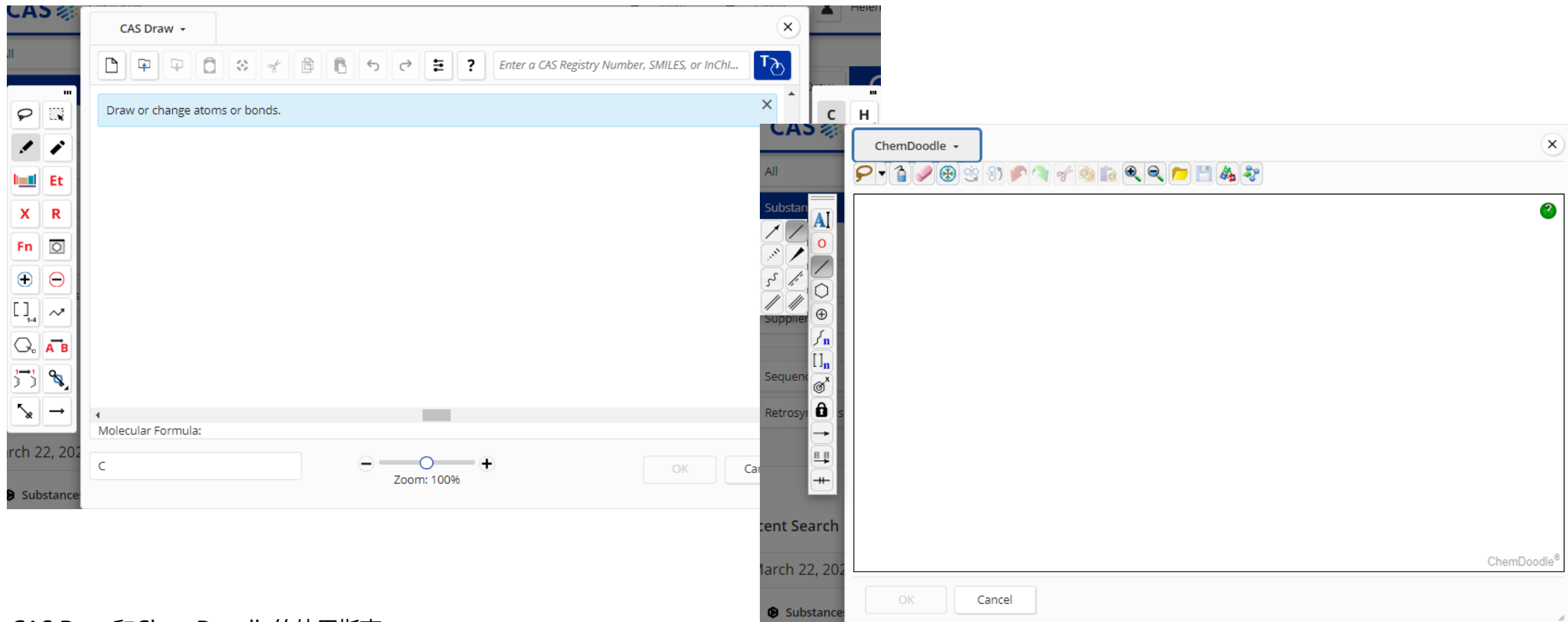
The NMR spectrum shows a complex pattern of peaks in the aromatic region (6.6-7.2 ppm) and a large cluster of aliphatic peaks between 1.0 and 2.0 ppm. The x-axis is labeled from 11.0 to -1.0 ppm.

物质检索—结构检索

The screenshot displays the SciFinder search interface. On the left, a sidebar lists search categories: All, Substances (selected), Reactions, References, Suppliers, Sequences, and Retrosynthesis. The main area is titled 'Substances' and includes a search bar with the placeholder 'Enter a query...'. Below the search bar is a dropdown menu for 'Molecular Formula' and a 'Draw' button. Examples of molecular formulas are provided: C6H6, [(C6H8)x], and C22H26CuN2O5.C2H3N. A 'CAS Draw' window is overlaid on the interface, showing a toolbar with various drawing tools and a panel with chemical symbols (C, H, O, S, N, P, Cl, Si, etc.). The 'CAS Draw' window also has a search bar for 'Enter a CAS Registry Number, SMILES, or InChI...' and a 'Molecular Formula' field containing 'c'. A zoom slider is visible at the bottom of the 'CAS Draw' window.

-  选择可变基团
-  自定义R基团
-  片段定义工具
-  重复片段工具
-  取代位点可变
-  锁工具

物质检索—结构绘图板



CAS Draw和ChemDoodle的使用指南

https://scifinder-n.cas.org/help/#t=Drawing_Search_Queries%2FDrawing_Structure_Queries.htm

<https://www.cas.org/support/training/scifinder-n/structure-search>

<https://www.cas.org/support/training/scifinder-n/chemdoodle-structure-search>

结构绘图工具的使用—同位素原子的绘制

The screenshot shows the CAS Draw software interface. The main window displays a chemical structure of a benzofuran derivative with a fluorine atom (F) attached to the side chain. A dialog box titled "Specify Atomic Mass" is open, allowing the user to select the type of fluorine isotope to use. The options are:

- Any
- Abnormal
- Specific: 19

The "Specific" option is selected, and the value "19" is entered in the input field. The dialog box has "OK" and "Cancel" buttons. At the bottom of the main window, there is a search bar containing "F", a zoom slider set to 100%, and another "OK" and "Cancel" button. The molecular formula is shown as $C_{10}H_{11}FO$ (166.20).

鼠标右键点击某原子，在弹出窗口中对F原子进行设置：

Any：获取所有F的同位素和非同位素标记物；

Abnormal：获取F的所有同位素标记物；

Specific：可输入具体的同位素质量数，点击OK，精准检索特定的F同位素标记物。

物质检索—结构检索

结构检索时，无需分步进行，一次检索即可得到As Drawn, Substructure和Similarity结果

CAS Draw

Enter a CAS Registry Number, SMILES, or InChI...

Draw or change atoms or bonds.

R1

Molecular Formula: Formula is not available

R1

Zoom: 100%

OK Cancel

R-Group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12 >

R1: Ni, Cu, Co

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	**																	

*Lanthanides La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu

**Actinides Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Isotopes D T

物质检索—检索结果集筛选

结构检索类别：
As Drawn
亚结构
相似结构
结构精准度筛选

Chemscape分析

Filter by & Exclude

物质筛选类别：
反应角色
文献角色
商业可用性
组分数目
分子量
立体化学
元素
物质类别
同位素
金属包含
实验物性数据
二次检索.....

Substances search for drawn structure

References Reactions Suppliers

Structure Match

- As Drawn (0)
- Substructure (732)**
- Similarity (9)
- Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

- Reaction Role
- Reference Role
- Commercial Availability
- Number of Components
- Molecular Weight
- Stereochemistry
- Element
- Substance Class
- Isotopes
- Metals
- Experimental Property
- Bioactivity Indicator
- Search Within Results

732 Results

Sort: Relevance View: Partial

1 685504-28-3

C31H35Cl3CoNP2
(7-4)-Trichloro[N-[2-(diphenylphosphino-κP)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

2 807307-30-8

C31H35Cl3CoNOP2
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino-κP)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

3 635299-07-9

C31H35Cl3CoNOP2.H
Components: 2
Component RN: 807307-30-8
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino-κP)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

4 635299-08-0

C31H35Cl3CoNP2.2/5C2H6O...
Components: 3
Cobaltate(1-), trichloro[N-[2-(diphenylphosphino-κP)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

5 16827-53-5

C34H33Co2N3O6P2
Cobalt, [μ-[2,2'-bis(diphenylphosphino)triethylamine]]tetracarbonyl(dinitrosyl)di...

6 635299-09-1

C31H35Cl2CoNOP2
(7-4)-Dichloro[N-[2-(diphenylphosphino-κP)ethyl]-N-[2-(diphenylphosphino)ethyl]]...

物质检索--结构检索

结构检索类别：

- As Drawn

可用可变基团X或R基团等可变工具定义，其他位点默认为原子锁定，环系默认为环锁定

- 亚结构

包括As Drawn检索结果，及被检索结构的修饰结构。位点默认为开放，环系未被环锁定

- 相似结构

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

注：如果关注相似结构检索结果，请不要绘制通式结构

物质检索-检索结果集筛选: Reaction Role

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Structure Match

- As Drawn (0)
- Substructure (732)**
- Similarity (9)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

- Product (216)
- Reactant (53)
- Reagent (3)
- Catalyst (36)

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Filtering: Reaction Role: Catalyst X Clear All Filters

36 Results Sort: Relevance View: Partial

Item ID	Chemical Name	References	Reactions	Suppliers
1879110-74-3	C ₃₃ H ₃₉ Cl ₂ CoNP ₂ (7-4)-[N,N-Bis[2-(diphenylphosphino-κP)ethyl]-1-pentanamine]dichlorocobalt	1	2	0
2332371-33-0	C ₃₀ H ₃₃ Cl ₂ CoNP ₂ (7-4)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]-N-ethyl...	1	3	0
1879110-75-4	C ₃₁ H ₃₅ Cl ₂ CoNP ₂ (7-4)-[N,N-Bis[2-(diphenylphosphino-κP)ethyl]-2-propanamine]dichlorocobalt	1	2	0
1087216-22-5	C ₂₈ H ₂₉ Cl ₂ CoNP ₂ Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethanamine-κN...	8	105	0
2170923-58-5	C ₂₈ H ₂₉ Cl ₂ CoNP ₂ (7B-5-13)-Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]eth...	1	32	0
1846596-28-8	C ₂₈ H ₃₃ Cl ₂ CoNP ₂ (7B-5-13)-Dichloro[2-(dicyclohexylphosphino-κP)-N-[2-(dicyclohexylphosphino-κP)ethyl]eth...	7	13	0

利用物质在反应中的角色精准定位相应的物质

物质检索—检索结果集筛选：Reference Role

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.
Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

- Preparation (489)
- Synthetic Preparation (488)
- Properties (245)
- Reactant (98)
- Reactant or Reagent (98)
- Industrial Manufacture (9)

View All

Commercial Availability

- Not Available (9)

Filtering: Reference Role: Industrial Manufacture X Clear All Filters

9 Results

Sort: Relevance View: Partial

1

1087216-22-5

C28H29Cl2CoNP2
Dichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]ethanamine-κN...

8 References 105 Reactions 0 Suppliers

2

1395056-63-9

C28H29Cl3CoNP2.H
Components: 2
Component RN: 1395144-60-1
Cobaltate(1-), trichloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)ethyl]...

3 References 8 Reactions 0 Suppliers

3

579490-65-6

C40H37NNiP2
(SP-4-1)-Butyl[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzen...

6 References 20 Reactions 0 Suppliers

4

579490-58-7

C37H31NNiP2
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzenamina...

7 References 22 Reactions 0 Suppliers

5

579490-62-3

C38H33NNiP2
(SP-4-1)-[2-(Diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzenamina...

6 References 21 Reactions 0 Suppliers

6

579490-55-4

C36H28ClNNiP2
(SP-4-3)-Chloro[2-(diphenylphosphino-κP)-N-[2-(diphenylphosphino-κP)phenyl]benzene...

8 References 52 Reactions 0 Suppliers

Reference Role

By Count Alphanumeric

5 Selected

- Preparation (489)
- Synthetic Preparation (488)
- Properties (245)
- Reactant (98)
- Reactant or Reagent (98)
- Uses (88)
- Catalyst Use (77)
- Process (32)
- Physical, Engineering, or Chemical Process (31)
- Industrial Manufacture (9)
- Technical or Engineered Material Use (8)
- Formation, Non-preparative (6)
- Biological Study (4)
- Pharmacological Activity (4)
- Therapeutic Use (4)
- Analytical Reagent Use (1)
- Analytical Study (1)
- Formation, Unclassified (1)

Apply Cancel

利用Reference Role
(物质的研究方向)
精准定位相应的物质

物质检索—检索结果集筛选：结构

^ Search Within Results


Search for up to 3 structures within the result set.

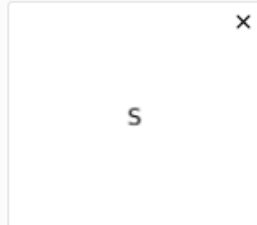
 Draw

Search

^ Search Within Results

Search for up to 3 structures within the result set.

 Edit






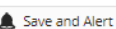
As Drawn

Substructure

Search

利用物质筛选工具
快速锁定目标物质

Substances search for drawn structure

References - Reactions - Suppliers -    

Structure Match

As Drawn (0)

Substructure (732)

Similarity (9)

Analyze Structure Precision

Chemscrape Analysis

Visually explore structure similarity with a powerful new tool.

[Learn more about Chemscrape.](#)

Create Chemscrape Analysis

Filter Behavior

Filter by Exclude

Reaction Role

Reference Role

Commercial Availability

Number of Components

Molecular Weight

Element

Substance Class

Isotopes

Metals





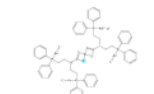

Experimental Property

Search Within Results

Search for up to 3 structures within the result set.

Filtering: Search Within Results: Drawn Structure X Clear All Filters

109 Results Sort: Relevance View: Partial

<p>1</p> <p>1698881-12-7</p>  <p>$C_{58}H_{52}N_2NiP_2S_4$ (SP-4-1)-Bis[<i>N,N</i>-bis[2-(diphenylphosphino)ethyl]carbomodithioato-κ₅,κ₅]nickel</p> <p>1 Reference 4 Reactions 0 Suppliers</p>	<p>2</p> <p>65120-45-8</p>  <p>$C_{34}H_{42}N_2NiP_2S$ Nickel(1+), [<i>N,N</i>-bis[2-(diphenylphosphino)ethyl]-<i>N,N</i>-diethyl-1,2-ethanediamine...</p> <p>0 References 0 Reactions 0 Suppliers</p>	<p>3</p> <p>65120-39-0</p>  <p>$C_{35}H_{45}N_2NiP_2S$ Nickel(1+), [<i>N,N</i>-bis[2-(diphenylphosphino)ethyl]-<i>N,N</i>-diethyl-1,2-ethanediamine...</p> <p>0 References 0 Reactions 0 Suppliers</p>
<p>4</p> <p>1698881-15-0</p>  <p>$C_{87}H_{84}CoN_3P_6S_6$ (OC-6-11)-Tris[<i>N,N</i>-bis[2-(diphenylphosphino)ethyl]carbomodithioato-κ₅,κ₅]cobalt</p> <p>1 Reference 3 Reactions 0 Suppliers</p>	<p>5</p> <p>1698881-21-8</p>  <p>$C_{58}H_{52}Au_4Cl_2N_2NiP_4S_4$ Bis[μ₂-[<i>N,N</i>-bis[2-(diphenylphosphino)ethyl]carbomodithioato-κ₅,κ₅]]tetrakis[...]</p> <p>1 Reference 4 Reactions 0 Suppliers</p>	<p>6</p> <p>65120-46-9</p>  <p>$C_{34}H_{43}N_2NiP_2S.ClO_4$ Components: 2 Nickel(1+), [<i>N,N</i>-bis[2-(diphenylphosphino)ethyl]-<i>N,N</i>-diethyl-1,2-ethanediamine...</p> <p>0 References 0 Reactions 0 Suppliers</p>

物质检索—检索结果集的保存

The screenshot displays the CAS search results page. On the left, there are navigation tabs for 'References', 'Reactions', and 'Suppliers'. Below these are filter options for 'Structure Match' (As Drawn, Substructure, Similarity), 'Chemscape Analysis', and 'Filter Behavior'. The main area shows a grid of search results, each with a chemical structure, a name, a formula, and counts for references, reactions, and suppliers. The results are sorted by 'Relevance' and shown in 'Partial' view. A 'Filtering' box at the top indicates 'Search Within Results: Drawn Structure'. A 'Save and Alert' button is visible in the top right corner of the main interface.

Result ID	Chemical Name	Formula	References	Reactions	Suppliers
1698881-12-7	Bis[<i>N,N</i> -bis[2-(diphenylphosphino)ethyl]carbamo...	$C_{68}H_{56}N_2NiP_4S_4$	1	4	0
65120-45-8	[<i>N,N</i> -bis[2-(diphenylphosphino)ethyl]- <i>N,N'</i> -diethyl-1,2-ethanediamine...	$C_{34}H_{43}N_2NiP_2S$	0	0	0
65120-39-0	Nickel(1+), [<i>N,N</i> -bis[2-(diphenylphosphino)ethyl]- <i>N,N'</i> -diethyl-1,2-ethanediamine...	$C_{35}H_{45}N_2NiP_2S$	0	0	0
1698881-15-0	(OC-6-11)-Tris[<i>N,N</i> -bis[2-(diphenylphosphino)ethyl]carbamo...	$C_{87}H_{84}CoN_3P_6S_6$	1	4	0
1698881-21-8	Bis[μ_3 -[<i>N,N</i> -bis[2-(diphenylphosphino)ethyl]carbamo...	$C_{58}H_{56}Au_4Cl_4N_2NiP_4S_4$	0	0	0
65120-46-9			0	0	0

获得文献信息

获得商品信息

获得反应信息

Save Results and Create Alert

Name: PNP-S

Save Options:
 Query Only
 Selected Answers
 All Answers (Up to 20,000)

Alert Frequency:
 No Alerts
 As Available
 Weekly
 Monthly

Add Existing Tags (Optional):
 catalyst
 Other fields
 Task
 Try

New Tag (Optional):
Tag Color:

Buttons: Save, Cancel

Download Substance Results

File Type: PDF

Select Quantity:
 All Results
 Selected Results
 Range (ex. 2 to 20)

Display:
 Structures Only
 Result Summary
 Result Details

File Name: Substance_20221121_1345


Include:
 Task History
 Substance Identifiers
 Experimental Spectra
 Predicted Spectra
 Regulatory Information
 Experimental Properties
 Predicted Properties
 Bioactivity Indicators
 Target Indicators

Buttons: Download, Cancel

[Learn more about downloads.](#)

CAS Markush检索

(19) 中华人民共和国国家知识产权局

 (12) 发明专利申请

(10) 申请公布号 CN 104945470 A
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38号 *A61P 35/02*(2006.01)
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A61P 37/02(2006.01)

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南小蓓

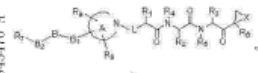
(74) 专利代理机构 杭州求是专利事务有限公司 33200
代理人 张法高 赵杭丽

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C07K 5/087(2006.01)
C07K 5/083(2006.01)

权利要求书3页 说明书24页 附图4页

(54) 发明名称
杂环构建的三肽环氧酮类化合物及制备和应用

(57) 摘要
本发明提供一种杂环构建的三肽环氧酮类化合物,以 Carfilzomib 为先导化合物,经缩合、酸性条件下脱去 Boc 保护基、碱性条件下反应得氨基酸甲酯异氰酸酯、水解、在缩合剂作用下获得。本发明是小分子短肽类蛋白酶抑制剂。本发明化合物具有极强的蛋白酶体抑制活性及细胞增殖抑制活性,是有前景的蛋白酶体抑制剂,为癌症治疗药物的研究提供了新的思路。本发明化合物的合成所需原料易得,路线设计合理,反应条件温和,各步产率高,操作简便,适合工业化生产。具有下述式 I 的结构通式:



CN 104945470 A

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

具体实施方式

[0026] 本发明结合附图和实施例作进一步的说明,以下实施例仅是说明本发明,而不是以任何方式限制本发明。

[0027] 制备实施例 1、4-(吡嗪-2-基氨基酰基)哌啶-1-甲酸叔丁酯(1a, 1b)

将 1-(叔丁氧羰基)哌啶-4-甲酸(2.75g, 12mmol)置于 50mL 三颈瓶中, N₂ 保护下加入 25mL 无水 CH₂Cl₂, 然后缓缓滴入吡啶(2.5mL, 30mmol)和二氯亚砷(1.1mL, 14mmol), 该反应液置于室温反应半小时。随后, 2-氨基吡嗪(0.95g, 10mmol)和三乙胺(5.7mL, 40mmol)溶于 15mL CH₂Cl₂ 后缓缓滴入上述反应液, 室温反应 6 小时。反应液加 30mL 饱和食盐水稀释, 分出有机层, 水层 CH₂Cl₂ 提取(15mL×3), 合并有机层, 无水硫酸钠干燥后减压除去溶剂, 柱层析分离得白色固体 2.3g, 收率 74%。m.p.: 134-136°C; ¹H NMR (500MHz, CDCl₃): δ = 9.55 (s, 1H, pyrazine-H), 8.35 (d, 1H, J=2.0Hz, pyrazine-H), 8.23 (s, 1H, pyrazine-H), 7.97 (s, 1H, NH), 4.20 (m, 2H, CH₂), 2.81 (m, 2H, CH₂), 2.48 (m, 1H, CH), 1.93 (d, 2H, J=12.5Hz, CH₂), 1.76 (m, 2H, CH₂), 1.47 (s, 9H, CH₃) ppm; ESI-MS: m/z = 307 [M+H]⁺。

[0028] 制备实施例 2、4-(吡嗪-2-酰基)哌啶-1-甲酸叔丁酯(1c, 1d)

吡嗪-2-羧酸(1.5g, 12mmol)置于 50mL 反应瓶中, 加入 35mL 无水 CH₂Cl₂ 溶解, 随即加入 1-羟基苯并三氮唑(1.6g, 12mmol)和 N-(3-二甲氨基丙基)-N'-乙基碳二亚胺盐酸盐(3.5g, 18mmol), 室温反应半小时。随后, 哌啶-1-甲酸叔丁酯(1.9g, 10mmol)加入反应液中, 室温反应 3 小时。反应液加入 30mL 饱和碳酸氢钠水溶液稀释, 分出有机层, 饱和食盐

CAS Markush检索

预测性物质[Prophetic Substance]:

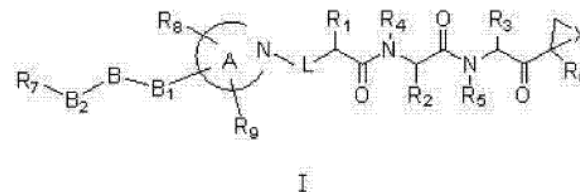
- 使用Markush结构陈述的预测物质，一个Markush可以陈述成百上千，甚至更多的结构
- 被Markush结构包含，但未被实施或呈现在表格、权利要求书或说明书中的结构，不会被CAS分配CAS Registry Number
- Markush检索，能检索到通过Substance可能检索不到的结构

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权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧酮类化合物，具有下述结构通式 I：



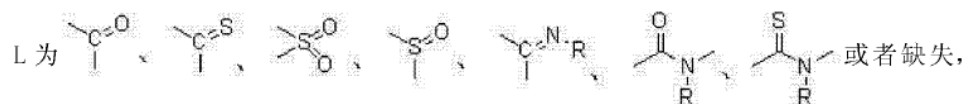
其中：

R_1, R_2, R_3 各自独立选自 H、 C_{1-6} 烷基 -D、卤代的 C_{1-6} 烷基 -D、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷氧基烷基、芳基、芳烷基、杂芳基或杂芳烷基；其中：D 为 $N(R_0)$ (R_0) 或缺失， R_0, R_0 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或 N 末端保护基；

R_4, R_5 各自独立选自 H、OH、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基或芳烷基；

R_6 选自 H、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 羟基烷基、 C_{1-6} 烷氧基、卤代的 C_{1-6} 烷氧基、 $C(O)O-C_{1-6}$ 烷基、 $C(O)NH-C_{1-6}$ 烷基、芳烷基；

X 为 O、S、NH、 $N-C_{1-6}$ 烷基或 N- 卤代的 C_{1-6} 烷基；



其中 R 选自 H、 C_{1-6} 烷基或卤代的 C_{1-6} 烷基；

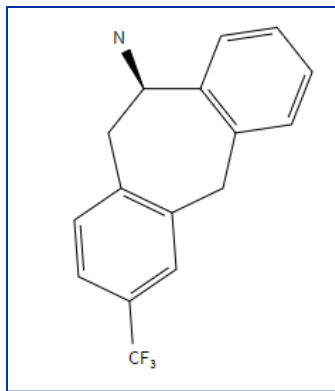
环 A 选自 5 ~ 7 元的饱和脂肪杂环、不饱和杂环、或者有取代的 5 ~ 7 元的饱和脂肪杂环、不饱和杂环，所述的杂环包含 0 ~ 3 个选自 O、N 和 S 的杂原子并任选地被 R_8, R_9 和 B_1 基团取代；

R_8, R_9 分别独立选自 H、OH、 C_{1-6} 烷基、 C_{1-6} 烷氧基、 C_{1-6} 羟基烷基、 C_{1-6} 巯基烷基、 C_{1-6} 烷基 -D、芳基、杂环芳基、环烷基和杂环基，这些基团可以被卤素、硝基、氨基、CN、 C_{1-6} 烷基、卤代的 C_{1-6} 烷基、 C_{1-6} 烷氧基或卤代的 C_{1-6} 烷氧基取代，每个基团可与一个或多个芳基或杂环

CAS Markush检索

第一步：物质结构检索

- As drawn结果为0
- Substructure结果为2
- Similarity相似度最高85-89%



Structure Match

As Drawn (0)

Substructure (2)

Similarity (5,664)

Chemscape Analysis

Visually explore structure similarity with a powerful new tool.

Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Similarity

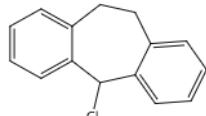
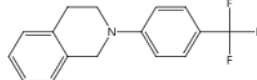
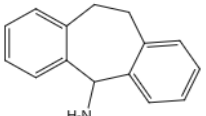
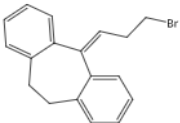
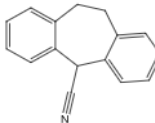
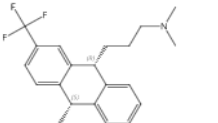
- 85-89 (1)
- 80-84 (2)
- 75-79 (20)
- 70-74 (140)
- 65-69 (958)
- 60-64 (4,211)

Reaction Role

Reference Role

Filtering: Number of Components: 1 X Clear All Filters

5,332 Results Sort: Number of References: Descending View: Partial

1	2	3
<p>1210-33-9</p>  <p>C₁₅H₁₃Cl 5-Chlorodibenzosuberene</p> <p>143 References 130 Reactions 61 Suppliers</p>	<p>1057277-76-5</p>  <p>C₁₆H₁₄F₃N 1,2,3,4-Tetrahydro-2-[4-(trifluoromethyl)phenyl]isoquinoline</p> <p>90 References 121 Reactions 2 Suppliers</p>	<p>7005-53-0</p>  <p>C₁₅H₁₅N IEM 2115</p> <p>58 References 78 Reactions 14 Suppliers</p>
4	5	6
<p>3436-04-2</p>  <p>C₁₈H₁₇Br 5-(3-Bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene</p>	<p>1729-63-1</p>  <p>C₁₆H₁₃N 10,11-Dihydro-5H-dibenzo[a,d]cycloheptene-5-carbonitrile</p>	<p>35764-73-9</p>  <p>C₂₁H₂₄F₃N Fluotracen</p> <p>Relative stereochemistry shown</p> <p>Feedback</p>

为了尽可能全面地获得公开的结构信息，需要同时进行Substance和Markush结构检索

CAS Markush检索

第二步：Markush结构检索
获得四件专利文献

直观呈现检索结构与专利原文
中Markush匹配部分的结构；
标引其在专利中出现的位置；
详细的结构取代信息描述。

The screenshot shows the CAS SciFinder interface for a Markush search. The search query is "Patent Markush search for drawn structure". The interface displays search filters, a list of results, and a table of patent options.

Patent Markush Match

- As Drawn (4)
- Substructure (33)

Filter Behavior

- Filter by
- Exclude

Patent Office

- World Intellectual Property Organization (3)
- European Patent Organization (1)

CA Section

- Agrochemical Bioregulators (1)
- Electric Phenomena (1)
- Heterocyclic Compounds (More Than One Hetero Atom) (1)
- Pharmacology (1)

Filter Content Report

Download filter data from this result set. [Download icon]

4 Results

1

WO2011025969

Compounds that treat malaria and prevent malaria transmission

By: Su, Xin-Zhuan; Yuan, Jing; Raj, Dipak; Pattaradilokrat, Sittiporn; Johnson, Ron; Huang, Ruili
World Intellectual Property Organization, WO2011025969 A1 2011-03-03 | Language: English, Database: CAplus
Assignee: United States Dept. of Health and Human Services

Patent claim 1

PatentPak | Full Text

Patent	Language	Kind Code	PatentPak Options
WO2011025969	English	A1	PDF PDF+ Viewer
CN102595894	Chinese	A	PDF
US20120196882	English	A1	PDF PDF+ Viewer
US9375424	English	B2	PDF
US20160303103	English	A1	PDF

2

EP502788

Patent claim 11

Full Text

There are no notes to display for this structure.

物质检索小结

1. 利用结构绘制工具合理扩大结构检索范围：R基团、可变基团、可变位置取代等
2. 利用结构绘制工具适当限定检索结构：环锁工具、原子锁工具、EZ构型限定等
3. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
4. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
5. 利用Structure Precision快速查找互变异构体/内盐
6. 利用CAS Markush检索尽可能全面的获得结构的公开信息

反应检索

- 反应检索方法
 - 结构式
 - 关键词
 - 物质名称、登记号
 - 文献标识符：专利号、收录号、DOI
- 常用获取方法推荐
 - 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

反应检索

Searching for...

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

Reactions

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

qinghaosu

X Draw Q

通过物质标识符、文献标识符进行检索

反应检索

CAS SciFinder® Reactions Semaglutide

Return to Home

Reactions search for "Semaglutide"

References - Save and Alert

Filter Behavior

- Filter by
- Exclude

Substance Role

- Product (222)
- Reactant (10)

Yield

- 90-100% (3)
- 80-89% (5)
- 70-79% (2)
- 50-69% (2)
- 10-29% (1)

View All

Number of Steps

Reaction Mapping

Experimental Protocols

- Synthetic Methods (11)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

228 Results Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (1 Reaction) Steps: 7

910463-68-2 Image Not Available Suppliers (28)

Suppliers (98) Suppliers (64)

Expand Scheme

Scheme 2 (5 Reactions) Steps: 5-7

910463-68-2 Image Not Available Suppliers (28)

Suppliers (79) Suppliers (37)

Expand Scheme

Scheme 3 (2 Reactions) Steps: 3-7

910463-68-2 Image Not Available Suppliers (28)

Suppliers (93) Suppliers (132)

CAS SciFinder® Reactions 175:621496

Return to Home

Reactions search for "175:621496"

References - Save and Alert

Filter Behavior

- Filter by
- Exclude

Yield

- 90-100% (3)
- 80-89% (5)
- 70-79% (2)
- 50-69% (3)
- No Yield Available (120)

Number of Steps

- 1 (25)
- 2 (29)
- 3 (27)
- 4 (21)
- 5 (16)
- 6-10 (15)

Non-Participating Functional Groups

- Amide (10)
- Carboxylic ester (10)
- Carboxylic acid (9)
- Ether (5)
- Amine (3)

View All

Reaction Mapping

Experimental Protocols

- Synthetic Methods (132)

Reaction Type

Stereochemistry

133 Results Group: By Scheme Sort: Number of Steps: Descending View: Collapsed

Scheme 1 (2 Reactions) Steps: 7-8

204656-20-2 Image Not Available Suppliers (37)

Suppliers (145) Suppliers (77)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 8

204656-20-2 Image Not Available Suppliers (37)

Suppliers (136)

Expand Scheme

Scheme 3 (1 Reaction) Steps: 7

204656-20-2 Image Not Available Suppliers (37)

Suppliers (32) Supplier (1)

Expand Scheme

反应检索

Searching for...

Reactions

通过结构式进行检索

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

Enter a query...

Draw

CAS Draw

Draw or change atoms or bonds.

Enter a CAS Registry Number, SMILES, or InChI...

X = Cl, Br

reactant

product

Molecular Formula: Formula is not available

C

Zoom: 100%

OK Cancel

C H
O S
N P
Cl Si
/ \
EZ
五 五
六 六
八 八

反应检索—结果集的分组与排序

Reactions search for drawn structure

References

Structure Match

As Drawn (32)

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (3)

Experimental Procedure (12)

Reaction Type

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Filtering: Reaction Mapping: Mapping Data Available

Clear All Filters

16 Results

Group: By Scheme

Sort: Yield

View: Collapsed

By Scheme

By Document

By Transformation

Relevance

Publication Date: Newest

Publication Date: Oldest

Yield

Number of Steps: Ascending

Number of Steps: Descending

Scheme 1 (5 Reactions)

Suppliers (85)

Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 76%

Suppliers (51)

Suppliers (3)

31-614-CAS-28968228 Steps: 1 Yield: 76%

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

1.1 Reagents: [O-Methylhydroxylamine hydrochloride](#)
Solvents: [Pyridine](#); rt; 1 h, 50 °C

1.2 Reagents: [\(7-4\)-Trihydro\(tetrahydrofuran\)boron](#)
Solvents: [Tetrahydrofuran](#); rt; 3 h, reflux; reflux → 0 °C

1.3 Reagents: [Sodium hydroxide](#)
Solvents: [Water](#); overnight, reflux; reflux → rt

By: Heidelbaugh, Todd M.; et al
World Intellectual Property Organization, WO2009091874 A1
2009-07-23

PatentPak Full Text

Experimental Protocols

反应分组Group:
按类型分组
按文献分组
按单步反应转化类型

反应排序Sort:
相关度
公布时间
产率
步数

反应检索—结果集筛选

As Drawn反应检索
亚结构反应检索
相似反应检索

反应筛选类别：
产率、反应步数
不参与反应的官能团
实验步骤
反应类型、立体化学
试剂、催化剂、溶剂
商业来源……

文献筛选类别：
文献类型、语言
出版年份、刊物名

The screenshot displays a search interface for chemical reactions. On the left is a sidebar with filter options: Structure Match (As Drawn (32), Substructure (8,521), Similarity (0)), Filter Behavior (Filter by, Exclude), and various filter categories like Yield, Number of Steps, Reaction Mapping, etc. The main area shows 8,521 results grouped by transformation. Four reaction types are visible: 1. Acylation of Nitrogen Nucleophiles by Carboxylic Acids; 2. Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters; 3. Acylation of Nitrogen Nucleophiles by Acyl/ Thioacyl/ Carbamoyl Halides and Analogs; 4. Formation of N/O/S Heterocycles. Each reaction is accompanied by a chemical equation diagram.

折叠菜单显示：

相同反应类型的反应放在一个菜单里，方便阅读和筛选

反应检索—结果集筛选：不参与反应官能团

Reactions search for drawn structure

References

Structure Match

- As Drawn (32)
- Substructure (8,521)
- Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

- Halide (290)
- Phenyl halide (286)
- Carboximidine (109)
- Alkene (84)
- Cyclic alkene (80)
- [View All](#)

Reaction Mapping

Experimental Protocols

Reaction Type

Stereochemistry

Filtering: Non-Participating Functional Groups: Halide X Clear All Filters

290 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 100%

Suppliers (107)

Expand Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 100%

Expand Scheme

Scheme 3 (1 Reaction) Steps: 1 Yield: 100%

Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

<input checked="" type="checkbox"/> Halide (282)	<input type="checkbox"/> Diene (45)	<input type="checkbox"/> Acetal (3)
<input type="checkbox"/> Phenyl halide (278)	<input type="checkbox"/> Ether (40)	<input type="checkbox"/> Acyclic alkene (3)
<input type="checkbox"/> Carboximidine (101)	<input type="checkbox"/> Cyclic ketone (29)	<input type="checkbox"/> Carbamate (3)
<input type="checkbox"/> Alkene (84)	<input type="checkbox"/> Urea (16)	<input type="checkbox"/> Carboxylic acid (3)
<input type="checkbox"/> Cyclic alkene (80)	<input type="checkbox"/> Tertiary amine (9)	<input type="checkbox"/> Alcohol (2)
<input type="checkbox"/> Amide (69)	<input type="checkbox"/> Imine (8)	<input type="checkbox"/> Primary alcohol (2)
<input type="checkbox"/> Amine (59)	<input type="checkbox"/> Thiocarbonyl (7)	<input type="checkbox"/> Unsaturated ester (2)
<input type="checkbox"/> Carboxylic ester (53)	<input type="checkbox"/> Acyclic ketone (5)	<input type="checkbox"/> Nitro (1)
<input type="checkbox"/> Secondary amine (50)	<input type="checkbox"/> Alkyl halide (4)	<input type="checkbox"/> Primary amine (1)
<input type="checkbox"/> Ketone (48)	<input type="checkbox"/> Nitrile (4)	<input type="checkbox"/> Unsaturated ketone (1)

Apply Cancel

不参与反应官能团：
出现在反应前后，但未发生变化的官能团

反应检索—结果集筛选: Synthetic Methods™

Structure Match

As Drawn (32)

Substructure (8,521)

Similarity (0)

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

Synthetic Methods (40)

Experimental Procedure (83)

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

Commercial Availability

Reaction Notes

Search Within Results

Source Reference

Filtering: Non-Participating Functional Groups: Halide X Clear All Filters

Experimental Protocols: Synthetic Methods X

40 Results Group: By Scheme Sort: Relevance View: Collapsed

Scheme 1 (1 Reaction) Steps: 1 Yield: 98%

Suppliers (15) Suppliers (89)

31-614-CAS-24450288 Steps: 1 Yield: 98%

1.1 Reagents: [Hydrochloric acid](#), [Titanium chloride \(TiCl₃\)](#)
Solvents: [Methanol](#), [Tetrahydrofuran](#), [Water](#); rt; 30 min; rt; 2 h, 30 - 50 °C

1.2 Reagents: [Water](#)

DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [¹⁸F]Talazoparib and its In Vivo Evaluation as a PARP Radiotracer

By: [Bowden, Gregory D.](#); et al
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701

Experimental Protocols Full Text

Collapse Scheme

Scheme 2 (1 Reaction) Steps: 1 Yield: 96%

Suppliers (9) Suppliers (97) Suppliers (91)

反应检索—结果集筛选: Synthetic Methods™

CAS Reaction Number: 31-614-CAS-24450288

Suppliers (15) Suppliers (89) 98%

Reaction Overview
Steps: 1 Yield: 98%

JOURNAL
DoE Optimization Empowers the Automated Preparation of Enantiomerically Pure [¹⁸F]Talazo parib and its In Vivo Evaluation as a PARP Radiotracer
By: Bowden, Gregory D.; et al
Journal of Medicinal Chemistry (2021), 64(21), 15690-15701
View PDF Full Text

Company/Organization
Werner Siemens Imaging Center, Department of Preclinical Imaging and Radiopharmacy
Eberhard Karls University Tuebingen 72076 Germany

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Hydrochloric acid Titanium chloride (TiCl ₃)	-	Methanol Tetrahydrofuran Water	rt; 30 min, rt; 2 h, 30 - 50 °C
2	Water	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

Products	Methyl 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-5-quinolinecarboxylate Yield: 98%
Reactants	4-Bromobenzaldehyde Benzoic acid, 5-fluoro-2-[2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl]-3-nitro-, methyl ester
Reagents	Hydrochloric acid Titanium chloride (TiCl ₃) Water

查看文献详情

Procedure

1. Suspend methyl 5-Fluoro-2-(2-(1-methyl-1H-1,2,4-triazol-5-yl)acetyl)-3-nitrobenzoate (8.1 g, 25.2 mmol) and 4-bromobenzaldehyde (8.9 g, 50.5 mmol) in THF (50 mL) and MeOH (10 mL).
2. Add titanium(III) chloride solution [20% wt solution in HCl (2 M), 130 mL, 6 equiv] to the resulting mixture in dropwise fashion over 30 minutes at room temperature.
3. Maintain the reaction temperature between 30 and 50°C for 2 hours.
4. Quench the mixture by the slow addition of water (260 mL).
5. Pour the reaction mixture into a separating funnel.
6. Extract the mixture with ethyl acetate (4 x 140 mL).
7. Pool the organic fractions.
8. Wash the organic fractions with NaHCO₃ (3 x 60 mL) and NaHSO₃ (3 x 100 mL).
9. Dry the organic fractions with sodium sulfate (Na₂SO₄).
10. Concentrate the solvent under reduced pressure to obtain a thick yellow syrup.
11. Wash the residue with aliquots of diethyl ether (3 x 10 mL), carefully.
12. Dry the resulting yellow syrup under high vacuum to obtain product.

Transformation
Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/
Knoevenagel Reaction
Reduction of Nitro Compounds to Amines

Scale gram

Characterization Data

5-Quinolinecarboxylic acid, 2-(4-bromophenyl)-7-fluoro-1,2,3,4-tetrahydro-3-(1-methyl-1H-1,2,4-triazol-5-yl)-4-oxo-, methyl ester

State yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

Transformations

1. Mannich Reaction/ Mannich-Type Reactions/ Biginelli Condensation
2. Condensation Reaction between Compounds with Active Hydrogen and Aldehydes or Ketones/
Knoevenagel Reaction
3. Reduction of Nitro Compounds to Amines

Synthetic Methods™:
分类显示详尽信息, 方便操作

联合检索—结构与关键词

Searching for...
References

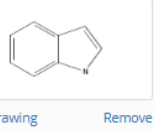
Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. [Learn More](#)

Friedel-crafts acylation

AND Author Name Enter last name, first name middle name.

+ Add Advanced Search Field [Learn more about Sci](#)

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



Reactions for AN 2011:601374

References

Filter Behavior: Filter by Exclude

Yield: 80-89% (1), 70-79% (8), 50-69% (12)

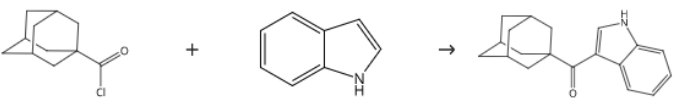
Number of Steps: 1 (21)

Non-Participating Functional Groups: Alkene (21), Amine (21), Cyclic alkene (21), Secondary amine (14), Tertiary amine (7)

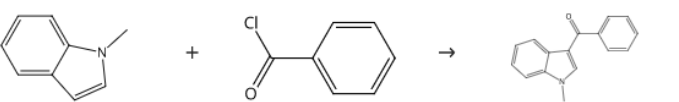
Reaction Mapping

21 Results

Scheme 1 (1 Reaction) Steps: 1 Yield: 82%



Scheme 2 (1 Reaction) Steps: 1 Yield: 78%



References search for "Friedel-crafts acylation" + drawn structure

Substances Reactions Citing Knowledge Graph

Structure Match: As Drawn (1,100), Substructure (2,270)

Filter Behavior: Filter by Exclude

Document Type: Journal (996), Patent (68), Review (31), Conference (27), Dissertation (1), Preprint (8)

Substance Role: Reactant or Reagent (1,067), Process (34), Properties (29)

1,100 Results

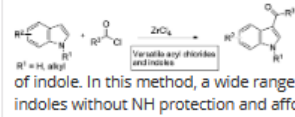
Sort: Relevance View: Partial Abstract

1

ZrCl₄-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole

By: Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad

Journal of Organic Chemistry (2011), 76(11), 4753-4758 | Language: English, Database: CAplus and MEDLINE



An efficient method for regio- and chemoselective Friedel-Crafts acylation of indoles using acyl chlorides in the presence of ZrCl₄ has been discovered. It minimizes/eliminates common competing reactions that occur due to high and multiatom-nucleophilic character of indole. In this method, a wide range of aroyl, heteroaroyl, alkenoyl, and alkanoyl chlorides undergo smooth acylation with various indoles without NH protection and afford 3-acylindoles in good to high yields.

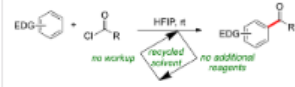
Full Text Substances (40) Reactions (21) Citing (99) Citation Map

2

Hexafluoro-2-propanol-Promoted Intermolecular Friedel-Crafts Acylation Reaction

By: Vekariya, Rakesh H.; Aube, Jeffrey

Organic Letters (2016), 18(15), 3534-3537 | Language: English, Database: CAplus and MEDLINE



The intermol. Friedel-Crafts acylation was carried out in hexafluoro-2-propanol to yield aryl and heteroaryl ketones at room temperature without any addnl. reagents.

Full Text Substances (50) Reactions (24) Citing (82) Citation Map

联合检索提高了检索速度

反应检索小结

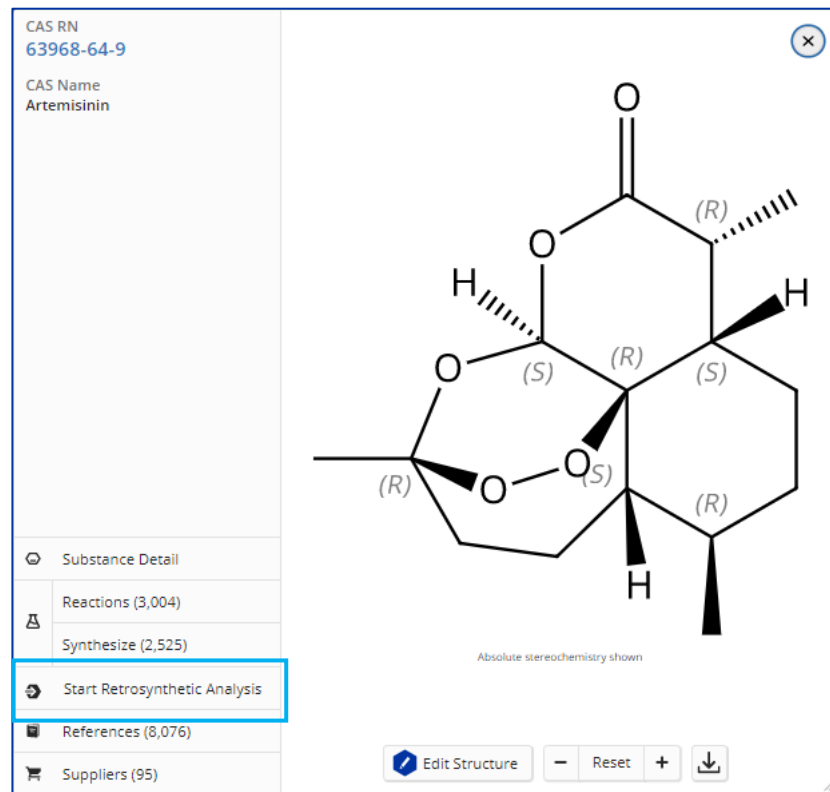
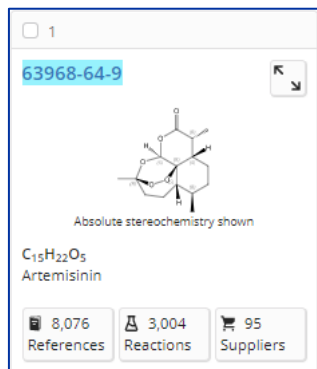
1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. 利用Synthetic Methods™查看文献中合成方法详情
4. 关键词与反应式的联合检索

大纲

- CAS Retrosynthesis Tool的使用
 - 获得已知化合物的逆合成反应路线
 - 获得未知化合物的逆合成反应路线



CAS Retrosynthesis Tool--由物质获得

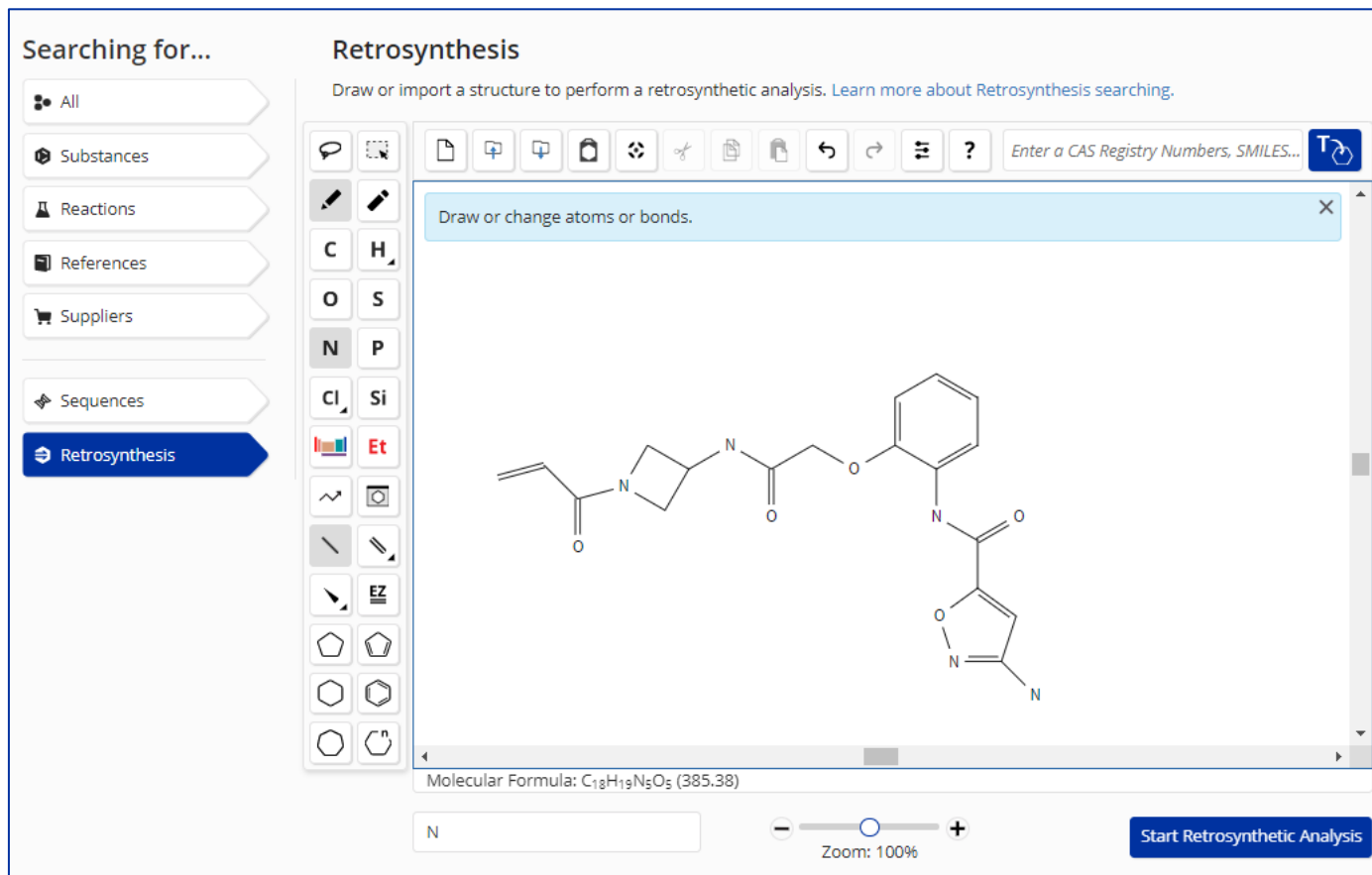


从已知化合物获得逆合成路线：

点击物质结构，弹出的物质菜单中点击Create Retrosynthesis

CAS Retrosynthesis Tool：
逆合成反应路线设计功能，
启发合成实验设计思路高效
获取逆合成反应路线

CAS Retrosynthesis Tool—直接绘制



绘制目标化合物：


从Retrosynthesis检索项打开绘图板，绘制目标化合物，获得实验路线

CAS Retrosynthesis Tool—预设参数

Retrosynthesis Plan Options for drawn structure Powered by ChemPlanner®

Select Synthetic Depth [Learn more.](#)

1 2 3 4



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

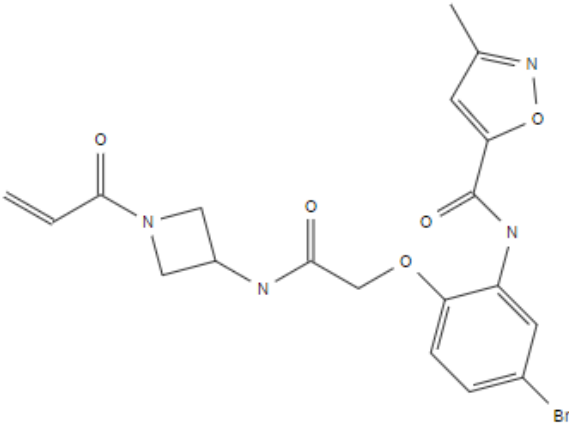
Common
 Uncommon (includes Common Rules)
 Rare (includes Common and Uncommon Rules)

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

1000

Email me when my plan is complete

Break and Protect Bonds [Learn more.](#)



预设反应路线参数：
反应深度
反应规则常见性
起始原料费用
设置断裂键或保护键

CAS Retrosynthesis Tool—路线概览

路线概览

重设参数

Retrosynthesis

Powered by ChemPlanner®

Predicted Results

Overview Steps

Plan Information

Estimated Yield: 15%
Overall Price: \$375.68
(USD per 100 grams)

Commercially Available:
B, C, D, F, G, H, I

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$1,000.00/mol

Scoring Profiles

Complexity Reduction

Convergence

Evidence

Cost

Yield

Atom Efficiency

Apply Reset Scoring

Retrosynthesis Step Key

Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

Experimental Steps

Predicted Steps

已报道的逆合成路线
预测的逆合成路线

Scoring Profiles: 每项有4个设置 (off, low, medium, high)

- Complexity Reduction: 可调整每一步原料结构的复杂性
- Convergence: 可调整逆合成路线中前体的数量
- Evidence: 表示预测路线支持的文献数量多少
- Cost: 表示预测路线大概的成本
- Yield: 表示每一步的产率
- Atom Efficiency: 表示每一步的原子转化效率

CAS Retrosynthesis Tool—路线详情

The screenshot displays the CAS Retrosynthesis Tool interface. At the top, it is titled "Retrosynthesis" and "Powered by ChemPlanner". The main area shows a retrosynthetic plan with steps A through H. Step A is highlighted with a blue box, and a blue arrow points from it to a detailed view of the reaction. The detailed view shows the reaction of three starting materials to form a product, with reagents, solvents, and conditions listed. The interface also includes a sidebar with "Overview" and "Steps" tabs, and a "Retrosynthesis Step Key" at the bottom left.

Overview Steps

View step specific evidence and alternate steps below or select the node between steps on the plan.

A ⇒ B + C + D

Average Yield: 37%

Evidence (1,181)

Alternative Steps (85)

B ⇒ E

Maximum Yield: 80%

Evidence (180,876)

Alternative Steps (20)

C ⇒ F + G

Maximum Yield: -

Evidence (1)

Alternative Steps (15)

E ⇒ H + I

Maximum Yield: -

Evidence (1)

Alternative Steps (24)

Click Evidence to view the specific synthesis conditions and literature for this step.

Retrosynthesis Step Key

Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

⇒ Experimental Steps

⇨ Predicted Steps

Reactions (1,181)

Group: By Scheme View: Expanded

Scheme 1 (1 Reaction) Steps: 1

Reaction Summary

Steps: 1

1.1 Reagents: 1-Ethyl-3-(3'-dimethylamino)propylcarbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine
Solvents: Dichloromethane; overnight, rt

1.2 Reagents: Zinc
Solvents: Acetic acid; 30 min, rt

1.3 Reagents: 4-Methylmorpholine, O-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate
Solvents: Dimethylformamide; 16 h, rt

Preparation of N-(heteroarylcarbonyl)amino acid amide compounds useful as matrix metalloproteinase 13 (MMP-13) inhibitors

By: Farrow, Neil Alexander; et al
World Intellectual Property Organization, WO2010056585 A2
2010-05-20

PatentPak Full Text

- 快速获取最优的逆合成路线
- 可查看每步路线的详细条件
- 可自定义选择替代路线
- 可获取预测逆合成路线

CAS Retrosynthesis Tool—路线详情

The screenshot displays the CAS Retrosynthesis Tool interface. On the left, a sidebar shows the overall retrosynthetic plan with steps A through I. The main window is titled "Retrosynthesis" and shows "A ⇒ B + C + D Alternative Steps (53)". It lists four alternative steps, each with a chemical reaction scheme, a "Predicted Step" label, and a "View Evidence" button. The first alternative step shows a reaction with an average yield of 40%. The second alternative step shows a reaction with an average yield of 63%. The third alternative step shows a reaction with an average yield of 63%. The fourth alternative step shows a reaction with an average yield of 63%. On the right, a retrosynthetic map shows the target molecule (A) and its precursors (B, C, D, E, F, G, H, I, J, K, L) connected by arrows. The map includes yield information for each step and a "Retrosynthesis Step Key" at the bottom.

Overview Steps

View step specific evidence and alternate steps below or select the node between steps on the plan.

A ⇒ B + C + D
Average Yield: 37%
Evidence (1,181)
Alternative Steps (85)

B ⇒ E
Maximum Yield: 80%
Evidence (180,876)
Alternative Steps (20)

C ⇒ F + G
Maximum Yield: -
Evidence (1)
Alternative Steps (15)

E ⇒ H + I
Maximum Yield: -
Evidence (1)
Alternative Steps (24)

Retrosynthesis

Hover on the experiment or predicted step to view this plan. View Evidence

Retrosynthesis Step Key
Hover on the options below to highlight experimental and predicted steps within this plan. View Steps Menu.

Experimental Steps

点击Alternative Steps查看并选择替换路线，
得到自定义的合成路线

逆合成路线小结

1. 通过物质结构获取已知化合物的逆合成路线
2. 获取预测的逆合成路线
3. 反应路线参数的预先设定与调节
4. 查看反应路线详情和文献支持，自定义选择替代路线

大纲

- CAS SciFinderⁿ中的序列检索
 - BLAST
 - CDR
 - Motif

视频链接:

https://american-chemical-society.zoom.us/rec/share/JPoebb74K7-dbzGw2Aj8vRqqeddGB5zzBnQTV8MYcW2E2QQqq2rkYWoBtkHy_tt2.ag1fUmL880MKBne3?startTime=1647943207000

[下一节：分析实验方法](#)



Sequences Search™ — Blast检索

Searching for...

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

Sequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

Enter a query or upload a file...

Sequence Type:
Nucleotide Protein

Search Within:
 Nucleotides Proteins

Include NCBI Sequences

Start Sequence Search

Advanced Sequence Search

可选择是否包含NCBI中的序列

支持四种检索选择：
Protein-Protein
Protein-Nucleotides
Nucleotide-Nucleotides
Nucleotide-Proteins

高级检索—设置相关参数

Sequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA

Sequence Type:
 Nucleotide Protein

Search Within:
 Nucleotides Proteins
 Include NCBI Sequences

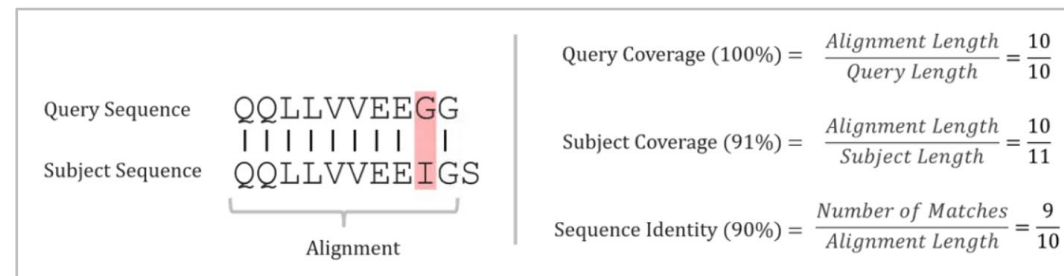
[Start Sequence Search](#)

Advanced Sequence Search Adjust Parameters for Short Sequences | Reset All

Alignment Identity % Match with Gaps? Yes No Gap Costs

Query Coverage % Word Size Reward for Match Penalty for Mismatch

BLAST Algorithm E-Value Exclude Low Complexity Regions Yes No



Recent Search History

[View All Search History](#)

February 13, 2023

Sequences 11:26 AM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA	View Results Edit Options Searching...
-----------------------	--	--	--

Results will expire on Mar 15, 2023.

Recent Search History

[View All Search History](#)

February 13, 2023

Sequences 11:26 AM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA	View Results Edit Search Complete
-----------------------	--	--	---

Results will expire on Mar 15, 2023.

BLAST检索结果

- 序列一致性详情
- 目标序列
- 披露序列的专利文献
- 可视化地图
- 结果筛选

Sequences search for your query

References

BLAST Search Details

Sequence Type: Nucleotide
Search Within: Nucleotides
BLAST Algorithm: BLASTn
NCBI Included: Yes
Alignment Identity: 80%
Query Coverage: 90%
E-Value: 10
Match with Gaps?: No
Gap Costs: Existence 5
Extension 2
Word Size: 11

Bioscape Analysis

Visually explore sequence similarity with a new tool.
Learn more about Bioscape.

Create Bioscape Analysis

Filter by

▼ E-Value

▲ Query Coverage %

0 to 100

▲ Subject Coverage %

0 to 100

▲ Alignment Identity %

0 to 100

▲ Sequence Length

Query Details AACAAACAATATCAAATCCTACTGGTGGCACAACCTTGA View More **序列结果排序**

Sort: Alignment Identity View: Expanded

170 Results

1 Alignment Identity: 100%

Query 1 39

Subject 1 595

Matches: 39
Mismatches: 0

View Less

Alignment Subject References

Alignment Data

BLAST Score: 78
E-Value: 7.79462e-12

Q 1 AACAAACA TATCAAATCC TACTGGTGGC ACAACTTGA 39
S 393 AACAAACA TATCAAATCC TACTGGTGGC ACAACTTGA 431

2 Alignment Identity: 100%

Query 1 39

Subject 1 813

Matches: 39
Mismatches: 0

View Less

Alignment Subject References

CAS Registry Number: 325380-52-7
NCBI Identifier: BG319743
Length: 813 nt
Organisms: Zea mays

Sequence

1 AAGAACAAA AGGATCAGCA GCCAGAGATG AGATGTAAGG TACTGATCCC CCATGCGCTT AGCTTAGCTT AACCCATGCC
81 CTAACATCTC GTACCCATAG CATAACAGGA ACACGGCAGGC AACTACTACA ACAACAAGGA CACCAGCAGC AAATTGTCTG
161 TCACGTCACG TACTAGAAAG AACAAACA TATCAAATCC TACTGGTGGC ACAACTTGAC AGAGGGTCTA GAACGAGCTA

Download Sequence Results

File Type

Excel (.xlsx)
 FASTA (.fasta)

Select Quantity

All Results
 Range (ex. 2 to 20)

File Name

Sequences_20230213_1132

Download Cancel Learn more about downloads.

下载结果:

- 比对详情
- 序列长度参数
- 相关专利号
- 专利中的序列编号等
(Excel或FASTA格式)

BLAST检索结果

6 Alignment Identity: 100%

Query 1 39

Subject 1 1,060

Matches: 39
Mismatches: 0

View Less ▾

Alignment Subject References

CAS Registry Number: **785872-37-9**
Length: 1,060 nt

Sequence

```

1  CATTGGGTAC CTCGAGGCCG GCCGGGAGCT CGCACTCACT CACTCACAAG TCACACAGCC AACTTGAAC CGTGCCCGC
81  AGCGGAGGGA GCTTGACGG GCCAACGCAC ACATAACACA AGTCGTCGT CGATGGCGCG GTGGCTGCG GTGCTGGCGC
161 TGGCCGCGGC CACGGCCATC GCCGTGGCGT CCGTGGCGGG CGGCGACATG AACCGGACA AGACGGAGTG CGCGGACCAG
241 CTGTGGGCC TGGCCCGTG CCTGCAGTAC GTGCAGGGG AGGCCCGCG GCCCGGCC GACTGTGCG GCGGCCTGCG
321 CCAGTGCTG GGAAGAGCC CCAAGTGCCT GTGCGTGCTC GTCAAGGACA AGGACGACCC CAACCTGGGC ATCAAGATCA
    
```

Alignment Subject References

Nucleic acid molecules and other molecules associated with plants
Assignees: LA ROSA, THOMAS J.; ZHOU, YIHUA; KOVALIC, DAVID K.; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS G.; HARDEMAN, KRISTINE J.; EDGERTON, MICHAEL D.; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY W.
US20120216318 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants
Assignees: LA ROSA, THOMAS; ZHOU, YIHUA; KOVALIC, DAVID; CAO, YONGWEI; LIU, JINGDONG; CHEIKH, NORDINE; SHUKLA, HRIDAYABHIRANJAN; RUFF, THOMAS; HARDEMAN, KRISTINE; EDGERTON, MICHAEL; VARAGONA, MARGUERITE; WU, WEI; CONNER, TIMOTHY
US20040214272 A1 | Seq ID No: 16999

Nucleic acid molecules and other molecules associated with plants

Substance Detail

Reference (1) Reactions (0) Suppliers (0)

CAS Registry Number
785872-37-9

Image Not Available

Unspecified
DNA (Zea mays clone MRT4577_11549C.1 protein fragment-specifying cDNA) (9CI)

Nucleic Acid Sequence
Sequence Length: 1060
204 a, 336 c, 311 g, 209 t

Other Names and Synonyms

1 Other Name for this Substance
1999: PN: US20040214272

Sequence Details

Sequence: DNA: linear

1	cattgggtac	ctcgagbccg	gccgggagct	cgcaactca	cactcacaag
51	tcacacagcc	aaccttgaac	cgctgcccgc	agcggagggg	gcttgacggg
101	gccaacgcac	acataacaca	agctcgtcgt	cgatggcgcg	gtggctgctg
151	gtgctggcgc	tggccgcgcc	cacggccatc	gccgtggcgt	ccgtggcggg
201	cgcgacatg	aacgcggaca	agacggagtg	cgcgaccag	ctgatggccc
251	tggcgccgtg	cctgcagtac	gtcaggggc	agcccgcgc	gcccgcgcc
301	gactgctgcg	gcggcctcgc	ccaggtcctg	gggaagacc	ccaagtgcct
351	gtcgtgctc	gtcaaggaca	aggacgacc	caacctggc	atcaagatca
401	agccaccct	cgctcgcgc	ctcccaacg	cctggggcg	caccgcgcc
451	aacgtctccc	actgcgtcca	gctcctgat	atcccccgg	gctccaaaga
501	cgccgcgctc	ttcagtcggc	gcagcgaaa	gggtccact	gctcctcag
551	ccaaggacaa	ctcagcgccg	acgaccgact	cccgcgctc	gcaggcgacc
601	accggacgcg	gctgtccttc	ctcggcgcg	accggggtg	ctgcaactca

Patent Annotations

Source: Zea mays
Reference: US20040214272. SEQID 16999: claimed

Feature	Location	Description
misc_feature		Clone ID: MRT4577_1154C.1

序列详情及相关的专利文献结果

References from your sequence

Substances Reactions Citing Knowledge Graph

Filter Behavior 38 Results Sort: Publication Date: Newest View: Full Abstract

1

Expressing Arabidopsis thaliana genes in plants for low low-nitrogen tolerance
By: Nadzan, Gregory; Schneeberger, Richard; Kim, Han Suk; Dang, David Van-Dinh; Feldmann, Kenneth A.; Pennell, Roger; Kwok, Shing; Zhang, Hongyu; Christensen, Cory; Okamura, Jack; et al
United States, US10815494 B2 2020-10-27 | Language: English, Database: CAplus

Methods and materials for modulating low-nitrogen tolerance levels in plants are disclosed. For example, nucleic acids encoding low nitrogen tolerance-modulating polypeptides are disclosed as well as methods for using such nucleic acids to transform plant cells. Also disclosed are plants having increased_{RLCL21} low-nitrogen tolerance levels and plant products produced from plants having increased low-nitrogen tolerance levels.

PatentPak Full Text Substance (1) Reactions (0) Citing (0) Citation Map

2

Functionally-defined, sequence-determined DNA fragments and their use in genetic engineering of plants
By: Alexandrov, Nickolai; Brover, Vyacheslav; Feldmann, Kenneth A.; Makarov, Vladimir; Swaller, Timothy J.; Nadzan, Gregory; Mascia, Peter; Troukhan, Maxim; Rarang, Joel; Burns, James; et al
United States, US20170037422 A1 2017-02-09 | Language: English, Database: CAplus

Libraries of plant genomic fragments that are functionally-defined and sequenced, included identification of open reading frames and gene products, are described for use in plant improvement. Members of the library contain extensive and 5'- and 3'-UTRs that will allow expression in a plant host. The DNA mols. are useful for specifying a gene product in cells, either as a promoter or as a protein coding sequence or as an UTR or as a 3' termination sequence, and are also useful in controlling the behavior of a gene in the chromosome, in controlling the expression of a gene or as tools for genetic mapping, recognizing or isolating identical or related DNA fragments, or identification of a particular individual organism, or for clustering of a group of organisms with a common trait.

PatentPak Full Text Substance (1) Reactions (0) Citing (0) Citation Map

Patent	Language	Kind Code	PatentPak Options
US20170037422	English	A1	PDF PDF+ Viewer
US20060107345	English	A1	PDF
US20120159672	English	A1	PDF
US20060150283	English	A1	PDF
US20060048240	English	A1	PDF
US20060168696	English	A1	PDF PDF+ Viewer

low nitrogen tolerance levels in plants
h; Feldmann, Kenneth A.; Pennell, Roger; Kwok,
plus
r example, nucleic acids encoding low nitrogen
ch nucleic acids to transform plant cells. Also
edute produced from plants having increased low-

Sequences Search™—Motif检索

Motif中有可变部分，可借助符号来表示：

“[]” 中括号：代表或者，表示出现在该位置的氨基酸或核苷酸是括号中的任意一个

“{ }” 大括号：代表氨基酸或核苷酸的重复次数。其中字段可用逗号开，{2, 6} 表示在大括号左边紧密相连的氨基酸可重复2-6次

Searching for...

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- Sequences**
- Retrosynthesis

Sequences

Enter a protein or nucleotide string. [Learn more about Sequence Search.](#)

BLAST CDR **Motif** [Clear Search](#)

[SG]x{4}GK[DT]

- X代表未指定氨基酸，可以是常见氨基酸、不常见氨基酸
- 对于核苷酸序列：N代表未指定核苷酸

[Advanced Sequence Search](#) [Reset All](#)

Query Coverage % E-Value Combine Motif Results

Sequence Type:

Include NCBI Sequences

Motif检索结果

Motif Search Details

Sequence Type: Protein
NCBI Included: Yes
Query Coverage: 90%
E-Value: 10

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Filter by

E-Value

Query Coverage %

Subject Coverage %

0 to 100

Alignment Identity %

0 to 100

Sequence Length

8 to 2060

Organisms

Homo sapiens (248)

synthetic construct (23)

unidentified (2)

Mus musculus (1)

Query Details [View More](#)

> Seq 1: 1 SXXXXGKD 8

248 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 75%

Query 1 8

Subject 1 114

Matches: 6
Mismatches: 2

[View Less](#)

Alignment Subject References

Alignment Data
BLAST Score: 77
E-Value: 0.00104148

```
Q 1 SXXXXGKD 8
   |||||++|
S 94 SXXXXXD 101
```

2 Alignment Identity: 75%

Query 1 8

Subject 1 643

Matches: 6
Mismatches: 2

[View Less](#)

Alignment Subject References

CAS Registry Number: -
Length: 643 aa
Organisms: Homo sapiens
Sequence

```
1 MEKSSSCESL GSQPAARPP SVDSLSSAST SHSENSVHTK SASVVSSDSI STSADNFSPD LRVLRNSNKL AEMEEPPLLP
```

Sequences Search™—CDR检索

CDR (complementarity—determining regions): 抗体或细胞中的互补决定区

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- Sequences**
- Retrosynthesis

Sequences

Enter a protein string, or upload a .txt or .fasta file. [Learn more about Sequence Search.](#)

BLAST **CDR** Motif [Clear Search](#)

CDR1	<input type="text" value="RASQSVSGSRFTYMH"/>	<input type="button" value="x"/>
CDR2	<input type="text" value="YASILES"/>	<input type="button" value="x"/>
CDR3	<input type="text" value="QHSWEIPPWT"/>	<input type="button" value="x"/>

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CDR检索结果

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References

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Select a segment below to view individual or intersecting CDR results.

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Filter by

E-Value

0 to 10⁶

Query Coverage %

0 to 100

Subject Coverage %

Query Details [View Less](#)

> CDR1
RASQSVSGSRFTYMH

> CDR2
YASILES

> CDR3
QHSWEIPPWT

21,934 Results Sort: Alignment Identity View: Expanded

Alignment Identity: 100%

Matches: 32
Mismatches: 0

View Less

Alignment Subject References

Alignment Data
BLAST Score: 84
E-Value: 7.45568461509489

CDR1	1	RASQSVSGSR	FTYMH	15
S	24	RASQSVSGSR	FTYMH	38
CDR2	1	YASILES		7
S	54	YASILES		60
CDR3	1	QHSWEIPPWT		10
S	93	QHSWEIPPWT		102

References

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CDR Segments:

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- 可根据已知信息和需求查看1-3个CDR被包含的序列结果

Reset segments:

- 重新选择查看匹配的序列结果

序列检索小结

- Sequences涵盖期刊、专利、NCBI当中的序列信息
- Sequences可以针对DNA/RNA的核苷酸序列、肽/蛋白的氨基酸序列进行检索
- 生物序列的获取方法：Sequences检索、物质名称/代码/结构式、关键词及文献-物质的数据关联
- Motif适合检索短序列，并支持可变部分输入
 - ✓ X代表未指定氨基酸，N代表未指定核苷酸
 - ✓ []表示出现在该位置的序列是括号里氨基酸/核苷酸中的任意一个
 - ✓ { } 代表氨基酸/核苷酸的重复次数，如重复次数是范围，用逗号将数字隔开，如 {2, 6}

大纲

- 分析实验方法
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分析实验方法的获取 – 从CAS SciFinder n结果集链接

方法一：在CAS SciFinderⁿ的文献结果集页面，点击CAS solutions中的 Analytical Methods获得有具体分析实验方法的文献，从文献详情页中链接至分析实验方法。

References search for "ginseng and biomarker"

Substances Reactions Citing Knowledge Graph Save and Alert

Based on your query, we've returned the most relevant results. Would you like to load the entire result set? [Learn about result relevance.](#) [Load More Results](#)

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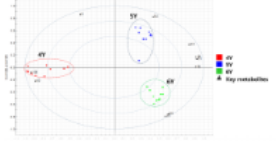
Document Type Language Publication Year Available at My Institution Author Organization Publication Name Concept CA Section CAS Solutions: Analytical Methods (47) Formula (4)

Filtering: CAS Solutions: Analytical Methods X Clear All Filters

47 Results Sort: Relevance View: Partial Abstract

1

Nontargeted metabolomics approach for age differentiation and structure interpretation of age-dependent key constituents in hairy roots of Panax ginseng
By: Kim, Nahyun; Kim, Kemok; Lee, Dong Hyuk; Shin, Yoo-Soo; Bang, Kyong-Hwan; Cha, Seon-Woo; Lee, Jae Won; Choi, Hyung-Kyoon; Hwang, Bang Yeon; Lee, Dongho
Journal of Natural Products (2012), 75(10), 1777-1784 | Language: English, Database: CAlupus and MEDLINE | Analytical Methods



The age of the **ginseng** plant has been considered as an important criterion to determine the quality of this species. For age differentiation and structure interpretation of age-dependent key constituents of Panax **ginseng**, hairy root (fine root) extracts aged from four to six years were analyzed using a nontargeted approach with ultraperformance liquid chromatog./quadrupole time-of-flight mass spectrometry (UPLC-QTOFMS). Various classification methods were used to determine an optimal method to best describe **ginseng** age by selecting influential metabolites of different ages. Through the metabol...

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Full Text Substances (5) Reactions (0) Citing (42) Citation Map

2

Anti-fatigue effects of small molecule oligopeptides isolated from Panax ginseng C. A. Meyer in mice
By: Bao, Lei; Cai, Xiaxia; Wang, Junbo; Zhang, Yuan; Sun, Bin; Li, Yong
Nutrients (2016), 8(12), 807/1-807/11 | Language: English, Database: CAlupus and MEDLINE | Analytical Methods

Panax **ginseng** C.A. Meyer (**ginseng**) is an edible and medicinal Chinese herb, which is often used in Asian countries for phys. fitness. **Ginseng** is reported to have a wide range of biol. activity and pharmaceutical properties. There were more studies on **ginsenosides** and **polysaccharides**, but fewer studies on **ginseng** oligopeptides (GOP), which are small mol. oligopeptides isolated

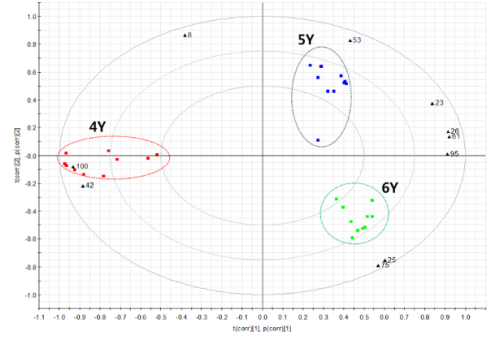
Nontargeted metabolomics approach for age differentiation and structure interpretation of age-dependent key constituents in hairy roots of Panax ginseng

Substances (5) Reactions (0) Citing (42) Citation Map Save

JOURNAL
Source: Journal of Natural Products, Volume: 75, Issue: 10, Pages: 1777-1784, Journal Article: Research Support, Non-U.S. Gov't, 2012, DOI: 10.1021/jp300499q
CODEN: JNPRDF, E-ISSN: 1520-6025, ISSN-L: 0163-3864
Database Information: AN: 2012:1395939, CAN: 157:558753, PubMed ID: 23002782, CAlupus and MEDLINE
Company/Organization: School of Life Sciences and Biotechnology, Korea University, Seoul 136-713, Korea, Republic of
Publisher: American Chemical Society-American Society of Pharmacognosy
Language: English

By: Kim, Nahyun; Kim, Kemok; Lee, Dong Hyuk; Shin, Yoo-Soo; Bang, Kyong-Hwan; Cha, Seon-Woo; Lee, Jae Won; Choi, Hyung-Kyoon; Hwang, Bang Yeon; Lee, Dongho

The age of the **ginseng** plant has been considered as an important criterion to determine the quality of this species. For age differentiation and structure interpretation of age-dependent key constituents of Panax **ginseng**, hairy root (fine root) extracts aged from four to six years were analyzed using a nontargeted approach with ultraperformance liquid chromatog./quadrupole time-of-flight mass spectrometry (UPLC-QTOFMS). Various classification methods were used to determine an optimal method to best describe **ginseng** age by selecting influential metabolites of different ages. Through the metabolite selection process, several age-dependent key constituents having the potential to be **biomarkers** were determined, and their structures were identified according to tandem mass spectrometry and accurate mass spectrometry by comparing them with an inhouse ginsenoside library and with literature data. This proposed method applied to the hairy roots of P. **ginseng** showed an improved efficiency of age differentiation when compared to previous results on the main roots and increases the possibility of the identification of key metabolites that can be used as **biomarker** candidates for quality assurance in **ginseng**.



Keywords: Panax root age metabolite analysis

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Concepts MEDLINE® Medical Subject Headings Substances Analytical Methods

Title	CAS Method Number
Analysis of Ginsenoside Re in Panax ginseng by Ultrasonic extraction	1-131-CAS-214718
Analysis of Malonyl-ginsenoside Rb ₁ in Panax ginseng by Ultrasonic extraction	1-131-CAS-217167



分析实验方法详情

Analysis of Ginsenoside Re in Panax ginseng by Ultrasonic extraction

CAS MN: 1-131-CAS-214718

Method Category: Natural Product Isolation Analysis

Technique: Ultra-performance liquid chromatography; Ultrasonic extraction; Quadrupole mass spectrometry; Time-of-flight mass spectrometry

实验原料

Materials	Role	Image	CAS RN
Ginsenoside Re	analyte	View Structure	52286-59-6
Ginsenoside Rg ₂	analyte	View Structure	52286-74-5
Ginsenoside Rb ₁	analyte	View Structure	41753-43-9
Ginsenoside Rd	analyte	View Structure	52705-93-8
Panax ginseng	matrix		
0.2 μm membrane filter	material		
Acquity UPLC BEH C18 column (i.d., 2.1 × 100 mm; particle size, 1.7 μm)	material		
Methanol	reagent	View Structure	67-56-1

Source

Nontargeted metabolomics approach for age differentiation and structure interpretation of age-dependent key constituents in hairy roots of Panax ginseng

Kim, Nahyun; Kim, Kemok; Lee, Dong Hyuk; Shin, Yoo-Soo; Bang, Kyong-Hwan; Cha, Seon-Woo; Lee, Jae Won; Choi, Hyung-Kyoon; Hwang, Bang Yeon; Lee, Dongho

Journal of Natural Products (2012), 75 (10), 1777 - 1784. American Chemical Society-American Society of Pharmacognosy

CODEN: JNPRDF | ISSN: 01633864 | DOI: 10.1021/np300499p

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[Abstract](#) ^

The age of the ginseng plant has been considered as an important criterion to determine the quality of this species. For age differentiation and structure interpretation of age-dependent key constituents of Panax ginseng, hairy root (fine root) extracts aged from four to six years were analyzed using a nontargeted approach with ultraperformance liquid chromatog./quadrupole time-of-flight mass spectrometry (UPLC-QTOFMS). Various classification methods were used to determine an optimal method to best describe ginseng age by selecting influential metabolites of different ages. Through the metabolite selection process, several age-dependent key constituents having the potential to be biomarkers were determined, and their structures were identified according to tandem mass spectrometry and accurate mass spectrometry by comparing them with an inhouse ginsenoside library and with literature data. This proposed method applied to the hairy roots of *P. ginseng* showed an improved efficiency of age differentiation when compared to previous results on the main roots and increases the possibility of the identification of key metabolites that can be used as biomarker candidates for quality assurance in ginseng.

Equipment Used

Freeze drier, Eyela, Tokyo, Japan

UPLC system, Acquity, Waters, Milford, MA, USA

Mass spectrometer, QTOF Micromass, Waters, Milford, MA, USA

文献详情

Conditions

Instrument

Mobile phase: 0.1% formic acid in water (A) and 0.1% formic acid in acetonitrile (B); flow rate: 350 μL/min

capillary voltage: 2800 V; cone voltage: 35 V; collision energy: 5 eV; source temperature: 100 °C; desolvation temperature: 250 °C; desolvation gas flow: 600 L/h; cone voltage and collision energy: 35-55 V and 30-50 eV, respectively.

Instructions

Collection of samples

1. Prepare *P. ginseng* samples and subject to analysis.

Preparation of standard solution

1. Prepare each ginsenoside standard in 50% methanol.
2. Store all the stock and working solutions at -20 °C before use.
3. Prepare stock solutions of ginsenosides and dilute to 0.08, 0.4, 2.0, 10.0 and 50.0 μg/mL to prepare the five-point calibration curves using the least-squares method.

Ultrasonic extraction

1. Cut and powder the hairy roots of *P. ginseng*.
2. Freeze dry (Eyela, Tokyo, Japan).
3. Powder.
4. Extract the samples ultrasonically with 70% methanol.
5. Centrifuge at 12000 rpm for 20 min.
6. Filter the supernatant through a 0.2 μm membrane filter.
7. Evaporate the solvent to dryness *in vacuo*.
8. Dilute the residue with 50% methanol to obtain a final concentration of 2 mg/mL.

Ultra-performance liquid chromatography quadrupole time of flight mass spectrometry (UPLC-QTOFMS) for the analysis of ginsenosides Rb₁, Rd, Re and Rg₂

1. Perform analysis using Acquity UPLC system (Waters, Milford, MA, USA) and a QTOF Micromass spectrometer (Waters, Manchester, UK).
2. Separate the analytes using Acquity UPLC BEH C18 column (i.d., 2.1 × 100 mm; particle size, 1.7 μm).
3. Use mobile phase consisting of 0.1% formic acid in water (A) and 0.1% formic acid in acetonitrile (B).
4. Maintain the following gradient elution program: 0.5 min 10% B, 3.0 min 25% B, 10.0 min 30% B, 16.0 min 35% B, 18.0 min 50% B, 21.0 min 65% B, 23.0 min 100% B for washing and 25.0 min 10% B to re-equilibrate the column with a flow rate of 350 μL/min.
5. Maintain the column and sample managers at 40 and 15 °C, respectively.
6. Inject 5 μL sample solution onto a column.
7. Perform mass spectral analysis in the negative-ion mode by scanning the m/z range of 200–1500.
8. Maintain the following mass spectral parameters: capillary voltage: 2800 V; cone voltage: 35 V; collision energy: 5 eV; source temperature: 100 °C; desolvation temperature: 250 °C; desolvation gas flow: 600 L/h; cone voltage and collision energy: 35-55 V and 30-50 eV, respectively.

Validation

Retention Time	3.76 min, Ginsenoside Re
	13.71 min, Ginsenoside Rd
	8.7 min, Ginsenoside Rg ₂
	3.43 min, Ginsenoside Re
	17.3 min, Ginsenoside derivative
	9.89 min, Ginsenoside derivative
Concentration	6.719 ± 0.491 mg/g (sample data), Ginsenoside Rb ₁
	0.060 ± 0.026 mg/g (sample data), Ginsenoside Rd
	8.338 ± 1.464 mg/g (sample data), Ginsenoside Re
	0.197 ± 0.098 mg/g (sample data), Ginsenoside Rg ₂

分析仪器

分析条件

操作步骤

数据有效性



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 - Flavonoids (72)
 - Phenols (54)
 - Caffeic acid (36)
 - Luteolin (26)
 - Polyphenols (nonpolymeric) (25)
- ^ Matrix (183)
 - Taraxacum officinale (183)
 - Leaf (70)
 - Root (42)
 - Betula (25)
 - Crataegus (25)
- ^ Method Category (117)
 - Food Analysis (117)
 - Natural Product Isolation Analysis (113)
 - Antioxidant Assay (54)
 - Suboptimal Analysis (35)
 - Element Detection (28)
- ^ Technique (117)
 - Solvent extraction (117)
 - Spectrophotometry (85)
 - UV-visible spectroscopy (55)
 - Ultrasonic extraction (35)
 - HPLC (29)
- ^ Year

Analysis of Chlorogenic acid in Taraxacum koksaghyz by Solvent extraction
CAS MN: 1-131-CAS-474927

View Details & Instructions Add to Compare

Analyte 4-Caffeoylquinic acid; Chicoric acid; Sinapic acid; Caffeic acid; 3',4'-Dimethoxycinnamic acid; Chlorogenic acid

Matrix Taraxacum koksaghyz; Leaf

Other Materials Reagent: Methanol
Material: Zorbax Eclipse plus C18 (250x4.6 mm, 5 µm) column

Method Category Natural Product Isolation Analysis

Technique Liquid chromatography diode array detectors; Reversed-phase HPLC; Solvent extraction

Equipment Used Freeze-dryer; HPLC system; Quaternary pump; Degasser; Column thermostat; Autosampler; Diode array detector

Source Antioxidant Sources from Leaves of Russian Dandelion
Molinu, Maria Giovanna; Piluzza, Giovanna; Campesi, Giuseppe; Sulas, Leonardo; Re, Giovanni Antonio
Chemistry & Biodiversity (2019), 16 (8), -. Verlag Helvetica Chimica Acta

Full Text View in CAS SciFinder

Abstract

Analysis of Flavonoids in Taraxacum officinale by UV-visible spectroscopy
CAS MN: 1-131-CAS-53490

View Details & Instructions Remove from Compare

Analyte Flavonoids

Matrix Taraxacum officinale

Other Materials Reagent: Aluminum chloride; Sodium hydroxide; Sodium nitrite; Carbon dioxide

分析方法的对比

Compare Methods

	1	2
Title	Analysis of Flavonoids in Taraxacum officinale by UV-visible spectroscopy	Analysis of Flavonoids in Taraxacum officinale by UV-visible spectroscopy
CAS Method Number	1-131-CAS-78532	1-131-CAS-44155
Method Category	Natural Product Isolation Analysis	Natural Product Isolation Analysis; Suboptimal Analysis
Technique	UV-visible spectroscopy	UV-visible spectroscopy
Analyte	Flavonoids	Flavonoids
Matrix	Taraxacum officinale	Taraxacum officinale
Other Materials	Aluminum chloride; Carbon dioxide; Sodium hydroxide; Sodium nitrite	Sodium nitrite; Carbon dioxide; Sodium hydroxide; Aluminum chloride
Equipment Used	Double-beam UV-Vis spectrophotometer, Shanghai Precision Scientific Instrument Co. Ltd.; High-speed grinder, Shanghai Precision Scientific Instrument Co. Ltd.; Ultrasonic View All	Double-beam UV-Vis spectrophotometer, Shanghai Precision Scientific Instrument Co. Ltd.; High-speed grinder, Shanghai Precision Scientific Instrument Co. Ltd.; Ultrasonic View All
Conditions	Instrument: detection wavelength-510 nm	Instrument: detection wavelength-510 nm
Source	Supercritical fluid extraction of flavonoids from dandelion Wu Jun; Luojun; Rong Shao View All	Supercritical fluid extraction of flavonoids from dandelion Wu Jun; Luojun; Rong Shao View All

Method

UV-VIS spectroscopy (Orthogonal experiments)

1. Obtain **dandelion** (*Taraxacum officinale*) herb for the study.
2. Pulverize the dried **dandelion** (baked at 45 °C for 12 h) in a high-speed mixer-grinder and sieve the powders over a 60-mesh screen.
3. Pack the 2 L extractor in with the dried **dandelion** powders.
4. Use CO₂ as the solvent.
5. Determined the flavonoids content in the extract using nitritealuminum nitrate method.
6. Use rutin to prepare a standard curve.
7. Add rutin samples of 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 mL, respectively to 25 mL volumetric flasks and dilute with 1 mL 5% NaNO₂, 1 mL 10% AlCl₃, 10 mL 4% NaOH and proper amount of water.
8. Dilute the parallel sample with the above chemicals but use containing no rutin for comparison.
9. Set the conditions for orthogonal experiment as follows: (a) pressure-35 MPa (b) temperature-50 °C (c) entrainer amount-4.0 mL/g (d) time-80 min.
10. Measure the absorbance at 510 nm using a double-beam UV-Vis spectrophotometer.
11. Calculate the concentration and the yield of flavonoids by the following equation: yield (mass of extract/mass of dry leaves,%) = $c \times v/m \times 100$, where c (g/mL)-the mass concentration of flavonoids, m (g)-the mass of **dandelion**, v (mL)-the volume of the extract.

[View Less](#)

Concentration

4.974%

UV-VIS spectroscopy (Orthogonal experiments)

1. Obtain **dandelion** (*Taraxacum officinale*) herb for the study.
2. Pulverize the dried **dandelion** (baked at 45 °C for 12 h) in a high-speed mixer-grinder and sieve the powders over a 60-mesh screen.
3. Pack the 2 L extractor in with the dried **dandelion** powders.
4. Use CO₂ as the solvent.
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6. Use rutin to prepare a standard curve.
7. Add rutin samples of 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 mL, respectively to 25 mL volumetric flasks and dilute with 1 mL 5% NaNO₂, 1 mL 10% AlCl₃, 10 mL 4% NaOH and proper amount of water.
8. Dilute the parallel sample with the above chemicals but use containing no rutin for comparison.
9. Set the conditions for orthogonal experiment as follows: (a) pressure-35 MPa (b) temperature-45 °C (c) entrainer amount-3.50 mL/g (d) time-100 min.
10. Measure the absorbance at 510 nm using a double-beam UV-Vis spectrophotometer.
11. Calculate the concentration and the yield of flavonoids by the following equation: yield (mass of extract/mass of dry leaves,%) = $c \times v/m \times 100$, where c (g/mL)-the mass concentration of flavonoids, m (g)-the mass of **dandelion**, v (mL)-the volume of the extract.

[View Less](#)

4.45%

分析实验方法小结

1. 通过CAS SciFinderⁿ中的文献结果集获得关联的分析方法
2. 在Analytical Methods平台中，直接通过主题检索或分类浏览获取分析实验方法
3. 查看分析实验方法操作详情，筛选分析目标物、介质、分析方法

大纲

- 配方/制剂信息检索
 - 通过文献获得配方/制剂信息
 - 通过检索式检索配方/制剂



获取配方或制剂 – 从CAS SciFinder n结果集链接

方法一：在CAS SciFinderⁿ的文献结果集页面，点击CAS solutions中的 Formulus 或勾选 Formulation Purpose选项，获得有具体配方或制剂信息的文献，从文献详情页中链接获取

References search for ""chronic heart failure" and "traditional chinese medicine""

Substances Reactions Citing Knowledge Graph Save and Alert

Filter Behavior: Filter by Exclude

Document Type Language Publication Year Available at My Institution Author Organization Publication Name Concept CA Section

CAS Solutions: Analytical Methods (5) Formulus (3)

Bioactivity Data Formulation Purpose Database

405 Results Sort: Publication Date: Newest View: Partial Abstract

1

XinLi formula, a traditional Chinese decoction, alleviates chronic heart failure via regulating the interaction of AGTR1 and AQP1
By: Wei, Xiao-Hong; Liu, Wen-Jing; Jiang, Wei; Lan, Tao-Hua; Pan, Hai'e; Ma, Ming-Yue; You, Liang-Zhen; Shang, Hong-Cai
Phytomedicine (2023), 113, 154722 | Language: English, Database: CPlus and MEDLINE

XinLi formula (XLF) is a traditional Chinese medicine used in clin. practice to treat chronic heart failure (CHF) in humans, with remarkable curative effect. However, the mechanism remains unknown. The goal of the current investigation was to determine how XLF affected CHF in a rat model of the condition brought on by ligation of the left anterior descending coronary artery, and to investigate the underlying mechanism. Cardiac function was detected by echocardiog. The contents of myocardial enzymes, Ang II, ALD, TGF-β1, and inflammatory factors were measured by ELISA. Myocardial injury and myo...
View More

Full Text Substances (0) Reactions (0) Citing (0) Citation Map

2

Comparative pharmacokinetics of seven bioactive components after oral administration of crude and processed Qixue Shuangbu Prescription in chronic heart failure rats by microdialysis combined with UPLC-MS/MS
By: Chen, Linwei; Wei, Nina; Jiang, Yong; Yuan, Chengye; Xu, Luwei; Li, Jindong; Kong, Min; Chen, Yan; Wang, Qin
Journal of Ethnopharmacology (2023), 303, 116035 | Language: English, Database: CPlus and MEDLINE

Qixue Shuangbu Prescription (QSP) is a classical traditional Chinese medicine prescription, which has widely used for the treatment of chronic heart failure (CHF). Preliminary clin. studies have shown that the efficacy of processed QSP (P-QSP) in treating CHF is greater than crude QSP (C-QSP). However, the pharmacokinetic characteristics of its major bioactive components under pathol. conditions are unclear. This study aims to compare pharmacokinetics of seven bioactive components after oral administration of C-QSP and P-QSP in CHF model rats. Ginsenoside Rb1, ginsenoside Re, ginsenoside Rg1, ...
View More

CAS Solutions

Analytical Methods (5)

Formulus (3)

Formulation Purpose

Cardiovascular agents (3)

定位配方或制剂的功能目标

获取制剂或配方相关信息

Application of a **traditional Chinese medicine** composition for preparing medicines for preventing and/or treating myocardial hypertrophy

Substances (0) Reactions (0) Citing (0) Citation Map

PATENT

Patent Number
CN112190652

Publication Date
2021-01-08

Application Number
CN2020-11207191

Application Date
2020-11-03

Kind Code
A

Assignee
Capital Medical University, China

Source
China
CODEN: CNXXEV

Database Information
AN: 2021:56481
CAN: 176:120018
CAplus

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. [View content from CAS Formulus®](#) in this document. [Learn more about Formulus®.](#)

By: Zhang, Minyu; Guo, Feifei; Wu, Hongwei; Yang, Hongjun; Wei, Junying; Wu, Sha

The invention relates to the field of medicines, in particular to an application of a **traditional Chinese medicine** composition to preparation of a medicine for preventing and/or treating myocardial hypertrophy and an application to preparation of a medicine for preventing pressure-loaded **chronic heart failure**, and expands new indications of Yixinshu capsules. Curative effect and action mechanism for myocardial hypertrophy resistance are studied. A new thought and a new choice are provided for treating myocardial hypertrophy and malignant heart diseases caused by further development of myocardial hypertrophy.

Keywords: myocardial hypertrophy prevention **traditional Chinese medicine** composition

PatentPak PDF Get Prior Art Analysis Full Text

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN112190652	Chinese	A	PDF	2021-01-08	CN2020-11207191	2020-11-03

Expand All | Collapse All

IPC Data

Concepts

Formulations

Formulations

Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents

[View CAS Formulus® Detail](#)

Location: Claim 1, 2, 3, 4, 5, 6, 7, 8, 9
Purpose: Cardiovascular agents
Target: myocardial hypertrophy, human

成份 Component	功能 Function	用量 Amount Reported
Panax ginseng	-	175-225 wt. parts
Ophiopogon japonicus	-	175-225 wt. parts
Schisandra chinensis	-	100-150 wt. parts
Astragalus membranaceus	-	175-225 wt. parts

Additional Components Reported in Full Text

Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents

[View CAS Formulus® Detail](#)

Location: Example
Purpose: Cardiovascular agents
Target: myocardial hypertrophy, human

Component	Function	Amount Reported
Panax ginseng	-	200 wt. parts

配方/制剂详情

Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents

Purpose	Target	Delivery Route	Physical Form	Source
Cardiovascular agents	ACTN2 protein level, ACTN2 protein level abnormal increase, Cardiac hypertrophy, Homo sapiens, TNNT2 protein level, TNNT2 protein level abnormal increase, interventricular septum thickness, interventricular septum thickness abnormal increase, left ventricle volume abnormal increase, left ventricular hypertrophy index, left ventricular hypertrophy index abnormal increase, left ventricular volume, malignant heart disease, myocardial cytoskeleton-related protein level, myocardial cytoskeleton-related protein level abnormal increase, posterior left ventricular wall thickness, posterior left ventricular wall thickness abnormal increase, stress-induced chronic heart failure	-	Capsules	View

制剂/配方的用途、靶点、递送途径及物理形式

制剂/配方的成分、功能及用量

Formulation Ingredients

Component	Function	Amount Reported	Optionality
Panax ginseng	-	200 wt. parts	Mandatory
Ophiopogon japonicus	-	200 wt. parts	Mandatory
Schisandra chinensis	-	133 wt. parts	Mandatory
Astragalus membranaceus	-	200 wt. parts	Mandatory
Salvia miltiorrhiza	-	267 wt. parts	Mandatory
Ligusticum striatum	-	133 wt. parts	Mandatory
Crataegus pinnatifida	-	200 wt. parts	Mandatory

More Formulations like this... NEW

相似的制剂/配方

Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents
Purpose: Cardiovascular agents
Target: ACTN2 protein level, ACTN2 pr...
Delivery Route: -
Physical Form: Capsules

Pharmaceutical Composition: Cardioprotective Agents or Cardiovascular Agents
Purpose: Cardioprotective agents, Car...
Target: Homo sapiens
Delivery Route: -
Physical Form: -

Pharmaceutical Composition: Containing Alantolactone: Angiogenesis Inhibitors or...
Purpose: Antiangiogenic agents, Antitu...
Target: Angiogenesis, Homo sapiens, ...
Delivery Route: Oral drug delivery syst...
Physical Form: Capsules, Pharmaceutic...

Antifungal Composition: Antifungal Agents
Purpose: Fungicides
Target: Aspergillus, Aspergillus clavat...
Delivery Route: -
Physical Form: -

Effective Dose

有效剂量

Descriptor	Solvent	Details
rate of administration of the capsules	-	0.16 g/kg/day
Experimental Activity		
Descriptor	Notes	Details
cardioprotective effect	cardioprotective effect of the composition on SPF SD rats with myocardial hypertrophy was assessed after 8 weeks of administration.	the composition has the protective effect on cardiac function in the rats.
rate of administration of the capsules	-	0.32 g/kg/day
Experimental Activity		
Descriptor	Notes	Details
cardioprotective effect	cardioprotective effect of the composition on SPF SD rats with myocardial hypertrophy was assessed after 8 weeks of administration.	the composition has the protective effect on cardiac function in the rats.
rate of administration of the capsules	-	0.64 g/kg/day
Experimental Activity		
Descriptor	Notes	Details
cardioprotective effect	cardioprotective effect of the composition on SPF SD rats with myocardial hypertrophy was assessed after 8 weeks of administration.	the composition has the protective effect on cardiac function in the rats.

Source Patent

查看或下载专利全文

Application of a traditional Chinese medicine composition for preparing medicines for preventing and/or treating myocardial hypertrophy

Assignee: Capital Medical University
CN112190652
Language: Chinese
Location: Example

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- 制剂或配方原料
- 相似的制剂或配方
- 制备工艺
- 制剂或配方实验评估
- 专利来源

检索配方或制剂 -- <https://formulus.cas.org>

方法二：

- 登录CAS Formulus主页
- 在检索框输入检索式，
如制剂或配方的原料、用途、物理形态、功能或文献识别符（包括专利号、DOI号和CA入库号）进行检索
- 支持高级检索

Searching for...

 Formulations

 Ingredients

 Formulation Designer

Design custom formulations
templates based on selections
and ingredients.

Formulations

Search for Formulations by Ingredient, Purpose, Form, Function, etc.

rehmannia and celiac 地黄与腹部



Try [Advanced Search](#) for a more precise search experience

- 制药、化妆品、食品、农化、油墨、涂料等多领域中的配方
- 工艺、成分、目标成分的常见配伍成分、设计配方、探索合规要求等

配方/制剂结果集

- 利用聚类项筛选结果：
行业、配方/制剂用途、物理形式、
物质状态、递送方式、涵盖信息、
文献类型、发表机构、发表年份
- 可查看制剂或配方成分，功能及用量
- 可查看原料详情
- 支持对比选中的制剂或配方
- 支持查看或下载专利全文
- 可查看制剂或配方详情

The screenshot shows a search results page for 'Formulations search for '+rehmannia' -Form:'Powder particle''. The interface includes a search bar, a filter sidebar on the left, and a main content area displaying search results. The filter sidebar has several sections with expandable/collapsible headers and checkboxes for various categories. The main content area shows two search results, each with a title, location, purpose, target, delivery route, and physical form. Below each result is a table of components with columns for Component, Function, and Amount Reported. A 'PATENT' section is also visible for each result, containing patent information and buttons for 'Patent PDF' and 'View in CAS SciFinder'. The interface also includes buttons for 'Add to Compare', 'View Formulation Detail', and '326 Similar Formulations - View All'.

Formulations search for "+rehmannia" -Form:"Powder particle"

Get Additional References Compare (0/3) Save

Filter by

- Industry
 - Pharmaceutical
- Purpose
 - Anti-inflammatory agents (56)
 - Pharmaceutical formulations (36)
 - Cardiovascular agents (26)
 - Antidiabetic agents (24)
 - Antitumor agents (21)
- Physical Form
 - Liquids (18)
 - Tablets (13)
 - Granular materials (8)
 - Pastes (6)
 - Capsules (5)
- State of Matter
- Delivery Route
 - Oral drug delivery systems (56)
 - Topical drug delivery systems (27)
 - Pharmaceutical sprays (4)
 - Vaginal drug delivery systems (3)
 - Transdermal drug delivery systems (2)
- Information Included
 - Component Amount (64)
 - Process (56)
 - Experimental Activity (7)
 - Effective Dose (5)
- Document Type
- Organization
- Publication Year

56 Results Sort: Relevance

1

Traditional Chinese Medicine Composition: Antiinflammatory Agents

Location: Example 2
Purpose: Anti-inflammatory agents
Target: Constipation, Homo sapiens, Intestinal microorganism
Delivery Route: Oral drug delivery systems
Physical Form: Granular materials, Tablets

Add to Compare

Component	Function	Amount Reported
Rehmannia	-	55 part
Eucommia	-	15 part
Angelica	-	15 part
Morus (plant)	-	15 part

PATENT

Composition, preparation method and preparation thereof for relieving constipation or regulating intestinal flora

Assignee: Beijing Aoteshuer Health Products Development Co., Ltd.
CN108498626
Language: Chinese

Patent PDF View in CAS SciFinder

View Formulation Detail

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

2

Dietary Supplements for Prevention and Treatment of Inflammatory Diseases: Antiinflammatory Agents

Location: Example 2
Purpose: Anti-inflammatory agents
Target: Acute inflammation, Allergy, Ankylosing spondylitis, Asthma, Atopy, Chronic inflammation, Colitis, Conjunctivitis, Crohn disease, Cystitis, Dermatitis, Fibromyalgia, Gastric ulcer, Gastritis, Gout, Hemorrhoid, Hepatitis, Homo sapiens, Lupus erythemat...
View More

Delivery Route: Oral drug delivery systems
Physical Form: Dietary supplements

Add to Compare

Component	Function	Amount Reported
Rehmannia	-	0.5 wt. parts
Hura crepitans extract	antiinflammatory agents	3 wt. parts

PATENT

Hura crepitans extracts for preventing and treating inflammatory diseases

Assignee: Korea Research Institute of Bioscience and Biotechnology
KR2011031691

不同制剂或配方信息的对比

Comparing your Formulations		
	Formulation 1	Formulation 2
Title	Dietary Supplements for Prevention and Treatment of Inflammatory Diseases: Antiinflammatory Agents	Health Food for Preventing Periodontal Disease: Antiinflammatory Agents
Purpose	Anti-inflammatory agents	Anti-inflammatory agents
Target	Acute inflammation, Allergy, Ankylosing spondylitis, Asthma, Atopy, Chronic inflammation, Colitis, Conjunctivitis, Crohn disease, Cystitis, Dermatitis, Fibromyalgia, Gastric ulcer, Gastritis, Gout, Hemorrhoid, Hepatitis, Homo sapiens, Lupus erythematosus, Multiple sclerosis, Myositis, Nephritis, Osteoarthritis, Otitis media, Periodontitis, Pharyngitis, Pneumonia, Psoriatic arthritis, Rheumatic fever, Rheumatoid arthritis, Rhinitis, Scapulohumeral peri-arthritis, Sjogren syndrome, Tendinitis, Tenosynovitis, Tonsillitis	Homo sapiens, Periodontal disease, Soluble tumor necrosis factors
Delivery Route	Oral drug delivery systems	Oral drug delivery systems
Physical Form	Dietary supplements	sunsik
Experimental Activity	Not Available	Not Available
Components	<p>Rehmannia Function: - Amount Reported: 0.5 wt. parts Optionality: -</p> <p>Hura crepitans extract Function: antiinflammatory agents Amount Reported: 3 wt. parts Optionality: -</p> <p>Group: Cereal (grain) Function: - Amount Reported: - Optionality: Mandatory</p> <p>Brown rice Function: - Amount Reported: 30 wt. parts Optionality: -</p> <p>Coix Function: - Amount Reported: 15 wt. parts Optionality: -</p>	<p>Rehmannia Function: - Amount Reported: 0.5 % by weight Optionality: -</p> <p>Panax notoginseng root extract Function: tumor necrosis factor-alpha inhibitors Amount Reported: 3 % by weight Optionality: -</p> <p>Group: Grains (particles) Function: - Amount Reported: - Optionality: Mandatory</p> <p>Brown rice Function: - Amount Reported: 30 % by weight Optionality: -</p> <p>Coix lacryma-jobi Function: - Amount Reported: 15 % by weight Optionality: -</p>

- 选择感兴趣的制剂或配方进行对比
- 一次最多可以比较三种不同制剂或配方的信息详情

<p>Group: Seed Function: - Amount Reported: - Optionality: Mandatory</p> <p>perilla seeds Function: - Amount Reported: 7 wt. parts Optionality: -</p> <p>black bean seeds Function: - Amount Reported: 8 wt. parts Optionality: -</p> <p>black sesame seeds Function: - Amount Reported: 7 wt. parts Optionality: -</p> <p>View More ></p>	<p>Group: Seed Function: - Amount Reported: - Optionality: Mandatory</p> <p>Perilla frutescens Function: - Amount Reported: 7 % by weight Optionality: -</p> <p>Glycine max Function: - Amount Reported: 8 % by weight Optionality: -</p> <p>Sesamum indicum Function: - Amount Reported: 7 % by weight Optionality: -</p>	
Source	<p>PATENT</p> <p>Hura crepitans extracts for preventing and treating inflammatory diseases</p> <p>Assignee : Korea Research Institute of Bioscience and Biotechnology KR2011031601 Language: Korean</p> <p>Formulation Location Example 2</p>	<p>PATENT</p> <p>Pharmaceutical compositions, health foods, and dentifrices containing Panax notoginseng root extracts for treatment of periodontal disease</p> <p>Assignee : Oscotec, Inc. JP2006022099 Language: Japanese</p> <p>Formulation Location Formulation Example 3</p>

高级检索

[← Return to Home](#)

Advanced Formulations Search ?

Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.

At least two search terms are required.

Search For Operator Enter one term

Function Anticorrosion
Ex: binder, surfactant, carrier

Search For Operator Enter one term

All Fields coating
General search of all fields

Add Another Term

 Search

All Fields

- All Fields
- Form
- Function
- Ingredient
- Purpose
- Route
- Target

Required
Optional
Excluded

Clear All

检索原料

Searching for...

Ingredients

Search by Ingredient Name, CAS Registry Number, or Function

Formulations

Ingredients

propylene glycol

Search

Ingredients search for "propylene glycol"

2 Selected 3 Results

Filter by

Industry

- Agrochemical
- Cleaning & Surfactant Products
- Cosmetics & Personal Care
- Food & Related
- Inks, Paints, & Coatings
- Pharmaceutical

View All

Regulatory Information

- REACH (5)
- Cosing: Cosmetic Ingredient Inventory (3)
- EPA Pesticide Inactive Ingredients (3)
- FDA Inactive Ingredients Database (3)
- ANMAT (1)

View All

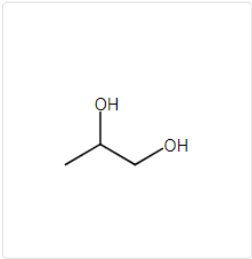
Experimental Properties

- Boiling Point (3)

1

CAS RN: 57-55-6

View Details



C3H8O2

(±)-Propylene glycol

Propylene glycol

Key Physical Properties	Value	Condition
Molecular Weight	76.09	-
Melting Point (Experimental)	-59 °C	-
Boiling Point (Experimental)	188.2 °C	-
Density (Experimental)	1.036 g/cm ³	Temp: 25 °C

Commonly Used As: Solvents; Carriers; Plasticizers; Humectants; Antifreeze...

Similar Ingredients with Regulatory Information

- 27194-74-7 Propylene glycol monolaurate
- 29387-86-8 Propylene glycol butyl ether
- 30136-13-1 Propylene glycol monopropyl ether

View 14 More

Commonly Formulated With | Regulatory Information | Experimental Properties

Formulations Suppliers Add to Designer

- 使用该原料的制剂或配方
- 原料供应商信息
- 可将原料添加至Formulation Designer

- 制剂或配方中，与该原料同时使用的其它配伍成分
- 管控信息及清单
- 实验属性

设计制剂或配方

Searching for...

 Formulations

 Ingredients

 Formulation Designer

Formulations

Search for Formulations by Ingredient, Purpose, Form, Function, etc.




Try [Advanced Search](#) for a more precise search experience

设计配方/制剂


Formulation Designer

* All fields are required


Industry

Cosmetics & Personal Care  Pharmaceutical
Cosmetics & Personal Care
Agrochemical
Cleaning & Surfactant Products
Food & Related
Inks, Paints, & Coatings

Purpose


Skin care products 

Physical Form


Gels 

Active or Featured Ingredient

Enter one term

Vitamin A 

Enter one term

polyethylene glycol 

At least 1 and up to 5 ingredients can be added.

Add Another Ingredient

Create! Clear All

Purposes (Showing top 100)

Top Count Alphanumeric Search

Select the purpose you would like to use:

Cosmetics and Personal care products	Skin care products	Antiarthritics
Skin conditioners	Analgesics	Bath preparations
Hair dyes	Antitumor agents	Transdermal drug delivery systems
Sunscreens	Allergy inhibitors	Insecticides
Hair preparations	Wetting agents	Hair care products
Antiperspirants	Wound healing promoters	Astringents
Cleaning compositions	Dyes	Semiconductor materials
Skin-lightening cosmetics	Fungicides	Insect repellents
Skin cleansers	Stabilizing agents	Sunless tanning products
Oral hygiene products	Whitening agents	Immunostimulants
Shampoos	Depilatories	Anti-Alzheimer agents
Makeup	Skin-darkening agents	Preservatives
Cosmetic fragrance products	Coating materials	Fabric softeners
Deodorants	Permeation enhancers	Food

Cancel

Physical Forms (Showing all 53)

Top Count Alphanumeric Search

Select the physical form you would like to use:

Emulsions	Sprays	Cosmetic sticks
Cream preparations	Pharmaceutical ointments	Eyeshadows
Cosmetic lotions	Powders	Films
Cosmetic packs	Cosmetic ointments	Hair conditioners
Gels	Essences	Lipsticks
Liquids	Hydrogels	Mascaras
Nanospheres	Oils	Milk
Solutions	Particles	Paper towels
Capsules	Effervescent materials	Pharmaceutical carriers
Pastes	Foundation cosmetics	Pharmaceutical lotions
Tablets	Pharmaceutical suppositories	Pharmaceutical pastes
Aerosols	Skin moisturizers	Skin cleansers
Foams	Freeze-dried drug delivery systems	Skin conditioners
Cosmetic gels	Coating materials	Skin toners

Cancel

查看制剂或配方设计结果详情

Base Selections			
Industry	Purpose	Physical Form	Active or Featured Ingredient
Cosmetics & Personal Care	Skin care products	Gels	Vitamin A polyethylene glycol
Edit	Edit	Edit	Edit

Template				
Function	Ingredient	Regulatory	Top Alternatives	Amounts
Active or Featured Ingredient:	Vitamin A	ANMAT	-	Amount not available ×
Active or Featured Ingredient:	polyethylene glycol	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	-	Amount not available ×
Function: Carriers	Polyethylene glycol View More Alternatives	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 181, Subpart B); FDA Inactive Ingredients Database	Water; Ethylene glycol	Approximate Range: 3 - 4% ×
Function: Skin conditioners	Glycerol View More Alternatives	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; FDA GRAS (Part 182,	Allantoin; Ethylene glycol; 1,2-Octanediol; Tricaprin; Palm-oil glycerides, monoglycerides, diglycerides and triglycerides, hydrogenated	Approximate Range: 3 - 11%

- 原料详情
- 原料管制信息
- 可替代的原料选项

Alternative Ingredients (Showing all 7)

Select the ingredient you would like to use:

Allantoin	Tricaprin	hydrogenated
Ethylene glycol	Palm-oil glycerides, monoglycerides,	Glyceryl polyacrylate
1,2-Octanediol	diglycerides and triglycerides,	N-(2-Hydroxyethyl)acetamide

配方/制剂信息检索小结

1. 通过检索原料、用途、物理形态、功能或文献识别符获得配方/制剂信息
2. 检索原料
3. 配方或制剂的设计
4. 通过文献结果集获得关联的配方/制剂信息
5. 查看配方/制剂详情
6. 对比不同配方/制剂信息

大纲

- CAS及CAS SciFinderⁿ简介
- 常见检索方式
 - 文献检索
 - 物质检索 (CAS Markush*)
 - 反应检索
 - 生物序列检索*
 - 逆合成反应路线设计 (CAS Retrosynthesis*)
 - 分析实验方法 (CAS Analytical Methods)
 - 配方/制剂信息检索 (CAS Formulus*)
- 常见问题及解答



如何获取CAS SciFinderⁿ账号

--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

Username: [Tips](#)

Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer: [Why?](#)

请注意：

1.必须输入真实姓名和邮箱。
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）。

填写个人信息后注册成功；之后直接点击<https://SciFinder-n.cas.org>访问。

检索浏览器推荐

浏览器推荐：

- Windows (7, 8.1, 10): Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)、Edge 15及更高版本
- Mac OS X (10.11, 10.12, 10.13): Safari 9.3及更高版本, Chrome 60及更高版本, Firefox 55及更高版本, Firefox 52 (ESR)
- 不建议使用360浏览器，相关功能或插件会被自动拦截

使用注意事项

- 一人注册一个帐号
- 实名注册，需提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（<https://www.cas.org/legal/infopolicy>）
- 不得账号分享
- 不得将账号用于非学术研究

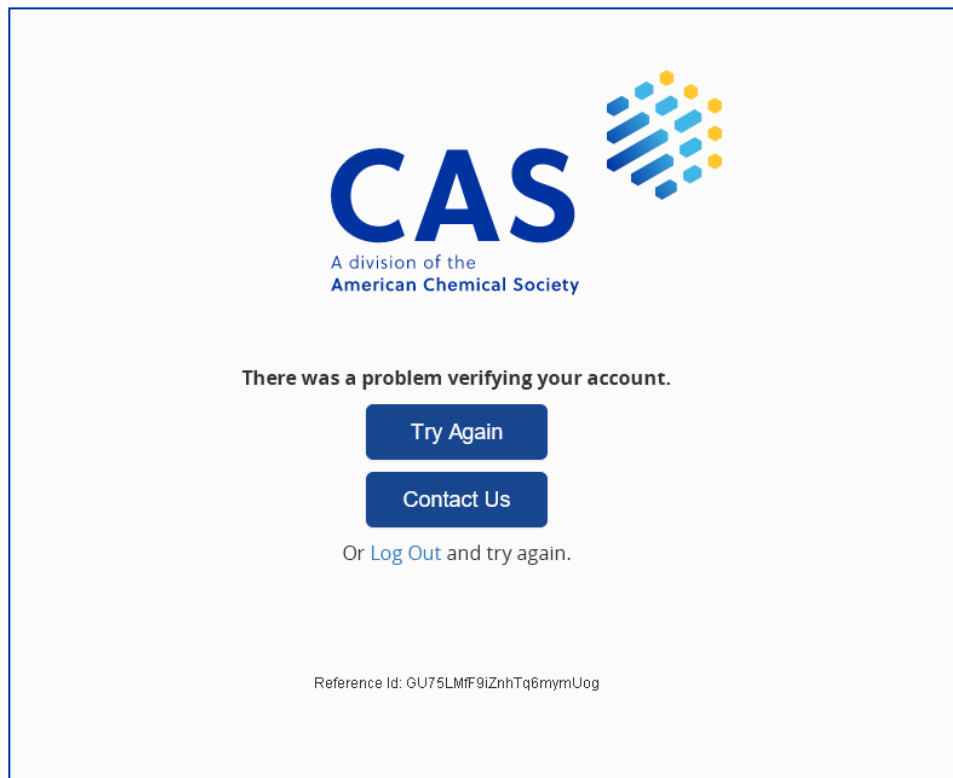
常见问题

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.

- 检查注册链接是否正确
- 确认连入校园网，且不是通过VPN连接
- 如果链接正确，且在校园内，请联系图书馆或china@acs-i.org

常见问题



- 确认账号密码是否正确
- 如果账号密码正确，请填写问题报告后联系图书馆或china@acs-i.org

学习资源



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ACS美国化学会

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Thursday 11:06

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2023年CAS SciFinder Discovery Platform论坛直播...

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预告: 2023 CAS SciFinder Discovery Platform 论坛



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CAS SCIFINDER DISCOVERY PLATFORM™
关注直播, 掌握科研利器!

新学期, 科研神器SciFinder升级了! 今年的直播将详细讲解CAS SciFinder Discovery Platform的新功能、检索技巧和科研应用, 为您的学业和科研生涯全程助力!

每次直播时间是18:00-19:00, 欢迎您带上问题, 我们将现场解答; 观看直播还有机会获得幸运纪念品!

<https://mp.weixin.qq.com/s/TGX0QrkeYySH76nBx1QSaw>

回顾: 2022 CAS SciFinder®论坛合集



2023 CAS 论坛直播时间表

- 3月1日** 解锁CAS SciFinder Discovery Platform新功能
收看回放 主讲人:钱欣
- 3月8日** 巧用CAS SciFinder Discovery Platform文献检索快速进阶
收看回放 主讲人:刘萌萌
- 3月15日** 万物互联 | CAS SciFinder Discovery Platform物质检索更高效
收看回放 主讲人:钱欣
- 3月22日** CAS SciFinder Discovery Platform反应检索,不止A to B
18:00-19:00 主讲人:刘子露
- 4月4日** 不止化学: CAS SciFinder Discovery Platform序列检索技巧
18:00-19:00 主讲人:刘萌萌
- 4月12日** 新手入门开题和文献综述?巧用CAS SciFinder Discovery Platform事半功倍
18:00-19:00 主讲人:刘子露
- 4月19日** 实验进展太慢?巧用CAS SciFinder Discovery Platform寻找启发
18:00-19:00 主讲人:钱欣
- 5月10日** 毕业季 | CAS SciFinder Discovery Platform助力论文写作及答辩准备
18:00-19:00 主讲人:刘子露
- 5月24日** 毕业季 | 巧用CAS SciFinder Discovery Platform做足升学与择业准备
18:00-19:00 主讲人:钱欣



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THANK YOU!



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