

CALIS第二十届培训周

CAS SciFinderⁿ

新一代科研创新信息工具

朱传娴（学术市场经理）
2022年5月



ACS
International



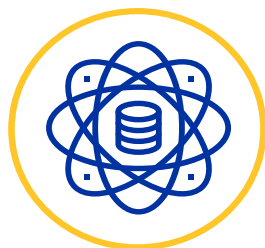
A division of the
American Chemical Society

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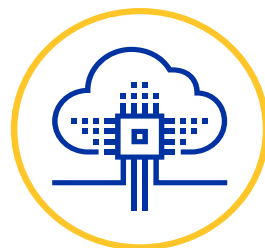
- CAS (美国化学文摘社)简介
- 新一代科研创新信息工具CAS SciFinderⁿ
- 分析方法解决方案CAS Analytical MethodsTM

美国化学文摘社 (CAS)隶属美国化学会(ACS)

- 拥有超过110年的经验；创立权威化学索引《化学文摘》（CA）
- 密切追踪、标引和提炼全球化学相关的文献（包括专利）
- 提供各种科学信息和相关技术产品与服务
- 协助创新和保护创新，助力于解决科研方面的难题与挑战



UNPARALLELED
SCIENTIFIC CONTENT



SPECIALIZED
TECHNOLOGY



UNMATCHED
HUMAN EXPERTISE

CAS数据覆盖学科

五大类80小类

- 生物化学：

- 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学

- 有机化学各领域：

- 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇

- 大分子化学各领域：

- 纤维素、木质素、造纸；涂料、墨水
- 染料、有机颜料；合成橡胶；纺织品、纤维

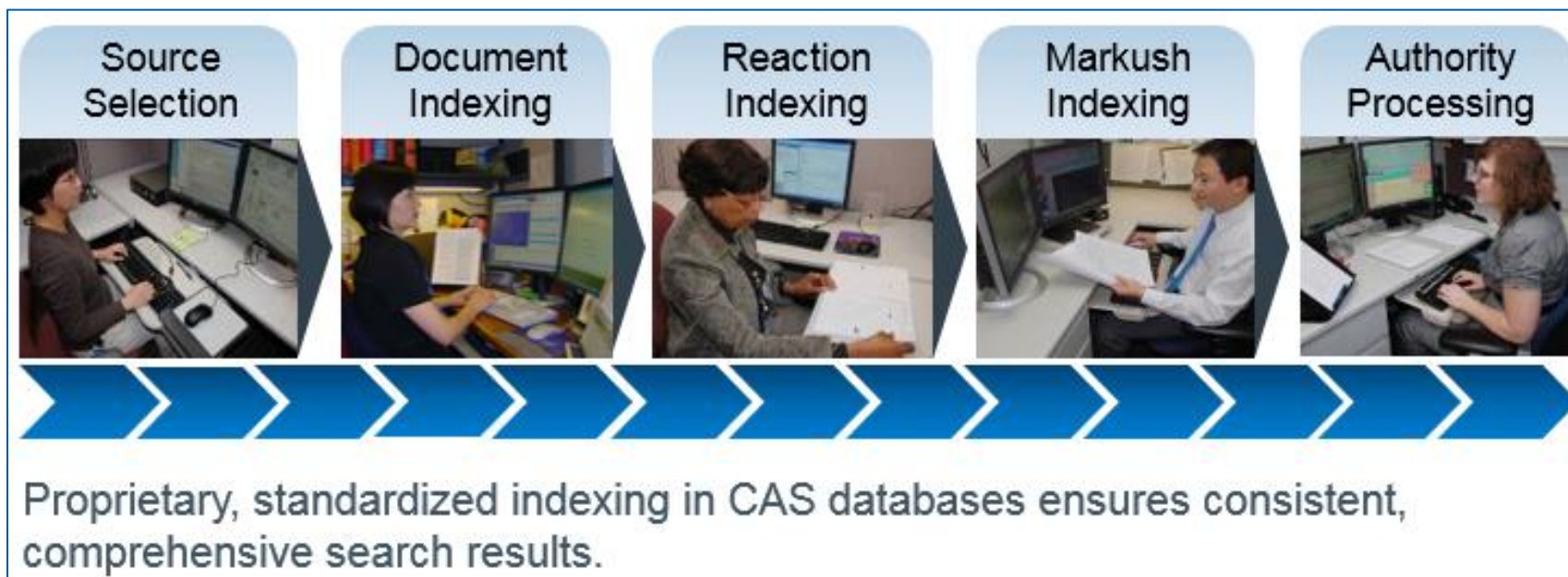
- 应用化学各领域：

- 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金

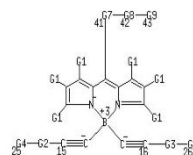
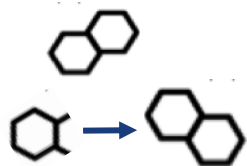
- 物理、无机、分析化学各领域：

- 表面化学、催化剂、相平衡、核现象、电化学

CAS科学家利用人类智慧对公开内容进行揭示



1990
Smith, M.
anthracene



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

经过CAS科学家的揭示相关信息更易被挖掘

- 人工标引——精准揭示关键技术信息
- 数千名科学家组成的编辑团队深刻理解客户的实际需求
- 审阅、筛选、摘要、标引以覆盖并揭示全球所有已公开的化学及相关信息
- CAS登记号——物质的黄金标准
- CAS Roles (CAS物质角色)——生物研究、性能用途、分析检测、合成制备
- CAS Index Terms (CAS技术词语标准)——揭示技术词语相互间的关联
- CA Sections (CAS学科分类, 80个类别)——精准定位具体研究领域

CAS解决方案与服务

DISCOVERY



CAS SciFinderⁿ

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大纲

- CAS (美国化学文摘社)简介
- 新一代科研创新信息工具CAS SciFinderⁿ
- 分析方法解决方案CAS Analytical MethodsTM

CAS SciFinderⁿ是来自CAS的全新产品

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CAS SciFinderⁿ中覆盖的内容合集

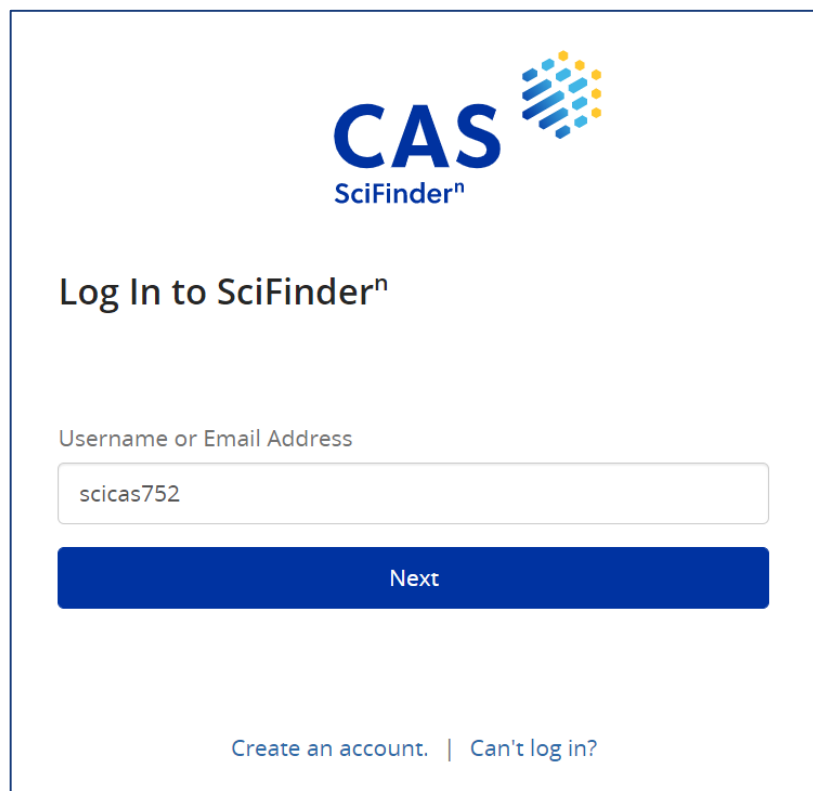


来源:

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

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

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



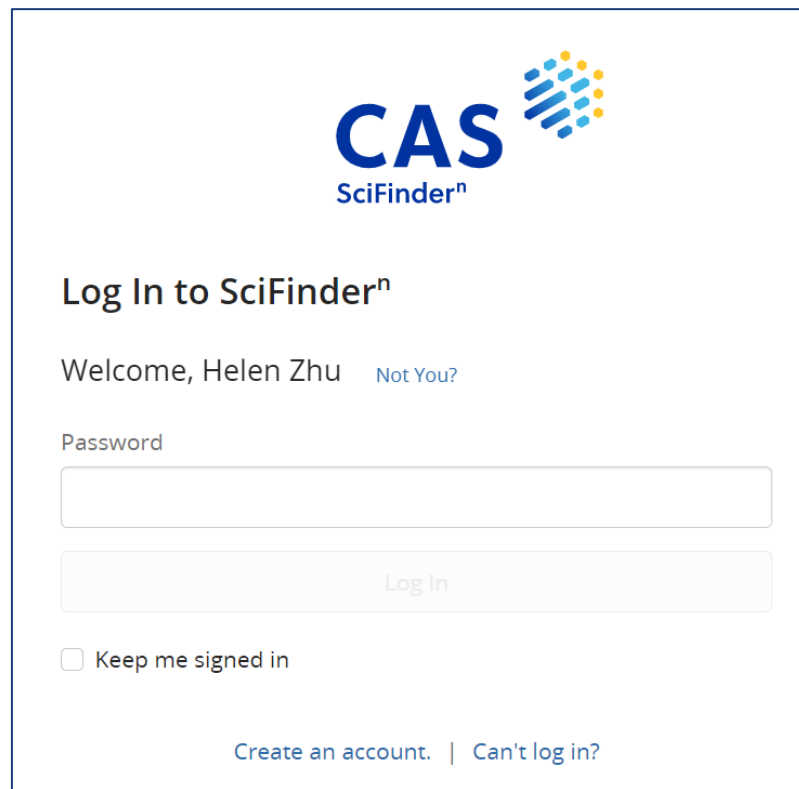
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账号与CAS SciFinder相同

简洁的界面，快速执行检索

灵活的
检索选项

Searching for...

- All
- Substances
- Reactions
- References
- Suppliers
- Biosequences
- Retrosynthesis

References

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

Heat treatment of materials

+ Add Advanced Search Field

Learn more about SciFinder

Edit Drawing Remove

Recent Search History

November 11, 2021
3:30 PM
Substances qinghaosu (1)

Rerun Search

Edit Search

便捷地合并文
本与结构检索

快速运行之前
的检索项目

文献检索—主题词

Searching for...

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

References

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

✕ Draw 🔍

- Toll like receptor (Chlamys farreri gene TLR)
- Toll like receptor 4 (Mus caroli strain C0423 gene Tlr4)
- Toll like receptor 4 (Mus caroli strain L0014 gene Tlr4)
- Toll like receptor 4 (Mus caroli strain L0211 gene Tlr4)
- Toll like receptor 4 (Mus caroli strain L0275 gene Tlr4)
- Toll like receptor 4 (Mus cookii strain L0103 gene Tlr4)
- Toll like receptor 4 (Mus cookii strain L0178 gene Tlr4)
- Toll like receptor 4 (Mus cookii strain R4106 gene Tlr4)

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；

支持布尔逻辑运算符(and, or, not)，默认运算顺序or > and > not；

() 优先运算；

“ ” 不允许词形变化，但可出现单数或复数；

支持通配符*或? (*代表0或多个字符；? 代表0或1个字符)。

高级检索--高效实现多字段组合检索

The screenshot displays the CAS SciFinder search interface. On the left, a sidebar titled "Searching for..." lists various search categories: All, Substances, Reactions, References (highlighted), Suppliers, Biosequences, and Retrosynthesis. The main area is titled "References" and includes a search bar with the text "G-protein coupled receptor". Below the search bar, there are fields for "Journal Name" (containing "journal of medid") and "Volume (Optional)". A dropdown menu is open under "Journal Name", listing several journals including "Journal of Medicinal Chemistry", "Journal of medical virology", "Journal of medical entomology", "Journal of medical education", "Journal of medical Internet research", "Journal of medical genetics", "Journal of medical case reports", "Journal of medical ethics", "Journal of medical microbiology", and "Journal of medical systems". To the left of the dropdown, there are buttons for "AND", "OR", and "NOT". At the bottom left, there is a list of search fields: Author Name, Journal Name, Organization Name, Title, Abstract/Keywords, Concept, Substances, Publication Year, Document Identifier, Patent Identifier, and Publisher. The top right of the interface shows "Saved", "History", and "Account" options.

可单独使用，也可联用下面的检索方法：

- 关键词、物质名称、CAS RN、文献号；
- 高级检索（刊物名、Concepts、物质等）；
- 结构检索

文献检索--主题词+结构联合检索

Searching for...

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

References

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

Antitumor

+ Add Advanced Search Field

[Learn more about Sci](#)

Structure Match

As Drawn (10)

Substructure (75)

Filter Behavior

Filter by Exclude

Document Type

- Journal (43)
- Patent (32)
- Review (2)

Substance Role

- Preparation (59)
- Reactant or Reagent (41)
- Biological Study (37)
- Uses (32)
- Properties (17)

View All

Language

- English (67)
- Czech (4)
- Chinese (3)
- Korean (1)

Publication Year

1998 to 2021

No Min to No Max Apply

View Larger

Available at My Institution

References (75)

Sort: Relevance View: Partial Abstract

Substances Reactions Citing Save

1

Antitumor Agents. 181. Synthesis and Biological Evaluation of 6,7,2',3',4'-Substituted-1,2,3,4-tetrahydro-2-phenyl-4-quinolones as a New Class of Antimitotic **Antitumor Agents**

By: Xia, Yi; Yang, Zheng-Yu; Xia, Peng; Bastow, Kenneth F.; Tachibana, Yoko; Kuo, Sheng-Chu; Hamel, Ernest; Hackl, Torben; Lee, Kuo-Hsiung

Journal of Medicinal Chemistry (1998), 41(7), 1155-1162 | Language: English, Database: CAPLUS and MEDLINE

A novel series of 6,7,2',3',4'-substituted-1,2,3,4-tetrahydro-2-phenyl-4-quinolones were synthesized and evaluated for interactions with tubulin and for cytotoxic activity against a panel of human tumor cell lines, including ileocecal carcinoma (HCT-8), breast cancer (MCF-7), lung carcinoma (A-549), epidermoid carcinoma of the nasopharynx (KB), renal cancer (CAKI-1), and melanoma cancer (SKMEL-2). Most compounds showed potent cytotoxic and antitubulin effects. The most active compounds demonstrated strong cytotoxic effects with ED₅₀ values in the nanomolar or subnanomolar range in almost all...

View More

Full Text

Substances (41) Reactions (26) Citing (256) Citation Map

2

aza-Flavanones as potent cross-species microRNA inhibitors that arrest cell cycle

By: Chandrasekhar, Srivari; Pushpavalli, Sreerangam N. C. V. L.; Chatla, Srinivas; Mukhopadhyay, Debasmita; Ganganna, Bogonda; Vijender, Kandi; Srihari, Pabbaraja; Reddy, Chada Raji; Janaki Ramalah, M.; Bhadra, Utpal

Bioorganic & Medicinal Chemistry Letters (2012), 22(1), 645-648 | Language: English, Database: CAPLUS and MEDLINE

Aza-Flavanones have been identified as a new class of selective microRNA inhibitors. These compounds were found to arrest cell cycle via a novel cross species microRNA-dependent regulatory pathway interpreting an unexpected link between cell cycle arrest and microRNA mediated control in cancer.

Full Text

Substances (18) Reactions (7) Citing (32) Citation Map

3

Relationship between structure and antiproliferative activity of 1-azaflavonones

By: Kawali, Satoru; Endo, Kotaro; Tokiwano, Tetsuo; Yoshizawa, Yuko

Anticancer Research (2012), 32(7), 2819-2826 | Language: English, Database: CAPLUS

The synthesis of 19 derivatives of 2-phenyl-3,4-dihydroquinolin-4(1H)-one, as aza analogs of flavanones, was carried out and these compounds were further screened for their antiproliferative activity toward HL60 promyelocytic leukemia cells. In comparison with flavanone the replacement of C-ring ether oxygen atom with a nitrogen atom potentiated activity by more than 100-fold. It was suggested that the aromaticity of the B-ring contributes greatly to the activity of 1-azaflavonones.

Full Text

Substances (40) Reactions (22) Citing (9) Citation Map

主题词+结构联合检索
大大提高检索的效率

直观的结果页面，丰富的聚类分析

文献类型语言
出版年份
作者
机构名
刊物名
Concept
CA Section
.....

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

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

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Filter Behavior

[Filter by](#) [Exclude](#)

- Document Type
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CA Section
- CAS Solutions
- Formulation Purpose
- Database
- Search Within Results

Filter Content Report

Download filter data from this result set. [Download](#)

73,996 Results Sort: Relevance View: Partial Abstract

1

Target validation of G-protein coupled receptors

By: Wise, Alan; Gearing, Katy; Rees, Stephen
Drug Discovery Today (2002), 7(4), 235-246 | Language: English, Database: CASplus and MEDLINE

A review with references **G-protein coupled receptors (GPCRs)** represent a large class of proteins for drug discovery. Over 30% of clin. marketed drugs are active at this receptor family; these drugs exhibit their activity at <10% of all known **GPCRs**. A major challenge for the pharmaceutical industry is to associate the many novel **GPCRs** with disease to identify the drugs of the future. This process consists of a collection of exptl. paradigms that together can be loosely labeled 'target validation'.

[Full Text](#) [Substances \(0\)](#) [Reactions \(0\)](#) [Citing \(343\)](#) [Citation Map](#)

2

The identification of ligands at orphan G-protein coupled receptors

By: Wise, Alan; Jupe, Steven C.; Rees, Stephen
Annual Review of Pharmacology and Toxicology (2004), 44, 43-66 | Language: English, Database: CASplus and MEDLINE

A review. The completion of the human genome sequencing project has identified ~720 genes that belong to the **G-protein coupled receptor (GPCR)** superfamily. Approx. half of these genes are thought to encode sensory receptors. Of the remaining 360 receptors, the natural ligand has been identified for ~210 receptors, leaving 150 so-called orphan **GPCRs** with no known ligand or function. The identification of ligands active at orphan **GPCRs** has been achieved through the development of a number of exptl. approaches, including the screening of putative small mol. and peptide ligands, reverse pharmacol...

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[Full Text](#) [Substances \(0\)](#) [Reactions \(0\)](#) [Citing \(183\)](#) [Citation Map](#)

3

A Brief History of G-Protein Coupled Receptors (Nobel Lecture)

By: Lefkowitz, Robert J.
Angewandte Chemie, International Edition (2013), 52(25), 6366-6378 | Language: English, Database: CASplus and MEDLINE

A review of studies made by the author and others in a form of Nobel lecture is presented.

[Full Text](#) [Substances \(0\)](#) [Reactions \(0\)](#) [Citing \(148\)](#) [Citation Map](#)

4

排序：
更快查找
相关信息

文献详情

被引文献

引文地图

The screenshot shows a CAS Reference Detail page for the article "Antiviral applications of Toll-like receptor agonists" by Horscroft, Nigel J.; Pryde, David C.; Bright, Helen. The page includes a left sidebar with journal information (Journal of Antimicrobial Chemotherapy, Volume 67, Issue 4, 2012) and database information (AN: 2012:423823, CAN: 156:387108, PubMed ID: 22258929). The main content area features the title, authors, abstract, and keywords. A navigation bar at the top includes "Citing (42)" and "Citation Map" buttons. A "Full Text" button is highlighted with a blue box and labeled "获取原文". Below the main text, there are expandable sections for "Concepts", "MEDLINE® Medical Subject Headings", "Substances", and "Cited Documents", with the "Cited Documents" section also highlighted and labeled "参考文献".

文献详情界面包括:

- 标题
- 摘要
- 原文关键词
- 文献中重要的技术术语 (含Caplus、Medline的关键词)
- 文献中重要的物质
- 书目信息
- 获得文献中的物质、反应
- 参考文献
- 链接原文
- 引文地图

CAS科学家增值标引的信息

参考文献

Citation Map: 便捷地获取关联文献

Citation Map

Filter By Cited By Citing

Filter Behavior

Filter by Exclude

Document Type

- Journal (72)
- Review (8)

Author

Concept

- Amino acids (25)
- Peptides (25)
- Maillard reaction (24)
- Maillard reaction products (24)
- Antioxidants (21)

View All

Language

- English (72)

Filter Content Report

Download filter data from this result set.

Transglutaminase cross-linking effect on sensory characteristics and antioxidant activities of Maillard reaction products from soybean protein hydrolysates

By: Song, Na; Tan, Chen; Huang, Meigui; Liu, Ping; Eric, Karangwa; Zhang, Xiaoming; Xia, Shuqin; Jia, Chengsheng
Food Chemistry (2013), 136(1), 144-151 | Language: English, Database: CPlus and MEDLINE

Full Text

Cited By 引用当前文献的文献

对引文做筛选

γ-Glutamylamine cyclotransferase: Specificity toward ε(L-γ-glutamyl)-L-lysine and related compounds

By: Fink, Mary Lynn; Chung, Soo Il; Folk, J. E.
Proceedings of the National Academy of Sciences of the United States of America (1980)

Expand Citations Create Map

Citations 参考文献

Citation Map Key

- Cited by Root Document
- References Citing Root Document

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- 在**CAS专利族文献**中找到你所熟悉语言的专利

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The screenshot displays the CAS PatentPak interface. At the top, there are navigation controls for PAGE (35/62), ZOOM, and DOWNLOAD (PDF, PDF+). The main content area shows a patent document titled "说明书" (Specification) for patent CN 109535200 A, page 21/48. The document contains several paragraphs of text and chemical reaction schemes. A blue arrow points from a chemical structure in the patent document to a detailed substance information panel on the right. This panel shows the CAS RN 2306115-70-6 and the CAS Name: 2H-Pyran, 2-[4-bromo-2-(trifluoromethyl)phenoxy]tetrahydro-. Below the name is a list of actions: Substance Detail, Reactions (2), Synthesize (1), Create Retrosynthesis Plan, References (1), and Suppliers (0). At the bottom of the panel are buttons for Edit Structure, Reset, and a download icon. The left sidebar shows a list of key substances in the patent, including CAS RN 2306115-70-6, 1003-68-5, and 1229705-85-4, each with a small chemical structure and analyst markup locations.

可在PatentPak浏览器中单击结构，打开物质菜单检索具体信息

Biosequences Search™—分子生物学解决方案

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Biosequences Search™ -- BLAST检索

CAS SciFinder[®] Saved History Account

Retrosynthesis plans now have a new rule-set trained on our full collection of single-step reactions, offering greater coverage of synthetic methods and added novelty. [Learn more about Retrosynthesis searching in CAS SciFinder[®].](#)

Searching for...

- All
- Substances
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- References
- Suppliers
- Biosequences**
- Retrosynthesis

Biosequences

Enter a protein or nucleotide string, or upload a .txt or .fasta file. [Learn more about Biosequence 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

Limit Total Sequence Results to:
1000

Start Biosequence Search

Advanced Biosequence Search ▾

BLAST:
用生物序列检索核酸或蛋白

四种检索选择:

Protein-Protein

Protein-Nucleotides

Nucleotide-Nucleotides

Nucleotide-Proteins

CAS SciFinder-n Help:

https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search.htm&rhsearch=biosequence&rhhlterm=biosequence&rhsyns=%20

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- Reactions
- References
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- Biosequences**
- Retrosynthesis

Biosequences

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

BLAST **CDR** Motif

CDR1	<input type="text" value="VFPLAPSSKS"/>	<input type="button" value="x"/>
CDR2	<input type="text" value="TSGGTAALGC"/>	<input type="button" value="x"/>
CDR3	<input type="text" value="LVKDYFPEPV"/>	<input type="button" value="x"/>

Include NCBI Sequences

Limit Total Sequence Results to:

CDR:
检索抗体或T细胞受体上的
互补决定区的氨基酸序列

CAS SciFinder-n Help:
https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search_-_CDR.htm&rhsearch=CDR&rhhlterm=CDR&rhsyns=%20

Biosequences Search™ -- Motif检索

Searching for...

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

Biosequences

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

BLAST CDR **Motif** Clear Search

[SG]x{4}GK[DT]

[] 或
{ } 重复次数

Sequence Type:
 Nucleotide Protein

Include NCBI Sequences

Limit Total Sequence Results to:
1000

Advanced Biosequence Search

Query Coverage % E-Value

Motif:
可用于检索序列中有不确定位点的DNA、RNA或蛋白;
推荐检索短序列

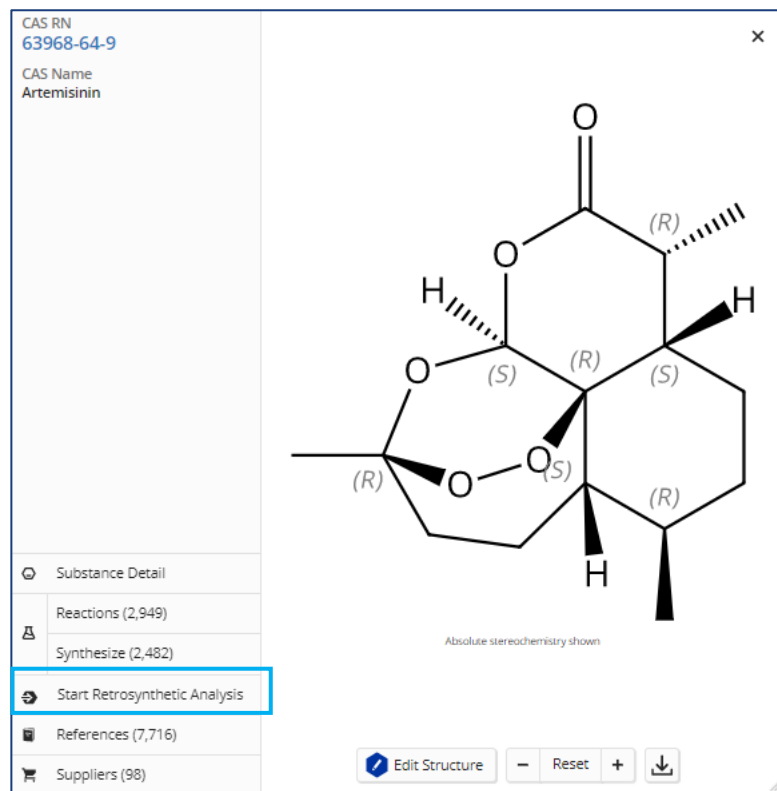
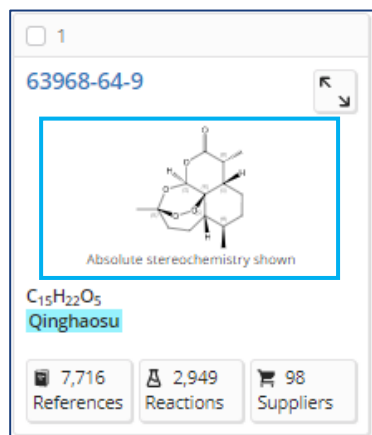
CAS SciFinder-n Help:

https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FBiosequence_Search%2FBiosequence_Search_-_Motif.htm&rhsearch=motif&rhhlterm=motif&rhsyns=%20

CAS Retrosynthesis Tool—逆合成工具

- 依据一个确定结构的物质进行设计
- 有报道且结构明确的物质，无论是否有反应信息报道
- 未有报道且结构明确的物质
- 节省设计、实施合成新方法所花费的时间

CAS Retrosynthesis Tool--由物质获得



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

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—直接绘制结构

Searching for...

Retrosynthesis

Draw or import a structure to perform a retrosynthetic analysis. [Learn more about Retrosynthesis searching.](#)

Enter a CAS Registry Numbers, SMILES...

Draw or change atoms or bonds.

Molecular Formula: C₁₉H₁₉BrN₄O₅ (463.29)

Start Retrosynthetic Analysis

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—对已知化合物

Retrosynthesis Powered by ChemPlanner®

Overview Steps Predicted Results

View Excluded Options [Download] [Email] [Save]

Plan Information

Estimated Yield: 87%
Overall Price: \$77.88
(USD per 100 grams)

Commercially Available: A, B, C

Plan Options

Synthetic Depth: 3
Predicted Rules: Common
Break & Protect Bonds: No
Starting Material Cost Limit: \$1,000.00/mol
[Edit Plan Options](#)

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

对已知化合物，CAS Retrosynthesis Tool既可以获取其已经报道的逆合成实验路线，也可以查看其预测的路线

A ⇒ B + C Alternative Steps (75)

Filter by

- Alternative Step Type
 - Experimental (26)
 - Predicted (49)
- Stereochemistry
 - Non-Selective (49)

1 of 27 Predicted Step

[Select](#) [View 1 similar Alternative](#) [View Evidence \(113\)](#) Average Yield: 75%

2 of 27 Predicted Step

[Select](#) [View 6 similar Alternatives](#) [View Evidence \(24\)](#) Average Yield: 75%

CAS Retrosynthesis Tool—对未知化合物

Retrosynthesis

Powered by ChemPlanner®

Overview Steps Predicted Results ON View Excluded Options Save

Plan Information
Estimated Yield: 44%
Overall Price: \$4,942.48
(USD per 100 grams)
Commercially Available: C, F

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

Scoring Profiles

- Complexity Reduction
- Convergence
- Evidence
- Cost
- Yield
- Atom Efficiency

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

- Experimental Steps
- Predicted Steps

Step A: Avg. Yield 65%

Step B: Avg. Yield 73%

Step D: Avg. Yield 73%

Step E: Avg. Yield 67%

预测新化合物的合成路线后，可继续通过Scoring灵活调整预测参数

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

Synthetic Methods™ -- 合成方法详情解决方案

- 迄今为止全球最大的为合成科学家提供的实验方法详情解决方案
- CAS科学家通过分析大量的顶级科技期刊及专利原文，收集、整理、筛选出来的实验方法
- 无需下载阅读全文，即可获得合成实验所需的所有信息
- 极大节省在期刊全文中查找信息的时间

Synthetic Methods™ -- 合成实验方法数据库



Suppliers (88) Suppliers (62)

Step 1

Alternative Steps (1)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	1,10-Phenanthroline Copper oxide (Cu ₂ O) Potassium bromide	Quinoline <i>N</i> -Methyl-2-pyrrolidone	6 h, 170 °C

CAS Reaction Number: 31-109-CAS-15004422

Experimental Protocols

Synthetic Methods Experimental Procedure

Products	Benzaldehyde, Yield: 67%
Reactants	2-Carboxybenzaldehyde
Catalysts	1,10-Phenanthroline Copper oxide (Cu ₂ O) Potassium bromide
Solvents	Quinoline <i>N</i> -Methyl-2-pyrrolidone
Procedure	<ol style="list-style-type: none">Charge an oven-dried vessel with 2-carboxybenzaldehyde (1.00 mmol), Cu₂O (10.7 mg, 0.075 mmol), phenanthroline (27.0 mg, 0.15 mmol) and potassium bromide (0.015 mmol).Flush the vessel with alternating vacuum and nitrogen purge cycles.Add a degassed solution of <i>n</i>-tetradecane in a mixture of NMP (1.5 mL) and quinoline (0.5 mL) to the reaction mixture <i>via</i> syringe.Stir the resulting mixture at 170 °C for 6 hours.Allow the reaction mixture to cool to room temperature.Dilute the reaction mixture with ethyl acetate (2 mL).Dissolve a sample of the reaction mixture (0.25 mL) in ethyl acetate (2 mL).Wash the reaction mixture with HCl (1 N, 2 mL).Dry the reaction mixture over MgSO₄/NaHCO₃.Analyze the product by GC.
Transformation	Decarboxylation of Aromatic Acids
Scale	milligram

CAS Method Number 3-109-CAS-15004422

物质信息
名称、角色

实验过程

Synthetic Methods中的实验详情不仅包含原文中描述的实验内容，还包括supporting information中涉及的实验内容

大纲

- CAS (美国化学文摘社)简介
- 新一代科研创新信息工具CAS SciFinderⁿ
- 分析方法解决方案CAS Analytical MethodsTM

CAS Analytical Methods™--分析实验方法数据库

Organic Compound Analysis: 天然产物分离分析, 手性分离, 活性药物成分及代谢产物分析...

Organometallics / Inorganics: 地质分析, 无机物分析, 金属有机化合物分析

Pharmacology / Toxicology: 成瘾药物检测, 有毒物检测...

Bioassays: 生物探针, 生物标定细胞实验, 生物标定药物实验, 生物医学材料分析, 生物分子/生物组织分离测定...

Water Analysis: 阴阳离子分析, 元素测定, 痕量元素分析, 废水分析, 生物标记公共卫生分析...

Historical Analysis / Dating: 考古分析, 同位素分析

Environmental Analysis: 土壤/空气/水分析, 农药残留分析...

Agricultural Applications / Analysis: 除草剂分析...

Food Analysis: 脂肪酸分析, 脂肪酸酯分析, 蛋白质分析...

Fuels / Geology / Biofuels: 生物燃料分析, 油气分析, 石油产品分析, 煤炭加工...

Miscellaneous: 化妆品分析, 爆炸物分析, 纳米材料分析...

Water: 阴阳离子分析、环境分析、废水分析、微量元素分析...

Polymer: 聚合物分析...

分析方法的类别:
13大类45小类;
某些子类属多个大类

分析方法的获取—Analytical Methods

<https://methods.cas.org> (与SciFinder-n登录账号相同)

The screenshot shows the CAS Analytical Methods website. At the top, there is a navigation bar with 'CAS Solutions' and 'Analytical Methods' logos, along with 'Saved' and 'Account' icons. Below this is a search bar with the text 'Enter keyword, matrix, analyte, etc.' and a search button. A blue box with white text is overlaid on the search bar, containing the Chinese text '输入感兴趣的检索词进行快速检索或高级检索'. Below the search bar is an 'Advanced Search' link. Further down is a 'Browse Method Categories' section with a grid of category links. A blue box with white text is overlaid on this section, containing the Chinese text '浏览丰富的分析方法目录，选择查看感兴趣的方法详情'. To the right of the main content, a dropdown menu is open, showing a list of method categories under 'Browse Method Categories > Pharmacology / Toxicology'. A blue arrow points from the 'Pharmacology / Toxicology' link in the main grid to this dropdown menu. The dropdown menu lists: Active Pharmaceutical Ingredient and Metabolite Analysis, Addictive Drug Assay, Forensic Analysis, Genetic Analysis, Nanomaterial Analysis, Organic Compound Analysis, and Toxin Assay. At the bottom of the page, there is a 'Recent Searches' section with two search history entries, each with a close button. The bottom right corner features the ACS International and CAS logos.

CAS Solutions

CAS Analytical Methods

★ Saved

Account

Search

Enter keyword, matrix, analyte, etc.

输入感兴趣的检索词进行快速检索或高级检索

Advanced Search

Browse Method Categories

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

浏览丰富的分析方法目录，选择查看感兴趣的方法详情

Browse Method Categories > Pharmacology / Toxicology

- Active Pharmaceutical Ingredient and Metabolite Analysis
- Addictive Drug Assay
- Forensic Analysis
- Genetic Analysis
- Nanomaterial Analysis
- Organic Compound Analysis
- Toxin Assay

Recent Searches

- Advanced : analyte : sofosbuvir, technique : hplc
- Advanced : analyte : sofosbuvir, technique : hplc, keyword : mass

分析方法详情

CAS Solutions Analytical Methods guajaverin

Return to Results

Method Detail (1 of 220)

Analysis of Garcimangosone D in Psidium guajava by Solvent extraction

CAS MN: 1-131-CAS-164363

Method Category: Natural Product Isolation Analysis
Technique: UV-visible spectroscopy; Adsorption liquid chromatography; HPLC

Materials	Role	View Structure	CAS Number
Garcimangosone D	analyte	View Structure	356055-68-0
Guajaverin	analyte	View Structure	22255-13-6
Guajaphenone A	analyte		
Psidium guajava	matrix		
Column (10 mm, 300_8 mm i.d.)	material		
Column (3 x 60 cm)	material		
Methanol	reagent		
Dichloromethane	reagent		
Hexane	reagent		
Chloroform	reagent		
Ethyl acetate	reagent		

方法分类、技术、所用材料/物质、角色、文献来源……

Source

A new antibacterial benzophenone glycoside from *Psidium guajava* (Linn.) leaves

Ukwueze, Stanley E.; Osadebe, Patience O.; Okoye, Festus B. C.

Natural Product Research (2015), 29 (18), 1728 - 1734. Taylor & Francis Ltd.

CODEN: NPRAAT | ISSN: 14786419 | DOI: 10.1080/14786419.2014.1003188

Full Text

Abstract

Bioactivity-guided fractionation of methanol extract from the leaves of *Psidium guajava* L. (Myrtaceae) yielded a new benzophenone glycoside, gajaphenone A (I) together with two known compounds, garcimangosone D and **guajaverin**. Their structures were elucidated by anal. of spectroscopic data including 1D and 2D NMR and electrospray ionisation mass spectrometry. The isolated compounds were screened against standard strains of Gram-pos. and Gram-neg. bacteria using broth dilution assay method, and the MIC values determined and compared with reference antibiotic ceftriaxone. They were found to have significant antibacterial activities against *Escherichia coli* and *Staphylococcus aureus* with all of them showing better activities against *S. aureus*, but displaying weaker activities, in comparison to ceftriaxone. However, despite reduced effect of these compounds against the organisms, this work opens the perspective to use these mols. as leads for the design of novel and selective drug candidates for some tropical infectious diseases.

Equipment Used

HPLC system, L-7100, Merck-Hitachi

UV detector, UV-L7400, Merck-Hitachi

Column chromatography system

Fraction collector, Retriever II, ISCO, Germany

Conditions

Instrument

Column: Eurospher C-18 column (10 mm, 300_8 mm i.d.; Knauer); mobile phase: methanol and nanopure water

Detection: 254 nm

Column: Sephadex LH-20 column (3 x 60 cm); mobile phase: dichloromethane:methanol (1:1); flow rate: 0.2 mL/min

Extraction of the sample

1. Defat the pulverized air-dried leaves (600 g) with n-hexane.
2. Extract the dried marc (450 g) with 5 L of 90% methanol for 4 days at room temperature (25 °C).
3. Concentrate the extract in vacuo with rotary evaporator.
4. Reconstitute the dried methanol extract (35 g, 7.7% w/w) in 20 mL of methanol.
5. Dilute to 200 mL with distilled water.
6. Shake for about 30 min.
7. Perform liquid-liquid extraction with chloroform (3 mL x 750 mL) and ethyl acetate (3 mL x 750 mL) to obtain PsG-WF (8.6 g; 1.9% w/w) and PsG-EF (4.5 g) fractions, respectively.

Semi-preparative HPLC analysis

1. Analyze the sample using a Merck-Hitachi L-7100 pump coupled to a Merck-Hitachi UV detector.
2. Perform separation with a Eurospher C-18 column (10 mm, 300_8 mm i.d.; Knauer).
3. Use methanol and nanopure water as the mobile phase.
4. Set the UV detector to 254 nm.

Validation

Concentration	Amount
	3.0 mg, Garcimangosone D
	3.5 mg, Guajaphenone A
	4.5 mg, Guajaverin

实验条件、实验步骤和数据有效性验证……

使用注意事项

- 一人注册一个帐号
- 实名注册， 请提供真实姓名信息（中文名用汉语拼音全拼）
- 不得过量下载（以电子形式存储不超过5,000条记录）
- 不得账号分享
- 不得将账号用于非学术研究

2022年CAS SciFinderⁿ论坛直播日程表

	日期	主题	主讲人
基础 培训	3月1日	文献信息的获取	刘萌萌
	3月8日	物质信息的获取	钱欣
	3月15日	反应信息的获取	程小燕
	3月22日	生物序列的获取	刘萌萌
	3月29日	利用CAS SciFinder ⁿ 顺利开题、进行文献综述	钱欣
检索 策略 详解	4月25日	聚合物相关信息获取策略	程小燕
	5月24日	无机与金属有机化合物相关信息获取策略	钱欣
	6月14日	光电材料相关信息获取策略	程小燕
	7月5日	农化相关信息获取策略	钱欣
	9月13日	药物结构设计与合成	程小燕
	10月11日	天然植物化学相关信息获取策略	钱欣
	11月8日	稀土材料相关信息获取策略	程小燕
	11月29日	纳米材料相关信息获取策略	钱欣
	12月20日	催化合成信息获取策略	程小燕

直播时间:

18:00 – 19:00

关注公众号：**ACS美国化学会**
随时观看回放，了解直播信息



2022 CAS SCIFINDERⁿ 检索技能大赛

参赛对象:

中国大陆地区高校和科研院所的CAS SciFinderⁿ用户

大赛时间:

第一阶段:2022年4月11日 - 5月8日

- 在线学习CAS SciFinderⁿ检索技能,并参加线上考试
- 可参加幸运抽奖,成绩优秀者将获得CAS官方证书

第二阶段:2022年5月9日 - 6月7日

- 提交CAS SciFinderⁿ检索体验PPT
- 赢取Macbook Air、投影仪、Airpods等大奖

(详情请参看ACS美国化学会微信公众号)

参赛方式:

大赛将于2022年4月11日开启,请扫描二维码参加:



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