

# CAS SciFinder Discovery Platform

## 全面高效获取科技信息



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美国化学文摘社(CAS)北京代表处

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# CAS SCIFINDER DISCOVERY PLATFORM™

## 2024专题论坛直播时间表

结合CAS信息科学家精心撰写的相关洞察报告，了解不同领域的研究进展、趋势与创新、挑战与机会，同时进行安全的专利布局和侵权风险管理，助力自信应对立项布局、研发流程和专利调研相关的信息挑战。

9月26日 | 药物立项调研策略



11月14日 | 电池及电化学能源材料



10月24日 | 聚合物的研发与应用



12月19日 | 专利查新与规避专利侵权风险



CAS SciFinder Discovery Platform  
9月至12月的四场专题论坛

直播时间为**周四15:00 - 16:00**。扫描二维码注册，观看直播有机会获得**CAS定制纪念品**，欢迎在直播中提问互动。

# 大纲

- CAS及CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A



# CAS 具有最全面的学科连接内容合集



Over  
**50K**  
scientific journals  
and documents  
超过5万种科技期刊

Over  
**279**  
million substances  
2.79亿种数据

Over  
**50**  
languages  
translated  
50多种语言

Over  
**109**  
patent offices  
worldwide  
109个专利授权机构

# CAS独特的内容合集



来源：

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

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

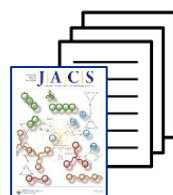
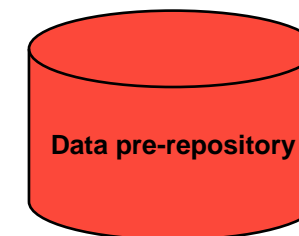
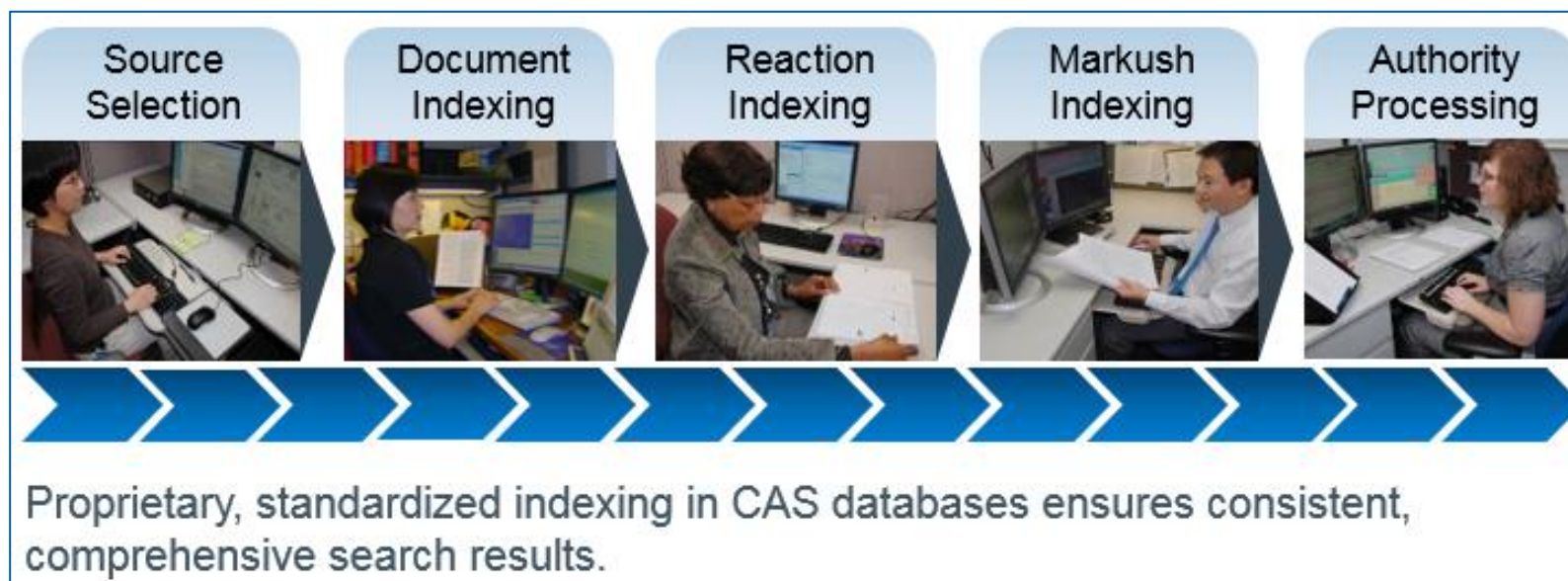
# CAS 内容合集来源于化学、超越化学

## 5大类80小类

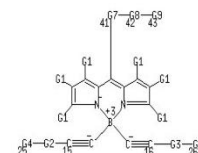
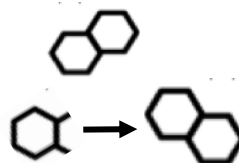
- 生物化学：
  - 药理学、农化产品管控信息、生化遗传学、发酵、免疫化学
- 有机化学各领域：
  - 有机金属化合物、脂肪/环族化合物、杂环化合物、生物分子、碳水化合物
- 大分子化学各领域：
  - 合成高聚物化学；塑料的制造、加工、成型与应用；涂料、墨水
  - 染料、有机颜料；合成橡胶；纺织品、纤维
- 应用化学各领域：
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- 物理、无机、分析化学各领域：
  - 电化学、表面化学、催化剂、相平衡、核现象

来源：<https://www.cas.org/support/documentation/references/ca-sections>

# 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科学家增值的文献研究

例: 专利WO2018152134

改写的标准和摘要，尽可能揭示专利核心价值

丰富的增值标引信息：

19 Concepts

163 Substances

625 Reactions

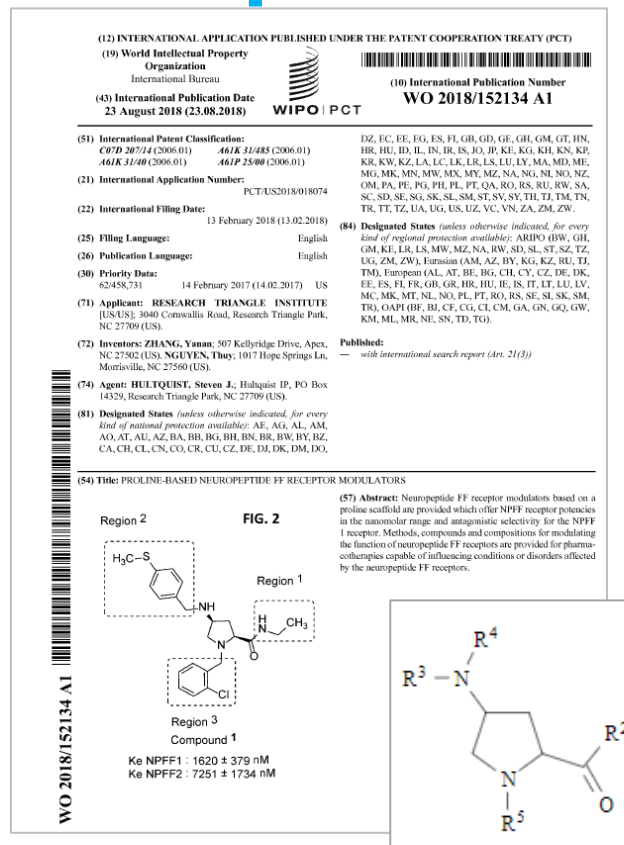
13 Patent Family Members

3 Formulations

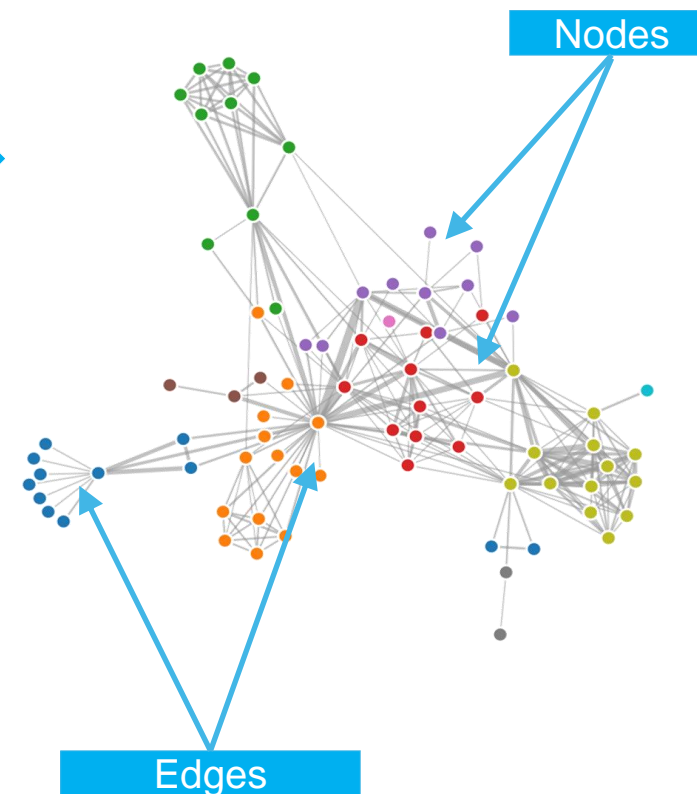
1 Markush structure

18 SAR data points

141 ADME data points



(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)  
(19) World Intellectual Property Organization  
(43) International Publication Date 23 August 2018 (23.08.2018)  
(51) International Patent Classification: A61K 31/485 (2006.01), A61K 31/40 (2006.01), A61P 25/00 (2006.01)  
(21) International Application Number: PCT/US2018/018074  
(22) International Filing Date: 13 February 2018 (13.02.2018)  
(25) Filing Language: English  
(26) Publication Language: English  
(30) Priority Data: 62/458,731 14 February 2017 (14.02.2017) US  
(71) Applicant: RESEARCH TRIANGLE INSTITUTE [US/US]; 3040 Cornwellis Road, Research Triangle Park, NC 27709 (US)  
(72) Inventors: ZHANG, Yanan; 507 Kellyridge Drive, Apex, NC 27502 (US); NGUYEN, Thuy; 1017 Hope Springs Ln, Morrisville, NC 27560 (US)  
(74) Agent: HULTQUIST, Steven J.; Hultquist IP, PO Box 14329, Research Triangle Park, NC 27709 (US)  
(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW  
(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW); Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM); European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR); OAPI (BF, BI, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG)  
(57) Abstract: Neuropeptide FF receptor modulators based on a proline scaffold are provided which offer NPFF receptor potencies in the nanomolar range and antagonistic selectivity for the NPFF1 receptor. Methods, compounds and compositions for modulating the function of neuropeptide FF receptors are provided for pharmacotherapies capable of influencing conditions or disorders affected by the neuropeptide FF receptors.  
(54) Title: PROLINE-BASED NEUROPEPTIDE FF RECEPTOR MODULATORS  
Region 2: CSC1=CC=C(NC1)C  
Region 1: CNC  
Region 3: ClC1=CC=C(NC1)C  
Compound 1: CNC1C(C(=O)N1)C2=CC=C(NC2)C  
Ke NPFF1 : 1620 ± 379 nM  
Ke NPFF2 : 7251 ± 1734 nM





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

## CAS SciFinder ——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。

# 如何获取CAS SciFinder账号

登录本校图书馆网站，查看注册相关的链接和说明

<https://lib.jiangnan.edu.cn/info/1131/1637.htm>

## 使用说明：

### 1、CAS SciFinder-n 账号注册须知

读者在使用CAS SciFindern之前须用江南大学的学校域名邮箱地址注册账号（如果已经注册了CAS SciFinder账号，请用该账号直接登录CAS SciFinder-n），根据提示输入相应信息，提交注册申请后系统将自动发送一个链接到您所填写的邮箱中，进入邮箱激活此链接即可完成注册。

### 2、SciFinder账号注册链接

<https://scifinder.cas.org/registration/index.html?corpKey=F1455EF5X86F35055X2E756CE85D18B16693>

### 3、CAS SciFinder-n检索网址

<https://scifinder-n.cas.org/>

### 4、CAS SciFinder-n培训材料及视频：

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

# 如何获取CAS SciFinder账号

登录本校图书馆网站，查看注册相关的链接和说明

请注意：

1. 必须输入真实姓名和**学校**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**：

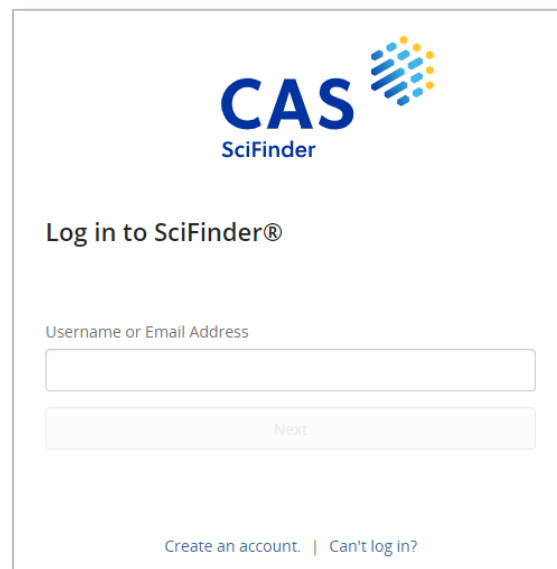
- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、\*)

例：abc@123

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

点击激活链接后注册成功

通过<https://SciFinder-n.cas.org>访问

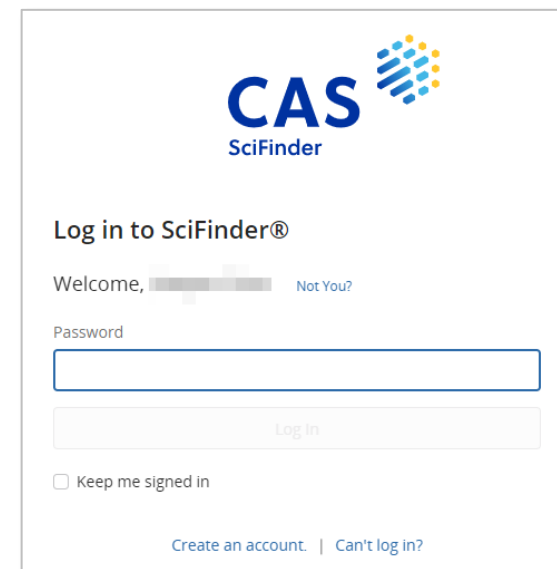


Log in to SciFinder®

Username or Email Address

Next

Create an account. | Can't log in?



Log in to SciFinder®

Welcome, [redacted] 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

检索结果管理和账号设置

The screenshot shows the CAS SciFinder main interface. On the left is a navigation sidebar with categories like 'DISCOVERY PLATFORM', 'STN IP PROTECTION SUITE', 'REGULATORY', and 'ACCOUNT MANAGEMENT'. The main header includes the CAS SciFinder logo, a user profile for Kaiqian Chen, and a '更新结果提醒' (Update Results Reminder) button. Below the header is a navigation bar with tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. A large search bar is present with a 'Draw' button highlighted. Below the search bar is an 'Author Name' field with an 'Add Advanced Search Field' button. Three feature tiles are shown: 'Retrosynthetic Analysis' (逆合成路线设计), 'Search CAS Lexicon' (CAS词库), and 'Search CAS Sequences' (CAS序列检索). At the bottom, a 'Recent Search History' section shows a search for 'fluoroketones' on July 31, 2024, with 'Rerun Search' and 'Edit Search' buttons.

更新结果提醒

Projects Saved

History Downloads You NEW

Submit Feedback

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

Draw

Author Name Enter last name, first name middle name. Example: Schubert, J A

高级检索选项

逆合成路线设计

Retrosynthetic Analysis  
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

CAS词库

Search CAS Lexicon  
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

CAS序列检索

Search CAS Sequences  
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

Recent Search History 近期检索历史 View All Search History

July 31, 2024

References fluoroketones (414 Results) 3:07 PM Rerun Search Edit Search

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A



# 您可能会感兴趣:

- 主题词怎么选择? 如何构建?
- 如何筛选文献? 追踪最新进展?
- 如何关注某篇文献的**被引文献**和**引文**?
- 如何快速获取**专利文献**中的关键信息?



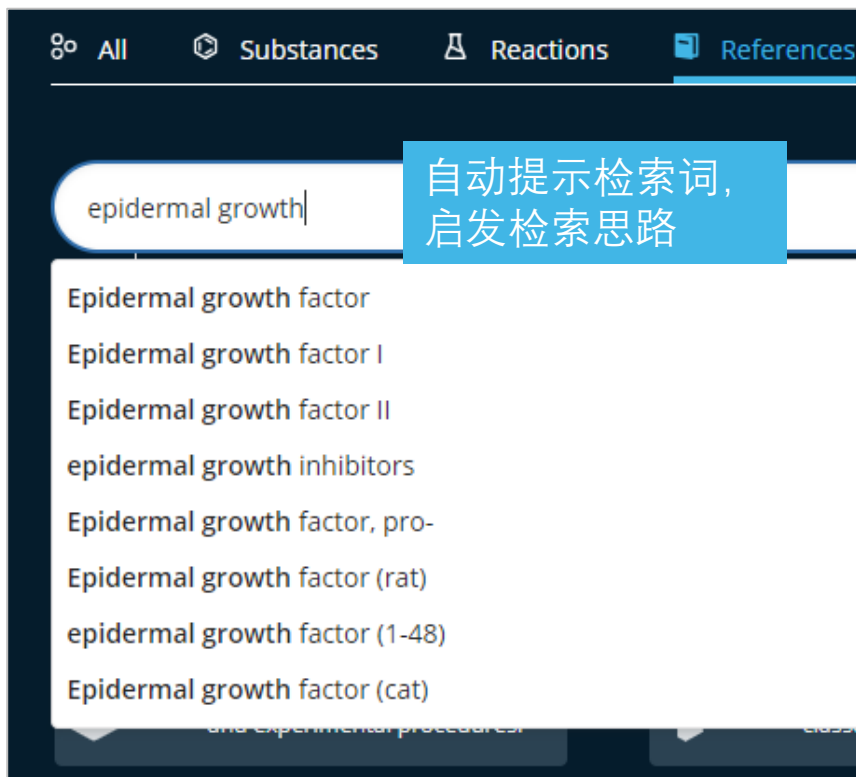
# 文献检索方式

The screenshot displays the CAS search interface. At the top, it says "Good Morning, Kaiqian" and has navigation tabs for "All", "Substances", "Reactions", "References", and "Suppliers". A search bar contains the text "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI." To the right of the search bar is a "Draw" button and a search icon. Below the search bar is a dropdown menu with the following options: "Author Name", "Publication Name", "Organization", "Title", "Abstract/Keywords", "Concept", "Substances", "Life Science Data", "Publication Year", "Document Identifier", "Patent Identifier", and "Publisher". A blue callout box labeled "结构绘制面板" (Structure Drawing Panel) points to the "Draw" button. A dropdown menu on the left side of the search bar shows the options "AND", "OR", and "NOT".

检索方法可单独使用，也可联用：

- 支持使用：关键词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
- 高级检索（刊物名、机构名、Concepts、标题等）；
- 结构检索（包括物质结构和反应式）

# 如何构建检索主题?



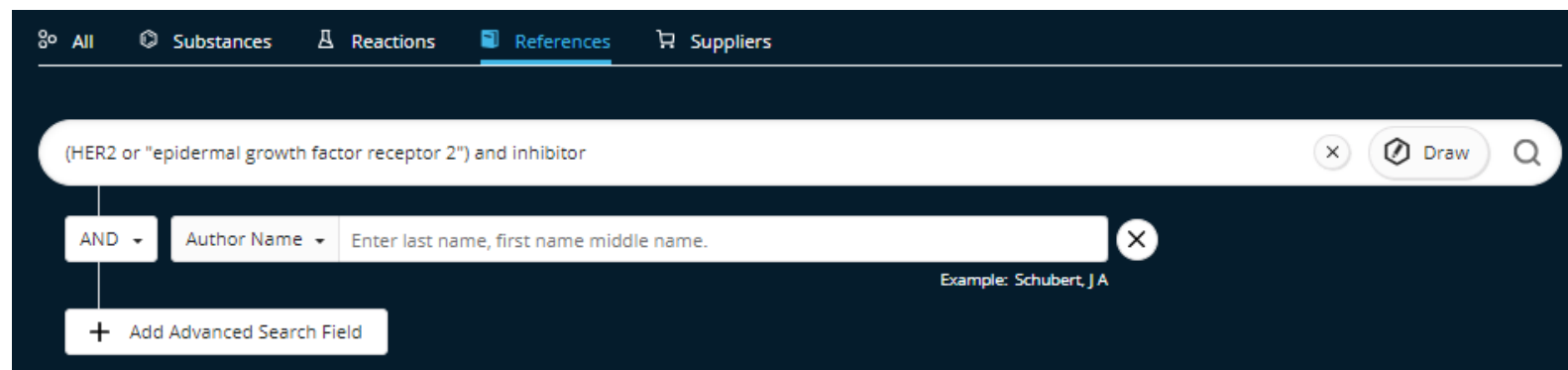
epidermal growth

自动提示检索词, 启发检索思路

- Epidermal growth factor
- Epidermal growth factor I
- Epidermal growth factor II
- epidermal growth inhibitors
- Epidermal growth factor, pro-
- Epidermal growth factor (rat)
- epidermal growth factor (1-48)
- Epidermal growth factor (cat)

- 支持布尔逻辑运算符(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? (\*代表0或多个字符; ? 代表0或1个字符)

e.g., (HER2 or "epidermal growth factor receptor 2") and inhibitor



(HER2 or "epidermal growth factor receptor 2") and inhibitor

AND Author Name Enter last name, first name middle name. Example: Schubert, J A

+ Add Advanced Search Field

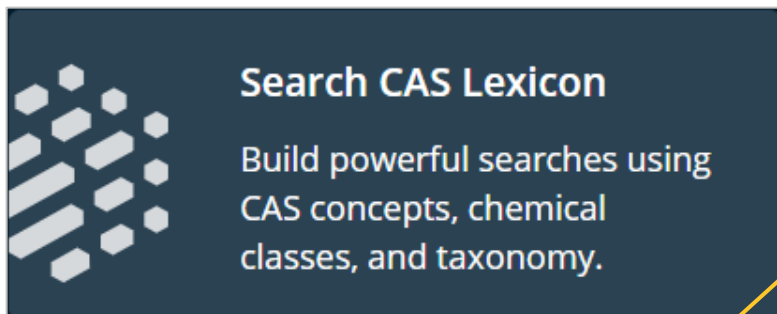


# CAS Lexicon 快速开启检索

对新的研究方向了解不深，不知道从何入手？

主题词示例：

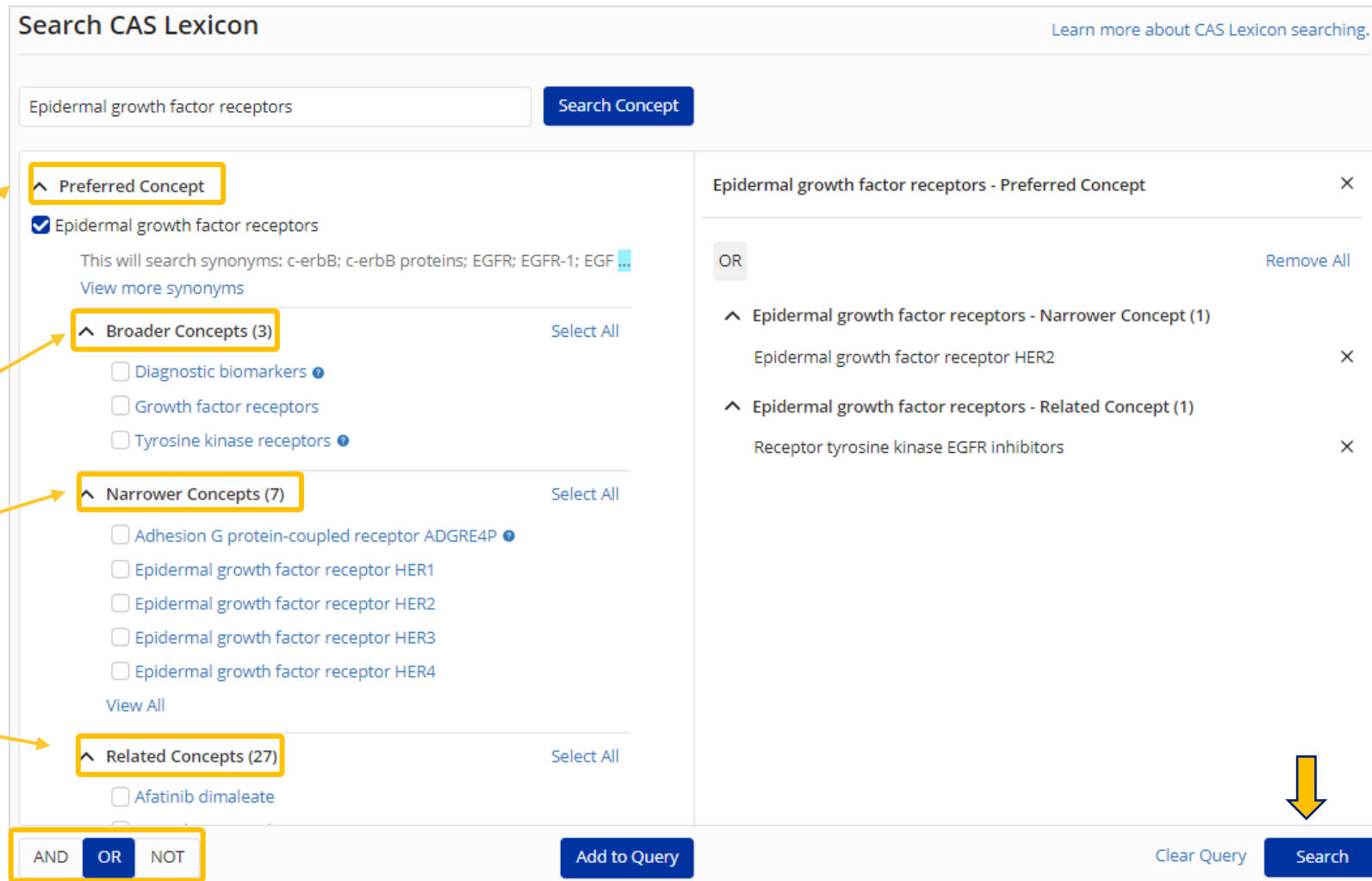
Epidermal growth factor receptors



**Search CAS Lexicon**  
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

在CAS Lexicon词库层中选择适合的主题词：

- 同义词
- 上位词
- 下位词
- 相关词



**Search CAS Lexicon** [Learn more about CAS Lexicon searching.](#)

Epidermal growth factor receptors

Preferred Concept

Epidermal growth factor receptors  
This will search synonyms: c-erbB; c-erbB proteins; EGFR; EGFR-1; EGF ...  
[View more synonyms](#)

Broader Concepts (3) [Select All](#)

- Diagnostic biomarkers
- Growth factor receptors
- Tyrosine kinase receptors

Narrower Concepts (7) [Select All](#)

- Adhesion G protein-coupled receptor ADGRE4P
- Epidermal growth factor receptor HER1
- Epidermal growth factor receptor HER2
- Epidermal growth factor receptor HER3
- Epidermal growth factor receptor HER4

[View All](#)

Related Concepts (27) [Select All](#)

- Afatinib dimaleate

Epidermal growth factor receptors - Preferred Concept

OR [Remove All](#)

- Epidermal growth factor receptors - Narrower Concept (1)  
Epidermal growth factor receptor HER2
- Epidermal growth factor receptors - Related Concept (1)  
Receptor tyrosine kinase EGFR inhibitors

AND  NOT

# 筛选文献结果

Document Type

- Journal (15K)
- Patent (4,258)
- Review (3,356)
- Biography (1)
- Clinical Trial (559)

[View All](#)

二次筛选  
文献类型  
文献语言  
发表年份  
作者  
发表机构  
期刊名称  
核心研究点  
学科研究方向  
CAS解决方案  
制剂/配方目的  
来源数据库  
.....

References search for "(HER2 or "epidermal growth factor receptor 2") and inhibitor"

Substances Reactions Citing Knowledge Graph

Sort: Relevance View: Partial Abstract

20,278 Results

1

**Celecoxib, a selective cyclooxygenase 2 inhibitor, protects against human epidermal growth factor receptor 2 (HER-2)/neu-induced breast cancer**

By: Howe, Louise R.; Subbaramaiah, Kotha; Patel, Jay; Masferrer, Jaime L.; Deora, Aparna; Hudis, Clifford; Thaler, Howard T.; Muller, William J.; Du, Baocheng; Brown, Anthony M. C.; et al

Cancer Research (2002), 62(19), 5405-5407 | Language: English, Database: CAlplus and MEDLINE

Cyclooxygenase 2 (HER-2) (Cox-2), an inducible form of Cox, is over-expressed in HER-2/neu-pos. human breast cancers. The aim of this study was to determine whether celecoxib, a selective Cox-2 inhibitor, protected against HER-2/neu-induced exptl. breast cancer. Cox-2 protein was detected in breast carcinomas from mouse mammary tumor virus (MMTV)/neu mice. Treatment with celecoxib (500 ppm) significantly reduced the incidence of mammary tumors in MMTV/neu mice (P = 0.003) and caused about a 50% reduction in mammary prostaglandin E<sub>2</sub> (PGE<sub>2</sub>) levels. Because mammary glands from MMTV/neu mice expe...

View More

Full Text

Substances (3) Reactions (0) Citing (179) Citation Map

2

**CUDC-101, a Multitargeted Inhibitor of Histone Deacetylase, Epidermal Growth Factor Receptor, and Human Epidermal Growth Factor Receptor 2, Exerts Potent Anticancer Activity**

By: Lai, Cheng-Jung; Bao, Rudi; Tao, Xu; Wang, Jing; Atoyán, Ruzanna; Qu, Hui; Wang, Da-Gong; Yin, Ling; Samson, Maria; Forrester, Jeffrey; et al

Cancer Research (2010), 70(9), 3647-3656 | Language: English, Database: CAlplus and MEDLINE

Receptor tyrosine kinase inhibitors have recently become important therapeutics for a variety of cancers. However, due to the heterogeneous and dynamic nature of tumors, the effectiveness of these agents is often hindered by poor response rates and acquired drug resistance. To overcome these limitations, we created a novel small mol., CUDC-101, which simultaneously inhibits histone deacetylase and the receptor kinases epidermal growth factor receptor (EGFR) and human epidermal growth factor receptor 2 (HER2) in cancer cells. Because of its integrated histone deacetylase inhibition, CUDC-101 sy...

View More

Full Text

Substances (7) Reactions (0) Citing (187) Citation Map

Sort: Relevance

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

排序方式:  
相关性  
引用次数  
收录号  
发表时间

# 筛选工具 CAS Section & Concept

## CAS标引的核心研究点

Concept

Top Count Alphanumeric Search

精准定位感兴趣的核心研究点

6 Selected

<input checked="" type="checkbox"/> Epidermal growth factor receptor HER2 (13K)	<input type="checkbox"/> Lung neoplasm (1,885)	<input type="checkbox"/> Antitumor agent resistance (1,106)
<input type="checkbox"/> Homo sapiens (13K)	<input type="checkbox"/> Antineoplastic Combined Chemotherapy Protocols (1,882)	<input type="checkbox"/> Insulin-like growth factor I receptors (1,093)
<input type="checkbox"/> Human (13K)	<input checked="" type="checkbox"/> Drug targets (1,879)	<input type="checkbox"/> Vascular endothelial growth factor receptor 2 (1,090)
<input type="checkbox"/> Humans (11K)	<input type="checkbox"/> Epidermal growth factor receptor HER3 (1,865)	<input type="checkbox"/> Bladder neoplasm (1,088)
<input checked="" type="checkbox"/> Antitumor agents (8,765)	<input type="checkbox"/> Antibodies and Immunoglobulins (1,785)	<input type="checkbox"/> Mammary gland neoplasm, metastasis (1,073)
<input type="checkbox"/> Female (7,862)	<input type="checkbox"/> Phosphorylation (1,740)	<input type="checkbox"/> Metastasis, mammary gland neoplasm (1,073)
<input checked="" type="checkbox"/> Mammary gland neoplasm (7,394)	<input type="checkbox"/> Progesterone receptors (1,678)	<input type="checkbox"/> Immunotherapy (1,072)
<input checked="" type="checkbox"/> Epidermal growth factor receptors (6,078)	<input type="checkbox"/> Metastasis (1,649)	<input type="checkbox"/> Antibodies, Monoclonal, Humanized (1,054)
<input checked="" type="checkbox"/> Breast Neoplasms (6,016)	<input type="checkbox"/> Prostate gland neoplasm (1,649)	<input type="checkbox"/> Head and neck neoplasm (1,039)
<input type="checkbox"/> Receptor, ErbB-2 (5,216)	<input type="checkbox"/> Drug Resistance, Neoplasm (1,628)	<input type="checkbox"/> Lung Neoplasms (1,032)
<input type="checkbox"/> Signal transduction (4,936)	<input type="checkbox"/> Gene Expression Regulation, Neoplastic (1,571)	<input type="checkbox"/> Protein sequences (1,026)
<input type="checkbox"/> Cell proliferation (3,867)	<input type="checkbox"/> Male (1,570)	<input type="checkbox"/> Immunohistochemistry (1,017)
<input type="checkbox"/> Cell Line, Tumor (3,531)		<input type="checkbox"/> Treatment Outcome (1,016)
<input type="checkbox"/> Animals (3,451)		
<input type="checkbox"/> Neoplasm (3,187)		

Apply Cancel

## CAS标引的学科研究方向

CA Section

By Count Alphanumeric

4 Selected

<input checked="" type="checkbox"/> Pharmacology (8,448)	<input type="checkbox"/> Nonmammalian Biochemistry (20)	<input type="checkbox"/> Aliphatic Compounds (2)
<input checked="" type="checkbox"/> Mammalian Pathological Biochemistry (4,190)	<input type="checkbox"/> Benzene, Its Derivatives, and Condensed Benzenoid Compounds (17)	<input type="checkbox"/> Alkaloids (2)
<input type="checkbox"/> Unavailable (2,669)	<input type="checkbox"/> Animal Nutrition (15)	<input type="checkbox"/> Inorganic Chemicals and Reactions (2)
<input checked="" type="checkbox"/> Immunochemistry (1,720)	<input type="checkbox"/> Carbohydrates (14)	<input type="checkbox"/> Agrochemical Bioregulators (1)
<input checked="" type="checkbox"/> Pharmaceuticals (864)	<input type="checkbox"/> Fermentation and Bioindustrial Chemistry (10)	<input type="checkbox"/> Air Pollution and Industrial Hygiene (1)
<input type="checkbox"/> Heterocyclic Compounds (More Than One Hetero Atom) (703)	<input type="checkbox"/> Plant Biochemistry (9)	<input type="checkbox"/> Chemistry of Synthetic High Polymers (1)
<input type="checkbox"/> Biochemical Methods (381)	<input type="checkbox"/> Heterocyclic Compounds (More Than One Hetero Atom, 7)	<input type="checkbox"/> Crystallography and Liquid Crystals (1)
<input type="checkbox"/> Biochemical Genetics (284)	<input type="checkbox"/> General Organic Chemistry (6)	<input type="checkbox"/> General Physical Chemistry (1)
<input type="checkbox"/> Mammalian Hormones (249)	<input type="checkbox"/> Microbial, Algal, and Fungal Biochemistry (6)	<input type="checkbox"/> Heterocyclic Compounds (One Hetero Atom, 1)
<input type="checkbox"/> Radiation Biochemistry (190)	<input type="checkbox"/> Organometallic and Organometalloidal Compounds (6)	<input type="checkbox"/> Industrial Inorganic Chemicals (1)
<input type="checkbox"/> Mammalian Biochemistry (123)	<input type="checkbox"/> Terpenes and Terpenoids (6)	<input type="checkbox"/> Industrial Organic Chemicals, Leather, Fats, and Waxes (1)
<input type="checkbox"/> Heterocyclic Compounds (One Hetero Atom) (94)	<input type="checkbox"/> Food and Feed Chemistry (4)	<input type="checkbox"/> Physical Organic Chemistry (1)
<input type="checkbox"/> Amino Acids, Peptides, and Proteins (58)		<input type="checkbox"/> Plastics Manufacture and Processing (1)
<input type="checkbox"/> Enzymes (49)		

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# 关注某作者的研究

高级检索选项，细化检索区域

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

Author Name | Ding, J

+ Add Advanced Search Field

Author

Top Count | Alphanumeric | Search

Author Name (Last, First Middle)

Ding, Jian

Ex: Schubert, J A

3 Selected

<input checked="" type="checkbox"/> Ding, J (257)	<input type="checkbox"/> Ding, Jian Hua (3)	<input type="checkbox"/> Ding, J. K. (2)
<input checked="" type="checkbox"/> Ding, J. (813)	<input type="checkbox"/> Ding, Jian Huan (1)	<input type="checkbox"/> Ding, J. L. (13)
<input type="checkbox"/> Ding, J A (16)	<input type="checkbox"/> Ding, Jian Hui (2)	<input type="checkbox"/> Ding, J. L. (68)
<input type="checkbox"/> Ding, J. A. (1)	<input type="checkbox"/> Ding, Jian Jun (2)	<input type="checkbox"/> Ding, J M (8)
<input type="checkbox"/> Ding, J B (3)	<input type="checkbox"/> Ding, Jian L. (18)	<input type="checkbox"/> Ding, J. M. (7)
<input type="checkbox"/> Ding, J. B. (4)	<input type="checkbox"/> Ding, Jian Liang (1)	<input type="checkbox"/> Ding, J N (4)
<input type="checkbox"/> ding, J. B. Har (1)	<input type="checkbox"/> Ding, Jian Ling (13)	<input type="checkbox"/> Ding, J. N. (47)
<input type="checkbox"/> Ding, J C (27)	<input type="checkbox"/> Ding, Jian M. (16)	<input type="checkbox"/> ding, J. N. Re (2)
<input type="checkbox"/> Ding, J. C. (4)	<input type="checkbox"/> Ding, Jian Mei (4)	<input type="checkbox"/> Ding, J P (20)
<input type="checkbox"/> Ding, J. D. (3)	<input type="checkbox"/> Ding, Jian Min (2)	<input type="checkbox"/> Ding, J. P. (16)
<input type="checkbox"/> Ding, J F (9)	<input type="checkbox"/> Ding, Jian Ming (1)	<input type="checkbox"/> Ding, J Q (6)
<input type="checkbox"/> Ding, J. F. (11)	<input type="checkbox"/> Ding, Jian NAME NOT TRANS.	<input type="checkbox"/> Ding, J. Q. (10)

OK | Cancel

References search for "Ding, J" Author Name

Substances | Reactions | Citing | Knowledge Graph

Filtering: Author: 3 Selected

4,126 Results | Sort: Relevance | View: Partial Abstract

1

**A kind of durable and easily degradable type colored woven cloth**

Assignee: Nantong Tongzhou District Tianchong Textile Co., Ltd. China, CN219405666 U 2023-07-25 | Language: Chinese, Database: CAPlus

[Machine Translation of Descriptors]. The utility model belongs to the yarn-dyed fabric technol. field, especially a kind of durable easily degradable type yarn-dyed fabric, including base fabric layer, the base fabric layer is sewed with the antimicrobial layer, the base fabric layer is made of woven warp and weft yarns, wherein the warp yarn and the weft yarn are can degrade the fiber strand, the weft yarn is made from bamboo charcoal fibers I and seaweed fiber by blending together, the warp yarn is composed of seaweed fiber II and chitin fibers blended together. The durable easily degradable...

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

2

**Manufacturing process of deep-light color interphase yarn-dyed fabric**

Assignee: Nantong Tongzhou District Tianchong Textile Co., Ltd. China, CN115961407 A 2023-04-14 | Language: Chinese, Database: CAPlus

[Machine Translation of Descriptors]. The present invention discloses a process for manufacturing a deep and light color interphase dyed fabric, which relates to the tech. field of weaving, comprising the following steps:(1) dividing the cotton yarn into two equal parts of Me Et, pre-treating the A part, and not pre-treating the B part;(2) dark dyeing the pre-treated A cotton yarn;(3) performing a light-color dyeing treatment on the B yarn, wherein the dye for the B dyeing is the same color as the dye for the A part dyeing;(4) soaping treatment was carried out on the A cotton yarn after dark c...

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

先全面检索，再筛选精炼

# 关注某作者的研究

## 机构名称的筛选

Organization

- Chinese Academy of Sciences (345)
- Shanghai Institute of Materia Medica, Chinese Academy of Sciences (263)
- National University of Singapore (207)
- Hebei University of Technology (96)
- Jiangnan University (61)

[View All](#)

Organization

Top Count Alphanumeric Search

102 Selected

- Chinese Academy of Sciences (345)
- Shanghai Institute of Materia Medica, Chinese Academy of Sciences (263)
- National University of Singapore (207)
- Hebei University of Technology (96)
- Jiangnan University (61)
- China ENFI Engineering Corporation (58)
- Northeast Agricultural University (50)
- [NAME NOT TRANSLATED] (47)
- Shanghai Jiaotong University (39)
- Hebei University of Technology (37)
- Inner Mongolia Energy Co., Ltd.
- Ningbo University
- Dalian Minzu University
- Hohai University
- Jiangsu University
- Nanyang Hanyuan Co., Ltd. (15)
- The Second Affiliated Hospital and Yuying Children's Hospital of Wenzhou Medical University (15)
- Institute of Process Engineering, Chinese Academy of Sciences (14)
- Institute of Process Engineering, Chinese Academy of Sciences (14)
- Jilin University

OK Cancel

Organization

Top Count Alphanumeric Search

Organization Name

Shanghai Institute of Materia Medica Search

231 Selected

- 1Division of Anti-Tumor Pharmacology, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 501 Haik Road, Shanghai, 201203 China. (1)
- 2Division of Anti-tumor Pharmacology, State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China. (1)
- Authors' Affiliations: Division of Antitumor Pharmacology and Division of Medicinal Chemistry, State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of
- Division of Anti-tumor Pharmacology, Institute of Materia Medica, Graduate School of the Chinese Academy of Sciences, Zhangjiang, Pu Dong, Shanghai, PR China. (1)
- Division of Anti-tumor Pharmacology, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 501 Haik Road, Shanghai, 201203, China. (1)
- Division of Anti-tumor Pharmacology, Shanghai Institute of Materia Medica, Chinese Academy of
- Division of Anti-tumor Pharmacology, State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zu Chong Zhi Road, Zhangjiang Hi-Tech Park, Shanghai 201203, Peoples' Republic of China. (1)
- Division of Anti-Tumor Pharmacology, State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zu Chong Zhi Road, Zhangjiang Hi-Tech Park, Shanghai 201203, P.R. China. (1)
- Division of Antitumor

← Prev 1 2 3 Next →

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# 文献详情

检索范围：标题，摘要，关键词，CAS标引的核心研究点、物质信息等

**BIBW2992, an irreversible EGFR/HER2 inhibitor highly effective in preclinical lung cancer models**

6 0 1,133 Citation Map 引文地图

**In this Reference**

- Concepts
- Substances
- Biomarkers
- Cited Documents

By: Li, D.; Ambrogio, L.; Shimamura, T.; Kubo, S.; Takahashi, M.; Chirieac, L. R.; Padera, R. F.; Shapiro, G. I.; Baum, A.; Himmelsbach, F.; et al  
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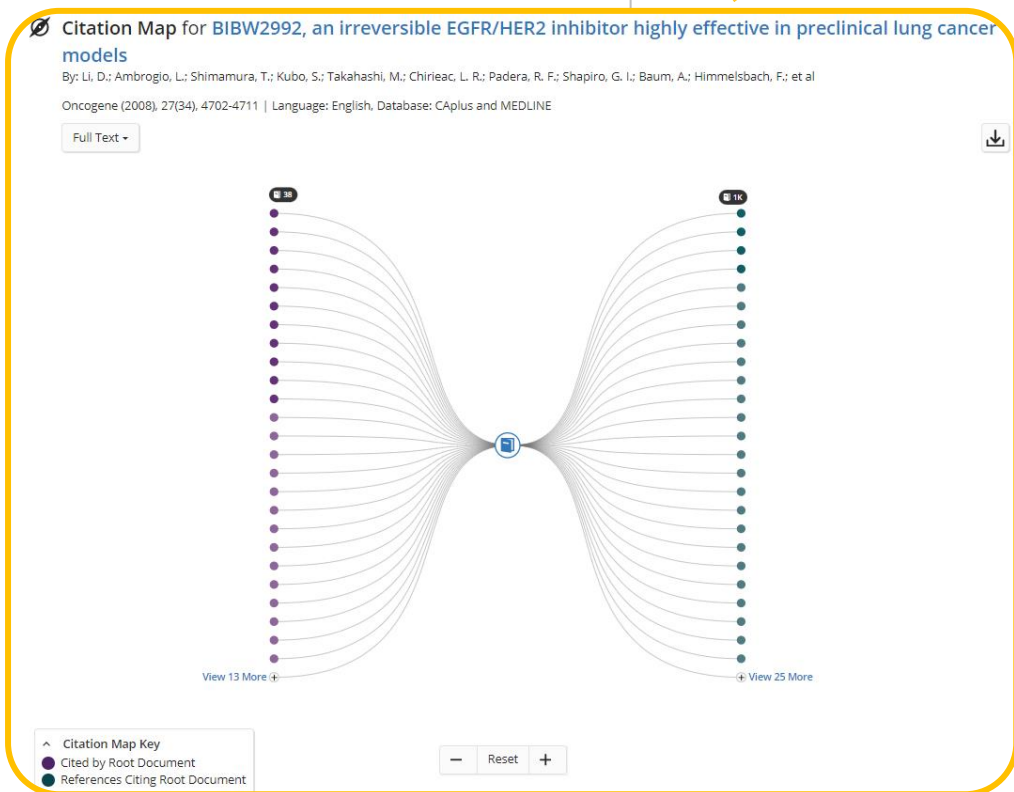
DOI: 10.1038/onc.2008.109

Genetic alterations in the kinase domain of the epidermal growth factor receptor (EGFR) in non-small cell lung cancer (NSCLC) patients are associated with sensitivity to treatment with small mol. tyrosine kinase inhibitors. Although first-generation reversible, ATP-competitive inhibitors showed encouraging clin. responses in lung adenocarcinoma tumors harboring such EGFR mutations, almost all patients developed resistance to these inhibitors over time. Such resistance to first-generation EGFR inhibitors was frequently linked to an acquired T790M point mutation in the kinase domain of EGFR, or upregulation of signaling pathways downstream of HER3. Overcoming these mechanisms of resistance, as well as primary resistance to reversible EGFR inhibitors driven by a subset of EGFR mutations, will be necessary for development of an effective targeted therapy regimen. Here, we show that BIBW2992, an anilinoquinazoline designed to irreversibly bind EGFR and HER2, potently suppresses the kinase activity of wild-type and activated EGFR and HER2 mutants, including erlotinib-resistant isoforms. Consistent with this activity, BIBW2992 suppresses transformation in isogenic cell-based assays, inhibits survival of cancer cell lines and induces tumor regression in xenograft and transgenic lung cancer models, with superior activity over erlotinib. These findings encourage further testing of BIBW2992 in lung cancer patients harboring EGFR or HER2 oncogenes. *Oncogene* (2008) 27, 4702-4711; doi:10.1038/onc.2008.109; published online 14 Apr. 2008.

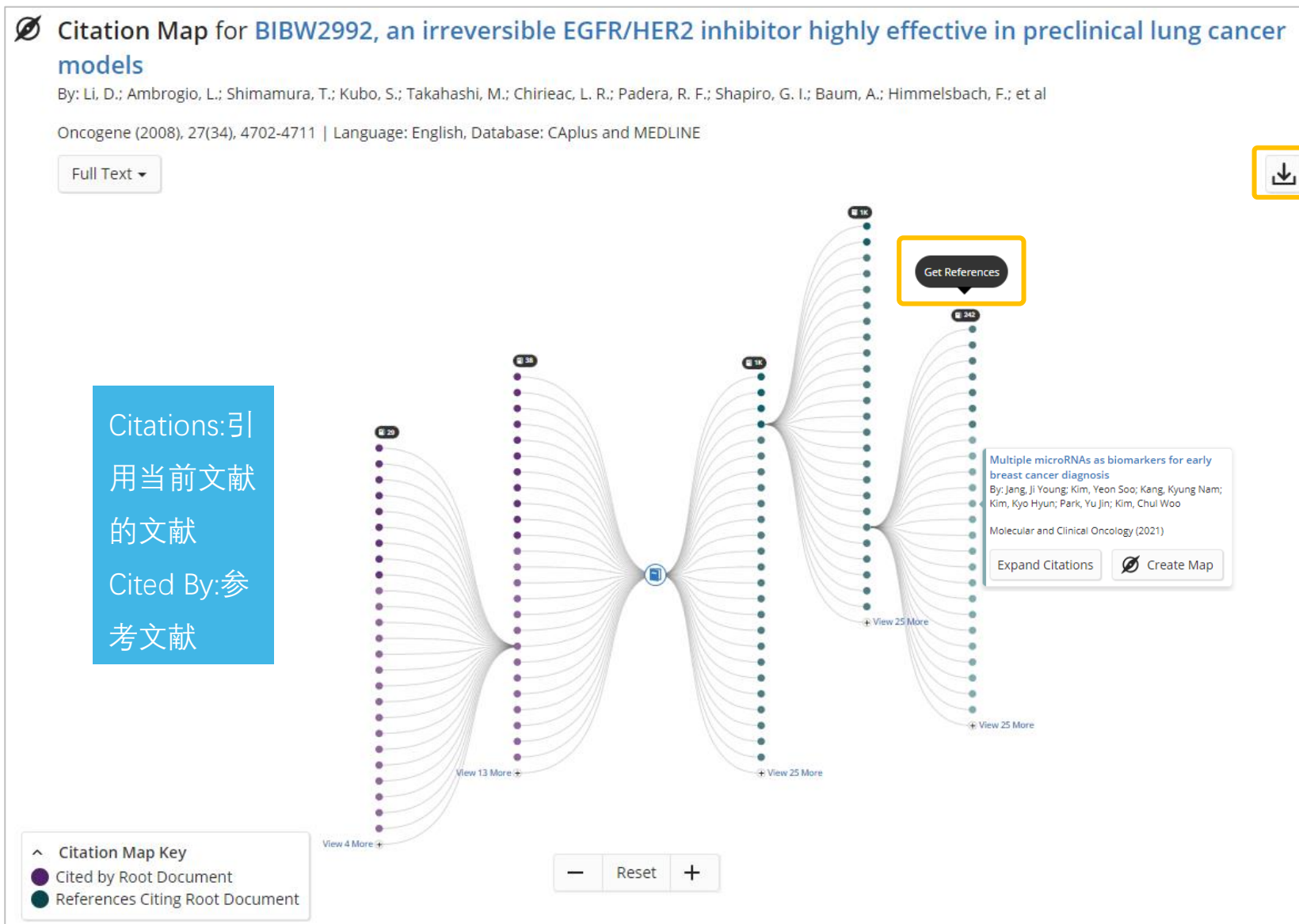
**Keywords:** antitumor resistance anilinoquinazoline derivative BIBW2992 EGFR HER2 lung cancer

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# 引文地图——便捷获取引文信息



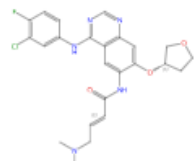
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- 可拓展
- 可下载
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# 文献详情

## Substances

原文中重点研究的物质信息

850140-72-6



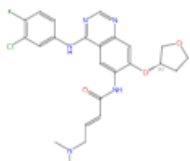
Absolute stereochemistry shown  
Double bond geometry shown

$C_{24}H_{25}ClFN_5O_3$   
Afatinib

Role: Unspecified

物质角色

439081-18-2

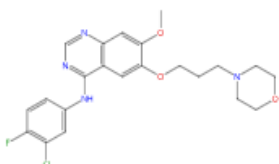


Absolute stereochemistry shown  
Double bond geometry unknown

$C_{24}H_{25}ClFN_5O_3$   
N-[4-[(3-Chloro-4-fluorophenyl)amino]-7-[[[(3S)-tetrahydro-3-furanyl]oxy]-6-quinazolin-2-ylamino]-3,4-dichlorobenzamide

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

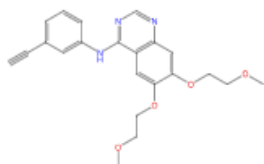
184475-35-2



$C_{22}H_{24}ClFN_4O_3$   
Gefitinib

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

183321-74-6



$C_{22}H_{23}N_3O_4$   
Erlotinib

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

## CAS Concepts

CAS标引的核心研究点

Antitumor agent resistance

Epidermal growth factor receptors  
Role: Biological Study, Unclassified

Antitumor agents

Homo sapiens

Covalent inhibitors

Human

Drug targets

Mutation  
Modifier: EGFR and HER2

Epidermal growth factor receptor HER2

Role: Biological Study, Unclassified

Non-small-cell lung carcinoma

Epidermal growth factor receptor HER3

Role: Biological Study, Unclassified

Protein phosphorylation

## Reactions

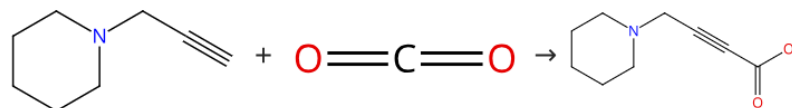
原文中重点研究的反应信息

244

31-320-CAS-11506461

Steps: 1 Yield: 100%

[View Experimental Protocols](#)

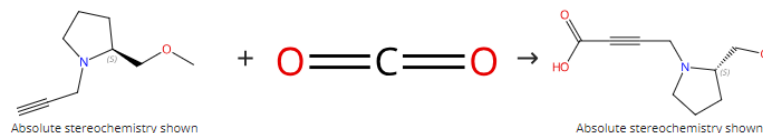


1.1 Reagents: [Butyllithium](#)  
Solvents: [Tetrahydrofuran](#), [Hexane](#)  
1.2 -

31-320-CAS-8784633

Steps: 1 Yield: 99%

[View Experimental Protocols](#)



1.1 Reagents: [Butyllithium](#)  
Solvents: [Tetrahydrofuran](#), [Hexane](#)  
1.2 -



# 专利文献详情

## Combination of a purine-based CDK inhibitor with a tyrosine kinase inhibitor and use thereof in the treatment of proliferative disorders

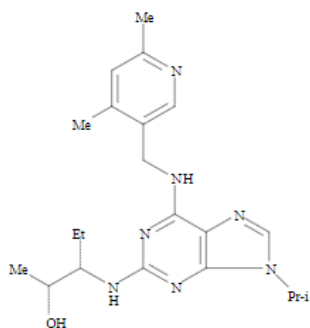
51 30 7 Citation Map

### In this Reference

By: Green, Simon; Frame, Sheelagh; Fleming, Ian

- IPC Data
- CAS Concepts
- Substances
- Reactions
- Formulations
- Cited Documents

The present invention relates to combination comprising (i) an ErbB inhibitor; and (ii) a CDK inhibitor, or a pharmaceutically acceptable salt thereof, selected from: (a) roscovitine; (b) 3-(9-isopropyl-6-((pyridin-3-yl-methyl)-amino)-9H-purin-2-yl-amino)-2-methyl-pentan-2-ol; (c) 3-(9-isopropyl-6-((pyridin-3-yl-methyl)-amino)-9H-purin-2-yl-amino)-pentan-2-ol; and (d) (2R,3S)-3-(6-(4,6-dimethyl-pyridin-3-yl-methylamino)-9-isopropyl-9H-purin-2-yl-amino)pentan-2-ol. Further aspects of the invention relate to pharmaceutical products and pharmaceutical compositions comprising combinations according to the invention, and methods of treatment using the same. Thus, the combination of trastuzumab (an ErbB2 inhibitor) and seliciclib (a CDK inhibitor) produced greater downregulation of the HER2 receptor in breast cancer cell lines than either single agent treatment alone, suggesting that the drugs synergistically downregulate the levels of this receptor.



Keywords: CDK kinase inhibitor, ErbB tyrosine kinase inhibitor, proliferative disorder; purine CDK kinase inhibitor, tyrosine kinase inhibitor

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Publication Information Patent

CAS PatentPak

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### Patent Family 专利家族

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
WO2008122779	English	A1	PDF   PDF+   <b>Viewer</b>	2008-10-16	WO2008-GB1189	2008-04-02
EP2139486	English	A1		2010-01-06	EP2008-718990	2008-04-02
CN101678029	Chinese	A		2010-03-24	CN2008-80018864	2008-04-02
JP2010523536	Japanese	T		2010-07-15	JP2010-501589	2008-04-02

### IPC Data

### IPC信息

Patent	Class	Patent Family Classification Codes
WO2008122779	IPC1	A61K 0031/52; A61K 0031/517; A61K 0045/00; A61K 0045/06; A61P 0035/00
EP2139486	IPC1	A61K 0031/52; A61K 0031/517; A61K 0045/00; A61K 0045/06; A61P 0035/00
CN101678029	IPC1	A61K 0031/52; A61K 0031/517; A61K 0045/00; A61K 0045/06; A61P 0035/00
JP2010523536	IPC1	A61K 0031/52; A61K 0045/00; A61K 0031/517; A61K 0039/395; A61K 0031/5377; A61P 0043/00; A61P 0035/00

### CAS Concepts

#### Antitumor agents

#### CAS标引的核心研究点

Head and neck neoplasm

#### Apoptosis

Homo sapiens

#### Combination chemotherapy

Human

#### Drug delivery systems Modifier: kits

Lung neoplasm

#### Drug interactions, synergistic

Mammary gland neoplasm

### 题录信息

### 物质信息

### Substances

1070912-92-3  
Image Not Available

Unidentified PKI

**PatentPak**

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

1070862-90-6

C<sub>20</sub>H<sub>29</sub>N<sub>7</sub>O  
2-Methyl-3-[[9-(1-methylethyl)-6-[[3-pyridinyl(methyl)amino]-9H-purin-2-yl]amino]...

**PatentPak**

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

1070791-10-4

C<sub>16</sub>H<sub>19</sub>FN<sub>6</sub>  
N-[[4,6-Dimethyl-3-pyridinyl]methyl]-2-fluoro-9-(1-methylethyl)-9H-purin-6-amine

**PatentPak**

Role: Properties, Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

1070791-09-1

C<sub>13</sub>H<sub>13</sub>FN<sub>6</sub>  
N-[[4,6-Dimethyl-3-pyridinyl]methyl]-2-fluoro-9H-purin-6-amine

**PatentPak**

Role: Properties, Reactant, Synthetic Preparation, Reactant or Reagent, Preparation

# CAS PatentPak: 高效浏览专利

一键定位专利原文中的核心研究物质

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The screenshot displays the CAS PatentPak interface. At the top, there are navigation controls for PAGE (8 / 81), ZOOM, and DOWNLOAD (PDF, PDF+). The main content area shows a patent document with two paragraphs of text. The first paragraph discusses H1650 cells and the combination of seliciclib and erlotinib. The second paragraph discusses cetuximab. On the left side, there are two sections for 'Key Substances in Patent'. The first section shows the CAS RN 183321-74-6 with a chemical structure and a yellow arrow pointing to a location in the first paragraph. The second section shows the CAS RN 231277-92-2 with a chemical structure and a blue location pin pointing to a location in the second paragraph. Below each chemical structure, there are 'Analyst Markup Locations' listed as Page 8, Page 8, and Page 64 for the first substance, and Page 9, Page 10, and Page 64 for the second substance.

# 小结

- **灵活构建检索主题：**布尔逻辑运算符支持的灵活主题词构建，全面精准获取最相关的研究文献，高效获取领域研究前沿及全貌信息。
- **CAS Lexicon：**便捷获取CAS科学家标引的层级词库，拓展领域标准词，简便快速开启自动检索。
- **检索结果的分析与精炼：**丰富的聚类分析选项，如Concept、CA Section等，快速缩小文献范围，细化研究热点及领域，多维度了解技术布局情况，并聚焦最感兴趣的文献，加速突破技术瓶颈。
- **文献详情速览：**基于CAS的数据关联，从最相关的研究文献中获取重要的信息。利用引文地图拓展文献检索。
- **CAS PatentPak：**高效阅读专利原文，定位其中的关键物质；重点专利现有技术分析。节省查阅全文所需的时间和精力，专注于研发与创新工作。

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A



# 您可能会感兴趣:

- 检索完整分子结构? 通式结构? 或含有某些片段的物质?
- 结构式信息不足该如何检索?
- 利用谱图数值确认产物或杂质? 从属性值出发, 调研某类材料?
- 如何确认结构新颖性和可专利性?



# 物质检索的方式

灵活的检索方式，满足各种物质类别的检索

通过物质标识符、文献标识符等关键词检索物质

自定义联合检索

使用结构绘制面板进行结构检索

AND  
OR  
NOT

Retrosynthetic Analysis  
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

Search CAS Lexicon  
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Search CAS Sequences  
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

## 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—物质/文献标识符

- 可同时检索多个物质识别符（物质名称或CAS RN）
- 不同物质使用空格隔开（<2000个字符）

- 迅速获得关注文献中的物质信息

The image displays two screenshots of the CAS SciFinder interface. The left screenshot shows a search for "polyformaldehyde" with 2 results. The first result is 9002-81-7, identified as Polyformaldehyde, with 8,752 references, 291 reactions, and 11 suppliers. The right screenshot shows a search for "10.1039/c3py00121k" with 15 results. The first three results are: 68-12-2 (Dimethylformamide, 181K references, 4.4M reactions, 336 suppliers), 109-72-8 (Butyllithium, 29K references, 581K reactions, 57 suppliers), and 128-08-5 (N-Bromosuccinimide, 21K references, 206K reactions, 110 suppliers). Both screenshots include a "Filter Behavior" panel with options for "Filter by" and "Exclude", and a "Search Within Results" section with checkboxes for Reaction Role (Product, Reactant, Reagent, Catalyst, Solvent) and Reference Role (Adverse Effect).

# 物质检索—CAS Draw: 结构绘制面板

重要结构绘制工具注释:

**X** 选择可变基团

**R** 自定义R基团

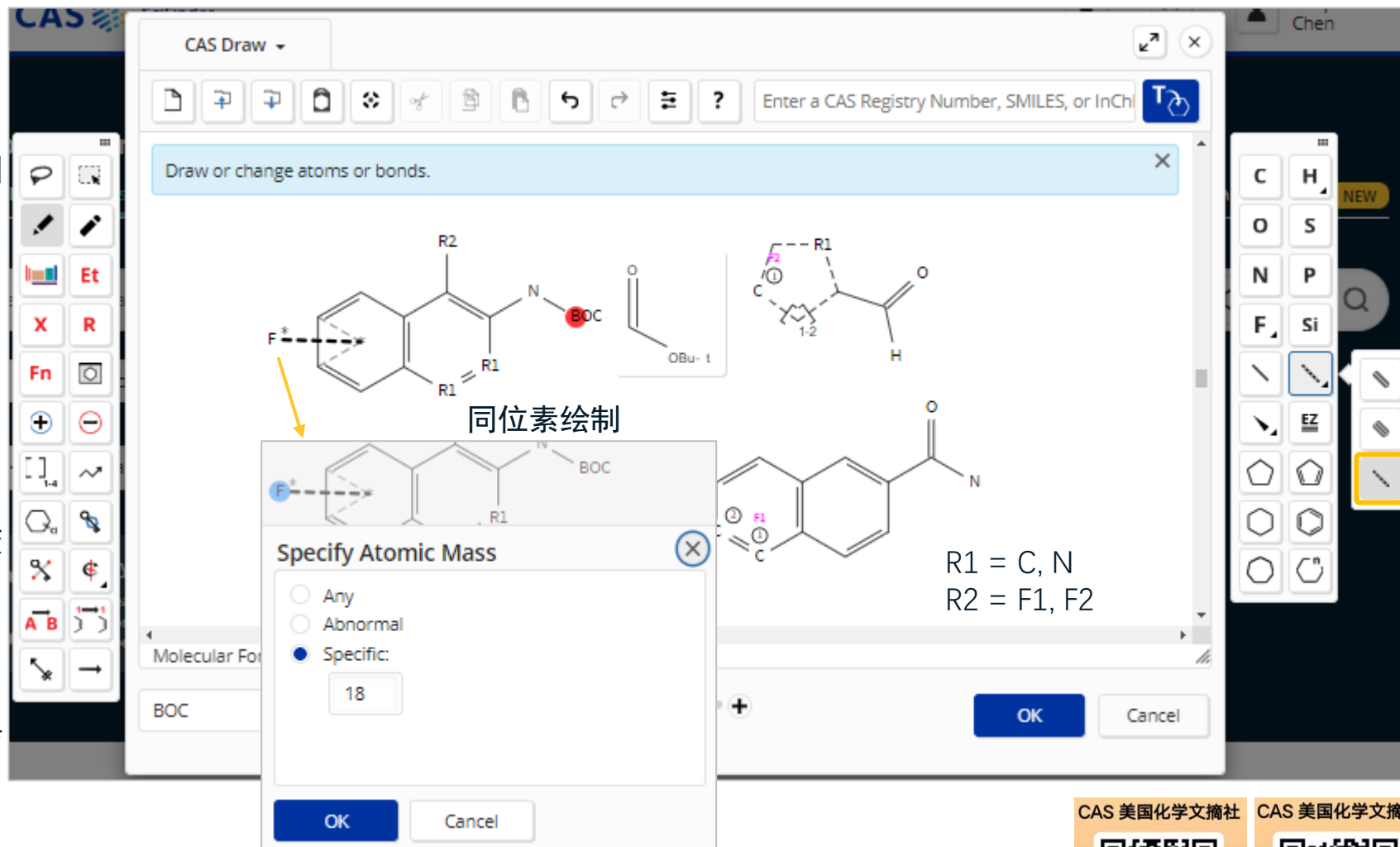
**Fn** 片段结构

[ ]<sub>1-4</sub> 重复工具

 取代位置可变

 环锁定工具

 原子锁定工具



CAS Draw

Enter a CAS Registry Number, SMILES, or InChI

Draw or change atoms or bonds.

同位素绘制

Specify Atomic Mass

Any

Abnormal

Specific:

18

OK Cancel

OK Cancel

R1 = C, N  
R2 = F1, F2

R-Group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10

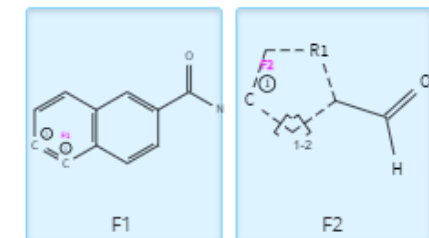
R2: F1 [1, 2], F2

Isotopes D T

> Variables

> Shortcuts

▼ Fragments



线上学习短视频:

CAS 美国化学文摘社

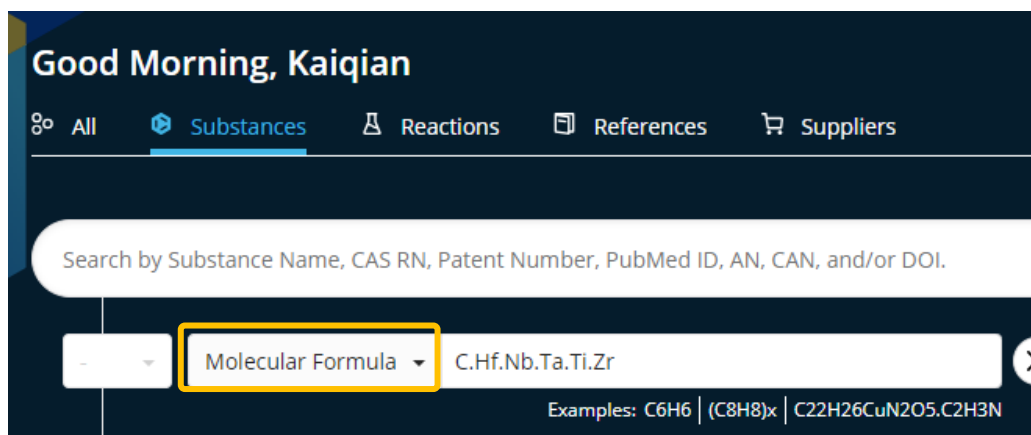


CAS 美国化学文摘社





# 物质检索—分子式检索



- 希尔(Hill)排序规则：C排首位，H排第二，其他元素符号按照首字母顺序进行排列。当化学式不含C时，所有元素（包括H）按字母顺序列出。
- 不同组分之间用“.”隔开，如：高熵碳化物 C.Hf.Nb.Ta.Ti.Zr
- 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

### Substances search for "C.Hf.Nb.Ta.Ti.Zr" Molecular Formula

示例：高熵碳化物

8 Results

Result ID	Component	Ratio
2304767-82-4	C	1
	Zr	0.20
	Hf	0.20
	Ti	0.20
	Ta	0.20
	Nb	0.20

Result ID	Component	Ratio
1427190-21-3	Zr	x
	Hf	x
	C	x
	Ti	x
	Ta	x
	Nb	x

Result ID	Component	Ratio
2649374-42-3	C	1
	Zr	0-1
	Hf	0-1
	Ti	0-1
	Ta	0-1
	Nb	0-1

### Substances search for "H2O4S.2Na" Molecular Formula

示例：硫酸钠

9 Results

Result ID	Chemical Structure	Component	Ratio
7757-82-6		H <sub>2</sub> O <sub>4</sub> S.2Na	• 2 Na
		Sulfate	

Result ID	Chemical Structure	Component	Ratio
13759-07-4		H <sub>2</sub> O <sub>4</sub> S.2Na	• 2 Na
		Thenardite (Na <sub>2</sub> (SO <sub>4</sub> ))	

Result ID	Chemical Structure	Component	Ratio
14262-80-7		H <sub>2</sub> O <sub>4</sub> S.2Na	• 2 Na
		Sulfuric- <sup>35</sup> S acid, disodium salt	

# 物质检索—属性值、谱图数值联用检索

The screenshot displays the CAS search interface. At the top, there are navigation tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. A search bar is present with the text 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' Below the search bar, a dropdown menu is open, showing various search criteria. The 'Molecular Formula' dropdown is selected, and a list of search fields is displayed. The fields are organized into two columns. The left column includes: Molecular Formula, CAS Registry Number, Chemical Identifier, Document Identifier, Patent Identifier, Experimental Spectra (highlighted), Life Science Data, Biological, Chemical Properties (highlighted), Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal (highlighted). The right column includes: Koc, logD, logP, Mass Intrinsic Solubility (g/L), Mass Solubility (g/L), Molar Intrinsic Solubility (mol/L), Molar Solubility (mol/L), Molecular Weight, pKa, Vapor Pressure (Torr), Proton NMR, Carbon-13 NMR, Nitrogen-15 NMR, Fluorine-19 NMR, Phosphorus-31 NMR, Boiling Point (°C), Enthalpy of Vaporization (kJ/mol), Flash Point (°C), Glass Transition Temperature (°C), and Melting Point (°C). Examples of molecular formulas are provided: C<sub>6</sub>H<sub>6</sub>, (C<sub>8</sub>H<sub>8</sub>)<sub>x</sub>, and C<sub>22</sub>H<sub>26</sub>CuN<sub>2</sub>O<sub>5</sub>.C<sub>2</sub>H<sub>3</sub>N.

## 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：<sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P NMR
- 化学标识符：化学名称、InChI key
- 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

# 快速筛选物质结果集

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (3)  
Substructure (36K)  
Similarity (704)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

36,294 Results

Sort: Relevance View: Partial

1 1822888-55-0  
C10H9NO3  
7-Hydroxy-6-methoxy-4(3H)-quinolinone

2 304904-61-8  
C11H11NO3  
6,7-Dimethoxy-4(3H)-quinolinone

3 1822733-79-8  
C11H8N2O2  
3,4-Dihydro-7-methoxy-4-oxo-6-quinolinecarbonitrile

4 5 6

多样的排序方式

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

Sort: Relevance View: Partial

Search Within Results

Reaction Role

Reference Role

Life Science Data

Commercial Availability

Number of Components

Molecular Weight

LogP

Stereochemistry

Element

Functional Group

Aromatic Rings

Substance Class

Isotopes

Metals

Experimental Property

Experimental Spectrum

Bioactivity Indicator

Target Indicator

Regulatory Data by Country/Region

Reference Availability

物质筛选类别:

二次筛选

反应角色

研究角色

生物活性数据

组分数量

分子量

立体化学

含有元素

取代基

芳环数量

物质类别

同位素

含有金属

实验属性

实验谱图

GHS危害信息

.....

结构检索类别:

- As Drawn: 可变结构可变, 其他位点锁环锁原子。
- Substructure 亚结构: 包含As Drawn结果, 有取代基。
- Similarity 相似结构: 母体结构可以被取代, 也可以被改变的相似结果。

# 聚类分析选项

## ^ Reaction Role

- Product (193K)
- Reactant (81K)
- Reagent (7,923)
- Catalyst (5,952)
- Solvent (2,374)

## ^ Substance Class

- Organic/Inorganic Small Molecule (227K)
- Manual Registration (150K)
- Nucleic Acid Sequence (94K)
- Protein/Peptide Sequence (81K)
- Salt and Compound With (11K)

[View All](#)

## ^ Life Science Data



- Pharmacological Data (1,951)
- ADME (242)
- Toxicity (50)

## Reference Role

By Count

Alphanumeric

物质在文献中的研究角色

0 Selected

- |   |  |  |
|---|--|--|
| <input type="checkbox"/> Preparation (25K)                      | <input type="checkbox"/> Adverse Effect (194)                            | <input type="checkbox"/> Diagnostic Use (18)             |
| <input type="checkbox"/> Synthetic Preparation (25K)            | <input type="checkbox"/> Agricultural Use (130)                          | <input type="checkbox"/> Formation, Non-preparative (18) |
| <input type="checkbox"/> Biological Study (20K)                 | <input type="checkbox"/> Purification or Recovery (113)                  | <input type="checkbox"/> Removal or Disposal (14)        |
| <input type="checkbox"/> Uses (20K)                             | <input type="checkbox"/> Process (105)                                   | <input type="checkbox"/> Byproduct (13)                  |
| <input type="checkbox"/> Therapeutic Use (20K)                  | <input type="checkbox"/> Physical, Engineering, or Chemical Process (75) | <input type="checkbox"/> Formation, Unclassified (13)    |
| <input type="checkbox"/> Pharmacological Activity (17K)         | <input type="checkbox"/> Technical or Engineered Material Use (70)       | <input type="checkbox"/> Cosmetic Use (12)               |
| <input type="checkbox"/> Reactant (5,173)                       | <input type="checkbox"/> Combinatorial Study (67)                        | <input type="checkbox"/> Food or Feed Use (10)           |
| <input type="checkbox"/> Reactant or Reagent (5,173)            | <input type="checkbox"/> Occurrence (58)                                 | <input type="checkbox"/> Pollutant (6)                   |
| <input type="checkbox"/> Biological Study, Unclassified (2,998) | <input type="checkbox"/> Natural Product Occurrence (52)                 | <input type="checkbox"/> Reagent (6)                     |
| <input type="checkbox"/> Prophetic Synthesis or Use (1,289)     | <input type="checkbox"/> Biological Use, Unclassified (42)               | <input type="checkbox"/> Analytical Matrix (4)           |
| <input type="checkbox"/> Properties (1,003)                     | <input type="checkbox"/> Modifier or Additive Use (31)                   | <input type="checkbox"/> Other Use, Unclassified (4)     |
| <input type="checkbox"/> Pharmacokinetics (445)                 | <input type="checkbox"/> Analytical Role, Unclassified (27)              | <input type="checkbox"/> Biosynthetic Preparation (3)    |
| <input type="checkbox"/> Industrial Manufacture (282)           | <input type="checkbox"/> Analytical Reagent Use (26)                     | <input type="checkbox"/> Polymer in Formulation (2)      |
| <input type="checkbox"/> Analytical Study (262)                 | <input type="checkbox"/> Nanoscale (24)                                  | <input type="checkbox"/> Biochemical Process (1)         |
| <input type="checkbox"/> Analyte (228)                          |  | <input type="checkbox"/> Miscellaneous (1)               |
|   |  | <input type="checkbox"/> Occurrence, Unclassified (1)    |

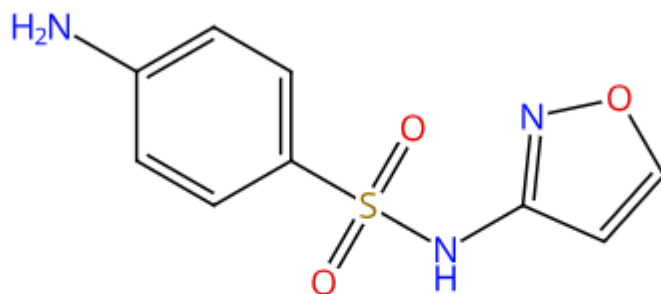
Apply

Cancel

# 物质检索—详情页面

CAS Registry Number: 723-46-6

28K 1,029 125



C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

Benzenesulfonamide, 4-amino-*N*-(5-methyl-3-isoxazolyl)- (9CI, ACI)

Key Physical Properties	重要物理性质	Value	Condit
Molecular Weight		253.28	-
Melting Point (Experimental)		167 °C	-
Boiling Point (Predicted)		482.1±55.0 °C	Press: 7
Density (Experimental)		1.08 g/cm <sup>3</sup>	-
pKa (Predicted)		5.81±0.50	Most A

Experimental Properties | Spectra

Other Names and **实验属性**

Experimental Properties

Experimental Spectra

Pharmacological Data

ADME

Toxicity

Predicted Properties

Predicted Spectra

Bioactivity Indicators

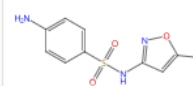
Target Indicators

Regulatory Information

GHS Hazard Statements

Additional Details

723-46-6



C<sub>10</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>S

CAS Name  
Sulfamethoxazole

Conditions

Working Frequency

400 MHz

Solvent

[Dimethyl sulfoxide \(67-68-5\)](#)

[Carbon tetrachloride \(56-23-5\)](#)

Temperature

20 °C

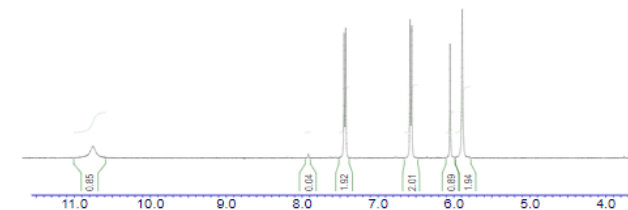
Spectrum Summary

Spectrum ID

F0175-0013

Source

Spectral data were obtained from Life Chemicals



实验谱图

Reset

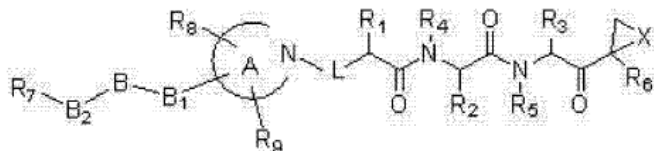
# CAS Markush检索，助力结构查新

CN 104945470 A

权 利 要 求 书

1/3 页

1. 一种杂环构建的三肽环氧化物类化合物，具有下述结构通式 I：



I

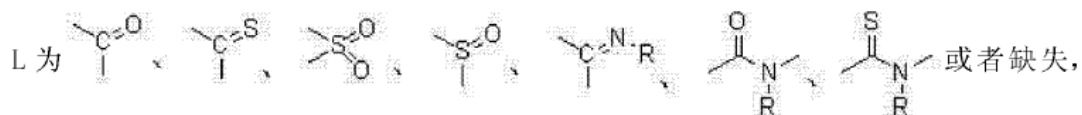
其中：

$R_1, R_2, R_3$  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  $N(R_a)$  ( $R_b$ ) 或缺失， $R_a, R_b$  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

## 具体物质[Specific Substance]

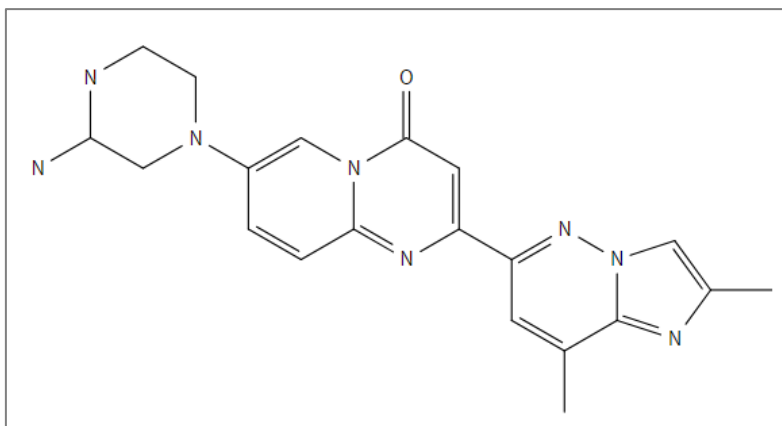
- 以具体化学结构陈述的特定物质，会被分配CAS 登记号

## 预测性物质[Prophetic Substance]

- 使用Markush结构陈述的预测物质，一个Markush可以陈述上千甚至更多的结构
- 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登记号
- Markush检索，能检索到通过Substance可能检索不到的结构

# CAS Markush检索

该结构进行精准结构，亚结构均无结果，能够确定它没有被公开吗？



此时您检索的是CAS REGISTRY数据合集，它是专利审查员的重要参考依据之一。

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (0)

Similarity (111K)

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Similarity

95-98 (2)

90-94 (54)

85-89 (229)

80-84 (261)

75-79 (291)

View All

Reaction Role

Product (253)

Reactant (20)

Filtering: Similarity: 3 Selected X Number of Components: 1 X Clear All Filters

285 Results Sort: Relevance View: Partial

1 95 ...

1825352-54-2

Absolute stereochemistry shown

$C_{21}H_{23}N_7O$   
2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-4H-...

5 References 25 Reactions 1 Supplier

2 95 ...

1825352-53-1

Absolute stereochemistry shown

$C_{21}H_{23}N_7O$   
2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-4H-...

5 References 25 Reactions 1 Supplier

3 95 ...

1825352-79-1

Absolute stereochemistry shown

$C_{21}H_{23}N_7O$   
9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R)-3-methyl-1-piperazinyl]-...

5 References 19 Reactions 1 Supplier

4 95 ...

1825352-78-0

Absolute stereochemistry shown

$C_{21}H_{23}N_7O$   
9-Methyl-2-(2-methylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S)-3-methyl-1-piperazinyl]-...

5 References 19 Reactions 0 Suppliers

5 95 ...

1825352-52-0

Relative stereochemistry shown

$C_{22}H_{25}N_7O$   
rel-2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3R,5S)-3,5-dimethyl-1-piperazinyl]-...

4 References 25 Reactions 1 Supplier

6 95 ...

2097817-67-7

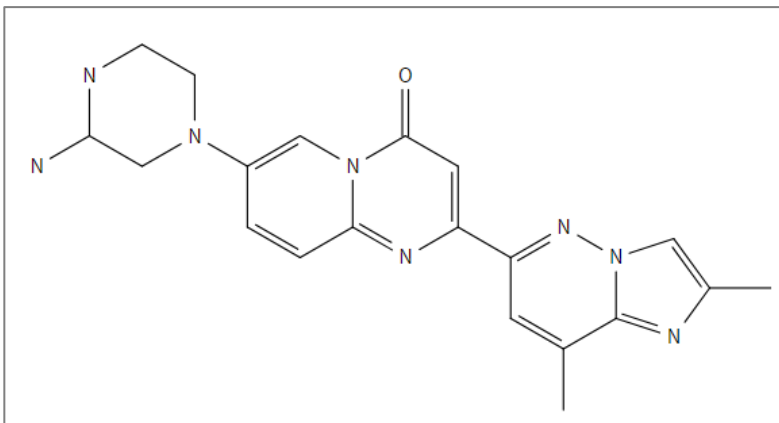
Absolute stereochemistry shown

$C_{22}H_{25}N_7O$   
2-(2,8-Dimethylimidazo[1,2-b]pyridazin-6-yl)-7-[(3S,5S)-3,5-dimethyl-1-piperazinyl]-...

3 References 16 Reactions 1 Supplier

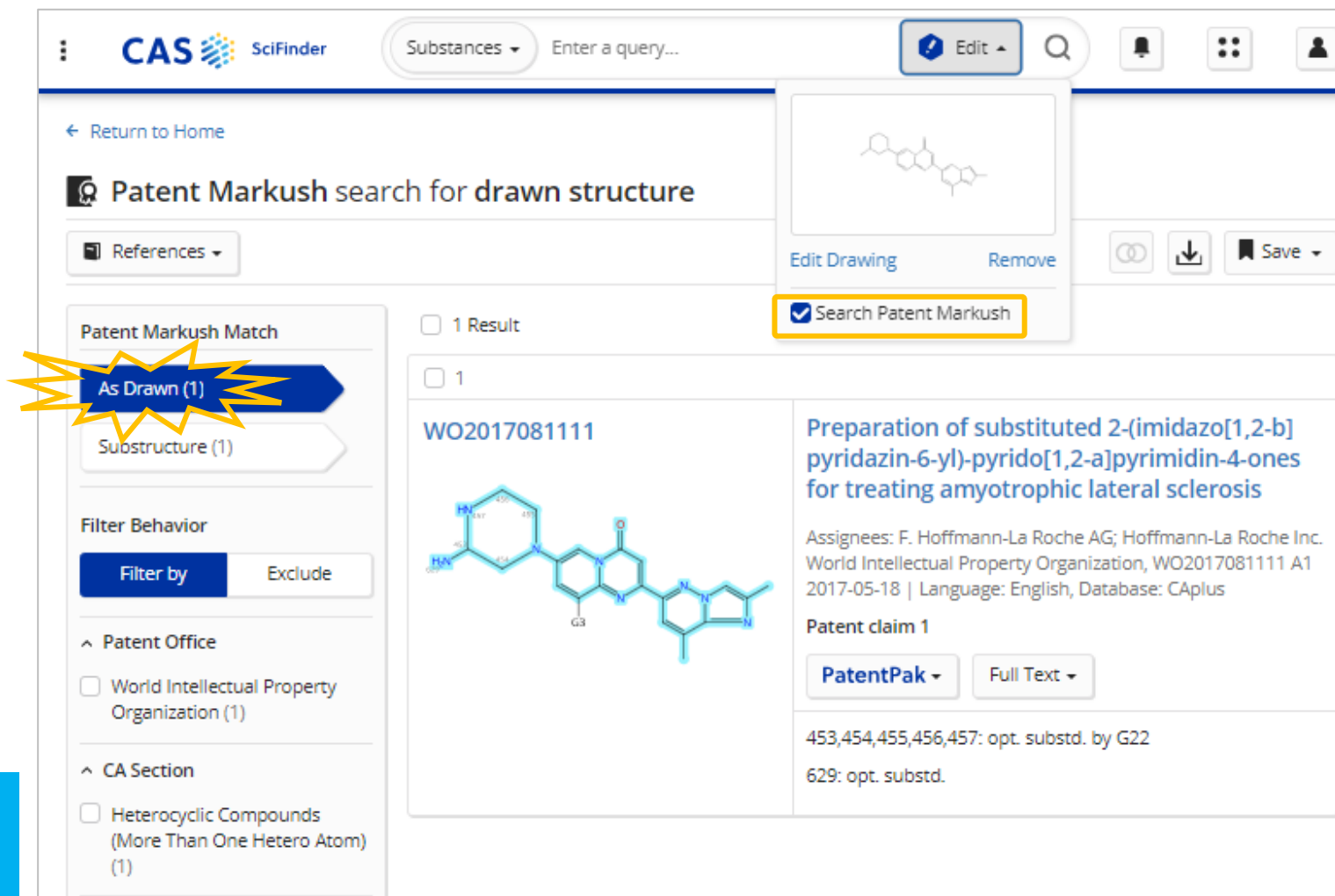
# CAS Markush检索

通过专利Markush结构检索，获得高度相关的专利结果



此时您检索的是Markush数据合集，它也是专利审查员的重要参考依据。

为了尽可能完整地获得公开的结构信息，需要同时进行Substance和Markush结构检索；根据需要，可进行文献检索补充。



CAS SciFinder interface showing a patent Markush search for a drawn structure. The search results show one result: WO2017081111, titled "Preparation of substituted 2-(imidazo[1,2-b]pyridazin-6-yl)-pyrido[1,2-a]pyrimidin-4-ones for treating amyotrophic lateral sclerosis". The interface includes a search bar, a "Search Patent Markush" button, and a list of filters.

Patent Markush Match

- As Drawn (1)
- Substructure (1)

Filter Behavior

Filter by  Exclude

Patent Office

- World Intellectual Property Organization (1)

CA Section

- Heterocyclic Compounds (More Than One Hetero Atom) (1)

1 Result

1

WO2017081111

Preparation of substituted 2-(imidazo[1,2-b]pyridazin-6-yl)-pyrido[1,2-a]pyrimidin-4-ones for treating amyotrophic lateral sclerosis

Assignees: F. Hoffmann-La Roche AG; Hoffmann-La Roche Inc. World Intellectual Property Organization, WO2017081111 A1 2017-05-18 | Language: English, Database: CAplus

Patent claim 1

PatentPak Full Text

453,454,455,456,457: opt. substd. by G22

629: opt. substd.



# 小结

- **物质的检索方式:** 灵活使用CAS科学家增值标引的信息, 充分利用结构绘制工具, 合理扩大或限定结构检索范围
- **检索结果的筛选:** 丰富的聚类分析选项, 如Substance Role、Reference Role、Substance Class等。
- **物质详情速览:** 物质详情页解读, 快速便捷地获取物质理化性质及实验谱图等。
- **CAS Markush (MARPAT):** REGISTRY与MARPAT等数据库是专利审查员进行专利实查的重要参考依据, 可以通过结构检索获取确切结构和预测结构两部分结果, 合并后即可获取结构查新全景。

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A

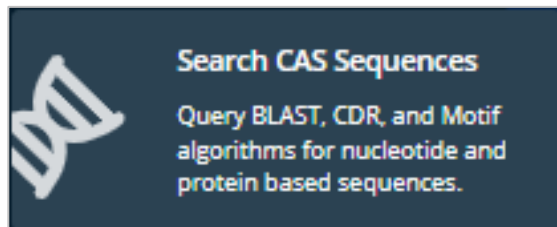


# 您可能会感兴趣：

- 如何从已知序列片段出发，检索**对应序列**？
- 如何获取序列相同但**修饰不同**的结果？
- 对含有**可变部分**的生物序列，如何进行检索？
- 如何对多个**CDR**序列进行检索？
- 如何通过**物质**或**文献**调研感兴趣的序列？
- .....



# CAS Sequences——序列检索



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

Your sequence search has been submitted. You can view the status of your query in your [Recent Search History](#) and on the [History Page](#).

### Recent Search History

[View All Search History](#)

August 1, 2024

Sequences 4:08 PM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTGA	<a href="#">View Results</a> <a href="#">Edit Options</a> Searching..
----------------------	--	---	---

Results will expire on September 1, 2024.

### Recent Search History

[View All Search History](#)

August 1, 2024

Sequences 4:08 PM	Sequence Type: Nucleotide Search Within: Nucleotides NCBI Included: Yes BLAST Algorithm: BLASTn Alignment Identity: 80% Query Coverage: 90%	AACAACAACATATCAAATCCTACTGGTGGCACAACCTGA	<a href="#">View Results</a> <a href="#">Edit Search</a> Complete
----------------------	--	---	---

Results will expire on September 1, 2024.

Search CAS Sequences CAS LIFE SCIENCES

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

BLAST CDR Motif 检索方式  
BLAST  
CDR  
Motif

AACAACAACATATCAAATCCTACTGGTGGCACAAC

上传fasta或txt格式序列

Clear Search

Upload Sequence (.fasta or .txt)

Sequence Type:  
Nucleotide Protein

Search Within:  
 Nucleotides  Proteins

Include NCBI Sequences

Search Sequences

包括来自期刊、专利和来自NCBI中的序列

Advanced Sequence Search

# CAS Sequences — BLAST检索结果

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

0 to 10<sup>6</sup>

Query Coverage %

0 to 100

Subject Coverage %

0 to 100

Alignment Identity %

0 to 100

Query Details AACAACAACATATCAAATCCTACTGGTGGCACAACCTTGA View More

170 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 100%

Query 1 39

Subject 1 528

Matches: 39 Mismatches: 0

View Less

Alignment Subject References

Alignment Data  
BLAST Score: 78  
E-Value: 7.79206e-12

```
Q 1 AACAACAACA TATCAAATCC TACTGGTGGC ACAACTTGA 39
   |||
S 23 AACAACAACA TATCAAATCC TACTGGTGGC ACAACTTGA 61
```

2 Alignment Identity: 100%

Query 1 39

Subject 1 455

Matches: 39 Mismatches: 0

View Less

Alignment Subject References

Alignment Data  
BLAST Score: 78  
E-Value: 7.79206e-12

```
Q 1 AACAACAACA TATCAAATCC TACTGG
   |||
S 393 AACAACAACA TATCAAATCC TACTGG
```

结果筛选

- 序列一致性详情
- 目标序列
- 披露序列的专利文献

Download Sequence Results

File Type

Excel (.xlsx)  
 FASTA (.fasta)

Select Quantity

All Results  
 Range (ex. 2 to 20)

File Name

Sequences\_20240801\_1638

Download Cancel Learn more about downloads.

检索结果下载:

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

# CAS Sequences — BLAST检索结果

Query ① Matches: 39  
Mismatches: 0

Subject ① 929

View Less ▾ **目标序列**

Alignment Subject References References

CAS Registry Number: 661510-85-6  
Length: 929 nt  
Organisms: Zea mays

可直接链接到文献结果集

Alignment Subject **References** **披露序列的专利文献** References

**Nucleic acid molecules and other molecules associated with plants and uses thereof for plant improvement**  
Assignees: LIU, JINGDONG; ZHOU, YIHUA; KOVALIC, DAVID; SCREEN, STEVEN; TABASKA, JACK; CAO, YONGWEI  
US20070011783 A1 | Seq ID No: 25627

**Nucleic acid molecules and other molecules associated with plants and uses thereof for plant improvement**  
Assignees: LIU, JINGDONG; ZHOU, YIHUA; KOVALIC, DAVID; SCREEN, STEVEN; TABASKA, JACK; CAO, YONGWEI; ANDERSEN, SCOTT; EDGERTON, MICHAEL; FINCHER, KAREN; HAMMOND-KOSACK, KIM; LA ROSA, THOMAS; MASUCCI, JAMES; URBAN, MARTIN; XIAO, JINHUA; ZIEGLER, TODD  
US20070283460 A9 | Seq ID No: 25627

# 序列详情及相关序列

CAS Registry Number: 2417899-77-3

4,229 0 2

Image Not Available

Unspecified

RNA (recombinant 5'-[1,2-[(3'-O-methyl)m<sup>7</sup>G-(5'→5')-ppp-Am]]-capped all uridine→N<sup>1</sup>-methylpseudouridine-substituted severe acute respiratory syndrome coronavirus 2 secretory signal peptide contg. spike glycoprotein S152-specifying plus 5'- and 3'-untranslated flanking region-contg. poly(A)-tailed messenger BNT162b2), inner salt (ACI)

Nucleic Acid Sequence  
Sequence Length: 4284  
1106 a, 1315 c, 1062 g, 801 u  
modified

Related Sequences (2)

获取序列一致、修饰不同或来自不同文献的相关序列

Other Names and Identifiers


Sequence Details **序列详情**

Sequence: RNA; linear

151	accagaggcg	uguacuacc	cgacaaggug	uucagaucca	gcgugcugca
201	cucuaccag	gaccuguucc	ugccuuucuu	cagcaacgug	accugguucc
251	acgcaucca	cgugucggc	accaauggca	ccaagagauu	cgacaacccc
301	gugcugcccu	ucaacgacgg	gguguauuuu	gccagcaccg	agaaguccaa
351	caucaucaga	ggcuggaucu	ucggcaccac	acuggacagc	aagaccaga
401	gcccugcugau	cgugaacaac	gccaccaacg	uggucauaa	agugugcgag
451	uuccaguucu	gcaacgacc	cuuccugggc	gucuacuacc	acaagaacaa
501	caagagcugg	auggaaagcg	aguuccgggu	guacagcagc	gccacaacu
551	gcaccuuga	guacgugucc	cagccuuucc	ugauggaccu	ggaggccaag
601	cagggcaacu	ucaagaaccu	gcgcgaguuc	guguuaaga	acaucgacgg
651	cuacucaag	aucuacagca	agcacacccc	uaucaaccuc	gugcgggauc
701	ugccucaggg	cuucucugcu	cuggaacccc	ugguggaucu	gcccaucggc
751	aucaacauca	cccguuua	aacacuecuc	ecccuecaca	aaacuaccu

Sequence Modifications **序列修饰详情**

Type		Description
modified base	guanosine-1	3'-me
modified base	guanosine-1	m7g
modified base	adenosine-2	am
uncommon link	guanosine-1 to adenosine-2	5'→5' triphosphate

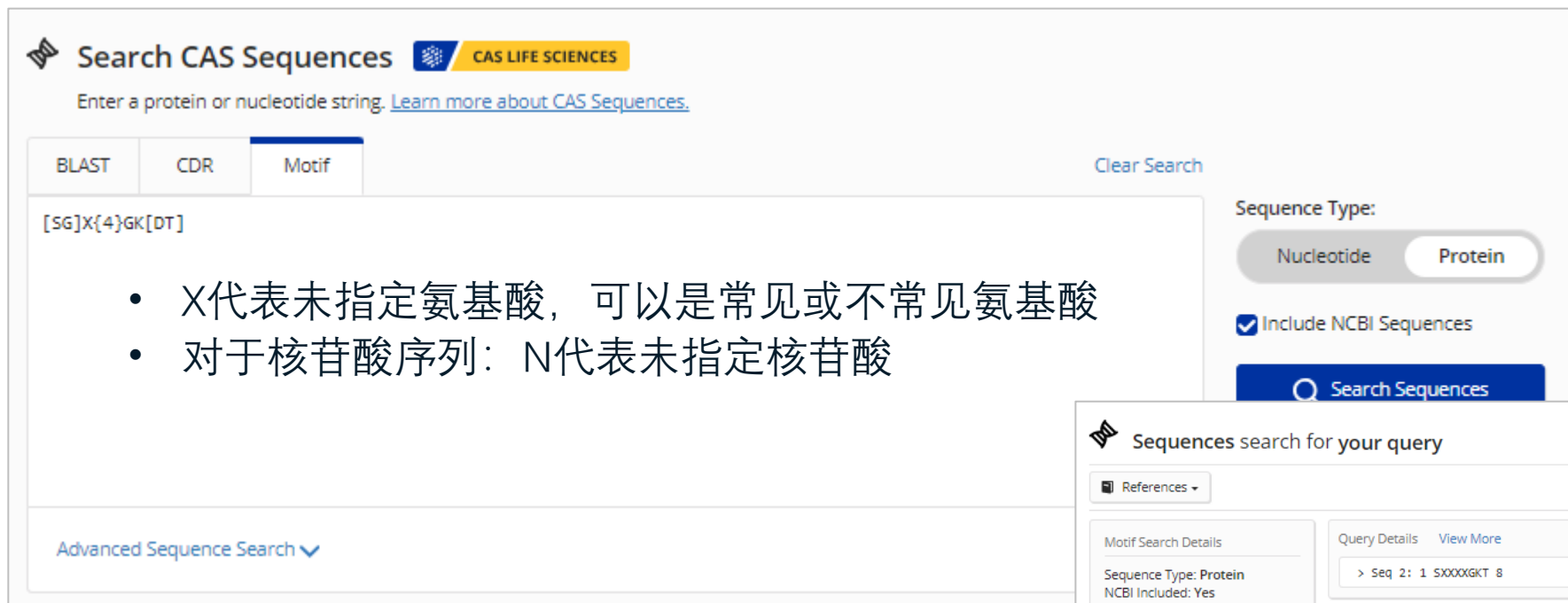
Pharmacological Data 

Bioactivity Indicators

Target Indicators

Regulatory Information

# CAS Sequences——Motif检索结果



Search CAS Sequences CAS LIFE SCIENCES

Enter a protein or nucleotide string. [Learn more about CAS Sequences.](#)

BLAST CDR Motif Clear Search

[SG]X{4}GK[DT]

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

Sequence Type: Nucleotide Protein

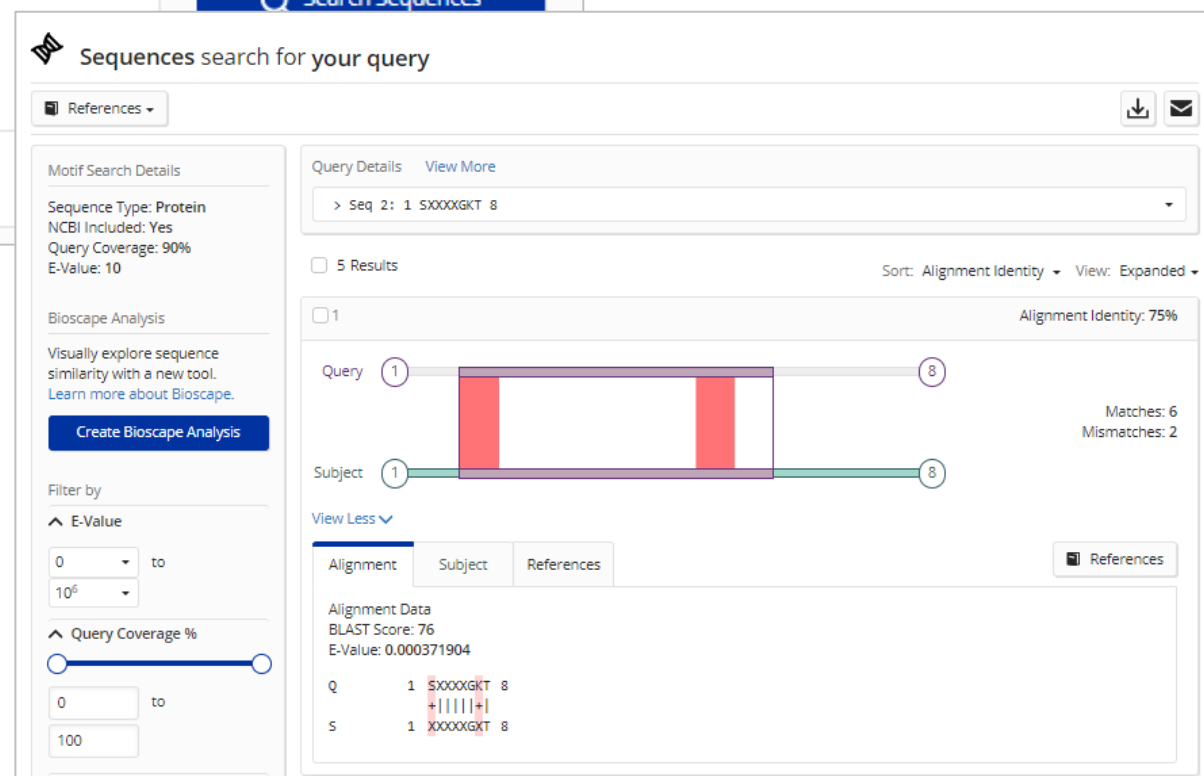
Include NCBI Sequences

Search Sequences

Advanced Sequence Search

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。其中字段可用逗号隔开，{2,6}表示在大括号左边紧密相连的氨基酸可重复2-6次



Sequences search for your query

References

Motif Search Details

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

Bioscope Analysis

Visually explore sequence similarity with a new tool. [Learn more about Bioscope.](#)

Create Bioscope Analysis

Filter by

E-Value

0 to 10<sup>6</sup>

Query Coverage %

0 to 100

Query Details View More

Seq 2: 1 SXXXXGKT 8

5 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 75%

Query 1 8

Subject 1 8

Matches: 6  
Mismatches: 2

View Less

Alignment Subject References

Alignment Data

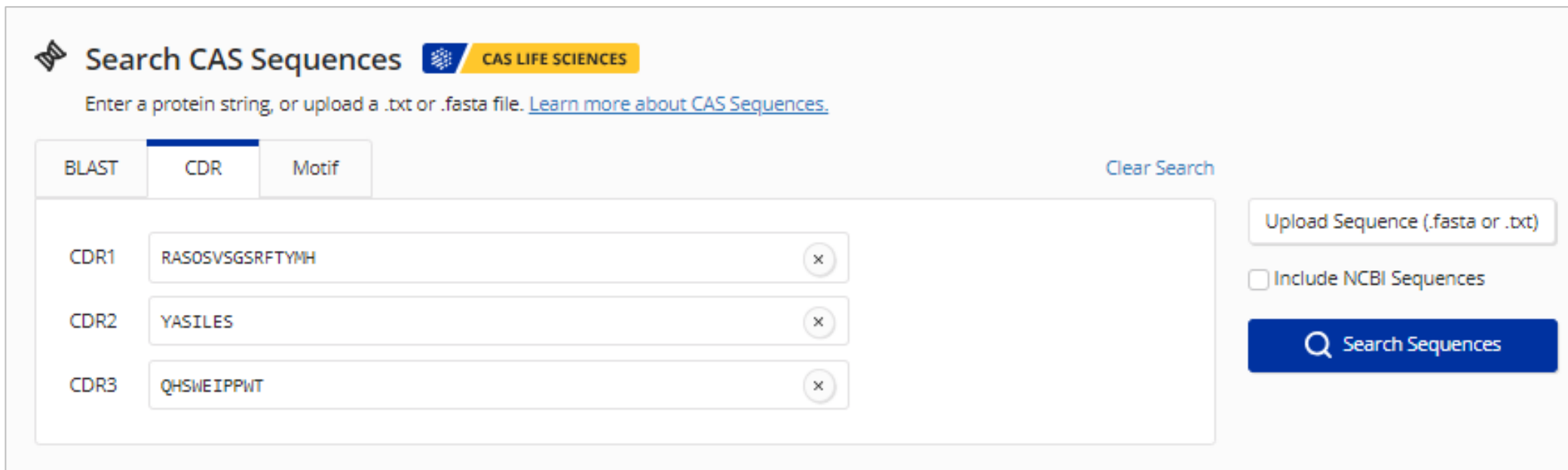
BLAST Score: 76  
E-Value: 0.000371904

Q	1	SXXXXGKT	8
		+ + + + +	
S	1	XXXXGKT	8



# CAS Sequences——CDR检索结果

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



The screenshot shows the 'Search CAS Sequences' interface. At the top, there is a search bar with the text 'Enter a protein string, or upload a .txt or .fasta file. [Learn more about CAS Sequences.](#)'. Below the search bar are three tabs: 'BLAST', 'CDR', and 'Motif', with 'CDR' selected. To the right of the tabs is a 'Clear Search' link. The main search area contains three input fields for CDR sequences: CDR1 with 'RASOSVSGSRFTYMH', CDR2 with 'YASILES', and CDR3 with 'QHSWEIPPWT'. Each field has a small 'x' icon to clear the text. On the right side of the interface, there is an 'Upload Sequence (.fasta or .txt)' button, a checkbox for 'Include NCBI Sequences', and a large blue 'Search Sequences' button with a magnifying glass icon.

支持单个或多个CDR序列检索并用

# CAS Sequences——CDR检索结果

**CDR Segments**

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

CDR1: 14,408  
CDR2: 16,727  
CDR3: 864  
Intersection (CDR1 & CDR2): 2,674  
Intersection (CDR1 & CDR3): 61  
Intersection (CDR2 & CDR3): 49  
Intersection (CDR1, CDR2 & CDR3): 200

**Query Details** [View Less](#)

> CDR1  
RASQSVSGSRFTYMH

> CDR2  
YASILES

> CDR3  
QHSWEIPPWT

34,983 Results Sort: Alignment Identity View: Expanded

1 Alignment Identity: 96.88%

Subject 1 112

CDR1: 1 15  
CDR2: 1 7  
CDR3: 1 10

Matches: 31  
Mismatches: 1

**Alignment Data**

BLAST Score: 81  
E-Value: 8.569987318855

Segment	Start	End	Sequence
CDR1	1	15	RASQSVSGSRFTYMH
S	24	38	RASQSVSGSRFTYMH
CDR2	1	7	YASILES
S	54	60	YASILES
CDR3	1	10	QHSWEIPPWT
S	93	102	QHSWEIPPWT

**CDR Segments**

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

CDR1: 14,408  
CDR2: 16,727  
CDR3: 864  
Intersection (CDR1 & CDR2): 2,674  
Intersection (CDR1 & CDR3): 61  
Intersection (CDR2 & CDR3): 49  
Intersection (CDR1, CDR2 & CDR3): 200

**Apply**  
Reset Segments

CDR Segments:

- 匹配到一个或者多个CDR的subject序列的序列数量
- 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

# 根据物质名称和识别符进行生物分子检索

- Common name: e.g. **Oxytocin**
- Brand name (drug name): e.g. **Rituxan**
- Generic name: e.g. **Adalimumab**
- CAS Registry Number: e.g. **219808-29-4**
- GenBank Number: e.g. **GenBank KT001084**
- EC number: e.g. **EC 3.2.1.83**

The screenshot displays two search results from the CAS Substances database. The top search is for "Oxytocin", showing 6 results. The first result, 50-56-6, includes a chemical structure and the formula  $C_{43}H_{66}N_{12}O_{12}S_2$ . The second result, 928036-04-8, is an unspecified WAY 162720. The third result, 1227568-68-4, is an unspecified Hirudotocin. The bottom search is for "GenBank KT001084" and "EC 3.2.1.83", showing 2 results. The first result, 37288-59-8, is an unspecified EC 3.2.1.83. The second result, 2092642-35-6, is an unspecified GenBank KT001084. Both search results include filter behavior options and buttons for references, reactions, and suppliers.

# 根据文献主题词检索，再获取物质信息

主题词示例：

("epidermal growth factor receptor-2" or HER2) and inhibitor

CA Section

- Pharmacology (7,056)
- Mammalian Pathological Biochemistry (3,547)
- Immunochemistry (1,537)
- Pharmaceuticals (800)
- Heterocyclic Compounds (More Than One Hetero Atom) (662)

[View All](#)

Concept

- Epidermal growth factor receptor HER2 (10K)
- Homo sapiens (10K)
- Human (10K)
- Humans (8,522)
- Antitumor agents (6,387)

[View All](#)

References search for "epidermal growth factor receptor-2" or HER2) and inhibitor"

Substances Reactions Citing Knowledge Graph

We are displaying the most relevant results. [Learn about result relevance.](#) [Load All Results](#)

Filtering: Concept: 2 Selected CA Section: 3 Selected [Clear All Filters](#)

11,403 Results Sort: Relevance View: Partial Abstract

1

**SAR and QSAR study on the bioactivities of human epidermal growth factor receptor-2 (HER2) inhibitors**

By: Qu, D.; Yan, A.; Zhang, J. S.  
SAR and QSAR in Environmental Research (2017), 28(2), 111-132 | Language: English, Database: CAlplus and MEDLINE

In this paper, structure-activity relationship (SAR, classification) and quant. structure-activity relationship (QSAR) models have been established to predict the bioactivity of human epidermal growth factor receptor-2 (HER2) inhibitors. For the SAR study, we established six SAR (or classification) models to distinguish highly and weakly active HER2 inhibitors. The dataset contained 868 HER2 inhibitors, which was split into a training set including 580 inhibitors and a test set including 288 inhibitors by a Kohonen's self-organizing map (SOM) or a random method. The SAR models were performed...

[View More](#)

Full Text Substances (0) Reactions (0) Citing (7) Citation Map

2

**A phase I trial of ganetespib in combination with paclitaxel and trastuzumab in patients with human epidermal growth factor receptor-2 (HER2)-positive metastatic breast cancer**

By: Jhaveri, Komal; Wang, Rui; Teplinsky, Eleonora; Chandrarapaty, Sarat; Solit, David; Cadoo, Karen; Speyer, James; D'Andrea, Gabriella; Adams, Sylvia; Patil, Sujata; et al  
Breast Cancer Research (2017), 19, 89/1-89/8 | Language: English, Database: CAlplus and MEDLINE

Background: Targeted therapies in HER2-pos. metastatic breast cancer significantly improve outcomes but efficacy is limited by therapeutic resistance. HER2 is an acutely sensitive Heat Shock Protein 90 (HSP90) client and HSP90 inhibition can overcome trastuzumab resistance. Preclin. data suggest that HSP90 inhibition is synergistic with taxanes with the potential for significant clin. activity. We therefore tested ganetespib, a HSP90 inhibitor, in combination with paclitaxel and trastuzumab in patients with trastuzumab-refractory HER2-pos. metastatic breast cancer. Methods: In this phase I dos...

[View More](#)

Full Text Substances (5) Reactions (0) Citing (46) Citation Map

# 根据文献主题词检索，再获取物质信息

**Substances from References**

References Reactions Suppliers

Filtering: Reference Role: Therapeutic Use Substance Class: Protein/Peptide Sequence Clear All Filters

23,551 Results Sort: Relevance View: Partial

**Filter Behavior**

Filter by Exclude

Search Within Results

Reaction Role

- Reference Role
  - Properties (31K)
  - Biological Study (30K)
  - Uses (24K)
  - Therapeutic Use (23K)
  - Biological Study, Unclassified (19K)

View All

Life Science Data

Commercial Availability

Number of Components

Molecular Weight

LogP

Stereochemistry

Element

**Substance Class**

- Organic/Inorganic Small Molecule (37K)
- Manual Registration (28K)
- Protein/Peptide Sequence (23K)
- Nucleic Acid Sequence (9,788)
- Salt and Compound With (2,755)

View All

1 180288-69-1  
Image Not Available  
Unspecified  
Trastuzumab  
Protein/Peptide Sequence  
Sequence Length: 1328  
21K References 234 Reactions 25 Suppliers

2 380610-27-5  
Image Not Available  
Unspecified  
Pertuzumab  
Protein/Peptide Sequence  
Sequence Length: 1326  
3,390 References 5 Reactions 23 Suppliers

3 62253-63-8  
Image Not Available  
 $C_{270}H_{395}N_{73}O_{83}S_7$   
Human epidermal growth factor  
Protein/Peptide Sequence  
Sequence Length: 53  
587 References 14 Reactions 31 Suppliers

4 1018448-65-1  
Image Not Available  
Unspecified  
Trastuzumab emtansine  
Protein/Peptide Sequence  
Sequence Length: 1328  
1,792 References 2 Reactions 22 Suppliers

5 205923-56-4  
Image Not Available  
Unspecified  
Cetuximab  
Protein/Peptide Sequence  
Sequence Length: 1326  
13K References 60 Reactions 68 Suppliers

6 1826843-81-5  
Image Not Available  
Unspecified  
Immunoglobulin G1, anti-(human tyrosine kinase receptor ErbB2) (human-Mus muscul...  
Protein/Peptide Sequence  
Sequence Length: 1328  
580 References 2 Reactions 15 Suppliers

# 小结

- **CAS Sequences检索**: BLAST, CDR, Motif, 可以针对DNA/RNA的核苷酸、多肽/蛋白的氨基酸序列进行检索, 也可以对相同序列不同修饰的结果进行拓展。Motif适合短序列检索, 并且支持可变部分输入。CDR可根据已知信息和需求查看1-3个CDR被包含的序列结果。
- **通过物质检索序列**: 通过常用名, 品牌名, 通用名, CAS登记号, GenBank编号, EC编号等直接检索序列。
- **通过文献间接获取序列**: 基于CAS的数据关联, 从相关的研究文献中获取序列相关信息, 并通过聚类分析选项进行筛选。

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A



# 您可能会感兴趣：

- 如何从我感兴趣的底物、产物或催化剂出发，找到**关联的反应**？
- 如何查找涉及**机理研究**的反应？或**人名反应**？
- 如何在大量反应结果中，**快速找到**最想要的反应？
- 如何设计新化合物的**逆合成**路线？
- 具体的**实验方案**怎么查、怎么选？
- .....





# 反应的获取方法——直接检索

Good Afternoon, Kaiqian

All Substances **Reactions** References Suppliers For You NEW

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

**Retrosynthetic Analysis**  
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

**Search CAS Lexicon**  
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Chemical drawing tool showing a reaction scheme with a benzene ring and a side chain.

Edit Drawing Remove

直接进行Reaction检索

Retrosynthetic Analysis  
Draw or import a structure.

Enter a CAS Registry Number, SMILES, or InChI

Draw or change atoms or bonds.

Buttons: C, H, O, S, N, P, Cl, Si, Et, and various bond types.

Molecular Formula:

Zoom: 100%

Start Retrosynthetic Analysis Cancel

通过Retrosynthesis Plan  
获取逆合成反应路线

# 反应的获取方法——间接检索

通过物质获取反应

**Substances**

References ▾ **Reactions ▾** Suppliers ▾

Filter Behavior

Filter by Exclude

Reaction Role

- Product (4)
- Reactant (4)
- Reagent (2)
- Catalyst (1)
- Solvent (1)

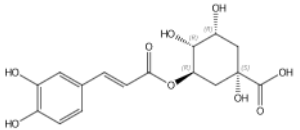
Reference Role

- Biological Study (9)
- Uses (9)
- Biological Study, Unclassified

9 Results Sort: Number of

1

327-97-9



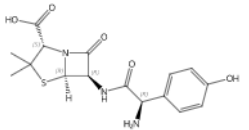
Absolute stereochemistry shown  
Double bond geometry unknown

$C_{16}H_{18}O_9$   
**Chlorogenic acid**

31K References **160 Reactions** 123 Suppliers

2

26787-78-0



Absolute stereochemistry shown

$C_{16}H_{19}N_3O_5S$   
**Amoxicillin**

31K References 461 Reactions 64 Suppliers

通过文献获取反应

**References**

Substances ▾ **Reactions ▾** Citing ▾

CAS Formulus®, the comprehensive formulations database and workflow solution, is now available for all SciFinder® users. Use the [CAS Solutions: Formulus filter](#) to view available content. [Learn more about Formulus.](#)

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](#)

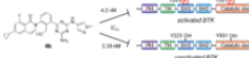
357 Results Sort: Relevance View: Partial Abstract ▾

1

**Design and Synthesis of Novel Amino-triazine Analogues as Selective Bruton's Tyrosine Kinase Inhibitors for Treatment of Rheumatoid Arthritis**

By: Kawahata, Wataru ; Asami, Tokiko; Kiyoi, Takao; Irie, Takayuki; Taniguchi, Haruka; Asamitsu, Yuko; Inoue, Tomoko; Miyake, Takahiro; Sawa, Masaaki

Journal of Medicinal Chemistry (2018), 61(19), 8917-8933 | Language: English, Database: CAPLUS and MEDLINE



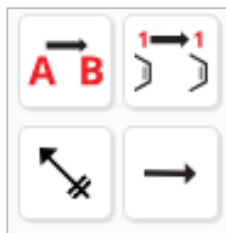
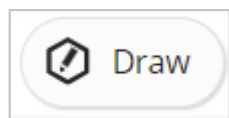
Bruton's tyrosine kinase (**BTK**) is a promising drug target for the treatment of multiple diseases, such as B-cell malignancies, asthma, and rheumatoid arthritis. A series of novel aminotriazines were identified as highly selective inhibitors of **BTK** by a scaffold-hopping approach. Subsequent **SAR** studies of this series using two conformationally different **BTK** proteins, an activated form of **BTK** and an unactivated form of **BTK**, led to the discovery of a highly selective **BTK inhibitor**, **1**. With significant efficacy in models in vivo and good ADME and safety profiles, **1** was advanced into preclinical studies...

[View More ▾](#)

Full Text ▾

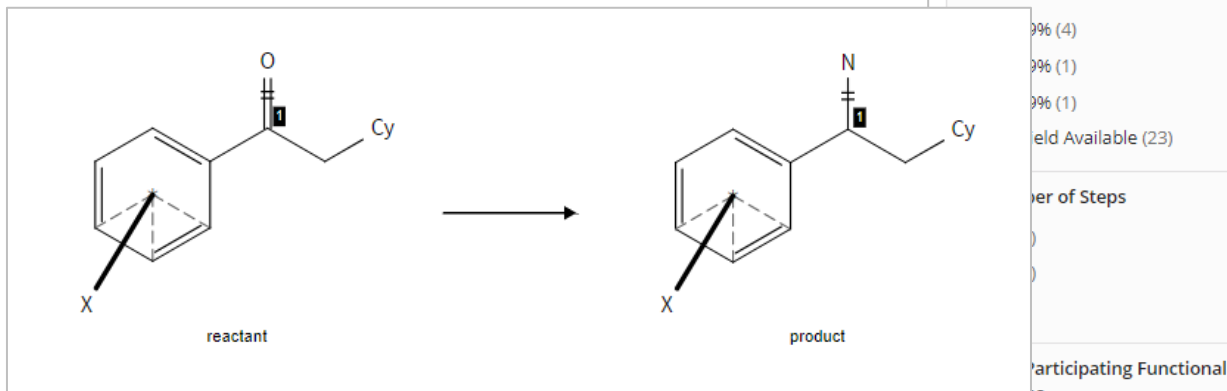
Substances (156) **Reactions (206)** Citing (18) Citation Map

# 使用绘制反应式、底物或产物检索反应



反应角色定义工具  
反应原子标记工具  
化学键标记工具  
反应箭头

结构匹配度



Reactions search for drawn structure

References -

分组、排序方式

29 Results

Structure Match

- As Drawn (29)
- Substructure (8,063)
- Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Participating Functional Groups

- Halide (12)
- Phenyl halide (12)
- Imine (1)

Reaction Mapping

Group: By Scheme Sort: Relevance 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 (86) Suppliers (18)

31-313-CAS-22352897 Steps: 1 Yield: 85% Reductive amination using cobalt-based nanoparticles for synthesis of amines

1.1 Reagents: Hydrogen, Ammonia  
Catalysts: Cobalt (compounds)  
Solvents: Tetrahydrofuran; 30 h, 40 bar, 120 °C

By: Murugesan, Kathiravan; et al  
Nature Protocols (2020), 15(4), 1313-1337

Experimental Protocols Full Text -

31-313-CAS-19925889 Steps: 1 Yield: 85% Simple ruthenium-catalyzed reductive amination enables the synthesis of a broad range of primary amines

1.1 Reagents: Hydrogen, Ammonia  
Catalysts: Dichlorotris(triphenylphosphine)ruthenium  
Solvents: 2-Methyl-2-butanol; 5 - 7 bar; 40 bar; 30 h, 130 °C

By: Senthamarai, Thirusangumurugan; et al  
Nature Communications (2018), 9(1), 1-12

Full Text -

31-313-CAS-18566400 Steps: 1 Yield: 85% MOF-derived cobalt nanoparticles catalyze a general synthesis of amines

1.1 Reagents: Hydrogen, Ammonia  
Catalysts: Cobalt  
Solvents: Tetrahydrofuran; 5 - 7 bar; 30 h, 40 bar, 120 °C

By: Jagadeesh, Rajenahally V. et al  
Science (Washington, DC, United States) (2017), 358(6361), 326-332

Full Text -

# 反应检索结果集的分组

Reactions search for drawn structure

References

按照文献分组

Structure Match

- As Drawn (29)
- Substructure (8,063)
- Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

- 80-89% (4)
- 70-79% (1)
- 50-69% (1)
- No Yield Available (23)

Number of Steps

- 1 (13)
- 2 (14)
- 3 (2)

Non-Participating Functional Groups

- Halide (12)
- Phenyl halide (12)
- Imine (1)

Reaction Mapping

- Mapping Data Available (29)

Reaction Scale

29 Results

Group: By Document Sort: Relevance View: Collapsed

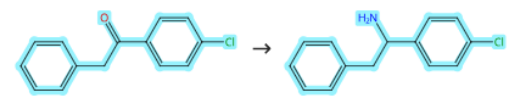
1

Reductive amination using cobalt-based nanoparticles for synthesis of amines

By: Murugesan, Kathiravan; Chandrashekar, Vishwas G.; Senthamarai, Thirusangumurugan; Jagadeesh, Rajenahally V.; Beller, Matthias

Nature Protocols (2020), 15(4), 1313-1337 | Language: English, Database: CPlus and MEDLINE

Full Text



Suppliers (86) Suppliers (18)

31-313-CAS-22352897 Steps: 1 Yield: 85%

1.1

Reagents: Hydrogen, Ammonia

Catalysts: Cobalt (compounds)

Solvents: Tetrahydrofuran; 30 h, 40 bar, 120 °C

Experimental Protocols

2

Simple ruthenium-catalyzed reductive amination enables the synthesis of a broad range of primary amines

By: Senthamarai, Thirusangumurugan; Murugesan, Kathiravan; Schneidewind, Jacob; Kalevaru, Narayana V.; Baumann, Wolfgang; et al

Nature Communications (2018), 9(1), 1-12 | Language: English, Database: CPlus

Full Text

Reactions search for drawn structure

References

按照反应类型分组

Structure Match

- As Drawn (133)
- Substructure (118K)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

- 90-100% (5)
- 80-89% (9)
- 70-79% (5)
- 50-69% (4)
- 30-49% (1)

View All

Number of Steps

- 1 (42)
- 2 (29)
- 3 (14)
- 4 (1)
- 5 (2)
- 6-10 (5)

Non-Participating Functional Groups

- Halide (39)
- Phenyl halide (39)
- Imine (5)
- Alkene (2)
- Amine (2)

View All


133 Results

Group: By Transformation Sort: Reaction Count: Descending View: Collapsed

1

Reduction of the Carbon-Nitrogen Double Bond

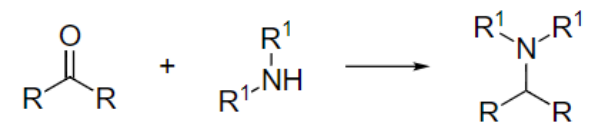
View 19 Related Reactions



2

Reductive Alkylation of Ammonia or Amines

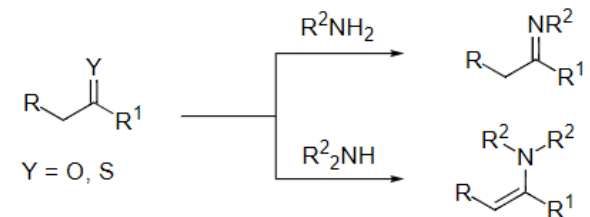
View 13 Related Reactions



3

Addition of Amines to Aldehydes, Ketones or Thiocarbonyls

View 2 Related Reactions



# 使用联用检索——结构与关键词检索反应

联用检索提高检索效率

The screenshot shows the search interface with 'Friedel-crafts acylation' entered in the search bar. Below the search bar, there are filters for 'AND', 'Author Name', and 'Add Advanced Search Field'. A pop-up window displays a drawn structure of indole with 'Edit Drawing' and 'Remove' buttons.

The screenshot displays search results for 'Friedel-crafts acylation' + drawn structure. It shows 21 results grouped by scheme. Each scheme includes a reaction diagram, the number of suppliers, and the yield percentage.

- Scheme 1 (1 Reaction): Steps: 1 Yield: 82%. Suppliers: (85), (117), (14).
- Scheme 2 (1 Reaction): Steps: 1 Yield: 78%. Suppliers: (104), (89), (9).
- Scheme 3 (1 Reaction): Steps: 1 Yield: 77%. Suppliers: (117), (73), (23).
- Scheme 4 (1 Reaction): Steps: 1 Yield: 77%. Suppliers: (46), (104), (33).

The screenshot shows the search results page for 'References search for "Friedel-crafts acylation" + drawn structure'. It includes filters for 'Substances', 'Reactions', 'Citing', and 'Knowledge Graph'. The main results section shows 1,280 results, sorted by Relevance, with a view of Partial Abstract. The first result is titled 'ZrCl<sub>4</sub>-Mediated Regio- and Chemoselective Friedel-Crafts Acylation of Indole' by Guchhait, Sankar K.; Kashyap, Maneesh; Kamble, Harshad. The abstract describes an efficient method for regio- and chemoselective Friedel-Crafts acylation of indoles using acyl chlorides in the presence of ZrCl<sub>4</sub>. The 'Reactions (21)' filter is highlighted in a yellow box.

# 反应结果的筛选

二次筛选  
产率  
反应步骤数  
不参与反应官能团  
反应原子标记  
反应规模  
实验步骤  
反应类型  
立体化学  
试剂  
催化剂  
溶剂  
.....

Reactions search for drawn structure

References

Structure Match

As Drawn (1.737)

Substructure (69K)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

Solvent

1,737 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (3 Reactions) Steps: 1 Yield: 89-97%

Suppliers (127) Suppliers (64) Suppliers (47)

<input type="checkbox"/>	31-614-CAS-27808800	Steps: 1 Yield: 97%	Organotin catalyzed transesterification.
	1.1 Reagents: <a href="#">Hydroquinone</a> , <a href="#">Sodium methoxide</a> , <a href="#">4-Methoxyphenol</a> Catalysts: <a href="#">Dimethyltin dichloride</a> Solvents: <a href="#">Heptane</a>	Assignee: CPS Chemical Co., Inc. European Patent Organization, EP646567 A2 1995-04-05	<a href="#">PatentPak</a> <a href="#">Full Text</a>
<input type="checkbox"/>	31-357-CAS-22382141	Steps: 1 Yield: 91%	Preparation method of 2-phenoxyethanol methacrylate
	1.1 Reagents: <a href="#">Phenothiazine</a> Catalysts: <a href="#">Potassium hydroxide</a> , <a href="#">Zinc oxide (ZnO)</a> , <a href="#">Magnesium alloy, nonbase</a> , <a href="#">Mg,Zn</a> ; 7 h, 130 °C	Assignee: Changzhou University China, CN111517949 A 2020-08-11	<a href="#">PatentPak</a> <a href="#">Full Text</a>
<input type="checkbox"/>	31-357-CAS-15789112	Steps: 1 Yield: 89%	Chemoselective Transesterification of Acrylate Derivatives for Functionalized Monomer Synthesis Using a Hard Zinc Alkoxide Generation Strategy
	1.1 Catalysts: <a href="#">4-(Dimethylamino)pyridine</a> , <a href="#">μ<sub>4</sub>-Oxohexakis[μ-(2,2,2-trifluoroacetato-κO;κO)]tetrazinc</a> ; 24 h, 80 °C	By: Nakatake, Daiki; et al European Journal of Organic Chemistry (2016), 2016(22), 3696-3699	

## Non-Participating Functional Groups

- Acyclic alkene (11)
- Alkene (11)
- Ether (11)

## Reaction Scale

- Milligram (9)
- Gram (6)
- No Scale Provided (1,760)

## Experimental Protocols

- Synthetic Methods (33)
- Experimental Procedure (107)

# 反应的详情页

Synthetic Methods——CAS科学家增值标引的合成制备详情

**CAS Reaction Number:** 31-177-CAS-21171434

Get Similar Reactions ↓ Save

Suppliers (5) Suppliers (41) 99%

Double bond geometry shown

### Reaction Overview

Steps: 1 Yield: 99%

### JOURNAL

Rhodium(III)-catalyzed mono- and dialkenylation of N-phenyl-7-azaindoles via regioselective C-H bond cleavage

By: Morioka, Ryosuke; et al  
View All  
Chemistry Letters (2016), 45(6), 682-684

View PDF Full Text

Company/Organization  
Department of Applied Chemistry,  
Graduate School of Engineering  
Osaka University  
Suita, Osaka 565-0871  
Japan

### Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Silver acetate	Tris(acetonitrile)((1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl)rhodium(2+)	1,2-Dimethoxyethane	3 h, 40 °C

Alternative Steps (0)

### Experimental Protocols

#### Synthetic Methods

Products	2-Methylpropyl (2E)-3-[2-(1H-pyrrolo[2,3-b]pyridin-1-yl)phenyl]-2-propenoate, Yield: 99%
Reactants	Isobutyl acrylate 1-Phenyl-1H-pyrrolo[2,3-b]pyridine
Reagents	Silver acetate
Catalysts	Tris(acetonitrile)((1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl)rhodium(2+)
Solvents	1,2-Dimethoxyethane

### Procedure

1. Stir a mixture of N-phenyl-7-azaindole (0.2 mmol), the corresponding alkene (0.2 mmol), [Cp\*Rh(MeCN)<sub>3</sub>][SbF<sub>6</sub>]<sub>2</sub> (0.008 mmol, 6.7 mg), AgOAc (0.4 mmol, 67 mg), and 1-methylnaphthalene (ca. 30 mg) as internal standard in DME (2 mL) under nitrogen at 40 °C for 3 hours.
2. Cool the mixture.
3. Extract the mixture with ethyl acetate (100 mL).
4. Dry the crude product over Na<sub>2</sub>SO<sub>4</sub>.
5. Evaporate the solvents under vacuum.
6. Purify the crude product by column chromatography on silica gel using hexane-ethyl acetate (10:1, v/v) as eluent to obtain isobutyl (E)-3-(2-(1H-Pyrrolo[2,3-b]pyridin-1-yl)phenyl)acrylate.

易于阅读的实验操作流程

### Transformation

Arylation and Alkylation of Alkenes/ Heck Reaction

### Characterization Data

### 产物表征数据

#### 2-Methylpropyl (2E)-3-[2-(1H-pyrrolo[2,3-b]pyridin-1-yl)phenyl]-2-propenoate

#### Proton NMR Spectrum

(400 MHz, CDCl<sub>3</sub>) δ 0.84 (d, *J* = 6.7 Hz, 6H), 1.85 (sep, *J* = 6.7 Hz, 1H), 3.85 (d, *J* = 6.8 Hz, 2H), 6.39 (d, *J* = 15.9 Hz, 1H), 6.67 (d, *J* = 3.5 Hz, 1H), 7.13 (dd, *J* = 7.7, 4.7 Hz, 1H), 7.28 (d, *J* = 3.5 Hz, 1H), 7.34 (d, *J* = 16.0 Hz, 1H), 7.43-7.58 (m, 3H), 7.82 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.99 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.32 (dd, *J* = 4.7, 1.5 Hz, 1H)

#### Carbon-13 NMR

(100 MHz, CDCl<sub>3</sub>) δ 19.0, 27.7, 70.5, 101.7, 116.7, 120.3, 120.7, 127.4, 128.4, 128.8, 129.2, 129.7, 130.8, 131.9, 137.6, 139.9, 144.0, 148.6, 166.5

#### HRMS

*m/z* calcd for C<sub>20</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub> ([M+H]<sup>+</sup>) 321.1598, found 321.1619

#### State

yellow oil

CAS Method Number 3-177-CAS-21171434

### 反应转化类型

#### Transformations

1. Arylation and Alkylation of Alkenes/ Heck Reaction

### 反应注释

#### Reaction Notes

regioselective, stereoselective

# Retrosynthetic Analysis——逆合成路线分析

结合先进的AI技术和CAS科学家标引的高质量反应数据，为已知/未知分子设计的合成路线

**Retrosynthesis Plan Options for drawn structure** Powered by ChemPlanner®

**Select Synthetic Depth** 合成深度 [Learn more.](#)

1  
 2  
 3  
 4

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

Common  
 Uncommon (includes Common Rules) 反应规则常见性  
 Rare (includes Common and Uncommon Rules)

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

1000 起始原料价格 USD/mol

Email me when my plan is complete

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

Break Bond 断裂键  
 Protect Bond 保护键  
[Clear All Bond Selections](#)

**Retrosynthetic Analysis**  
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

**Retrosynthetic Analysis**  
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

**Retrosynthetic Analysis**  
Draw or import a structure.

Molecular Formula: C<sub>18</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>3</sub> (298.27)

[Start Retrosynthetic Analysis](#) [Cancel](#)



# Retrosynthetic Analysis——路线结果呈现

可查看每步反应的文献支持与详细条件

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

## Retrosynthesis Plan for drawn structure

Key Experimental Steps Predicted Steps Edit Plan Options

View Excluded Options Save

Plan Information  
Estimated Yield: 25%  
Overall Price: \$32.51 (USD per 100 grams)

Scoring Profiles  
Complexity Reduction  
Convergence  
Evidence  
Cost  
Yield

已知反应 预测反应

可自由拖动、缩放的路线图

支持文献

可调节的评分维度

反应中心一致，周边化学结构相似的反应方法

Recent Search History  
August 2, 2024  
Retrosynthesis 4:12 AM  
Synthetic Depth: 3  
Predicted Rules: Common  
Break & Protect Bonds: No  
Starting Material Cost Limit: \$1,000.00/mol  
Retrosynthesis Plan will expire on September 1, 2024.  
Open Plan Edit Search Searching.

Step	Evidence
$A \Rightarrow B + C$ Average Yield: 77% Evidence Alternative steps (39)	1.1 Catalysts: 反应条件 Tantalum, tetraaquadodeca- $\mu$ -chlorodichlorohexa-, octahedro, hydrate (1:4); 3 h, 350 °C
$C \Rightarrow D + E$ Maximum Yield: 32% Evidence Alternative steps (31)	Predicted Step Only No reaction summary

# CAS Analytical Methods - 分析方法

- 访问网址: <https://methods.cas.org/>

The screenshot shows the homepage of the CAS Analytical Methods website. At the top, it greets the user with "Good Morning, Kaiqian". Below this is a search bar with the placeholder text "Search for keywords, matrices or analyte." and a blue button labeled "直接检索" (Direct Search). To the left of the search bar are two main navigation options: "Explore Methods" (浏览不同类别分析方法) and "Advanced Search" (高级检索). The "Explore Methods" section includes a grid icon and the text "Search methods using criteria like method categories and subcategories." The "Advanced Search" section includes a magnifying glass icon and the text "Search methods using criteria like keywords, analytes, matrices and more." Below these is a "Recent Searches" section (近期检索历史) which lists "cannabinol" and "Parkinson", each with a close button (x).

# 分析方法结果集

示例：莠去津

分析物

基质

方法类别

所用技术  
发表年份

Results for Atrazine

3,819 Results    Sort: Relevance    Group: By Method

Filter By

- Analyte
  - Atrazine (3191)
  - Simazine (1353)
  - Terbutylazine (705)
  - Alachlor (644)
  - Chlorpyrifos (638)
  - View All
- Matrix
  - River waters (423)
  - Drinking waters (326)
  - Soils (281)
  - Water (270)
  - Surface waters (256)
  - View All
- Method Category
  - Pesticide Residue Analysis (2008)
  - Water / Wastewater / Sludge Analysis (1339)
  - Herbicide Analysis (1166)
  - Food Analysis (1154)
  - Suboptimal Analysis (809)
  - View All
- Technique
- Year

1    [Click title, can enter analysis method details.](#)

**Analysis of Simazine by Liquid chromatography**    [Compare](#)

By: Matsui, Jun; Fujiwara, Kuniyuki; Takeuchi, Toshifumi  
**Atrazine**-selective polymers prepared by molecular imprinting of trialkylmelamines as dummy template species of **atrazine**  
Analytical Chemistry (2000), 72 (8), 1810-1813. American Chemical Society

**Analyte** Simazine; Ametryn; 1,3,5-Triazine; Terbutylazine; Cyanazine; Terbutryn; **Atrazine**; Prometryn; Propazine  
**Other Materials** Reagent: Triethylmelamine; Acetonitrile; Chloroform  
Material: UV lamp; Cooling circular bath; Stainless sieves; Stainless steel column (100 mm x 4.6 mm, i.d.)  
**Method Category** Herbicide Analysis  
**Technique** Liquid chromatography; Liquid chromatography spectrometric detectors  
**Equipment Used** Mechanical mortar; Liquid chromatographic system; Pump; Photodiode-array detector; Autosampler injector

[View Abstract](#)    [Full Text](#)    [View in CAS SciFinder](#)

2    [Can link to SciFinder, view literature details page.](#)

**Analysis of Atrazine in Urine by Solvent extraction**    [Compare](#)

By: Mendas, Gordana; Vuletic, Marko; Galic, Nives; Drevenkar, Vlasta  
Urinary metabolites as biomarkers of human exposure to **atrazine**: **Atrazine** mercapturate in agricultural workers  
Toxicology Letters (2012), 210 (2), 174-181. Elsevier Ireland Ltd.

**Analyte** Atrazine mercapturate; **Atrazine**  
**Matrix** Urine  
**Other Materials** Material: Hypersil ODS column (100 mm x 2.1 mm I.D., of 5 µm particle size)  
**Method Category** Biomarker Public Health Analysis  
**Technique** HPLC-tandem mass spectrometry; Solvent extraction

# 分析方法详情

示例：利用液液微萃取技术分析废水中残余的莠去津

### Analysis of Atrazine in Wastewater by Liquid-liquid microextraction

Download Save

CAS Method Number	Method Category	Technique
1-143-CAS-148147	Water / Wastewater / Sludge Analysis; Herbicide Analysis	Liquid-liquid microextraction; Liquid chromatography spectrometric detectors; HPLC

<b>Analyte</b>	<b>Matrix</b>	<b>Material</b>	<b>Reagent</b>	<b>Biological Reagent</b>
Deethylatrazine Atrazine Desisopropylatrazine	Wastewater Groundwaters	Hollow fibers 150 × 4.6mm I.D. C <sub>18</sub> column (Zorbax RX-C18, 5 μm particles)	Hydrochloric acid Acetonitrile 1-Octanol Sodium chloride	

分析物  
分析基质  
所用材料

## 所用仪器

### Equipment Used

Liquid chromatographic instrument, LC-VP, Shimadzu, Japan

Diode array detector, SPD-M10Avp, Shimadzu, Japan

HPLC system controller, SCL-10Avp, Shimadzu, Japan

HPLC pump, LC-10ATvp, Shimadzu, Japan

## Source

### 文献来源

#### JOURNAL

Determination of atrazine, desethyl atrazine and desisopropyl atrazine in environmental water samples using hollow fiber-protected liquid-phase microextraction and high performance liquid chromatography

Peng, Jinfeng; Lue, Jianxia; Hu, Xialin; Liu, Jingfu; Jiang, Guibin

Microchimica Acta (2007), 158 (1-2), 181 - 186. Springer Wien

CODEN : MIACAQ | ISSN : 00263672 | DOI : 10.1007/s00604-006-0692-9

View Abstract

Full Text

Instructions 无需阅读原文，即可获取方法详情。

### Preparation of water samples

1. Collect wastewater and ground water samples.
2. Store the samples at 4 °C.

### Preparation of atrazine stock solutions

1. Prepare standard stock solutions (100 mg/L) of atrazine (ATR), desethylatrazine (DEA) and desisopropyl atrazine (DIA) by dissolving 0.25 mg of the compounds in 2.5 mL acetonitrile.
2. Store the solutions in brown glass bottles at 4 °C.
3. Prepare fresh working solutions daily by appropriate dilution of the stock solutions.

### Preparation of polyvinylidene fluoride (PVDF) fiber

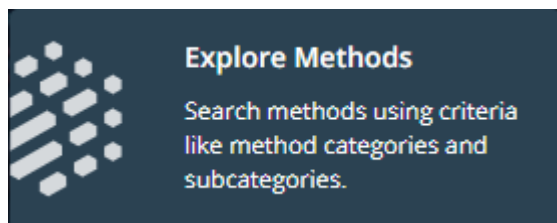
1. Cut PVDF porous hollow fiber membrane (inner diameter 450 μm, wall thickness 125 μm, pore size 2.5 μm) manually into 5.1 cm length.
2. Immerse the fiber in 1-octanol for 10 min.
3. Take out the hollow fiber.
4. Flush the outside and inside of the fiber five times with water in a washing bottle and water in a 0.5 mL microsyringe, respectively.
5. Connect the hollow fiber with the needle of the microsyringe holding ~20 μL acceptor solution (4 M HCl).
6. Depress the plunger of the microsyringe to flush out ~20 μL acceptor solution to wash and fill the lumen of the hollow fiber without any air bubbles.
7. Seal the two ends of the fiber with heated tweezers.
8. Obtain the hollow fiber protected liquid-phase microextraction device with an effective fiber length of ~5.0 cm with acceptor phase volume of ~8 μL ready for extraction.

### Liquid-phase microextraction procedure

1. Perform extraction with PVDF fiber at a middle-stirring rate.
2. Extract 50 mL volume of aqueous solution in a 100 mL petri dish with addition of 20% sodium chloride.
3. Cover the petri dish with glass cap.
4. After extracting for 30 min, take out the hollow fiber from the aqueous solution.
5. Cut open one sealed end of the fiber for connecting with the microsyringe.
6. Cut open the other sealed end to facilitate flushing out the acceptor solution into 200 μL glass vial with the microsyringe.
7. Add 8 μL of sodium hydroxide into the glass vial to neutralize the acid acceptor solution.
8. Finally, retract the total solution of ~16 μL into an 25 μL HPLC microsyringe.

详细直观的实验步骤

# 浏览分析方法分类



[Return to Home](#)

## Explore Methods

Category	Category Name	Include Keywords (Optional)
Agricultural Applications / Analysis	<b>Active Pharmaceutical Ingredient</b>	Crizotinib
Bioassays	Addictive Drug Assay	<a href="#">+ Add Another Keyword</a>
Biomolecule Isolation	Forensic Analysis	
Environmental Analysis	Genetic Analysis	
Food Analysis	Nanomaterial Analysis	
Fuels / Geology / Biofuels	Organic Compound Analysis	
Historical Analysis / Dating	Toxin Assay	
Miscellaneous		
Organic Compound Analysis		
Organometallics / Inorganics		
<b>Pharmacology / Toxicology</b>		
Polymer Analysis		
Water Analysis		

[Search Methods](#)

## Results for Active Pharmaceutical Ingredient and Metabolite Analysis +1 Keyword

39 Results | Sort: Relevance | Group: By Method

1

### Analysis of Crizotinib in Pharmaceutical capsules by Spectrophotometry

By: Darwish, Ibrahim A.; Alshehri, Jamilah M.; Alzoman, Nourah Z.; Khalil, Nasr Y.; Abdel-Rahman, Hamdy M. Charge-transfer reaction of 1,4-benzoquinone with crizotinib: Spectrophotometric study, computational molecular modeling and use in development of microwell assay for crizotinib. Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (2014), 131, 347-354. Elsevier B.V.

Analyte: Crizotinib  
Matrix: Pharmaceutical capsules  
Other Materials: Reagent: Methanol; Quinone; Ethanol; Material: 96-microwell assay plates  
Method Category: Active Pharmaceutical Ingredient and Metabolite Analysis  
Technique: Spectrophotometry  
Equipment Used: Microwell-plate reader

[View Abstract](#) [Full Text](#) [View in CAS SciFinder](#)

2

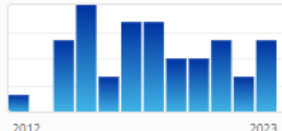
### Analysis of Crizotinib in Drugs by HPLC

By: Vijayakumar, Bontha; Samhitha, Bontha Laxmi; Ramu, Adepu; Krishna, Madishetty Vamshi; Sreekanth, Gandhe. Enantioselective analysis of crizotinib by chiral LC method. Pharma Chemica (2017), 9 (22), 18-24. Scholars Research Library

Analyte: Crizotinib  
Matrix: Drugs  
Other Materials: Reagent: Diethylamine; Isopropanol; Methanol; Hexane; Material: Injector; Chiralcel OD-H (250 mm x 4.6 mm, 5 μm) column; Membrane filter (0.45 μm)  
Method Category: Chiral Separation; Active Pharmaceutical Ingredient and Metabolite Analysis  
Technique: UV-visible spectroscopy; HPLC  
Equipment Used: High pressure liquid chromatography; HPLC pump; UV-Visible detector; Electronic balance

[View Abstract](#) [Full Text](#) [View in CAS SciFinder](#)

**Filter By**

- Analyte
  - Crizotinib (28)
  - Erlotinib (8)
  - Afatinib (7)
  - Alectinib (7)
  - Ceritinib (6)
  - [View All](#)
- Matrix
  - Blood plasma (32)
  - Drugs (2)
  - Brain (1)
  - Drug delivery systems (1)
  - Pharmaceutical capsules (1)
  - [View All](#)
- Method Category
- Technique
- Year
  - 
  - No Min to No Max [Apply](#)



# CAS Formulus - 制剂/配方

- 访问网址: <https://formulus.cas.org/>

The screenshot shows the CAS Formulus website interface. At the top, it says "Good Morning, Kaiqian" and "配方或主要成分检索" (Formulation or main component search). Below this are tabs for "Formulations" and "Ingredients", and a "直接检索" (Direct search) button. A search bar contains the text "Search by Formulations by Ingredients, Purpose, Form, Functions, etc." with a magnifying glass icon. Below the search bar are two main sections: "Formulation Designer" (制剂/配方设计) and "Advanced Search" (高级检索). The "Formulation Designer" section describes designing custom templates based on selections. The "Advanced Search" section describes searching for formulations using criteria like ingredients and target. Below these sections is a "Recent Search History" (近期检索历史) section, which includes a "View Search History" link. The history shows a search from July 26, 2024, at 5:16 PM, for "Formulations" with the query "+Ingredient:'Olaparib' +Form:'Tablets' (136)". There are "Rerun Search" and "Edit Search" buttons for this entry.

# 制剂/配方结果集

领域

用途

物理形态

物质状态

递送途径

所含信息

文献类型

机构/组织

语言

发表年份

Formulations search for "Lutein"

Get Additional References

Filter by

- Industry
  - Agrochemical
  - Cleaning & Surfactant Products
  - Cosmetics & Personal Care
  - Food & Related
  - Inks, Paints, & Coatings
- Purpose
  - Ophthalmic agents (1,101)
  - Dietary supplement formulations (781)
  - Pharmaceutical formulations (588)
  - Drug delivery systems (425)
  - Cosmetics and Personal care products (200)
- Physical Form
  - Capsules (1,089)
  - Tablets (802)
  - Powders (651)
  - Liquids (407)
  - Solutions (379)
- State of Matter

6,901 Results

Sort: Relevance Group: By Family

1 [Click title, you can enter the formulation/recipe details.](#)

**Lutein Concentrate Composition: Dermatological Agents** [Compare](#)

Location: Example 10  
Purpose: Dermatological agents  
Physical Form: Capsules

Component	Function	Amount Reported
Group: <a href="#">lutein concentrate</a>	-	3.2 mg
<a href="#">Lutein A</a>	-	8.5 %
<a href="#">Zeaxanthin</a>	-	8.5 %
fat content	-	19.2 %
Iron	-	0.863 %

Additional group components reported

Group: Additional ingredients	-	-
<a href="#">Vegetable oils</a>	-	250.0 mg/capsule

**PATENT**  
[Lutein concentrate from plant sources by aqueous method](#)  
Assignee : Ajanta Pharma Ltd.  
IN1999MU00604  
Language: English

Patent PDF [View in CAS SciFinder](#)

[View Formulation Detail](#)

[16 Similar Formulations - View All](#)

可同时对比3种制剂/配方

可链接至SciFinder, 查看文献详情页

# 制剂/配方详情

## Soft Capsule Formulation: Food

### 配方用途

Purpose	Target	Delivery Route	Physical Form	Source
Food	Homo sapiens, reaggregation	Oral drug delivery systems	Capsules	

Predicted value

### 配方成分

#### Formulation Ingredients

Component	Function
Group: hardly soluble component	Formulation active agents
Lutein A	-
Capsanthin	pigment <sup>®</sup>
Diacetyl/tartaric acid	-
saffron oil	-
Group: Coating materials	Coating materials
gelatin BCN 200 S	Coating materials
Glycerol	Food additives
caramel BD-2	pigments



Save

无需阅读原文，即可获取配方详情

#### Process

hardly soluble component, organic acid monoglyceride, hydrophilic emulsifier, glycerin fatty acid ester/polyglycerin fatty acid ester and other components were mixed and then each component as a film was coated to obtain a soft capsule preparation

详细、直观的操作步骤  
与实验数据

#### Effective Dose

Descriptor	Solvent	Details
separation of oily components containing sparingly soluble components is slight, but to the first solution of disintegration test dispersibility is uniform good	Water	-

#### Experimental Activity

Descriptor	Notes	Details
dispersibility test	visual observation of dispersibility in water were evaluated	-

#### Experimental Activity

#### Source Patent

Pharmaceutical oral agent comprising sparingly soluble component with organic acid monoglyceride and hydrophilic emulsifier

Assignee : Lion Corporation  
WO2018101267  
Language: Japanese  
Location: Table 5, Example 29

文献来源

Patent PDF

View in CAS SciFinder



# Formulation Designer 辅助设计制剂、配方

启发制剂配方设计



Formulation Designer

Industry	Purpose	Physical Form	Add up to 5 Ingredients
Pharmaceutical	Drug delivery systems	Tablets	Water
Cosmetics & Personal Care	Pharmaceutical formulations	Solutions	Crizotinib
Agrochemical	Antitumor agents	Capsules	+ Add Another Ingredient
Cleaning & Surfactant Products	Anti-inflammatory agents	Particles	
Inks, Paints, & Coatings	Analgesics	Liquids	
Food & Related	Antibacterial agents	Powders	
	Ophthalmic agents	Gels	
	Antidiabetic agents	Suspensions	
	Antiviral agents	Pharmaceutical injections	
	Antihypertensives	Pharmaceutical liposomes	
	- View More Purposes -	- View More Physical Forms -	

Create Template

Formulation Designer

Industry	Purpose	Physical Form	Active or Featured Ingredient
Pharmaceutical	Antitumor agents Pharmaceutical formulations	Solutions	Water Crizotinib

Edit Selections Save Download

Your Template Unit Size mg Go Clear

Function	Ingredient	Regulatory Lists	Top Alternatives	Amounts
Active or Featured Ingredient:	Water	ANMAT; CosIng: Cosmetic Ingredient Inventory; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; NMPA	-	Amount not available
Active or Featured Ingredient:	Crizotinib	EMA EPARS; FDA Orange Book; Japanese Approved Drugs List	-	Amount not available
Preservatives	Glycerol View More Alternatives	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 182, Subpart A); FDA GRAS (Part 182, Subpart B); FDA Inactive Ingredients Database; NMPA	(±)-Propylene glycol; Ethanol; Boric acid (H <sub>3</sub> BO <sub>3</sub> ); Benzyl alcohol; Phenol	Approximate Range: 12 - 22%
Stabilizing agents	Glycerol View More Alternatives	ANMAT; CosIng: Cosmetic Ingredient Inventory; Drug Master File List; EMA Excipients List; EPA Pesticide Inactive Ingredients; EPA Safer Chemical Ingredients; FDA GRAS (Part 182, Subpart A); FDA GRAS (Part 182, Subpart B); FDA Inactive Ingredients Database; NMPA	Sucrose; (±)-Propylene glycol; Mannitol; Polyoxyethylene sorbitan monooleate; Poly(vinylpyrrolidone)	Approximate Range: 12 - 21%

基于期刊、专利和产品说明书中标引的制剂、配方数据，获得见解。

# 小结

- **反应的检索方式**: 使用标识符, 结构绘制以及关键词联用等方式, 关注筛选目标反应信息。
- **信息之间的深度关联**: 从关注的物质/文献, 一键链接到相关反应, 高效完成信息检索。
- **反应检索及路线设计**: 多元的检索方式, 逆合成路线分析, 反应结果的筛选和详情查看。
- **反应检索结果筛选及详情速览**: Synthetic Methods, 通过CAS科学家的标引, 无需阅读原文, 直接获取实验步骤详情及产物表征信息。
- **CAS Analytical Methods**: 分析方法解决方案, 支持直接检索、高级检索及按不同类别浏览, 提供分析方法详情和方法对比。
- **CAS Formulus**: 制剂/配方解决方案, 支持制剂/配方及成分的检索, 提供详情和详情对比, 以及协助设计制剂/配方。

# 总结

- CAS 内容合集来源于化学并超越于化学，支持多学科、跨学科研发创新
- 全面覆盖的内容确保不遗漏任何重要的信息
- CAS 科学家人工智慧与先进专有技术结合标引的数据，能够揭示隐藏在数据间的隐秘关联
- 强大的功能确保降低文献检索和分析的时间，将更多宝贵的时间应用于创新工作中，提升科研创新效率

# 大纲

- CAS及CAS SciFinder Discovery Platform (Academic)简介
- 科研信息的高效查阅
  - 全面的文献调研与拓展助力开题
  - 多角度出发检索物质结构及相关属性
  - 生物序列检索方法与结果分析
  - 探索实验方案以获取制备及其他实验详情
- 常见问题Q&A



# CAS SciFinder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

# 常见登录问题

## 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



There was a problem verifying your account.

Try Again

Contact Us

Or Log Out and try again.

Reference Id: GU75LMF9iZnhTq6mymUog

- 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

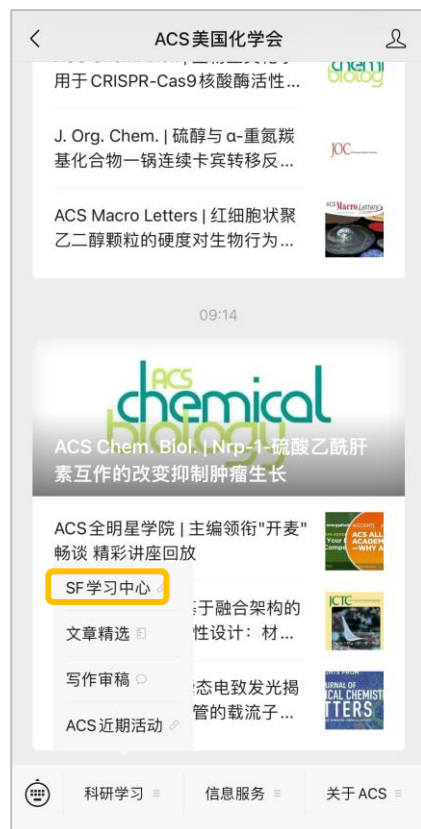
# 使用注意事项

- 一人注册一个帐号
- 不得账号分享
- 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（<https://www.cas.org/legal/infopolicy>）
- 不得将账号用于非学术研究

# 线上学习资源

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CAS SciFinder 学习中心



<https://space.bilibili.com/630784162>



Between problems  
and progress  
are connections  
that matter

谢谢!

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