

# 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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# 大纲

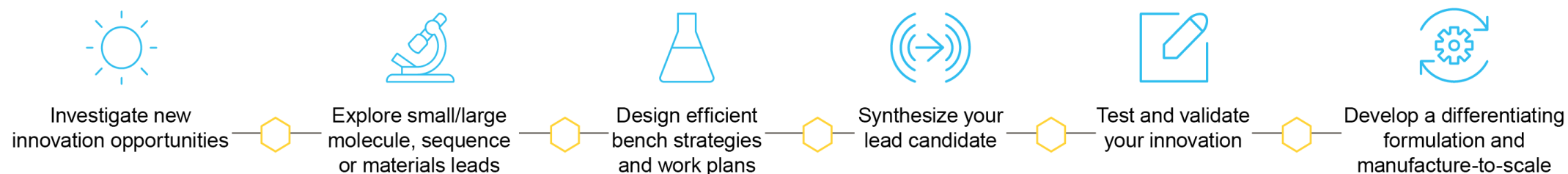
- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A



# CAS 独特的解决方案和能力

助您加速创新之旅

Informing and accelerating the innovation process end-to-end



## CAS SciFinder Discovery Platform™

为研究人员提供他们所需要的信息，加速科学发现市场化并优化利润率

## STN IP Protection Suite™

确保知识产权得到保护，并找到机会拓展新市场

## CAS Custom Services<sup>SM</sup>

定制数据、分析和见解，最大化信息资产的价值，推动数字化成功

**独特的内容** | 最大科学数据合集

**专业技术** | 为整个创新之旅提供信息

**专业知识** | 多学科背景的科学家和技术专家

# CAS SciFinder Discovery Platform 涵盖的工作流程解决方案



新一代的权威科学研究工具，是化学及相关学科智能研究平台，提供全球全面、可靠的化学及相关学科研究信息和分析工具



独特的分析方法详情数据库，有助于分析科学家快速获取详尽的分析方法信息、直接用于实验，并启发新方法的建立



专业的制剂/配方数据库，助力配方研究科学家快速评估配方、寻找可替代供应商和探索监管信息



# CAS 独特的内容合集

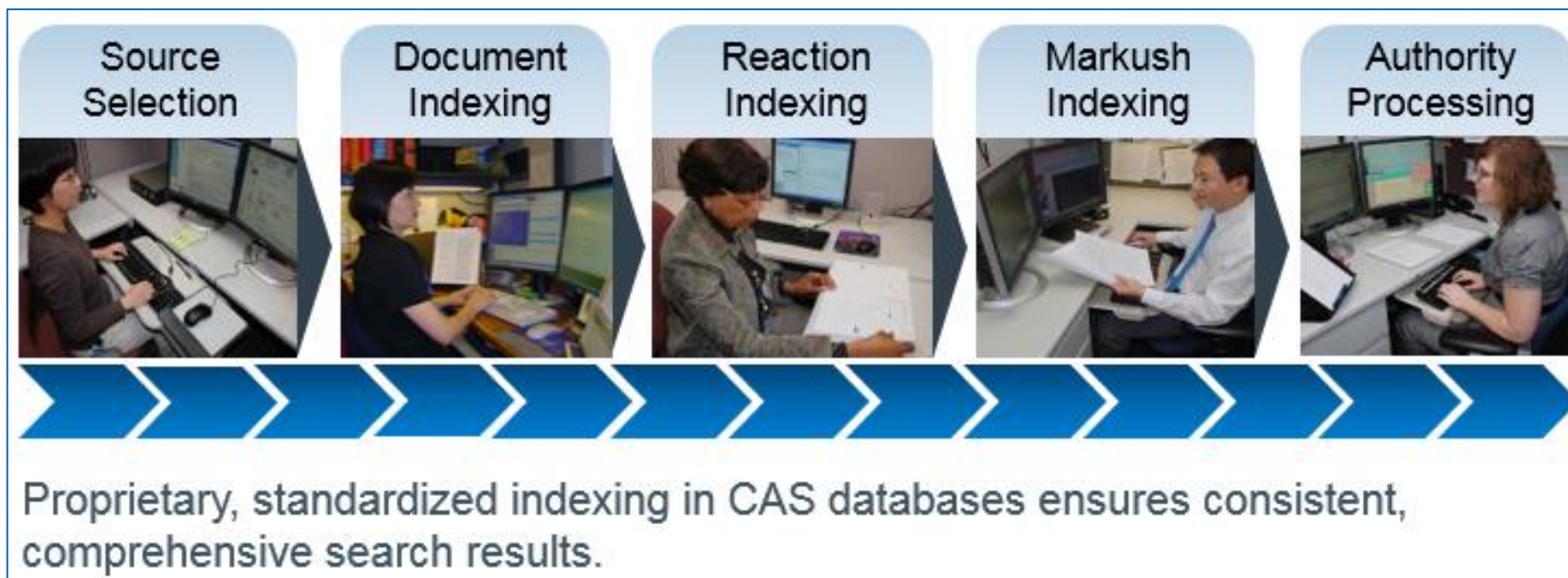


来源：

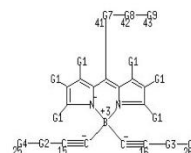
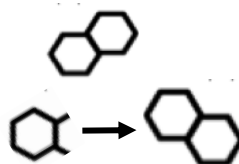
<https://www.cas.org/cas-data>

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

# CAS 科学家的智力标引




1990  
Smith, M.  
anthracene



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

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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




Log in to SciFinder®

Username or Email Address

Next

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

By using CAS SciFinder®, you agree to the [License Agreements and Policies](#), including but not limited to the [End User License Agreement](#)



Log in to SciFinder®

Welcome, npan@acs-i.org [Not You?](#)

Password

Log In

☐ Keep me signed in

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

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使用CAS SciFinder账号登录

# CAS SciFinder 主界面

The screenshot displays the CAS SciFinder main interface. On the left is a sidebar menu titled 'SCIFINDER DISCOVERY PLATFORM' containing links to 'CAS SciFinder', 'CAS Analytical Methods', 'CAS Formulus', 'STN IP PROTECTION SUITE', 'STNext', 'CAS Scientific Patent Explorer', 'REGULATORY', 'CAS Chemical Compliance Index', 'ACCOUNT MANAGEMENT', and 'CAS Profile'. The main header includes the CAS SciFinder logo, a '更新结果提醒' (Update Results Reminder) button, and user account icons. Below the header is a navigation bar with 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The central search area features a large search bar with the placeholder 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' and a 'Draw' button for chemical structure input. Below the search bar is a 'Molecular Formula' input field with a dropdown menu and an 'Add Advanced Search Field' button. Three main functional tiles are visible: 'Retrosynthetic Analysis' (labeled '逆合成路线设计'), 'Search CAS Lexicon' (labeled 'CAS词库'), and 'Search CAS Sequences' (labeled 'CAS序列检索'). At the bottom, there is a 'Recent Search History' section (labeled '近期检索历史') and a 'View All Search History' link. Annotations in blue boxes with white text point to specific features: '高级检索选项' (Advanced Search Options) points to the 'Add Advanced Search Field' button; '结构绘制面板' (Structure Drawing Panel) points to the 'Draw' button; and '近期检索历史' (Recent Search History) points to the 'Recent Search History' section.

CAS SciFinder

更新结果提醒

Good Morning, [User]

Substances Reactions References Suppliers

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

Draw

Molecular Formula

Examples: C<sub>6</sub>H<sub>6</sub> | (C<sub>8</sub>H<sub>8</sub>)<sub>x</sub> | 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

+ Add Advanced Search Field

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.

逆合成路线设计

CAS词库

CAS序列检索

Recent Search History 近期检索历史

View All Search History

# 大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研？
  - 如何聚焦某类物质？
  - 如何调研反应信息？
  - 怎么查、怎么选具体的实验方案？
- 常见问题Q&A



# 1. 如何开展文献检索？

- 主题词怎么选择？如何构建检索主题？
- 想要研究某结构相关的文献？
- 如何筛选文献？追踪最新进展？
- 如何纵览关注的研究方向？
- 专利内容繁杂，如何高效获取信息？



# 1.1 如何精准构建检索主题？

- 支持使用：主题词、物质名称、CAS登记号、专利号、PubMed ID、文献号、DOI
- 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

The screenshot displays the CAS search interface. At the top, there are navigation tabs: All, Substances, Reactions, References (selected), and Suppliers. The main search bar contains the query: ("natural product" not camptothecin) and synthesis. Below the search bar, there are fields for AND, Author Name, and a text input field with the placeholder "Enter last name, first name middle name.". A button labeled "+ Add Advanced Search Field" is also visible. On the right side, a dropdown menu is open, showing suggestions for the query "natural pro". The suggestions include: Natural product, Natural products, Natural protein fiber, Natural protein fibers, Natural products, chiral, Natural product nomenclature, Natural products, CapsiAlil, and Natural products nomenclature. To the right of the dropdown menu, there are two bullet points: "自动提示检索词" (Automatic search suggestions) and "基于科学家创建的叙词表" (Based on the thesaurus created by scientists).

# 1.1 如何精准构建检索主题？

主题词示例：

（“natural product” not camptothecin) and synthesis （天然产物排除喜树碱，合成）

References search for **"natural product" not camptothecin**

Substances Reactions Citing Knowledge Graph

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

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Solutions

Bioactivity Data

Formulation Purpose

Database

630,863 Results

1

Natural products in crop protection

By: Dayan, Franck E.; Cantrell, Charles L.; Duke, Stephen O.  
Bioorganic & Medicinal Chemistry (2009), 17(12), 4022-4034 | Language: English

A review. The tremendous increase in crop yields associated with the growth and utilization of chems. for pest control. However, concerns over the potential environmental impact of pesticides has led to the introduction of new pesticide registration procedures in the United States. These new regulations have reduced the number of synthetic pesticides currently in use. The current paradigm of relying almost exclusively on chems. for pest control is being challenged. View More

Full Text

Substances (0)

2

Natural product isolation

By: Sticher, Otto  
Natural Product Reports (2008), 25(3), 517-554 | Language: English, Database: CAS

A review. Covering: 2000 to mid-2007. Since the 1990s, interest in natural product research has gained new attention for providing novel chemical structures and purification, recent extraction techniques used for natural product isolation, as well as multi-step chromatographic operations. It covers examples of natural product isolation. View More

Full Text

Substances (0)

3

Marine natural products

By: Faulkner, D. John  
Natural Product Reports (2002), 19(1), 1-48 | Language: English, Database: CAS

References search for **"natural product" not camptothecin) and synthesis**

Substances Reactions Citing Knowledge Graph

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

Load All Results

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Content

Life Science Data

Formulation Purpose

Database

162,825 Results

Sort: Relevance View: Partial Abstract

1

Natural product synthesis in the age of scalability

By: Kuttruff, Christian A.; Eastgate, Martin D.; Baran, Phil S.  
Natural Product Reports (2014), 31(4), 419-432 | Language: English, Database: CAPLUS and MEDLINE

A review. The ability to procure useful quantities of a mol. by simple, scalable routes is emerging as an important goal in natural product synthesis. Approaches to mols. that yield substantial material enable collaborative investigations (such as SAR studies or eventual com. production) and inherently spur innovation in chem. As such, when evaluating a natural product synthesis, scalability is becoming an increasingly important factor. This highlight discussed recent examples of natural product synthesis from the authors' laboratory and others, where the preparation of gram-scale quantities of... View More

Full Text

Substances (0)

Reactions (0)

Citing (138)

Citation Map

2

Synthesis of natural product inspired compound collections

By: Kumar, Kamal; Waldmann, Herbert  
Angewandte Chemie, International Edition (2009), 48(18), 3224-3242 | Language: English, Database: CAPLUS and MEDLINE

A review. Natural products, their derivatives, and their analogs are among the most important sources for new drug candidates and tools for chem. biol. and medicinal chem. research. Therefore, there is a need for the development of efficient synthesis methods which give access to natural product derived and inspired compound collections. To meet this challenge, the requirements of multistep stereoselective syntheses, and the logic and methodol. of natural product total synthesis need to be translated and adapted to the methods and formats for the synthesis of compound collections. Recent developments... View More

Full Text

Substances (0)

Reactions (0)

Citing (249)

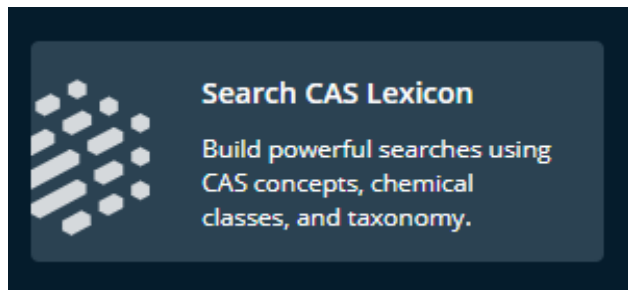
Citation Map

3

Application of donor/acceptor-carbenoids to the synthesis of natural products

By: Davies, Huw M. L.; Denton, Justin R.

# 如何选择概念词？借助CAS Lexicon词库



- CAS科学家标引的概念词 (Concepts) 和重要物质
- 选择感兴趣的技术词来建立检索式（最多可用1000个词）

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

Search a concept to start (ex. Biomass)...

**Search Concept**

**Preferred Concept**

☒ Steroids

This will search synonyms: MeSH ID: D013256; Natural **steroids**; **Ster...**

[View more synonyms](#)

**Broader Concepts (2)** [Select All](#)

- ☐ Alicyclic compounds
- ☐ Lipids

**Narrower Concepts (94)** [Select All](#)

- ☒ 11-Deoxycortisol
- ☒ 17-Hydroxyprogesterone
- ☐ 17 $\alpha$ ,20 $\beta$ -Dihydroxyprogesterone
- ☐ 17 $\alpha$ -Trenbolone
- ☐ 3 $\beta$ -[N-(N',N'-Dimethylaminoethyl)carbamoyl]cholesterol

[View All](#)

**Related Concepts (10)** [Select All](#)

- ☐ Isoprenoids
- ☐ Proteins, steroid-binding
- ☒ Steroid synthesis inhibitors

AND OR NOT

**Add to Query**

**Steroids - Preferred Concept** [X](#)

OR [Remove All](#)

**Steroids - Narrower Concepts (2)**

- 11-Deoxycortisol [X](#)
- 17-Hydroxyprogesterone [X](#)

**Steroids - Related Concept (1)**

- Steroid synthesis inhibitors [X](#)

Clear Query **Search**

主题词示例：  
Steroids (甾体)

- 甾体的上位词
- 甾体的下位词
- 甾体相关词汇

# 自定义组合检索

The screenshot displays the CAS search interface with the 'References' tab selected. The search bar prompts users to search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Below the search bar, there is a section for 'Author Name' with a text input field and an example 'Schubert, J A'. A button labeled '+ Add Advanced Search Field' is highlighted with a yellow box. A dropdown menu is open from this button, listing various search criteria: Authors, Publication Name, Organization, Title, Abstract/Keywords, Concept, Substances, Bioactivity Data (marked as NEW), Publication Year, Document Identifier, Patent Identifier, and Publisher. Another dropdown menu is shown below the main search bar, containing logical operators: AND, OR, and NOT.

检索方法可单独使用，也可联用：

- 关键词、物质名称、CAS RN、文献号
- 高级检索（刊物名、机构名、Concepts、标题等）

## 1.2 如何获得结构相关的文献？

示例：关注植物或药物中特定的结构骨架化合物

策略：从References出发，主题词+结构联用检索

## 定位物质在文献中的研究角色

References search for "herb and medic\*" + drawn structure

Substances ▾ Reactions ▾ Citing ▾ Knowledge Graph

Structure Match

As Drawn (0)

Substructure (368)

Filter Behavior

Filter by Exclude

Document Type

Substance Role

Biological Study (334)

Uses (214)

Analytical Study (83)

Preparation (49)

Occurrence (33)

View All

Language

368 Results

1

Pentacyclic triterpenoids from the medicinal herb, *Centella asiatica* (L.) Urban

By: James, Jacinda T.; Dubery, Ian A.

Molecules (2009), 14(10), 3922-3941 | Language: English, Database: CAPLUS and MEDLINE

A review. *Centella asiatica* accumulates large quantities of pentacyclic triterpenoid saponins, collectively known as centelloids. Triterpenoids include asiaticoside, centelloside, madecassoside, brahmoside, brahminoside, thankunside, scelefoleoside, centello- asiatic-, brahmic-, centellic- and madecassic acids. The triterpene saponins are common secondary plant metabolites and are synthesized via the isoprenoid pathway to produce a hydrophobic triterpenoid structure (aglycon) containing a hydrophilic sugar chain (glycone). The bioactivity of saponins has been attributed to these charac...

View More

Full Text ▾

Substances (6) Reactions (0) Citing (204) Citation

2

Effects of *Gymnema sylvestre* extract on the pharmacokinetics and pharmacodynamics of glimepiride in streptozotocin induced diabetic rats

By: Kamble, Bhagyashree; Gupta, Ankur; Moothedath, Ismail; Khatal, Laxman; Janrao, Shirish; Jadhav, Amol; Duraiswamy, B.

Chemico-Biological Interactions (2016), 245, 30-38 | Language: English, Database: CAPLUS and MEDLINE

Analytical Methods

*Gymnema sylvestre*, important Indian traditional herbal medicine has been used for diabetes from several years and marketed as single or multi-herb formulations globally. People are consuming *G. sylvestre* along with conventional hypoglycemic drugs.

By Count Alphanumeric

8 Selected

Biological Study (334)

Uses (214)

Therapeutic Use (204)

Pharmacological Activity (132)

Biological Study, Unclassified (127)

Analyte (83)

Analytical Study (83)

Preparation (49)

Purification or Recovery (43)

Natural Product Occurrence (33)

Occurrence (33)

Properties (23)

Food or Feed Use (16)

Cosmetic Use (15)

Pharmacokinetics (15)

Adverse Effect (6)

Reactant (6)

Reactant or Reagent (6)

Apply Cancel

# 1.3 文献结果分析与筛选

References search for "(“natural product” not camptothecin) and synthesis"

Substances Reactions Citing Knowledge Graph

We are displaying the most relevant results. Learn about result relevance. Load All Results

Filter Behavior Filter by Exclude

Search Within Results

Document Type Language Publication Year Author Organization Publication Name Concept CA Section CAS Content Life Science Data Formulation Purpose Database

162,825 Results

Sort: Relevance View: Partial Abstract

1

Natural product synthesis in the age of scalability

By: Kuttruff, Christian A.; Eastgate, Martin D.; Baran, Phil S. Natural Product Reports (2014), 31(4), 419-432 | Language: English, Database: CPlus and MEDLINE

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View More

Full Text

Substances (0) Reactions (0) Citing (138) Citation Map

2

Synthesis of natural product inspired compound collections

By: Kumar, Kamal; Waldmann, Herbert Angewandte Chemie, International Edition (2009), 48(18), 3224-3242 | Language: English, Database: CPlus and MEDLINE

A review. Natural products, their derivatives, and their analogs are among the most important sources for new drug candidates and tools for chem. biol. and medicinal chem. research. Therefore, there is a need for the development of efficient synthesis methods which give access to natural product derived and inspired compound collections. To meet this challenge, the requirements of multistep stereoselective syntheses, and the logic and methodol. of natural product total synthesis need to be translated and adapted to the methods and formats for the synthesis of compound collections. Recent devel...

View More

Full Text

Substances (0) Reactions (0) Citing (249) Citation Map

3

Application of donor/acceptor-carbenoids to the synthesis of natural products

By: Davies, Huw M. L.; Denton, Justin R.

AI技术支持的相关度排序

Sort: Relevance

Save and Alert

Share Results

Copy Search to Clipboard

定题追踪

Save Results

Name Natural & synthesis

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

Add Existing Tags (Optional)

Agriculture Chinese Medicine Cigarette Diabetes Food

New Tag (Optional) Tag Color Add tag name Light Blue

Alerts

Frequency As Available

Add Email(s) Add Recipient(s)

Save Cancel

Relevance

Times Cited

Accession Number: Ascending

Accession Number: Descending

Publication Date: Newest

Publication Date: Oldest

排序方式

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

结果集的二次检索



# 筛选工具 CA Section, Concept

## 聚焦核心研究点

^ Concept

- ☐ Pharmaceutical natural products (113K)
- ☐ Homo sapiens (29K)
- ☐ Human (29K)
- ☐ Pharmaceutical tablets (16K)
- ☐ Pharmaceutical capsules (14K)
- [View All](#)

^ CA Section

- ☐ Pharmaceuticals (59K)
- ☐ Unavailable (39K)
- ☐ Pharmacology (10K)
- ☐ Biomolecules and Their Synthetic Analogs (8,826)
- ☐ Food and Feed Chemistry (5,025)
- [View All](#)

## 纵览学科研究方向

Concept

Top Count Alphanumeric Search

3 Selected

<input type="checkbox"/> Pharmaceutical natural products (113K)	<input type="checkbox"/> Safflower (5,231)
<input type="checkbox"/> Homo sapiens (29K)	<input checked="" type="checkbox"/> Oral drug delivery systems (5,162)
<input type="checkbox"/> Human (29K)	<input type="checkbox"/> Humans (5,125)
<input type="checkbox"/> Pharmaceutical tablets (16K)	<input type="checkbox"/> Astragalus membranaceus (5,110)
<input type="checkbox"/> Pharmaceutical capsules (14K)	<input type="checkbox"/> Zingiber officinale (4,999)
<input type="checkbox"/> Angelica sinensis (11K)	<input type="checkbox"/> Plant extracts (4,718)
<input type="checkbox"/> Food (11K)	<input type="checkbox"/> Rehmannia (4,712)
<input checked="" type="checkbox"/> Natural products (11K)	<input type="checkbox"/> Fermentation (4,676)
<input type="checkbox"/> Pharmaceutical granules (11K)	<input type="checkbox"/> Citrus reticulata (4,665)
<input type="checkbox"/> Pharmaceutical powders (10K)	<input type="checkbox"/> Mandarin (4,665)
<input type="checkbox"/> Glycyrrhiza (9,431)	<input type="checkbox"/> Panax (4,621)
<input type="checkbox"/> Pharmaceutical natural products, licorice (8,994)	<input type="checkbox"/> Topical drug delivery systems (4,612)
<input checked="" type="checkbox"/> Antitumor agents (8,564)	<input type="checkbox"/> Panax notoginseng (4,537)
<input type="checkbox"/> Ligusticum chuanxiong (8,153)	<input type="checkbox"/> Scutellaria baicalensis (4,537)

OK Cancel

Concept

Top Count Alphanumeric **Search** 精准定位核心研究点

Concept Name

支持使用通配符

☒ 4 Selected

<input type="checkbox"/> Biodegradable polymeric drug delivery systems (1)	<input type="checkbox"/> Intradermal drug delivery systems (5)	<input type="checkbox"/> Parenteral drug delivery systems (162)
<input type="checkbox"/> Bolus drug delivery systems (1)	<input type="checkbox"/> Intrahepatic drug delivery systems (55)	<input type="checkbox"/> Parenteral drug delivery systems, intraadiposal (1)
<input type="checkbox"/> Buccal drug delivery systems (199)	<input type="checkbox"/> Intrahepatic drug delivery systems (1)	<input type="checkbox"/> Parenteral drug delivery systems, intralesional (3)
<input type="checkbox"/> Chewable drug delivery systems (36)	<input type="checkbox"/> Intrapericardial drug delivery systems (1)	<input type="checkbox"/> Parenteral drug delivery systems, intrapleural (2)
<input type="checkbox"/> Colon specific drug delivery systems (5)	<input type="checkbox"/> Intraperitoneal drug delivery systems (22)	<input type="checkbox"/> Parenteral drug delivery systems, intraprostatic (1)
<input type="checkbox"/> Controlled-release drug delivery systems (922)	<input type="checkbox"/> Intrathecal drug delivery systems (21)	<input type="checkbox"/> Parenteral drug delivery systems, intravesical (4)
<input type="checkbox"/> Controlled-release floating drug delivery systems (11)	<input type="checkbox"/> Intrathoracic drug delivery systems (1)	<input type="checkbox"/> Pharmaceutical injections, freeze-dried injectable drug delivery systems (573)
<input type="checkbox"/> Delivery of Health Care (2)	<input type="checkbox"/> Intratracheal drug delivery	

OK Cancel

# 1.4 可视化分析——检索结果趋势分析

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Content

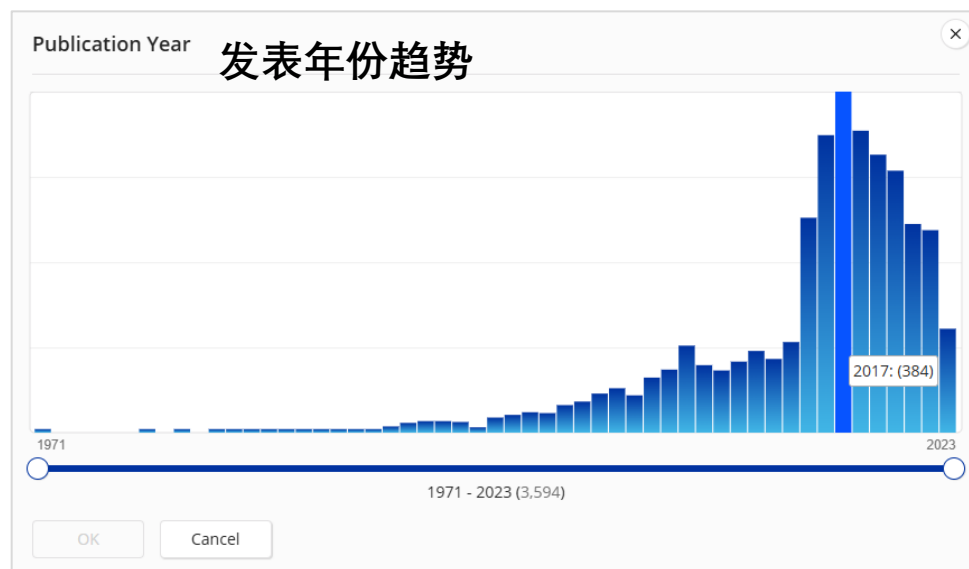
Life Science Data

Formulation Purpose

Database

Filter Content Report

Download filter data from this result set.



Download Reference Filter Content

File Type: Excel (.xlsx)

Select Quantity: All Filter Values

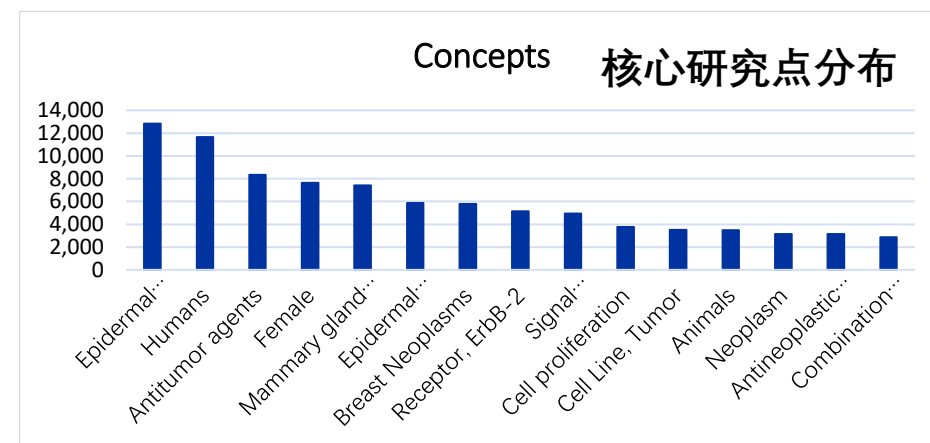
File Name: Reference\_Filters\_20241121\_1455

Only the top 1,000 filter values will be downloaded.

Filters:

<input type="checkbox"/> Document Type	<input checked="" type="checkbox"/> Concept
<input type="checkbox"/> Language	<input type="checkbox"/> CA Section
<input type="checkbox"/> Publication Year	<input type="checkbox"/> CAS Content
<input type="checkbox"/> Author	<input type="checkbox"/> Life Science Data
<input type="checkbox"/> Organization	<input type="checkbox"/> Formulation Purpose
<input type="checkbox"/> Publication Name	<input type="checkbox"/> Database

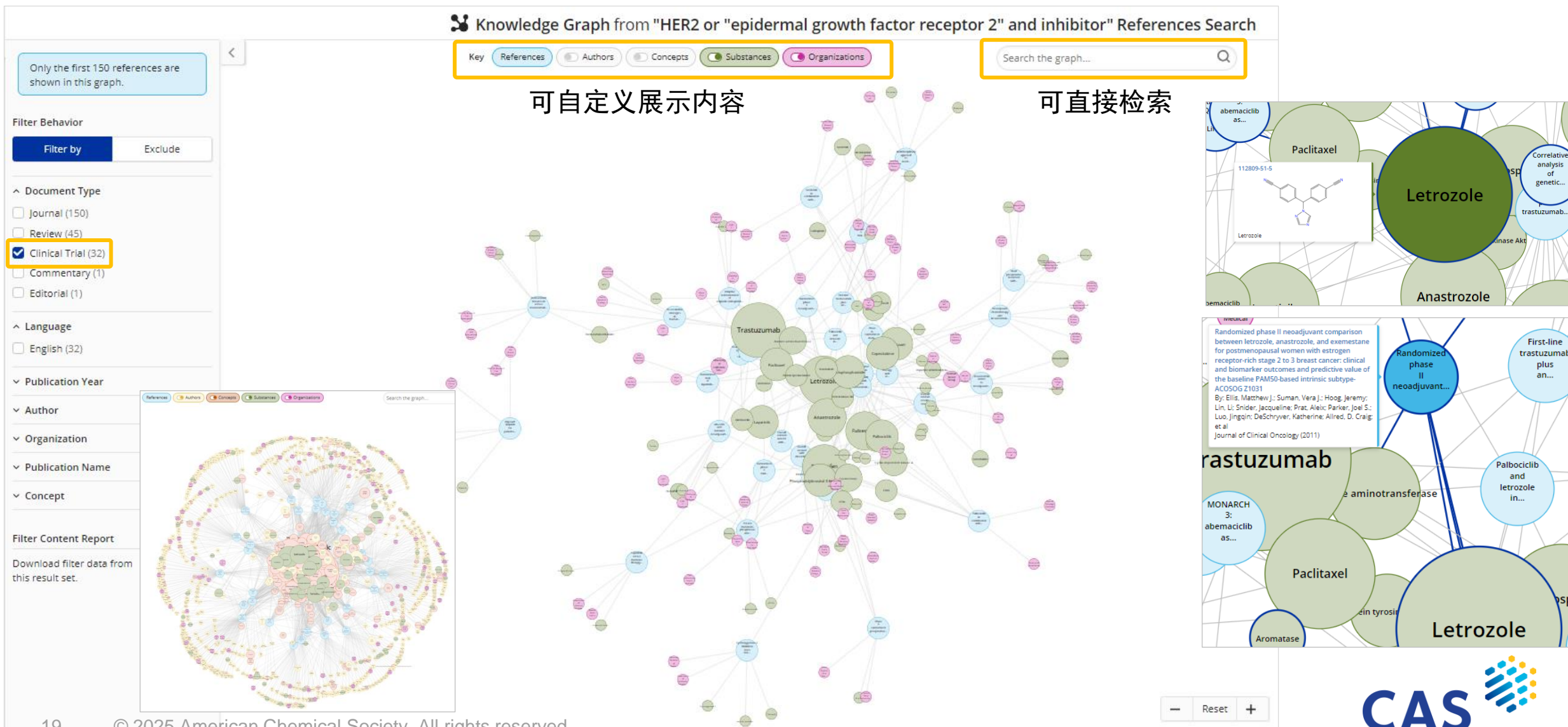
Download Cancel Learn more about downloads.



自主选择下载分析栏目

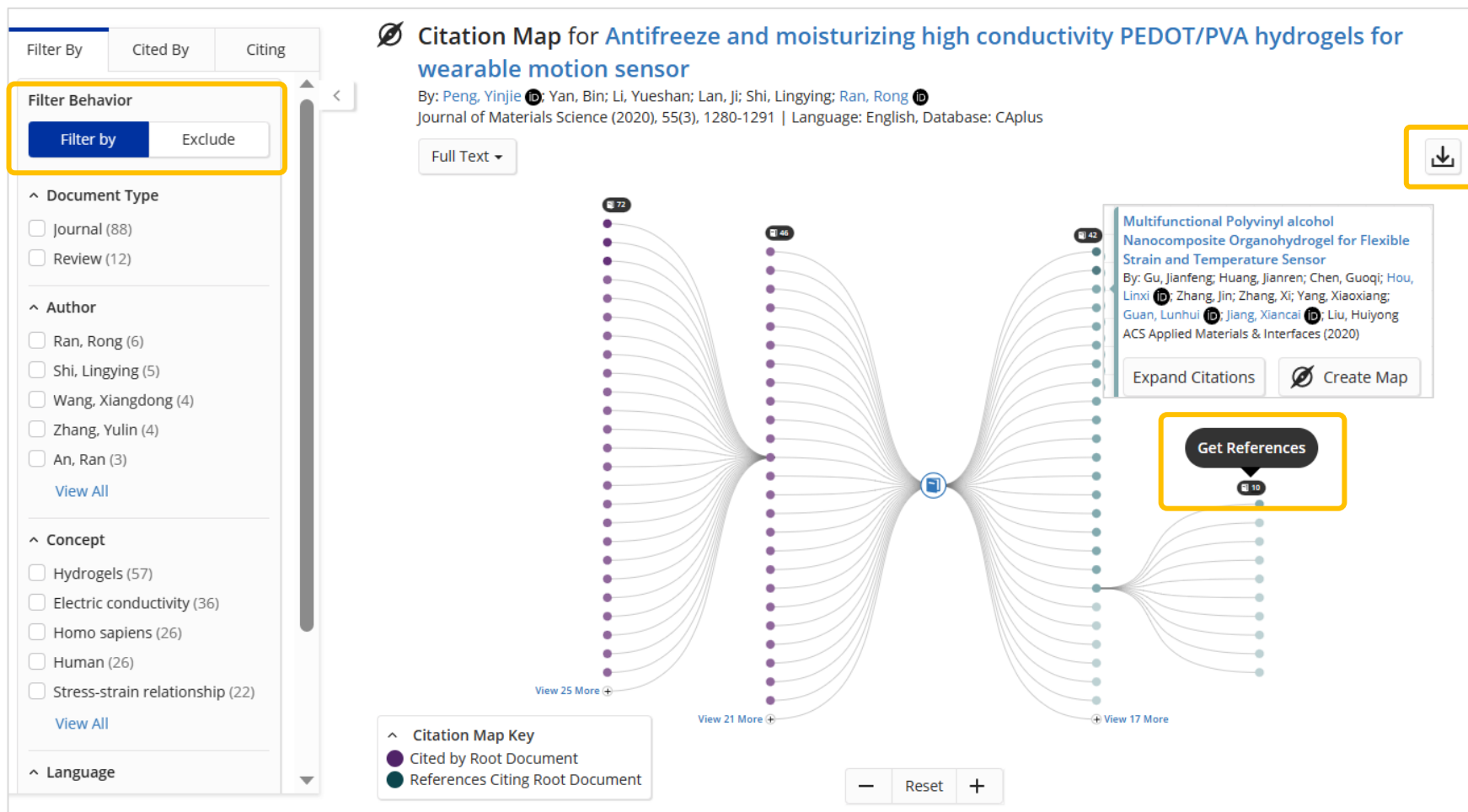
# 1.4 可视化分析——知识图谱

Knowledge Graph



# 1.4 可视化分析——引文地图

便捷获得相关文献



Citation Map

- Cited By: 参考文献
- Citing: 引用当前文献的文献
- 通过聚类选项筛选引文
- 可下载引文地图
- 显示引文和被引文献的数量，点击可链接至对应的文献结果页面

# 1.5 深入文献详情

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

3 0 180 Citation Map

## In this Reference

- [Concepts](#)
- [Substances](#)
- [Biomarkers](#)
- [Cited Documents](#)

By: Howe, Louise R.; Subbaramaiah, Kotha; Patel, Jay; Masferrer, Jaime L.; Deora, Aparna; Hudis, Clifford; Thaler, H. J.; Du, Baoheng; Brown, Anthony M. C.; et al  
[View All](#)

Cyclooxygenase 2 (HER-2) (Cox-2), an inducible form of Cox, is over-expressed in HER-2/neu-pos. human breast cancer. A study was to determine whether celecoxib, a selective Cox-2 inhibitor, protected against HER-2/neu-induced epidermal growth factor receptor 2 (HER-2) protein was detected in breast carcinomas from mouse mammary tumor virus (MMTV)/neu mice. Treatment with celecoxib significantly reduced the incidence of mammary tumors in MMTV/neu mice (P = 0.003) and caused about a 50% reduction in prostaglandin E<sub>2</sub> (PGE<sub>2</sub>) levels. Because mammary glands from MMTV/neu mice expressed all four PGE<sub>2</sub> receptors, that signaling through PGE<sub>2</sub> receptors is important for mammary tumorigenesis. These results strengthen the rationale for clinical trials to determine whether selective Cox-2 inhibitors possess anticancer properties in humans at risk for breast cancer.

Keywords: COX2 inhibitor celecoxib HER2 neu breast cancer

Full Text

## Publication Information • Journal

### Source

Cancer Research  
Volume: 62  
Issue: 19  
Pages: 5405-5407  
Journal; Article;  
Research Support, Non-U.S. Gov't; Research Support, U.S. Gov't, P.H.S.  
2002

### Database Information

AN: 2002:779608  
CAN: 138:280829  
PubMed ID: 12359744  
CAplus and MEDLINE

### Company/Organization

Departments of Cell and Developmental Biology  
Weill Medical College of Cornell University  
New York, New York 10021  
United States

### Email

lrhowe@med.cornell.edu

### Publisher

American Association for Cancer Research

## Concepts

## CAS科学家提供的标准技术术语

### Antitumor agents

Prostaglandin EP2 receptors

Role: Biological Study, Unclassified

### Epidermal growth factor receptor HER2

Role: Biological Study, Unclassified

Prostanoid receptor PTGER4

Role: Biological Study, Unclassified

### Homo sapiens

Prostanoid receptors, type EP<sub>1</sub>

Role: Biological Study, Unclassified

### Human

### Mammary gland neoplasm

Prostanoid receptors, type EP<sub>3</sub>

Role: Biological Study, Unclassified

## 内容导航速览

## Substances

Substances (3)

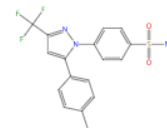
329900-75-6

Image Not Available

Unspecified  
Cyclooxygenase 2

Role: Biological Study, Unclassified, Biological Study

169590-42-5

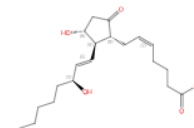


C<sub>17</sub>H<sub>14</sub>F<sub>3</sub>N<sub>3</sub>O<sub>2</sub>S  
Celecoxib

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

## 物质的研究角色

363-24-6



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

C<sub>20</sub>H<sub>32</sub>O<sub>5</sub>  
Prostaglandin E<sub>2</sub>

Role: Biological Study, Unclassified, Biological Study



# 1.5 深入文献详情

CAS PatentPak 快速定位专利中的物质

1

Intermediates for the preparation of halichondrin B

By: Austad, Brian; Chase, Charles E.; Fang, Francis G.

World Intellectual Property Organization, WO2005118565 A1 2005-12-15 | Language: English, Data

The present invention provides macrocyclic compounds I [PG<sup>1</sup>, PG<sup>2</sup>, PG<sup>3</sup> = H, protecting group (esp silylene, cyclic acetal, cyclic ketal, cyclic carbonate, cyclic boronate; R<sup>1</sup> = R, OR; R = H, C<sub>1-4</sub>-haloalkyl, Me, CH<sub>2</sub>Ph); LG<sup>1</sup> = leaving group (e.g., sulfonyloxy, (un)substituted alkylsulfonyloxy, alkenylsulfonyl, mesyloxy or tosyloxy)], especially diastereomer II, synthesis of the same and intermediates thereto. [Chemical structures and reaction schemes are shown, including the synthesis of ER-812930, ER-812933, ER-812934, ER-812935, ER-816961, and ER-818937.]

View More ▾

PatentPak ▾

Full Text ▾

Substances (152)

Reactions (1,160)

Reactions (0)

Citing (13)

Patent	Language	Kind Code	PatentPak Options
WO2005118565	English	A1	PDF   PDF+   <b>Viewer</b>
AU2005250487	English	A1	PDF
CA2935786	English	A1	PDF
CA3028453	English	A1	PDF
CN1993342	Chinese	A	PDF
AU2005250487	English	B2	PDF
EP2522663	English	A1	PDF
JP5226304	Japanese	B2	PDF
KR1434673	Korean	B1	PDF
EP2522663	English	B1	PDF

View All on Reference Detail

CAS PatentPak

PAGE 19 / 97

ZOOM

DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 871358-21-3

Analyst Markup Locations (2)

Page 19

Page 65

CAS RN 871358-49-5

Analyst Markup Locations (1)

Page 20

CAS RN 871358-60-0

Analyst Markup Locations (2)

Page 20

Page 67

CAS PatentPak

PAGE 65 / 97

ZOOM

DOWNLOAD PDF PDF+

Key Substances in Patent

CAS RN 871358-21-3

Analyst Markup Locations (2)

Page 19

Page 65

CAS RN 871358-49-5

Analyst Markup Locations (1)

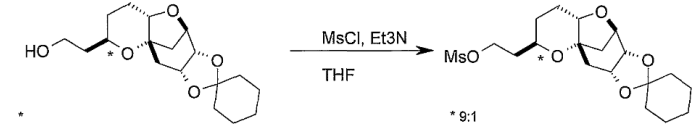
Page 20

CAS RN 871358-60-0

Analyst Markup Locations (2)

WO 2005/118565

PCT/US2005/019669



**[00156]** The previously prepared solution of ER-816961 (1 wt in 5 v THF) was diluted with THF (5 v), cooled to 5 °C and Et<sub>3</sub>N (3 eq., 0.94 wt) was added. MsCl (1.05 eq, 0.25 v) was added at a rate that maintained the T below 10 °C. The reaction was quenched by addition of water (5 wt). Heptane (8 v) was added and the mixture allowed to partition. The aqueous phase was separated and extracted with MTBE (2 v). The combined organic extracts were washed with saturated sodium bicarbonate (5 v) and water (1-9 v). The organic layer was concentrated and solvent exchanged with EtOH to prepare a solution of ER-818937 (1.23 wt calcd. based on 100% conversion) in EtOH (1 v) which was used directly in the next stage.



# 文献检索小结

1. 检索主题的构建：利用CAS Lexicon精准选词，使用布尔逻辑算符及通配符连接主题词，利用高级检索选项进行自定义组合检索
2. 主题词+结构联合检索，快速获得文献
3. 利用丰富的筛选工具，缩小范围，锁定目标文献
4. 检索结果趋势分析、知识图谱、引文地图
5. 文献详情，CAS PatentPak浏览专利详情

# 大纲

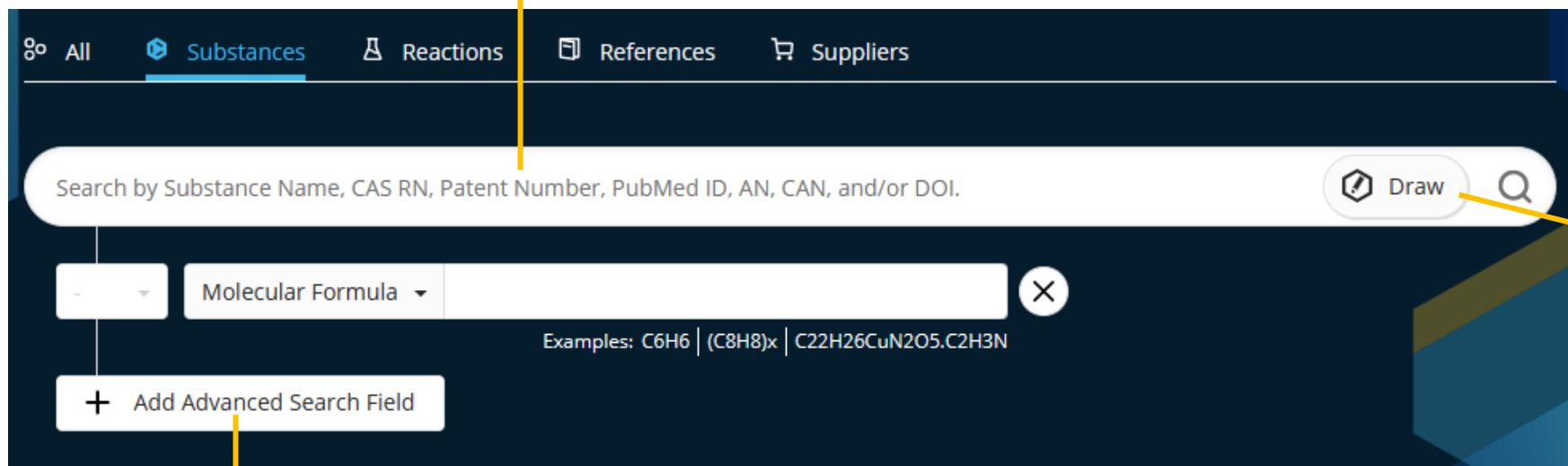
- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研？
  - 如何聚焦某类物质？
  - 如何调研反应信息？
  - 怎么查、怎么选具体的实验方案？
- 常见问题Q&A

## 2. 如何聚焦某类物质？

- 快速检索聚合物或无机化合物？
- 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？
- 检索完整分子结构？通式结构？或含有某些片段的物质？
- 如何确认结构新颖性？
- 如何查找相似的序列？

# 研究某种/某类物质？

- 通过物质标识符、文献标识符检索物质



The screenshot shows the CAS search interface. At the top, there are tabs for 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. Below these is a search bar with the text 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' To the right of the search bar is a 'Draw' button with a chemical structure icon. Below the search bar is a dropdown menu for 'Molecular Formula' with a search icon. Below that is a button labeled '+ Add Advanced Search Field'. An orange arrow points from the text '通过物质标识符、文献标识符检索物质' to the search bar. Another orange arrow points from the text '使用结构绘制面板进行结构检索' to the 'Draw' button. A third orange arrow points from the text '高级检索' to the '+ Add Advanced Search Field' button.

- 使用结构绘制面板进行结构检索

- 高级检索

## 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——物质标识符

Substances search for "Paxlovid 2628280-40-8"

- 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）

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Product (2)

Reactant (1)

Reference Role

Adverse Effect (2)

Analyte (2)

Analytical Study (2)

Biological Study (2)

Biological Study, Unclassified (2)

View All

Life Science Data

Commercial Availability

2 Results

1

2628280-40-8

Absolute stereochemistry shown

C23H32F3N5O4  
3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli...

999 References 320 Reactions 42 Suppliers

2

2803933-60-8

Absolute stereochemistry shown

Absolute stereochemistry shown

C37H48N6O5S2.C23H32F3N5O4  
Components: 2  
Paxlovid

283 References 3 Reactions 0 Suppliers

Sort: Relevance

Relevance

CAS RN: Ascending

CAS RN: Descending

Molecular Formula: Ascending

Molecular Formula: Descending

Molecular Weight: Ascending

Molecular Weight: Descending

Number of References: Ascending

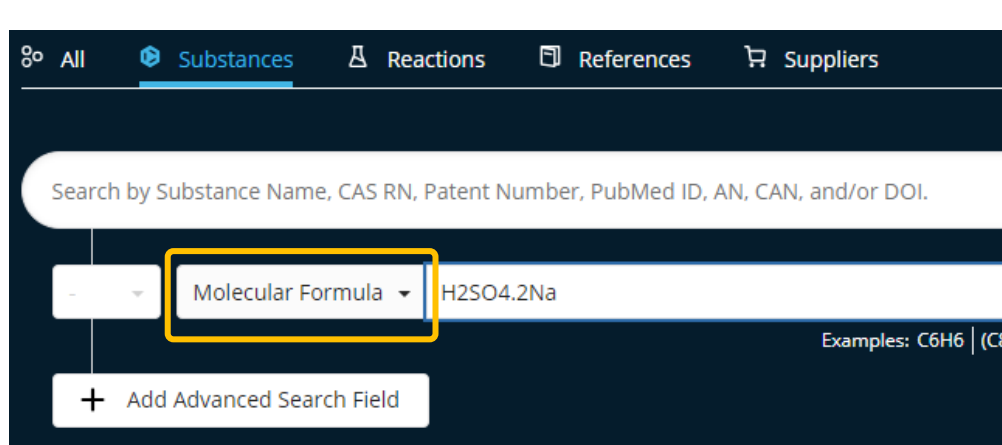
Number of References: Descending

Number of Suppliers

物质排序：相关度、CAS RN、分子式、分子量、文献量、供应商数量

## 2.1 分子式检索：高效检索聚合物或无机化合物

- 含碳化合物，C排第一位，H排第二位，其他元素符号按照首字母顺序进行排列
- 不含碳化合物，按照元素符号的首字母顺序进行排列
- 不同组分之间用“.”隔开，如：铁钴镍合金 Fe.Co.Ni
- 无机含氧盐：阳离子和阴离子用点 (.) 分开；阴离子以氢补齐至电中性  $\text{Na}_2\text{SO}_4$ :  $\text{H}_2\text{O}_4\text{S} \cdot 2\text{Na}$



Substances search for "H2SO4.2Na" Molecular Formula

References Reactions Suppliers

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Product (2)

Reagent (2)

Catalyst (1)

Reference Role

Process (6)

Uses (6)

Biological Study (5)

Properties (5)

9 Results

Sort: Relevance View: Partial

1 7757-82-6

$\text{H}_2\text{O}_4\text{S} \cdot 2\text{Na}$

Components: 2

Component RN: 7664-93-9

Sodium sulfate

118K References 58K Reactions 206 Suppliers

2 13759-07-4

$\text{H}_2\text{O}_4\text{S} \cdot 2\text{Na}$

Components: 2

Component RN: 7664-93-9

Thenardite ( $\text{Na}_2(\text{SO}_4)$ )

978 References 0 Reactions 0 Suppliers

3 14262-80-7

$\text{H}_2\text{O}_4\text{S} \cdot 2\text{Na}$

Components: 2

Component RN: 13770-01-9

Sulfuric- $^{35}\text{S}$  acid, disodium salt

73 References 1 Reaction 2 Suppliers

适用于分子式检索的物质类型包括：

- 无机化合物：合金，无机表格化合物，多氧簇金属化合物等
- 聚合物



## 2.2 属性值联用检索物质

The screenshot shows the CAS search interface with the 'Experimental Spectra' dropdown menu open. The menu lists various search criteria: Molecular Formula, CAS Registry Number, Chemical Identifier, Document Identifier, Patent Identifier, Experimental Spectra (selected), Bioactivity Data (NEW), Biological, Chemical Properties, Density, Electrical, Lipinski, Magnetic, Mechanical, Optical and Scattering, Structure Related, and Thermal. The 'Experimental Spectra' sub-menu is also visible, listing: Proton NMR, Carbon-13 NMR, Nitrogen-15 NMR, Fluorine-19 NMR, and Phosphorus-31 NMR. The background shows the search bar with the text 'Search by Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.' and examples: C6H6, (C8H8)x, C22H26CuN2O5.C2H3N. Below the search bar, there are sections for 'Recent Searches' and 'Substances'.

### 实验核磁谱图数值助力结构解析

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:  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  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

Chemical Properties	Koc
Density	logD
Electrical	logP
Lipinski	Mass Intrinsic Solubility (g/L)
Magnetic	Mass Solubility (g/L)
Mechanical	Molar Intrinsic Solubility (mol/L)
Optical and Scattering	Molar Solubility (mol/L)
Structure Related	Molecular Weight
Thermal	pKa
	Vapor Pressure (Torr)

# 属性值、谱图数值联用检索物质

Substances

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

Molecular Weight 220 to 280  
Predicted values only. Examples: 46.07 | 125 to 350 | >300

AND pKa 1.3 to 1.8  
Predicted values only. Examples: -1.77 | <9.25 | >2.4 | 5.25 to 8.25

AND Carbon-13 NMR 114 to 171, 96, 11.5  
Allowance of  $\pm 2$  ppm. Examples: 152.3, 127.6, 133.1 | 155.02 to 207.59 | 187

+ Add Advanced Search Field

Substances search for 3 Advanced Fields

References Reactions Suppliers

Filter Behavior  
Filter by Exclude

Search Within Results

Reaction Role

Reference Role

☐ Preparation (13)  
☐ Synthetic Preparation (13)  
☐ Biological Study (12)  
☐ Uses (12)  
☐ Pharmacological Activity (11)  
[View All](#)

Life Science Data

☒ Pharmacological Data (13)  
☒ ADME (3)  
☒ Toxicity (1)

Commercial Availability

Number of Components

Molecular Weight

LogP

Stereochemistry

Element

Functional Group

Filtering: Life Science Data: 3 Selected X

13 Results

Sort: Molecular Formula: Ascending View: Partial

1 1628224-40-7  
  
Absolute stereochemistry shown, Rotation (-)  
C9H13N3O5  
( $\alpha$ S)- $\alpha$ -Amino-3-(carboxymethoxy)-5-methyl-1H-pyrazole-4-propanoic acid  
1 Reference 4 Reactions 0 Suppliers

2 296262-16-3  
  
C10H10N2O2S2  
2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]acetic acid  
5 References 42 Reactions 48 Suppliers

3 723-46-6  
  
C10H11N3O3S  
Sulfamethoxazole  
30K References 1,047 Reactions 112 Suppliers

4 1631737-39-7  
  
Absolute stereochemistry shown, Rotation (-)  
C10H15N3O5  
(2R,3R,4S,5R)-4,5-Dihydro-5-(hydroxymethyl)-3'-methylspiro[furan-2(3H),7'(6'H)-[...]]  
2 References 22 Reactions 0 Suppliers

5 442571-27-9  
  
C11H12N2O2S2  
2-[(5,6-Dimethylthieno[2,3-d]pyrimidin-4-yl)thio]propanoic acid  
2 References 4 Reactions 27 Suppliers

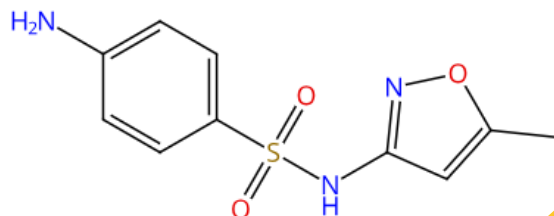
6 1927010-88-5  
  
C11H16ClNO3  
3-Chloro-4-[(1-methylpropyl)amino]-5-(2-propen-1-yloxy)-2(5H)-furanone  
1 Reference 3 Reactions 0 Suppliers

- 分子量：220至280之间
- pKa：1.3至1.8之间
- C谱特征峰：114至171之间，96，11.5

# 物质详情

CAS Registry Number: 723-46-6

30K 1,047 112 View in CAS BioFinder



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	Value	Condition
Molecular Weight	253.28	-
Melting Point (Experimental)	167 °C	-
Boiling Point (Predicted)	482.145±55.00 °C	Press: 760.00 Torr
Density (Experimental)	1.08 g/cm <sup>3</sup>	-
pKa (Predicted)	5.811±0.50	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Other Names and Identifiers

Experimental Properties

Experimental Spectra

## Experimental Properties

实验属性

Biological	Chemical	Density	Electrical	Lipinski	Structure Related	Thermal
Property	Value	Condition	Source			
Crystal Structure - 1 Source	See Full Text		(1) CAS			
Molecular Structure - 2 Sources	See Full Text		(2-3) CAS			
Particle Size - 1 Source	See Full Text		(4) CAS			
Specific Surface Area - 1 Source	See Full Text		(5) IC			
X-Ray Diffraction Pattern - 2 Sources	See Full Text		(6-7) CAS			

Sources

(1) Perlovich, German L.; Crystal Growth & Design, (2013), 13(9), 4002-4016, Caplus

## Experimental Spectra

实验谱图

<sup>1</sup> H NMR	<sup>13</sup> C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible
				Solvent	Source	
<a href="#">View Carbon-13 NMR Spectrum (Image Available)</a>				DMSO- <i>d</i> <sub>6</sub>	<a href="#">(1) WSS</a>	
<a href="#">View Carbon-13 NMR Spectrum (Image Available)</a>				DMSO- <i>d</i> <sub>6</sub>	<a href="#">(2) WSS</a>	
<a href="#">View Carbon-13 NMR Spectrum (Image Available)</a>				-	<a href="#">(2) WSS</a>	
<a href="#">View Carbon-13 NMR Spectrum (Image Available)</a>				-	<a href="#">(3) BIORAD</a>	
<a href="#">View Carbon-13 NMR Spectrum (Image Available)</a>				DMSO- <i>d</i> <sub>6</sub>	<a href="#">(4) AIST</a>	
<a href="#">View Carbon-13 NMR Spectrum</a>				DMSO- <i>d</i> <sub>6</sub>	<a href="#">(5) CAS</a>	
<a href="#">View Carbon-13 NMR Spectrum</a>				Methanol- <i>d</i> <sub>4</sub>	<a href="#">(6) CAS</a>	
Carbon-13 NMR Spectrum - 1 Source				-	<a href="#">(7) CAS</a>	

Sources

- (1) Kartashov, V. S.; Khimiko-Farmatsevticheskii Zh
- (2) Fruttero, Roberta; Journal of the Chemical Socie
- (3) Copyright Bio-Rad Laboratories. All Rights Reser
- (4) "Integrated Spectral Data Base System of Organ
- (5) Sunduru, Naresh; European Journal of Medicina
- (6) Ham, Won Seok; Angewandte Chemie, Internati
- (7) Blasioli, Sonia; Journal of Colloid and Interface S

723-46-6

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

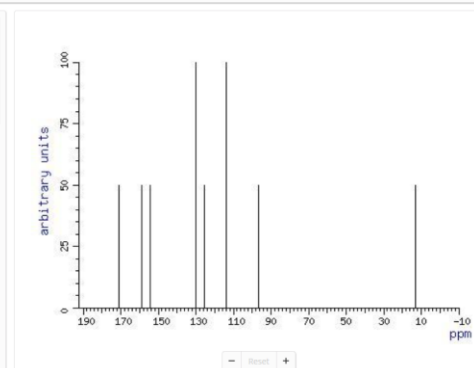
CAS Name  
Sulfamethoxazole

Conditions  
Solvent  
DMSO-d<sub>6</sub> (2206-27-1)  
Temperature  
30 °C

Spectrum Summary  
Spectrum ID  
CC-03-C\_SPC-17694

Spectrometer  
BRUKER WH-90

Source  
Spectral data were obtained from John Wiley & Sons, Inc.



Technology (Japan)

## 2.3 结构检索

灵活构建通式结构，提高物质/反应信息的检索效率

X

选择可变基团

R

自定义R基团

Fn

片段结构

[ ]  
1-4

重复工具

取代位置可变

环锁定工具

原子锁定工具

CAS Draw

Draw or change atoms or bonds.

Enter a CAS Registry Number, SMILES, or InChI.

Molecular Formula: Formula is not available

R2

Zoom: 100%

OK

R-Group Definitions

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

R2: F1 [1, 2], F2

> Atoms

> Variables

> Shortcuts

▼ Fragments

F1

F2

Unspecified Bond

利用绘图工具自定义相似结构：

1. 化学键型键级不确定
2. 骨架结构上指定出现的原子
3. 环系范围的定义

# 片段结构的检索

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (2)

Substructure (62K)

Similarity (596)

Analyze Structure Precision

Chemscape Analysis

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

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Life Science Data

Commercial Availability

Number of Components

1 (57K)

Filtering: Number of Components: 1 X

57,950 Results

Sort: Relevance View: Partial

1 1890344-49-6 C10H13NO 4-(1H-Pyrrol-3-yl)cyclohexanone

2 1391324-41-6 C10H13NO 2-(1H-Pyrrol-3-yl)cyclohexanone

3 1391209-36-1 C10H13NO 3-(1H-Pyrrol-3-yl)cyclohexanone

4 1894439-09-8 C10H13NO 4-(1H-Pyrrol-2-yl)cyclohexanone

5 1528461-22-4 C10H13NO 4-(1H-Pyrrol-1-yl)cyclohexanone

6 1391339-47-1 C10H13NO 2-(1H-Pyrrol-2-yl)cyclohexanone

物质筛选类别:

二次检索

反应角色

文献角色

生命科学数据

是否商业可得

组分数目

分子量

油水分配系数

立体化学

所含元素

所含官能团

芳环数量

物质类别

聚合物类别

同位素

是否含金属

实验属性

实验谱图

.....

Filter Behavior

Filter by Exclude

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

Polymer Class

Isotopes

Metals

Experimental Property

Experimental Spectrum

# 物质检索结果的筛选



思考：如何锁定尚未合成的天然产物结果？

Similarity (596)

Structure Precision

- ☒ Conventional Results (13)
- ☐ Tautomers and Zwitterions (47)

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

Reaction Role

- ☒ Product (13)
- ☐ Reactant (3)

Reference Role

- ☐ Preparation (8,818)
- ☐ Synthetic Preparation (8,698)
- ☐ Uses (4,407)
- ☐ Biological Study (2,397)
- ☐ Technical or Engineered Material Use (2,187)
- ☒ Natural Product Occurrence (13)

[View All](#)

1 1239178-39-2

Absolute stereochemistry shown, Rotation (-)

$C_{23}H_{29}NO$   
(4aR,6aR,13aS,13bS)-1,4a,5,6,6a,13,13a,13b-Octahydro-4,4,6a,13b-tetramethyl-2H-b...

15 References 28 Reactions 2 Suppliers

2 1845745-84-7

Absolute stereochemistry shown, Rotation (+)

$C_{24}H_{25}NO_4$   
1H-Naphtho[2,1-b]carbazole-4-carboxylic acid, 2,3,4,4a,5,6,8,13b-octahydro-3-hyd...

4 References 213 Reactions 1 Supplier

3 201214-57-5

Absolute stereochemistry shown

$C_{38}H_{53}NO_5$   
Lolicine A

8 References 1 Reaction 0 Suppliers

4 679395-52-9

Absolute stereochemistry shown, Rotation (-)

$C_{33}H_{45}NO_4$   
(4aS,6aS,12bS,12cR)-9-[(S)-[(2R)-3,3-Dimethyl-2-oxiranyl]hydroxymethyl]-1,4,4a,5...

24 References 3 Reactions 0 Suppliers

5 468733-27-9

Absolute stereochemistry shown

$C_{29}H_{35}NO_7$   
(2'S,4aS,5'S,6aS,12bS,12cR)-5'-[1-(Acetyloxy)-1-methylethyl]-1,2,4a,5,6,6a,7,12,...

2 References 1 Reaction 0 Suppliers

6 138605-81-9

Absolute stereochemistry shown

$C_{37}H_{49}NO_7$   
Lolitolol

18 References 1 Reaction 0 Suppliers

7 1432622-95-1

8 81771-19-9

9 179464-13-2

## Bioactivity Indicator

- ☐ Enzyme inhibitors (2)
- ☐ Nervous system agents (2)
- ☐ Membrane transport modulators (1)

## Target Indicator

- ☐ Enzymes (2)
- ☐ Membrane proteins (1)
- ☐ Transport proteins (1)

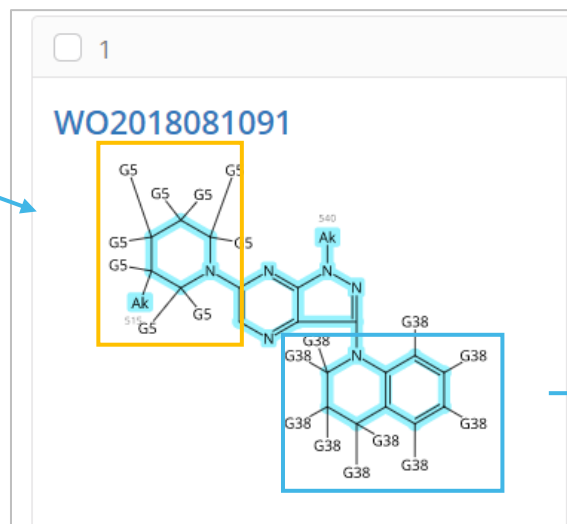
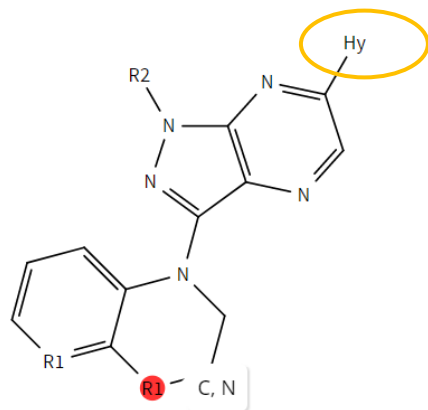
Reaction Role:  
物质在反应中的角色

Reference Role:  
物质在文献中的研究角色



# 2.4 CAS Markush 检索，助力结构查新

## CAS科学家对文献的标引和解读



### 命中的Markush结构及解读

WO2018081091

☒ Search Patent Markush

**Pyrazolo[3,4-b]pyrazine derivatives as SHP2 phosphatase inhibitors and their preparation**

By: Giordanetto, Fabrizio; Greisman, Jack Benjamin; Maragakis, Paul; Taylor, Alexander M.; DiPietro, Lucian V.; Kelley, Elizabeth H.; Lescarbeau, Andre; Murcko, Mark Andrew; Pierce, Levi Charles Thomas; Shortsleeves, Kelley C.; Walters, W. Patrick; Bhat, Sathesh; Therrien, Eric; Dahlgren, Markus Kristofer

World Intellectual Property Organization, WO2018081091 A1 2018-05-03 | Language: English, Database: Cplus

Assignees: Relay Therapeutics, Inc., D.E. Shaw Research, LLC

**Patent claim 1**

[PatentPak](#) [Full Text](#)

515: alkyl <containing 1-6 C> (opt. subst. by G17)

WO 2018/081091

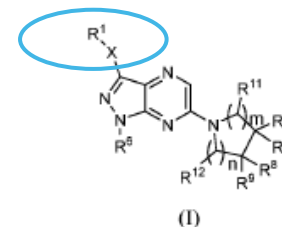
PCT/US2017/058048

### 原文中Markush结构及描述

136

What is claimed is:

1. A compound of formula (I), or a pharmaceutically acceptable salt thereof,



5

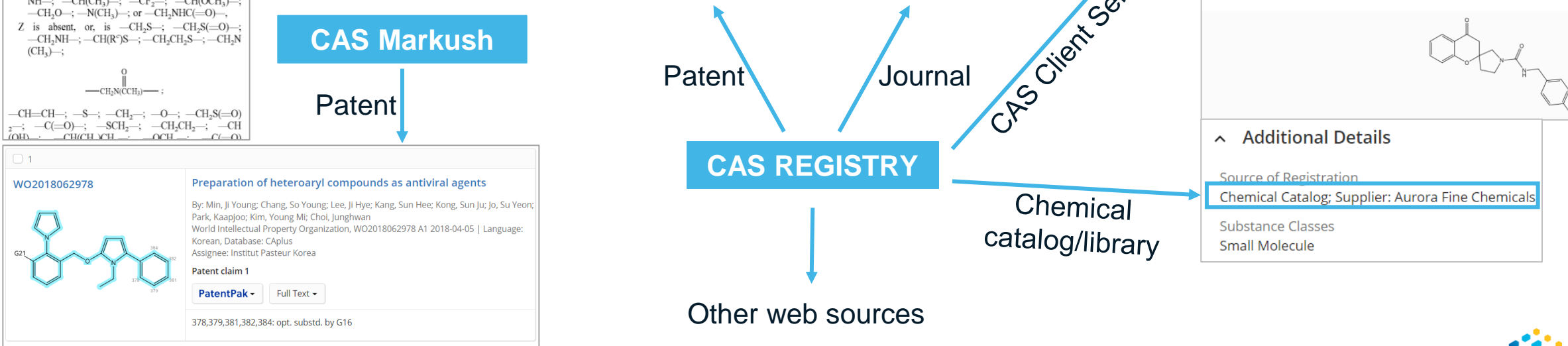
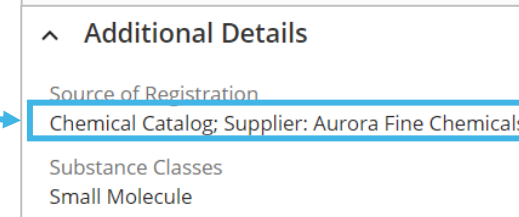
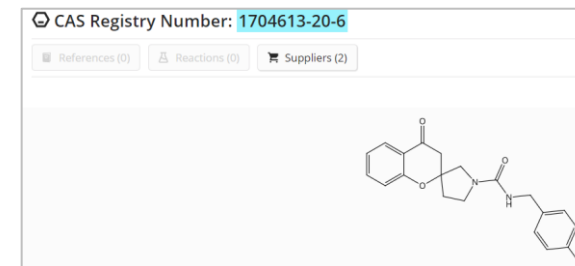
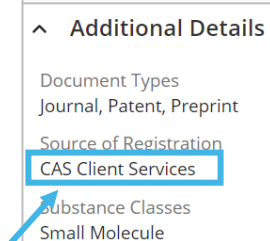
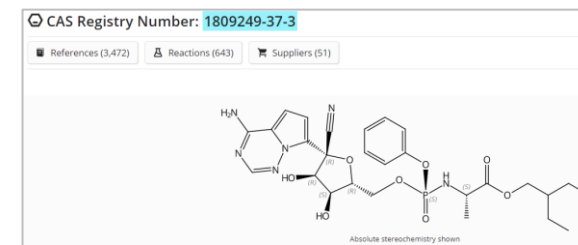
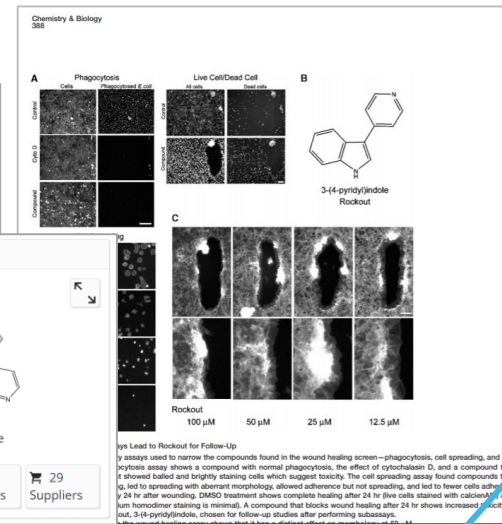
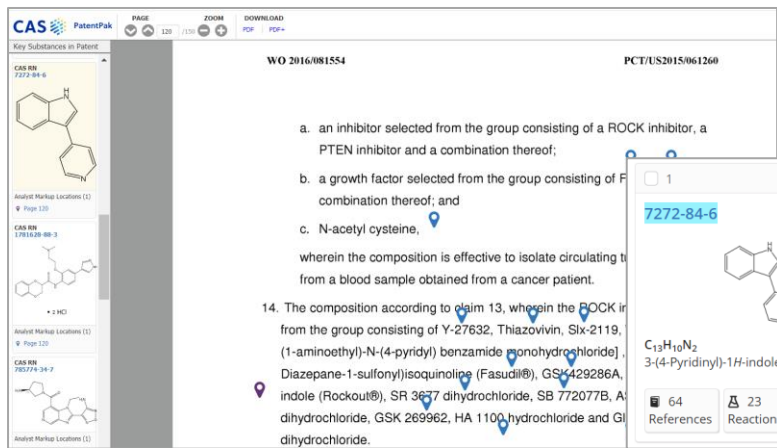
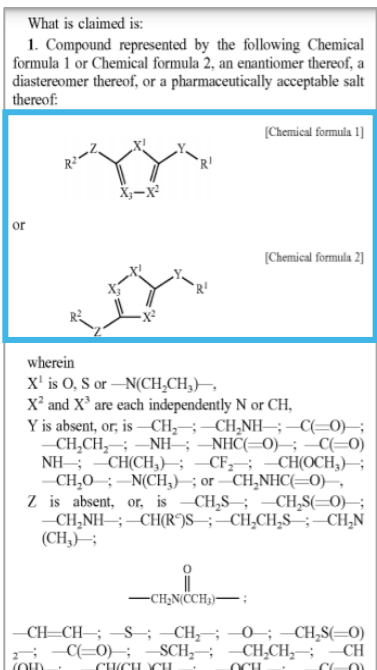
wherein

X is N-R<sup>66</sup>, O, S, S(O), SO<sub>2</sub>, CR<sup>13</sup>R<sup>14</sup>, -O-C(R<sup>13</sup>R<sup>14</sup>)-, -C(R<sup>13</sup>R<sup>14</sup>)O-, C(O), or C=C(R<sup>13</sup>R<sup>14</sup>);

- 15 R<sup>66</sup> is selected from the group consisting of H, -(C<sub>1</sub>-C<sub>6</sub>)alkyl and phenyl, or together with R<sup>1</sup> bicyclic aryl or
- and the nitrogen to which they are attached form a nitrogen ring moiety selected from the group substituted with one or
- consisting of 5-7 membered monocyclic heteroaryl, a 8-12 membered bicyclic moiety with one
- saturated ring and one aromatic or heteroaromatic ring, a 8-12 membered bicyclic heteroaryl,
- and a 4-7 membered heterocycle, wherein the nitrogen ring moiety is optionally substituted
- 20 with one, two or more substituents each independently selected from the group consisting of
- R<sup>10</sup>, -OR<sup>10</sup>, -S(O)<sub>w</sub>R<sup>10</sup> (wherein w is 0, 1 or 2), -N(R<sup>10</sup>)<sub>2</sub>, -OS(O)<sub>w</sub>R<sup>10</sup> (wherein w is 0, 1, or
- 2), -S(O)<sub>w</sub>-N(R<sup>10</sup>)<sub>2</sub> (wherein w is 0, 1 or 2), -S(O)(NH)R<sup>10</sup>, -P(O)(R<sup>10</sup>)<sub>2</sub>, -C(O)R<sup>10</sup>, -
- C(O)N(R<sup>10</sup>)<sub>2</sub>, oxo, halogen, nitrile, phenyl (optionally substituted with one, two or three halo,
- C<sub>1-3</sub>alkyl or C<sub>1-3</sub>haloalkyl), C<sub>1-3</sub>alkyl, C<sub>1-3</sub>haloalkyl, and heteroaryl (optionally substituted with
- 25 one, two or three halo, C<sub>1-3</sub>alkyl or C<sub>1-3</sub>haloalkyl);

### 专利中的定位，专利权人、命中结构的特点等等

## CAS结构层面的数据集



# 如何进行完整的分子结构检索？

**Substances search for drawn structure**

References ▾ Reactions ▾ Suppliers ▾

Structure Match

As Drawn (0)

Substructure (0)

Similarity (101K)

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

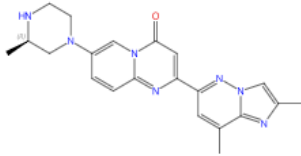
Filtering: Similarity: 3 Selected ✕ Number of Components: 1 ✕ [Clear All Filters](#)

286 Results

Sort: Relevance ▾ View: Partial ▾

1 95 ...

1825352-54-2



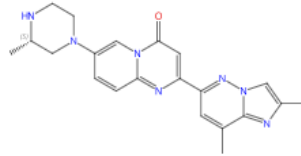
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

2 95 ...

1825352-53-1



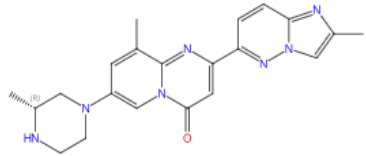
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

3 95 ...

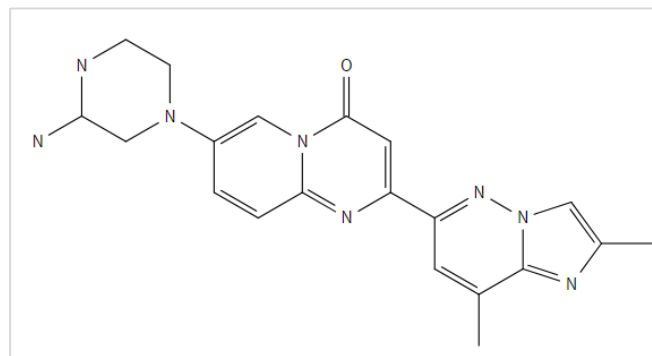
1825352-79-1



Absolute stereochemistry shown

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

5 References 19 Reactions 1 Supplier



CAS 物质数据集 CAS REGISTRY® 是专利审查员进行新颖性判断的重要依据，此例中的物质在 Registry 中 As Drawn 检索结果为 0，初步判断此分子比较新，同时用户可以根据必要性来选择性查看相似检索结果

# 如何进行完整的分子结构检索？

**Substances search for drawn structure**

References ▾ Reactions ▾ Suppliers ▾

Structure Match

As Drawn (0)

Substructure (0)

**Similarity (101K)**

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

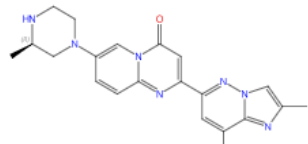
Filtering: Similarity: 3 Selected ✕ Number of Components: 1 ✕ [Clear All Filters](#)

286 Results

Sort: Relevance ▾ View: Partial ▾

1 95 ...

**1825352-54-2**



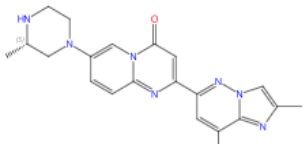
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

2 95 ...

**1825352-53-1**



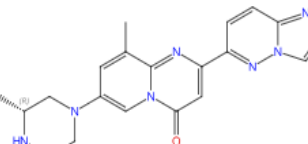
Absolute stereochemistry shown

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

5 References 25 Reactions 1 Supplier

3 95 ...

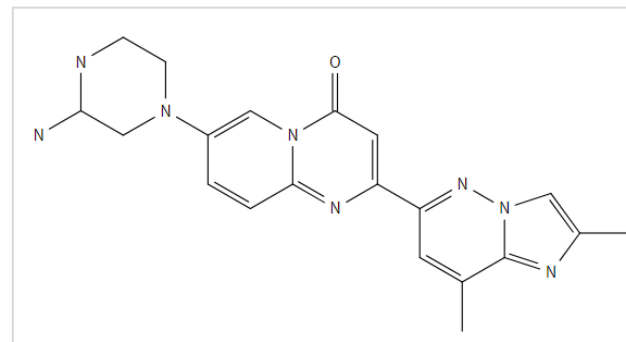
**1825352-79-1**



Absolute stereochemistry shown

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

5 References 19 Reactions 1 Supplier



查看相似结构，可参考  
Similarity score

<https://cas-product-help.zendesk.com/hc/en-us/articles/11112258474125-What-are-similarity-scores>

# 如何进行完整的分子结构检索？

CAS SciFinder

Substances Enter a query...

Edit

Return to Home

Patent Markush search for drawn structure

References

Patent Markush Match

As Drawn (1)

Substructure (1)

Filter Behavior

Filter by Exclude

Patent Office

World Intellectual Property Organization (1)

CA Section

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: 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.

Chemical structure diagram of a complex molecule, likely a pyrido-pyrimidine derivative, with various substituents and labels (e.g., G3, G22, G29).

- CAS 专利马库什数据集是专利审查员进行可专利性检索的重要参考依据
- 马库什检索可以使用具体结构、骨架结构和通式结构来进行迭代检索，确保获得完整的公开结构信息

用户可以根据必要性使用 CAS 文献数据集 CAplus 进行文本检索补充

# 物质检索小结

1. 物质检索方法：物质、文献标识符检索；分子式、物性参数、谱图数据检索；及结构式检索，充分利用结构绘制工具，合理扩大或限定结构检索范围
2. 正确理解As Drawn、Substructure、Similarity检索结果集的意义和范围
3. 充分利用物质筛选项准确定位目标物质：Reaction Role、Reference Role等
4. 利用CAS Markush检索尽可能全面的获得结构的公开信息



# 大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研？
  - 如何聚焦某类物质？
  - 如何调研反应信息？
  - 怎么查、怎么选具体的实验方案？
- 常见问题Q&A



### 3. 如何进行反应调研？

- 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？
- 如何查找相似反应？
- 如何关注特定转化类型的反应？
- 如何在大量反应结果中，快速找到最想要的反应？
- 如何查找涉及机理研究的反应？或人名反应？
- 如何设计新化合物的逆合成路线？

# 使用标识符直接检索

支持使用：CAS反应登记号、物质名称、CAS登记号、文献号等

🔍 All Substances Reactions References Suppliers

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

## 示例：丙烯酸异丁酯的相关反应

Reactions search for "106-63-8"

References

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

1,262 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (4 Reactions)

Steps: 1 Yield: 85-100%

Suppliers (36)

Suppliers (73)

Supplier (1)

31-320-CAS-19339297 Steps: 1 Yield: 100%  
1.1 Catalysts: [Dabco](#); 7 - 14 h, rt  
A cascade synthesis of 5-allyl benzoylcarbamothioates via Mumm-type rearrangement  
By: Dahiya, Anjali; et al  
Organic & Biomolecular Chemistry (2018), 16(42), 7787-7791  
Full Text

31-320-CAS-4790587 Steps: 1 Yield: 85%  
1.1 Reagents: [Dabco](#)  
The catalyzed  $\alpha$ -hydroxyalkylation and  $\alpha$ -aminoalkylation of activated olefins (the Morita-Baylis-Hillman reaction)

点击反应的CAS登记号  
可进入反应详情页

Reactions search for "Suzuki coupling reaction"

References

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

1,395,346 Results

Scheme 1 (20 Reactions)

Suppliers (112)

Suppliers (58)

Suppliers (40)

31-179-CAS-12086025 Steps: 1 Yield: 100%  
1.1 Reagents: [Potassium carbonate](#)  
Catalysts: [\(SP-4-1\)-Bis\(acetato- \$\kappa\$ O\)bis\(N"-butyl-N,N,N',N'-tetramethylguanidine- \$\kappa\$ N'\)palladium...](#)  
Solvents: [Ethanol](#), [Water](#); 20 h, 80 °C  
Guanidine/Pd(OAc)<sub>2</sub>-Catalyzed Room Temperature Suzuki Cross-Coupling Reaction in Aqueous Media under Aerobic Conditions  
By: Li, Shenghai; et al  
Journal of Organic Chemistry (2007), 72(11), 4067-4072  
Full Text

31-179-CAS-10541130 Steps: 1 Yield: 99%  
1.1 Reagents: [Potassium hydroxide](#)  
Catalysts: [Palladium\(1+\), \(acetonitrile\)chloro\[oxylbis\(2,1-ethanedithioxy-2,1-ethanedithiol\[3-\(1-...\]](#)  
Solvents: [1,4-Dioxane](#); 5 h, 75 °C  
Synthesis, characterization of N-heterocyclic carbene metallocrown palladium complex and catalytic activities in Suzuki and Heck coupling reaction  
By: Wang, Jun-Wen; et al  
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2012), 73(1-4), 119-128  
Full Text

31-179-CAS-8409485 Steps: 1 Yield: 98%  
1.1 Reagents: [Potassium hydroxide](#)  
Catalysts: [Palladium\(1+\), \(acetonitrile\)chloro\[1,2-ethanedithiolbis\(oxo-2,1-ethanedithiol\[3-\(1-na...\]](#)  
Synthesis, characterization of N-heterocyclic carbene metallocrown palladium complex and catalytic activities in Suzuki and Heck coupling reaction  
By: Wang, Jun-Wen; et al  
Journal of Inclusion Phenomena and Macrocyclic Chemistry (2012), 73(1-4), 119-128

910463-68-2

Image Not Available

Unspecified  
[Semaglutide](#)

Protein/Peptide Sequence  
Sequence Length: 34

1,527 References 259 Reactions 32 Suppliers

# 3.1 使用自然语言，检索某类反应

Reactions search for "Preparation of aldehyde from primary alcohol in THF"

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Milligram (1,105)

Gram (591)

Kilogram (2)

No Scale Provided (6,030)

Experimental Protocols

Reaction Type

Stereochemistry

Reagent

Catalyst

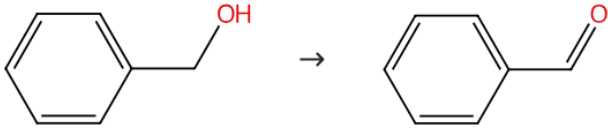
Solvent

Commercial Availability

7,682 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (68 Reactions) Steps: 1 Yield: 100%



Suppliers (166) Suppliers (80)

31-614-CAS-41356630 Steps: 1 Yield: 100% A cooperative nanoscale ZnO-NiO-Ni heterojunction for sustainable catalytic amidation of aldehydes with secondary amines

1.1 Reagents: [tert-Butyl hydroperoxide](#), [Morpholine](#)  
Catalysts: [Nickel monoxide](#), [Zinc oxide \(ZnO\)](#), [Nickel](#)  
Solvents: [Tetrahydrofuran](#), [Dodecane](#); 24 h, 90 °C

Experimental Protocols Full Text

31-480-CAS-16653494 Steps: 1 Yield: 100% Copper(II) complex of new non-innocent O-aminophenol-based ligand as biomimetic model for galactose oxidase enzyme in aerobic oxidation of alcohols

1.1 Reagents: [Cesium carbonate](#), [Oxygen](#)  
Catalysts: [1648843-87-1](#)  
Solvents: [Tetrahydrofuran](#); 4 h, rt

Experimental Protocols Full Text

31-480-CAS-16606643 Steps: 1 Yield: 100% Redox potential tuning by redox-inactive anions in copper(I) complexes of non-innocent o-aminophenol-based ligand containing benzoxazole: Learning from nature

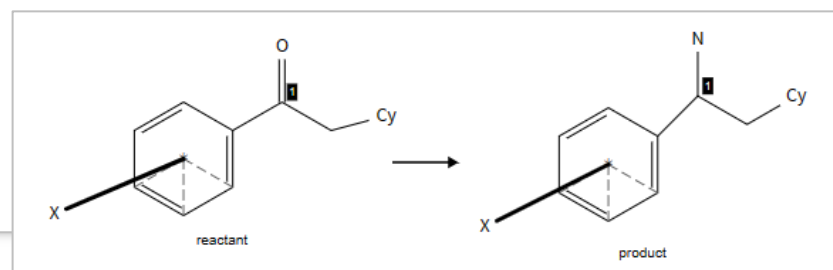
1.1 Reagents: [Cesium carbonate](#), [Oxygen](#)  
Catalysts: [2058233-98-8](#)  
Solvents: [Tetrahydrofuran](#); 12 h, 298 K

Experimental Protocols Full Text

- 产物: synthesis / preparation / manufacture of
- 底物: from
- 溶剂: in
- 催化剂: catalyzed by
- 试剂: mediated by

## 3.2 查找亚结构反应

As Drawn  
亚结构反应  
相似反应



Reactions search for drawn structure

References

Structure Match

- As Drawn (34)
- Substructure (8,044)
- Similarity (0)

Filter Behavior

Filter by Exclude

Search Within Results

Yield

- 80-89% (4)
- 70-79% (2)
- 50-69% (1)
- No Yield Available (9)

Reaction Scale

- Milligram (2)
- Gram (1)
- No Scale Provided (13)

Non-Participating Functional Groups

Filtering: Reaction Mapping: Mapping Data Available

16 Results

Group: By Scheme

- By Scheme
- By Document
- By Transformation

Sort: Relevance

- Relevance
- Publication Date: Newest
- Publication Date: Oldest
- Yield
- Number of Steps: Ascending
- Number of Steps: Descending

View: Collapsed

Scheme 1 (5 Reactions)

Suppliers (93) Suppliers (15)

Expand Scheme

Scheme 2 (1 Reaction)

Steps: 1 Yield: 76%

Suppliers (53) Suppliers (3)

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

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

Preparation of heterocyclic compounds as selective subtype alpha 2 adrenergic agents

By: Heidelbaugh, Todd M.; et al

反应分组:

- 按反应式
- 按文献
- 按转化类型

反应排序:

- 相关度
- 公布时间
- 产率
- 步数

## 3.3 高效筛选目标反应

折叠菜单：相同反应类型的反应在同一菜单里，方便阅读和筛选

反应筛选类别：  
产率、规模、步数  
不参与反应的官能团  
实验步骤  
反应类型、立体化学  
试剂、催化剂、溶剂  
商品信息……

文献筛选类别：  
文献类型、语言  
出版年份、刊物名

The screenshot displays the CAS Reaxys reaction search interface. On the left, a sidebar contains filters for 'Structure Match' (As Drawn (34), Substructure (8,044), Similarity (0)), 'Filter Behavior' (Filter by, Exclude), and a 'Search Within Results' section with expandable categories: Commercial Availability, Reaction Notes, Source Reference, Document Type, Language, Publication Year, Organization, Publication Name, CA Section, Filter Content Report, and Download filter data from this result set. The main panel shows search results for '8,044 Results', grouped by 'By Transformation' and sorted by 'Reaction Count: Descending'. The first result is 'Reductive Alkylation of Ammonia or Amines' (View 108 Related Reactions), showing a chemical reaction between a carbonyl compound and an amine. The second result is 'Formation of N/O/S Heterocycles' (View 47 Related Reactions), showing two reaction schemes for the formation of heterocycles. The third result is '1,3-Dipolar Addition' (View 37 Related Reactions).



# 筛选工具：不参与反应官能团

不参与反应官能团：出现在反应前后，但未发生变化的官能团

Structure Match

As Drawn (34)

Substructure (8,044)

Similarity (0)

Filter Behavior

Filter by

Exclude

Search Within Results

Yield

Reaction Scale

Non-Participating Functional Groups

☒ Halide (205)

☐ Phenyl halide (203)

☐ Amide (66)

☐ Alkene (62)

☐ Cyclic alkene (58)

View All

Number of Steps

Reaction Mapping

Experimental Protocols

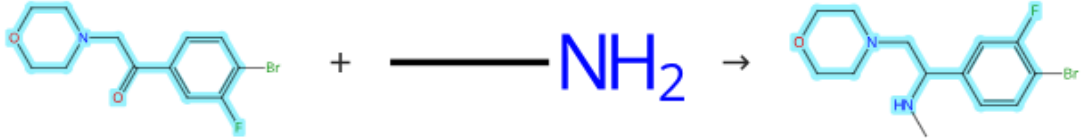
Filtering: Non-Participating Functional Groups: Halide X

Clear All Filters

205 Results

Group: By Scheme Sort: Relevance View: C

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



Suppliers (122)

☐ 31-313-CAS-11425767 Steps: 1 Yield: 100%

1.1 Solvents: [Tetrahydrofuran](#); 15 min, rt

1.2 Reagents: [Acetic acid](#), [Sodium cyanoborohydride](#); rt → 40 °C; 24 h, 40 °C

1.3 Reagents: [Sodium carbonate](#)  
Solvents: [Water](#)

Experimental Protocols


Preparation of N-[1-biphenyl(morpholinyl- and pyridinyl)ethyl]glycinamide derivatives as antagonists of urotensin II

By: Neeb, Michael J.; et al  
World Intellectual Property Organization, WO2008011  
2008-01-24

PatentPak Full Text

Collapse Scheme

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



Non-Participating Functional Groups

By Count Alphanumeric

1 Selected

☒ Halide (205)

☐ Phenyl halide (203)

☐ Amide (66)

☐ Alkene (62)

☐ Cyclic alkene (58)

☐ Diene (45)

☐ Ether (37)

☐ Amine (15)

☐ Tertiary amine (15)

☐ Carboxamidine (14)

☐ Urea (12)

☐ Carboxylic ester (9)

☐ Carbamate (8)

☐ Imine (8)

☐ Acyclic ketone (7)

☐ Ketone (7)

OK

Cancel

# 4.1 直观的合成实验详情 Synthetic Methods™

- CAS科学家标引的合成详情
- 节省阅读全文的时间，高效获得所需的合成实验信息

CAS Reaction Number: 31-614-CAS-24450288

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

☒ Synthetic Methods (40)

☐ Experimental Procedure (83)

Suppliers (15)

Suppliers (89)

98%

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	<a href="#">Hydrochloric acid</a> <a href="#">Titanium chloride (TiCl<sub>3</sub>)</a>	-	<a href="#">Methanol</a> <a href="#">Tetrahydrofuran</a> <a href="#">Water</a>	rt; 30 min, rt; 2 h, 30 - 50 °C
2	<a href="#">Water</a>	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

Products

[Methyl 2-\(4-bromophenyl\)-7-fluoro-1,2,3,4-tetrahydro-3-\(1-methyl-1H-1,2,4-triazol-5-yl\)-4-oxo-5-quinolinecarboxylate](#), Yield: 98%

Reactants

[4-Bromobenzaldehyde](#)  
[Benzoic acid, 5-fluoro-2-\[\(1-methyl-1H-1,2,4-triazol-5-yl\)acetyl\]-3-nitro-, methyl ester](#)

Reagents

[Hydrochloric acid](#)  
[Titanium chloride \(TiCl<sub>3</sub>\)](#)  
[Water](#)

View PDF Full Text

Company/Organization

Werner Siemens Imaging Center,  
Department of Preclinical Imaging  
and Radiopharmacy  
Eberhard Karls University  
Tübingen 72076  
Germany

Procedure

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

Transformation

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

Scale

gram

## Characterization Data

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

State

yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

## Transformations

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

# 直观的合成实验详情 Synthetic Methods™

- CAS科学家标引的合成详情
- 节省阅读全文的时间，高效获得所需的合成实验信息

CAS Reaction Number: 31-614-CAS-24450288

Filter Behavior

Filter by Exclude

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Experimental Protocols

☒ Synthetic Methods (40)

☐ Experimental Procedure (83)

Suppliers (15)

Suppliers (89)

98%

Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	<a href="#">Hydrochloric acid</a> <a href="#">Titanium chloride (TiCl<sub>3</sub>)</a>	-	<a href="#">Methanol</a> <a href="#">Tetrahydrofuran</a> <a href="#">Water</a>	rt; 30 min, rt; 2 h, 30 - 50 °C
2	<a href="#">Water</a>	-	-	-

Alternative Steps (2)

Experimental Protocols

Synthetic Methods

Products [Methyl 2-\(4-bromophenyl\)-7-fluoro-1,2,3,4-tetrahydro-3-\(1-methyl-1H-1,2,4-triazol-5-yl\)-4-oxo-5-quinolinecarboxylate](#), Yield: 98%

Reactants [4-Bromobenzaldehyde](#)  
[Benzoic acid, 5-fluoro-2-\[\(1-methyl-1H-1,2,4-triazol-5-yl\)acetyl\]-3-nitro-, methyl ester](#)

Reagents [Hydrochloric acid](#)  
[Titanium chloride \(TiCl<sub>3</sub>\)](#)  
[Water](#)

View PDF Full Text

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

## Procedure

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

## Transformation

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

## Scale

gram

## Characterization Data

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

## State

yellow amorphous solid

CAS Method Number 3-315-CAS-33168860

## Transformations

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

## 3.4 如何获得逆合成路线?

先进AI技术与CAS科学家标引的丰富反应信息相结合

(1) 已知化合物：点击物质结构，弹出的物质菜单中点击 Start Retrosynthetic Analysis

The screenshot displays the CAS Retrosynthesis Tool interface. On the left, a search bar shows the CAS RN 2628280-40-8. Below it, the chemical structure of 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-cyano-2-[(3S)-2-oxo-3-pyrroli... is shown with absolute stereochemistry. The molecular formula is C<sub>23</sub>H<sub>32</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>. Below the structure, there are buttons for 236 References, 53 Reactions, and 39 Suppliers. On the right, a sidebar lists various options: Substance Detail, Reactions (53), Synthesize (52), Start Retrosynthetic Analysis (highlighted with a yellow box), References (236), and Suppliers (39). The main area shows the chemical structure with absolute stereochemistry and a close button (X). At the bottom, there are buttons for Edit Structure, Reset, and a download icon.

CAS Retrosynthesis Tool:

- 逆合成反应路线设计功能
- 启发合成实验设计思路
- 高效获取逆合成反应路线

(2) 已知/未知化合物：点击Retrosynthesis检索项，打开绘图板，绘制目标化合物，获得实验路线

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

# 逆合成分析的预设参数

## Retrosynthesis Plan Options for drawn structure

### Set Rules Supporting Predicted Reactions

[Learn more](#)

☒ Common **反应规则常见性**

☐ Uncommon (includes common rules)

☐ Rare (includes common and uncommon rules)

### Set Starting Materials Cost Limit

[Learn more](#)

Set Starting Materials Cost Limit **起始原料费用**

☐ Email me when my plan is complete

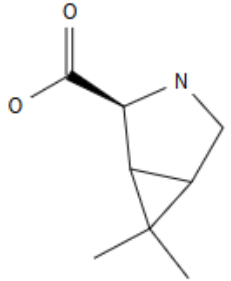
[Continue to Retrosynthesis Plan](#)

### Break and Protect Bonds (Optional)

Select a bond within the box to break or protect. You may break a single bond or protect multiple bonds in the target molecule. [Learn more](#)

**断裂键或保护键**

[Clear All Bond Selections](#)



# 逆合成路线详情

## Retrosynthesis Plan for drawn structure

Powered by ChemPlanner®

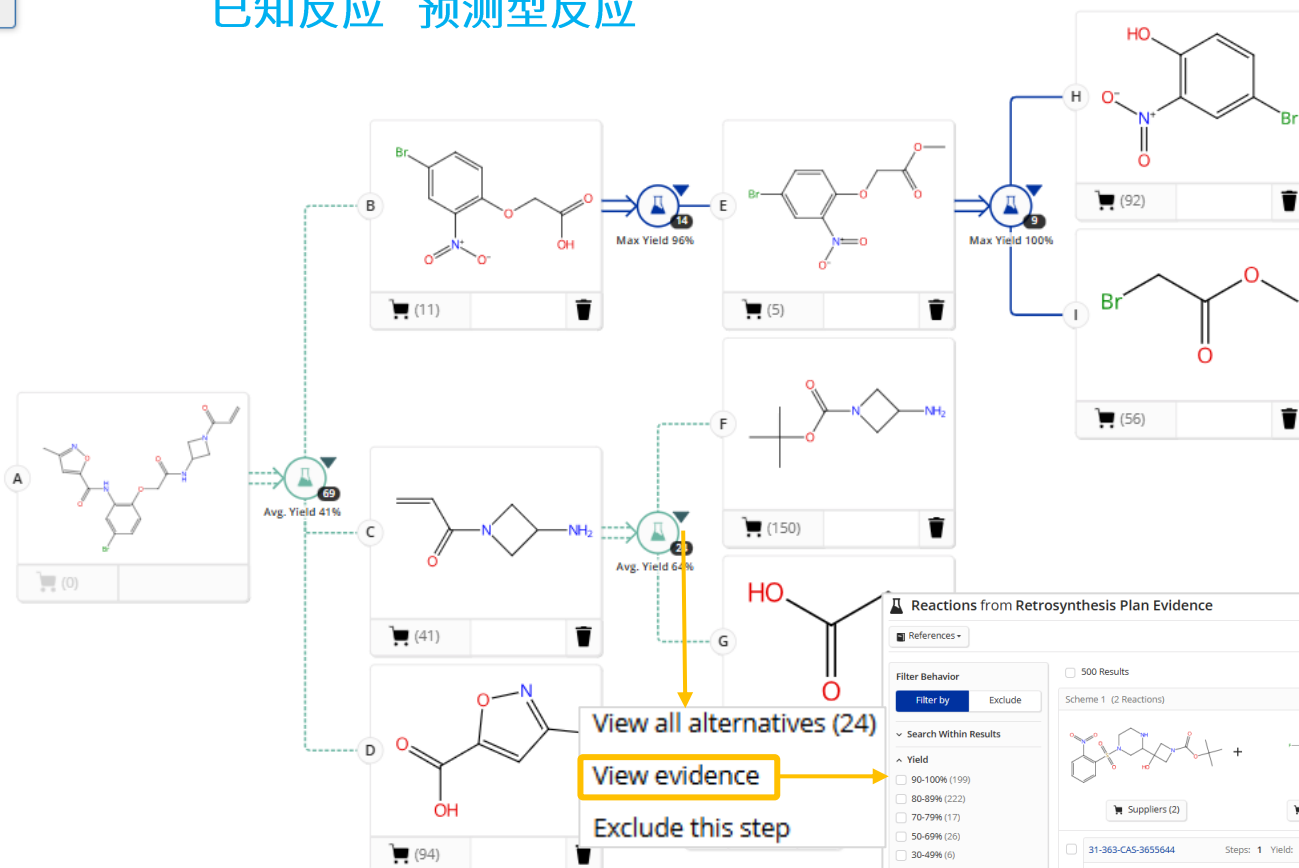
Key Experimental Steps Predicted Steps Edit Plan Options

View Excluded Options Save

### Plan Information

Estimated Yield: 26%  
Overall Price: \$631.59  
(USD per 100 grams)

已知反应 预测型反应



Step	Evidence
A → B + C + D	1.1 Reagents: 1-Ethyl-3-(3'-dimethylaminopropyl) carbodiimide, 1-Hydroxybenzotriazole, Diisopropylethylamine Average Yield: 41% Solvents: Dichloromethane; overnight, rt View All Experimental Protocols
B → E	1.1 Reagents: Tetramethylammonium hydroxide Maximum Yield: 96% Solvents: Tetrahydrofuran, Water; 12 h, reflux View All Experimental Protocols
C → F + G	1.1 Reagents: Triethylamine, 1-Ethyl-3-(3'-dimethylaminopropyl) carbodiimide, 1-Hydroxybenzotriazole Average Yield: 64% Solvents: Dichloromethane; 2 h, rt View All Experimental Protocols
	1.1 Reagents: Potassium carbonate Solvents: Acetone; overnight, reflux View All Experimental Protocols

可查看每步反应的详细条件与文献支持

Reactions from Retrosynthesis Plan Evidence

References

Filter Behavior

Filter by Exclude

Search Within Results

Yield

90-100% (199)

80-89% (222)

70-79% (17)

50-69% (26)

30-49% (6)

View All

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Milligram (125)

Gram (23)

No Scale Provided (352)

Experimental Protocols

Synthetic Methods (242)

Experimental Procedure (59)

500 Results

Group: By Scheme Sort: Relevance View: Expanded

Scheme 1 (2 Reactions)

Steps: 1 Yield: 90%

Suppliers (2)

Suppliers (18)

31-363-CAS-3655644

Steps: 1 Yield: 90%

1.1 Reagents: Hydrochloric acid  
Solvents: Methanol; 1,4-Dioxane; 30 min, rt → 60 °C

1.2 Reagents: Diisopropylethylamine  
Solvents: Dichloromethane; 16 h, rt

Experimental Protocols

Full Text

31-363-CAS-5805337

Steps: 1 Yield: 90%

1.1 Reagents: Hydrochloric acid  
Solvents: Methanol; 1,4-Dioxane; 30 min, rt → 60 °C

1.2 Reagents: Diisopropylethylamine  
Solvents: Dichloromethane; 16 h, rt

Experimental Protocols

Full Text

PatentPak

Full Text

Collapse Scheme



# 路线优化，考虑替换路线？

The screenshot displays a chemical synthesis software interface. On the left, a reaction scheme shows a starting material (C) reacting to form a product (F). A dropdown menu is open, showing options: "View all alternatives (24)", "View evidence", and "Exclude this step". A yellow box highlights "Alternative steps (24)" in the dropdown, and an arrow points to a detailed view of these alternatives.

Maximum Yield: 96%  
Evidence  
Alternative steps (14)

Tetramethylammonium hydroxide  
Solvents: Tetrahydrofuran, Water;  
12 h, reflux

1.1 Reagents: Triethylamine,  
1-Ethyl-3-(3'-dimethylaminopropyl)  
carbodiimide  
1-Hydroxybenzotriazole  
Solvents: Dichloromethane; 2 h, rt

Average Yield: 64%  
Evidence  
Alternative steps (24)

C ⇒ F + G Alternative Steps (24)

Filter by  
Alternative Step Type  
Predicted (24)

1 of 12  
Predicted Step  
Selected  
View 4 similar Alternatives  
View evidence  
Average yield: 64%

2 of 12  
Predicted Step  
Select  
View 2 similar Alternatives  
View evidence  
Average yield: 78%

3 of 12  
Predicted Step

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

# 反应检索小结

1. 通过物质标识符、文献标识符、结构式进行反应信息检索
2. 反应结果集的浏览与筛选
3. Synthetic Methods™——查看文献中合成方法详情
4. 关键词与反应式的联合检索
5. 获取已知化合物或新化合物的逆合成路线，查看文献支持，自定义选择替代路线

# 大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A



## 4. 怎么查找分析实验方法和制剂/配方详情?

- 能一键获取从原文中提取的分析操作和数据详情吗?
- 如何对多种分析方法进行充分评估?
- 我研究的物质有什么具体的配方应用?
- 专利配方的组成和制备工艺是什么? 如何进行实验评估?

# 关注文献关联的分析方法？

方法 (1): 在CAS SciFinder的文献结果集页面，点击CAS Content中的 Analytical Methods筛选含有具体分析实验方法的文献，从文献详情页中链接至分析方法

References search for "lapatinib and cancer"

Substances Reactions Citing Knowledge Graph

We are displaying the most relevant results. Learn about result relevance. Load All Results

Filtering: CAS Content: Analytical Methods X Clear All Filters

28 Results Sort: Relevance View: Partial Abstract

1

**Therapeutic Drug Monitoring of the new targeted anticancer agents imatinib, nilotinib, dasatinib, sunitinib, sorafenib and lapatinib by LC tandem mass spectrometry**  
By: Haouala, A.; Zanolari, B.; Rochat, B.; Montemurro, M.; Zaman, K.; Duchosal, M. A.; Ris, H. B.; Leyvraz, S.; Widmer, N.; Decosterd, L. A.  
Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2009), 877(22), 1982-1996 | Language: English, Database: CAlus and MEDLINE

The treatment of some cancer patients has shifted from traditional, non-specific cytotoxic chemotherapy to chronic treatment with mol. targeted therapies. Imatinib mesylate, a selective inhibitor of tyrosine kinases (TKIs) is the most prominent example of this new era and has opened the way to the development of several addnl. TKIs, including sunitinib, nilotinib, dasatinib, sorafenib and lapatinib, in the treatment of various hematol. malignancies and solid tumors. All these agents are characterized by an important inter-individual pharmacokinetic variability, are at risk for drug interaction...

View More

Full Text Substances (7) Reactions (0) Citing (180) Citation Map

2

**Determination of lapatinib (GW572016) in human plasma by liquid chromatography electrospray tandem mass spectrometry (LC-ESI-MS/MS)**  
By: Bai, Feng; Freeman, Burgess B.; Fraga, Charles H.; Fouladi, Maryam; Stewart, Clinton F.  
Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2006), 831(1-2), 169-175 | Language: English, Database: CAlus and MEDLINE

A sensitive method for the determination of lapatinib (GW572016) in human plasma was developed using high-performance liquid chromatog. separation with tandem mass spectrometric detection. Plasma samples (100 µL) were prepared using solid phase extraction (SPE) columns, and 6.0 µL of the reconstituted eluate was injected onto a Phenomenex CuroSil-PFP 3 µ anal. column (50 mm × 2.0 mm) with an isocratic mobile phase. Analytes were detected with a PE SCIEX API-365 LC-MS/MS system at unit (Q1) and low (Q3) resolution in pos. multiple reaction monitoring mode (m/z 581 (precursor ion) to m/z 364 (pr...

# 含有分析方法的文献详情页

## Therapeutic Drug Monitoring of the new targeted anticancer agents imatinib, nilotinib, dasatinib, sunitinib, sorafenib and lapatinib by LC tandem mass spectrometry

7

0

180



Citation Map



### In this Reference

- [Concepts](#)
- [Substances](#)
- [Analytical Methods](#)
- [Cited Documents](#)

By: Haouala, A.; Zanolari, B.; Rochat, B.; Montemurro, M.; Zaman, K.; Duchosal, M. A.; Ris, H. B.; Levvraz, S.; Widmer, N.; Decosterd, L. A.

DOI: 10.1016/j.jchromb.2009.04.045

The treatment of some **cancer** patients has shifted from traditional, non-specific cytotoxic chemotherapy to targeted therapies. Imatinib mesylate, a selective inhibitor of tyrosine kinases (TKIs) is the most commonly used TKI. It has opened the way to the development of several additional TKIs, including sunitinib, nilotinib, dasatinib, and sorafenib. The treatment of various hematological **malignancies** and solid tumors. All these agents are characterized by high pharmacokinetic variability, are at risk for drug interactions, and are not devoid of toxicity. Anticipating the careful monitoring of their plasma exposure via Therapeutic Drug Monitoring (TDM) is a key component of patients' follow-up. We have developed a liquid chromatography-tandem mass spectrometry (LC-MS/MS) method for the simultaneous determination of the six major TKIs currently in use. Plasma supernatant is diluted in ammonium formate 20 mM (pH 4.0) 1:2. Reverse-phase chromatography with gradient elution of 20 mM ammonium formate pH 2.2 and acetonitrile containing 1% formic acid to the initial solvent composition up to 20 min. Analyte quantification, using matrix-matched calibration and electrospray ionization-triple quadrupole mass spectrometry by selected reaction monitoring (SRM) was validated according to FDA recommendations, including assessment of extraction yield, matrix effect, accuracy, precision, efficiency (87.1-104.2%), as well as TKIs short- and long-term stability in plasma. The method is linear (-9.2 to +9.9%) and sensitive (lower limits of quantification comprised between 1 and 10 ng/mL) for all six TKIs. It is an improvement over previous methods in terms of convenience (a single extraction procedure for six major TKIs, reducing significantly the analysis time), sensitivity, selectivity and throughput. It may contribute to filling the current knowledge gaps in the pharmacokinetics/pharmacodynamics of these anticancer drugs, to define their therapeutic ranges in different patient populations, and to optimize the lasting therapeutic response.

**Keywords:** imatinib nilotinib dasatinib sunitinib sorafenib lapatinib drug monitoring



View Source

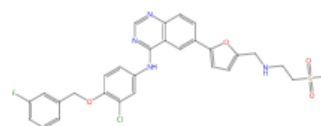
Full Text

View in CAS Analytical Methods

### Substances

Substances (7)

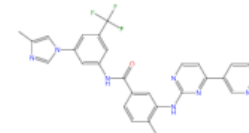
231277-92-2



$C_{29}H_{26}ClFN_4O_4S$   
**Lapatinib**

Role: Analyte, Therapeutic Use, Analytical Study, Biological Study, Uses

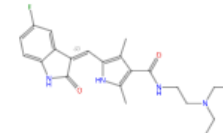
641571-10-0



$C_{28}H_{22}F_3N_7O$   
**Nilotinib**

Role: Analyte, Therapeutic Use, Analytical Study, Biological Study, Uses

557795-19-4



$C_{22}H_{27}FN_4O_2$   
**Sunitinib**

Role: Analyte, Therapeutic Use, Analytical Study, Biological Study, Uses

### Analytical Methods

Method Title

Analysis of Imatinib mesylate in Blood plasma by HPLC-tandem mass spectrometry

View All Methods



# CAS Analytical Methods 分析方法详情

Analysis of Imatinib mesylate in Blood plasma by HPLC-tandem mass spectrometry

CAS Method Number

1-101-CAS-181855

Method Category

Active Pharmaceutical Ingredient and Metabolite Analysis

Technique

HPLC-tandem mass spectrometry; Extraction

Analyte

Dasatinib  
Imatinib mesylate  
Lapatinib  
Nilotinib  
Sorafenib  

View All

Matrix

Blood plasma

Material

2.1 mm x 50 mm XTerra dC18 5 µm analytical column

Reagent

-

Biological Reagent

-

Equipment Used

LC system, Flux Instruments, AG, Thermo Fischer Scientific Inc, Waltham, MA  
  
triple quadrupole (TSQ) Quantum Discovery mass spectrometer (MS), Thermo Fisher Scientific, Inc, Waltham, MA  
  
thermostated column heater, Croco-Cil, Cluzeau Info Laboratory, Courbevoie, France  
  
Centrifuge, J6B, Beckmann  
  
benchtop Centrifuge, 16R, Hettich, Bach, Switzerland

Conditions

Chromatographic

mobile phase:20 mM ammonium formate in ultrapure water adjusted to pH 2.2 with formic acid (FA) 98-100% (solution A), and acetonitrile with 1% FA (solution B);flow rate:0.3-0.5 mL/min;

Instrument

ESI:positive mode;capillary temperature:350 °C;in source induced dissociation:10 V;tube lens voltages range:86-129 V;spray voltage:4 kV;sheath and auxiliary gas:nitrogen;flow-rate:60 psi and 5;Q2 collision gas (argon) pressure:1 mTorr (0.13 Pa)

Validation

Linearity Range

1-10000 ng/mL, Imatinib  
1-200 ng/mL, Dasatinib  
1-500 ng/mL, Nilotinib  
100-15000 ng/mL, Sunitinib  
1-5000 ng/mL, Sorafenib  
5-5000 ng/mL, Lapatinib

Limit of Detection

0.3 ng/mL, Imatinib  
0.3 ng/mL, Dasatinib  
0.4 ng/mL, Nilotinib  
0.1 ng/mL, Sunitinib  
1 ng/mL, Sorafenib  
0.4 ng/mL, Lapatinib

Limit of Quantitation

1 ng/mL, Imatinib  
1 ng/mL, Dasatinib  
1 ng/mL, Nilotinib  
1 ng/mL, Sunitinib  
10 ng/mL, Sorafenib  
5 ng/mL, Lapatinib

Accuracy

7.2%, -7.6% and -1.9% (Intra-assay bias, in 3, 2000 and 8000 ng/mL concentrations respectively);6.5%, -9.2% and -2.9% (Inter-assay bias, in 3, 2000 and 8000 ng/mL concentrations respectively), Imatinib  
-2.1%, -8.7% and -0.5% (Intra-assay bias, in 3, 60 and 150 ng/mL concentrations respectively);2.4%, -5.3% and -1.2% (Inter-assay bias, in 3, 60 and 150 ng/mL concentrations respectively), Dasatinib  
5.2%, 2.1% and 1.8% (Intra-assay bias, in 3, 800 and 3000 ng/mL concentrations respectively);4.2%, 4.0% and 9.9% (Inter-assay bias, in 3, 800 and 3000 ng/mL concentrations respectively), Nilotinib  
-8.7%, -1.4% and 0.1% (Intra-assay bias, in 3, 80 and 400 ng/mL concentrations respectively);-5.4%, -1.2% and -0.3% (Inter-assay bias, in 3, 80 and 400 ng/mL concentrations respectively), Sunitinib  
-0.2%, -7.3% and -1.2% (Intra-assay bias, in 15, 800 and 4000 ng/mL concentrations respectively);4.5%, -7.0% and 2.2% (Inter-assay bias, in 15, 800 and 4000 ng/mL concentrations respectively), Lapatinib  
-7.8%, 5.8% and -7.7% (Intra-assay bias, in 300, 1500 and 6000 ng/mL concentrations respectively);-6.6%, 5.6% and -8.1% (Inter-assay bias, in 300, 1500 and 6000 ng/mL concentrations respectively), Sorafenib

Precision

6.8%, 4.4% and 4.1% (Intra-assay CV, in 3, 2000 and 8000 ng/mL concentrations respectively);6.1%, 3.7% and 4.8% (Inter-assay CV, in 3, 2000 and 8000 ng/mL concentrations respectively), Imatinib

Source

JOURNAL

Therapeutic Drug Monitoring of the new targeted anticancer agents imatinib, nilotinib, dasatinib, sunitinib, sorafenib and lapatinib by LC tandem mass spectrometry  
Haouala, A.; Zanolari, B.; Rochat, B.; Montemurro, M.; Zaman, K.; Duchosal, M. A.; Ris, H. B.; Leyvraz, S.; Widmer, N.; Decosterd, L. A.  
  
Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2009), 877 (22), 1982 - 1996.  
Elsevier B.V.  
  
CODEN : JCBAAI | ISSN : 15700232 | DOI : 10.1016/j.jchromb.2009.04.045  

View Abstract

Full Text

Instructions

Preparation of plasma samples

1. Collect blood samples (5 mL) at random time after last drug intake in Monovettes (Sarstedt, Numbrecht, Germany, with K-EDTA as anticoagulant) from patients treated with one of the six analytes.

2. Centrifuge (1850 x g 3000rpm, + 4 °C, 10 min) (Beckmann Centrifuge, Model J6B) blood samples without delay and separate and transfer the plasma into polypropylene test tubes before storage at -20 °C.

Preparation of stock and standard solutions

1. Prepare stock solutions of imatinib and nilotinib at 1 mg/mL and dasatinib at 0.05 mg/mL by dissolution of 59.7 mg imatinib mesylate, 50 mg nilotinib base and 10 mg dasatinib base in 50.0 mL, 50.0 mL and 200.0 mL MeOH respectively.

2. Prepare sunitinib stock solution (1 mg/mL) in MeOH by extraction of Sutent capsules with MeOH.

3. Prepare sorafenib and lapatinib stock solutions after careful grounding in a mortar and extraction with MeOH of one Nexavar 200 mg tablet and one Tyverb 250 mg.Filter the resulting MeOH suspension and complete to the volume of 200 and 250 mL of MeOH respectively.

4. Store the stock solutions at 4 °C in glass flasks, with caps tightly wrapped with Parafilm.

5. Dilute the stock solutions with MeOH to obtain working solutions.

Plasma sample extraction

1. Mix a plasma sample aliquot (100 µL) with a 100 µL of internal standard solution.

2. Subject the resulting sample to protein precipitation with acetonitrile (600 µL) and carefully vortex-mix.

3. Centrifuge the mixture at 4 °C for 10 min at 20,000 x g (14000 rpm) on a benchtop Hettich Centrifuge (Benchtop Universal 16R centrifuge, Bach, Switzerland).

4. Add a 200 µL aliquot of the supernatant and 400 µL of buffer ammonium formate 20 mM pH adjusted to 4.0 with formic acid into 1.5 mL glass HPLC microvials and vortex-mix after secure closing with aluminium crimp seals.

5. Maintain processed samples at +10 °C in the thermostated autosampler rack.

LC-MS/MS analysis of the extracted plasma samples

1. Carry out chromatography on a LC system consisting of a Rheos 2200 quaternary pumps, equipped with an online degasser and a HTS PAL autosampler (CTC Analytics AG, Zwingen, Switzerland) controlled by Janeiro-CNS software (Flux Instruments, AG, Thermo Fischer Scientific Inc, Waltham, MA).

2. Separate the analytes on a 2.1 mm x 50 mm XTerra dC18 5 µm analytical column (Waters, Milford, MA, USA) placed in a thermostated column heater at 25 °C (Croco-Cil, Cluzeau Info Laboratory, Courbevoie, France).

3. Use 20 mM ammonium formate in ultrapure water adjusted to pH 2.2 with formic acid (FA) 98-100% (solution A), and acetonitrile with 1% FA (solution B) as the mobile phase.

4. Set up a gradient elution program as follows:5% of B at 0 min, 50% of B at 11 min, 100% of B at 14 min with a flow rate of 0.3 mL/min.

5. In the second part of the run carry out 3 min of intensive rinsing (100% B with 0.5 mL/min) and re-equilibration step to the initial solvent up to 20 min (at 17.01 with 0.3 mL/min).

6. Set the thermostated column heater at 25 °C and maintain the autosampler at 10 °C.

7. Carry out detection using a triple quadrupole (TSQ) Quantum Discovery mass spectrometer (MS) from Thermo Fisher Scientific, Inc. equipped with an Ion Max electrospray ionization (ESI) interface and operated with Xcalibur 2.0 software (Thermo Fischer Scientific Inc, Waltham, MA).

8. Set the MS conditions as follows: ESI in positive mode, capillary temperature: 350 °C, in source induced dissociation: 10 V, tube lens voltages range: 86-129 V, spray voltage: 4 kV and sheath and auxiliary gas (nitrogen) flow-rate: 60 psi and 5 respectively.Set the Q2 collision gas (argon) pressure at 1 mTorr (0.13 Pa).

9. Acquire the MS in selected reaction monitoring (SRM).

10. Perform chromatographic data acquisition, peak integration and quantification using the Xcalibur LC-Quan software package (version 2.0) (ThermoQuest, San Jose. CA, USA).

59

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CAS

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# 直接检索感兴趣的分析实验方法

方法(2): 登录<https://methods.cas.org>, 主题检索或分类浏览

The screenshot shows the homepage of the CAS Analytical Methods website. At the top, there is a navigation bar with the CAS logo, the text 'Analytical Methods', and links for 'Support', 'Saved', and a user profile icon. Below the navigation bar, a large banner area features a dark background with a network-like pattern. On the left, it says 'Good Afternoon,' followed by a placeholder for a user name. In the center, there is a large search bar with the placeholder text 'Search for keywords, matrices or analyte.' and a magnifying glass icon. Below the search bar, there are two main sections: 'Explore Methods' and 'Advanced Search'. 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 sections, there is a 'Recent Searches' section. It contains two search entries: 'graphene' and 'Advanced : analyte : chlorogenic acid, matrix : coffee beans'. Each entry has a close button (an 'x' in a circle) to its right. The entire interface is framed by a dark blue border.

CAS Analytical Methods

Support Saved

Good Afternoon, [User Name]

Search for keywords, matrices or analyte. **直接检索**

**Explore Methods**  
Search methods using criteria like method categories and subcategories.

**Advanced Search**  
Search methods using criteria like keywords, analytes, matrices and more.

**浏览不同类别分析方法** **高级检索**

Recent Searches **近期检索**

graphene

Advanced : analyte : chlorogenic acid, matrix : coffee beans

# CAS Analytical Methods 分析方法类别

目前涵盖13个大类，45个小类；某些子分类属于多种方法分类。

**Agricultural Applications / Analysis:** 除草剂分析…

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

**Biomolecule Isolation:** 天然产物分离分析，蛋白质分析…

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

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

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

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

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

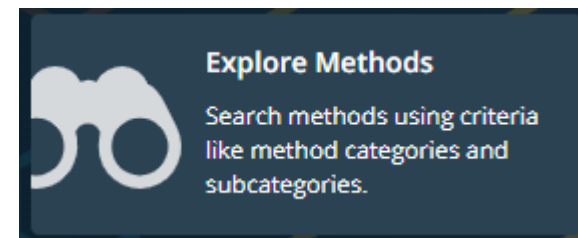
**Organic Compound Analysis:** 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…

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

**Pharmacology / Toxicology:** 活性药物成分及代谢物，成瘾药物检测，有毒物检测…

**Polymer:** 塑料加工

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

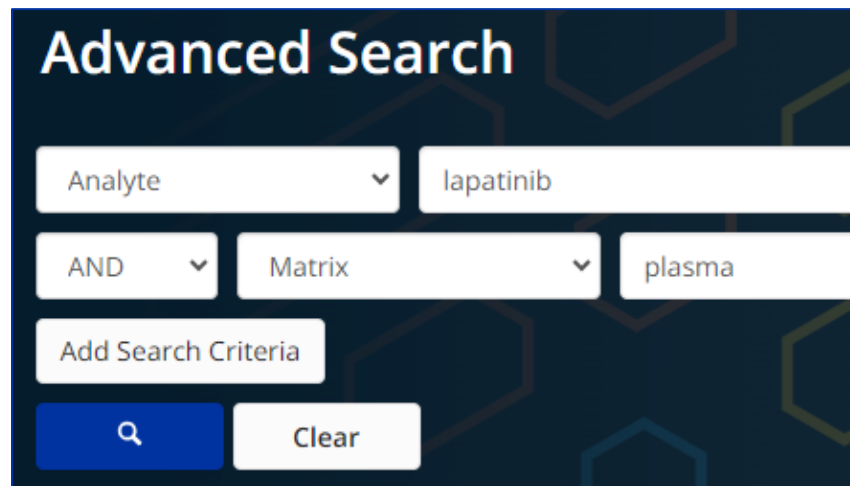


# 关键词检索分析方法

- 直接检索示例：  
lapatinib 拉帕替尼



- 高级检索示例：  
分析拉帕替尼血药浓度的方法





# 检索结果分析与精炼

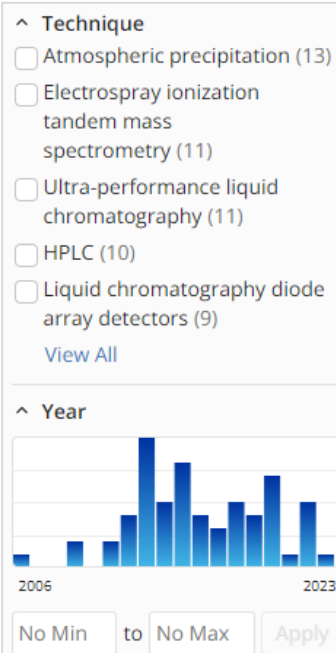
分析物

基质

方法分类

技术&仪器

年份



## Results for lapatinib

### Filter By

#### ^ Analyte

- ☐ Lapatinib (49)
- ☐ Sorafenib (17)
- ☐ Erlotinib (15)
- ☐ Dasatinib (12)
- ☐ Nilotinib (12)

View All

#### ^ Matrix

- ☐ Blood plasma (35)
- ☐ Pharmaceutical tablets (6)
- ☐ Urine (4)
- ☐ Blood (3)
- ☐ Animal tissue (2)

View All

#### ^ Method Category

- ☐ Active Pharmaceutical Ingredient and Metabolite Analysis (59)
- ☐ Bioassay (2)
- ☐ Biomolecule Isolation Assay (1)
- ☐ Nanomaterial Analysis (1)

#### ^ Technique

#### ^ Year

62 Results

Sort: Relevance

Group: By Method

1

### Analysis of Lapatinib in Pharmaceutical tablets by Ultra-performance liquid chromatography

By: Biswal, Sabyasachi; Mondal, Sumanta

Analytical method validation report for assay of Lapatinib by UPLC  
Pharmaceutical Methods (2019), 10 (1), 9-14. EManuscript Services

Analyte Lapatinib

Matrix Pharmaceutical tablets

Other Materials Material: BHEL UPLC Column; Filter (4.5  $\mu$ )

Method Category Active Pharmaceutical Ingredient and Metabolite Analysis

Technique Ultra-performance liquid chromatography; Photodiode array detectors

Equipment Used Ultra performance liquid chromatography (UPLC) system; Autosampler; Phtodiode array (PDA) detector; pH meter; Ultra Sonicator; Analytical balance

View Abstract

Full Text

View in CAS SciFinder

JOURNAL

Compare

对比不同分析方法

2

### Analysis of Lapatinib by Microplate spectroscopy

By: Murata, Akihiro; Nakata, Bunzo; Komoto, Masahiro; Hirata, Keiichiro; Kimura, Kenjiro; Amano, Ryosuke; Hirakawa, Kosei

In vitro effects of lapatinib with gemcitabine for pancreatic cancer cells  
Hepato-Gastroenterology (2013), 60 (126), 1484-1487. H.G.E. Update Medical Publishing S.A.

Analyte Lapatinib; Gemcitabine

Other Materials Reagent: Methanol; [3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]; Dimethyl sulfoxide; Phosphate-buffered saline solutions

Material: Human cell line PANC-1; Dulbecco's modified Eagle's medium (DMEM); MiaPaca-2 cell line; 96-well

View All

Method Category Bioassay

JOURNAL

Compare

# 对照多个感兴趣的分析方法详情

## Comparing your 2 selected Methods

	Method 1 <span>×</span>	Method 2 <span>×</span>
	Analysis of <b>Lapatinib</b> by Microplate spectroscopy	Analysis of <b>Lapatinib</b> in Pharmaceutical tablets by Ultra-performance liquid chromatography
CAS Method Number	2-107-CAS-164891	1-101-CAS-446826
Method Category	Bioassay	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Microplate spectroscopy	Ultra-performance liquid chromatography; Photodiode array detectors
Analyte	<b>Lapatinib</b> ; Gemcitabine	<b>Lapatinib</b>
Matrix	-	Pharmaceutical tablets
Other Materials	Dimethyl sulfoxide; [3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide]; Methanol; Phosphate-buffered saline solutions; Human cell line PANC-1; Dulbecco's modified Eagle's medium (DMEM); MiaPaca-2 cell line; 96-well tissue culture plates	BHEL UPLC Column; Filter (4.5 µ)
Equipment Used	Microplate reader, 550, Bio-Rad Laboratories, Hercules, CA, USA	Ultra performance liquid chromatography (UPLC) system, SHIMADZU; Autosampler, SHIMADZU; Photodiode array (PDA) detector, SHIMADZU; pH meter, Labindia; Ultra Sonicator; Analytical balance, SHIMADZU
Conditions	Instrument: detection wavelength: 570 nm	-
Preparation	Collection of <b>lapatinib</b> and gemcitabine sample 1. Collect <b>lapatinib</b> and gemcitabine samples. 2. Dissolve <b>lapatinib</b> in methanol and dissolve gemcitabine in phosphate buffered saline (PBS). 3. Dilute in Dulbecco's modified Eagle's medium (DMEM) to the required concentrations immediately before use.	Preparation of 0.1% ortho phosphoric acid (OPA) buffer pH 3 1. Add 1 mL of ortho phosphoric acid in 1000 mL water. 2. Adjust this solution to pH 3 by using sodium hydroxide.  Preparation of mobile phase 1. Mix a mixture of 0.1% OPA buffer 300 mL (30%) and 700 mL acetonitrile (70%) and degas in ultrasonic water bath for 5 min. 2. Filter through 4.5 µ filter under vacuum filtration.  Diluents preparation 1. Prepare the diluents with 0.1% OPA buffer:acetonitrile (30:70) ratio.



Format

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 ☐ XLS

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Instructions	<p><b>Cell culture</b></p> <ol style="list-style-type: none"> <li>1. Maintain pancreatic cancer cell lines MiaPaca-2 and PANC-1 at 37 °C in a humidified atmosphere of 5% CO<sub>2</sub>.</li> <li>2. Grow cell line continuously in Dulbecco's modified Eagle's medium (DMEM) (Nikken Bio., Kyoto, Japan) supplemented with 10% fetal bovine serum, penicillin, streptomycin and sodium pyruvate.</li> </ol> <p><b>Determination of cell growth inhibition by 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl tetrazolium bromide (MTT) assay</b></p> <ol style="list-style-type: none"> <li>1. Seed cells in 96-well tissue culture plates (Costar, Corning, NY, USA) at a density of <math>1 \times 10^4</math> per 100 µL/well.</li> <li>2. Expose the cell to drugs for 48 h.</li> <li>3. Add 10 µL of MTT solution (2 mg/mL) to each well.</li> <li>4. Incubate cells for a further 2 h.</li> <li>5. Stop the reaction by removing MTT.</li> <li>6. Dissolve formazan crystals in dimethyl sulfoxide (DMSO) (100 µL/well).</li> <li>7. Record absorbance at 570 nm using a 96-well microplate reader (model 550; Bio-Rad Laboratories, Hercules, CA, USA).</li> <li>8. Determine the IC<sub>50</sub> values for the drugs by plotting the rate of growth inhibition versus the drug concentration.</li> </ol>	<p><b>Ultra performance liquid chromatography-Photodiode array detection (UPLC-PDA)</b></p> <ol style="list-style-type: none"> <li>1. Perform the analysis using Ultra performance liquid chromatography (UPLC) equipped with Auto Sampler and PDA detector.</li> <li>2. Carry out the separation on a BHEL UPLC Column.</li> <li>3. Use .1% OPA Buffer:acetonitrile (30:70 v/v) as the mobile phase at 0.25 mL/min.</li> <li>4. Inject 5 µL of the sample into the column.</li> <li>5. Carry out the detection at 309 nm.</li> </ol>
Bioactivity	7.5 µM (IC <sub>50</sub> , MiaPaca-2 cell line), <b>Lapatinib</b> , 4.5 µM (IC <sub>50</sub> , PANC-1 cell line), <b>Lapatinib</b> , 2.7 µM (IC <sub>50</sub> , MiaPaca-2 cell line), Gemcitabine, 0.25 µM (IC <sub>50</sub> , PANC-1 cell line), Gemcitabine	-
Linearity Range	-	10-50 µg/mL
Limit of Detection	-	0.06 µg/mL
Limit of Quantitation	-	0.18 µg/mL
Accuracy	-	100.38, 99.35 and 99.34% (recovery) in 10, 100 and 150% added concentrations, respectively
Precision	-	0.7% (RSD)
Source	<p>JOURNAL</p> <p>In vitro effects of <b>lapatinib</b> with gemcitabine for pancreatic cancer cells</p> <p>By: Murata, Akihiro; Nakata, Bunzo; Komoto, Masahiro; Hirata, Keiichiro; Kimura, Kenjiro; Amano, Ryosuke; Hirakawa, Kosei</p> <p>Hepato-Gastroenterology (2013), 60 (126), 1484 - 1487.</p> <p>Full Text -</p>	<p>JOURNAL</p> <p>Analytical method validation report for assay of <b>Lapatinib</b> by UPLC</p> <p>By: Biswal, Sabyasachi; Mondal, Sumanta</p> <p>Pharmaceutical Methods (2019), 10 (1), 9 - 14.</p> <p>Full Text -</p>



# 文献关联的制剂/配方

方法（1）：在CAS SciFinder的文献结果集页面，点击CAS Content中的 Formulations获得有具体制剂/配方信息的文献，从文献详情页中链接获取

References search for "'chronic heart failure' and 'traditional Chinese medicine'"

Substances Reactions Citing Knowledge Graph

Filter Behavior

Filter by Exclude

Search Within Results

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

CA Section

CAS Content

Analytical Methods (8)

Formulations (3)

Life Science Data

Formulation Purpose

Database

519 Results

Sort: Relevance View: Partial Abstract

1

Prevention and treatment of chronic heart failure through traditional Chinese medicine: Role of the gut microbiota

By: Jia, Qiuji; Wang, Lirong; Zhang, Xiaonan; Ding, Yuejia; Li, Hao; Yang, Yingxi; Zhang, Ao; Li, Yanyang; Lv, Shichao; Zhang, Junping  
Pharmacological Research (2020), 151, 104552 | Language: English, Database: CAlplus and MEDLINE

A review. In recent years, although the concept and means of modern treatment of chronic heart failure (CHF) are continually improving, the readmission rate and mortality rate are still high. At present, there is evidence that there is a link between gut microbiota and heart failure, so the intervention of gut microbiota and its metabolites is expected to become a potential new therapeutic target in heart failure. Traditional Chinese medicine (TCM) has apparent advantages in stabilizing the disease, improving heart function, and improving the quality of life. It can exert its effect by operating...

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Full Text

Substances (0) Reactions (0) Citing (63) Citation Map

2

Progress in treatment of chronic heart failure in Western medicine and treatment strategies in traditional Chinese medicine

By: Chen, Chang-xun; Gao, Jian-ping; Wu, Qi; Guo, Juan; Gu, Wei-liang  
Zhongxiyi Jiehe Xuebao (2010), 8(1), 7-14 | Language: Chinese, Database: CAlplus and MEDLINE

A review. The concept of modern medicine in treating chronic heart failure (CHF) has changed markedly in recent years. To improve the quality of life and prolong life, the treatment goal is no longer just temporary improvement of symptoms, more importantly, is to prevent and delay the occurrence and development of ventricular remodeling. Long-term chronic over-activation of sympathetic system, renin-angiotensin-aldosterone system and other neuroendocrine factors promotes myocardial remodeling, increases myocardial injury and deteriorates cardiac function. Despite short-term use can significant...

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定位制剂/配方的功能目标

# 文献关联的制剂/配方

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



### In this Reference

- [IPC Data](#)
- [CAS Concepts](#)
- [Formulations](#)

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

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

Keywords: myocardial hypertrophy prevention traditional Chinese medicine composition

PatentPak PDF

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### Publication Information • Patent

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Patent Number  
CN112190652

Publication Date  
2021-01-08

Assignee  
Capital Medical University,  
China

Source  
China  
CODEN: CNXXEV

### Formulations

[View All Formulations](#)

#### Formulation Title

[Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents](#)

[Traditional Chinese Medicine for Preventing and/or Treating Myocardial Hypertrophy: Cardiovascular Agents](#)

### Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
CN112190652	Chinese	A	<a href="#">PDF</a>	2021-01-08	CN2020-11207191	2020-11-03

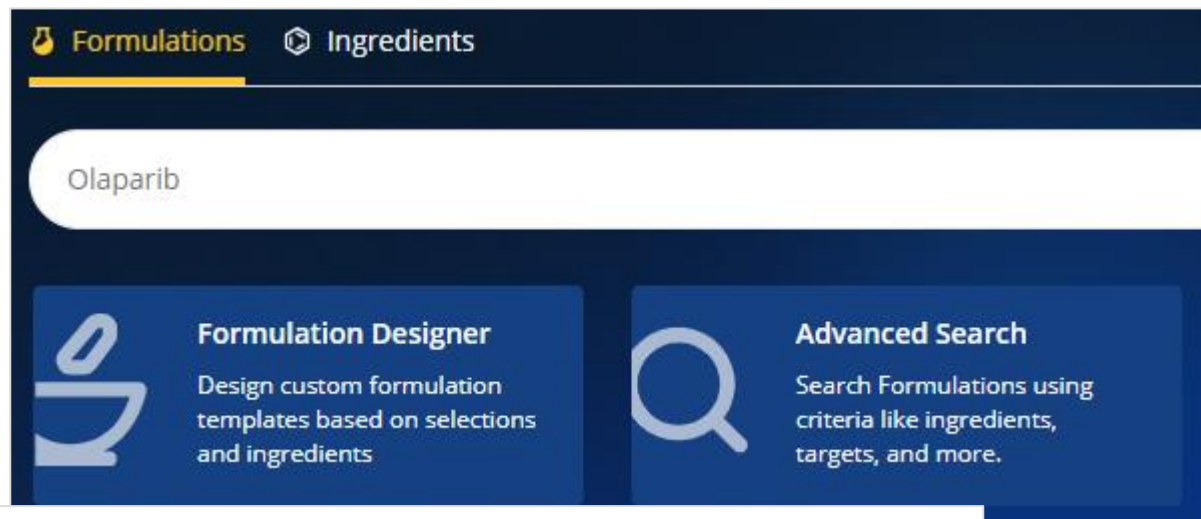
# 直接检索制剂/配方或配方成分

方法（2）：登录CAS Formulus主页 (<https://formulus.cas.org>) 进行直接检索或高级检索

The screenshot displays the CAS Formulus web interface. At the top, the navigation bar includes the CAS Formulus logo, a menu icon, and links for Help & Support, Alerts, Saved, and a user profile. Below the navigation bar, a greeting "Good Afternoon," is followed by tabs for "Formulations" and "Ingredients". A large search bar is present with the placeholder text "Search by Formulations by Ingredients, Purpose, Form, Functions, etc." and a magnifying glass icon. The text "直接检索" (Direct Search) is overlaid on the search bar. Below the search bar, there are two main sections: "Formulation Designer" with a flask icon and the description "Design custom formulation templates based on selections and ingredients", and "Advanced Search" with a magnifying glass icon and the description "Search Formulations using criteria like ingredients, targets, and more." The text "制剂/配方设计" (Formulation Design) is overlaid on the Formulation Designer section, and "高级检索" (Advanced Search) is overlaid on the Advanced Search section. At the bottom, there is a "Recent Search History" section with the text "近期检索" (Recent Search) overlaid. It shows a search from November 20, 2024, at 12:41 PM for "Formulations" with the query "PEG (1020195)". There are buttons for "Rerun Search" and "Edit Search". A link "View Search History" is also visible.

# 关键词检索制剂/配方

- 直接检索示例：  
Olaparib 奥拉帕尼



- 高级检索示例：  
奥拉帕尼片剂

**Advanced Formulations Search** ?

Searches the following content fields: Ingredient, Function, Purpose, Physical Form, Delivery Route, and Target.  
At least two search terms are required.

Search For	Operator	Enter one term
Ingredient	Required	Olaparib <small>Ex: caffeine, sodium, 50-00-0</small>
Form	Required	Tablets <small>Ex: spray, granule, powder</small>

[Add Another Term](#)

[Search](#) [Clear All](#)

# 检索结果分析与精炼

应用领域

目的/用途

物理形态

物质状态

作用方式

制剂信息

文献类型

机构名

发表年份

Document Type

☐ Journal (7)  
☐ Article (7)

☐ Patent (627)  
☐ Claim (392)  
☐ Comparative Example (30)  
☐ Example (203)  
☐ Table (2)

☐ Product Insert (5)

Organization

☐ CSPC Zhongqi Pharmaceutical Technology (Shijiazhuang) Co., Ltd. (34)

☐ Shanghai Institute of Materia Medica, Chinese Academy of Sciences (33)

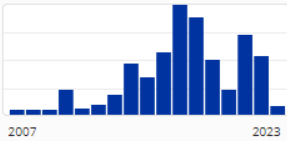
☐ Sunshine Lake Pharma Co., Ltd. (29)

☐ AstraZeneca UK Ltd. (22)

☐ Immunomedics, Inc. (21)

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Publication Year



No Min to No Max Apply

State of Matter

☐ Solid (100)  
☐ Liquid (26)  
☐ Semisolid (5)

Delivery Route

☐ Oral drug delivery systems (128)  
☐ Pharmaceutical intravenous injections (35)  
☐ Intraperitoneal injections (34)  
☐ Mucosal drug delivery systems (30)  
☐ Intramuscular injections (26)

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Information Included

☐ Component Amount (269)  
☐ Process (196)  
☐ Experimental Activity (162)  
☐ Effective Dose (49)

Filter by

Industry

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Purpose

☐ Antitumor agents (415)  
☐ Drug delivery systems (86)  
☐ Pharmaceutical formulations (34)  
☐ Antiproliferative agents (23)  
☐ Anti-inflammatory agents (22)

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Physical Form

☐ Tablets (128)  
☐ Capsules (66)  
☐ Pharmaceutical injections (19)  
☐ Particles (18)  
☐ Powders (15)

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Formulations search for "Olaparib"

Get Additional References 一键获取相关文献

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639 Results Sort: Relevance

1

Mixture: Pharmaceutical Mixture

Location: Article page 2

Purpose: pharmaceutical mixture

Add to Compare

Component	Function	Amount Reported
Group: olaparib capsule	active agent	50 mg
Olaparib	-	50 mg
Pharmaceutical capsules	carriers	-
Water	vehicles	-

View Formulation Detail

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JOURNAL

Evaluation of the pharmacodynamics and pharmacokinetics of the PARP inhibitor olaparib: a Phase I multicentre trial in patients scheduled for elective breast cancer surgery


Investigational New Drugs



Language: English

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# 制剂、配方详情

 **Olaparib** Solid Dispersion: Antitumor Agents

Purpose	Target	Delivery Route	Physical Form	Source
Antitumor agents	Homo sapiens, Ovary neoplasm	-	Capsules, Particles, Pharmaceutical solid dispersions, Powders	<a href="#">View</a>

 Predicted value

Formulation Ingredients

制剂成分、功能、用量

Component	Function	Amount Reported	Optionality
<b>Olaparib</b>	poly(ADP-ribose) polymerase inhibitor <sup>Ⓢ</sup>	200 g	Mandatory
Vinyl acetate-vinylpyrrolidone copolymer	carrier <sup>Ⓢ</sup> , polymeric stabilizer <sup>Ⓢ</sup>	800 g	Mandatory

More Formulations like this...

Lincomycin Solid Dispersion: Veterinary Drug

Purpose: Veterinary drugs

Target: Homo sapiens, Livestock, Poultry

Delivery Route: -

Physical Form: Pharmaceutical solid di...

Olaparib Dispersible Tablets: Antitumor Agents

Purpose: Antitumor agents

Target: Homo sapiens, Mammary glan...

Delivery Route: Oral drug delivery syst...

Physical Form: Pharmaceutical orally d...

Olaparib Dispersible Tablets: Antitumor Agents

Purpose: Antitumor agents

Target: Homo sapiens, Mammary glan...

Delivery Route: Oral drug delivery syst...

Physical Form: Pharmaceutical orally d...

Lincomycin Solid Dispersion: Veterinary Drug

Purpose: Veterinary drugs

Target: Homo sapiens, Livestock, Poultry



Delivery Route: -

Physical Form: Pharmaceutical solid di...

Source Patent

Olaparib solid dispersion and preparation method therefor

Assignee : Farmasino Pharmaceuticals (Jiangsu) Co., Ltd.  
CN106692066  
Language: Chinese  
Location: Example 4

Process

工艺信息

preparation of olaparib solid dispersions and capsules. olaparib (50 g) and copolyvidone VA64 (950 g) were passed through a 60 mesh sieve, and the sieved olaparib and copolyvidone VA64 were uniformly mixed to obtain a raw material mixture (1000 g). the extrusion temperature of the twin-screw extruder was set to 150 °C. after the temperature was reached, the raw material mixture was added to the extruder, melted, extruded, and finally extruded in a strip shape to obtain a strip shape. extrudate (960 g). the above strip-like extrudate was cooled to room temperature, pulverized and passed through a 20 mesh sieve to obtain a granulated olaparib solid dispersion (960 g). the above granulated olaparib solid dispersion was placed in a hard capsule shell according to the loading amount of 50 mg of the solid dispersion per granule to obtain a corresponding capsule.



# 分析方法及制剂/配方检索小结

1. 利用CAS Analytical Methods进行主题检索或分类浏览获得分析方法，或通过文献查看关联的分析实验及数据详情
2. 利用CAS Formulus检索制剂/配方、原料，或通过文献结果集获得关联的制剂/配方信息；利用配方设计工具启发产品配方的开发

# 大纲

- CAS SciFinder Discovery Platform 简介
- 科研信息的高效查阅
  - 如何开展文献调研?
  - 如何聚焦某类物质?
  - 如何调研反应信息?
  - 怎么查找分析实验方法和制剂/配方详情?
- 常见问题Q&A



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

例：abc@123

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--CONTACT INFORMATION--

First Name:

Last Name:

Email:

Confirm Email:

Phone Number:

Fax Number:

Area of Research:

Job Title:

--USERNAME AND PASSWORD--

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Password:

Re-enter Password:

--SECURITY INFORMATION--

Security Question:

Answer:  [Why?](#)

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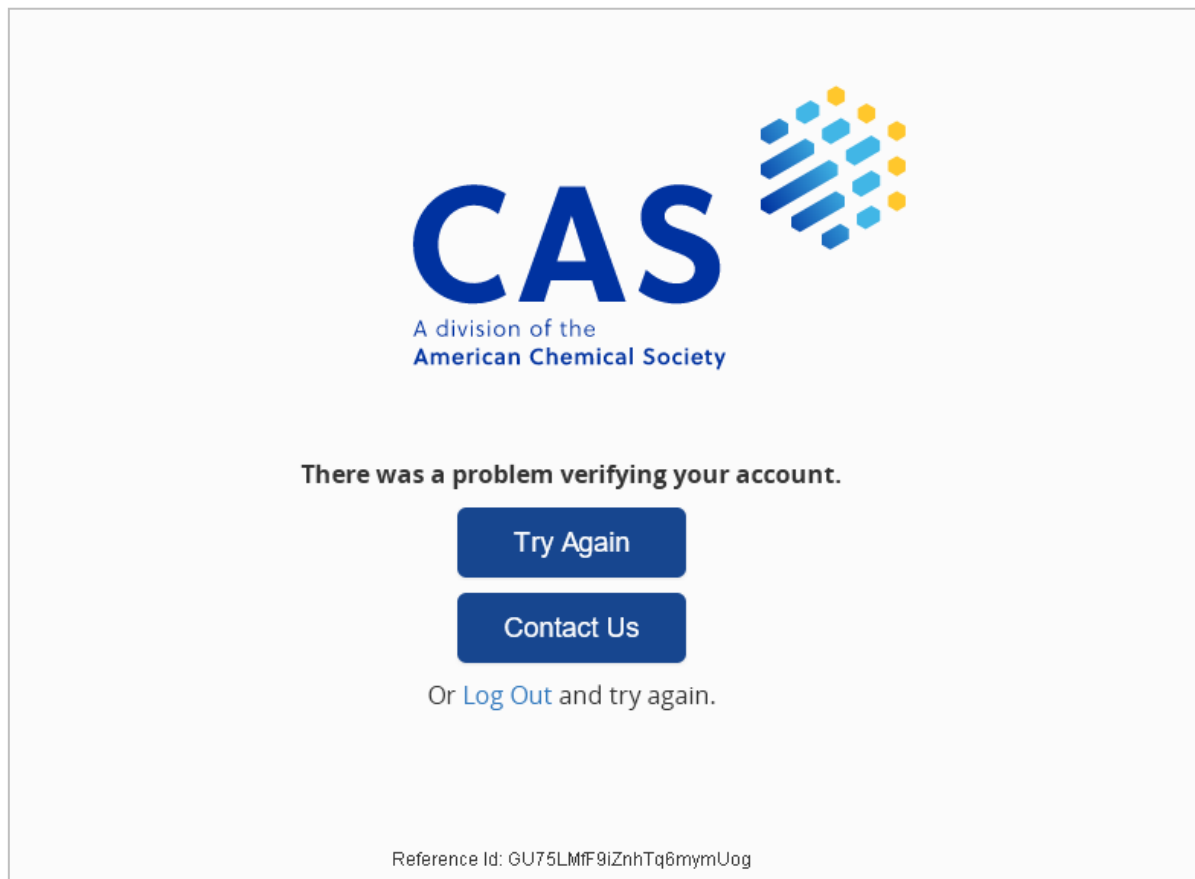
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演讲人：潘娜 博士



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演讲人：钱欣 博士



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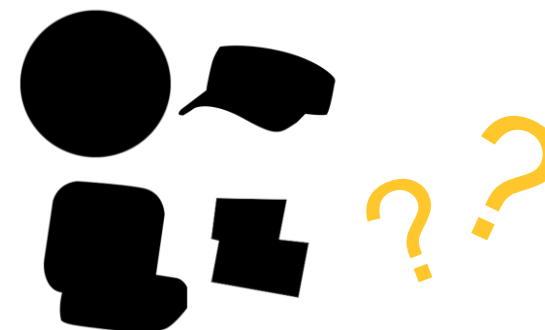
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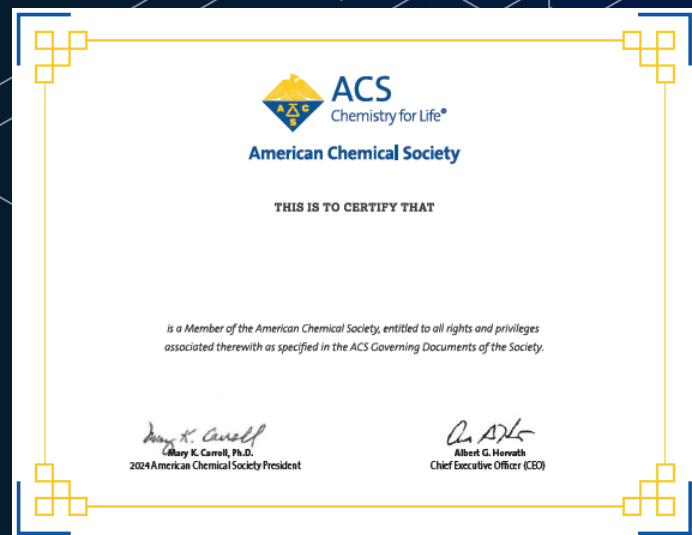
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